Full wwPDB EM Validation Report (i)

Sep 20, 2026 – 02:50 pm BST

PDB ID	:	8BD3 / pdb_00008bd3
EMDB ID	:	EMD-15973
Title	:	Cryo-EM structure of the Photosystem II - LHCII supercomplex from Chlorella ohadi
Authors	:	Fadeeva, M.; Klaiman, D.; Caspy, I.; Nelson, N.
Deposited on	:	2022-10-18
Resolution	:	2.73 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

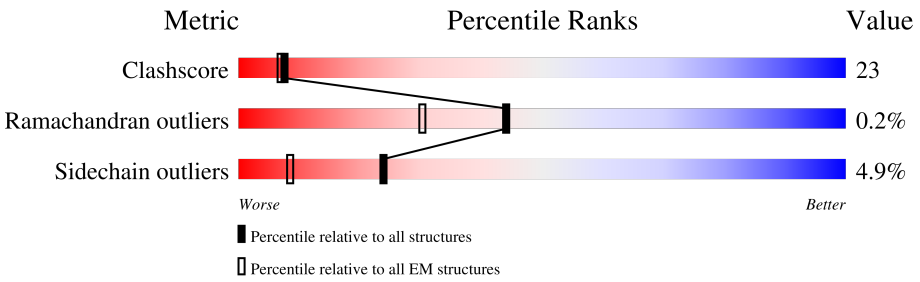
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

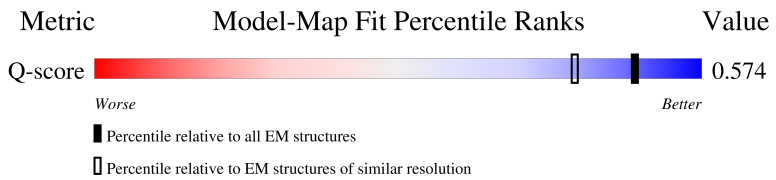
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10432 (2.23 - 3.23)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	214	61% 36% •
1	7	214	68% 30% •
2	2	222	• 50% 46% •
2	4	222	• 44% 50% 6%

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Mol	Chain	Length	Quality of chain
2	9	222	59% 39%
2	G	222	67% 32%
2	g	222	73% 26%
2	q	222	46% 51%
3	3	221	44% 52% 5%
3	5	221	5% 35% 60%
3	8	221	63% 34%
3	N	221	62% 34%
3	n	221	64% 33%
3	p	221	6% 52% 44%
4	0	217	66% 31%
4	6	217	66% 31%
5	A	336	76% 22%
5	a	336	77% 21%
6	B	504	80% 19%
6	b	504	77% 22%
7	C	448	73% 24%
7	c	448	71% 26%
8	D	342	75% 24%
8	d	342	75% 23%
9	E	81	74% 25%
9	e	81	67% 33%
10	F	37	54% 46%
10	f	37	59% 41%
11	H	67	84% 15%

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Mol	Chain	Length	Quality of chain
11	h	67	79% 21%
12	I	34	79% 21%
12	i	34	79% 21%
13	J	38	92% 5%
13	j	38	84% 13%
14	K	37	59% 38%
14	k	37	70% 27%
15	L	37	68% 32%
15	l	37	70% 27%
16	M	57	11% 77% 21%
16	m	57	11% 82% 18%
17	O	240	74% 23%
17	o	240	81% 18%
18	R	236	74% 25%
18	r	236	75% 24%
19	S	257	74% 25%
19	s	257	74% 26%
20	T	30	70% 30%
20	t	30	57% 40%
21	V	32	84% 16%
21	v	32	88% 12%
22	W	60	60% 38%
22	w	60	68% 32%
23	X	37	70% 30%
23	x	37	81% 19%

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Mol	Chain	Length	Quality of chain
24	Y	221	78% 21% •
24	y	221	72% 25% •
25	Z	62	89% 11%
25	z	62	74% 26%
26	U	144	86% 14%
26	u	144	83% 16% •
27	Q1	34	76% 24%
27	q1	34	62% 38%
28	P1	108	88% 12%
28	p1	108	82% 16% •
29	F1	188	79% 18% •
29	f1	188	80% 20% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	5	610	-	-	X	-
31	CLA	p	613	-	-	X	-
31	CLA	q	312	-	-	X	-
32	LUT	5	616	-	-	X	-
35	RRX	G	614	-	-	X	-
37	XAT	G	620	-	-	X	-
43	BCR	c	614	-	X	-	-
45	DGD	C	620	-	-	X	-
45	DGD	c	619	-	-	X	-

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 117990 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	214	1630	1056	265	304	5	0	0
1	7	214	1630	1056	265	304	5	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	195	LEU	PHE	conflict	UNP A0A2P6TPU9
1	225	GLU	ASP	conflict	UNP A0A2P6TPU9
1	250	ASN	THR	conflict	UNP A0A2P6TPU9
7	195	LEU	PHE	conflict	UNP A0A2P6TPU9
7	225	GLU	ASP	conflict	UNP A0A2P6TPU9
7	250	ASN	THR	conflict	UNP A0A2P6TPU9

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	222	1686	1089	271	321	5	0	0
2	4	222	1685	1088	271	321	5	0	0
2	G	222	1686	1089	271	321	5	0	0
2	9	222	1686	1089	271	321	5	0	0
2	q	222	1685	1088	271	321	5	0	0
2	g	222	1686	1089	271	321	5	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	74	THR	SER	conflict	UNP A0A2P6TDA6
4	74	THR	SER	conflict	UNP A0A2P6TDA6
G	74	THR	SER	conflict	UNP A0A2P6TDA6
9	74	THR	SER	conflict	UNP A0A2P6TDA6
q	74	THR	SER	conflict	UNP A0A2P6TDA6
g	74	THR	SER	conflict	UNP A0A2P6TDA6

- Molecule 3 is a protein called Chlorophyll a-b binding of LHCII.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	5	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	N	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	8	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	p	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	n	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		

- Molecule 4 is a protein called Chlorophyll a-b binding of LHCII.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	217	Total	C	N	O	S	0	0
			1657	1070	271	311	5		
4	0	217	Total	C	N	O	S	0	0
			1657	1070	271	311	5		

- Molecule 5 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		
5	a	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		

- Molecule 6 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	504	3954	2583	667	692	12	0	0
6	b	504	3954	2583	667	692	12	0	0

- Molecule 7 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	448	3482	2280	584	603	15	0	0
7	c	448	3482	2280	584	603	15	0	0

- Molecule 8 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	342	2730	1806	449	464	11	0	0
8	d	342	2730	1806	449	464	11	0	0

- Molecule 9 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E	81	652	423	106	123	0	0
9	e	81	652	423	106	123	0	0

- Molecule 10 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	37	302	206	49	46	1	0	0
10	f	37	302	206	49	46	1	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	67	507	336	73	95	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	h	67	507	336	73	95	3	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	34	274	187	41	45	1	0	0
12	i	34	274	187	41	45	1	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	J	38	270	182	42	46	0	0
13	j	38	270	182	42	46	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	K	37	295	204	43	48	0	0
14	k	37	295	204	43	48	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	L	37	303	203	48	52	0	0
15	l	37	303	203	48	52	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	M	57	370	242	60	67	1	0	0
16	m	57	370	242	60	67	1	0	0

- Molecule 17 is a protein called Chloroplast oxygen-evolving enhancer protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O	240	1789	1134	287	362	6	0	0
17	o	240	1789	1134	287	362	6	0	0

- Molecule 18 is a protein called Chlorophyll a b binding CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	236	1818	1148	311	352	7	0	0
18	r	236	1818	1148	311	352	7	0	0

- Molecule 19 is a protein called Chlorophyll a b-binding CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	257	1934	1242	323	364	5	0	0
19	s	257	1934	1242	323	364	5	0	0

- Molecule 20 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	30	246	172	36	37	1	0	0
20	t	30	246	172	36	37	1	0	0

- Molecule 21 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	V	32	233	155	38	40	0	0
21	v	32	233	155	38	40	0	0

- Molecule 22 is a protein called Photosystem II reaction center W protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	W	60	468	301	74	93	0	0
22	w	60	468	301	74	93	0	0

- Molecule 23 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	X	37	247	156	43	48	0	0
23	x	37	247	156	43	48	0	0

- Molecule 24 is a protein called Multifunctional fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	221	1688	1099	270	314	5	0	0
24	y	221	1688	1099	270	314	5	0	0

- Molecule 25 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	62	478	335	68	74	1	0	0
25	z	62	478	335	68	74	1	0	0

- Molecule 26 is a protein called Chloroplast oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	U	144	1122	701	207	214	0	0
26	u	144	1122	701	207	214	0	0

- Molecule 27 is a protein called Chloroplast PsbY.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Q1	34	260	171	44	44	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	q1	34	260	171	44	44	1	0	0

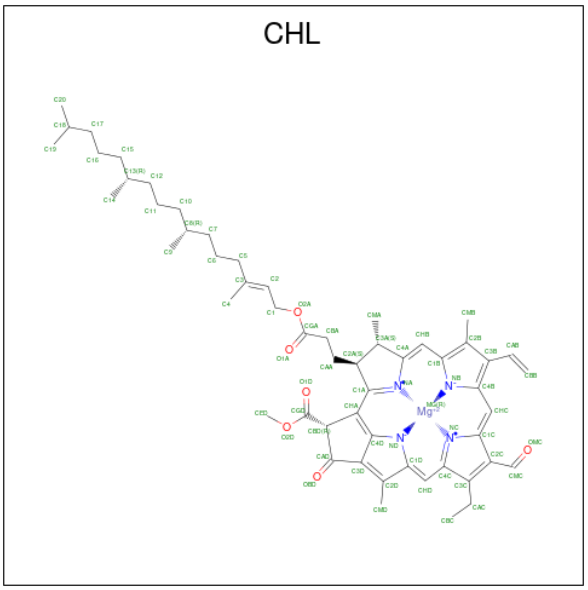
- Molecule 28 is a protein called Chloroplast photosystem II 10 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	P1	108	820	524	137	157	2	0	0
			Total	C	N	O	S		
28	p1	108	820	524	137	157	2	0	0

- Molecule 29 is a protein called Photosystem II oxygen evolving enhancer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	F1	188	1443	918	245	279	1	0	0
			Total	C	N	O	S		
29	f1	188	1443	918	245	279	1	0	0

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	1	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	1	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	2	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	2	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	2	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	2	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	4	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	63	52	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	56	45	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	R	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	R	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	R	1	55	44	1	4	6	0
			Total	C	Mg	N	O	
30	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	S	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
30	S	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
30	S	1	49	38	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	63	52	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	59	48	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	0	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	0	1	52	41	1	4	6	0
			Total	C	Mg	N	O	
30	0	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	0	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	0	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	0	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	7	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	7	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	7	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	7	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	7	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	7	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	7	1	63	52	1	4	6	0
			Total	C	Mg	N	O	
30	8	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	8	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	8	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
30	8	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	8	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	9	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	9	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	9	1	52	41	1	4	6	0
			Total	C	Mg	N	O	
30	9	1	53	42	1	4	6	0
			Total	C	Mg	N	O	
30	9	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	9	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	p	1	51	40	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	p	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	p	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	p	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	p	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	p	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	q	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	q	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	q	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
30	q	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	q	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	63	52	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	63	52	1	4	6	0

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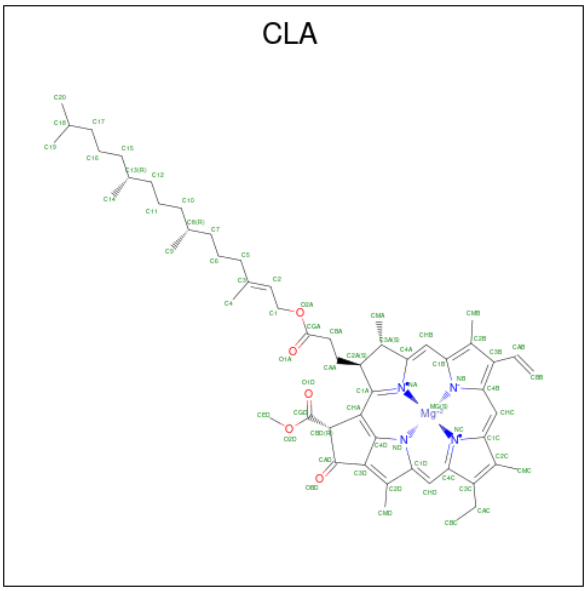
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	n	1	50	39	1	4	6	0
30	n	1	66	55	1	4	6	0
30	r	1	56	45	1	4	6	0
30	r	1	56	45	1	4	6	0
30	r	1	55	44	1	4	6	0
30	s	1	46	35	1	4	6	0
30	s	1	44	35	1	4	4	0
30	s	1	43	34	1	4	4	0
30	s	1	49	38	1	4	6	0
30	y	1	66	55	1	4	6	0
30	y	1	46	35	1	4	6	0
30	y	1	59	48	1	4	6	0
30	y	1	66	55	1	4	6	0
30	y	1	50	39	1	4	6	0
30	y	1	66	55	1	4	6	0

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	1	1	60	50	1	4	5	0
31	1	1	55	45	1	4	5	0
31	1	1	65	55	1	4	5	0
31	1	1	65	55	1	4	5	0
31	1	1	65	55	1	4	5	0
31	1	1	65	55	1	4	5	0
31	1	1	65	55	1	4	5	0
31	1	1	54	44	1	4	5	0
31	2	1	65	55	1	4	5	0
31	2	1	55	45	1	4	5	0
31	2	1	54	44	1	4	5	0
31	2	1	60	50	1	4	5	0
31	2	1	60	50	1	4	5	0
31	2	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	2	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	43	33	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	5	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	A	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	A	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	B	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	C	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
31	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	N	1	65	55	1	4	5	0
31	N	1	49	39	1	4	5	0
31	N	1	45	35	1	4	5	0
31	N	1	65	55	1	4	5	0
31	N	1	49	39	1	4	5	0
31	N	1	54	44	1	4	5	0
31	N	1	54	44	1	4	5	0
31	R	1	49	39	1	4	5	0
31	R	1	60	50	1	4	5	0
31	R	1	60	50	1	4	5	0
31	R	1	48	38	1	4	5	0
31	R	1	48	38	1	4	5	0
31	R	1	58	48	1	4	5	0
31	R	1	57	47	1	4	5	0
31	R	1	49	39	1	4	5	0
31	R	1	49	39	1	4	5	0
31	R	1	55	45	1	4	5	0
31	R	1	65	55	1	4	5	0
31	S	1	65	55	1	4	5	0
31	S	1	42	34	1	4	3	0
31	S	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	S	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	0	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	0	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	0	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	0	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	0	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	0	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	0	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	0	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	0	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	7	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
31	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	8	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	8	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	8	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	9	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	9	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	9	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	9	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
31	9	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	9	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
31	p	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	q	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	q	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	q	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
31	q	1	43	33	1	4	5	0
			Total	C	Mg	N	O	
31	q	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	a	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	d	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	g	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
31	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	58	48	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	r	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	65	55	1	4	5	0

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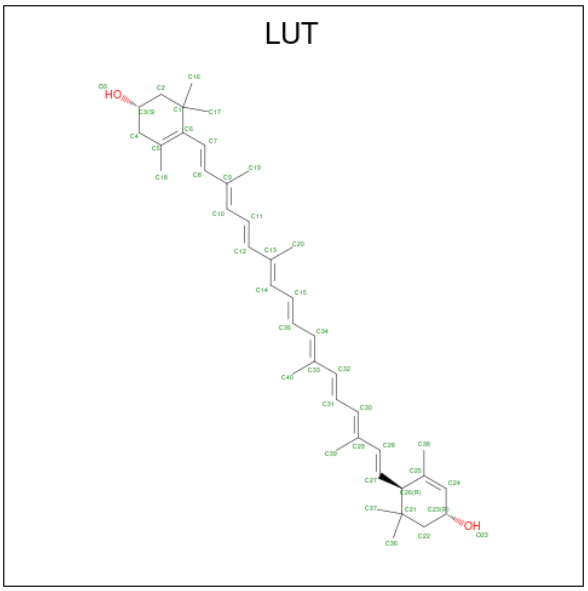
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	54	44	1	4	5	0

- Molecule 32 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	1	1	42	40	2	0
			Total	C	O	
32	1	1	42	40	2	0
			Total	C	O	
32	2	1	42	40	2	0
			Total	C	O	
32	3	1	42	40	2	0
			Total	C	O	
32	3	1	42	40	2	0
			Total	C	O	
32	4	1	42	40	2	0
			Total	C	O	
32	5	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	5	1	42	40	2	0
32	6	1	42	40	2	0
32	6	1	42	40	2	0
32	G	1	42	40	2	0
32	N	1	42	40	2	0
32	N	1	42	40	2	0
32	R	1	42	40	2	0
32	S	1	42	40	2	0
32	S	1	42	40	2	0
32	Y	1	42	40	2	0
32	Y	1	42	40	2	0
32	0	1	42	40	2	0
32	0	1	42	40	2	0
32	7	1	42	40	2	0
32	7	1	42	40	2	0
32	8	1	42	40	2	0
32	8	1	42	40	2	0
32	9	1	42	40	2	0
32	p	1	42	40	2	0
32	p	1	42	40	2	0
32	q	1	42	40	2	0

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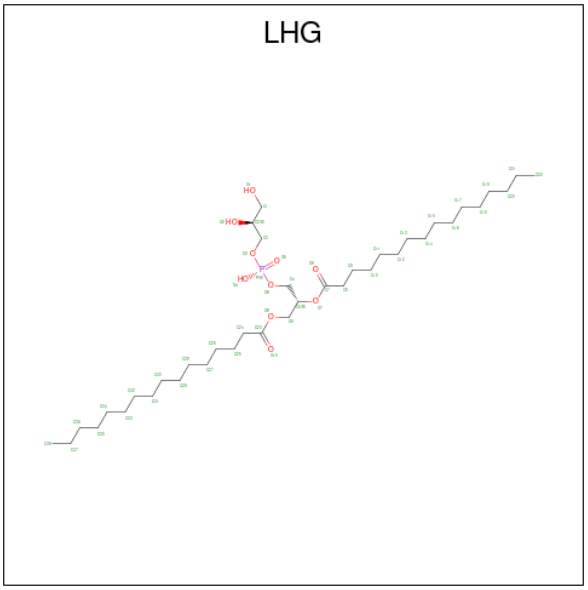
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
32	g	1	42	40	2		0
			Total	C	O		
32	n	1	42	40	2		0
			Total	C	O		
32	n	1	42	40	2		0
			Total	C	O		
32	r	1	42	40	2		0
			Total	C	O		
32	s	1	42	40	2		0
			Total	C	O		
32	s	1	42	40	2		0
			Total	C	O		
32	y	1	42	40	2		0
			Total	C	O		
32	y	1	42	40	2		0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	1	1	35	24	10	1	0
			Total	C	O	P	
33	2	1	49	38	10	1	0
			Total	C	O	P	
33	3	1	33	22	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	4	1	47	36	10	1	0
33	5	1	35	24	10	1	0
33	6	1	37	26	10	1	0
33	A	1	44	33	10	1	0
33	A	1	39	28	10	1	0
33	B	1	49	38	10	1	0
33	C	1	40	29	10	1	0
33	D	1	44	33	10	1	0
33	D	1	49	38	10	1	0
33	G	1	44	33	10	1	0
33	K	1	36	25	10	1	0
33	L	1	49	38	10	1	0
33	M	1	41	30	10	1	0
33	N	1	49	38	10	1	0
33	R	1	38	27	10	1	0
33	S	1	41	30	10	1	0
33	S	1	44	33	10	1	0
33	Y	1	42	31	10	1	0
33	0	1	36	25	10	1	0
33	7	1	35	24	10	1	0
33	8	1	49	38	10	1	0

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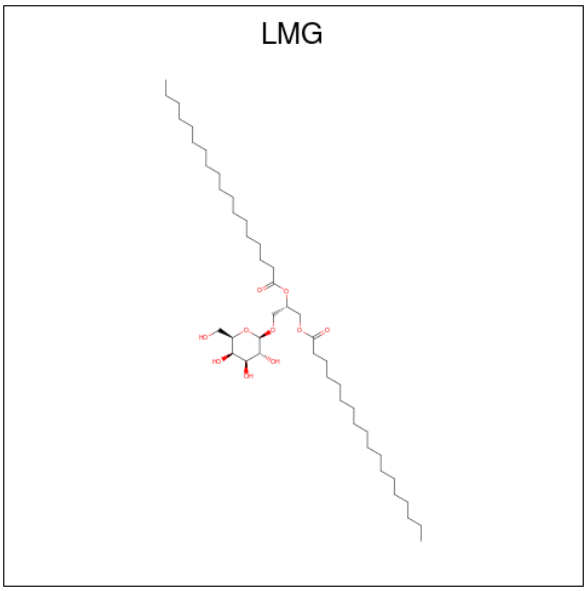
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	9	1	33	22	10	1	0
33	p	1	35	24	10	1	0
33	q	1	46	35	10	1	0
33	a	1	39	28	10	1	0
33	b	1	44	33	10	1	0
33	b	1	49	38	10	1	0
33	c	1	47	36	10	1	0
33	d	1	49	38	10	1	0
33	e	1	44	33	10	1	0
33	g	1	44	33	10	1	0
33	j	1	49	38	10	1	0
33	l	1	49	38	10	1	0
33	n	1	49	38	10	1	0
33	r	1	38	27	10	1	0
33	s	1	41	30	10	1	0
33	s	1	44	33	10	1	0
33	t	1	41	30	10	1	0
33	y	1	46	35	10	1	0
33	z	1	36	25	10	1	0
33	F1	1	35	24	10	1	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	1	1	38	28	10	0
34	2	1	38	28	10	0
34	2	1	51	41	10	0
34	2	1	40	30	10	0
34	3	1	38	28	10	0
34	4	1	51	41	10	0
34	4	1	40	30	10	0
34	5	1	38	28	10	0
34	6	1	42	32	10	0
34	6	1	39	29	10	0
34	6	1	38	28	10	0
34	A	1	41	31	10	0
34	A	1	38	28	10	0
34	A	1	38	28	10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	B	1	51	41	10	0
			Total	C	O	
34	B	1	38	28	10	0
			Total	C	O	
34	B	1	38	28	10	0
			Total	C	O	
34	C	1	51	41	10	0
			Total	C	O	
34	C	1	38	28	10	0
			Total	C	O	
34	C	1	32	22	10	0
			Total	C	O	
34	C	1	44	34	10	0
			Total	C	O	
34	D	1	46	36	10	0
			Total	C	O	
34	D	1	46	36	10	0
			Total	C	O	
34	D	1	51	41	10	0
			Total	C	O	
34	D	1	48	38	10	0
			Total	C	O	
34	G	1	38	28	10	0
			Total	C	O	
34	G	1	51	41	10	0
			Total	C	O	
34	G	1	40	30	10	0
			Total	C	O	
34	I	1	38	28	10	0
			Total	C	O	
34	J	1	51	41	10	0
			Total	C	O	
34	J	1	38	28	10	0
			Total	C	O	
34	N	1	38	28	10	0
			Total	C	O	
34	R	1	38	28	10	0
			Total	C	O	
34	S	1	41	31	10	0
			Total	C	O	
34	W	1	55	45	10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	W	1	38	28	10	0
			Total	C	O	
34	W	1	38	28	10	0
			Total	C	O	
34	X	1	38	28	10	0
			Total	C	O	
34	X	1	38	28	10	0
			Total	C	O	
34	Y	1	38	28	10	0
			Total	C	O	
34	0	1	42	32	10	0
			Total	C	O	
34	0	1	38	28	10	0
			Total	C	O	
34	7	1	39	29	10	0
			Total	C	O	
34	7	1	38	28	10	0
			Total	C	O	
34	7	1	38	28	10	0
			Total	C	O	
34	9	1	51	41	10	0
			Total	C	O	
34	9	1	40	30	10	0
			Total	C	O	
34	9	1	38	28	10	0
			Total	C	O	
34	p	1	38	28	10	0
			Total	C	O	
34	q	1	51	41	10	0
			Total	C	O	
34	q	1	40	30	10	0
			Total	C	O	
34	a	1	38	28	10	0
			Total	C	O	
34	a	1	38	28	10	0
			Total	C	O	
34	a	1	38	28	10	0
			Total	C	O	
34	b	1	45	35	10	0
			Total	C	O	
34	b	1	51	41	10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	b	1	38	28	10	0
			Total	C	O	
34	b	1	38	28	10	0
			Total	C	O	
34	b	1	46	36	10	0
			Total	C	O	
34	b	1	38	28	10	0
			Total	C	O	
34	c	1	38	28	10	0
			Total	C	O	
34	c	1	38	28	10	0
			Total	C	O	
34	c	1	44	34	10	0
			Total	C	O	
34	d	1	41	31	10	0
			Total	C	O	
34	d	1	51	41	10	0
			Total	C	O	
34	d	1	48	38	10	0
			Total	C	O	
34	f	1	38	28	10	0
			Total	C	O	
34	g	1	38	28	10	0
			Total	C	O	
34	g	1	49	39	10	0
			Total	C	O	
34	j	1	43	33	10	0
			Total	C	O	
34	k	1	48	38	10	0
			Total	C	O	
34	k	1	38	28	10	0
			Total	C	O	
34	m	1	45	35	10	0
			Total	C	O	
34	n	1	38	28	10	0
			Total	C	O	
34	n	1	40	30	10	0
			Total	C	O	
34	r	1	38	28	10	0
			Total	C	O	
34	s	1	41	31	10	0

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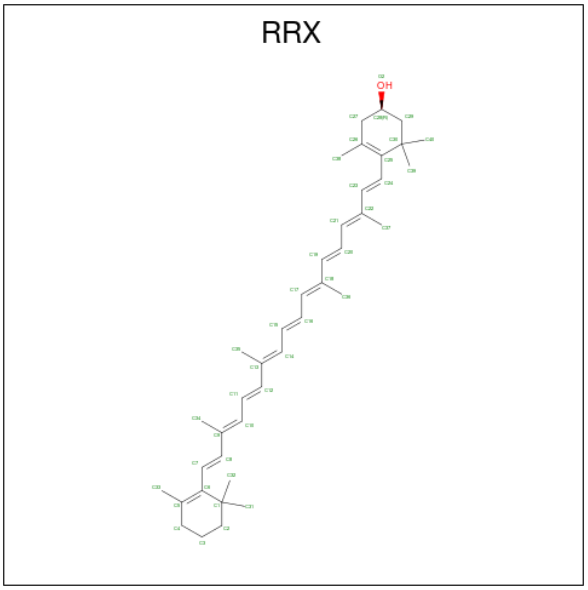
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	w	1	48	38	10	0
34	w	1	55	45	10	0
34	w	1	38	28	10	0
34	w	1	38	28	10	0
34	w	1	38	28	10	0
34	x	1	38	28	10	0
34	y	1	38	28	10	0
34	Q1	1	38	28	10	0
34	q1	1	38	28	10	0

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	2	1	41	40	1	0
35	4	1	41	40	1	0

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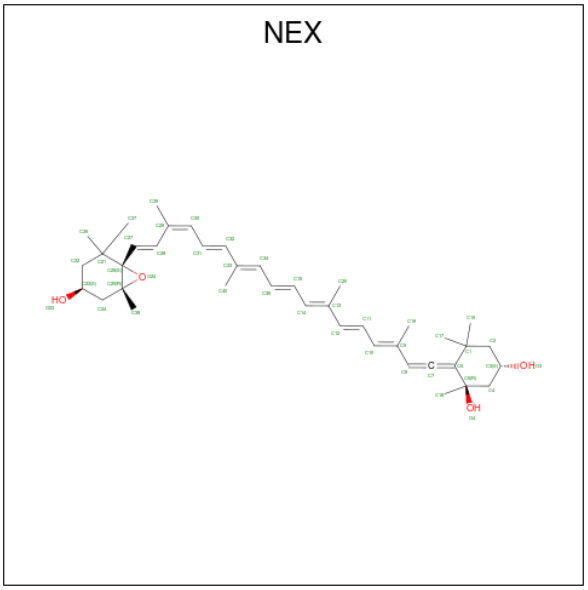
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	G	1	41	40	1	0
35	9	1	41	40	1	0
35	q	1	41	40	1	0
35	g	1	41	40	1	0

- Molecule 36 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	2	1	44	40	4	0
36	3	1	44	40	4	0
36	4	1	44	40	4	0
36	5	1	44	40	4	0
36	6	1	44	40	4	0
36	G	1	44	40	4	0

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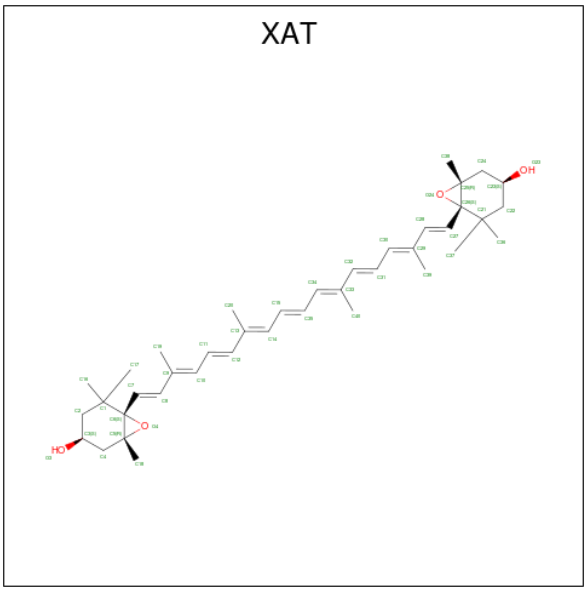
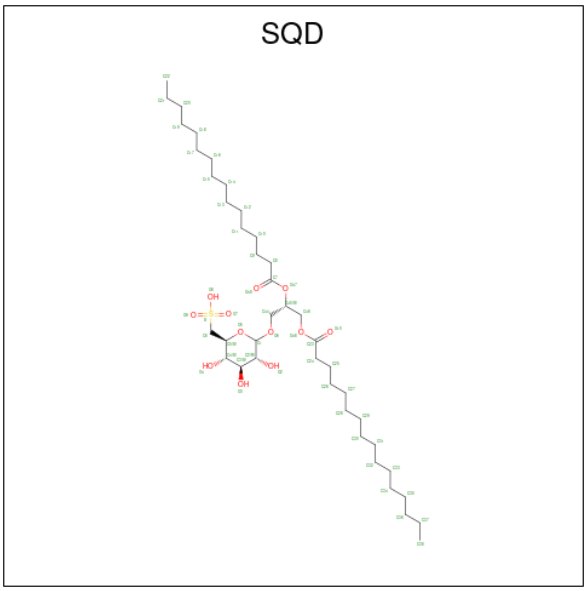
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	N	1	44	40	4	0
36	R	1	44	40	4	0
36	R	1	44	40	4	0
36	S	1	44	40	4	0
36	Y	1	44	40	4	0
36	0	1	44	40	4	0
36	8	1	44	40	4	0
36	9	1	44	40	4	0
36	p	1	44	40	4	0
36	q	1	44	40	4	0
36	g	1	44	40	4	0
36	n	1	44	40	4	0
36	r	1	44	40	4	0
36	r	1	44	40	4	0
36	s	1	44	40	4	0
36	y	1	44	40	4	0

- Molecule 37 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	2	1	44	40	4	0
37	4	1	44	40	4	0
37	G	1	44	40	4	0
37	R	1	44	40	4	0
37	9	1	44	40	4	0
37	q	1	44	40	4	0
37	g	1	44	40	4	0
37	r	1	44	40	4	0

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
38	6	1	Total	C	O	S	0
			42	29	12	1	
38	A	1	Total	C	O	S	0
			51	38	12	1	
38	A	1	Total	C	O	S	0
			45	32	12	1	
38	B	1	Total	C	O	S	0
			54	41	12	1	
38	B	1	Total	C	O	S	0
			52	39	12	1	
38	G	1	Total	C	O	S	0
			42	29	12	1	
38	G	1	Total	C	O	S	0
			38	25	12	1	
38	M	1	Total	C	O	S	0
			50	37	12	1	
38	R	1	Total	C	O	S	0
			51	38	12	1	
38	S	1	Total	C	O	S	0
			51	38	12	1	
38	X	1	Total	C	O	S	0
			38	25	12	1	
38	Y	1	Total	C	O	S	0
			42	29	12	1	
38	0	1	Total	C	O	S	0
			42	29	12	1	
38	a	1	Total	C	O	S	0
			48	35	12	1	

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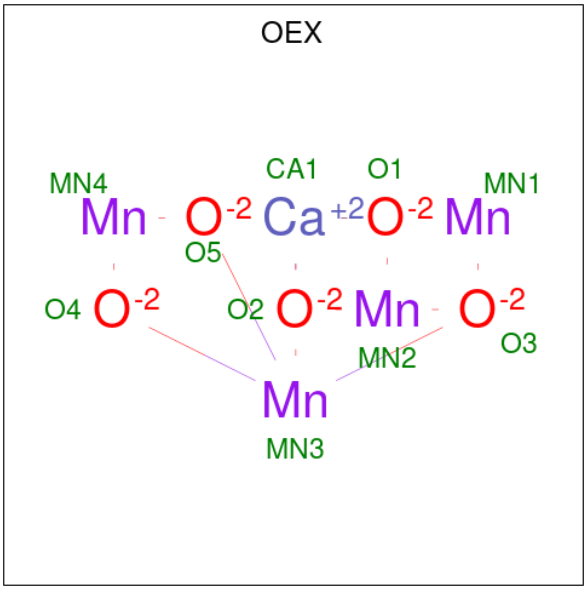
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
38	a	1	45	32	12	1	0
38	b	1	54	41	12	1	0
38	b	1	52	39	12	1	0
38	g	1	38	25	12	1	0
38	g	1	42	29	12	1	0
38	m	1	50	37	12	1	0
38	r	1	51	38	12	1	0
38	s	1	51	38	12	1	0
38	x	1	42	29	12	1	0
38	y	1	42	29	12	1	0

- Molecule 39 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
39	A	1	10	1	4	5	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
39	a	1	10	1	4	5	0

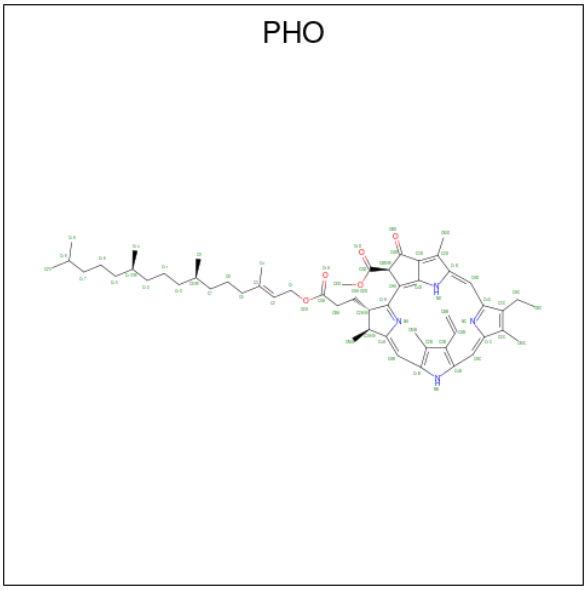
- Molecule 40 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
40	A	1	1	1	0
40	a	1	1	1	0

- Molecule 41 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
41	A	2	2	2	0
41	a	2	2	2	0

- Molecule 42 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
42	A	1	64	55	4	5	0
42	D	1	64	55	4	5	0

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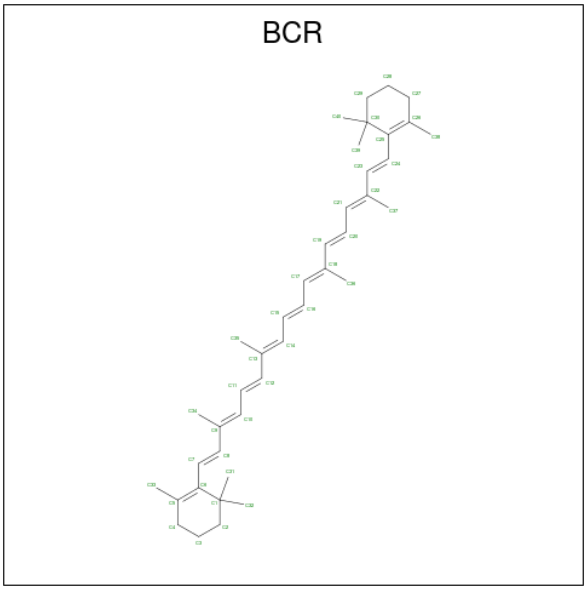
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
42	a	1	64	55	4	5	0
42	d	1	64	55	4	5	0

- Molecule 43 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
43	A	1	40	40	0
43	B	1	40	40	0
43	B	1	40	40	0
43	B	1	40	40	0
43	C	1	40	40	0
43	C	1	40	40	0
43	D	1	40	40	0
43	H	1	40	40	0
43	T	1	40	40	0

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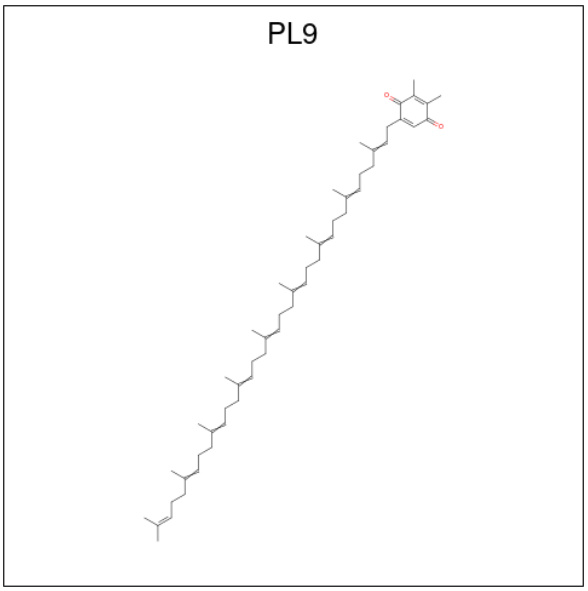
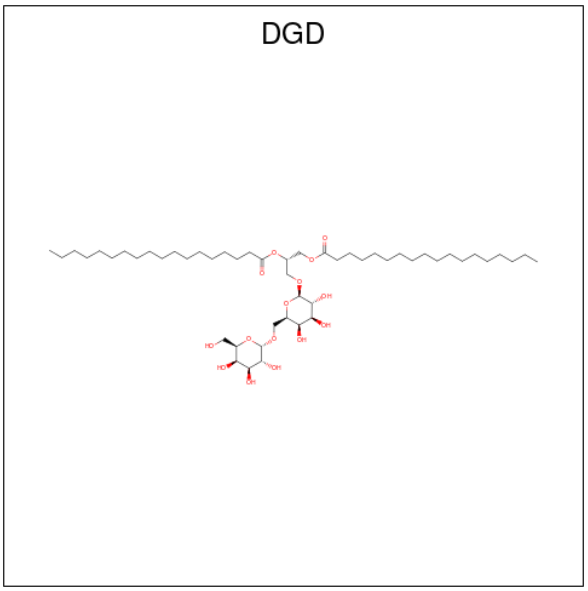
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
43	V	1	40	40	0
43	Z	1	40	40	0
43	a	1	40	40	0
43	b	1	40	40	0
43	b	1	40	40	0
43	b	1	40	40	0
43	c	1	40	40	0
43	c	1	40	40	0
43	d	1	40	40	0
43	h	1	40	40	0
43	t	1	40	40	0
43	v	1	40	40	0
43	z	1	40	40	0

- Molecule 44 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



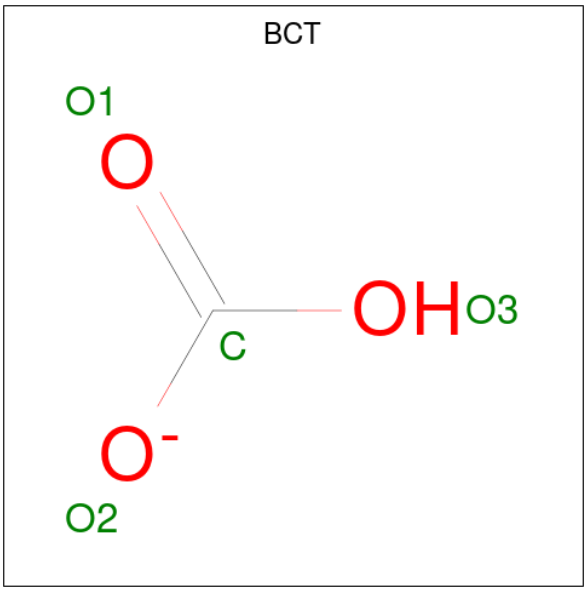
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
44	A	1	55	53	2	0
44	D	1	55	53	2	0
44	a	1	55	53	2	0
44	d	1	55	53	2	0

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



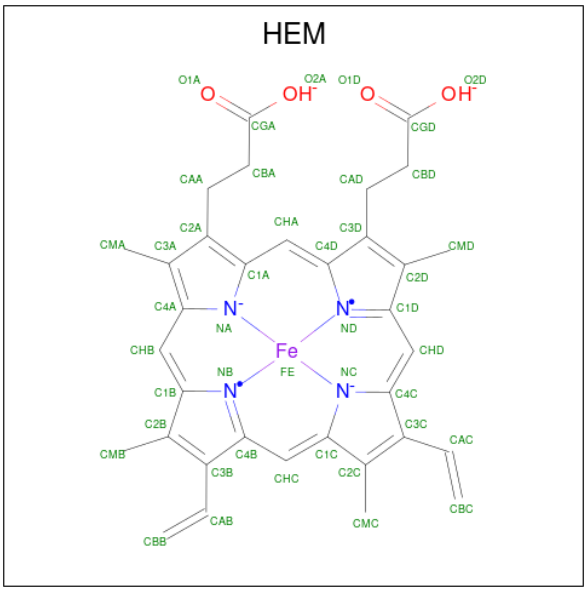
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	C	1	50	35	15	0
45	C	1	66	51	15	0
45	C	1	66	51	15	0
45	C	1	66	51	15	0
45	c	1	66	51	15	0
45	c	1	62	47	15	0
45	c	1	66	51	15	0
45	c	1	66	51	15	0

- Molecule 46 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



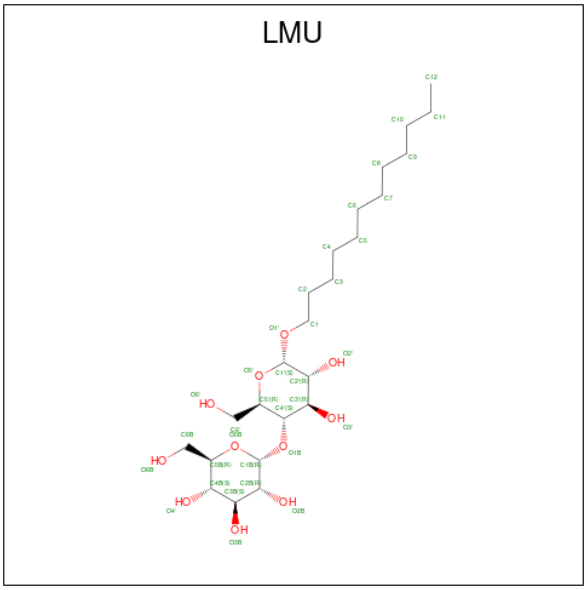
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	D	1	4	1	3	0
46	d	1	4	1	3	0

- Molecule 47 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
47	E	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
47	e	1	43	34	1	4	4	0

- Molecule 48 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	K	1	35	24	11	0
			Total	C	O	
48	R	1	35	24	11	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	c	1	28	17	11	0
48	r	1	35	24	11	0

- Molecule 49 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
49	1	3	3	3	0
49	2	3	3	3	0
49	3	1	1	1	0
49	4	1	1	1	0
49	5	1	1	1	0
49	6	4	4	4	0
49	A	21	21	21	0
49	B	6	6	6	0
49	C	15	15	15	0
49	D	12	12	12	0
49	E	1	1	1	0
49	G	5	5	5	0
49	I	1	1	1	0
49	J	1	1	1	0
49	N	5	5	5	0
49	O	6	6	6	0
49	R	4	4	4	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
49	S	3	3	3	0
			Total	O	
49	T	4	4	4	0
			Total	O	
49	Y	8	8	8	0
			Total	O	
49	0	7	7	7	0
			Total	O	
49	7	6	6	6	0
			Total	O	
49	8	4	4	4	0
			Total	O	
49	9	2	2	2	0
			Total	O	
49	q	1	1	1	0
			Total	O	
49	a	14	14	14	0
			Total	O	
49	b	6	6	6	0
			Total	O	
49	c	15	15	15	0
			Total	O	
49	d	15	15	15	0
			Total	O	
49	e	2	2	2	0
			Total	O	
49	f	1	1	1	0
			Total	O	
49	g	4	4	4	0
			Total	O	
49	j	1	1	1	0
			Total	O	
49	m	2	2	2	0
			Total	O	
49	n	7	7	7	0
			Total	O	
49	o	6	6	6	0
			Total	O	
49	r	4	4	4	0
			Total	O	
49	s	3	3	3	0

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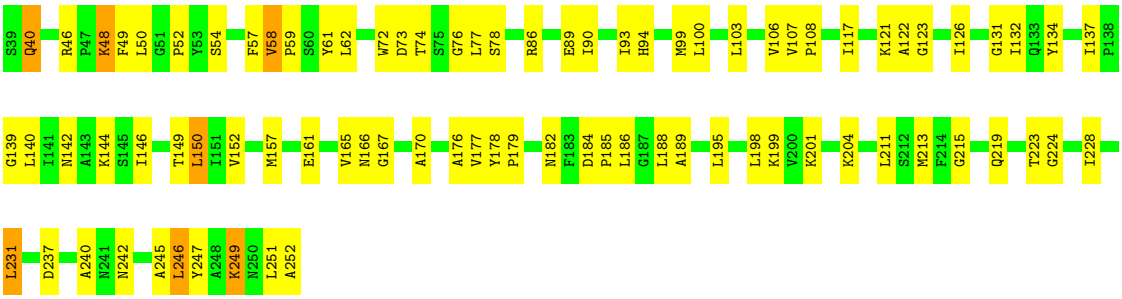
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
49	t	2	2	2	0
			Total	O	
49	w	2	2	2	0
			Total	O	
49	y	8	8	8	0
			Total	O	
49	F1	4	4	4	0
			Total	O	
49	f1	3	3	3	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

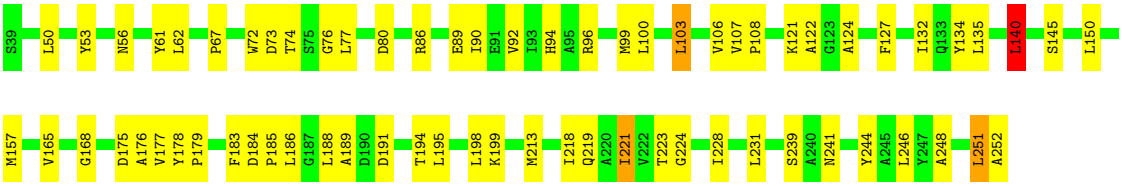
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



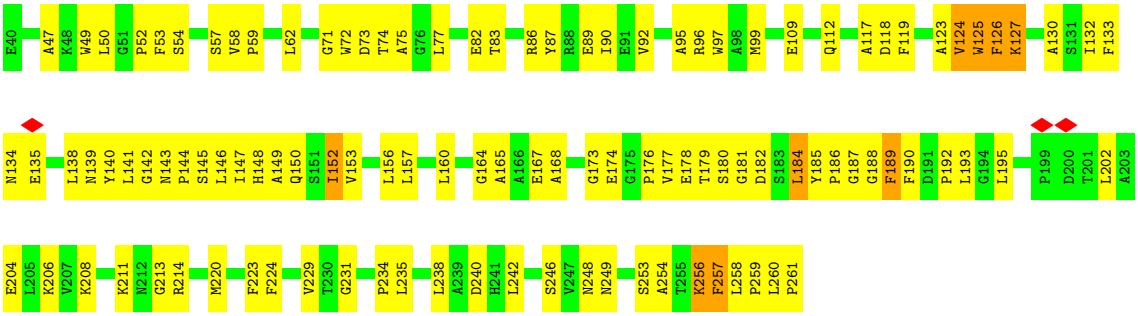
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



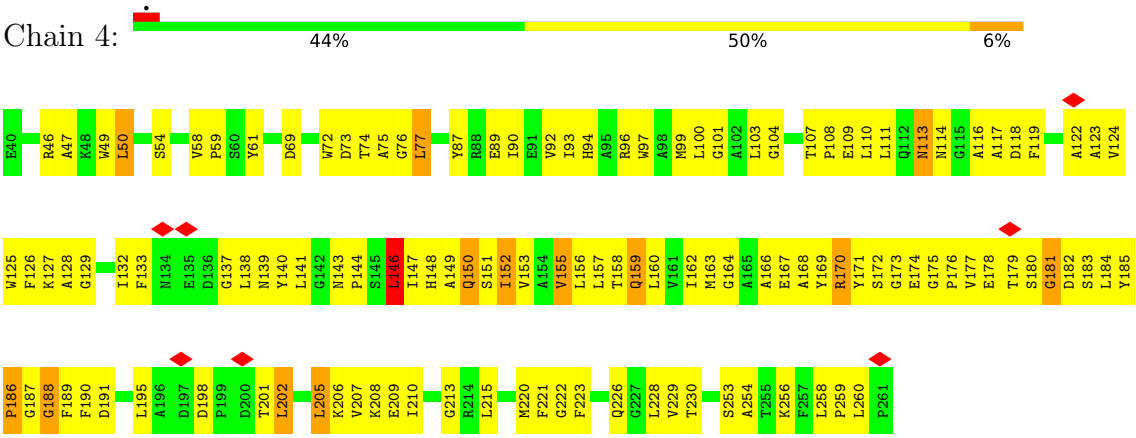
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



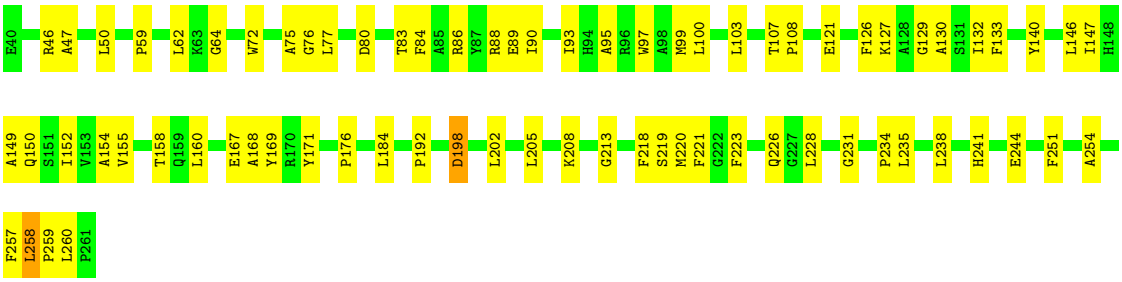
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



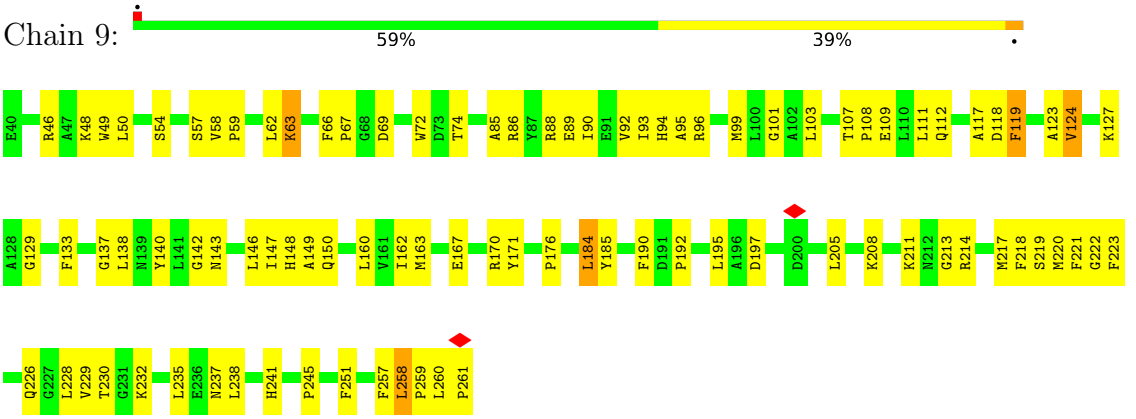
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain G:



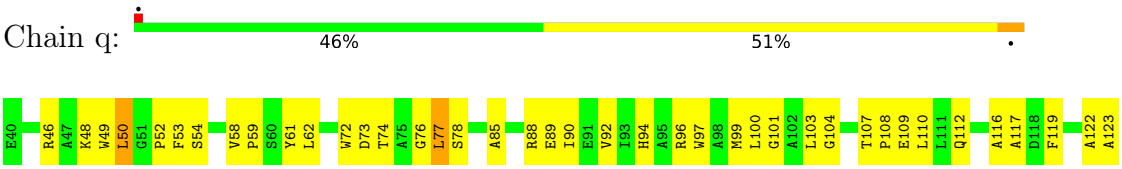
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

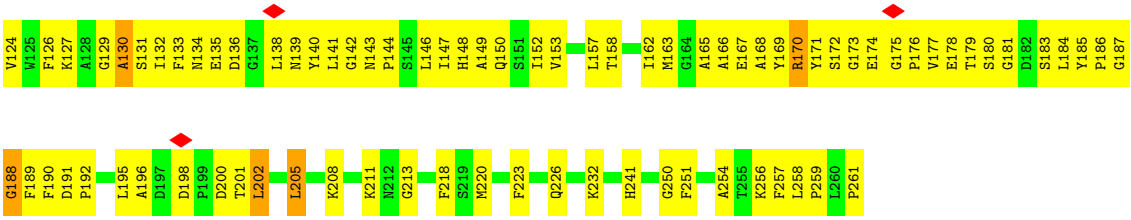
Chain 9:



• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

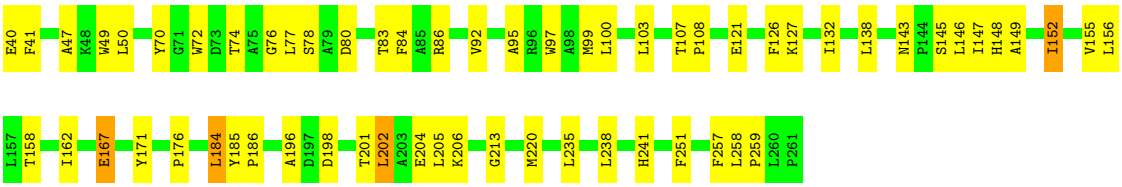
Chain q:





• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain g:

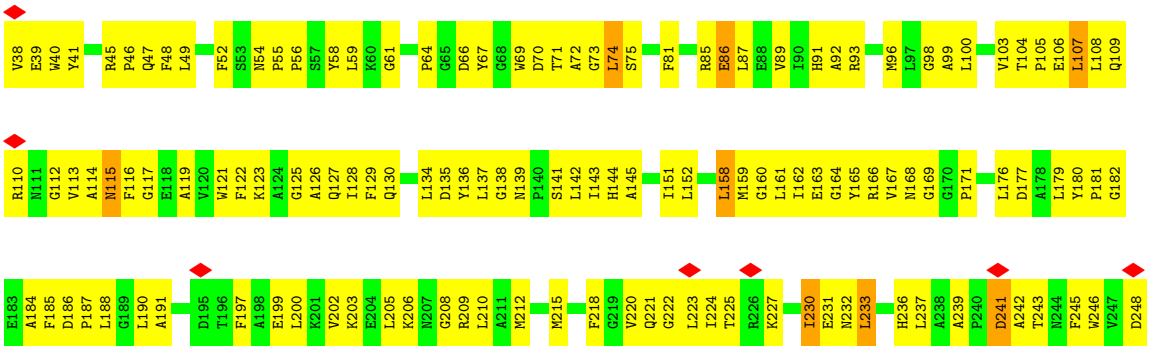


• Molecule 3: Chlorophyll a-b binding of LHCII

Chain 3:

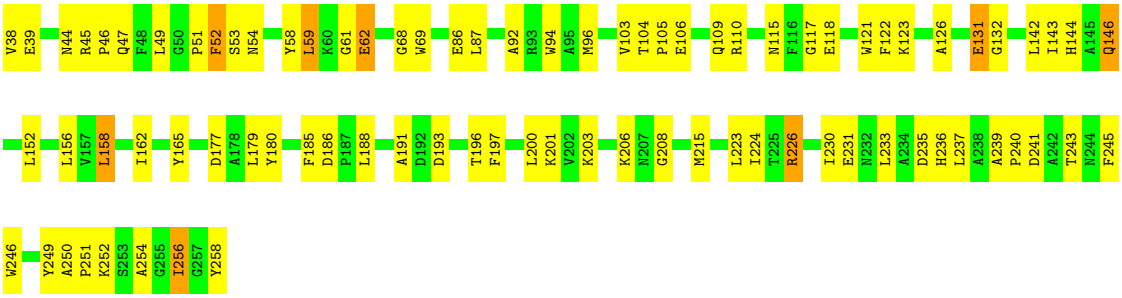
• Molecule 3: Chlorophyll a-b binding of LHCII

Chain 5:



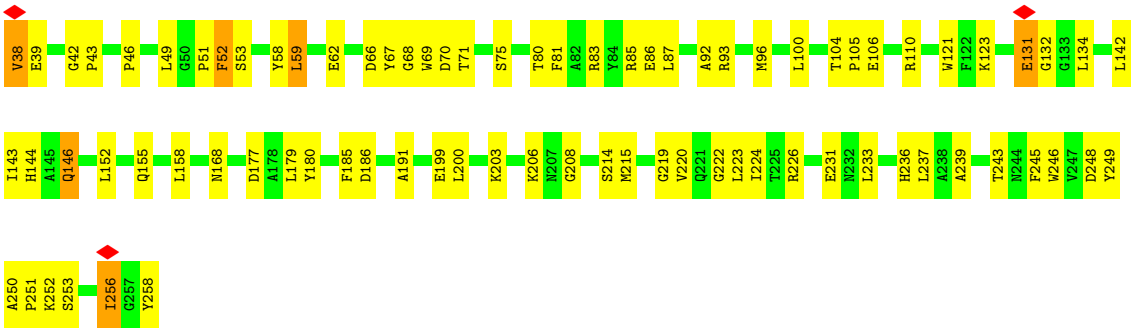
• Molecule 3: Chlorophyll a-b binding of LHCII

Chain N:



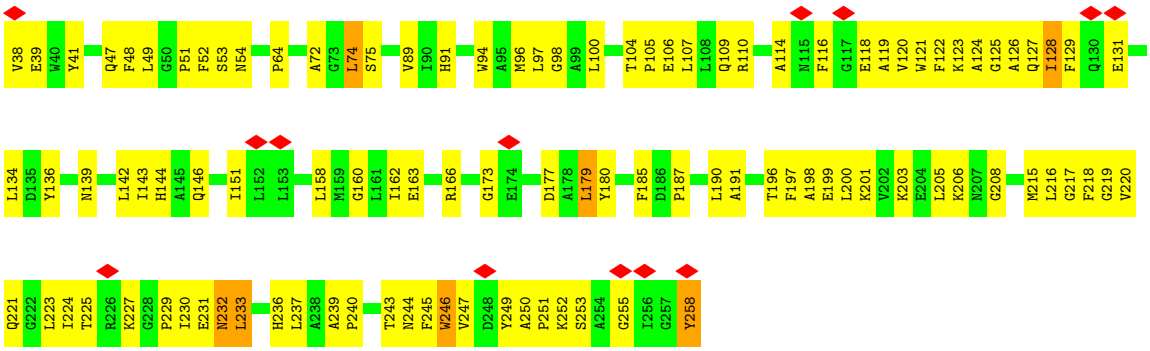
• Molecule 3: Chlorophyll a-b binding of LHCII

Chain 8:



• Molecule 3: Chlorophyll a-b binding of LHCII

Chain p:



• Molecule 3: Chlorophyll a-b binding of LHCII

Chain n:

V38 E39 G42 P43 P46 L49 G50 P51 F52 Y58 L59 E62 D66 Y67 G68 W69 D70 G73 L74 S75 F81 R85 E86 L87 A92 R93 M96 L100 G101 C102 V103 T104 P105 E106 R110 W121 F122 K123 E131 G132 G133 L134 L142 I143

H144 A145 Q146 S147 L152 Q155 L158 I162 N168 G175 L176 D177 A178 L179 Y180 F185 D186 A191 E199 L200 K203 K206 N207 G208 S214 M215 G222 L223 I224 T225 R226 E231 N232 L233 H236 L237 A238 A239 T243 N244 F245 W246 V247 D248

Y249 A250 P251 K252 S253 A254 G255 I256 G257 Y258

- Molecule 4: Chlorophyll a-b binding of LHCII

Chain 6: 66% 31%

E40 D45 F49 L50 F53 S54 Y69 G70 W71 D72 L76 S77 R85 H93 A94 M98 L99 C104 V105 T106 P107 E108 L109 L110 N113 G114 A115 A121 V122 K125 L136 L139 L144 V145 H146 A147 Q148 T156 M161 E165 R168

G172 P173 V177 V178 D179 Y182 D188 G191 L192 A193 L199 L202 K203 V204 K205 K208 N209 G210 M217 F218 G219 F220 F221 I222 Q223 A224 I225 K229 Q233 N234 L235 T244 D245 N246 F247 Y248 S249 L250 Y251 A252 K253 T254 L255 A256

- Molecule 4: Chlorophyll a-b binding of LHCII

Chain 0: 66% 31%

E40 V47 K48 F49 P58 L61 G67 G70 W71 D72 L76 S77 R85 H93 A94 M98 T106 Q111 N117 F118 G119 E120 A121 V122 K125 Q129 I130 F131 Q132 E133 G134 L144 V145 H146 A147 Q148 S149 I150 V151 L154 M161 I164

E165 V169 N170 P173 A174 G175 E176 V177 Y182 P183 D188 P189 L190 G191 L192 A193 D194 D197 T198 L199 L202 K203 V204 K205 E206 I207 G210 M217 F218 G219 F220 F221 I222 Q223 T227 G228 K229 N234 L235 A240 S249 L250 Y251 A252 K253 T254 L255 A256

- Molecule 5: Photosystem II protein D1

Chain A: 76% 22%

E9 R27 L28 V35 L36 M37 I38 P39 T40 L41 L42 T43 V47 P57 R64 Y73 I77 I82 I83 P84 F93 I96 W97 L102 W105 L106 Y107 Y112 Q113 L114 H118 L121 W131 E132 L133 R136 L137 R140 T155 I160

Y161 P162 F168 S169 D170 L174 A188 I192 L193 M194 F197 L210 M214 H215 L218 S221 T228 E229 N230 A250 F255 G256 R257 L258 I259 F260 Q261 Y262 A263 S264 L275 W278 P279 I283 T286 A287 L288 T292 M293 G299 N303

Q304 V307 D308 R312 V313 W317 A324 N325 L326 G327 M328 E333 R334 N335 A336 L341 D342 L343 A344

- Molecule 5: Photosystem II protein D1

Chain a: 77% 21%

E9 S10 A15 C18 E19 L28 W32 V35 I38 L41 S46 V47 F48 I49 I50 A51 A54 A55 I60 L72 I77 I82 I83 P84 F93 S101 L106 Y112 Q113 L114 H118 F119 F120 L121 W131 E132 L133 R136 L137

R140 P141 V151 T155 I159 I160 Y161 P162 Q165 F168 L174 A188 N191 I192 L193 M194 H198 G201 S221 S222 L223 T227 E235 R257 L258 I259 A263 M266 N267 L275 W278 P279 I283 T286 M293 N296 Q304

V307 R312 V313 A324 M328 R334 L341 D342 L343 A344

• Molecule 6: Photosystem II CP47 reaction center protein

Chain B: 80% 19% •

G2 Y6 T10 V11 V12 L13 V22 H23 L24 M25 H26 L29 V30 W33 A34 G35 S36 M37 A38 F39 A43 V51 L52 R57 F65 S74 W75 W91 E94 I101 I102 L103 H114 F123 R124 P131 H142 L145 L148 L149

F156 T159 G160 L161 F162 V181 D186 H201 H202 I203 A204 L214 F215 H216 R224 L225 Y226 R230 M231 T236 V237 A243 A244 V245 F246 W247 V252 W257 R272 D276 L292 S297 Q300 E307 F311 N317 G322 I336

W340 V345 D348 K349 F362 T365 V368 V369 K373 P382 F383 R384 R385 S391 I392 E393 D413 R422 R423 F430 L437 D440 T445 F462 F463 F464 G465 H466 H469 T473 D477 D485 L486 D487 V490 E491 F492 L498

R505

• Molecule 6: Photosystem II CP47 reaction center protein

Chain b: 77% 22% •

G2 L3 Y6 R7 T10 V11 V12 L13 V22 H23 L24 M25 H26 L29 V30 W33 A34 G35 S36 F39 D46 V51 L52 N53 P54 M55 W56 R57 Q58 S74 W75 G82 W91 E94 A99 H100 I101 I112 W113 H114 W115 E121 R124

H142 L149 F156 T159 G160 L161 A180 V181 H201 H202 I203 A204 I207 L214 F215 H216 L217 C218 R224 L225 R230 T236 V237 L238 A243 F246 W247 V252 Y258 P270 T271 R272 W275 F280 I284 Q289 L292 E307

Y312 D313 Y314 I315 G316 N317 N318 K321 G328 N331 S332 G333 D334 W340 L341 D348 K349 R357 T361 F362 F366 P367 V368 V369 D374 R385 S391 V395 V399 D413 V417 R422 R423 A424 Q425 I429 F430 S439 D440 T445

W450 F451 A454 F458 F462 F463 F464 G465 H466 H469 D477 Q489 L496 K497 L498 T503 R504 R505

• Molecule 7: Photosystem II CP43 reaction center protein

Chain C: 73% 24% •

G13 R14 W23 G26 L30 K36 A40 H41 N56 L74 L77 L83 V101 L105 A111 V112 L113 H120 V123 E126 F132 P133 F134 F135 G136 K142 N143 K144 H145 T146 L149 G150 I151 H152 L153 I154 Y155 L156 G157 L158 V164

W165 K166 I173 Y174 D175 D183 V184 R185 I186 I187 P194 G195 G199 Y200 L201 F202 R203 S204 P205 D209 G210 W211 I212 D216 E219 T222 H225 I228 H239 K243 P244 W245 A246 W247 A248 R249 R250 W254 S261 L264 M270 A274

S287 E296 Q299 T302 F303 T304 F305 L306 V307 R308 D309 Q320 G326 K327 Y328 E336 I337 I338 T343 M344 R345 F346 W347 D348 P356 L357 R358 N361 L368 K369 I372 Q373 P374 R378 A381 M384 T385 S391 L392 N393 S394 V398 E401

I402 N403 N406 Y407 V408 S412 W413 T416 S417 H418 F419 F426 H429 H432 A433 A440 R449 V454 L460

- Molecule 7: Photosystem II CP43 reaction center protein

Chain c: 71% 26% •

G13 R14 W23 W24 A25 G26 L30 G35 K36 A40 H41 W51 M55 N56 A61 P68 E71 L74 I75 L76 L77 D95 T96 Y97 P98 Y99 F100 V101 V104 L105 V112 L113 G117 V118 Y119 H120 S121 L122 V123 G124 P125 E126 E129 E130 S131

F132 P133 F134 F135 G136 K142 I151 H152 L153 I154 V155 L156 L162 L163 V164 W165 K166 F170 I173 W177 D183 V184 V192 F198 L201 F202 R203 S204 P205 F206 W211 E219 H225 W238 H239 I240 V253 W254 S261 L264 G265 A266 I267

M270 A274 C275 Y285 E296 T302 L306 Q310 V316 T323 G324 L325 G326 K327 Y328 R331 T334 G335 E336 I337 I338 F339 T343 W347 D348 F349 R350 G351 E355 P356 L357 N361 D364 K367 I372 Q373 P388 L389 L392 N393

S394 V398 A399 V408 S409 P410 R411 S412 W413 H418 F419 F425 F426 L430 W431 H432 A433 G434 R437 R449 E452 R458 P459 L460

- Molecule 8: Photosystem II D2 protein

Chain D: 75% 24% •

K11 R12 F15 D16 D20 F27 V28 L35 L36 P39 T40 A41 G46 F49 T50 G51 T52 T53 F54 V55 T56 Y67 L74 H87 L90 F91 L92 A97 L107 F113 H117 G118 S121 L122 I123 M126 L127 F130 E131 R134

R139 A143 A148 P149 I150 S155 V156 F157 L158 I159 G166 P171 I178 F179 R180 Q186 H189 N190 W191 T192 L193 M199 G200 V201 A202 L210 I213 A216 N220 F223 R233 Q239 A240 E241 E242 T243 Y244 R251 Q255 I256 F257 G258

F261 K264 V274 P275 V276 L279 L289 L293 R294 D297 R304 Y315 T316 K317 L320 R326 L352

- Molecule 8: Photosystem II D2 protein

Chain d: 75% 23% •

K11 R12 D16 D20 R24 V28 W32 P39 T40 A41 L45 F49 T50 G51 V55 T56 S66 L74 L90 F91 L92 W93 Q98 T102 L107 L110 H117 I123 M126 L127 F130 R134 S135 V136 K137 I138 R139 P140

A145 F146 S147 A148 P149 F153 F157 L158 I159 Y160 P161 L162 G163 Q164 P171 I178 Q186 H189 N190 W191 T192 L193 H197 M198 M199 G200 I213 N220 R233 P237 T238 Q239 A240 E241 S245 T248 W253 S254 Q255 I256 F257 F261 W266

L272 F273 V274 P275 V276 L279 S282 L289 A290 L291 N292 L293 R294 E312 K317 L320 E323 V340 V345 A351 L352

• Molecule 9: Cytochrome b559 subunit alpha

Chain E: 74% 25%

S2 E7 R8 D12 I13 L14 R18 Y19 I22 H23 S24 I25 T26 I27 P28 D45 P50 E62 T63 P64 T67 L79 V82

• Molecule 9: Cytochrome b559 subunit alpha

Chain e: 67% 33%

S2 R8 P9 F10 S11 D12 I13 Y19 H23 S24 I25 T26 I27 P28 F37 T40 Y44 F47 G48 S49 P50 Y55 R60 Q61 L65 I66 T67 D68 N71 E74 K78 V82

• Molecule 10: Cytochrome b559 subunit beta

Chain F: 54% 46%

K8 I14 F15 R18 W19 L20 H23 A24 L25 A26 V27 P28 T29 V30 F31 F32 L33 M39 Q43 R44

• Molecule 10: Cytochrome b559 subunit beta

Chain f: 59% 41%

K8 Y12 P13 I14 F15 R18 L25 A26 V27 P28 T29 V30 F31 F32 A35 M39 Q43 R44

• Molecule 11: Photosystem II reaction center protein H

Chain H: 84% 15%

D19 W44 V62 E66 N69 L74 D75 D76 V77 T78 S83 L84 A85

• Molecule 11: Photosystem II reaction center protein H

Chain h: 79% 21%

D19 I22 K31 Y37 P42 G43 W44 G45 T46 L56 F57 V62 E66 N69 L74 D75 D76 V77 A85

• Molecule 12: Photosystem II reaction center protein I

Chain I: 79% 21%

M1 L2 T3 L4 K5 I6 S25 N26 D27 P28 Q34

• Molecule 12: Photosystem II reaction center protein I

Chain i: 79% 21%

M1 L4 Y9 V12 L24 D27 P28 G29 R30 Q34

• Molecule 13: Photosystem II reaction center protein J

Chain J: 92% • 5%

G5 T6 L12 L42

• Molecule 13: Photosystem II reaction center protein J

Chain j: 84% 13% •

G5 R9 L12 G28 I29 F30 S40 S41 L42

• Molecule 14: Photosystem II reaction center protein K

Chain K: 59% 38% •

K10 Y15 A16 P17 F18 D19 P20 I21 V22 D23 V24 L25 P26 V27 V30 L33 L34 L35 A36 L37 V38 R46

• Molecule 14: Photosystem II reaction center protein K

Chain k: 70% 27% •

K10 L11 P12 Y15 A16 P17 L25 P26 L33 L34 L35 A36 L37 V38 R46

• Molecule 15: Photosystem II reaction center protein L

Chain L: • 68% 32%

A2 K8 E12 L13 N14 R15 T16 W20 L23 L24 V27 L28 A29 V30 Y35 I36 F37 N38

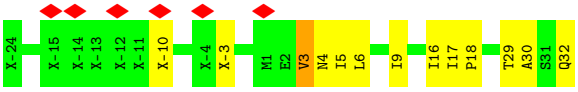
• Molecule 15: Photosystem II reaction center protein L

Chain l: • 70% 27% •

A2 K3 T16 W20 G21 L22 L23 L24 I25 F26 V27 L28 A29 V30 Y35 I36 F37 N38

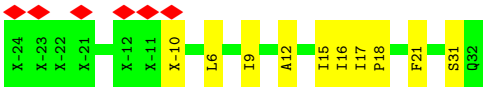
• Molecule 16: Photosystem II reaction center protein M

Chain M:



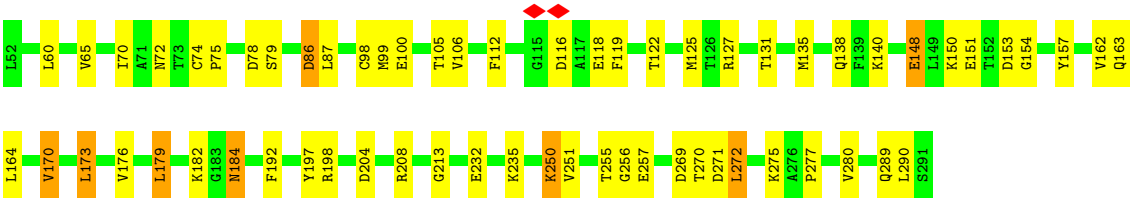
• Molecule 16: Photosystem II reaction center protein M

Chain m:



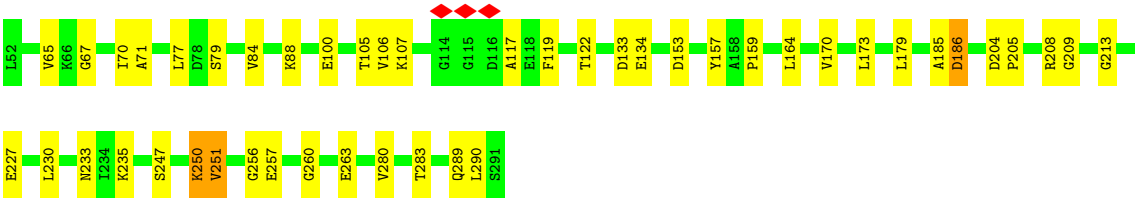
• Molecule 17: Chloroplast oxygen-evolving enhancer protein 1

Chain O:



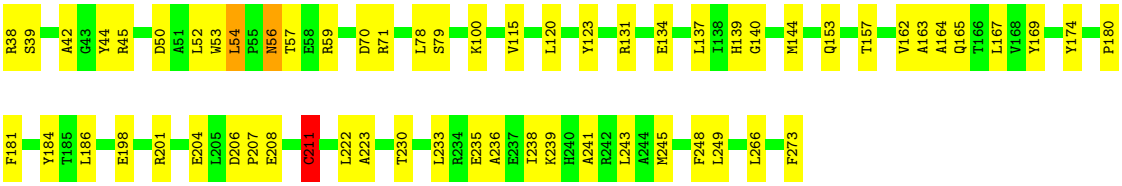
• Molecule 17: Chloroplast oxygen-evolving enhancer protein 1

Chain o:



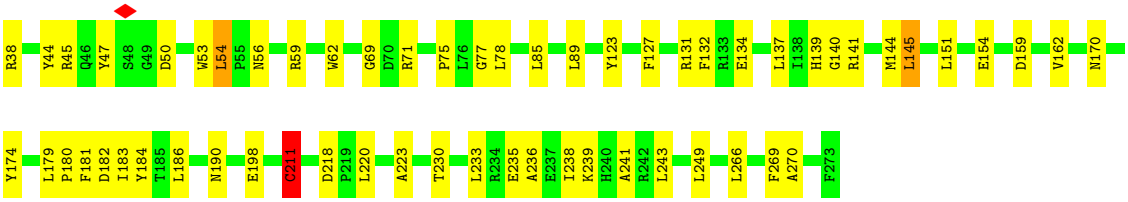
• Molecule 18: Chlorophyll a b binding CP29

Chain R:



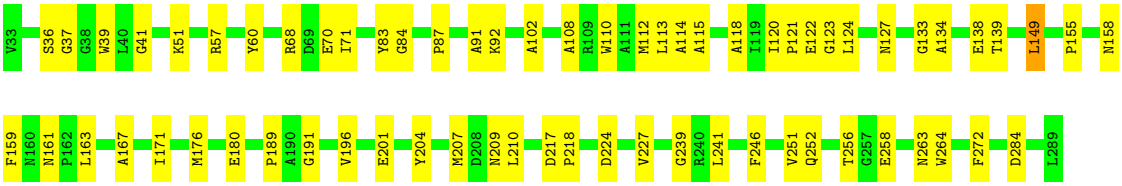
• Molecule 18: Chlorophyll a b binding CP29

Chain r:



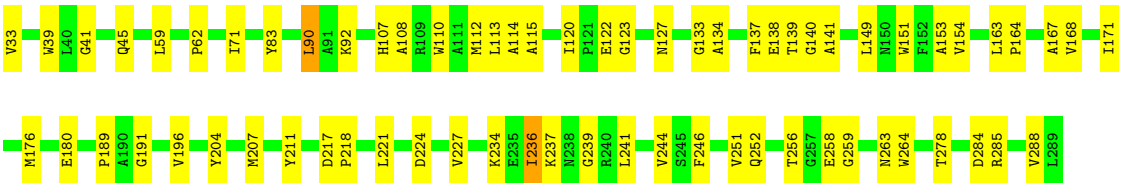
• Molecule 19: Chlorophyll a b-binding CP26

Chain S: 74% 25%



• Molecule 19: Chlorophyll a b-binding CP26

Chain s: 74% 26%

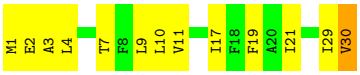


• Molecule 20: Photosystem II reaction center protein T

Chain T: 70% 30%

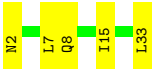
• Molecule 20: Photosystem II reaction center protein T

Chain t: 57% 40%



• Molecule 21: Photosystem II reaction center protein Ycf12

Chain V: 84% 16%



• Molecule 21: Photosystem II reaction center protein Ycf12

Chain v: 88% 12%

N2 I5 L9 I15 L33

• Molecule 22: Photosystem II reaction center W protein

Chain W: 60% 38%

L60 V61 D62 E68 G71 K72 I73 I76 N77 D78 L81 A84 I85 T86 I87 V88 F89 T90 I91 V92 W93 T100 I103 S107 D108 R109 E110 N111 D112 G116 L117 T118 L119

• Molecule 22: Photosystem II reaction center W protein

Chain w: 68% 32%

L60 G67 T70 I73 S80 A84 I85 T86 F89 T90 W93 G94 V98 S99 T100 R101 E102 R109 E110 N111 F115 G116 L117 T118 L119

• Molecule 23: Photosystem II reaction center protein X

Chain X: 70% 30%

A64 L72 V76 G79 V82 L83 I86 A87 G88 A89 I90 T91 F96 R100

• Molecule 23: Photosystem II reaction center protein X

Chain x: 81% 19%

A64 V76 G79 V82 I86 A87 G88 T91 F96 R100

• Molecule 24: Multifunctional fusion protein

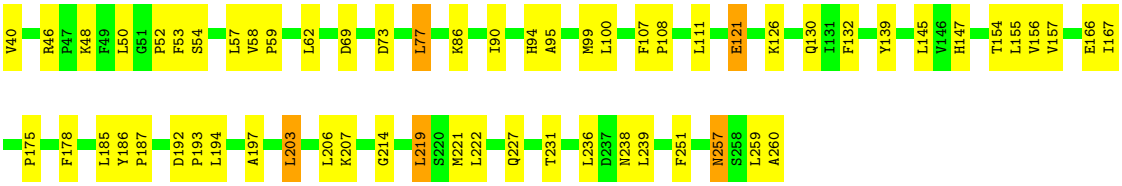
Chain Y: 78% 21%

V40 P47 L50 G51 P52 F53 S54 D55 G56 L57 L62 Y70 L77 K86 I90 H94 A95 R96 W97 A98 M99 L100 F107 P108 G116 K126 F132 N142 L145 V146 H147 T154 L155 V156 V157 I167 Y168 P175 N176 G177 F178 L185

Y186 P187 D192 P193 L194 A197 L203 L206 K209 G214 L219 L222 L236 L239 Y252 A260

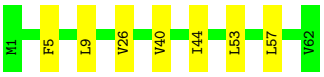
• Molecule 24: Multifunctional fusion protein

Chain y: 72% 25%



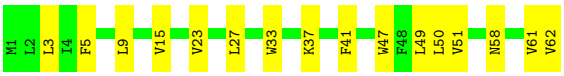
• Molecule 25: Photosystem II reaction center protein Z

Chain Z: 89% 11%



• Molecule 25: Photosystem II reaction center protein Z

Chain z: 74% 26%

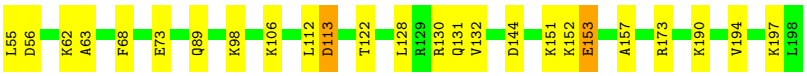


• Molecule 26: Chloroplast oxygen-evolving enhancer protein 3

Chain U: 86% 14%

• Molecule 26: Chloroplast oxygen-evolving enhancer protein 3

Chain u: 83% 16%

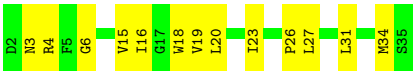


• Molecule 27: Chloroplast PsbY

Chain Q1: 76% 24%

• Molecule 27: Chloroplast PsbY

Chain q1: 62% 38%

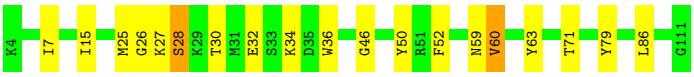


• Molecule 28: Chloroplast photosystem II 10 kDa protein

Chain P1: 88% 12%

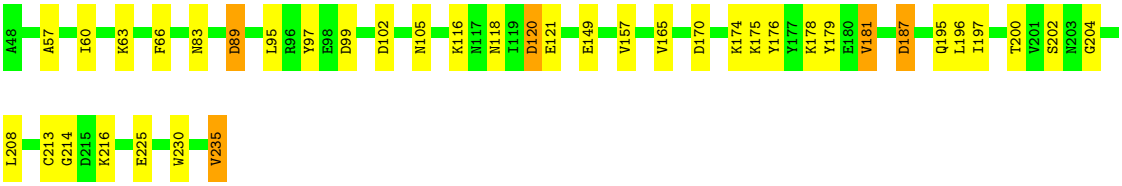
• Molecule 28: Chloroplast photosystem II 10 kDa protein

Chain p1: 82% 16% •



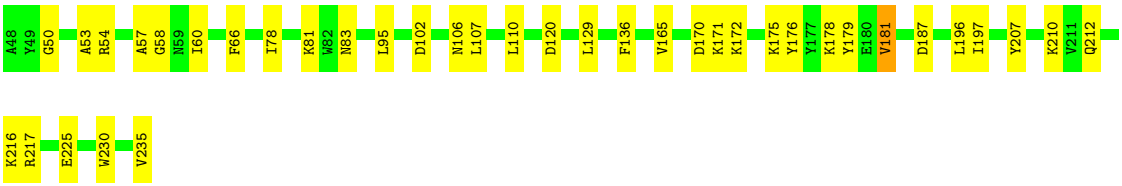
• Molecule 29: Photosystem II oxygen evolving enhancer 2

Chain F1: 79% 18% •



• Molecule 29: Photosystem II oxygen evolving enhancer 2

Chain f1: 80% 20% •



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94893	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	460.8, 460.8, 460.8	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9216, 0.9216, 0.9216	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, BCR, CSU, RRX, DGD, FE2, PL9, BCT, NEX, CL, LHG, XAT, CLA, SQD, LMG, OEX, PHO, HEM, LMU, LUT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1	0.72	1/1675 (0.1%)	0.89	0/2283
1	7	0.68	0/1675	0.88	0/2283
2	2	0.70	0/1734	0.91	1/2359 (0.0%)
2	4	0.76	0/1732	0.98	1/2355 (0.0%)
2	9	0.64	0/1734	0.85	0/2359
2	G	0.50	0/1734	0.66	0/2359
2	g	0.53	0/1734	0.69	0/2359
2	q	0.76	0/1732	0.98	1/2355 (0.0%)
3	3	0.67	0/1734	0.90	1/2362 (0.0%)
3	5	0.90	0/1734	1.14	1/2362 (0.0%)
3	8	0.73	0/1734	0.91	0/2362
3	N	0.72	0/1734	0.92	0/2362
3	n	0.72	0/1734	0.91	0/2362
3	p	0.57	0/1734	0.75	0/2362
4	0	0.42	0/1701	0.60	0/2315
4	6	0.49	0/1701	0.65	0/2315
5	A	0.33	0/2714	0.40	0/3701
5	a	0.38	0/2714	0.47	0/3701
6	B	0.32	0/4085	0.37	0/5564
6	b	0.38	0/4085	0.48	0/5564
7	C	0.35	0/3602	0.42	1/4910 (0.0%)
7	c	0.41	0/3602	0.50	0/4910
8	D	0.42	0/2825	0.53	0/3849
8	d	0.43	0/2825	0.52	0/3849
9	E	0.55	0/670	0.69	0/913
9	e	0.71	0/670	0.87	0/913
10	F	0.71	0/312	0.89	0/426
10	f	0.79	0/312	1.02	0/426
11	H	0.24	0/518	0.30	0/708
11	h	0.24	0/518	0.32	0/708
12	I	0.64	0/282	0.76	0/382

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	i	0.60	0/282	0.75	0/382
13	J	0.18	0/276	0.24	0/377
13	j	0.28	0/276	0.30	0/377
14	K	0.27	0/305	0.40	0/420
14	k	0.24	0/305	0.42	0/420
15	L	0.41	0/311	0.53	0/422
15	l	0.42	0/311	0.54	0/422
16	M	0.27	0/248	0.45	0/338
16	m	0.24	0/248	0.39	0/338
17	O	0.36	0/1823	0.48	0/2466
17	o	0.35	0/1823	0.46	0/2466
18	R	0.51	0/1850	0.64	0/2515
18	r	0.60	0/1850	0.75	0/2515
19	S	0.44	0/1985	0.61	0/2711
19	s	0.45	0/1985	0.62	0/2711
20	T	0.25	0/253	0.32	0/343
20	t	0.45	0/253	0.57	0/343
21	V	0.13	0/234	0.28	0/319
21	v	0.13	0/234	0.25	0/319
22	W	0.74	0/477	0.90	0/650
22	w	0.74	0/477	0.91	0/650
23	X	0.55	0/248	0.76	0/339
23	x	0.61	0/248	0.79	0/339
24	Y	0.34	0/1735	0.43	1/2359 (0.0%)
24	y	0.32	0/1735	0.39	0/2359
25	Z	0.19	0/491	0.31	0/672
25	z	0.18	0/491	0.28	0/672
26	U	0.24	0/1132	0.35	0/1521
26	u	0.21	0/1132	0.31	0/1521
27	Q1	0.55	0/265	0.69	0/362
27	q1	0.55	0/265	0.75	0/362
28	P1	0.36	0/835	0.47	0/1127
28	p1	0.34	0/835	0.45	0/1127
29	F1	0.49	0/1473	0.60	0/1991
29	f1	0.57	0/1473	0.68	0/1991
All	All	0.51	1/85454 (0.0%)	0.65	7/116284 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	1
18	r	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	VAL	N-CA	5.14	1.49	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	126	PHE	CA-CB-CG	6.76	120.56	113.80
3	5	112	GLY	CA-C-O	-5.73	118.32	122.45
3	3	122	PHE	CA-CB-CG	5.68	119.48	113.80
2	q	130	ALA	N-CA-C	-5.51	106.46	114.12
24	Y	55	ASP	N-CA-C	-5.25	108.64	114.62
7	C	211	TRP	CB-CA-C	-5.17	110.60	116.54
2	4	150	GLN	N-CA-C	-5.10	108.81	114.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	211	CSU	Mainchain
18	r	211	CSU	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1630	0	1583	90	0
1	7	1630	0	1583	85	0
2	2	1686	0	1616	136	0
2	4	1685	0	1612	187	0
2	9	1686	0	1616	116	0
2	G	1686	0	1616	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	g	1686	0	1616	49	0
2	q	1685	0	1612	161	0
3	3	1686	0	1635	163	0
3	5	1686	0	1635	219	0
3	8	1686	0	1635	86	0
3	N	1686	0	1635	84	0
3	n	1686	0	1635	78	0
3	p	1686	0	1635	146	0
4	0	1657	0	1612	76	0
4	6	1657	0	1612	91	0
5	A	2632	0	2532	62	0
5	a	2632	0	2532	67	0
6	B	3954	0	3823	83	0
6	b	3954	0	3823	98	0
7	C	3482	0	3375	97	0
7	c	3482	0	3375	112	0
8	D	2730	0	2630	73	0
8	d	2730	0	2630	69	0
9	E	652	0	636	20	0
9	e	652	0	636	25	0
10	F	302	0	311	15	0
10	f	302	0	311	16	0
11	H	507	0	520	8	0
11	h	507	0	520	12	0
12	I	274	0	280	6	0
12	i	274	0	280	6	0
13	J	270	0	282	3	0
13	j	270	0	282	7	0
14	K	295	0	311	11	0
14	k	295	0	311	10	0
15	L	303	0	311	10	0
15	l	303	0	311	13	0
16	M	370	0	302	10	0
16	m	370	0	301	7	0
17	O	1789	0	1759	46	0
17	o	1789	0	1759	29	0
18	R	1818	0	1737	59	0
18	r	1818	0	1736	57	0
19	S	1934	0	1879	62	0
19	s	1934	0	1879	67	0
20	T	246	0	262	8	0
20	t	246	0	262	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	233	0	263	4	0
21	v	233	0	263	4	0
22	W	468	0	450	26	0
22	w	468	0	450	24	0
23	X	247	0	260	7	0
23	x	247	0	260	5	0
24	Y	1688	0	1637	43	0
24	y	1688	0	1637	56	0
25	Z	478	0	513	5	0
25	z	478	0	513	11	0
26	U	1122	0	1151	16	0
26	u	1122	0	1151	13	0
27	Q1	260	0	269	9	0
27	q1	260	0	269	16	0
28	P1	820	0	834	9	0
28	p1	820	0	834	14	0
29	F1	1443	0	1408	25	0
29	f1	1443	0	1408	34	0
30	0	336	0	282	43	0
30	1	441	0	437	52	0
30	2	270	0	219	43	0
30	3	311	0	236	69	0
30	4	327	0	268	67	0
30	5	305	0	221	58	0
30	6	330	0	275	48	0
30	7	443	0	441	53	0
30	8	296	0	270	34	0
30	9	328	0	269	50	0
30	G	344	0	302	50	0
30	N	346	0	306	52	0
30	R	167	0	138	15	0
30	S	182	0	121	16	0
30	Y	350	0	318	49	0
30	g	278	0	233	34	0
30	n	409	0	366	59	0
30	p	305	0	221	44	0
30	q	326	0	265	60	0
30	r	167	0	138	17	0
30	s	182	0	123	20	0
30	y	353	0	327	42	0
31	0	512	0	481	46	0
31	1	494	0	513	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	2	468	0	451	57	0
31	3	559	0	506	82	0
31	4	435	0	386	66	0
31	5	481	0	410	88	0
31	6	535	0	523	67	0
31	7	545	0	552	69	0
31	8	512	0	489	79	0
31	9	437	0	392	62	0
31	A	239	0	242	22	0
31	B	1024	0	1116	92	0
31	C	818	0	870	61	0
31	D	130	0	144	16	0
31	G	457	0	444	55	0
31	N	566	0	539	95	0
31	R	598	0	536	42	0
31	S	627	0	608	65	0
31	Y	484	0	491	56	0
31	a	190	0	203	20	0
31	b	1024	0	1117	98	0
31	c	826	0	888	72	0
31	d	179	0	183	12	0
31	g	457	0	441	44	0
31	n	512	0	489	86	0
31	p	478	0	408	89	0
31	q	432	0	383	63	0
31	r	598	0	534	46	0
31	s	627	0	606	71	0
31	y	538	0	539	68	0
32	0	84	0	112	12	0
32	1	84	0	112	12	0
32	2	42	0	56	8	0
32	3	84	0	112	24	0
32	4	42	0	56	11	0
32	5	84	0	112	38	0
32	6	84	0	112	19	0
32	7	84	0	112	16	0
32	8	84	0	112	18	0
32	9	42	0	56	15	0
32	G	42	0	56	8	0
32	N	84	0	112	22	0
32	R	42	0	56	3	0
32	S	84	0	112	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	84	0	112	12	0
32	g	42	0	56	8	0
32	n	84	0	112	18	0
32	p	84	0	112	24	0
32	q	42	0	56	12	0
32	r	42	0	56	4	0
32	s	84	0	112	24	0
32	y	84	0	112	16	0
33	0	36	0	42	3	0
33	1	35	0	40	5	0
33	2	49	0	74	4	0
33	3	33	0	36	7	0
33	4	47	0	67	5	0
33	5	35	0	40	9	0
33	6	37	0	44	2	0
33	7	35	0	40	3	0
33	8	49	0	74	4	0
33	9	33	0	36	9	0
33	A	83	0	109	8	0
33	B	49	0	74	6	0
33	C	40	0	53	7	0
33	D	93	0	135	12	0
33	F1	35	0	40	1	0
33	G	44	0	61	15	0
33	K	36	0	42	6	0
33	L	49	0	74	4	0
33	M	41	0	55	1	0
33	N	49	0	74	3	0
33	R	38	0	46	1	0
33	S	85	0	113	11	0
33	Y	42	0	57	4	0
33	a	39	0	48	4	0
33	b	93	0	135	21	0
33	c	47	0	67	8	0
33	d	49	0	74	13	0
33	e	44	0	61	7	0
33	g	44	0	61	12	0
33	j	49	0	74	5	0
33	l	49	0	74	11	0
33	n	49	0	74	3	0
33	p	35	0	40	3	0
33	q	46	0	65	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	r	38	0	46	3	0
33	s	85	0	113	11	0
33	t	41	0	55	1	0
33	y	46	0	65	11	0
33	z	36	0	42	3	0
34	0	80	0	100	13	0
34	1	38	0	46	2	0
34	2	129	0	168	14	0
34	3	38	0	46	13	0
34	4	91	0	122	21	0
34	5	38	0	46	11	0
34	6	119	0	148	21	0
34	7	115	0	140	12	0
34	9	129	0	168	32	0
34	A	117	0	144	9	0
34	B	127	0	164	16	0
34	C	165	0	210	17	0
34	D	191	0	262	16	0
34	G	129	0	168	25	0
34	I	38	0	46	5	0
34	J	89	0	118	5	0
34	N	38	0	46	2	0
34	Q1	38	0	46	14	0
34	R	38	0	46	0	0
34	S	41	0	52	2	0
34	W	131	0	178	15	0
34	X	76	0	92	6	0
34	Y	38	0	46	5	0
34	a	114	0	138	12	0
34	b	256	0	332	21	0
34	c	120	0	150	17	0
34	d	140	0	190	11	0
34	f	38	0	46	1	0
34	g	87	0	114	10	0
34	j	43	0	56	4	0
34	k	86	0	112	5	0
34	m	45	0	60	5	0
34	n	78	0	96	20	0
34	p	38	0	46	5	0
34	q	91	0	122	10	0
34	q1	38	0	46	11	0
34	r	38	0	46	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	s	41	0	52	4	0
34	w	217	0	290	35	0
34	x	38	0	46	5	0
34	y	38	0	44	4	0
35	2	41	0	56	12	0
35	4	41	0	56	17	0
35	9	41	0	56	13	0
35	G	41	0	56	28	0
35	g	41	0	56	3	0
35	q	41	0	56	20	0
36	0	44	0	54	10	0
36	2	44	0	54	6	0
36	3	44	0	54	10	0
36	4	44	0	54	8	0
36	5	44	0	54	16	0
36	6	44	0	54	11	0
36	8	44	0	54	4	0
36	9	44	0	54	9	0
36	G	44	0	54	1	0
36	N	44	0	55	7	0
36	R	88	0	108	15	0
36	S	44	0	54	4	0
36	Y	44	0	54	2	0
36	g	44	0	54	2	0
36	n	44	0	54	2	0
36	p	44	0	54	2	0
36	q	44	0	54	4	0
36	r	88	0	108	9	0
36	s	44	0	54	4	0
36	y	44	0	54	5	0
37	2	44	0	56	11	0
37	4	44	0	56	9	0
37	9	44	0	56	3	0
37	G	44	0	56	22	0
37	R	44	0	56	7	0
37	g	44	0	56	20	0
37	q	44	0	56	16	0
37	r	44	0	56	4	0
38	0	42	0	47	2	0
38	6	42	0	47	4	0
38	A	96	0	121	4	0
38	B	106	0	147	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	G	80	0	86	13	0
38	M	50	0	63	3	0
38	R	51	0	68	6	0
38	S	51	0	68	4	0
38	X	38	0	39	1	0
38	Y	42	0	47	5	0
38	a	93	0	112	8	0
38	b	106	0	147	11	0
38	g	80	0	86	21	0
38	m	50	0	63	2	0
38	r	51	0	68	4	0
38	s	51	0	68	6	0
38	x	42	0	47	3	0
38	y	42	0	47	3	0
39	A	10	0	0	1	0
39	a	10	0	0	0	0
40	A	1	0	0	0	0
40	a	1	0	0	0	0
41	A	2	0	0	1	0
41	a	2	0	0	1	0
42	A	64	0	74	7	0
42	D	64	0	74	9	0
42	a	64	0	74	3	0
42	d	64	0	74	5	0
43	A	40	0	56	3	0
43	B	120	0	168	20	0
43	C	80	0	112	6	0
43	D	40	0	56	13	0
43	H	40	0	56	4	0
43	T	40	0	56	6	0
43	V	40	0	56	1	0
43	Z	40	0	56	3	0
43	a	40	0	56	4	0
43	b	120	0	168	16	0
43	c	80	0	112	15	0
43	d	40	0	56	5	0
43	h	40	0	56	4	0
43	t	40	0	56	13	0
43	v	40	0	56	3	0
43	z	40	0	56	4	0
44	A	55	0	80	5	0
44	D	55	0	80	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	a	55	0	80	9	0
44	d	55	0	80	9	0
45	C	248	0	346	34	0
45	c	260	0	373	51	0
46	D	4	0	0	0	0
46	d	4	0	1	0	0
47	E	43	0	30	10	0
47	e	43	0	30	11	0
48	K	35	0	46	1	0
48	R	35	0	46	8	0
48	c	28	0	29	3	0
48	r	35	0	46	11	0
49	0	7	0	0	0	0
49	1	3	0	0	0	0
49	2	3	0	0	0	0
49	3	1	0	0	0	0
49	4	1	0	0	0	0
49	5	1	0	0	0	0
49	6	4	0	0	0	0
49	7	6	0	0	0	0
49	8	4	0	0	0	0
49	9	2	0	0	0	0
49	A	21	0	0	1	0
49	B	6	0	0	0	0
49	C	15	0	0	1	0
49	D	12	0	0	0	0
49	E	1	0	0	0	0
49	F1	4	0	0	0	0
49	G	5	0	0	0	0
49	I	1	0	0	1	0
49	J	1	0	0	0	0
49	N	5	0	0	0	0
49	O	6	0	0	0	0
49	R	4	0	0	0	0
49	S	3	0	0	0	0
49	T	4	0	0	0	0
49	Y	8	0	0	0	0
49	a	14	0	0	0	0
49	b	6	0	0	0	0
49	c	15	0	0	0	0
49	d	15	0	0	0	0
49	e	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	f	1	0	0	0	0
49	f1	3	0	0	0	0
49	g	4	0	0	0	0
49	j	1	0	0	0	0
49	m	2	0	0	0	0
49	n	7	0	0	0	0
49	o	6	0	0	0	0
49	q	1	0	0	0	0
49	r	4	0	0	0	0
49	s	3	0	0	0	0
49	t	2	0	0	0	0
49	w	2	0	0	0	0
49	y	8	0	0	0	0
All	All	117990	0	117879	5329	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (5329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:223:PHE:HE1	35:4:615:RRX:C32	1.41	1.31
2:4:223:PHE:HE1	35:4:615:RRX:H50	1.09	1.17
2:4:223:PHE:CE1	35:4:615:RRX:C32	2.31	1.13
2:G:223:PHE:HE1	35:G:614:RRX:C32	1.61	1.13
38:g:301:SQD:C13	37:g:321:XAT:H362	1.78	1.11
30:9:310:CHL:H42	35:9:317:RRX:H9	1.33	1.11
3:8:53:SER:HA	2:9:171:TYR:HE2	1.11	1.09
3:8:53:SER:HA	2:9:171:TYR:CE2	1.88	1.08
31:N:311:CLA:HHC	31:N:311:CLA:HBB1	1.29	1.07
3:5:171:PRO:HG3	36:5:618:NEX:H8	1.38	1.05
30:1:619:CHL:HBD	30:1:619:CHL:HBA1	1.38	1.04
31:7:311:CLA:H2	32:7:317:LUT:H28	1.39	1.03
19:S:138:GLU:HA	30:S:308:CHL:HED1	1.37	1.03
4:6:110:LEU:CD2	34:6:322:LMG:H331	1.88	1.02
34:0:622:LMG:HC62	34:x:202:LMG:H112	1.37	1.02
2:4:147:ILE:HG12	31:4:604:CLA:H41	1.42	1.01
4:6:217:MET:HG2	32:6:318:LUT:H12	1.43	1.00
33:9:320:LHG:HC92	33:9:320:LHG:H272	1.43	1.00
3:n:147:SER:HB2	34:n:321:LMG:HC4	1.41	0.99
2:4:223:PHE:CE1	35:4:615:RRX:H48	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:621:LMG:H172	31:3:301:CLA:H43	1.43	0.98
2:q:176:PRO:HG2	30:q:310:CHL:HBB2	1.42	0.98
37:g:321:XAT:H361	37:g:321:XAT:H28	1.46	0.98
37:9:322:XAT:H28	37:9:322:XAT:H361	1.46	0.97
37:2:619:XAT:H28	37:2:619:XAT:H361	1.46	0.97
3:3:220:VAL:HG21	31:3:314:CLA:HAC2	1.46	0.97
45:c:619:DGD:HA32	45:c:619:DGD:HB21	1.47	0.97
31:G:609:CLA:O2A	35:G:614:RRX:H6	1.63	0.97
4:6:205:LYS:HD3	31:6:313:CLA:HBA1	1.46	0.96
37:G:620:XAT:H28	37:G:620:XAT:H361	1.46	0.96
31:6:304:CLA:HAC2	30:6:308:CHL:H171	1.48	0.96
31:3:306:CLA:H11	36:3:319:NEX:H241	1.46	0.96
37:q:321:XAT:H28	37:q:321:XAT:H361	1.46	0.96
31:g:311:CLA:O1A	38:g:318:SQD:H92	1.66	0.95
2:2:235:LEU:HD22	34:2:618:LMG:HC91	1.47	0.95
37:4:619:XAT:H28	37:4:619:XAT:H361	1.46	0.95
2:G:223:PHE:CE1	35:G:614:RRX:C32	2.50	0.95
2:9:214:ARG:HB3	31:9:304:CLA:HBC3	1.47	0.94
47:e:102:HEM:HHD	47:e:102:HEM:HBC2	1.50	0.94
3:8:236:HIS:HA	3:8:243:THR:HG21	1.49	0.94
3:n:236:HIS:HA	3:n:243:THR:HG21	1.49	0.93
3:5:215:MET:HE2	32:5:617:LUT:H10	1.51	0.93
1:7:244:TYR:HE2	30:7:321:CHL:H41	1.33	0.93
3:3:147:SER:HB2	34:3:321:LMG:H291	1.51	0.93
31:7:311:CLA:H92	32:7:317:LUT:H371	1.52	0.92
2:4:223:PHE:CE1	35:4:615:RRX:H50	1.97	0.92
19:s:90:LEU:HD22	32:s:318:LUT:H221	1.51	0.91
31:6:305:CLA:H61	30:6:307:CHL:HBA1	1.51	0.91
2:q:169:TYR:HD1	2:q:174:GLU:HG3	1.34	0.91
1:7:56:ASN:HB2	3:8:168:ASN:OD1	1.71	0.91
2:9:192:PRO:HD2	35:9:317:RRX:H14	1.52	0.91
3:5:139:ASN:HB3	3:5:142:LEU:HB2	1.50	0.91
47:E:101:HEM:HHD	47:E:101:HEM:HBC2	1.52	0.90
3:3:186:ASP:HA	32:3:317:LUT:H24	1.53	0.90
3:3:252:LYS:HA	3:3:256:ILE:HG23	1.51	0.90
30:q:303:CHL:HED1	33:q:320:LHG:H292	1.53	0.90
31:n:304:CLA:HAC1	30:n:308:CHL:HBB2	1.54	0.90
2:4:146:LEU:HD12	2:4:147:ILE:HD12	1.53	0.89
31:q:305:CLA:HHC	31:q:305:CLA:HBB1	1.52	0.89
1:7:121:LYS:HA	30:7:308:CHL:HED3	1.52	0.89
43:D:405:BCR:H16C	10:F:29:THR:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:122:ALA:HB1	31:7:305:CLA:HED1	1.55	0.88
2:4:146:LEU:HA	30:4:605:CHL:HED3	1.55	0.88
43:B:617:BCR:HC21	34:B:621:LMG:HC91	1.53	0.88
17:O:138:GLN:HG2	17:O:150:LYS:HE3	1.56	0.88
6:b:230:ARG:HH22	38:b:627:SQD:H1	1.38	0.88
31:1:610:CLA:H2	32:1:615:LUT:H28	1.53	0.88
33:C:623:LHG:H251	31:S:312:CLA:HAB	1.55	0.88
31:4:603:CLA:HBB1	31:4:603:CLA:HHC	1.55	0.88
7:c:254:TRP:HB2	22:w:118:THR:HG22	1.55	0.88
2:G:223:PHE:HE1	35:G:614:RRX:H50	1.37	0.88
30:4:608:CHL:HAA1	31:4:610:CLA:HMD1	1.56	0.87
3:8:49:LEU:HD12	2:9:171:TYR:CD2	2.09	0.87
31:b:609:CLA:H142	34:d:410:LMG:C43	2.05	0.87
31:9:305:CLA:HHC	31:9:305:CLA:HBB1	1.56	0.87
2:q:117:ALA:HA	34:q1:101:LMG:H311	1.55	0.87
34:4:620:LMG:H382	3:5:223:LEU:HD11	1.57	0.86
31:1:611:CLA:CAB	38:g:318:SQD:H242	2.05	0.86
34:9:321:LMG:H321	34:9:321:LMG:HC1	1.57	0.86
2:2:214:ARG:HB3	31:2:602:CLA:HBC3	1.56	0.86
1:7:244:TYR:HE2	30:7:321:CHL:C4	1.87	0.85
2:4:101:GLY:HA3	32:4:616:LUT:H10	1.57	0.85
31:9:312:CLA:H72	31:9:314:CLA:HMA2	1.58	0.85
31:6:304:CLA:HMC2	30:6:308:CHL:H121	1.58	0.85
4:6:110:LEU:HD23	34:6:322:LMG:H331	1.56	0.85
31:2:603:CLA:HHC	31:2:603:CLA:HBB1	1.57	0.85
31:9:314:CLA:HHC	31:9:314:CLA:HBB1	1.58	0.85
19:S:155:PRO:HG2	31:S:306:CLA:NB	1.91	0.85
3:5:200:LEU:HA	3:5:203:LYS:HD2	1.57	0.84
2:2:176:PRO:HD2	30:2:607:CHL:HBB2	1.59	0.84
34:q:302:LMG:H132	34:q:302:LMG:HC91	1.56	0.84
30:7:321:CHL:HBB2	31:8:603:CLA:HAC1	1.58	0.84
2:4:143:ASN:HD22	2:4:146:LEU:HD23	1.40	0.84
31:G:612:CLA:C12	37:G:620:XAT:H34	2.06	0.84
4:6:110:LEU:HD21	34:6:322:LMG:H331	1.59	0.84
38:g:301:SQD:C13	37:g:321:XAT:C36	2.56	0.84
31:p:613:CLA:HMB3	32:p:616:LUT:H162	1.60	0.84
30:5:607:CHL:HBA2	4:6:255:LEU:HB2	1.57	0.83
2:q:169:TYR:CD1	2:q:174:GLU:HG3	2.11	0.83
33:l:101:LHG:HC31	33:l:101:LHG:HC62	1.58	0.83
1:7:244:TYR:CE2	30:7:321:CHL:C4	2.61	0.83
4:6:202:LEU:HB3	31:6:311:CLA:CMA	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:163:MET:HE3	30:9:308:CHL:HMB3	1.59	0.83
2:4:155:VAL:HG12	30:4:605:CHL:HAC1	1.60	0.83
3:5:104:THR:HB	3:5:105:PRO:HD3	1.58	0.83
31:s:304:CLA:HHC	31:s:304:CLA:HBB1	1.60	0.83
31:s:311:CLA:H42	31:s:313:CLA:HBA1	1.61	0.83
30:n:308:CHL:H152	30:y:601:CHL:H52	1.60	0.83
34:4:621:LMG:H132	34:4:621:LMG:HC91	1.60	0.83
2:G:223:PHE:CE1	35:G:614:RRX:H48	2.13	0.83
2:9:103:LEU:HB3	31:9:306:CLA:HBC2	1.60	0.83
31:s:305:CLA:H92	30:s:307:CHL:HBA2	1.60	0.82
2:q:258:LEU:HD22	2:q:259:PRO:HD2	1.60	0.82
3:3:159:MET:HE3	30:3:308:CHL:HMB1	1.62	0.82
3:3:239:ALA:HB3	3:3:243:THR:HG22	1.60	0.82
31:G:602:CLA:H91	31:Y:304:CLA:H61	1.62	0.82
19:s:285:ARG:HE	38:s:301:SQD:H3	1.44	0.82
4:0:217:MET:HG2	32:0:617:LUT:H12	1.61	0.82
3:5:136:TYR:HB3	3:5:142:LEU:HB3	1.61	0.82
8:d:98:GLN:HB3	34:d:410:LMG:HC5	1.60	0.81
1:1:149:THR:HG22	30:1:605:CHL:HAC1	1.63	0.81
31:1:611:CLA:HAB	38:g:318:SQD:H242	1.60	0.81
30:y:607:CHL:H102	30:y:609:CHL:H172	1.62	0.81
2:4:137:GLY:HA2	2:4:150:GLN:HG2	1.63	0.81
4:6:217:MET:HE2	32:6:318:LUT:H10	1.61	0.81
3:p:106:GLU:HA	3:p:119:ALA:HB1	1.63	0.81
31:1:610:CLA:H92	32:1:615:LUT:H371	1.61	0.81
3:n:226:ARG:NH2	34:n:322:LMG:HC61	1.96	0.81
4:6:50:LEU:HB3	4:6:54:SER:HB3	1.62	0.80
3:n:226:ARG:HH22	34:n:322:LMG:C6	1.94	0.80
31:G:610:CLA:HAA2	38:G:617:SQD:H441	1.63	0.80
2:q:140:TYR:HB3	2:q:146:LEU:HD23	1.62	0.80
2:G:223:PHE:CE1	35:G:614:RRX:H50	2.14	0.80
24:Y:175:PRO:HG2	38:Y:320:SQD:H441	1.64	0.80
31:8:609:CLA:H52	32:8:615:LUT:H30	1.64	0.80
31:6:311:CLA:H51	32:6:317:LUT:H30	1.63	0.80
31:p:602:CLA:HAC2	33:p:619:LHG:H262	1.61	0.80
38:a:412:SQD:H92	34:a:413:LMG:H111	1.63	0.80
34:b:626:LMG:HC92	38:b:627:SQD:H2	1.64	0.80
45:C:620:DGD:HAV1	34:C:624:LMG:H151	1.62	0.80
2:2:52:PRO:HB2	18:R:42:ALA:HB1	1.64	0.80
7:C:155:VAL:HG12	34:C:621:LMG:H362	1.64	0.80
31:0:614:CLA:HBA2	34:p:620:LMG:H111	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:308:CHL:HBB2	30:q:309:CHL:CBB	2.12	0.79
27:Q1:6:GLY:HA3	34:Q1:101:LMG:HC62	1.64	0.79
30:4:609:CHL:HAA2	3:5:71:THR:HG21	1.65	0.79
1:7:56:ASN:CB	3:8:168:ASN:OD1	2.30	0.79
31:8:614:CLA:H11	34:9:302:LMG:HC92	1.64	0.79
31:q:315:CLA:H102	37:q:321:XAT:H34	1.63	0.79
8:d:192:THR:HG23	31:d:404:CLA:HBC2	1.64	0.79
2:9:138:LEU:HD21	31:9:306:CLA:HAA2	1.63	0.79
2:4:179:THR:H	2:4:188:GLY:HA3	1.47	0.79
4:6:188:ASP:HA	32:6:317:LUT:H24	1.65	0.79
3:8:236:HIS:HA	3:8:243:THR:CG2	2.13	0.79
31:b:611:CLA:HHC	31:b:611:CLA:HBB1	1.64	0.79
3:3:159:MET:HE1	36:3:319:NEX:H30	1.63	0.79
31:c:606:CLA:H151	43:c:615:BCR:H363	1.64	0.79
3:n:236:HIS:HA	3:n:243:THR:CG2	2.13	0.79
30:5:608:CHL:HBB2	36:5:618:NEX:H10	1.64	0.79
3:5:252:LYS:HA	3:5:256:ILE:HG23	1.63	0.79
37:G:620:XAT:H362	38:G:624:SQD:C13	2.13	0.79
3:N:245:PHE:HB3	31:N:313:CLA:H11	1.65	0.79
38:g:301:SQD:H92	37:g:321:XAT:H222	1.64	0.79
8:D:192:THR:HG23	31:D:403:CLA:HBC2	1.64	0.78
6:b:142:HIS:HE1	31:b:616:CLA:ND	1.80	0.78
2:4:254:ALA:HA	37:4:619:XAT:H22	1.63	0.78
2:q:103:LEU:HD21	31:q:314:CLA:HBB2	1.65	0.78
31:5:612:CLA:HBB1	31:5:612:CLA:HMB3	1.66	0.78
31:R:304:CLA:HBA1	37:R:318:XAT:H382	1.64	0.78
3:p:54:ASN:H	2:q:171:TYR:HE2	1.29	0.78
18:r:170:ASN:HA	48:r:302:LMU:H2B	1.65	0.78
3:p:247:VAL:HG13	2:q:133:PHE:HE2	1.48	0.78
24:y:126:LYS:HA	30:y:607:CHL:HED3	1.64	0.78
31:4:602:CLA:H61	32:4:616:LUT:H30	1.64	0.78
3:5:86:GLU:HA	3:5:179:LEU:HD11	1.66	0.78
18:R:164:ALA:HB1	31:R:306:CLA:HED1	1.66	0.78
1:7:213:MET:HE2	32:7:318:LUT:H10	1.65	0.78
3:n:59:LEU:HD23	3:n:68:GLY:HA2	1.66	0.78
2:2:220:MET:HE2	32:2:615:LUT:H10	1.66	0.78
1:7:165:VAL:HG11	2:9:57:SER:HB3	1.63	0.78
34:g:322:LMG:H111	30:y:607:CHL:H11	1.66	0.78
1:1:50:LEU:HB2	1:1:54:SER:HB2	1.66	0.78
31:3:306:CLA:H52	30:3:308:CHL:HAA2	1.66	0.77
3:3:191:ALA:HB2	31:3:311:CLA:HAA2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:176:PRO:HD2	30:G:607:CHL:HBB2	1.64	0.77
19:S:189:PRO:HD2	30:S:309:CHL:HBB2	1.66	0.77
1:7:241:ASN:HA	1:7:246:LEU:HD11	1.66	0.77
3:8:59:LEU:HD23	3:8:68:GLY:HA2	1.66	0.77
22:w:80:SER:HB3	34:w:205:LMG:HC4	1.65	0.77
30:N:306:CHL:H171	31:S:315:CLA:HMC3	1.66	0.77
18:R:169:TYR:CE2	48:R:302:LMU:H6D	2.20	0.77
19:s:189:PRO:HD2	30:s:309:CHL:HBB2	1.66	0.77
3:n:226:ARG:NH2	34:n:322:LMG:C6	2.48	0.77
31:1:611:CLA:CAB	38:g:318:SQD:C24	2.63	0.77
45:c:619:DGD:HAW1	45:c:619:DGD:HBE1	1.66	0.77
31:G:612:CLA:H121	37:G:620:XAT:H34	1.67	0.77
30:p:607:CHL:HBD	30:p:607:CHL:HBA1	1.67	0.77
3:3:38:VAL:HA	3:3:42:GLY:HA3	1.66	0.76
7:C:246:ALA:HB1	22:W:111:ASN:ND2	2.00	0.76
31:9:305:CLA:HED2	31:9:305:CLA:H12	1.67	0.76
6:b:230:ARG:NH2	38:b:627:SQD:H1	2.00	0.76
30:0:605:CHL:HBD	30:0:605:CHL:HBA1	1.66	0.76
31:B:611:CLA:H61	31:B:613:CLA:HED3	1.65	0.76
31:8:614:CLA:H2	2:9:228:LEU:HD12	1.66	0.76
3:n:147:SER:CB	34:n:321:LMG:HC4	2.13	0.76
31:4:604:CLA:H43	30:4:606:CHL:CAD	2.16	0.76
30:1:601:CHL:HHC	30:1:601:CHL:HBB1	1.68	0.76
2:4:178:GLU:HG2	2:4:189:PHE:HB3	1.65	0.76
8:d:123:ILE:HD11	34:d:411:LMG:H402	1.66	0.76
31:N:310:CLA:H92	32:N:316:LUT:H371	1.68	0.76
1:7:244:TYR:CE2	30:7:321:CHL:H41	2.18	0.76
3:p:120:VAL:HG23	3:p:123:LYS:HB2	1.66	0.76
30:5:608:CHL:CBB	36:5:618:NEX:H10	2.16	0.76
31:N:312:CLA:HHC	31:N:312:CLA:HBB1	1.67	0.76
2:9:230:THR:HG23	2:9:232:LYS:H	1.51	0.76
3:5:186:ASP:HA	32:5:616:LUT:H24	1.68	0.76
32:S:318:LUT:H371	32:S:318:LUT:H28	1.68	0.76
2:q:178:GLU:HG2	2:q:189:PHE:HD1	1.51	0.76
45:c:619:DGD:HBH1	45:c:619:DGD:HBV2	1.67	0.76
8:D:49:PHE:CG	43:D:405:BCR:H15C	2.21	0.75
30:2:605:CHL:HHC	30:2:605:CHL:HBB1	1.69	0.75
31:7:304:CLA:HAC1	30:7:308:CHL:HBB2	1.66	0.75
30:S:307:CHL:HBB2	30:S:308:CHL:CBB	2.16	0.75
2:2:149:ALA:HA	30:2:605:CHL:CHC	2.17	0.75
31:s:303:CLA:HMB3	31:s:303:CLA:HBB1	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:G:622:LMG:H172	31:N:321:CLA:H43	1.69	0.75
31:g:305:CLA:HBB1	31:g:305:CLA:HMB1	1.68	0.75
48:R:302:LMU:H101	31:R:307:CLA:HED1	1.69	0.75
2:9:162:ILE:HG23	36:9:319:NEX:H15	1.68	0.75
31:n:311:CLA:H52	32:n:317:LUT:H30	1.67	0.75
31:2:609:CLA:H2	35:2:614:RRX:H6	1.66	0.75
2:4:133:PHE:HE1	30:4:607:CHL:HMD3	1.51	0.75
3:5:106:GLU:HB3	3:5:230:ILE:HD11	1.69	0.75
4:6:202:LEU:HB3	31:6:311:CLA:HMA2	1.66	0.75
33:c:622:LHG:H312	33:s:320:LHG:HC92	1.69	0.75
2:2:153:VAL:HA	2:2:156:LEU:HD12	1.69	0.74
3:5:115:ASN:HD22	3:5:115:ASN:H	1.34	0.74
31:b:612:CLA:H8	31:b:614:CLA:H51	1.67	0.74
31:6:315:CLA:HMB1	31:6:315:CLA:HBB1	1.68	0.74
3:p:126:ALA:H	30:p:607:CHL:HED1	1.52	0.74
31:S:303:CLA:HMB3	31:S:303:CLA:HBB1	1.66	0.74
30:q:310:CHL:HHC	30:q:310:CHL:HBB1	1.69	0.74
4:0:202:LEU:HB3	31:0:610:CLA:HMA2	1.67	0.74
2:9:109:GLU:HA	2:9:123:ALA:HB1	1.69	0.74
30:9:303:CHL:HAC1	33:9:320:LHG:HC32	1.68	0.74
30:g:306:CHL:HBB1	30:g:306:CHL:HHC	1.69	0.74
34:w:202:LMG:H211	31:y:612:CLA:H141	1.69	0.74
31:5:610:CLA:H2	32:5:616:LUT:H28	1.69	0.74
31:B:607:CLA:HBB1	31:B:607:CLA:HMB1	1.69	0.74
4:0:164:ILE:HD11	36:0:618:NEX:C34	2.18	0.74
8:d:312:GLU:HG2	17:o:205:PRO:HB3	1.68	0.74
24:y:77:LEU:HD23	31:y:602:CLA:H42	1.70	0.74
6:B:142:HIS:HE1	31:B:615:CLA:ND	1.85	0.74
24:Y:50:LEU:HB2	24:Y:54:SER:HB3	1.68	0.74
6:b:216:HIS:HE1	31:b:610:CLA:C1A	2.01	0.74
34:d:410:LMG:H402	23:x:79:GLY:HA2	1.68	0.74
30:6:306:CHL:HHC	30:6:306:CHL:HBB1	1.69	0.74
7:C:245:TRP:HB3	45:C:620:DGD:HD2	1.68	0.74
31:N:311:CLA:HHC	31:N:311:CLA:CBB	2.13	0.74
2:9:223:PHE:CZ	35:9:317:RRX:H48	2.23	0.74
33:g:319:LHG:H282	37:g:321:XAT:C33	2.17	0.74
31:c:603:CLA:H203	31:c:610:CLA:HAB	1.69	0.74
4:0:205:LYS:HG3	31:0:611:CLA:HED2	1.69	0.74
31:g:310:CLA:HBA1	35:g:315:RRX:H18	1.70	0.74
31:7:311:CLA:HMB3	31:7:311:CLA:HBB1	1.70	0.73
31:2:609:CLA:H12	31:2:609:CLA:H3A	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:247:PHE:HB2	31:6:314:CLA:CAD	2.18	0.73
3:N:110:ARG:HH21	3:N:231:GLU:HA	1.53	0.73
3:p:225:THR:HB	3:p:249:TYR:CE2	2.24	0.73
3:3:236:HIS:HB2	31:3:314:CLA:HAA2	1.70	0.73
2:4:177:VAL:HA	2:4:189:PHE:HD2	1.54	0.73
3:5:185:PHE:HA	30:5:608:CHL:H2	1.70	0.73
41:A:403:CL:CL	8:D:317:LYS:NZ	2.57	0.73
31:S:311:CLA:H42	31:S:313:CLA:HBA1	1.68	0.73
31:8:611:CLA:HBB1	31:8:611:CLA:HMB3	1.70	0.73
31:b:611:CLA:H102	31:b:616:CLA:HAA1	1.71	0.73
31:n:305:CLA:H152	31:s:306:CLA:CHB	2.19	0.73
2:4:228:LEU:HD21	34:4:621:LMG:H341	1.70	0.73
31:4:603:CLA:HMC3	32:4:616:LUT:H191	1.69	0.73
3:5:236:HIS:HA	3:5:243:THR:OG1	1.88	0.73
3:N:245:PHE:HB2	31:N:313:CLA:CAD	2.18	0.73
24:Y:77:LEU:HD23	31:Y:303:CLA:H42	1.69	0.73
31:p:612:CLA:HHC	31:p:612:CLA:HBB1	1.70	0.73
2:4:152:ILE:H	2:4:152:ILE:HD12	1.54	0.73
31:N:305:CLA:H121	31:S:306:CLA:H3A	1.69	0.73
31:p:611:CLA:H43	31:p:612:CLA:HMD2	1.68	0.73
3:n:226:ARG:HH22	34:n:322:LMG:HC61	1.54	0.73
3:3:215:MET:HE2	32:3:318:LUT:H10	1.71	0.73
3:p:245:PHE:HZ	30:q:309:CHL:H11	1.52	0.73
4:0:202:LEU:HB3	31:0:610:CLA:CMA	2.18	0.73
31:7:305:CLA:HMA2	30:7:307:CHL:C3C	2.19	0.73
30:p:605:CHL:HHC	30:p:605:CHL:HBB1	1.69	0.73
31:7:313:CLA:HBB1	31:7:313:CLA:HHC	1.71	0.73
31:s:303:CLA:H61	32:s:318:LUT:H28	1.70	0.73
3:3:245:PHE:HB3	31:3:314:CLA:H11	1.71	0.72
33:D:408:LHG:H312	20:T:21:ILE:HD11	1.71	0.72
33:G:618:LHG:C6	37:G:620:XAT:H382	2.18	0.72
31:Y:310:CLA:HBB1	31:Y:310:CLA:HMB3	1.71	0.72
3:8:215:MET:HE2	32:8:616:LUT:H10	1.70	0.72
3:p:191:ALA:HB2	3:p:200:LEU:HD12	1.71	0.72
30:q:307:CHL:HHC	30:q:307:CHL:HBB1	1.70	0.72
45:c:619:DGD:HBG3	32:y:616:LUT:H193	1.70	0.72
8:d:56:THR:HG21	9:e:50:PRO:HD3	1.71	0.72
30:3:303:CHL:HHC	30:3:303:CHL:HBB1	1.71	0.72
7:C:83:LEU:O	7:C:166:LYS:NZ	2.22	0.72
30:G:605:CHL:HHC	30:G:605:CHL:HBB1	1.70	0.72
31:b:614:CLA:H43	33:b:625:LHG:H371	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:629:LMG:H302	30:r:309:CHL:H42	1.70	0.72
30:6:309:CHL:HHC	30:6:309:CHL:HBB1	1.71	0.72
31:7:305:CLA:HBB1	31:7:305:CLA:HMB3	1.70	0.72
5:a:38:ILE:HG23	34:a:401:LMG:H362	1.72	0.72
5:a:141:PRO:O	8:d:220:ASN:ND2	2.23	0.72
1:7:77:LEU:HD23	31:7:303:CLA:H42	1.70	0.72
31:n:303:CLA:H61	32:n:318:LUT:H30	1.71	0.72
31:5:602:CLA:HBB1	31:5:602:CLA:HMB3	1.72	0.72
30:R:309:CHL:HHC	30:R:309:CHL:HBB1	1.71	0.72
3:8:87:LEU:HD13	31:8:603:CLA:HBA1	1.71	0.72
1:7:178:TYR:HB3	31:7:311:CLA:HED3	1.70	0.72
2:q:176:PRO:CG	30:q:310:CHL:HBB2	2.18	0.72
31:n:313:CLA:HBB1	31:n:313:CLA:HMB3	1.70	0.72
30:2:607:CHL:HHC	30:2:607:CHL:HBB1	1.72	0.72
5:A:192:ILE:HG13	5:A:293:MET:HE1	1.72	0.72
30:N:306:CHL:HHC	30:N:306:CHL:HBB1	1.72	0.72
4:0:149:SER:HB2	34:0:622:LMG:HC92	1.72	0.72
45:c:617:DGD:HBW2	45:c:618:DGD:HAG2	1.70	0.72
31:7:316:CLA:HBD	31:7:316:CLA:HBA1	1.72	0.72
3:n:87:LEU:HD13	31:n:304:CLA:HBA1	1.72	0.72
31:b:613:CLA:HMB1	31:b:613:CLA:HBB1	1.72	0.72
34:b:629:LMG:H342	30:r:309:CHL:H61	1.71	0.72
31:1:603:CLA:HAC1	30:1:607:CHL:HBB2	1.71	0.71
2:2:259:PRO:HA	34:2:620:LMG:HC5	1.72	0.71
30:4:605:CHL:HBB1	30:4:605:CHL:HHC	1.71	0.71
31:5:610:CLA:H52	32:5:616:LUT:H30	1.72	0.71
31:N:304:CLA:HAC1	30:Y:301:CHL:HBB2	1.70	0.71
34:n:321:LMG:H311	34:n:321:LMG:H151	1.72	0.71
2:4:177:VAL:HA	2:4:189:PHE:CD2	2.25	0.71
3:5:191:ALA:HB2	31:5:610:CLA:HAA2	1.72	0.71
30:G:607:CHL:HBB1	30:G:607:CHL:HHC	1.72	0.71
30:7:302:CHL:HHC	30:7:302:CHL:HBB1	1.72	0.71
3:8:96:MET:SD	31:8:609:CLA:HAB	2.31	0.71
31:b:616:CLA:H2	31:b:617:CLA:HBB2	1.73	0.71
30:5:605:CHL:HHC	30:5:605:CHL:HBB1	1.70	0.71
31:9:314:CLA:CHC	35:9:317:RRX:H37	2.19	0.71
31:q:313:CLA:C3C	33:q:320:LHG:HC61	2.21	0.71
2:g:155:VAL:HG12	30:g:306:CHL:HAC1	1.72	0.71
34:4:621:LMG:HC91	34:4:621:LMG:C13	2.21	0.71
30:N:302:CHL:HBB1	30:N:302:CHL:HHC	1.73	0.71
3:p:223:LEU:HD11	34:q:301:LMG:H382	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:244:ASN:HB3	3:p:246:TRP:HD1	1.55	0.71
24:Y:154:THR:HG22	30:Y:306:CHL:HAC1	1.72	0.71
4:0:170:ASN:HD22	2:q:53:PHE:HA	1.56	0.71
2:q:119:PHE:HB3	2:q:122:ALA:HB3	1.73	0.71
3:n:215:MET:HE2	32:n:318:LUT:H10	1.72	0.71
30:0:601:CHL:HBB1	30:0:601:CHL:HHC	1.73	0.71
31:3:311:CLA:H52	32:3:317:LUT:H30	1.71	0.71
31:4:610:CLA:H72	35:4:615:RRX:H25	1.72	0.71
31:5:610:CLA:H2	32:5:616:LUT:H26	1.72	0.71
8:d:145:ALA:HB2	8:d:272:LEU:HD11	1.71	0.71
3:3:104:THR:HB	3:3:105:PRO:HD3	1.73	0.71
2:4:59:PRO:HA	4:6:85:ARG:HH22	1.56	0.71
2:4:171:TYR:HE2	3:5:54:ASN:H	1.39	0.71
3:5:123:LYS:HA	30:5:607:CHL:HED3	1.72	0.71
3:N:233:LEU:HD13	31:N:314:CLA:HBC2	1.71	0.71
34:q1:101:LMG:H132	34:q1:101:LMG:H352	1.73	0.71
30:1:619:CHL:HBA1	30:1:619:CHL:CBD	2.17	0.71
30:p:608:CHL:HHC	30:p:608:CHL:HBB1	1.71	0.71
31:p:614:CLA:HHC	31:p:614:CLA:HBB1	1.73	0.71
34:n:322:LMG:H321	31:y:615:CLA:H61	1.73	0.71
18:r:184:TYR:HA	48:r:302:LMU:H31	1.70	0.71
1:1:195:LEU:HG	1:1:199:LYS:HE2	1.71	0.71
33:G:618:LHG:H281	37:G:620:XAT:C32	2.21	0.71
30:S:307:CHL:HHC	30:S:307:CHL:HBB1	1.72	0.71
34:c:624:LMG:H341	33:y:619:LHG:H101	1.71	0.71
8:d:126:MET:HG3	8:d:146:PHE:HD2	1.56	0.71
30:n:302:CHL:HHC	30:n:302:CHL:HBB1	1.72	0.71
30:4:608:CHL:HBB1	30:4:608:CHL:HHC	1.71	0.70
3:N:47:GLN:HG3	3:N:53:SER:HB2	1.73	0.70
3:8:246:TRP:HH2	30:9:309:CHL:H62	1.54	0.70
30:9:303:CHL:HBB1	30:9:303:CHL:HHC	1.72	0.70
16:m:31:SER:HA	38:m:101:SQD:H2	1.73	0.70
24:y:197:ALA:HB1	24:y:203:LEU:HG	1.72	0.70
30:2:608:CHL:HHC	30:2:608:CHL:HBB1	1.73	0.70
30:4:609:CHL:HHC	30:4:609:CHL:HBB1	1.72	0.70
3:5:151:ILE:HD13	30:5:605:CHL:HAC1	1.72	0.70
30:5:601:CHL:HHC	30:5:601:CHL:HBB1	1.72	0.70
30:7:310:CHL:HAA2	2:9:74:THR:HG21	1.72	0.70
32:p:617:LUT:H363	31:q:305:CLA:HED3	1.73	0.70
30:r:309:CHL:HHC	30:r:309:CHL:HBB1	1.72	0.70
3:5:106:GLU:HB3	3:5:230:ILE:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:609:CHL:HAA2	2:q:74:THR:HG21	1.73	0.70
2:G:260:LEU:H	34:G:621:LMG:HC61	1.57	0.70
30:Y:309:CHL:HHC	30:Y:309:CHL:HBB1	1.73	0.70
30:0:609:CHL:HHC	30:0:609:CHL:HBB1	1.73	0.70
30:g:308:CHL:HHC	30:g:308:CHL:HBB1	1.72	0.70
19:s:241:LEU:HD21	31:s:313:CLA:HBC2	1.72	0.70
43:B:617:BCR:HC22	34:B:621:LMG:H292	1.73	0.70
31:2:603:CLA:HED2	31:2:603:CLA:H12	1.73	0.70
30:3:307:CHL:HHC	30:3:307:CHL:HBB1	1.72	0.70
30:8:601:CHL:HBB1	30:8:601:CHL:HHC	1.72	0.70
30:q:310:CHL:H42	35:q:317:RRX:H9	1.73	0.70
31:q:312:CLA:H2	35:q:317:RRX:C40	2.21	0.70
34:D:411:LMG:H402	23:X:79:GLY:HA2	1.72	0.70
3:N:87:LEU:HD13	31:N:304:CLA:HBA1	1.73	0.70
3:8:53:SER:CA	2:9:171:TYR:HE2	1.98	0.70
2:9:211:LYS:HE3	33:9:320:LHG:HC61	1.73	0.70
9:e:55:TYR:O	9:e:60:ARG:NH2	2.24	0.70
30:3:307:CHL:HBB2	34:3:321:LMG:H322	1.74	0.70
4:6:205:LYS:HD3	31:6:313:CLA:CBA	2.22	0.70
31:C:603:CLA:H203	31:C:610:CLA:HAB	1.74	0.70
3:N:59:LEU:HD23	3:N:68:GLY:HA2	1.74	0.70
30:0:607:CHL:HHC	30:0:607:CHL:HBB1	1.74	0.70
30:6:308:CHL:H122	30:6:308:CHL:HMB3	1.72	0.70
31:B:610:CLA:HHC	31:B:610:CLA:HBB1	1.72	0.70
3:N:252:LYS:HA	3:N:256:ILE:HG23	1.73	0.70
18:R:139:HIS:HD2	37:R:318:XAT:H15	1.56	0.70
31:R:304:CLA:CAB	37:R:318:XAT:H32	2.22	0.70
31:8:614:CLA:HBB1	31:8:614:CLA:HMB3	1.74	0.70
30:5:609:CHL:HHC	30:5:609:CHL:HBB1	1.74	0.70
31:B:611:CLA:HMB1	31:B:611:CLA:HBB1	1.72	0.70
31:8:602:CLA:H61	32:8:616:LUT:H30	1.73	0.70
6:b:53:ASN:HD21	6:b:331:ASN:HD21	1.39	0.70
19:s:207:MET:HE3	30:s:309:CHL:HBC3	1.71	0.70
30:s:307:CHL:HHC	30:s:307:CHL:HBB1	1.72	0.70
2:2:130:ALA:H	30:3:302:CHL:HED1	1.56	0.69
2:4:117:ALA:H	34:Q1:101:LMG:H121	1.57	0.69
3:5:72:ALA:HB3	3:5:74:LEU:HD21	1.74	0.69
3:8:186:ASP:HA	32:8:615:LUT:H24	1.74	0.69
31:5:615:CLA:HBD	31:5:615:CLA:HBA1	1.74	0.69
31:C:606:CLA:H41	34:W:201:LMG:H331	1.73	0.69
2:q:122:ALA:HB1	31:q:306:CLA:HED2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:303:CHL:HHC	30:q:303:CHL:HBB1	1.74	0.69
3:n:186:ASP:HA	32:n:317:LUT:H24	1.74	0.69
30:9:308:CHL:HHC	30:9:308:CHL:HBB1	1.74	0.69
2:q:223:PHE:CD1	35:q:317:RRX:H48	2.27	0.69
34:2:621:LMG:H132	34:2:621:LMG:HC91	1.73	0.69
3:5:225:THR:HG23	3:5:227:LYS:H	1.57	0.69
30:6:302:CHL:HBB1	30:6:302:CHL:HHC	1.74	0.69
3:p:180:TYR:HB3	31:p:610:CLA:HED3	1.73	0.69
2:q:132:ILE:HB	2:q:138:LEU:HD12	1.74	0.69
31:q:312:CLA:H2	35:q:317:RRX:H6	1.73	0.69
10:f:14:ILE:HD11	27:q1:26:PRO:HB2	1.73	0.69
3:3:96:MET:SD	31:3:311:CLA:HAB	2.32	0.69
6:B:216:HIS:HE1	31:B:609:CLA:C1A	2.04	0.69
31:B:615:CLA:H2	31:B:616:CLA:HBB2	1.75	0.69
19:S:207:MET:HE3	30:S:309:CHL:HBC3	1.75	0.69
22:W:119:LEU:HD21	28:P1:42:ARG:HG2	1.74	0.69
31:8:614:CLA:H42	34:9:302:LMG:H112	1.73	0.69
3:p:220:VAL:HG11	31:p:613:CLA:HAC2	1.75	0.69
30:1:605:CHL:HBB1	30:1:605:CHL:HHC	1.73	0.69
2:2:133:PHE:HE2	30:3:302:CHL:HMD3	1.56	0.69
30:3:302:CHL:HBB1	30:3:302:CHL:HHC	1.74	0.69
3:5:251:PRO:HG2	3:5:252:LYS:HD2	1.75	0.69
31:5:615:CLA:HBA1	31:5:615:CLA:CHA	2.22	0.69
45:C:620:DGD:HBH2	45:C:620:DGD:HBV2	1.73	0.69
3:5:158:LEU:HG	36:5:618:NEX:H15	1.75	0.69
33:D:407:LHG:HC91	33:L:101:LHG:HC81	1.74	0.69
2:q:254:ALA:HA	37:q:321:XAT:H22	1.75	0.69
30:g:309:CHL:HHC	30:g:309:CHL:HBB1	1.74	0.69
30:y:608:CHL:HHC	30:y:608:CHL:HBB1	1.73	0.69
31:1:604:CLA:HMA2	30:1:606:CHL:HBC3	1.72	0.69
30:4:601:CHL:HHC	30:4:601:CHL:HBB1	1.75	0.69
30:5:609:CHL:HMB2	30:6:302:CHL:HHB	1.75	0.69
31:6:316:CLA:HBB1	31:6:316:CLA:HMB3	1.75	0.69
8:D:186:GLN:HB2	31:D:403:CLA:HBC1	1.75	0.69
30:7:306:CHL:HBB1	30:7:306:CHL:HHC	1.74	0.69
2:g:205:LEU:HB3	31:g:310:CLA:HMA2	1.74	0.69
34:w:202:LMG:H182	34:w:202:LMG:H431	1.73	0.69
3:3:110:ARG:HH11	3:3:230:ILE:HG22	1.58	0.69
1:1:213:MET:HE2	32:1:616:LUT:H10	1.74	0.69
30:4:607:CHL:HAA2	3:5:253:SER:HB2	1.75	0.69
45:C:620:DGD:HBN2	31:Y:311:CLA:H142	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:140:LYS:HB2	17:O:148:GLU:HG3	1.75	0.69
30:q:311:CHL:HBB1	30:q:311:CHL:HHC	1.74	0.69
4:6:115:ALA:O	34:6:321:LMG:HC2	1.93	0.68
34:7:322:LMG:H291	34:7:322:LMG:H332	1.74	0.68
2:q:196:ALA:HB2	31:q:312:CLA:HAA2	1.74	0.68
45:c:617:DGD:HBH1	45:c:618:DGD:HAT1	1.74	0.68
3:n:96:MET:SD	31:n:311:CLA:HAB	2.33	0.68
30:y:609:CHL:HHC	30:y:609:CHL:HBB1	1.74	0.68
34:6:321:LMG:H111	34:6:322:LMG:H111	1.76	0.68
19:S:241:LEU:HD21	31:S:313:CLA:HBC2	1.75	0.68
5:a:267:ASN:HD22	38:a:411:SQD:H3	1.58	0.68
34:q1:101:LMG:H312	34:q1:101:LMG:C10	2.23	0.68
1:1:107:VAL:HB	1:1:108:PRO:HD3	1.73	0.68
31:3:306:CLA:H92	30:3:308:CHL:HBA2	1.74	0.68
5:A:188:ALA:HB2	5:A:328:MET:HB2	1.76	0.68
30:g:302:CHL:H161	33:g:319:LHG:H372	1.73	0.68
1:1:251:LEU:HB3	30:1:619:CHL:HBA2	1.74	0.68
3:5:143:ILE:HA	30:5:605:CHL:C4D	2.23	0.68
6:B:365:THR:HG22	8:D:326:ARG:HH21	1.57	0.68
45:C:620:DGD:HBV2	31:Y:311:CLA:H51	1.76	0.68
2:4:149:ALA:HA	30:4:605:CHL:CHC	2.24	0.68
3:5:246:TRP:O	3:5:251:PRO:HD3	1.94	0.68
42:D:401:PHO:H3A	31:D:403:CLA:H142	1.76	0.68
3:p:206:LYS:HD3	31:p:611:CLA:O1D	1.93	0.68
24:y:50:LEU:HB2	24:y:54:SER:HB3	1.74	0.68
2:2:59:PRO:HG2	2:2:73:ASP:HB3	1.76	0.68
3:N:96:MET:SD	31:N:310:CLA:HAB	2.33	0.68
24:Y:116:GLY:HA3	34:Y:319:LMG:HC3	1.75	0.68
30:7:309:CHL:HHC	30:7:309:CHL:HBB1	1.76	0.68
30:9:309:CHL:C4B	30:9:309:CHL:H43	2.24	0.68
3:p:200:LEU:HA	3:p:203:LYS:HD2	1.75	0.68
2:2:165:ALA:HB3	36:2:616:NEX:H203	1.74	0.68
2:2:223:PHE:HE1	35:2:614:RRX:H48	1.58	0.68
31:6:305:CLA:HBB1	31:6:305:CLA:HMB3	1.74	0.68
31:G:609:CLA:H72	35:G:614:RRX:C21	2.24	0.68
31:N:310:CLA:H2	32:N:316:LUT:H28	1.76	0.68
30:Y:308:CHL:HHC	30:Y:308:CHL:HBB1	1.76	0.68
31:p:602:CLA:H11	32:p:617:LUT:H373	1.76	0.68
30:0:607:CHL:H12	2:q:259:PRO:HD3	1.74	0.68
19:S:176:MET:HE2	19:S:176:MET:HA	1.76	0.68
24:y:175:PRO:HD2	30:y:608:CHL:HBB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p1:34:LYS:HG2	28:p1:46:GLY:HA2	1.75	0.68
4:0:125:LYS:HE2	2:q:258:LEU:HD11	1.76	0.68
17:O:99:MET:SD	17:O:176:VAL:HG11	2.34	0.67
5:a:133:LEU:HD12	8:d:256:ILE:HG12	1.76	0.67
19:s:176:MET:HE2	19:s:176:MET:HA	1.75	0.67
30:y:606:CHL:HHC	30:y:606:CHL:HBB1	1.76	0.67
30:2:601:CHL:HHC	30:2:601:CHL:HBB1	1.74	0.67
36:Y:317:NEX:H402	38:Y:320:SQD:H162	1.75	0.67
1:7:74:THR:O	3:8:83:ARG:NE	2.26	0.67
30:9:310:CHL:HHC	30:9:310:CHL:HBB1	1.76	0.67
3:p:245:PHE:HB2	31:p:613:CLA:CAD	2.24	0.67
3:n:252:LYS:HA	3:n:256:ILE:HG23	1.76	0.67
30:1:609:CHL:HHC	30:1:609:CHL:HBB1	1.76	0.67
4:6:253:LYS:HD2	4:6:254:THR:N	2.10	0.67
31:N:305:CLA:H191	31:S:306:CLA:ND	2.10	0.67
4:0:205:LYS:HD3	31:0:612:CLA:HBA1	1.74	0.67
3:p:91:HIS:HE1	31:p:603:CLA:ND	1.91	0.67
6:b:29:LEU:HD11	43:b:618:BCR:H19C	1.75	0.67
31:B:612:CLA:HMB1	31:B:612:CLA:HBB1	1.75	0.67
45:C:620:DGD:HAV2	33:Y:318:LHG:H361	1.76	0.67
33:c:622:LHG:H242	31:s:312:CLA:HAB	1.76	0.67
2:4:152:ILE:O	2:4:156:LEU:HG	1.95	0.67
3:5:220:VAL:HG21	31:5:613:CLA:HAC2	1.77	0.67
31:g:312:CLA:HBB1	31:g:312:CLA:HMB3	1.76	0.67
31:5:610:CLA:H12	31:5:610:CLA:H3A	1.77	0.67
30:G:608:CHL:HBB1	30:G:608:CHL:HHC	1.76	0.67
30:Y:307:CHL:HHC	30:Y:307:CHL:HBB1	1.76	0.67
30:p:607:CHL:HHC	30:p:607:CHL:HBB1	1.76	0.67
1:1:185:PRO:HD2	32:1:615:LUT:H23	1.77	0.67
4:6:172:GLY:O	18:R:56:ASN:ND2	2.28	0.67
30:6:310:CHL:HHC	30:6:310:CHL:HBB1	1.77	0.67
5:A:140:ARG:HH22	33:A:417:LHG:HC41	1.58	0.67
2:9:86:ARG:NH1	2:9:86:ARG:HA	2.10	0.67
3:p:52:PHE:CG	2:q:168:ALA:HB1	2.29	0.67
3:p:198:ALA:HA	3:p:201:LYS:HD3	1.76	0.67
3:8:252:LYS:HA	3:8:256:ILE:HG23	1.76	0.67
30:9:307:CHL:HHC	30:9:307:CHL:HBB1	1.75	0.67
3:p:225:THR:HB	3:p:249:TYR:HE2	1.60	0.67
6:b:216:HIS:HE1	31:b:610:CLA:NA	1.90	0.67
7:c:357:LEU:HD21	7:c:372:ILE:HG12	1.77	0.67
30:1:608:CHL:HHC	30:1:608:CHL:HBB1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:606:CHL:HBB1	30:4:606:CHL:HMB1	1.76	0.67
44:A:416:PL9:H453	8:D:39:PRO:HA	1.76	0.67
30:G:601:CHL:HHC	30:G:601:CHL:HBB1	1.76	0.67
31:Y:304:CLA:CAD	30:Y:309:CHL:H2	2.24	0.67
1:7:106:VAL:HG13	1:7:228:ILE:HD11	1.76	0.67
31:p:610:CLA:H52	32:p:616:LUT:H28	1.76	0.67
30:g:302:CHL:HHC	30:g:302:CHL:HBB1	1.75	0.67
3:3:95:ALA:HA	32:3:318:LUT:H11	1.77	0.67
30:6:308:CHL:HHC	30:6:308:CHL:HBB1	1.76	0.67
3:N:200:LEU:HB3	31:N:310:CLA:HMA2	1.76	0.67
31:9:304:CLA:H102	32:9:318:LUT:H371	1.76	0.67
5:a:188:ALA:HB2	5:a:328:MET:HB2	1.76	0.67
2:g:258:LEU:HD22	2:g:259:PRO:HD2	1.76	0.67
2:4:73:ASP:HA	32:4:616:LUT:H24	1.78	0.66
30:Y:301:CHL:H93	30:Y:302:CHL:H8	1.77	0.66
1:7:107:VAL:HB	1:7:108:PRO:HD3	1.76	0.66
2:9:190:PHE:HE2	30:9:310:CHL:NA	1.93	0.66
31:9:304:CLA:HBC2	31:9:304:CLA:HMC1	1.76	0.66
3:p:215:MET:HA	3:p:218:PHE:CD2	2.30	0.66
2:4:117:ALA:HA	34:Q1:101:LMG:H351	1.75	0.66
38:B:620:SQD:H372	43:t:101:BCR:H362	1.75	0.66
30:R:308:CHL:HBB1	30:R:308:CHL:HHC	1.78	0.66
35:2:614:RRX:H55	34:2:618:LMG:H322	1.76	0.66
33:G:618:LHG:H362	37:G:620:XAT:H12	1.77	0.66
5:a:41:LEU:HD22	42:a:408:PHO:H61	1.77	0.66
45:c:617:DGD:HA22	34:k:101:LMG:H351	1.77	0.66
3:5:164:GLY:O	3:5:167:VAL:HG22	1.96	0.66
38:B:623:SQD:H351	23:X:83:LEU:HD21	1.78	0.66
15:L:8:LYS:HZ2	15:L:8:LYS:HB3	1.60	0.66
30:N:309:CHL:H52	30:Y:302:CHL:H51	1.77	0.66
30:7:310:CHL:HHC	30:7:310:CHL:HBB1	1.76	0.66
3:8:110:ARG:HH21	3:8:231:GLU:HA	1.61	0.66
13:j:40:SER:O	13:j:42:LEU:HD22	1.96	0.66
3:n:92:ALA:HB1	3:n:208:GLY:HA3	1.78	0.66
4:0:183:PRO:HD2	31:0:610:CLA:OBD	1.94	0.66
30:p:609:CHL:HBB1	30:p:609:CHL:HHC	1.76	0.66
22:w:86:THR:HG21	34:w:202:LMG:H221	1.77	0.66
2:4:223:PHE:CZ	35:4:615:RRX:H48	2.30	0.66
30:5:607:CHL:HHC	30:5:607:CHL:HBB1	1.76	0.66
30:0:608:CHL:HHC	30:0:608:CHL:HBB1	1.77	0.66
3:8:92:ALA:HB1	3:8:208:GLY:HA3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:89:VAL:HG21	3:p:179:LEU:HD11	1.78	0.66
27:q1:3:ASN:HD22	34:q1:101:LMG:HC72	1.60	0.66
4:6:156:THR:HG21	30:6:307:CHL:HED3	1.78	0.66
34:6:321:LMG:O2	18:R:273:PHE:HB3	1.96	0.66
4:0:255:LEU:HD12	31:0:615:CLA:HED1	1.78	0.66
30:8:605:CHL:HHC	30:8:605:CHL:HBB1	1.78	0.66
2:4:208:LYS:HG3	31:4:611:CLA:HED2	1.78	0.66
3:5:110:ARG:HH12	3:5:231:GLU:CD	2.04	0.66
3:5:227:LYS:HB2	3:5:232:ASN:HD21	1.61	0.66
5:A:255:PHE:HD2	5:A:264:SER:HB3	1.61	0.66
8:D:233:ARG:HH21	28:P1:26:GLY:HA2	1.60	0.66
33:G:618:LHG:HC61	37:G:620:XAT:H382	1.76	0.66
34:W:202:LMG:H371	31:Y:311:CLA:H171	1.77	0.66
31:c:606:CLA:H52	34:w:202:LMG:H331	1.77	0.66
19:s:163:LEU:HD21	19:s:171:ILE:HD12	1.78	0.66
29:F1:187:ASP:N	29:F1:187:ASP:OD1	2.29	0.66
1:1:186:LEU:HD12	32:1:615:LUT:H222	1.78	0.66
31:3:315:CLA:H2	31:3:315:CLA:HBA2	1.77	0.66
30:4:605:CHL:HHD	30:4:606:CHL:HED2	1.77	0.66
30:4:607:CHL:H11	3:5:250:ALA:HA	1.77	0.66
33:A:417:LHG:HC2	31:C:608:CLA:HED2	1.78	0.66
2:G:220:MET:HE2	32:G:615:LUT:H10	1.75	0.66
1:7:107:VAL:HG21	31:7:305:CLA:HAC2	1.78	0.66
2:9:220:MET:HE2	32:9:318:LUT:H10	1.78	0.66
6:b:12:VAL:HG23	31:b:613:CLA:HMC2	1.78	0.66
31:n:314:CLA:H13	33:n:320:LHG:H321	1.78	0.66
6:B:162:PHE:CE1	48:R:302:LMU:H1'	2.31	0.66
31:N:310:CLA:H52	32:N:316:LUT:H30	1.78	0.66
31:8:609:CLA:H2	32:8:615:LUT:H28	1.77	0.66
33:q:320:LHG:HC92	37:q:321:XAT:H393	1.77	0.66
30:s:308:CHL:HBB2	31:s:310:CLA:HBC3	1.76	0.66
30:y:607:CHL:HHC	30:y:607:CHL:HBB1	1.78	0.66
2:4:133:PHE:CE1	30:4:607:CHL:HMD3	2.32	0.65
2:4:223:PHE:CE1	35:4:615:RRX:C31	2.79	0.65
32:5:617:LUT:H12	32:5:617:LUT:H191	1.77	0.65
1:7:53:TYR:HA	3:8:168:ASN:HD22	1.60	0.65
30:7:307:CHL:HBB1	30:7:307:CHL:HHC	1.78	0.65
31:2:613:CLA:H62	31:2:613:CLA:NB	2.11	0.65
2:4:229:VAL:HG13	2:4:256:LYS:HZ2	1.61	0.65
8:D:123:ILE:HD11	34:D:412:LMG:H402	1.79	0.65
2:G:99:MET:SD	31:G:609:CLA:HAB	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:164:ILE:HD11	36:0:618:NEX:C35	2.27	0.65
31:9:304:CLA:HBC1	33:9:320:LHG:H262	1.77	0.65
1:1:178:TYR:HB3	31:1:610:CLA:HED3	1.78	0.65
30:1:606:CHL:HBB1	30:1:606:CHL:HHC	1.77	0.65
30:1:607:CHL:H12	2:2:259:PRO:HD3	1.78	0.65
2:2:192:PRO:HD2	35:2:614:RRX:H14	1.78	0.65
30:4:607:CHL:HBB1	30:4:607:CHL:HHC	1.77	0.65
38:A:411:SQD:H352	31:C:608:CLA:H72	1.79	0.65
2:G:223:PHE:HE1	35:G:614:RRX:H48	1.44	0.65
3:N:224:ILE:HD12	3:N:258:TYR:HE2	1.60	0.65
31:N:304:CLA:H2	31:N:304:CLA:HMA1	1.78	0.65
31:n:311:CLA:H2	32:n:317:LUT:H28	1.77	0.65
31:4:613:CLA:H12	31:4:614:CLA:HED2	1.79	0.65
3:5:253:SER:HA	3:5:258:TYR:CE1	2.31	0.65
31:Y:305:CLA:HMA3	30:Y:307:CHL:C2C	2.26	0.65
2:9:218:PHE:HE1	31:9:315:CLA:HAB	1.60	0.65
2:g:176:PRO:HD2	30:g:308:CHL:HBB2	1.78	0.65
19:s:137:PHE:HE1	19:s:259:GLY:HA2	1.61	0.65
2:4:258:LEU:HD22	2:4:259:PRO:HD2	1.78	0.65
30:0:607:CHL:HED3	2:q:258:LEU:HD23	1.77	0.65
7:c:204:SER:HB3	34:w:201:LMG:HC72	1.79	0.65
19:s:123:GLY:O	19:s:127:ASN:ND2	2.27	0.65
22:w:93:TRP:CZ2	34:w:202:LMG:H131	2.32	0.65
34:w:202:LMG:H252	31:y:612:CLA:H162	1.79	0.65
3:8:131:GLU:OE1	3:8:132:GLY:N	2.30	0.65
31:8:612:CLA:H13	33:8:618:LHG:H321	1.78	0.65
7:c:202:PHE:CZ	31:c:606:CLA:H13	2.31	0.65
3:5:115:ASN:HD22	3:5:115:ASN:N	1.94	0.65
4:6:202:LEU:HB3	31:6:311:CLA:HMA1	1.77	0.65
30:7:308:CHL:HBB1	30:7:308:CHL:HMB3	1.78	0.65
33:q:320:LHG:HC5	37:q:321:XAT:H382	1.77	0.65
33:b:628:LHG:H251	33:b:628:LHG:H132	1.78	0.65
30:n:306:CHL:HHC	30:n:306:CHL:HBB1	1.78	0.65
31:s:316:CLA:HBB1	31:s:316:CLA:HHC	1.79	0.65
31:y:610:CLA:H52	32:y:616:LUT:H30	1.76	0.65
30:3:302:CHL:H52	30:3:302:CHL:H93	1.78	0.65
30:G:606:CHL:HBB1	30:G:606:CHL:HHC	1.79	0.65
18:R:236:ALA:HB2	31:R:313:CLA:HED2	1.76	0.65
31:8:604:CLA:H92	30:8:606:CHL:HBA2	1.78	0.65
2:9:112:GLN:HA	2:9:117:ALA:HA	1.77	0.65
3:n:233:LEU:HD13	31:n:315:CLA:HBC2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:112:MET:SD	31:s:311:CLA:HAB	2.36	0.65
30:3:309:CHL:HHC	30:3:309:CHL:HBB1	1.79	0.65
3:5:64:PRO:HB2	3:5:205:LEU:HD12	1.79	0.65
30:5:606:CHL:HMB1	30:5:606:CHL:HBB1	1.79	0.65
45:C:617:DGD:HA42	34:J:101:LMG:H381	1.78	0.65
31:0:614:CLA:C4B	31:0:614:CLA:H71	2.27	0.65
31:7:304:CLA:HBB1	31:7:304:CLA:HHC	1.78	0.65
3:p:163:GLU:HG3	30:p:609:CHL:C4B	2.27	0.65
2:2:238:LEU:HD13	34:2:618:LMG:HC92	1.79	0.65
31:B:606:CLA:H72	43:B:619:BCR:H342	1.79	0.65
31:n:316:CLA:H11	34:n:322:LMG:C9	2.27	0.65
31:1:612:CLA:HMD2	38:g:301:SQD:H251	1.79	0.64
6:B:124:ARG:NH1	11:H:19:ASP:O	2.29	0.64
31:y:604:CLA:HMA3	30:y:606:CHL:C2C	2.27	0.64
33:B:624:LHG:H122	30:R:309:CHL:HBA2	1.77	0.64
9:E:14:LEU:HD11	34:J:102:LMG:H372	1.79	0.64
22:W:86:THR:HG21	34:W:201:LMG:H221	1.79	0.64
4:0:98:MET:SD	31:0:610:CLA:HAB	2.37	0.64
2:9:221:PHE:HB2	32:9:318:LUT:H401	1.79	0.64
2:2:125:TRP:CG	2:2:126:PHE:H	2.15	0.64
2:2:144:PRO:O	2:2:148:HIS:HB2	1.97	0.64
3:3:38:VAL:HA	3:3:42:GLY:CA	2.27	0.64
30:3:308:CHL:CBB	32:3:318:LUT:H161	2.27	0.64
19:S:112:MET:SD	31:S:311:CLA:HAB	2.38	0.64
4:0:125:LYS:HA	30:0:607:CHL:HED2	1.78	0.64
31:8:604:CLA:HMA3	30:8:606:CHL:C2C	2.27	0.64
3:p:185:PHE:HZ	30:p:608:CHL:NB	1.95	0.64
3:p:199:GLU:HG2	3:p:203:LYS:HE2	1.79	0.64
31:q:312:CLA:HBA1	35:q:317:RRX:C40	2.27	0.64
3:n:110:ARG:HH21	3:n:231:GLU:HA	1.61	0.64
38:s:301:SQD:H282	31:s:315:CLA:HAA2	1.78	0.64
22:w:80:SER:HB2	34:w:205:LMG:H302	1.79	0.64
29:f1:197:ILE:C	29:f1:230:TRP:HE1	2.04	0.64
2:2:126:PHE:CD2	2:2:127:LYS:HG3	2.32	0.64
2:4:92:VAL:HB	2:4:184:LEU:HD11	1.78	0.64
2:4:163:MET:HE2	30:4:606:CHL:HMA3	1.79	0.64
9:e:8:ARG:HD3	9:e:13:ILE:HG12	1.79	0.64
31:3:313:CLA:HHC	31:3:313:CLA:HBB1	1.79	0.64
2:4:124:VAL:HB	2:4:127:LYS:HB3	1.79	0.64
3:5:185:PHE:HB3	31:5:610:CLA:HMD3	1.78	0.64
31:B:607:CLA:C4A	31:B:607:CLA:HBA2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:5:608:CHL:H12	32:5:616:LUT:H383	1.78	0.64
31:5:615:CLA:HBA1	31:5:615:CLA:CBD	2.27	0.64
10:F:14:ILE:HD11	27:Q1:26:PRO:HB2	1.79	0.64
3:N:86:GLU:HA	3:N:179:LEU:HD11	1.78	0.64
9:e:25:ILE:HD12	27:q1:18:TRP:CD1	2.32	0.64
31:y:610:CLA:H62	31:y:612:CLA:HMA2	1.79	0.64
31:1:611:CLA:C3B	38:g:318:SQD:H241	2.28	0.64
3:3:258:TYR:CE2	31:3:316:CLA:HHD	2.32	0.64
2:4:157:LEU:HA	2:4:160:LEU:HD12	1.79	0.64
37:4:619:XAT:H163	34:4:620:LMG:H172	1.80	0.64
30:Y:302:CHL:HBB1	30:Y:302:CHL:HMB3	1.80	0.64
4:0:76:LEU:HD23	31:0:602:CLA:H42	1.80	0.64
2:9:86:ARG:HA	2:9:86:ARG:HH11	1.62	0.64
2:g:72:TRP:CZ2	30:g:302:CHL:HBA1	2.32	0.64
19:s:218:PRO:HD2	32:s:317:LUT:H23	1.80	0.64
2:2:186:PRO:HG3	30:2:607:CHL:CHD	2.28	0.64
30:3:307:CHL:CBB	34:3:321:LMG:H322	2.27	0.64
7:C:368:LEU:HA	7:C:372:ILE:HD11	1.77	0.64
31:S:305:CLA:H171	31:S:305:CLA:H141	1.79	0.64
2:9:129:GLY:H	30:9:309:CHL:HED1	1.63	0.64
3:n:131:GLU:OE1	3:n:132:GLY:N	2.30	0.64
2:2:149:ALA:HA	30:2:605:CHL:C1C	2.28	0.64
2:2:223:PHE:HE1	35:2:614:RRX:C32	2.10	0.64
3:3:185:PHE:HZ	30:3:309:CHL:NB	1.95	0.64
31:G:609:CLA:H102	35:G:614:RRX:H26	1.80	0.64
30:Y:301:CHL:HBB1	30:Y:301:CHL:HMB1	1.79	0.64
4:0:111:GLN:HG3	4:0:121:ALA:HB2	1.80	0.64
30:n:301:CHL:HHC	30:n:301:CHL:HBB1	1.79	0.64
30:n:308:CHL:HMB1	30:n:308:CHL:HBB1	1.80	0.64
19:s:204:TYR:HA	19:s:207:MET:HE2	1.79	0.64
30:y:601:CHL:HBB1	30:y:601:CHL:HMB1	1.80	0.64
3:3:134:LEU:HD21	31:3:306:CLA:HAA2	1.79	0.64
3:5:177:ASP:HB3	3:5:180:TYR:O	1.98	0.64
3:5:245:PHE:HB2	31:5:613:CLA:CAD	2.27	0.64
5:A:133:LEU:HD12	8:D:256:ILE:HG12	1.78	0.64
6:B:464:PHE:HD2	31:B:611:CLA:HAC2	1.63	0.64
19:S:217:ASP:HA	32:S:317:LUT:H24	1.79	0.64
30:Y:301:CHL:H121	30:Y:301:CHL:H91	1.80	0.64
8:d:257:PHE:HE2	33:d:408:LHG:H112	1.63	0.64
29:F1:170:ASP:HB2	29:F1:176:TYR:HE1	1.63	0.64
1:1:249:LYS:H	1:1:249:LYS:HD2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:125:GLY:HA2	30:5:606:CHL:HAC2	1.80	0.63
5:A:341:LEU:HB3	5:A:343:LEU:HD13	1.80	0.63
30:G:606:CHL:HBB2	30:N:301:CHL:HBB1	1.80	0.63
1:7:186:LEU:HD12	32:7:317:LUT:H222	1.80	0.63
30:9:309:CHL:HHC	30:9:309:CHL:HBB1	1.80	0.63
6:b:413:ASP:N	6:b:413:ASP:OD1	2.31	0.63
7:c:302:THR:HG21	7:c:343:THR:HG21	1.79	0.63
8:d:233:ARG:HH21	28:p1:26:GLY:HA2	1.63	0.63
33:d:408:LHG:HC91	15:l:20:TRP:HZ2	1.63	0.63
31:n:305:CLA:HMA3	30:n:307:CHL:C2C	2.28	0.63
2:2:112:GLN:HB3	2:2:119:PHE:HD2	1.63	0.63
3:8:233:LEU:HD13	31:8:613:CLA:HBC2	1.80	0.63
15:l:27:VAL:HG11	33:l:101:LHG:H201	1.79	0.63
31:Y:310:CLA:H2	32:Y:315:LUT:H28	1.81	0.63
1:7:176:ALA:HB2	18:r:38:ARG:HH21	1.63	0.63
31:p:602:CLA:H111	32:p:617:LUT:H361	1.80	0.63
31:q:312:CLA:HBA1	35:q:317:RRX:H7	1.81	0.63
3:n:86:GLU:HA	3:n:179:LEU:HD11	1.79	0.63
31:y:612:CLA:HHC	31:y:612:CLA:HBB1	1.80	0.63
1:1:121:LYS:HA	30:1:607:CHL:HED2	1.79	0.63
30:G:606:CHL:HBB2	30:N:301:CHL:CBB	2.28	0.63
3:p:110:ARG:HH22	3:p:230:ILE:HG21	1.63	0.63
44:a:414:PL9:H102	44:a:414:PL9:HC2	1.81	0.63
18:r:236:ALA:HB2	31:r:313:CLA:HED2	1.80	0.63
34:Q1:101:LMG:H161	34:Q1:101:LMG:H372	1.80	0.63
30:2:606:CHL:HMB1	30:2:606:CHL:HBB1	1.80	0.63
3:3:122:PHE:CD1	3:3:123:LYS:HG3	2.33	0.63
30:5:608:CHL:HMB1	30:5:608:CHL:HBB1	1.81	0.63
34:B:625:LMG:H372	30:R:309:CHL:C10	2.29	0.63
10:F:43:GLN:HB3	29:F1:57:ALA:HB3	1.79	0.63
31:G:603:CLA:H2	31:G:603:CLA:HMA3	1.81	0.63
34:G:621:LMG:H411	30:N:309:CHL:H161	1.81	0.63
12:I:26:ASN:ND2	49:I:201:HOH:O	2.30	0.63
2:9:226:GLN:O	2:9:230:THR:HG22	1.99	0.63
34:9:321:LMG:HC1	34:9:321:LMG:H292	1.81	0.63
3:p:143:ILE:HA	30:p:605:CHL:C4D	2.28	0.63
31:p:611:CLA:HAA1	31:p:612:CLA:OBD	1.99	0.63
7:c:112:VAL:HG12	33:s:322:LHG:H342	1.80	0.63
33:d:408:LHG:H312	20:t:21:ILE:HD11	1.79	0.63
3:5:203:LYS:HG3	31:5:611:CLA:HED2	1.78	0.63
34:5:620:LMG:HC62	31:6:315:CLA:CMA	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:8:614:CLA:CHC	34:9:302:LMG:H362	2.27	0.63
3:p:151:ILE:HG22	30:p:605:CHL:HAC1	1.80	0.63
3:p:247:VAL:HG13	2:q:133:PHE:CE2	2.30	0.63
31:q:312:CLA:C2	35:q:317:RRX:H6	2.29	0.63
30:g:307:CHL:HHC	30:g:307:CHL:HBB1	1.79	0.63
2:2:86:ARG:HA	2:2:86:ARG:HH11	1.62	0.63
3:3:245:PHE:HB2	31:3:314:CLA:CAD	2.28	0.63
2:4:144:PRO:O	2:4:148:HIS:HB2	1.98	0.63
31:4:610:CLA:H2	35:4:615:RRX:H6	1.81	0.63
6:B:423:ARG:NH2	6:B:430:PHE:O	2.31	0.63
10:F:20:LEU:HD11	34:X:203:LMG:H292	1.79	0.63
30:N:307:CHL:HBB2	30:Y:301:CHL:HAB	1.81	0.63
3:p:233:LEU:HA	31:p:613:CLA:CMA	2.28	0.63
34:d:411:LMG:O10	11:h:69:ASN:ND2	2.32	0.63
2:g:235:LEU:HD22	34:g:320:LMG:HC91	1.81	0.63
19:s:217:ASP:HA	32:s:317:LUT:H24	1.81	0.63
1:1:99:MET:SD	31:1:610:CLA:HAB	2.39	0.63
30:3:302:CHL:HMA2	31:3:316:CLA:C3B	2.28	0.63
30:7:307:CHL:HBB2	30:7:308:CHL:HAB	1.80	0.63
3:p:136:TYR:HB3	3:p:142:LEU:HB3	1.81	0.63
31:c:613:CLA:HBA1	31:c:613:CLA:HBD	1.80	0.63
3:p:197:PHE:CE2	3:p:201:LYS:HD2	2.33	0.63
30:p:605:CHL:CBB	34:p:620:LMG:H321	2.28	0.63
30:q:308:CHL:HAA2	30:q:308:CHL:HBD	1.81	0.63
30:q:309:CHL:C4B	30:q:309:CHL:H102	2.29	0.63
5:a:118:HIS:HE1	31:a:409:CLA:C4D	2.12	0.63
31:c:611:CLA:H42	21:v:33:LEU:HA	1.79	0.63
3:n:254:ALA:HB3	30:n:301:CHL:HED3	1.81	0.63
30:n:307:CHL:H52	31:s:313:CLA:H102	1.81	0.63
31:y:603:CLA:HMA1	31:y:603:CLA:H2	1.81	0.63
30:3:310:CHL:HMB3	30:3:310:CHL:HBB1	1.80	0.62
30:N:301:CHL:HBB1	30:N:301:CHL:HHC	1.79	0.62
31:Y:310:CLA:H62	31:Y:312:CLA:HMA2	1.80	0.62
3:n:203:LYS:HD3	31:n:313:CLA:HAA2	1.81	0.62
31:n:315:CLA:HBA1	31:n:315:CLA:CHA	2.28	0.62
30:r:309:CHL:HBD	30:r:309:CHL:HAA1	1.81	0.62
24:y:186:TYR:HB3	31:y:610:CLA:HED3	1.81	0.62
31:y:613:CLA:H93	33:y:619:LHG:H152	1.80	0.62
30:3:303:CHL:HAC1	33:3:320:LHG:HC32	1.81	0.62
2:4:132:ILE:HA	2:4:138:LEU:HB2	1.81	0.62
2:4:147:ILE:CG1	31:4:604:CLA:H41	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:86:GLU:HA	3:8:179:LEU:HD11	1.79	0.62
31:8:613:CLA:CHA	31:8:613:CLA:HBA1	2.28	0.62
2:9:185:TYR:HB3	31:9:312:CLA:HED3	1.80	0.62
31:q:306:CLA:H62	36:q:319:NEX:H373	1.80	0.62
31:c:603:CLA:H161	31:c:610:CLA:HBB2	1.80	0.62
19:s:256:THR:HG23	19:s:258:GLU:H	1.62	0.62
24:y:192:ASP:HA	32:y:616:LUT:H24	1.79	0.62
3:3:246:TRP:O	3:3:251:PRO:HD3	1.99	0.62
4:6:106:THR:OG1	4:6:107:PRO:HD3	1.99	0.62
6:B:272:ARG:NH1	6:B:276:ASP:OD2	2.33	0.62
6:B:322:GLY:HA3	6:B:445:THR:HG23	1.80	0.62
45:C:620:DGD:HBH2	31:Y:311:CLA:H51	1.81	0.62
33:G:618:LHG:HC62	37:G:620:XAT:H382	1.80	0.62
31:c:605:CLA:H201	45:c:616:DGD:HAN1	1.81	0.62
4:6:235:LEU:HD23	32:6:317:LUT:H163	1.80	0.62
43:B:618:BCR:HC41	34:B:621:LMG:H331	1.81	0.62
8:D:117:HIS:HE1	31:D:404:CLA:C4D	2.13	0.62
30:8:607:CHL:HBB1	30:8:607:CHL:HMB3	1.81	0.62
1:1:122:ALA:HB1	31:1:604:CLA:HED1	1.80	0.62
30:1:607:CHL:HBB1	30:1:607:CHL:HMB3	1.80	0.62
31:1:611:CLA:H2	31:1:612:CLA:OBD	1.98	0.62
2:2:118:ASP:HB3	2:2:142:GLY:HA3	1.82	0.62
30:3:308:CHL:HBB1	32:3:318:LUT:H161	1.80	0.62
2:4:132:ILE:HB	2:4:138:LEU:HD12	1.80	0.62
31:N:305:CLA:HMA3	30:N:307:CHL:C2C	2.29	0.62
8:d:186:GLN:HB2	31:d:404:CLA:HBC1	1.82	0.62
43:C:614:BCR:H11C	38:S:301:SQD:H281	1.81	0.62
2:G:231:GLY:HA2	31:N:315:CLA:HMA2	1.82	0.62
31:N:314:CLA:CHA	31:N:314:CLA:HBA1	2.29	0.62
5:A:118:HIS:HE1	31:A:409:CLA:C4D	2.13	0.62
6:B:382:PRO:HG2	6:B:385:ARG:HG2	1.81	0.62
7:C:264:LEU:HD21	31:C:608:CLA:HAB	1.80	0.62
30:S:308:CHL:HHC	30:S:308:CHL:HBB1	1.80	0.62
1:7:252:ALA:HB2	30:7:321:CHL:HAA2	1.80	0.62
3:p:245:PHE:CD1	3:p:249:TYR:HB2	2.34	0.62
30:p:606:CHL:HMB1	30:p:606:CHL:HBB1	1.81	0.62
30:p:608:CHL:HBD	30:p:608:CHL:HAA1	1.82	0.62
31:r:305:CLA:HBC1	31:r:311:CLA:CBC	2.30	0.62
19:s:138:GLU:HA	30:s:308:CHL:CED	2.30	0.62
2:2:47:ALA:HB1	30:2:601:CHL:HBC1	1.82	0.62
2:4:180:SER:O	2:4:181:GLY:C	2.41	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:50:LEU:CB	4:6:54:SER:HB3	2.30	0.62
24:Y:175:PRO:HD2	30:Y:308:CHL:HBB2	1.81	0.62
44:d:407:PL9:H502	20:t:10:LEU:HD13	1.82	0.62
31:n:305:CLA:H92	30:n:307:CHL:HBA2	1.79	0.62
2:4:143:ASN:ND2	2:4:146:LEU:HD23	2.15	0.62
2:4:205:LEU:HD11	31:4:610:CLA:H43	1.82	0.62
2:4:229:VAL:HG13	2:4:256:LYS:NZ	2.14	0.62
31:G:604:CLA:H2	30:G:606:CHL:HBD	1.80	0.62
31:0:610:CLA:H2	32:0:616:LUT:H28	1.82	0.62
3:8:203:LYS:HD3	31:8:611:CLA:HAA2	1.81	0.62
2:9:137:GLY:HA3	2:9:150:GLN:HG2	1.81	0.62
3:p:225:THR:CG2	31:p:613:CLA:HED2	2.29	0.62
31:q:304:CLA:H61	32:q:318:LUT:H28	1.81	0.62
45:c:619:DGD:HBT2	31:y:611:CLA:HBC3	1.82	0.62
30:3:307:CHL:C1C	34:3:321:LMG:H371	2.29	0.62
2:G:155:VAL:HG12	30:G:605:CHL:HAC1	1.81	0.62
38:g:301:SQD:H92	37:g:321:XAT:C22	2.30	0.62
30:r:308:CHL:HHC	30:r:308:CHL:HBB1	1.82	0.62
24:y:154:THR:HG22	30:y:605:CHL:HAC1	1.82	0.62
30:1:605:CHL:C4A	34:6:321:LMG:H302	2.30	0.61
3:5:237:LEU:HD21	31:5:614:CLA:HMC3	1.81	0.61
30:5:606:CHL:CBB	30:5:609:CHL:HBC1	2.29	0.61
4:6:208:LYS:NZ	33:6:320:LHG:O5	2.33	0.61
7:C:203:ARG:HG2	7:C:209:ASP:HB3	1.82	0.61
31:R:304:CLA:CBB	37:R:318:XAT:H32	2.30	0.61
30:7:321:CHL:HBB1	30:7:321:CHL:HMB3	1.80	0.61
3:8:180:TYR:HB3	31:8:609:CLA:HED3	1.81	0.61
2:9:72:TRP:CE3	32:9:318:LUT:H383	2.35	0.61
30:9:310:CHL:HMB1	36:9:319:NEX:C12	2.30	0.61
30:p:601:CHL:HHC	30:p:601:CHL:HBB1	1.82	0.61
2:g:171:TYR:CD2	3:n:49:LEU:HD12	2.35	0.61
30:3:308:CHL:HBB1	30:3:308:CHL:HHC	1.82	0.61
2:4:205:LEU:HB3	31:4:610:CLA:HMA2	1.82	0.61
30:5:607:CHL:HED1	4:6:256:ALA:HA	1.82	0.61
3:p:225:THR:HG21	31:p:613:CLA:HED2	1.80	0.61
1:1:251:LEU:CB	30:1:619:CHL:HBA2	2.31	0.61
30:1:619:CHL:HBD	30:1:619:CHL:CBA	2.24	0.61
2:4:59:PRO:HB3	2:4:61:TYR:CZ	2.34	0.61
31:B:612:CLA:H171	31:B:613:CLA:HBB2	1.81	0.61
31:C:601:CLA:H192	31:C:607:CLA:H152	1.82	0.61
11:h:42:PRO:HG3	18:r:85:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:n:304:CLA:HAC1	30:n:308:CHL:CBB	2.29	0.61
19:s:122:GLU:HA	19:s:134:ALA:HB1	1.83	0.61
2:2:133:PHE:HE1	3:3:247:VAL:HG22	1.65	0.61
31:4:602:CLA:H2	31:4:602:CLA:CHB	2.31	0.61
3:5:246:TRP:HA	3:5:250:ALA:HB3	1.82	0.61
18:R:139:HIS:CD2	37:R:318:XAT:H15	2.36	0.61
34:9:301:LMG:H411	34:9:301:LMG:H372	1.82	0.61
2:q:147:ILE:HG22	2:q:149:ALA:HB2	1.82	0.61
2:q:173:GLY:HA2	30:q:310:CHL:HMC	1.82	0.61
6:b:91:TRP:CD2	31:b:607:CLA:HBA2	2.36	0.61
24:y:99:MET:SD	31:y:610:CLA:HAB	2.41	0.61
30:y:607:CHL:C10	30:y:609:CHL:H172	2.31	0.61
31:2:610:CLA:H61	31:2:611:CLA:C4D	2.30	0.61
2:9:190:PHE:HB3	30:9:310:CHL:H11	1.83	0.61
2:g:99:MET:SD	31:g:310:CLA:HAB	2.40	0.61
31:y:613:CLA:H18	31:y:614:CLA:O1A	2.01	0.61
3:3:191:ALA:HB1	3:3:197:PHE:CD1	2.35	0.61
2:4:139:ASN:HB3	2:4:143:ASN:O	2.01	0.61
30:4:601:CHL:HED1	33:4:618:LHG:H292	1.83	0.61
30:5:607:CHL:HBD	30:5:607:CHL:HBA1	1.81	0.61
44:A:416:PL9:H33	10:F:25:LEU:HD21	1.82	0.61
34:G:622:LMG:H132	34:G:622:LMG:HC91	1.82	0.61
30:G:623:CHL:H93	30:Y:309:CHL:H193	1.81	0.61
31:N:304:CLA:HMD2	30:N:309:CHL:H2	1.81	0.61
30:N:308:CHL:HMB1	30:N:308:CHL:HBB1	1.81	0.61
17:O:269:ASP:O	17:O:275:LYS:NZ	2.34	0.61
30:7:302:CHL:C1D	33:7:319:LHG:HC81	2.31	0.61
31:a:409:CLA:H101	34:w:201:LMG:H142	1.82	0.61
18:r:44:TYR:HB2	36:r:301:NEX:O3	2.01	0.61
34:5:620:LMG:C6	31:6:315:CLA:HMA2	2.31	0.61
19:s:171:ILE:HG21	30:s:307:CHL:HED3	1.82	0.61
2:4:187:GLY:O	2:4:188:GLY:C	2.43	0.61
31:4:604:CLA:NA	36:4:617:NEX:H242	2.14	0.61
31:S:303:CLA:H203	31:S:304:CLA:HBB1	1.83	0.61
2:q:186:PRO:HG3	30:q:310:CHL:HBC2	1.82	0.61
30:s:308:CHL:HHC	30:s:308:CHL:HBB1	1.83	0.61
43:t:101:BCR:H382	43:t:101:BCR:H23C	1.82	0.61
3:3:143:ILE:HA	30:3:307:CHL:C4D	2.30	0.61
3:3:188:LEU:HD12	32:3:317:LUT:H222	1.83	0.61
3:5:45:ARG:HB2	3:5:46:PRO:HD2	1.82	0.61
5:A:215:HIS:HA	44:A:416:PL9:HC2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:S:301:SQD:H302	31:S:315:CLA:HBD	1.83	0.61
30:7:309:CHL:HBD	30:7:309:CHL:HAA1	1.82	0.61
31:c:606:CLA:H41	34:w:202:LMG:H331	1.83	0.61
30:n:307:CHL:HHC	30:n:307:CHL:HBB1	1.83	0.61
29:f1:66:PHE:CZ	29:f1:225:GLU:HA	2.36	0.61
30:1:619:CHL:CBB	30:3:308:CHL:HBB2	2.31	0.61
30:3:309:CHL:HAA1	30:3:309:CHL:HBD	1.83	0.61
2:4:183:SER:O	30:4:608:CHL:HMD1	2.01	0.61
5:A:303:ASN:O	7:C:403:ASN:ND2	2.29	0.61
31:0:604:CLA:H52	30:0:606:CHL:HBA1	1.83	0.61
30:0:605:CHL:O2D	30:0:605:CHL:H2A	2.01	0.61
1:7:189:ALA:HB1	1:7:195:LEU:HD13	1.82	0.61
3:8:69:TRP:O	32:8:616:LUT:H24	2.01	0.61
42:d:402:PHO:H72	31:d:404:CLA:H111	1.82	0.61
30:n:309:CHL:HMB1	30:n:309:CHL:HBB1	1.82	0.61
31:y:603:CLA:ND	30:y:609:CHL:H8	2.16	0.61
3:N:38:VAL:HG13	3:N:44:ASN:HB2	1.83	0.60
31:7:304:CLA:HED2	31:7:304:CLA:H12	1.82	0.60
30:8:601:CHL:HED1	33:8:618:LHG:H292	1.83	0.60
2:q:185:TYR:HA	31:q:312:CLA:O1D	2.00	0.60
7:c:253:VAL:HG21	7:c:437:ARG:HG2	1.83	0.60
31:Y:310:CLA:H52	32:Y:315:LUT:H30	1.83	0.60
31:q:312:CLA:H72	35:q:317:RRX:H25	1.82	0.60
2:2:90:ILE:HG21	31:2:603:CLA:HAA2	1.82	0.60
31:2:604:CLA:HMA2	30:2:606:CHL:C3C	2.30	0.60
3:5:107:LEU:HD22	3:5:230:ILE:HD13	1.83	0.60
34:C:624:LMG:H111	33:Y:318:LHG:HC31	1.83	0.60
30:N:308:CHL:H12	32:N:316:LUT:H383	1.83	0.60
5:a:334:ARG:HD3	8:d:320:LEU:HD23	1.83	0.60
31:a:409:CLA:HMA2	45:c:616:DGD:HBH1	1.82	0.60
3:n:147:SER:HB2	34:n:321:LMG:C4	2.25	0.60
17:o:256:GLY:O	17:o:290:LEU:N	2.30	0.60
30:y:608:CHL:H2	32:y:616:LUT:H383	1.84	0.60
2:2:95:ALA:HB1	2:2:213:GLY:HA3	1.82	0.60
2:2:185:TYR:HA	31:2:609:CLA:O1D	2.01	0.60
3:3:103:VAL:HG13	3:3:230:ILE:HD11	1.83	0.60
30:6:307:CHL:HBB1	30:6:307:CHL:HMB1	1.83	0.60
30:6:309:CHL:HMA2	36:6:319:NEX:H30	1.83	0.60
3:N:215:MET:HG3	32:N:317:LUT:H12	1.83	0.60
31:b:612:CLA:HMB1	31:b:612:CLA:HBB1	1.83	0.60
45:c:619:DGD:HA32	45:c:619:DGD:C2B	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:173:GLY:HA2	30:2:607:CHL:HBC1	1.83	0.60
3:5:224:ILE:HG23	3:5:258:TYR:CE2	2.36	0.60
31:5:610:CLA:H122	31:5:612:CLA:HMB2	1.83	0.60
2:G:59:PRO:HD2	2:G:62:LEU:HD12	1.84	0.60
17:O:106:VAL:HG22	17:O:280:VAL:HG22	1.83	0.60
4:0:93:HIS:HE1	31:0:603:CLA:C4D	2.14	0.60
3:p:123:LYS:HA	30:p:607:CHL:HED2	1.83	0.60
3:p:250:ALA:HB3	3:p:251:PRO:HD3	1.84	0.60
2:q:196:ALA:HB1	2:q:202:LEU:HG	1.84	0.60
8:d:117:HIS:HE1	31:d:405:CLA:ND	1.99	0.60
17:o:263:GLU:HG3	17:o:283:THR:HG22	1.81	0.60
31:y:603:CLA:CAD	30:y:609:CHL:H2	2.32	0.60
31:1:611:CLA:HBA1	38:g:301:SQD:H462	1.83	0.60
30:N:309:CHL:HMB1	30:N:309:CHL:HBB1	1.84	0.60
30:Y:306:CHL:HHC	30:Y:306:CHL:HBB1	1.83	0.60
19:s:39:TRP:HE1	34:s:321:LMG:HC4	1.66	0.60
31:S:305:CLA:H92	30:S:307:CHL:HBA2	1.83	0.60
30:9:308:CHL:HBB2	30:9:309:CHL:CBB	2.31	0.60
30:q:308:CHL:HMB1	30:q:308:CHL:HBB1	1.83	0.60
33:d:408:LHG:HC91	15:l:20:TRP:CZ2	2.36	0.60
31:y:610:CLA:H2	32:y:616:LUT:H28	1.81	0.60
28:P1:50:TYR:CZ	28:P1:52:PHE:HB2	2.36	0.60
6:B:12:VAL:HG23	31:B:612:CLA:HMC2	1.83	0.60
31:D:404:CLA:H43	23:X:76:VAL:HA	1.83	0.60
2:9:241:HIS:CG	31:9:315:CLA:HAA2	2.37	0.60
31:b:604:CLA:HMB2	31:b:604:CLA:H51	1.83	0.60
14:k:17:PRO:HB2	33:z:102:LHG:H241	1.84	0.60
36:r:319:NEX:H161	38:r:322:SQD:H92	1.84	0.60
6:B:159:THR:HG22	6:B:161:LEU:H	1.67	0.60
18:R:52:LEU:HD23	18:R:57:THR:HG23	1.83	0.60
2:9:218:PHE:CE1	31:9:315:CLA:HAB	2.36	0.60
31:q:312:CLA:H92	31:q:314:CLA:HMA1	1.83	0.60
2:g:143:ASN:OD1	2:g:145:SER:OG	2.20	0.60
30:n:310:CHL:HBB1	30:n:310:CHL:HMB1	1.84	0.60
3:5:75:SER:HB3	3:5:81:PHE:CD1	2.37	0.60
4:6:122:VAL:HG23	4:6:125:LYS:HB2	1.84	0.60
2:G:219:SER:OG	35:G:614:RRX:H45	2.02	0.60
31:G:609:CLA:O2A	35:G:614:RRX:C40	2.44	0.60
30:N:309:CHL:HBA2	30:Y:302:CHL:H12	1.84	0.60
33:S:320:LHG:H111	33:S:320:LHG:H321	1.84	0.60
31:0:611:CLA:H12	38:0:621:SQD:O10	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:0:620:LMG:H341	30:7:306:CHL:CHA	2.31	0.60
1:7:244:TYR:CE2	30:7:321:CHL:H43	2.37	0.60
6:b:496:LEU:HB2	6:b:503:THR:HB	1.84	0.60
45:c:619:DGD:HAG1	31:y:614:CLA:H51	1.84	0.60
33:d:408:LHG:H191	20:t:17:ILE:HD11	1.84	0.60
2:g:72:TRP:CE3	32:g:316:LUT:H383	2.37	0.60
31:r:305:CLA:HBC1	31:r:311:CLA:HBC2	1.83	0.60
30:r:308:CHL:HBB2	30:r:309:CHL:HMB2	1.82	0.60
30:3:309:CHL:H42	32:3:317:LUT:H383	1.82	0.59
30:4:607:CHL:H102	30:4:607:CHL:C4B	2.32	0.59
7:C:249:ARG:NH2	22:W:111:ASN:O	2.35	0.59
30:G:623:CHL:HHC	30:G:623:CHL:HBB1	1.82	0.59
3:n:69:TRP:O	32:n:318:LUT:H24	2.01	0.59
34:n:322:LMG:H141	31:y:615:CLA:H42	1.84	0.59
31:y:604:CLA:H61	36:y:618:NEX:H23	1.84	0.59
39:A:401:OEX:O4	7:C:345:ARG:NH2	2.36	0.59
31:B:613:CLA:H43	33:D:407:LHG:H362	1.85	0.59
3:8:185:PHE:HA	30:8:607:CHL:H43	1.84	0.59
31:q:312:CLA:HAA1	31:q:312:CLA:HED2	1.83	0.59
7:c:264:LEU:HD21	31:c:608:CLA:HAB	1.84	0.59
18:r:144:MET:SD	31:r:312:CLA:HAB	2.42	0.59
4:6:205:LYS:HG3	31:6:312:CLA:HED2	1.83	0.59
31:N:313:CLA:H172	31:N:314:CLA:C1D	2.32	0.59
4:0:193:ALA:HB1	4:0:199:LEU:HD13	1.84	0.59
4:0:251:TYR:O	4:0:253:LYS:N	2.35	0.59
4:0:255:LEU:HB2	30:p:607:CHL:HBA2	1.84	0.59
31:p:615:CLA:HBC3	34:q:302:LMG:H321	1.84	0.59
31:b:608:CLA:H203	15:l:36:ILE:HG13	1.82	0.59
2:2:168:ALA:HB1	3:3:52:PHE:CG	2.36	0.59
19:S:41:GLY:HA3	24:Y:52:PRO:HB2	1.85	0.59
30:S:309:CHL:HHC	30:S:309:CHL:HBB1	1.83	0.59
4:0:169:VAL:HG21	2:q:50:LEU:HD23	1.84	0.59
31:9:312:CLA:HBA1	35:9:317:RRX:H7	1.84	0.59
3:p:236:HIS:HA	3:p:243:THR:HG21	1.85	0.59
6:b:25:MET:HG2	43:b:618:BCR:H23C	1.85	0.59
33:b:625:LHG:H302	33:b:625:LHG:H251	1.84	0.59
7:c:30:LEU:HD21	31:c:611:CLA:H2A	1.82	0.59
9:e:26:THR:HB	47:e:102:HEM:HAB	1.82	0.59
28:p1:28:SER:O	28:p1:32:GLU:HG2	2.02	0.59
1:1:107:VAL:HG21	31:1:604:CLA:HAC2	1.83	0.59
3:3:145:ALA:HA	30:3:307:CHL:C1C	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:163:GLU:HG3	30:3:310:CHL:C4B	2.32	0.59
3:5:206:LYS:HD3	31:5:611:CLA:O1D	2.02	0.59
30:N:307:CHL:HHC	30:N:307:CHL:HBB1	1.84	0.59
30:n:302:CHL:HED1	33:n:320:LHG:H292	1.83	0.59
17:o:204:ASP:HB3	17:o:235:LYS:HE3	1.84	0.59
31:5:611:CLA:H12	31:5:612:CLA:OBD	2.02	0.59
31:p:610:CLA:H2	32:p:616:LUT:C25	2.32	0.59
3:n:236:HIS:CA	3:n:243:THR:HG21	2.28	0.59
30:y:605:CHL:HHC	30:y:605:CHL:HBB1	1.84	0.59
3:3:165:TYR:HA	3:3:169:GLY:O	2.03	0.59
2:G:72:TRP:CZ2	30:G:601:CHL:HBA1	2.37	0.59
43:H:101:BCR:H21C	34:X:202:LMG:H311	1.83	0.59
22:w:90:THR:HG21	34:w:202:LMG:H261	1.84	0.59
2:2:231:GLY:HA2	31:3:316:CLA:HMA3	1.85	0.59
30:2:608:CHL:HAA2	3:3:71:THR:HG21	1.85	0.59
2:4:75:ALA:HB3	2:4:77:LEU:CD2	2.33	0.59
3:5:250:ALA:N	3:5:251:PRO:HD2	2.18	0.59
30:5:606:CHL:HBA1	36:5:618:NEX:C32	2.33	0.59
34:D:409:LMG:H142	34:D:409:LMG:H292	1.84	0.59
31:Y:304:CLA:C1B	30:Y:309:CHL:H121	2.33	0.59
30:0:607:CHL:HBB2	30:0:609:CHL:HBC1	1.84	0.59
18:r:50:ASP:HB3	18:r:59:ARG:HH21	1.67	0.59
2:4:156:LEU:O	2:4:160:LEU:HG	2.03	0.59
30:5:608:CHL:HBD	30:5:608:CHL:HAA1	1.85	0.59
7:C:134:PHE:HA	34:C:621:LMG:HC4	1.83	0.59
18:R:139:HIS:HE1	31:R:305:CLA:C4D	2.16	0.59
30:8:601:CHL:H93	2:9:160:LEU:HD21	1.85	0.59
31:c:612:CLA:HBB2	34:c:620:LMG:H312	1.84	0.59
29:f1:197:ILE:HG12	29:f1:210:LYS:HG3	1.84	0.59
1:1:167:GLY:N	18:R:38:ARG:HB3	2.18	0.59
2:2:187:GLY:HA3	31:2:609:CLA:HED2	1.85	0.59
2:4:77:LEU:HD22	2:4:77:LEU:H	1.67	0.59
2:4:100:LEU:HB3	31:4:604:CLA:HAB	1.84	0.59
3:5:143:ILE:HA	30:5:605:CHL:ND	2.18	0.59
4:6:108:GLU:HA	4:6:121:ALA:HB1	1.85	0.59
8:D:189:HIS:HA	8:D:294:ARG:HD2	1.85	0.59
35:G:614:RRX:H55	34:G:619:LMG:H322	1.85	0.59
31:R:307:CLA:HBA1	31:R:316:CLA:H172	1.84	0.59
19:S:155:PRO:HG3	31:S:306:CLA:NA	2.18	0.59
30:8:606:CHL:HHC	30:8:606:CHL:HBB1	1.83	0.59
30:q:307:CHL:HAA1	30:q:307:CHL:HBD	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:c:619:DGD:HD1	31:y:611:CLA:HBA1	1.85	0.59
9:e:10:PHE:CZ	10:f:18:ARG:HD3	2.37	0.59
34:g:322:LMG:H411	34:g:322:LMG:H372	1.85	0.59
36:s:319:NEX:H193	36:s:319:NEX:H161	1.83	0.59
1:1:166:ASN:ND2	2:2:53:PHE:HA	2.18	0.58
31:4:610:CLA:HMB3	31:4:610:CLA:HBB1	1.84	0.58
30:5:607:CHL:HMA2	4:6:256:ALA:O	2.03	0.58
7:C:247:TRP:CZ2	45:C:620:DGD:HA21	2.38	0.58
31:C:604:CLA:HMB1	31:C:604:CLA:HBB1	1.85	0.58
19:S:138:GLU:HA	30:S:308:CHL:CED	2.23	0.58
31:Y:304:CLA:H2	31:Y:304:CLA:HMA3	1.83	0.58
30:7:321:CHL:HAA1	30:7:321:CHL:HBD	1.84	0.58
30:1:601:CHL:HMB3	30:3:310:CHL:HBB1	1.84	0.58
2:2:202:LEU:HG	2:2:206:LYS:HE3	1.84	0.58
3:3:122:PHE:HE1	3:3:123:LYS:HE2	1.68	0.58
31:B:604:CLA:HBB1	31:B:604:CLA:HMB1	1.86	0.58
31:N:314:CLA:HBC1	32:N:316:LUT:H162	1.85	0.58
31:8:603:CLA:HMD2	30:8:608:CHL:H2	1.85	0.58
2:9:163:MET:HE1	36:9:319:NEX:H30	1.85	0.58
2:9:257:PHE:CB	34:9:301:LMG:H152	2.32	0.58
30:9:303:CHL:HAA2	30:9:303:CHL:HBD	1.84	0.58
1:1:165:VAL:HG11	2:2:57:SER:HB3	1.85	0.58
2:2:133:PHE:HE2	30:3:302:CHL:CMD	2.16	0.58
3:5:70:ASP:HB2	31:5:602:CLA:HBA2	1.85	0.58
6:B:204:ALA:CB	31:B:602:CLA:HAB	2.33	0.58
31:N:310:CLA:HBB1	31:N:310:CLA:HMB3	1.85	0.58
24:Y:99:MET:SD	31:Y:310:CLA:HAB	2.43	0.58
4:0:235:LEU:HB2	32:0:616:LUT:H22	1.84	0.58
2:2:253:SER:O	2:2:256:LYS:HG3	2.03	0.58
31:4:610:CLA:HBB1	31:4:612:CLA:H3A	1.85	0.58
30:6:308:CHL:HAA2	30:6:308:CHL:HBD	1.85	0.58
30:G:606:CHL:HMB1	30:G:608:CHL:HMC	1.85	0.58
4:0:221:PHE:CD1	30:0:607:CHL:H71	2.39	0.58
2:9:245:PRO:HG2	31:9:316:CLA:HMB2	1.85	0.58
2:q:149:ALA:HA	30:q:307:CHL:CHC	2.34	0.58
2:q:177:VAL:HG22	2:q:189:PHE:CE2	2.38	0.58
7:c:23:TRP:HD1	48:c:623:LMU:H6'1	1.68	0.58
2:g:259:PRO:HD3	30:y:607:CHL:H12	1.83	0.58
31:g:304:CLA:C4D	30:g:309:CHL:H71	2.34	0.58
2:2:86:ARG:HA	2:2:86:ARG:NH1	2.19	0.58
30:R:310:CHL:HHC	30:R:310:CHL:HBB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:100:THR:OG1	34:W:201:LMG:HC5	2.02	0.58
30:7:306:CHL:HBA2	31:r:315:CLA:HMA3	1.86	0.58
31:8:614:CLA:H43	2:9:257:PHE:CE1	2.38	0.58
9:e:8:ARG:HE	9:e:12:ASP:CG	2.11	0.58
2:g:138:LEU:HD11	30:g:307:CHL:HAC1	1.84	0.58
30:s:309:CHL:HBB1	30:s:309:CHL:HHC	1.86	0.58
24:y:48:LYS:HD3	24:y:58:VAL:HG21	1.85	0.58
2:2:125:TRP:CG	2:2:126:PHE:N	2.71	0.58
31:5:604:CLA:HMA3	30:5:606:CHL:C2C	2.34	0.58
31:G:610:CLA:C1C	38:G:617:SQD:H142	2.34	0.58
30:N:308:CHL:HMB3	36:N:318:NEX:H35	1.85	0.58
26:U:100:ARG:NH2	26:U:138:ASP:OD1	2.36	0.58
30:0:608:CHL:HMA3	36:0:618:NEX:H402	1.84	0.58
30:7:308:CHL:O1A	2:9:259:PRO:HD2	2.03	0.58
31:b:612:CLA:H152	31:b:614:CLA:O1D	2.03	0.58
43:d:406:BCR:H20C	34:d:409:LMG:H301	1.83	0.58
31:p:613:CLA:H12	31:p:614:CLA:HMD2	1.86	0.58
2:q:169:TYR:HD1	2:q:174:GLU:CG	2.10	0.58
19:s:264:TRP:HB2	32:s:317:LUT:H22	1.86	0.58
3:3:122:PHE:HD1	3:3:123:LYS:HG3	1.68	0.58
2:4:139:ASN:HA	2:4:148:HIS:H	1.67	0.58
2:4:170:ARG:HA	30:4:608:CHL:C4C	2.33	0.58
3:5:110:ARG:NH1	3:5:230:ILE:HB	2.19	0.58
6:B:145:LEU:HB3	31:B:604:CLA:H161	1.85	0.58
3:N:226:ARG:NH2	31:N:321:CLA:H3A	2.19	0.58
31:N:305:CLA:H101	31:S:306:CLA:CMA	2.34	0.58
19:S:155:PRO:CG	31:S:306:CLA:NB	2.66	0.58
2:q:59:PRO:HB3	2:q:61:TYR:CZ	2.39	0.58
38:b:627:SQD:H91	8:d:130:PHE:HB3	1.86	0.58
31:1:611:CLA:H52	31:1:612:CLA:C3D	2.34	0.58
2:4:179:THR:HB	2:4:188:GLY:HA2	1.86	0.58
34:5:620:LMG:HC62	31:6:315:CLA:HMA1	1.86	0.58
34:5:620:LMG:H302	34:5:620:LMG:H342	1.85	0.58
38:6:301:SQD:H462	31:6:312:CLA:HHB	1.86	0.58
31:6:305:CLA:HMA3	30:6:307:CHL:C2C	2.34	0.58
9:E:8:ARG:HD3	9:E:13:ILE:HG12	1.85	0.58
2:G:223:PHE:CE1	35:G:614:RRX:C31	2.86	0.58
3:N:246:TRP:O	3:N:251:PRO:HD3	2.03	0.58
33:a:415:LHG:HC2	31:c:608:CLA:HED2	1.84	0.58
45:c:619:DGD:HBE1	45:c:619:DGD:CCA	2.33	0.58
2:g:149:ALA:HA	30:g:306:CHL:CHC	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:307:CHL:HBB2	30:n:301:CHL:CBB	2.34	0.58
33:g:319:LHG:H312	37:g:321:XAT:C35	2.33	0.58
30:n:306:CHL:H191	31:s:313:CLA:HAC1	1.85	0.58
5:A:317:TRP:CZ3	8:D:180:ARG:HD2	2.39	0.58
31:A:406:CLA:CHA	31:A:406:CLA:HBA1	2.34	0.58
30:9:310:CHL:HMB3	36:9:319:NEX:H14	1.85	0.58
31:9:314:CLA:C1C	35:9:317:RRX:H37	2.34	0.58
3:p:232:ASN:HB3	31:p:613:CLA:O2D	2.04	0.58
7:c:192:VAL:HG22	34:n:321:LMG:H131	1.85	0.58
30:n:308:CHL:HAA1	30:n:308:CHL:HBD	1.84	0.58
31:n:315:CLA:H2A	31:n:315:CLA:HED3	1.86	0.58
30:r:310:CHL:HHC	30:r:310:CHL:HBB1	1.85	0.58
2:4:147:ILE:HD11	31:4:604:CLA:H51	1.86	0.57
31:7:311:CLA:H52	32:7:317:LUT:H30	1.86	0.57
3:p:236:HIS:HB2	31:p:613:CLA:HAA2	1.86	0.57
31:g:313:CLA:H191	24:y:156:VAL:HG23	1.84	0.57
31:1:611:CLA:HAB	38:g:318:SQD:C24	2.32	0.57
3:3:200:LEU:HA	3:3:203:LYS:HD2	1.86	0.57
3:5:236:HIS:ND1	31:5:613:CLA:HAA2	2.19	0.57
4:6:93:HIS:HE1	31:6:304:CLA:C4D	2.16	0.57
6:B:336:ILE:HD13	16:m:-10:UNK:HA	1.86	0.57
11:H:62:VAL:O	11:H:66:GLU:HG2	2.03	0.57
3:p:118:GLU:OE1	3:p:127:GLN:NE2	2.37	0.57
3:p:125:GLY:HA3	30:p:607:CHL:C3D	2.34	0.57
2:q:223:PHE:CE1	35:q:317:RRX:H48	2.39	0.57
2:g:238:LEU:HD23	34:g:320:LMG:HC92	1.86	0.57
31:n:305:CLA:HMB1	31:n:305:CLA:HBB1	1.86	0.57
31:n:315:CLA:HBC1	32:n:317:LUT:H162	1.86	0.57
31:s:303:CLA:H172	31:s:303:CLA:H141	1.86	0.57
34:Q1:101:LMG:O7	34:Q1:101:LMG:HC1	2.04	0.57
6:B:114:HIS:HE1	31:B:616:CLA:C1D	2.17	0.57
2:G:257:PHE:CE1	31:N:315:CLA:H12	2.40	0.57
3:N:186:ASP:HA	32:N:316:LUT:H24	1.86	0.57
31:N:304:CLA:HED2	31:N:304:CLA:H12	1.84	0.57
18:R:140:GLY:HA3	18:R:241:ALA:HB1	1.86	0.57
34:0:620:LMG:H331	34:7:301:LMG:H161	1.85	0.57
1:7:198:LEU:HB3	31:7:311:CLA:HMA2	1.86	0.57
3:p:255:GLY:H	31:p:615:CLA:HMA3	1.69	0.57
2:q:77:LEU:HD23	31:q:304:CLA:H42	1.85	0.57
7:c:201:LEU:HD13	31:c:606:CLA:H141	1.86	0.57
2:g:103:LEU:HD13	31:g:312:CLA:HBB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:n:316:CLA:H11	34:n:322:LMG:HC92	1.86	0.57
29:f1:170:ASP:HB2	29:f1:176:TYR:HE1	1.69	0.57
4:6:106:THR:HG22	34:6:322:LMG:C36	2.34	0.57
31:6:305:CLA:HBA1	30:6:307:CHL:CHD	2.35	0.57
5:A:47:VAL:HG11	5:A:114:LEU:HD22	1.87	0.57
43:B:618:BCR:H19C	38:B:620:SQD:H223	1.85	0.57
8:D:244:TYR:OH	8:D:264:LYS:HD2	2.04	0.57
30:9:311:CHL:HMB1	30:9:311:CHL:HBB1	1.87	0.57
3:p:247:VAL:HG22	2:q:133:PHE:CD2	2.40	0.57
2:q:167:GLU:HG3	30:q:311:CHL:C4B	2.34	0.57
5:a:266:ASN:HD22	5:a:266:ASN:H	1.50	0.57
31:c:612:CLA:HBB1	31:c:612:CLA:HMB3	1.85	0.57
31:g:304:CLA:H2	31:g:304:CLA:HED2	1.84	0.57
31:n:304:CLA:HMD2	30:n:310:CHL:H2	1.85	0.57
31:2:602:CLA:HBC1	33:2:617:LHG:H252	1.86	0.57
3:5:218:PHE:CZ	32:5:616:LUT:H8	2.40	0.57
6:B:156:PHE:HZ	33:B:624:LHG:H282	1.68	0.57
19:S:120:ILE:HD11	31:S:311:CLA:H193	1.86	0.57
24:Y:206:LEU:HD23	24:Y:209:LYS:HD2	1.86	0.57
34:0:622:LMG:HC72	34:0:622:LMG:O10	2.05	0.57
1:7:198:LEU:HB3	31:7:311:CLA:CMA	2.35	0.57
31:7:315:CLA:HBA1	31:7:315:CLA:CHA	2.32	0.57
31:9:305:CLA:HHC	31:9:305:CLA:CBB	2.33	0.57
3:p:106:GLU:OE2	3:p:231:GLU:HG3	2.05	0.57
31:p:611:CLA:H92	31:p:612:CLA:HED1	1.86	0.57
45:c:619:DGD:HD5	31:y:611:CLA:HMA2	1.86	0.57
3:n:110:ARG:NH2	3:n:231:GLU:HA	2.19	0.57
31:n:305:CLA:H152	31:s:306:CLA:C4A	2.35	0.57
17:o:133:ASP:OD1	17:o:134:GLU:N	2.37	0.57
22:w:93:TRP:CE2	34:w:202:LMG:H131	2.40	0.57
24:y:221:MET:HE2	32:y:617:LUT:H10	1.84	0.57
30:y:607:CHL:H121	30:y:609:CHL:H152	1.86	0.57
29:F1:116:LYS:O	29:F1:204:GLY:HA2	2.04	0.57
2:2:140:TYR:HB3	2:2:146:LEU:HB3	1.87	0.57
33:A:417:LHG:O3	33:A:417:LHG:O1	2.16	0.57
6:B:74:SER:OG	6:B:94:GLU:OE2	2.22	0.57
8:D:216:ALA:O	8:D:220:ASN:ND2	2.27	0.57
38:G:617:SQD:H251	31:7:312:CLA:HAB	1.86	0.57
30:G:623:CHL:CBB	30:Y:307:CHL:HBB2	2.34	0.57
20:T:15:GLY:HA3	38:b:621:SQD:H321	1.86	0.57
8:d:189:HIS:HA	8:d:294:ARG:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f1:196:LEU:HB3	29:f1:230:TRP:CD2	2.40	0.57
31:4:604:CLA:CHB	36:4:617:NEX:H383	2.34	0.57
31:C:611:CLA:H42	21:V:33:LEU:HA	1.86	0.57
2:G:254:ALA:HA	37:G:620:XAT:H172	1.86	0.57
30:N:307:CHL:H92	36:N:318:NEX:H202	1.85	0.57
31:7:316:CLA:HBB2	3:8:121:TRP:CZ2	2.40	0.57
2:9:149:ALA:HA	30:9:307:CHL:CHC	2.35	0.57
3:p:162:ILE:HD13	30:p:608:CHL:HMA2	1.86	0.57
31:p:613:CLA:H51	31:p:613:CLA:C4B	2.34	0.57
31:q:313:CLA:C1C	38:x:201:SQD:H142	2.34	0.57
31:n:304:CLA:H43	24:y:77:LEU:HD21	1.86	0.57
31:r:303:CLA:HBD	33:r:320:LHG:HC82	1.86	0.57
30:4:601:CHL:CMC	37:4:619:XAT:H23	2.35	0.57
31:5:613:CLA:ND	31:5:613:CLA:H52	2.20	0.57
32:5:617:LUT:H191	32:5:617:LUT:C12	2.34	0.57
5:A:292:THR:HG22	7:C:416:THR:HG23	1.85	0.57
31:G:609:CLA:H52	35:G:614:RRX:H25	1.85	0.57
24:Y:186:TYR:HB3	31:Y:310:CLA:HED3	1.86	0.57
24:Y:194:LEU:HD12	32:Y:315:LUT:H222	1.85	0.57
34:0:620:LMG:H341	30:7:306:CHL:C4D	2.34	0.57
1:7:145:SER:HB2	34:7:301:LMG:HC5	1.87	0.57
31:7:316:CLA:H2	34:9:301:LMG:HC72	1.85	0.57
2:9:241:HIS:HB2	31:9:315:CLA:HAA2	1.86	0.57
2:g:80:ASP:HB3	2:g:83:THR:HG22	1.86	0.57
17:o:100:GLU:OE2	22:w:60:LEU:N	2.38	0.57
24:y:94:HIS:HE1	31:y:603:CLA:C4D	2.18	0.57
2:2:140:TYR:CD1	2:2:141:LEU:HG	2.40	0.57
31:0:614:CLA:H91	34:p:620:LMG:H131	1.86	0.57
2:q:89:GLU:HA	2:q:184:LEU:HD21	1.86	0.57
2:q:139:ASN:CG	2:q:144:PRO:HA	2.30	0.57
2:q:175:GLY:N	2:q:176:PRO:HD2	2.20	0.57
6:b:374:ASP:OD1	6:b:374:ASP:N	2.37	0.57
7:c:113:LEU:HD13	43:c:614:BCR:H19C	1.85	0.57
2:4:195:LEU:HB2	31:4:610:CLA:O1A	2.04	0.57
3:5:87:LEU:HD13	31:5:603:CLA:HBA1	1.87	0.57
6:B:162:PHE:CD1	48:R:302:LMU:H1'	2.39	0.57
34:B:625:LMG:H342	30:R:309:CHL:H42	1.86	0.57
34:C:624:LMG:H162	33:Y:318:LHG:HC92	1.87	0.57
42:D:401:PHO:H72	31:D:403:CLA:H111	1.87	0.57
34:G:622:LMG:H112	31:N:315:CLA:H11	1.87	0.57
3:N:191:ALA:HB2	31:N:310:CLA:HAA2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:173:PRO:HB3	18:r:54:LEU:HG	1.87	0.57
3:p:142:LEU:HA	30:p:605:CHL:HED3	1.86	0.57
31:q:305:CLA:HHC	31:q:305:CLA:CBB	2.32	0.57
31:c:606:CLA:H8	43:c:615:BCR:H12C	1.85	0.57
45:c:619:DGD:HAS1	33:y:619:LHG:H332	1.86	0.57
30:g:308:CHL:HBD	30:g:308:CHL:HAA1	1.86	0.57
17:o:257:GLU:HG2	17:o:289:GLN:HG2	1.87	0.57
19:s:41:GLY:HA3	24:y:52:PRO:HB2	1.85	0.57
34:3:321:LMG:O6	34:3:321:LMG:HC92	2.05	0.56
3:5:107:LEU:HD22	3:5:230:ILE:CD1	2.35	0.56
7:C:306:LEU:HD12	7:C:328:TYR:HB3	1.87	0.56
2:G:149:ALA:HA	30:G:605:CHL:CHC	2.35	0.56
34:G:622:LMG:H141	31:N:315:CLA:H71	1.86	0.56
19:S:252:GLN:HE21	19:S:263:ASN:HD22	1.53	0.56
24:Y:192:ASP:HA	32:Y:315:LUT:H24	1.87	0.56
3:8:223:LEU:HD21	34:9:302:LMG:H172	1.87	0.56
2:q:220:MET:HE2	32:q:318:LUT:H10	1.87	0.56
31:b:605:CLA:HBB1	31:b:605:CLA:HMB1	1.87	0.56
45:c:618:DGD:HE4	13:j:42:LEU:HD21	1.86	0.56
9:e:26:THR:HB	47:e:102:HEM:CAB	2.35	0.56
2:2:59:PRO:HD2	2:2:62:LEU:HD12	1.87	0.56
3:5:224:ILE:HG23	3:5:258:TYR:CD2	2.40	0.56
3:5:255:GLY:H	31:5:615:CLA:H2A	1.70	0.56
45:C:620:DGD:HB22	45:C:620:DGD:HG11	1.86	0.56
34:D:412:LMG:O10	11:H:69:ASN:ND2	2.37	0.56
3:N:235:ASP:C	3:N:243:THR:HG21	2.30	0.56
19:S:272:PHE:HD1	38:S:301:SQD:H461	1.70	0.56
1:7:124:ALA:HB2	30:7:308:CHL:HED2	1.87	0.56
30:8:608:CHL:HMB1	30:8:608:CHL:HBB1	1.87	0.56
3:p:196:THR:O	3:p:200:LEU:HG	2.05	0.56
31:p:613:CLA:H41	31:p:613:CLA:H72	1.86	0.56
31:p:614:CLA:NC	31:p:614:CLA:H51	2.20	0.56
14:k:46:ARG:NH2	21:v:33:LEU:O	2.38	0.56
19:s:252:GLN:HE21	19:s:263:ASN:HD22	1.53	0.56
2:2:208:LYS:HD3	31:2:611:CLA:HAA2	1.87	0.56
31:2:609:CLA:HBA1	35:2:614:RRX:H7	1.85	0.56
30:4:606:CHL:HBB2	30:4:607:CHL:CBB	2.35	0.56
3:5:74:LEU:HD22	3:5:74:LEU:H	1.70	0.56
34:6:321:LMG:H111	34:6:322:LMG:C11	2.35	0.56
31:A:405:CLA:H122	42:A:408:PHO:H3A	1.88	0.56
31:B:611:CLA:C3B	31:B:613:CLA:HMA2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:26:GLY:HA3	31:C:611:CLA:HMD2	1.88	0.56
33:G:618:LHG:HC61	37:G:620:XAT:C38	2.34	0.56
37:G:620:XAT:O23	38:G:624:SQD:H81	2.05	0.56
3:N:58:TYR:CD1	3:N:59:LEU:HD13	2.40	0.56
31:N:305:CLA:H112	31:S:306:CLA:HHB	1.86	0.56
17:O:235:LYS:HD3	17:O:272:LEU:HD23	1.87	0.56
18:R:144:MET:SD	31:R:312:CLA:HAB	2.45	0.56
30:R:308:CHL:HBB2	30:R:309:CHL:HMB2	1.85	0.56
6:b:24:LEU:HD21	31:b:617:CLA:CAB	2.35	0.56
3:n:185:PHE:HA	30:n:309:CHL:H43	1.87	0.56
31:r:305:CLA:H2	31:r:305:CLA:HED2	1.86	0.56
22:w:89:PHE:CD2	34:w:202:LMG:H432	2.41	0.56
34:w:203:LMG:H122	34:w:203:LMG:HC91	1.87	0.56
34:w:205:LMG:O9	34:w:205:LMG:HC91	2.06	0.56
26:u:144:ASP:HA	26:u:151:LYS:HE3	1.87	0.56
30:2:605:CHL:HAA1	30:2:605:CHL:HBD	1.87	0.56
2:4:182:ASP:OD2	2:4:185:TYR:HB2	2.06	0.56
31:4:603:CLA:HHC	31:4:603:CLA:CBB	2.33	0.56
7:C:326:GLY:HA2	17:O:157:TYR:OH	2.06	0.56
30:G:623:CHL:HED2	24:Y:126:LYS:HA	1.87	0.56
6:b:114:HIS:HE1	31:b:617:CLA:C1D	2.19	0.56
9:e:24:SER:O	9:e:28:PRO:HG2	2.06	0.56
2:2:130:ALA:HA	2:2:133:PHE:HD2	1.70	0.56
2:2:132:ILE:HG23	2:2:152:ILE:HD12	1.87	0.56
31:3:314:CLA:C4C	31:3:314:CLA:H62	2.35	0.56
31:4:604:CLA:O2A	36:4:617:NEX:H241	2.05	0.56
3:5:209:ARG:HB2	33:5:619:LHG:H262	1.88	0.56
6:B:237:VAL:HG22	31:B:610:CLA:HBC2	1.87	0.56
7:C:432:HIS:HE1	31:C:608:CLA:NA	1.99	0.56
3:N:223:LEU:HD21	31:N:321:CLA:H41	1.86	0.56
30:N:307:CHL:H41	30:N:307:CHL:H72	1.88	0.56
31:8:609:CLA:H92	32:8:615:LUT:H371	1.87	0.56
3:p:232:ASN:HB3	31:p:613:CLA:CED	2.36	0.56
2:q:162:ILE:HG22	36:q:319:NEX:H34	1.86	0.56
30:q:303:CHL:HBC1	33:q:320:LHG:C3	2.36	0.56
5:a:77:ILE:HD13	15:l:30:VAL:HG13	1.86	0.56
30:g:306:CHL:HBA1	30:g:306:CHL:CHA	2.34	0.56
31:s:304:CLA:HHC	31:s:304:CLA:CBB	2.34	0.56
31:4:602:CLA:HMB2	31:4:602:CLA:H52	1.86	0.56
31:5:602:CLA:H11	32:5:617:LUT:H26	1.86	0.56
33:5:619:LHG:HC62	33:5:619:LHG:O5	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:6:322:LMG:H301	34:6:322:LMG:HC92	1.85	0.56
7:C:356:PRO:HB3	26:U:130:ARG:HB2	1.88	0.56
3:N:69:TRP:O	32:N:317:LUT:H24	2.06	0.56
3:N:226:ARG:HH22	31:N:321:CLA:H3A	1.70	0.56
30:N:307:CHL:HBB2	30:Y:301:CHL:CAB	2.34	0.56
17:O:148:GLU:HB3	17:O:182:LYS:HG3	1.87	0.56
1:7:178:TYR:CZ	1:7:199:LYS:HE3	2.40	0.56
3:8:38:VAL:HG11	3:8:43:PRO:HD2	1.88	0.56
2:q:97:TRP:CE2	30:q:310:CHL:HED3	2.41	0.56
2:q:172:SER:O	2:q:174:GLU:HG2	2.06	0.56
34:b:624:LMG:H321	34:b:624:LMG:H361	1.87	0.56
8:d:55:VAL:O	8:d:66:SER:HB3	2.06	0.56
3:n:46:PRO:HB2	30:n:302:CHL:CBC	2.36	0.56
17:o:105:THR:HB	17:o:119:PHE:HB3	1.87	0.56
29:f1:78:ILE:HD11	29:f1:95:LEU:HD21	1.88	0.56
3:3:87:LEU:HD13	31:3:305:CLA:HBA1	1.88	0.56
3:3:159:MET:CE	36:3:319:NEX:H30	2.34	0.56
3:3:258:TYR:CD1	3:3:258:TYR:C	2.83	0.56
2:4:254:ALA:O	37:4:619:XAT:H42	2.06	0.56
2:4:258:LEU:HD21	4:6:125:LYS:HG3	1.87	0.56
3:N:92:ALA:HB1	3:N:208:GLY:HA3	1.86	0.56
3:N:254:ALA:HB3	30:N:301:CHL:HED3	1.87	0.56
19:S:91:ALA:HB2	31:S:303:CLA:HBA1	1.87	0.56
31:S:313:CLA:H92	31:S:313:CLA:H41	1.88	0.56
22:W:86:THR:CG2	34:W:201:LMG:H221	2.35	0.56
1:7:76:GLY:HA3	3:8:80:THR:HA	1.87	0.56
1:7:90:ILE:HG21	31:7:304:CLA:HAA2	1.87	0.56
3:8:46:PRO:HB2	30:8:601:CHL:CBC	2.36	0.56
43:c:615:BCR:H332	12:i:24:LEU:HD21	1.88	0.56
3:n:46:PRO:HB2	30:n:302:CHL:HBC1	1.88	0.56
30:s:307:CHL:HBD	30:s:307:CHL:HAA2	1.88	0.56
31:1:611:CLA:HBB1	31:1:611:CLA:HHC	1.88	0.56
3:3:252:LYS:CA	3:3:256:ILE:HG23	2.30	0.56
31:4:610:CLA:H2	35:4:615:RRX:C40	2.35	0.56
30:5:608:CHL:HMB1	36:5:618:NEX:H14	1.88	0.56
5:A:41:LEU:HD22	42:A:408:PHO:H61	1.88	0.56
7:C:429:HIS:CE1	31:C:605:CLA:ND	2.73	0.56
8:D:12:ARG:NH1	8:D:20:ASP:OD2	2.39	0.56
30:G:601:CHL:H13	33:G:618:LHG:H371	1.87	0.56
18:R:186:LEU:HD13	30:R:308:CHL:HMD1	1.88	0.56
2:9:107:THR:OG1	31:9:306:CLA:HBC3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:221:GLN:HB2	31:p:613:CLA:CED	2.36	0.56
3:p:245:PHE:CZ	30:q:309:CHL:H11	2.37	0.56
2:q:205:LEU:HB3	31:q:312:CLA:HMA2	1.88	0.56
44:a:414:PL9:H261	33:e:101:LHG:H361	1.88	0.56
31:b:615:CLA:H161	34:b:622:LMG:H411	1.87	0.56
31:c:613:CLA:H13	33:c:622:LHG:H171	1.88	0.56
13:j:28:GLY:HA3	34:j:101:LMG:H321	1.87	0.56
30:n:308:CHL:O1A	24:y:259:LEU:HD12	2.05	0.56
31:2:602:CLA:H8	32:2:615:LUT:H371	1.87	0.56
3:3:67:TYR:HB2	31:3:304:CLA:HMD1	1.87	0.56
3:3:146:GLN:HB2	30:3:307:CHL:CBB	2.36	0.56
30:4:607:CHL:H102	30:4:607:CHL:CHC	2.36	0.56
3:5:40:TRP:HH2	33:5:619:LHG:O4	1.89	0.56
3:5:72:ALA:HB3	3:5:74:LEU:CD2	2.36	0.56
17:O:79:SER:O	17:O:250:LYS:NZ	2.37	0.56
3:8:110:ARG:NH2	3:8:231:GLU:HA	2.19	0.56
31:9:312:CLA:H2	35:9:317:RRX:H8	1.87	0.56
3:p:89:VAL:HG22	3:p:205:LEU:HD21	1.88	0.56
5:a:133:LEU:HD22	5:a:137:LEU:HG	1.88	0.56
31:c:606:CLA:H51	31:c:607:CLA:H192	1.88	0.56
31:2:610:CLA:CGA	38:6:301:SQD:H441	2.35	0.56
2:4:93:ILE:HG23	2:4:170:ARG:HH21	1.70	0.56
7:C:432:HIS:HE1	31:C:608:CLA:C1A	2.19	0.56
47:E:101:HEM:HMC2	10:F:30:VAL:HG21	1.88	0.56
18:R:59:ARG:NH1	18:R:70:ASP:OD1	2.39	0.56
19:S:83:TYR:HB2	31:S:303:CLA:HMD1	1.88	0.56
3:8:46:PRO:HB2	30:8:601:CHL:HBC1	1.88	0.56
30:8:607:CHL:HAA1	30:8:607:CHL:HBD	1.87	0.56
31:9:305:CLA:HMA3	31:9:305:CLA:H2	1.88	0.56
31:p:602:CLA:H42	32:p:617:LUT:H371	1.88	0.56
30:p:606:CHL:CBB	30:p:609:CHL:HBC1	2.36	0.56
6:b:334:ASP:N	6:b:334:ASP:OD1	2.36	0.56
31:g:305:CLA:H52	30:g:307:CHL:HAA2	1.87	0.56
22:w:109:ARG:HH21	22:w:115:PHE:HA	1.71	0.56
28:p1:30:THR:HG22	28:p1:36:TRP:CD1	2.41	0.56
31:1:610:CLA:HMB2	31:1:612:CLA:HBA2	1.88	0.55
2:4:139:ASN:OD1	2:4:148:HIS:HA	2.06	0.55
2:4:253:SER:HB2	2:4:256:LYS:HD3	1.88	0.55
3:5:168:ASN:ND2	4:6:53:PHE:HA	2.22	0.55
3:5:225:THR:O	3:5:227:LYS:HG3	2.06	0.55
3:5:252:LYS:HB3	3:5:258:TYR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:304:GLN:HG2	5:A:313:VAL:HG21	1.88	0.55
2:G:103:LEU:HD13	31:G:611:CLA:HBB2	1.87	0.55
3:N:200:LEU:HB3	31:N:310:CLA:CMA	2.35	0.55
19:S:256:THR:HG23	19:S:258:GLU:H	1.71	0.55
30:0:605:CHL:HHC	30:0:605:CHL:HBB1	1.88	0.55
3:8:199:GLU:OE2	3:8:203:LYS:HE3	2.06	0.55
5:a:296:ASN:HB3	7:c:389:LEU:HA	1.87	0.55
6:b:423:ARG:NH2	6:b:430:PHE:O	2.39	0.55
47:e:102:HEM:HBD2	47:e:102:HEM:HHA	1.87	0.55
30:n:309:CHL:HBD	30:n:309:CHL:HAA1	1.88	0.55
28:p1:59:ASN:N	28:p1:59:ASN:OD1	2.39	0.55
2:2:139:ASN:HB3	2:2:143:ASN:O	2.07	0.55
3:3:182:GLY:HA2	3:3:186:ASP:HB2	1.88	0.55
3:3:200:LEU:HD22	31:3:311:CLA:HHB	1.88	0.55
4:6:250:LEU:O	4:6:251:TYR:C	2.49	0.55
31:6:314:CLA:ND	31:6:314:CLA:H2	2.21	0.55
7:C:394:SER:HA	7:C:408:VAL:HG23	1.88	0.55
8:D:257:PHE:CE1	33:D:408:LHG:H331	2.41	0.55
18:R:201:ARG:NH1	31:R:311:CLA:O1D	2.32	0.55
5:a:342:ASP:HB2	8:d:352:LEU:HG	1.88	0.55
44:a:414:PL9:H353	33:e:101:LHG:H322	1.87	0.55
7:c:356:PRO:HB3	26:u:130:ARG:HB2	1.88	0.55
34:c:624:LMG:H311	33:y:619:LHG:HC92	1.88	0.55
18:r:123:TYR:CD2	18:r:131:ARG:HG3	2.42	0.55
19:s:224:ASP:HB3	19:s:227:VAL:HB	1.89	0.55
31:s:312:CLA:C4C	33:s:320:LHG:HC62	2.37	0.55
1:1:231:LEU:HG	32:1:615:LUT:H163	1.89	0.55
3:3:246:TRP:HA	3:3:250:ALA:CB	2.36	0.55
2:4:126:PHE:CE1	31:5:615:CLA:HMA3	2.41	0.55
19:S:204:TYR:HA	19:S:207:MET:HE2	1.87	0.55
30:0:607:CHL:C1	2:q:259:PRO:HD3	2.35	0.55
7:c:75:ILE:HG13	7:c:76:LEU:HD12	1.87	0.55
7:c:432:HIS:HE1	31:c:608:CLA:C1A	2.19	0.55
9:e:68:ASP:OD2	9:e:71:ASN:ND2	2.39	0.55
20:t:4:LEU:HG	33:t:102:LHG:H282	1.87	0.55
2:2:127:LYS:HG2	3:3:254:ALA:O	2.06	0.55
30:2:601:CHL:HBC1	33:2:617:LHG:HC31	1.88	0.55
34:5:620:LMG:O10	34:5:620:LMG:H361	2.07	0.55
7:c:123:VAL:HG21	25:z:27:LEU:HD22	1.88	0.55
30:2:606:CHL:CBB	30:2:608:CHL:HBC1	2.36	0.55
3:3:240:PRO:HB2	31:3:315:CLA:CHB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:205:LEU:CD1	31:4:610:CLA:H43	2.36	0.55
2:4:208:LYS:HD3	31:4:612:CLA:O1A	2.05	0.55
34:G:621:LMG:H351	3:N:223:LEU:HD22	1.88	0.55
19:S:138:GLU:CA	30:S:308:CHL:HED1	2.25	0.55
31:7:304:CLA:HAC1	30:7:308:CHL:CBB	2.35	0.55
31:g:312:CLA:HAB	34:g:320:LMG:H361	1.89	0.55
31:n:311:CLA:H12	31:n:311:CLA:CHB	2.37	0.55
18:r:218:ASP:HA	32:r:317:LUT:H24	1.89	0.55
31:s:314:CLA:HMA1	32:s:317:LUT:H162	1.88	0.55
38:x:201:SQD:H45	38:x:201:SQD:O5	2.07	0.55
30:1:606:CHL:O2A	36:R:301:NEX:H31	2.06	0.55
5:A:334:ARG:HD3	8:D:320:LEU:HD23	1.88	0.55
7:C:111:ALA:HB1	33:S:322:LHG:H383	1.89	0.55
7:C:185:ARG:NH1	7:C:219:GLU:OE2	2.36	0.55
7:C:381:ALA:HB1	26:U:75:ARG:HG3	1.87	0.55
3:N:146:GLN:HB2	30:N:306:CHL:CBB	2.37	0.55
2:q:59:PRO:HG2	2:q:73:ASP:HB3	1.89	0.55
31:b:608:CLA:HBB1	31:b:608:CLA:HMB1	1.89	0.55
32:g:316:LUT:H28	32:g:316:LUT:H361	1.86	0.55
3:3:120:VAL:HG23	3:3:123:LYS:HB2	1.88	0.55
2:4:140:TYR:HD1	2:4:146:LEU:HG	1.70	0.55
3:5:227:LYS:HB2	3:5:232:ASN:ND2	2.20	0.55
31:8:612:CLA:H172	31:8:613:CLA:C1D	2.37	0.55
3:p:246:TRP:CD1	3:p:246:TRP:H	2.23	0.55
2:q:250:GLY:HA3	37:q:321:XAT:H193	1.89	0.55
34:c:624:LMG:H292	30:y:601:CHL:HAC1	1.89	0.55
31:n:311:CLA:H92	32:n:317:LUT:H371	1.88	0.55
3:3:38:VAL:HA	3:3:42:GLY:H	1.72	0.55
31:4:611:CLA:C4C	33:4:618:LHG:HC62	2.37	0.55
3:5:99:ALA:HB1	32:5:616:LUT:H12	1.89	0.55
9:E:26:THR:HB	47:E:101:HEM:HAB	1.89	0.55
30:0:605:CHL:HED3	31:r:315:CLA:O1A	2.07	0.55
1:7:62:LEU:HD11	1:7:73:ASP:HB2	1.89	0.55
1:7:134:TYR:O	1:7:140:LEU:HD12	2.07	0.55
31:8:613:CLA:HBC1	32:8:615:LUT:H162	1.87	0.55
3:p:191:ALA:HB3	31:p:610:CLA:HAA2	1.89	0.55
2:q:258:LEU:O	34:q:301:LMG:HC4	2.07	0.55
31:a:407:CLA:HBA1	31:a:407:CLA:CHA	2.36	0.55
31:a:409:CLA:H12	34:w:201:LMG:H112	1.87	0.55
3:n:250:ALA:N	3:n:251:PRO:HD2	2.21	0.55
19:s:252:GLN:O	19:s:256:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:610:CLA:HMA3	38:6:301:SQD:H5	1.89	0.55
30:3:302:CHL:HBD	30:3:302:CHL:HAA1	1.88	0.55
2:4:132:ILE:HG13	2:4:152:ILE:HG13	1.89	0.55
3:5:89:VAL:HG21	3:5:179:LEU:HD13	1.89	0.55
15:L:27:VAL:HG11	33:L:101:LHG:H182	1.88	0.55
24:Y:178:PHE:HA	38:Y:320:SQD:H2	1.89	0.55
31:Y:313:CLA:H121	33:Y:318:LHG:H332	1.89	0.55
4:0:133:GLU:OE1	4:0:134:GLY:N	2.40	0.55
3:8:250:ALA:N	3:8:251:PRO:HD2	2.21	0.55
7:c:452:GLU:OE2	8:d:248:THR:OG1	2.25	0.55
2:2:179:THR:C	2:2:181:GLY:H	2.15	0.55
31:5:604:CLA:H43	30:5:606:CHL:HAA2	1.88	0.55
31:A:409:CLA:H12	34:A:412:LMG:H121	1.88	0.55
30:0:608:CHL:CMA	36:0:618:NEX:H30	2.37	0.55
1:7:157:MET:HB3	30:7:310:CHL:CBB	2.36	0.55
30:8:606:CHL:HAA2	30:8:606:CHL:HBD	1.89	0.55
5:a:28:LEU:HB2	34:a:401:LMG:H292	1.88	0.55
7:c:162:LEU:HD22	31:c:602:CLA:H202	1.89	0.55
33:g:319:LHG:H371	37:g:321:XAT:H10	1.89	0.55
3:n:38:VAL:HG11	3:n:43:PRO:HD2	1.88	0.55
3:n:199:GLU:OE2	3:n:203:LYS:HE3	2.06	0.55
31:n:316:CLA:H11	34:n:322:LMG:HC91	1.88	0.55
30:y:607:CHL:H143	30:y:609:CHL:H112	1.89	0.55
2:2:89:GLU:HA	2:2:184:LEU:HD11	1.90	0.54
3:3:159:MET:HE3	30:3:308:CHL:CMB	2.36	0.54
31:3:313:CLA:HHC	31:3:313:CLA:CBB	2.37	0.54
31:3:314:CLA:H8	31:3:314:CLA:C1C	2.37	0.54
2:4:254:ALA:HB1	37:4:619:XAT:H183	1.89	0.54
3:5:81:PHE:CZ	3:5:85:ARG:HD3	2.41	0.54
3:5:167:VAL:HG21	4:6:50:LEU:HD23	1.89	0.54
31:5:614:CLA:HBA2	31:5:614:CLA:CHA	2.37	0.54
5:A:160:ILE:HG12	7:C:419:PHE:CZ	2.42	0.54
33:G:618:LHG:C6	37:G:620:XAT:C38	2.85	0.54
30:0:607:CHL:HAA2	30:0:607:CHL:HBD	1.88	0.54
1:7:127:PHE:HZ	2:9:251:PHE:HB3	1.73	0.54
2:q:158:THR:O	2:q:162:ILE:HG12	2.06	0.54
6:b:161:LEU:O	48:r:302:LMU:H6E	2.07	0.54
29:F1:66:PHE:CZ	29:F1:225:GLU:HA	2.42	0.54
1:1:94:HIS:HE1	31:1:603:CLA:C4D	2.20	0.54
3:5:161:LEU:CD1	36:5:618:NEX:H11	2.38	0.54
30:5:606:CHL:HBB2	30:5:607:CHL:CBB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:229:LYS:HB2	4:6:234:ASN:OD1	2.07	0.54
6:B:35:GLY:HA3	6:B:101:ILE:HG12	1.89	0.54
7:C:202:PHE:HB2	22:W:73:ILE:HG23	1.89	0.54
31:0:604:CLA:HMA2	30:0:606:CHL:C3C	2.38	0.54
31:8:604:CLA:O1A	36:8:617:NEX:H241	2.07	0.54
2:9:109:GLU:OE2	2:9:235:LEU:HB2	2.07	0.54
3:p:203:LYS:HG3	31:p:611:CLA:HED2	1.88	0.54
31:p:610:CLA:C2	32:p:616:LUT:H26	2.37	0.54
5:a:54:ALA:HB2	5:a:72:LEU:HD12	1.88	0.54
6:b:348:ASP:OD1	6:b:349:LYS:N	2.38	0.54
45:c:617:DGD:HB32	34:j:101:LMG:H142	1.89	0.54
8:d:117:HIS:HE1	31:d:405:CLA:C4D	2.20	0.54
8:d:213:ILE:HG21	44:d:407:PL9:HC8	1.89	0.54
3:n:200:LEU:HB3	31:n:311:CLA:HMA2	1.89	0.54
34:2:618:LMG:O8	34:2:618:LMG:H122	2.07	0.54
3:3:143:ILE:HA	30:3:307:CHL:CHA	2.38	0.54
3:5:96:MET:SD	31:5:610:CLA:HAB	2.47	0.54
3:5:249:TYR:HA	3:5:252:LYS:HD3	1.89	0.54
4:6:110:LEU:CD2	34:6:322:LMG:C33	2.77	0.54
6:B:224:ARG:NH1	34:D:410:LMG:O3	2.41	0.54
2:G:80:ASP:HB3	2:G:83:THR:HG22	1.87	0.54
3:N:236:HIS:HA	3:N:243:THR:CG2	2.38	0.54
17:O:198:ARG:HB2	17:O:272:LEU:HD13	1.89	0.54
19:S:252:GLN:O	19:S:256:THR:HG22	2.07	0.54
22:W:109:ARG:HH22	22:W:116:GLY:H	1.55	0.54
30:0:607:CHL:HAA1	37:q:321:XAT:H41	1.88	0.54
3:p:122:PHE:CD2	3:p:123:LYS:HG2	2.42	0.54
6:b:35:GLY:HA3	6:b:101:ILE:HG12	1.87	0.54
3:n:168:ASN:HD22	24:y:53:PHE:HA	1.72	0.54
3:n:180:TYR:HB3	31:n:311:CLA:HED3	1.88	0.54
31:n:311:CLA:HBB1	31:n:311:CLA:HMB3	1.88	0.54
19:s:138:GLU:HA	30:s:308:CHL:HED2	1.89	0.54
2:4:228:LEU:HD22	34:4:621:LMG:H322	1.88	0.54
9:E:13:ILE:HG21	47:E:101:HEM:HAD2	1.88	0.54
2:G:127:LYS:HA	30:N:301:CHL:HED2	1.89	0.54
14:K:18:PHE:CE1	33:K:102:LHG:H242	2.43	0.54
3:N:246:TRP:HD1	31:N:314:CLA:HED2	1.72	0.54
31:N:312:CLA:HHC	31:N:312:CLA:CBB	2.36	0.54
17:O:232:GLU:O	17:O:235:LYS:NZ	2.40	0.54
33:S:322:LHG:H282	25:Z:44:ILE:HG21	1.90	0.54
31:9:312:CLA:H2	35:9:317:RRX:C40	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:314:CLA:O2A	31:9:314:CLA:H2A	2.07	0.54
3:p:139:ASN:HB3	3:p:142:LEU:HB2	1.88	0.54
6:b:204:ALA:CB	31:b:603:CLA:HAB	2.38	0.54
6:b:422:ARG:O	6:b:425:GLN:HG2	2.08	0.54
7:c:270:MET:HE1	31:c:607:CLA:H11	1.89	0.54
47:e:102:HEM:HMB1	27:q1:19:VAL:HG21	1.88	0.54
2:2:97:TRP:CE2	30:2:607:CHL:HED2	2.42	0.54
2:2:167:GLU:HG3	30:2:608:CHL:C4B	2.38	0.54
31:2:613:CLA:HED2	37:2:619:XAT:H202	1.89	0.54
3:3:99:ALA:HB1	32:3:317:LUT:H12	1.90	0.54
2:4:75:ALA:HB3	2:4:77:LEU:HD21	1.89	0.54
30:4:607:CHL:C4A	30:4:607:CHL:HBA2	2.38	0.54
3:5:187:PRO:HD2	32:5:616:LUT:C24	2.38	0.54
31:5:603:CLA:HBC1	30:5:609:CHL:HAC2	1.90	0.54
4:6:99:LEU:HB3	31:6:305:CLA:HAB	1.90	0.54
31:6:314:CLA:H2	31:6:314:CLA:C4D	2.37	0.54
31:B:609:CLA:HMA3	31:B:610:CLA:C1C	2.38	0.54
8:D:41:ALA:HB1	42:D:401:PHO:H42	1.89	0.54
34:J:101:LMG:HC91	34:J:101:LMG:H121	1.88	0.54
3:8:200:LEU:HB3	31:8:609:CLA:HMA2	1.88	0.54
34:9:321:LMG:H321	34:9:321:LMG:HC8	1.89	0.54
3:p:240:PRO:HG3	31:p:614:CLA:HMB3	1.89	0.54
31:q:314:CLA:HAB	35:q:317:RRX:C14	2.38	0.54
5:a:10:SER:HA	22:w:102:GLU:OE1	2.08	0.54
6:b:156:PHE:HZ	33:b:628:LHG:H282	1.72	0.54
6:b:275:TRP:HB3	6:b:318:ASN:HD22	1.72	0.54
38:b:627:SQD:H151	8:d:127:LEU:HD13	1.89	0.54
18:r:223:ALA:HB3	31:r:312:CLA:HAA2	1.89	0.54
19:s:151:TRP:NE1	36:s:319:NEX:O23	2.30	0.54
24:y:219:LEU:HD12	33:y:619:LHG:H271	1.89	0.54
3:3:49:LEU:HB3	3:3:52:PHE:O	2.06	0.54
6:B:247:TRP:HB2	31:B:608:CLA:HBC1	1.90	0.54
31:B:610:CLA:HHC	31:B:610:CLA:CBB	2.37	0.54
7:C:74:LEU:HD13	7:C:77:LEU:HD22	1.89	0.54
30:N:306:CHL:H193	31:S:315:CLA:HBC3	1.90	0.54
18:R:174:TYR:HD2	31:R:306:CLA:HBA1	1.73	0.54
1:7:94:HIS:HE1	31:7:304:CLA:C4D	2.20	0.54
7:c:325:LEU:HD23	17:o:159:PRO:HG2	1.89	0.54
3:n:246:TRP:O	3:n:251:PRO:HD3	2.08	0.54
31:n:304:CLA:HED2	31:n:304:CLA:H2	1.90	0.54
24:y:206:LEU:HB3	31:y:610:CLA:CMA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:614:CLA:HMB3	31:B:614:CLA:HBB1	1.90	0.54
2:G:133:PHE:CE2	2:G:152:ILE:HG12	2.43	0.54
2:G:152:ILE:HD12	2:G:152:ILE:H	1.72	0.54
3:N:121:TRP:CH2	31:N:321:CLA:HBB2	2.42	0.54
4:0:188:ASP:HA	32:0:616:LUT:H24	1.88	0.54
1:7:77:LEU:HD21	31:8:603:CLA:H43	1.89	0.54
31:8:612:CLA:H192	31:8:613:CLA:C4C	2.38	0.54
3:p:49:LEU:HD12	2:q:171:TYR:CD2	2.42	0.54
30:p:606:CHL:HAA2	30:p:606:CHL:HBD	1.88	0.54
6:b:30:VAL:HG13	31:b:614:CLA:HMC2	1.89	0.54
43:c:614:BCR:H12C	38:s:301:SQD:H311	1.89	0.54
14:k:38:VAL:HG21	43:v:101:BCR:H19C	1.88	0.54
3:3:109:GLN:HA	3:3:114:ALA:O	2.07	0.54
31:A:405:CLA:H152	42:A:408:PHO:H11	1.89	0.54
31:A:406:CLA:HMB1	31:A:406:CLA:HBB1	1.90	0.54
6:B:75:TRP:HB2	6:B:94:GLU:HG3	1.90	0.54
6:B:413:ASP:N	6:B:413:ASP:OD1	2.41	0.54
31:N:305:CLA:HMA3	30:N:307:CHL:C3C	2.38	0.54
4:0:125:LYS:HG2	2:q:258:LEU:HD21	1.89	0.54
1:7:184:ASP:HA	32:7:317:LUT:H24	1.90	0.54
3:8:246:TRP:O	3:8:251:PRO:HD3	2.08	0.54
31:b:606:CLA:HMA3	31:b:607:CLA:H3A	1.90	0.54
33:b:628:LHG:H152	30:r:309:CHL:HBA2	1.88	0.54
31:c:612:CLA:CBB	34:c:620:LMG:H312	2.38	0.54
31:n:305:CLA:H121	31:s:306:CLA:H3A	1.90	0.54
31:n:311:CLA:H52	32:n:317:LUT:C30	2.37	0.54
34:w:202:LMG:C21	31:y:612:CLA:H141	2.38	0.54
31:y:604:CLA:HBB1	31:y:604:CLA:HMB3	1.89	0.54
4:6:202:LEU:CB	31:6:311:CLA:HMA2	2.37	0.54
5:A:221:SER:HA	8:D:139:ARG:HB2	1.89	0.54
2:G:198:ASP:N	2:G:198:ASP:OD1	2.32	0.54
3:N:250:ALA:N	3:N:251:PRO:HD2	2.23	0.54
31:N:313:CLA:H2	31:N:313:CLA:C4D	2.38	0.54
31:N:313:CLA:H192	31:N:314:CLA:C4C	2.38	0.54
1:7:134:TYR:CD2	1:7:135:LEU:HG	2.43	0.54
31:8:609:CLA:H52	32:8:615:LUT:C30	2.37	0.54
31:8:612:CLA:H202	31:8:613:CLA:CGA	2.38	0.54
3:p:215:MET:HA	3:p:218:PHE:HD2	1.72	0.54
5:a:82:ILE:HB	5:a:174:LEU:HB2	1.89	0.54
7:c:239:HIS:HE1	31:c:606:CLA:C1A	2.19	0.54
31:3:311:CLA:CBB	32:3:317:LUT:H32	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:4:620:LMG:H322	31:6:316:CLA:NC	2.22	0.54
3:5:221:GLN:O	3:5:225:THR:HG22	2.07	0.54
43:B:617:BCR:HC22	34:B:621:LMG:H321	1.88	0.54
2:G:150:GLN:HB2	30:G:605:CHL:CBB	2.37	0.54
2:G:228:LEU:HD11	34:G:622:LMG:H361	1.90	0.54
16:M:4:ASN:C	16:M:6:LEU:H	2.15	0.54
16:M:6:LEU:HD12	16:M:9:ILE:HD12	1.91	0.54
22:W:109:ARG:NH2	22:W:116:GLY:H	2.06	0.54
1:7:239:SER:OG	34:7:322:LMG:HC62	2.07	0.54
3:p:139:ASN:OD1	3:p:142:LEU:N	2.41	0.54
38:a:412:SQD:H262	34:a:413:LMG:H312	1.89	0.54
2:g:220:MET:HE2	32:g:316:LUT:H10	1.90	0.54
31:g:313:CLA:HBB1	31:g:313:CLA:HMB3	1.88	0.54
3:n:86:GLU:HA	3:n:179:LEU:HD21	1.90	0.54
18:r:137:LEU:HD12	18:r:211:CSU:HB2	1.89	0.54
31:r:311:CLA:HMA2	31:r:316:CLA:HHD	1.90	0.54
20:t:11:VAL:HG23	43:t:101:BCR:H14C	1.89	0.54
24:y:206:LEU:HB3	31:y:610:CLA:HMA2	1.89	0.54
30:y:606:CHL:HBB2	30:y:607:CHL:CBB	2.38	0.54
31:y:613:CLA:H111	33:y:619:LHG:H311	1.88	0.54
30:1:606:CHL:HAA2	30:1:606:CHL:HBD	1.90	0.53
3:3:109:GLN:HB2	3:3:116:PHE:HD1	1.72	0.53
3:3:223:LEU:HD23	31:3:301:CLA:C1B	2.38	0.53
3:5:39:GLU:O	3:5:45:ARG:HA	2.08	0.53
31:G:610:CLA:H3A	38:G:617:SQD:H441	1.90	0.53
18:R:169:TYR:OH	48:R:302:LMU:H4'	2.08	0.53
31:8:604:CLA:HMB1	31:8:604:CLA:HBB1	1.90	0.53
3:p:245:PHE:C	3:p:247:VAL:H	2.16	0.53
34:q:302:LMG:H132	34:q:302:LMG:C9	2.33	0.53
38:b:627:SQD:H5	8:d:134:ARG:HE	1.73	0.53
7:c:334:THR:OG1	7:c:336:GLU:OE1	2.25	0.53
18:r:69:GLY:HA2	18:r:71:ARG:NH2	2.23	0.53
3:5:92:ALA:HB1	3:5:208:GLY:HA3	1.89	0.53
31:B:614:CLA:H62	43:B:617:BCR:H20C	1.90	0.53
30:N:307:CHL:HMB1	30:N:309:CHL:HMC	1.90	0.53
31:7:315:CLA:C8	31:7:315:CLA:H2	2.38	0.53
31:p:610:CLA:H2	32:p:616:LUT:H26	1.91	0.53
31:p:614:CLA:HHC	31:p:614:CLA:CBB	2.37	0.53
2:q:109:GLU:HA	2:q:123:ALA:HB1	1.90	0.53
2:q:175:GLY:O	2:q:176:PRO:C	2.50	0.53
7:c:425:PHE:HA	31:c:608:CLA:HMC2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:c:619:DGD:HAV2	33:y:619:LHG:H351	1.90	0.53
8:d:266:TRP:HH2	33:l:101:LHG:H102	1.72	0.53
1:1:117:ILE:HD11	1:1:122:ALA:HA	1.90	0.53
1:1:189:ALA:HB1	1:1:195:LEU:HD13	1.90	0.53
2:2:229:VAL:HG22	2:2:257:PHE:CZ	2.43	0.53
3:3:118:GLU:HG2	3:3:124:ALA:HA	1.89	0.53
3:3:121:TRP:CH2	31:3:301:CLA:HBB2	2.43	0.53
45:C:617:DGD:HAS2	45:C:618:DGD:HAV2	1.90	0.53
34:C:624:LMG:H142	31:Y:311:CLA:HAB	1.90	0.53
22:W:93:TRP:CZ2	34:W:201:LMG:H112	2.43	0.53
30:7:321:CHL:CBB	31:8:603:CLA:HAC1	2.32	0.53
2:q:177:VAL:HA	2:q:189:PHE:CD1	2.43	0.53
2:q:178:GLU:HG2	2:q:189:PHE:CD1	2.38	0.53
5:a:106:LEU:HD11	43:a:410:BCR:H402	1.89	0.53
45:c:619:DGD:HE1	31:y:611:CLA:HMA2	1.90	0.53
2:g:76:GLY:HA3	24:y:86:LYS:HD2	1.88	0.53
26:u:56:ASP:OD1	26:u:56:ASP:N	2.42	0.53
1:1:139:GLY:HA2	1:1:142:ASN:HD21	1.73	0.53
30:2:607:CHL:H2	35:2:614:RRX:H12	1.89	0.53
31:3:304:CLA:H62	31:3:305:CLA:HMA3	1.89	0.53
2:4:147:ILE:HG23	30:4:605:CHL:C1D	2.39	0.53
3:5:249:TYR:HB3	3:5:258:TYR:CD2	2.44	0.53
3:5:254:ALA:O	3:5:256:ILE:HG22	2.08	0.53
31:5:603:CLA:H43	4:6:76:LEU:HD21	1.90	0.53
6:B:114:HIS:HE1	31:B:616:CLA:ND	2.01	0.53
2:G:205:LEU:HD23	2:G:208:LYS:HD2	1.89	0.53
2:G:251:PHE:HB3	24:Y:132:PHE:HZ	1.73	0.53
31:8:614:CLA:C4D	34:9:302:LMG:H292	2.39	0.53
31:p:612:CLA:HHC	31:p:612:CLA:CBB	2.36	0.53
9:e:13:ILE:HG21	47:e:102:HEM:HAD2	1.91	0.53
30:n:307:CHL:HAA2	30:n:307:CHL:HBD	1.89	0.53
30:n:308:CHL:HAA2	24:y:260:ALA:HB2	1.90	0.53
22:w:67:GLY:O	34:w:201:LMG:O5	2.25	0.53
31:1:611:CLA:H8	31:1:612:CLA:ND	2.22	0.53
2:4:170:ARG:HA	30:4:608:CHL:C3C	2.39	0.53
34:4:620:LMG:O7	34:4:621:LMG:H121	2.09	0.53
31:C:606:CLA:H52	34:W:201:LMG:H352	1.91	0.53
47:E:101:HEM:HBD2	47:E:101:HEM:HHA	1.90	0.53
31:N:314:CLA:HBA1	31:N:314:CLA:HBD	1.90	0.53
31:7:316:CLA:CHC	30:7:321:CHL:HMA2	2.38	0.53
3:8:86:GLU:HA	3:8:179:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:245:PHE:HB2	31:8:612:CLA:CAD	2.38	0.53
3:p:98:GLY:HA2	32:p:617:LUT:H181	1.89	0.53
8:d:136:VAL:HG12	8:d:138:ILE:HG23	1.90	0.53
48:r:302:LMU:H52	31:r:307:CLA:HAB	1.90	0.53
43:T:101:BCR:HC8	43:b:618:BCR:H341	1.90	0.53
31:7:316:CLA:C4D	34:9:301:LMG:H301	2.37	0.53
31:8:613:CLA:HMB1	31:8:613:CLA:HBB1	1.89	0.53
30:9:309:CHL:HAA1	30:9:309:CHL:HBD	1.91	0.53
3:p:240:PRO:HB2	31:p:614:CLA:CHB	2.38	0.53
30:p:606:CHL:HBB2	30:p:607:CHL:CBB	2.39	0.53
31:b:603:CLA:HBD	31:b:603:CLA:HBA2	1.91	0.53
34:c:621:LMG:H111	34:c:621:LMG:H292	1.91	0.53
26:u:112:LEU:HD21	26:u:128:LEU:HD13	1.89	0.53
34:Q1:101:LMG:HC71	34:Q1:101:LMG:O2	2.08	0.53
29:F1:178:LYS:HB3	29:F1:230:TRP:CZ2	2.43	0.53
31:2:602:CLA:HMC1	32:2:615:LUT:C32	2.38	0.53
3:3:109:GLN:HB2	3:3:116:PHE:CD1	2.43	0.53
3:3:216:LEU:HD23	31:3:305:CLA:HBB2	1.91	0.53
2:4:158:THR:HG21	30:4:606:CHL:HED3	1.90	0.53
7:C:175:ASP:OD2	7:C:185:ARG:NH2	2.22	0.53
12:I:25:SER:HB3	22:W:103:ILE:HD13	1.91	0.53
31:R:311:CLA:HMA2	31:R:316:CLA:HHD	1.90	0.53
24:Y:157:VAL:HG11	30:Y:307:CHL:HED2	1.91	0.53
30:9:310:CHL:CMB	36:9:319:NEX:H14	2.39	0.53
6:b:30:VAL:HG12	31:b:606:CLA:HHD	1.91	0.53
43:b:618:BCR:HC32	16:m:6:LEU:HB3	1.90	0.53
7:c:238:TRP:HA	34:c:624:LMG:H141	1.91	0.53
45:c:619:DGD:HAN2	45:c:619:DGD:HBE2	1.89	0.53
27:q1:6:GLY:HA3	34:q1:101:LMG:HC4	1.89	0.53
30:1:606:CHL:HBB2	30:1:607:CHL:HAB	1.90	0.53
2:2:99:MET:SD	31:2:609:CLA:HAB	2.48	0.53
31:2:610:CLA:H2	31:2:611:CLA:HMD2	1.90	0.53
3:5:188:LEU:HD12	32:5:616:LUT:H222	1.89	0.53
3:5:252:LYS:HA	3:5:256:ILE:CG2	2.36	0.53
38:M:102:SQD:H112	31:b:615:CLA:H42	1.90	0.53
19:S:102:ALA:HA	19:S:210:LEU:HD11	1.90	0.53
31:Y:303:CLA:H101	32:Y:316:LUT:H371	1.91	0.53
2:9:49:TRP:CE2	2:9:50:LEU:HG	2.44	0.53
34:9:321:LMG:H112	34:9:321:LMG:H322	1.91	0.53
2:q:135:GLU:O	2:q:136:ASP:C	2.52	0.53
5:a:84:PRO:HA	5:a:112:TYR:CG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:a:414:PL9:H453	8:d:39:PRO:HA	1.91	0.53
6:b:114:HIS:HE1	31:b:617:CLA:ND	2.04	0.53
6:b:161:LEU:HD22	33:b:628:LHG:H242	1.91	0.53
9:e:44:TYR:HE2	29:f1:53:ALA:HB2	1.74	0.53
31:g:305:CLA:HMA3	30:g:307:CHL:C2C	2.38	0.53
3:n:245:PHE:HB2	31:n:314:CLA:CAD	2.38	0.53
19:s:278:THR:HG22	38:s:301:SQD:H1	1.89	0.53
2:2:229:VAL:HA	2:2:257:PHE:HZ	1.73	0.53
31:2:609:CLA:H3A	31:2:609:CLA:C1	2.38	0.53
2:4:49:TRP:HE3	30:4:601:CHL:HAA1	1.72	0.53
7:C:144:LYS:HD3	34:C:621:LMG:HC61	1.91	0.53
31:G:604:CLA:HBB1	31:G:604:CLA:HMB3	1.91	0.53
4:0:67:GLY:HA3	4:0:207:ILE:HG21	1.91	0.53
3:8:236:HIS:CA	3:8:243:THR:HG21	2.29	0.53
31:9:313:CLA:C4D	31:9:314:CLA:HMD3	2.38	0.53
34:9:321:LMG:H292	34:9:321:LMG:C1	2.39	0.53
2:q:97:TRP:CD1	30:q:311:CHL:HMD3	2.44	0.53
2:q:107:THR:N	2:q:108:PRO:HD2	2.24	0.53
7:c:166:LYS:HA	7:c:170:PHE:HB2	1.91	0.53
13:j:28:GLY:HA2	34:j:101:LMG:H171	1.91	0.53
3:n:233:LEU:HD22	32:n:317:LUT:H163	1.91	0.53
31:n:314:CLA:H172	31:n:315:CLA:C1D	2.39	0.53
18:r:123:TYR:OH	18:r:134:GLU:OE1	2.21	0.53
31:y:610:CLA:H62	31:y:612:CLA:CMA	2.38	0.53
31:1:603:CLA:HAC2	30:1:607:CHL:H193	1.91	0.53
3:5:40:TRP:CE3	3:5:46:PRO:HG3	2.44	0.53
30:G:623:CHL:H121	30:Y:309:CHL:H112	1.91	0.53
24:Y:94:HIS:HE1	31:Y:304:CLA:C4D	2.22	0.53
30:7:308:CHL:HMB1	30:7:308:CHL:H101	1.91	0.53
2:9:140:TYR:HB2	2:9:147:ILE:HD12	1.91	0.53
31:9:304:CLA:H52	32:9:318:LUT:H28	1.91	0.53
30:9:308:CHL:HAA2	30:9:308:CHL:HBD	1.91	0.53
3:p:125:GLY:O	3:p:128:ILE:HG22	2.09	0.53
31:p:614:CLA:H2	31:p:614:CLA:HBA2	1.91	0.53
5:a:283:ILE:HA	5:a:286:THR:HG22	1.91	0.53
31:1:614:CLA:HBA1	31:1:614:CLA:CHA	2.32	0.52
5:A:84:PRO:HA	5:A:112:TYR:CG	2.44	0.52
8:D:46:GLY:HA2	43:D:405:BCR:H11C	1.90	0.52
31:G:612:CLA:C11	37:G:620:XAT:H34	2.39	0.52
38:G:617:SQD:H61	38:G:617:SQD:O6	2.09	0.52
31:7:316:CLA:C4C	34:9:301:LMG:H341	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:321:CHL:HMC	3:8:155:GLN:OE1	2.09	0.52
30:9:310:CHL:HAB	36:9:319:NEX:H10	1.90	0.52
31:b:610:CLA:HMA3	31:b:611:CLA:C1C	2.39	0.52
43:b:619:BCR:HC41	34:b:622:LMG:H322	1.90	0.52
20:t:3:ALA:O	20:t:7:THR:HG23	2.08	0.52
22:w:86:THR:CG2	34:w:202:LMG:H221	2.39	0.52
1:1:198:LEU:HB3	31:1:610:CLA:CMA	2.39	0.52
34:3:321:LMG:C10	34:3:321:LMG:H141	2.39	0.52
6:B:39:PHE:CD1	34:m:102:LMG:HC92	2.44	0.52
6:B:216:HIS:HE1	31:B:609:CLA:NA	1.96	0.52
3:N:123:LYS:HA	30:Y:301:CHL:HED3	1.91	0.52
4:0:164:ILE:CD1	36:0:618:NEX:C34	2.88	0.52
3:p:89:VAL:HB	3:p:179:LEU:HD21	1.92	0.52
3:p:120:VAL:CG2	3:p:123:LYS:HB2	2.36	0.52
30:q:309:CHL:H8	30:q:309:CHL:C1C	2.39	0.52
31:b:612:CLA:C3B	31:b:614:CLA:HMA2	2.39	0.52
7:c:118:VAL:HG12	25:z:27:LEU:HD12	1.91	0.52
30:g:302:CHL:H11	30:y:609:CHL:C1B	2.39	0.52
18:r:139:HIS:HE1	31:r:305:CLA:C4D	2.22	0.52
18:r:223:ALA:HB1	18:r:230:THR:HG23	1.92	0.52
31:S:305:CLA:H52	30:S:307:CHL:HBA2	1.90	0.52
31:8:603:CLA:H2	31:8:603:CLA:HED2	1.91	0.52
7:c:68:PRO:HG2	7:c:71:GLU:HG3	1.91	0.52
45:c:619:DGD:O3E	34:c:624:LMG:HC5	2.10	0.52
8:d:239:GLN:OE1	28:p1:50:TYR:OH	2.23	0.52
34:s:321:LMG:O5	34:s:321:LMG:O4	2.23	0.52
31:y:604:CLA:HMA3	30:y:606:CHL:C3C	2.40	0.52
31:2:603:CLA:HHC	31:2:603:CLA:CBB	2.33	0.52
3:3:147:SER:HB2	34:3:321:LMG:H321	1.91	0.52
4:6:98:MET:SD	31:6:311:CLA:HAB	2.49	0.52
31:C:606:CLA:H92	31:C:607:CLA:H193	1.92	0.52
33:S:322:LHG:H161	33:S:322:LHG:H262	1.92	0.52
4:0:131:PHE:HZ	2:q:251:PHE:HB3	1.75	0.52
2:q:165:ALA:O	2:q:168:ALA:N	2.42	0.52
33:g:319:LHG:H312	37:g:321:XAT:C34	2.40	0.52
3:n:155:GLN:OE1	30:n:308:CHL:HMC	2.09	0.52
30:1:609:CHL:HAA2	2:2:74:THR:HG21	1.91	0.52
3:3:165:TYR:HB3	30:3:309:CHL:CMC	2.39	0.52
3:5:163:GLU:O	3:5:167:VAL:HG13	2.10	0.52
31:B:615:CLA:H2	31:B:616:CLA:CBB	2.39	0.52
7:C:320:GLN:HG2	17:O:157:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:604:CLA:HMA3	30:G:606:CHL:C3C	2.39	0.52
3:N:142:LEU:O	3:N:144:HIS:N	2.41	0.52
24:Y:90:ILE:HG21	31:Y:304:CLA:HAA2	1.91	0.52
31:8:602:CLA:H92	31:9:305:CLA:H52	1.90	0.52
5:a:93:PHE:HZ	31:a:409:CLA:HAA1	1.75	0.52
3:n:175:GLY:HA3	19:s:33:VAL:HA	1.91	0.52
31:r:306:CLA:CHA	31:r:306:CLA:HBA1	2.38	0.52
3:3:143:ILE:HD12	3:3:145:ALA:H	1.74	0.52
30:5:605:CHL:HAA1	30:5:605:CHL:HBD	1.91	0.52
34:A:412:LMG:HC72	7:C:204:SER:HB2	1.90	0.52
7:C:195:GLY:HA3	34:W:203:LMG:HC2	1.91	0.52
31:C:613:CLA:HBA1	31:C:613:CLA:HBD	1.90	0.52
8:D:148:ALA:HB2	8:D:276:VAL:HG13	1.90	0.52
36:N:318:NEX:H10	19:S:39:TRP:CZ3	2.44	0.52
3:8:233:LEU:HD22	32:8:615:LUT:H163	1.91	0.52
30:8:606:CHL:HMB2	30:8:608:CHL:HMC	1.91	0.52
3:p:233:LEU:HA	31:p:613:CLA:HMA3	1.91	0.52
6:b:53:ASN:HD21	6:b:331:ASN:ND2	2.05	0.52
31:n:314:CLA:H71	31:n:315:CLA:HMD3	1.92	0.52
2:2:185:TYR:HB3	31:2:609:CLA:HED3	1.91	0.52
30:4:607:CHL:HBB2	30:4:609:CHL:HBC1	1.91	0.52
4:6:193:ALA:HB1	4:6:199:LEU:HD13	1.92	0.52
31:6:311:CLA:H51	32:6:317:LUT:C30	2.37	0.52
38:A:413:SQD:H441	6:b:75:TRP:CE2	2.45	0.52
2:G:90:ILE:HG21	31:G:603:CLA:HAA2	1.91	0.52
2:9:176:PRO:HD2	30:9:310:CHL:HBB2	1.91	0.52
31:q:313:CLA:C4D	31:q:314:CLA:HMD3	2.39	0.52
5:a:50:ILE:HD12	34:m:102:LMG:H161	1.91	0.52
31:d:405:CLA:CHA	31:d:405:CLA:HBA1	2.40	0.52
31:g:305:CLA:HMA3	30:g:307:CHL:C3C	2.40	0.52
4:6:173:PRO:HB3	18:R:54:LEU:HG	1.92	0.52
31:6:304:CLA:HHC	31:6:304:CLA:HBB1	1.90	0.52
9:E:24:SER:O	9:E:28:PRO:HG2	2.10	0.52
31:G:609:CLA:HBA1	35:G:614:RRX:H7	1.91	0.52
3:N:246:TRP:O	3:N:250:ALA:HB3	2.09	0.52
18:R:120:LEU:O	31:R:316:CLA:ND	2.42	0.52
4:0:122:VAL:HG23	4:0:125:LYS:HB2	1.92	0.52
2:9:59:PRO:HD2	2:9:62:LEU:HD12	1.91	0.52
3:p:218:PHE:CD1	3:p:229:PRO:HB3	2.44	0.52
31:b:615:CLA:H171	43:b:618:BCR:C12	2.40	0.52
7:c:205:PRO:HD3	34:w:201:LMG:H332	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:c:617:DGD:HBG1	43:d:406:BCR:H402	1.91	0.52
31:y:604:CLA:H91	34:y:620:LMG:H372	1.91	0.52
1:1:179:PRO:HD2	31:1:610:CLA:OBD	2.09	0.52
31:1:612:CLA:CMD	38:g:301:SQD:H251	2.40	0.52
2:2:164:GLY:HA2	30:2:608:CHL:CAB	2.40	0.52
31:5:603:CLA:H2	31:5:603:CLA:H2A	1.92	0.52
5:A:64:ARG:O	17:O:198:ARG:NH2	2.42	0.52
7:C:41:HIS:CD2	31:C:609:CLA:NA	2.77	0.52
2:G:95:ALA:HB1	2:G:213:GLY:HA3	1.91	0.52
2:G:221:PHE:CD2	31:G:612:CLA:HAC1	2.43	0.52
3:N:240:PRO:HG3	31:N:314:CLA:HMB2	1.91	0.52
31:N:313:CLA:H122	31:N:314:CLA:HMD3	1.92	0.52
31:0:610:CLA:H51	32:0:616:LUT:H30	1.90	0.52
2:q:140:TYR:CE2	31:q:306:CLA:H2	2.44	0.52
5:a:131:TRP:CH2	31:c:605:CLA:HAA2	2.45	0.52
9:e:74:GLU:O	9:e:78:LYS:HG2	2.10	0.52
18:r:174:TYR:CD1	31:r:306:CLA:H2	2.45	0.52
26:u:113:ASP:N	26:u:113:ASP:OD1	2.38	0.52
29:F1:196:LEU:HB3	29:F1:230:TRP:CD2	2.45	0.52
29:f1:129:LEU:HD11	29:f1:136:PHE:HZ	1.75	0.52
3:3:219:GLY:HA2	31:3:301:CLA:HBB2	1.90	0.52
3:3:239:ALA:HB1	3:3:242:ALA:HB3	1.92	0.52
2:4:122:ALA:O	2:4:128:ALA:HB2	2.10	0.52
2:4:169:TYR:HB3	2:4:174:GLU:HG3	1.92	0.52
3:5:222:GLY:O	31:6:316:CLA:HMB3	2.09	0.52
42:A:408:PHO:H202	44:D:406:PL9:H453	1.92	0.52
2:G:76:GLY:N	24:Y:86:LYS:HD2	2.25	0.52
3:N:131:GLU:OE1	3:N:132:GLY:N	2.41	0.52
3:N:239:ALA:O	3:N:243:THR:HG22	2.10	0.52
1:7:86:ARG:HD3	2:9:74:THR:O	2.10	0.52
30:7:307:CHL:HBB2	30:7:308:CHL:CAB	2.40	0.52
31:8:612:CLA:H71	31:8:613:CLA:HMD3	1.91	0.52
3:p:218:PHE:HD1	3:p:229:PRO:HB3	1.75	0.52
5:a:192:ILE:HG13	5:a:293:MET:HE1	1.92	0.52
6:b:454:ALA:HB2	34:b:622:LMG:H181	1.91	0.52
34:b:601:LMG:H371	43:b:619:BCR:H371	1.91	0.52
31:b:615:CLA:HBB1	31:b:615:CLA:HMB3	1.91	0.52
30:r:309:CHL:HAA1	30:r:309:CHL:CBD	2.40	0.52
29:F1:105:ASN:HD22	29:F1:213:CYS:HA	1.75	0.52
1:1:59:PRO:HG2	1:1:62:LEU:HD12	1.91	0.51
1:1:78:SER:OG	31:1:602:CLA:O1A	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:165:VAL:CG1	2:2:57:SER:HB3	2.40	0.51
1:1:245:ALA:HB3	1:1:246:LEU:HD13	1.91	0.51
2:2:238:LEU:O	2:2:242:LEU:HG	2.09	0.51
3:3:253:SER:OG	30:3:302:CHL:HBA1	2.10	0.51
32:3:318:LUT:H191	32:3:318:LUT:C12	2.40	0.51
2:4:206:LYS:O	2:4:209:GLU:HB3	2.10	0.51
3:5:45:ARG:HG3	3:5:66:ASP:O	2.11	0.51
3:5:89:VAL:HG22	3:5:205:LEU:HD21	1.91	0.51
4:6:161:MET:HE3	36:6:319:NEX:H31	1.92	0.51
4:6:229:LYS:HB3	4:6:233:GLN:HG2	1.91	0.51
6:B:91:TRP:HE1	34:B:622:LMG:HC91	1.74	0.51
8:D:304:ARG:NH1	16:M:-3:UNK:O	2.43	0.51
2:G:235:LEU:HD22	34:G:619:LMG:HC91	1.91	0.51
33:M:101:LHG:HC62	20:T:1:MET:HB2	1.92	0.51
31:Y:305:CLA:HBB1	31:Y:305:CLA:HMB3	1.92	0.51
31:8:614:CLA:H43	2:9:257:PHE:CD1	2.45	0.51
2:9:49:TRP:CE3	30:9:303:CHL:HAA1	2.45	0.51
2:9:147:ILE:HA	30:9:307:CHL:C4D	2.40	0.51
3:p:187:PRO:HD2	32:p:616:LUT:H23	1.93	0.51
3:p:245:PHE:C	3:p:247:VAL:N	2.68	0.51
30:p:607:CHL:HBA1	30:p:607:CHL:CBD	2.40	0.51
31:p:610:CLA:H12	31:p:610:CLA:H3A	1.92	0.51
6:b:247:TRP:HB2	31:b:609:CLA:HBC1	1.92	0.51
9:e:2:SER:OG	28:p1:63:TYR:O	2.27	0.51
9:e:27:ILE:HB	9:e:28:PRO:HD3	1.92	0.51
1:1:49:PHE:HD2	30:1:601:CHL:HAA1	1.74	0.51
31:1:611:CLA:H101	31:1:612:CLA:NB	2.25	0.51
2:2:146:LEU:HD23	30:2:605:CHL:HED3	1.92	0.51
3:3:215:MET:HE2	32:3:318:LUT:C10	2.39	0.51
3:3:227:LYS:HB2	3:3:232:ASN:OD1	2.10	0.51
3:5:145:ALA:HA	30:5:605:CHL:CHC	2.40	0.51
45:C:620:DGD:HBW1	31:Y:312:CLA:HBC3	1.92	0.51
9:E:26:THR:HB	47:E:101:HEM:CAB	2.40	0.51
3:N:58:TYR:HD1	3:N:59:LEU:HD13	1.74	0.51
31:N:314:CLA:C2	31:N:314:CLA:HAA2	2.40	0.51
18:R:184:TYR:CE1	48:R:302:LMU:H21	2.46	0.51
31:S:311:CLA:H51	32:S:317:LUT:H373	1.93	0.51
33:S:320:LHG:H282	33:S:320:LHG:HC92	1.91	0.51
24:Y:100:LEU:HB3	31:Y:305:CLA:HAB	1.91	0.51
31:Y:310:CLA:H62	31:Y:312:CLA:CMA	2.39	0.51
30:7:308:CHL:H101	30:7:308:CHL:CMB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:63:LYS:NZ	2:9:63:LYS:HB2	2.25	0.51
31:p:604:CLA:NB	36:p:618:NEX:H242	2.25	0.51
31:p:613:CLA:CGA	31:p:613:CLA:C1A	2.88	0.51
5:a:307:VAL:HG23	10:f:44:ARG:HD2	1.91	0.51
43:b:618:BCR:H12C	34:b:622:LMG:H421	1.91	0.51
18:r:75:PRO:HD2	37:r:318:XAT:H242	1.92	0.51
18:r:233:LEU:HB3	31:r:312:CLA:HMA2	1.93	0.51
1:1:73:ASP:HA	32:1:616:LUT:H24	1.92	0.51
30:5:606:CHL:HAB	32:5:617:LUT:H161	1.93	0.51
30:6:308:CHL:HBB2	30:6:310:CHL:HBC1	1.92	0.51
7:C:239:HIS:HE1	31:C:606:CLA:C1A	2.23	0.51
8:D:279:LEU:HD11	42:D:401:PHO:HMC3	1.92	0.51
2:G:257:PHE:CE1	31:N:315:CLA:H43	2.45	0.51
17:O:72:ASN:O	17:O:131:THR:HG21	2.10	0.51
4:0:222:ILE:HG13	31:0:613:CLA:HAC2	1.93	0.51
33:p:619:LHG:O10	33:p:619:LHG:H272	2.11	0.51
2:q:100:LEU:HG	31:q:312:CLA:HMC3	1.92	0.51
45:c:616:DGD:HAH1	45:c:616:DGD:HA82	1.91	0.51
38:g:301:SQD:C9	37:g:321:XAT:H222	2.36	0.51
31:g:311:CLA:HMA2	38:g:318:SQD:H61	1.92	0.51
2:4:163:MET:HE3	30:4:606:CHL:HMB3	1.93	0.51
2:4:186:PRO:HD2	31:4:610:CLA:OBD	2.10	0.51
4:6:248:TYR:HA	4:6:252:ALA:HB2	1.93	0.51
2:G:130:ALA:HA	2:G:133:PHE:HD1	1.75	0.51
34:I:101:LMG:H322	22:W:84:ALA:HA	1.92	0.51
31:7:304:CLA:HHC	31:7:304:CLA:CBB	2.40	0.51
3:p:216:LEU:HB2	32:p:617:LUT:H402	1.93	0.51
31:p:614:CLA:O1A	2:q:157:LEU:HD21	2.11	0.51
2:q:72:TRP:O	32:q:318:LUT:H24	2.10	0.51
6:b:399:VAL:HG23	6:b:417:VAL:HG22	1.90	0.51
33:b:625:LHG:HC91	33:l:101:LHG:HC81	1.92	0.51
30:n:301:CHL:HMA3	31:n:316:CLA:CAB	2.40	0.51
30:n:310:CHL:HBA2	30:y:601:CHL:H12	1.92	0.51
22:w:86:THR:HG23	34:w:202:LMG:H442	1.91	0.51
3:3:200:LEU:HB3	31:3:311:CLA:HMA2	1.92	0.51
3:5:136:TYR:HD1	3:5:142:LEU:HD13	1.75	0.51
8:D:193:LEU:O	15:L:35:TYR:OH	2.24	0.51
2:G:171:TYR:CD2	3:N:49:LEU:HD12	2.45	0.51
30:S:307:CHL:HAA2	30:S:307:CHL:HBD	1.93	0.51
31:8:602:CLA:H61	32:8:616:LUT:H28	1.91	0.51
31:8:609:CLA:H8	32:8:615:LUT:C30	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:195:LEU:HB2	31:9:312:CLA:O1A	2.10	0.51
3:p:232:ASN:HB3	31:p:613:CLA:HED1	1.92	0.51
31:q:306:CLA:H2A	31:q:306:CLA:HED3	1.92	0.51
30:q:308:CHL:CBB	30:q:309:CHL:CBB	2.87	0.51
5:a:28:LEU:HB2	34:a:401:LMG:C29	2.40	0.51
7:c:26:GLY:HA3	31:c:611:CLA:HMD2	1.92	0.51
44:d:407:PL9:H421	33:d:408:LHG:H222	1.92	0.51
3:n:146:GLN:HB2	30:n:306:CHL:CBB	2.41	0.51
31:n:314:CLA:H202	31:n:315:CLA:CGA	2.40	0.51
3:3:118:GLU:HB3	3:3:124:ALA:HA	1.92	0.51
3:3:136:TYR:CD1	3:3:137:LEU:HG	2.45	0.51
3:3:162:ILE:HD11	36:3:319:NEX:C34	2.40	0.51
3:3:246:TRP:HZ3	30:3:302:CHL:CHD	2.24	0.51
2:4:103:LEU:HG	35:4:615:RRX:H28	1.92	0.51
3:5:143:ILE:N	30:5:605:CHL:O1D	2.43	0.51
3:5:161:LEU:HD13	36:5:618:NEX:H11	1.93	0.51
30:5:601:CHL:HBD	30:5:601:CHL:HAA1	1.92	0.51
43:B:617:BCR:H383	38:B:620:SQD:H121	1.91	0.51
31:C:603:CLA:H161	31:C:610:CLA:HBB2	1.93	0.51
9:E:45:ASP:OD2	27:Q1:4:ARG:NH2	2.38	0.51
30:G:606:CHL:HBB1	32:G:615:LUT:H161	1.92	0.51
30:G:623:CHL:H171	31:Y:304:CLA:HAC2	1.91	0.51
31:N:310:CLA:H62	31:N:312:CLA:HMA3	1.93	0.51
19:S:158:ASN:OD1	19:S:159:PHE:N	2.40	0.51
31:0:615:CLA:C1C	34:q:301:LMG:H341	2.40	0.51
3:p:109:GLN:HB3	3:p:110:ARG:HD3	1.92	0.51
6:b:464:PHE:CZ	33:b:625:LHG:H252	2.46	0.51
7:c:151:ILE:HG12	34:c:620:LMG:H322	1.93	0.51
45:c:619:DGD:C1D	31:y:611:CLA:HBA1	2.40	0.51
2:g:121:GLU:HB3	2:g:127:LYS:HE2	1.93	0.51
31:n:314:CLA:H192	31:n:315:CLA:C4C	2.39	0.51
18:r:62:TRP:CZ2	18:r:77:GLY:HA2	2.46	0.51
30:s:307:CHL:HBB2	30:s:308:CHL:CBB	2.41	0.51
22:w:100:THR:OG1	34:w:202:LMG:HC5	2.10	0.51
34:q1:101:LMG:H152	34:q1:101:LMG:H361	1.93	0.51
28:p1:34:LYS:HG2	28:p1:46:GLY:CA	2.40	0.51
31:3:315:CLA:H62	31:3:315:CLA:NB	2.26	0.51
3:5:86:GLU:HA	3:5:179:LEU:HD21	1.93	0.51
31:B:614:CLA:H72	38:m:101:SQD:H141	1.93	0.51
38:B:620:SQD:H192	38:B:620:SQD:H362	1.92	0.51
7:C:302:THR:HG21	7:C:343:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:449:ARG:NH2	8:D:241:GLU:HB2	2.26	0.51
33:D:408:LHG:H271	15:L:23:LEU:HD22	1.93	0.51
31:N:313:CLA:HBB1	32:N:316:LUT:H8	1.92	0.51
1:7:90:ILE:HD13	31:7:304:CLA:HBA1	1.92	0.51
1:7:134:TYR:CE1	31:7:305:CLA:H2	2.46	0.51
1:7:179:PRO:HD2	31:7:311:CLA:OBD	2.10	0.51
2:9:54:SER:O	2:9:58:VAL:HG23	2.10	0.51
2:q:179:THR:H	2:q:189:PHE:HB2	1.76	0.51
34:g:322:LMG:H292	31:y:615:CLA:HBD	1.93	0.51
30:1:607:CHL:C1	2:2:259:PRO:HD3	2.41	0.51
2:2:153:VAL:O	2:2:157:LEU:HG	2.10	0.51
3:3:165:TYR:HB3	30:3:309:CHL:C2C	2.40	0.51
3:3:225:THR:O	3:3:227:LYS:HD3	2.11	0.51
2:4:140:TYR:CD1	2:4:146:LEU:HG	2.45	0.51
3:5:176:LEU:HB3	3:5:181:PRO:HA	1.93	0.51
5:A:57:PRO:HD3	5:A:73:TYR:CE2	2.46	0.51
33:A:415:LHG:H152	33:A:415:LHG:H101	1.92	0.51
7:C:146:THR:HG21	7:C:244:PRO:HD3	1.91	0.51
8:D:91:PHE:CE1	31:D:404:CLA:HAA1	2.46	0.51
3:8:146:GLN:HB2	30:8:605:CHL:CBB	2.41	0.51
2:9:260:LEU:HD12	34:9:301:LMG:HC62	1.92	0.51
2:q:186:PRO:O	31:q:312:CLA:HED3	2.11	0.51
2:g:205:LEU:HB3	31:g:310:CLA:CMA	2.39	0.51
31:g:311:CLA:HBD	31:g:311:CLA:HBA1	1.92	0.51
33:l:101:LHG:H251	33:l:101:LHG:HC91	1.92	0.51
1:1:106:VAL:HG13	1:1:228:ILE:HD11	1.92	0.51
31:3:305:CLA:HBD	31:3:305:CLA:HBA2	1.92	0.51
2:4:132:ILE:HD13	30:4:606:CHL:HMD3	1.91	0.51
31:4:613:CLA:HBB1	31:4:613:CLA:HHC	1.92	0.51
3:5:91:HIS:HE1	31:5:603:CLA:ND	2.08	0.51
3:5:158:LEU:HA	36:5:618:NEX:H201	1.91	0.51
31:5:610:CLA:O2A	32:5:616:LUT:H221	2.10	0.51
30:6:307:CHL:CBB	30:6:310:CHL:HBC1	2.41	0.51
7:C:136:GLY:O	7:C:144:LYS:NZ	2.39	0.51
2:G:126:PHE:HB2	30:N:301:CHL:HMA3	1.92	0.51
30:G:606:CHL:CBB	32:G:615:LUT:H161	2.41	0.51
3:N:197:PHE:CZ	3:N:201:LYS:HD3	2.46	0.51
24:Y:239:LEU:HD22	32:Y:315:LUT:H163	1.91	0.51
3:p:200:LEU:HB2	31:p:610:CLA:HMA2	1.91	0.51
3:p:243:THR:O	3:p:244:ASN:C	2.53	0.51
2:q:143:ASN:HB3	2:q:146:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:602:CLA:H62	31:c:603:CLA:NB	2.26	0.51
18:r:183:ILE:CG2	48:r:302:LMU:H3'	2.40	0.51
24:y:166:GLU:HG3	30:y:609:CHL:C4B	2.41	0.51
27:q1:4:ARG:NH1	29:f1:50:GLY:HA2	2.26	0.51
1:1:231:LEU:HD21	31:1:614:CLA:HMC2	1.92	0.51
31:3:306:CLA:HBB1	32:3:318:LUT:H8	1.93	0.51
2:4:61:TYR:OH	2:4:76:GLY:HA2	2.11	0.51
3:5:64:PRO:HB2	3:5:205:LEU:CD1	2.41	0.51
4:6:182:TYR:HB3	31:6:311:CLA:HED3	1.92	0.51
5:A:82:ILE:HB	5:A:174:LEU:HB2	1.91	0.51
7:C:413:TRP:CD1	31:C:604:CLA:HMA2	2.46	0.51
34:C:622:LMG:HC92	34:N:320:LMG:HC4	1.92	0.51
31:G:603:CLA:C1C	30:G:608:CHL:H111	2.41	0.51
19:S:246:PHE:CZ	32:S:318:LUT:H10	2.46	0.51
26:U:56:ASP:OD1	26:U:56:ASP:N	2.43	0.51
4:0:229:LYS:HE3	4:0:234:ASN:ND2	2.26	0.51
1:7:73:ASP:HA	32:7:318:LUT:H24	1.93	0.51
31:9:306:CLA:H12	30:9:308:CHL:CAD	2.41	0.51
2:q:143:ASN:HD22	34:q1:101:LMG:H362	1.76	0.51
6:b:466:HIS:HE1	31:b:609:CLA:C4D	2.23	0.51
31:g:313:CLA:H172	31:g:314:CLA:HBD	1.92	0.51
17:o:107:LYS:NZ	17:o:117:ALA:O	2.44	0.51
31:s:314:CLA:H91	33:s:320:LHG:H301	1.93	0.51
34:4:620:LMG:H112	34:4:621:LMG:H122	1.93	0.50
31:B:606:CLA:H61	43:B:619:BCR:H311	1.91	0.50
2:G:192:PRO:HD2	35:G:614:RRX:H14	1.94	0.50
15:L:24:LEU:O	15:L:28:LEU:HB2	2.12	0.50
30:Y:301:CHL:H161	30:Y:302:CHL:H52	1.93	0.50
31:q:306:CLA:HMA3	30:q:308:CHL:C2C	2.41	0.50
7:c:432:HIS:HE1	31:c:608:CLA:NA	2.04	0.50
31:c:613:CLA:HMC2	43:c:614:BCR:H20C	1.93	0.50
15:l:21:GLY:O	15:l:25:ILE:HG12	2.12	0.50
3:5:203:LYS:HD3	31:5:612:CLA:CGA	2.41	0.50
5:A:278:TRP:HB3	5:A:279:PRO:HD3	1.91	0.50
6:B:462:PHE:HA	31:B:611:CLA:HMC2	1.92	0.50
38:B:620:SQD:H372	43:t:101:BCR:C36	2.39	0.50
14:K:17:PRO:HB2	33:K:102:LHG:H241	1.92	0.50
17:O:122:THR:HG22	17:O:164:LEU:HD23	1.93	0.50
19:S:224:ASP:HB3	19:S:227:VAL:HB	1.93	0.50
30:0:608:CHL:HAA1	30:0:608:CHL:HBD	1.94	0.50
34:0:620:LMG:H122	34:7:301:LMG:HC91	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:601:CHL:HED2	33:8:618:LHG:H122	1.92	0.50
2:9:49:TRP:CZ3	30:9:303:CHL:HAA1	2.45	0.50
3:p:109:GLN:HA	3:p:114:ALA:HB3	1.92	0.50
34:b:629:LMG:H112	34:r:321:LMG:H291	1.91	0.50
8:d:199:MET:HG2	44:d:407:PL9:H321	1.93	0.50
43:t:101:BCR:H23C	43:t:101:BCR:C38	2.41	0.50
1:1:224:GLY:HA3	2:2:261:PRO:HA	1.92	0.50
31:1:611:CLA:CAB	38:g:318:SQD:H241	2.37	0.50
31:2:610:CLA:H61	31:2:611:CLA:C3D	2.41	0.50
3:3:38:VAL:HA	3:3:42:GLY:N	2.25	0.50
30:3:309:CHL:HMB2	36:3:319:NEX:H14	1.94	0.50
7:C:154:ILE:HG22	34:C:621:LMG:H361	1.93	0.50
43:D:405:BCR:H373	10:F:33:LEU:HD21	1.93	0.50
2:G:86:ARG:NE	2:G:86:ARG:HA	2.26	0.50
30:G:601:CHL:HED3	33:G:618:LHG:H291	1.93	0.50
16:M:17:ILE:HB	16:M:18:PRO:HD3	1.92	0.50
30:N:301:CHL:HMA2	31:N:315:CLA:C3B	2.41	0.50
31:N:314:CLA:HBA1	31:N:314:CLA:CBD	2.41	0.50
31:R:306:CLA:HBA1	31:R:306:CLA:CHA	2.40	0.50
19:S:87:PRO:HD2	32:S:318:LUT:H23	1.93	0.50
1:7:231:LEU:HB2	32:7:317:LUT:H22	1.93	0.50
31:8:603:CLA:HBC1	30:8:608:CHL:HAC2	1.92	0.50
2:9:108:PRO:HB2	2:9:123:ALA:HA	1.93	0.50
30:q:303:CHL:ND	33:q:320:LHG:HC81	2.26	0.50
31:a:409:CLA:HMA2	45:c:616:DGD:CDB	2.41	0.50
8:d:291:LEU:HB2	8:d:293:LEU:HD23	1.92	0.50
30:n:302:CHL:HED2	33:n:320:LHG:H122	1.92	0.50
31:n:304:CLA:HBC1	30:n:310:CHL:HAC2	1.91	0.50
18:r:71:ARG:HD2	31:r:303:CLA:HED3	1.93	0.50
29:F1:197:ILE:C	29:F1:230:TRP:HE1	2.19	0.50
3:3:94:TRP:CE2	30:3:309:CHL:HED3	2.46	0.50
3:5:116:PHE:CZ	3:5:137:LEU:HD23	2.47	0.50
3:5:151:ILE:CD1	30:5:605:CHL:HAC1	2.41	0.50
3:5:162:ILE:HD11	36:5:618:NEX:C34	2.41	0.50
5:A:210:LEU:HD23	5:A:214:MET:HG3	1.92	0.50
31:B:605:CLA:HMA3	31:B:606:CLA:H3A	1.94	0.50
7:C:36:LYS:HE2	7:C:126:GLU:HG3	1.93	0.50
2:G:47:ALA:HB1	30:G:601:CHL:HBC1	1.93	0.50
31:G:603:CLA:HBB1	31:G:603:CLA:HHC	1.94	0.50
19:S:123:GLY:O	19:S:127:ASN:ND2	2.28	0.50
24:Y:90:ILE:HD13	31:Y:304:CLA:HBA1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:142:ASN:HD22	34:Y:319:LMG:H292	1.76	0.50
30:Y:301:CHL:H121	30:Y:301:CHL:C9	2.41	0.50
1:7:80:ASP:OD1	1:7:80:ASP:N	2.41	0.50
30:7:307:CHL:O2A	36:r:301:NEX:H403	2.11	0.50
31:p:613:CLA:HMB2	31:p:613:CLA:H43	1.93	0.50
5:a:15:ALA:O	5:a:19:GLU:HG2	2.11	0.50
30:n:308:CHL:H2	30:y:601:CHL:H152	1.93	0.50
2:2:178:GLU:HB3	2:2:188:GLY:C	2.36	0.50
34:3:321:LMG:H332	34:3:321:LMG:HC72	1.93	0.50
3:5:69:TRP:HZ3	31:5:602:CLA:HBC2	1.75	0.50
31:5:604:CLA:CHB	36:5:618:NEX:H383	2.41	0.50
43:D:405:BCR:H21C	34:D:409:LMG:H361	1.92	0.50
31:N:310:CLA:H8	32:N:316:LUT:C30	2.42	0.50
17:O:105:THR:HB	17:O:119:PHE:HB3	1.94	0.50
19:S:133:GLY:O	19:S:139:THR:HG22	2.11	0.50
30:0:606:CHL:CBB	30:0:609:CHL:HBC1	2.42	0.50
30:0:608:CHL:HMB1	36:0:618:NEX:H401	1.93	0.50
2:9:208:LYS:HG3	31:9:313:CLA:HED2	1.94	0.50
2:q:166:ALA:HB1	30:q:310:CHL:CHB	2.42	0.50
31:b:609:CLA:HMB1	31:b:609:CLA:HBB1	1.93	0.50
7:c:198:PHE:HD2	7:c:202:PHE:HE2	1.59	0.50
7:c:302:THR:HG21	7:c:339:PHE:HB3	1.92	0.50
7:c:413:TRP:CD1	31:c:604:CLA:HMA2	2.47	0.50
17:o:84:VAL:HG21	17:o:185:ALA:HB1	1.94	0.50
31:y:603:CLA:C3D	30:y:609:CHL:H2	2.42	0.50
1:1:219:GLN:HG2	31:1:613:CLA:C1D	2.41	0.50
2:2:156:LEU:O	2:2:160:LEU:HG	2.11	0.50
3:3:106:GLU:HA	3:3:119:ALA:HB1	1.93	0.50
3:3:196:THR:O	3:3:200:LEU:HB2	2.12	0.50
3:5:233:LEU:HB2	32:5:616:LUT:H22	1.94	0.50
3:5:252:LYS:HD2	3:5:252:LYS:N	2.26	0.50
31:B:614:CLA:H122	34:B:621:LMG:H422	1.94	0.50
31:G:609:CLA:CGA	35:G:614:RRX:H6	2.40	0.50
34:G:622:LMG:H151	31:N:321:CLA:C1	2.41	0.50
31:Y:304:CLA:NB	30:Y:309:CHL:H121	2.26	0.50
4:0:223:GLN:HG2	31:0:613:CLA:C1D	2.41	0.50
3:8:253:SER:HB2	30:9:309:CHL:CAA	2.42	0.50
3:p:246:TRP:HA	3:p:250:ALA:HB2	1.92	0.50
33:c:622:LHG:H241	33:s:320:LHG:HC2	1.93	0.50
33:d:408:LHG:HC62	15:l:16:THR:OG1	2.12	0.50
31:s:311:CLA:H51	32:s:317:LUT:H373	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:y:621:SQD:H81	38:y:621:SQD:O10	2.10	0.50
3:5:40:TRP:O	3:5:45:ARG:HB2	2.12	0.50
3:5:93:ARG:HA	3:5:96:MET:HE3	1.93	0.50
3:5:220:VAL:O	3:5:224:ILE:HG13	2.11	0.50
43:D:405:BCR:H383	34:D:409:LMG:H182	1.93	0.50
31:7:316:CLA:C1C	34:9:301:LMG:H361	2.42	0.50
3:8:142:LEU:O	3:8:144:HIS:N	2.44	0.50
31:9:313:CLA:CHD	33:9:320:LHG:HC62	2.42	0.50
3:p:94:TRP:HB3	32:p:617:LUT:H191	1.94	0.50
3:p:203:LYS:CG	31:p:611:CLA:HED2	2.42	0.50
2:q:143:ASN:HB2	34:q1:101:LMG:H362	1.94	0.50
31:b:611:CLA:HHC	31:b:611:CLA:CBB	2.36	0.50
16:m:17:ILE:HB	16:m:18:PRO:HD3	1.94	0.50
1:1:152:VAL:HG11	30:1:606:CHL:HED2	1.93	0.50
1:1:252:ALA:HA	31:3:301:CLA:CHB	2.42	0.50
2:2:173:GLY:HA2	30:2:607:CHL:CBC	2.42	0.50
2:2:256:LYS:HD3	2:2:257:PHE:CZ	2.47	0.50
3:3:42:GLY:O	3:3:45:ARG:HG3	2.11	0.50
2:4:202:LEU:HD13	2:4:206:LYS:HG3	1.93	0.50
2:4:205:LEU:HB3	31:4:610:CLA:CMA	2.41	0.50
30:4:607:CHL:H42	3:5:245:PHE:HE2	1.75	0.50
30:6:307:CHL:HMC	32:6:318:LUT:H163	1.93	0.50
30:G:601:CHL:H11	30:Y:309:CHL:CHB	2.42	0.50
3:N:39:GLU:O	3:N:46:PRO:HD3	2.12	0.50
3:N:62:GLU:CD	3:N:62:GLU:H	2.20	0.50
3:N:188:LEU:HD12	32:N:316:LUT:H222	1.93	0.50
3:N:224:ILE:HD12	3:N:258:TYR:CE2	2.45	0.50
31:N:305:CLA:H92	30:N:307:CHL:HBA2	1.93	0.50
18:R:131:ARG:NH2	31:R:305:CLA:O1A	2.45	0.50
31:S:303:CLA:H91	32:S:318:LUT:H363	1.93	0.50
31:0:615:CLA:HMC3	30:p:607:CHL:HHB	1.93	0.50
1:7:89:GLU:HG3	1:7:177:VAL:HG22	1.93	0.50
31:8:612:CLA:H151	31:8:613:CLA:C2D	2.41	0.50
31:9:314:CLA:HHC	31:9:314:CLA:CBB	2.35	0.50
3:p:224:ILE:HG22	3:p:249:TYR:CD2	2.46	0.50
31:p:610:CLA:H12	31:p:610:CLA:C4A	2.42	0.50
7:c:51:TRP:CE2	7:c:55:MET:HG3	2.47	0.50
8:d:193:LEU:O	15:l:35:TYR:OH	2.26	0.50
10:f:27:VAL:N	10:f:28:PRO:HD2	2.25	0.50
33:j:102:LHG:H262	21:v:9:LEU:HD11	1.93	0.50
34:k:102:LMG:HC61	28:p1:15:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:x:96:PHE:CZ	27:q1:34:MET:HG3	2.46	0.50
1:1:195:LEU:O	1:1:199:LYS:HG3	2.11	0.50
31:2:604:CLA:NA	36:2:616:NEX:H242	2.27	0.50
3:5:127:GLN:HA	3:5:130:GLN:HG3	1.93	0.50
5:A:312:ARG:NH1	29:F1:83:ASN:OD1	2.44	0.50
30:G:623:CHL:H111	30:Y:309:CHL:H172	1.94	0.50
12:I:28:PRO:HB3	22:W:117:LEU:HD12	1.93	0.50
31:S:305:CLA:H161	31:S:316:CLA:HMB2	1.93	0.50
3:8:233:LEU:O	3:8:237:LEU:HG	2.12	0.50
30:8:608:CHL:HAA1	30:8:608:CHL:HBD	1.94	0.50
30:p:605:CHL:HAA1	30:p:605:CHL:HBD	1.94	0.50
31:q:304:CLA:H61	32:q:318:LUT:C28	2.41	0.50
43:b:618:BCR:H383	38:b:621:SQD:H91	1.94	0.50
45:c:619:DGD:HBT2	45:c:619:DGD:HBF2	1.92	0.50
34:c:620:LMG:H162	34:c:620:LMG:H342	1.94	0.50
34:g:322:LMG:O9	34:g:322:LMG:HC1	2.11	0.50
31:s:311:CLA:O2A	32:s:317:LUT:H26	2.12	0.50
3:3:46:PRO:HB2	30:3:303:CHL:HBC1	1.93	0.49
2:4:47:ALA:HB1	30:4:601:CHL:CBC	2.42	0.49
2:4:147:ILE:HG22	2:4:149:ALA:HB2	1.94	0.49
3:5:180:TYR:HB3	31:5:610:CLA:HED3	1.93	0.49
43:B:618:BCR:H382	43:t:101:BCR:H361	1.94	0.49
26:U:116:ILE:HD12	26:U:184:LEU:HD22	1.94	0.49
2:q:61:TYR:OH	2:q:76:GLY:HA2	2.12	0.49
5:a:267:ASN:ND2	38:a:411:SQD:H3	2.24	0.49
10:f:43:GLN:HB3	29:f1:57:ALA:HB3	1.94	0.49
48:r:302:LMU:H22	31:r:307:CLA:CAB	2.42	0.49
29:f1:216:LYS:HZ2	29:f1:217:ARG:HH12	1.60	0.49
2:2:176:PRO:HB3	36:2:616:NEX:H163	1.93	0.49
31:3:301:CLA:H72	31:3:316:CLA:HAC1	1.93	0.49
2:4:156:LEU:HD22	3:5:246:TRP:CH2	2.47	0.49
3:5:224:ILE:HD11	31:5:615:CLA:HBC1	1.92	0.49
30:5:606:CHL:HAA2	30:5:606:CHL:HBD	1.94	0.49
30:5:607:CHL:CED	4:6:256:ALA:HA	2.43	0.49
10:F:27:VAL:N	10:F:28:PRO:HD2	2.27	0.49
13:J:6:THR:HG23	28:P1:79:TYR:HB3	1.92	0.49
3:N:206:LYS:HE3	33:N:319:LHG:HC62	1.94	0.49
17:O:271:ASP:HB2	17:O:275:LYS:HE3	1.95	0.49
24:Y:193:PRO:HD2	32:Y:315:LUT:H23	1.94	0.49
31:0:611:CLA:H2	31:0:612:CLA:OBD	2.12	0.49
31:g:310:CLA:H52	35:g:315:RRX:H25	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f1:207:TYR:HB2	29:f1:235:VAL:HG21	1.95	0.49
1:1:90:ILE:HG21	31:1:603:CLA:HAA2	1.94	0.49
2:4:125:TRP:CE2	2:4:126:PHE:HD2	2.30	0.49
3:5:188:LEU:HB2	3:5:190:LEU:HD13	1.94	0.49
3:5:200:LEU:HB3	31:5:610:CLA:HMA1	1.94	0.49
4:6:148:GLN:HB2	30:6:306:CHL:CBB	2.42	0.49
4:6:192:LEU:HD12	31:6:311:CLA:O2A	2.13	0.49
30:6:309:CHL:HAA1	30:6:309:CHL:HBD	1.93	0.49
5:A:43:THR:O	5:A:47:VAL:HG12	2.12	0.49
5:A:283:ILE:HA	5:A:286:THR:HG22	1.94	0.49
30:G:601:CHL:H192	30:G:623:CHL:CHB	2.42	0.49
31:7:311:CLA:H8	32:7:317:LUT:C30	2.42	0.49
2:9:214:ARG:HA	2:9:217:MET:HE2	1.93	0.49
2:9:257:PHE:HB2	34:9:301:LMG:H152	1.94	0.49
30:9:307:CHL:HBD	30:9:307:CHL:HAA1	1.94	0.49
3:p:72:ALA:HA	2:q:90:ILE:HD11	1.94	0.49
31:q:313:CLA:HBD	31:q:314:CLA:OBD	2.12	0.49
5:a:223:LEU:HD12	8:d:139:ARG:NH1	2.28	0.49
6:b:54:PRO:HD2	6:b:57:ARG:HB2	1.92	0.49
34:d:409:LMG:H112	13:j:30:PHE:HB3	1.92	0.49
31:g:312:CLA:HMC3	35:g:315:RRX:H44	1.93	0.49
15:l:27:VAL:HG21	33:l:101:LHG:H182	1.93	0.49
34:w:205:LMG:H312	34:w:205:LMG:O10	2.12	0.49
1:1:166:ASN:C	18:R:38:ARG:HB3	2.38	0.49
2:2:138:LEU:HD13	30:2:606:CHL:HMD3	1.94	0.49
30:3:307:CHL:HAA1	30:3:307:CHL:HBD	1.93	0.49
34:3:321:LMG:HC71	34:3:321:LMG:O10	2.12	0.49
2:4:113:ASN:C	2:4:113:ASN:HD22	2.21	0.49
3:5:126:ALA:HA	3:5:129:PHE:HD2	1.76	0.49
31:6:314:CLA:NC	31:6:314:CLA:H51	2.27	0.49
2:G:257:PHE:CD2	34:G:621:LMG:H162	2.47	0.49
3:N:104:THR:HB	3:N:105:PRO:HD3	1.95	0.49
31:S:305:CLA:HMA3	30:S:307:CHL:C4C	2.42	0.49
30:8:601:CHL:H71	2:9:160:LEU:HD23	1.95	0.49
30:8:605:CHL:H141	30:8:605:CHL:H18	1.94	0.49
30:8:606:CHL:OMC	32:8:616:LUT:H163	2.13	0.49
2:9:90:ILE:HG21	31:9:305:CLA:HAA2	1.93	0.49
3:p:97:LEU:HB3	31:p:604:CLA:HAB	1.93	0.49
5:a:162:PRO:HB3	5:a:168:PHE:HA	1.94	0.49
30:n:307:CHL:HMB2	30:n:310:CHL:HMC	1.94	0.49
48:r:302:LMU:H82	31:r:307:CLA:C1B	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:91:HIS:HE1	31:3:305:CLA:C4D	2.25	0.49
2:4:260:LEU:HB2	34:4:620:LMG:O5	2.12	0.49
3:5:100:LEU:HA	3:5:103:VAL:HG22	1.95	0.49
3:5:159:MET:HG3	30:5:609:CHL:CMC	2.42	0.49
31:5:610:CLA:C4D	32:5:616:LUT:H382	2.42	0.49
31:A:406:CLA:H203	42:A:408:PHO:H91	1.93	0.49
8:D:16:ASP:OD1	34:D:410:LMG:O3	2.30	0.49
3:N:103:VAL:HB	3:N:230:ILE:HD11	1.95	0.49
17:O:257:GLU:HG2	17:O:289:GLN:HG2	1.95	0.49
30:8:601:CHL:HAA2	30:8:601:CHL:HBD	1.95	0.49
31:8:603:CLA:HBC2	30:8:608:CHL:HHD	1.94	0.49
31:8:612:CLA:H172	31:8:613:CLA:C4D	2.42	0.49
3:p:124:ALA:O	3:p:127:GLN:HG2	2.12	0.49
42:a:408:PHO:H202	44:d:407:PL9:H453	1.95	0.49
8:d:41:ALA:HB1	42:d:402:PHO:H42	1.94	0.49
3:n:142:LEU:O	3:n:144:HIS:N	2.44	0.49
30:n:301:CHL:HMA3	31:n:316:CLA:C3B	2.42	0.49
31:n:305:CLA:H201	31:s:305:CLA:HBC1	1.94	0.49
36:y:618:NEX:H161	36:y:618:NEX:H193	1.93	0.49
34:Q1:101:LMG:HC1	34:Q1:101:LMG:C10	2.42	0.49
2:2:72:TRP:H	31:2:602:CLA:CAD	2.26	0.49
3:3:143:ILE:HG22	30:3:307:CHL:C3D	2.42	0.49
30:5:607:CHL:HBA1	30:5:607:CHL:CHA	2.42	0.49
31:A:406:CLA:H172	44:D:406:PL9:H512	1.94	0.49
7:C:264:LEU:HD21	31:C:608:CLA:CAB	2.42	0.49
8:D:27:PHE:HB2	9:E:7:GLU:HG3	1.93	0.49
3:N:106:GLU:O	3:N:110:ARG:HG2	2.12	0.49
31:Y:304:CLA:H2	31:Y:304:CLA:CMA	2.43	0.49
4:0:249:SER:H	3:p:129:PHE:HE1	1.59	0.49
30:7:308:CHL:HED1	2:9:258:LEU:CD1	2.43	0.49
30:7:310:CHL:HAA1	30:7:310:CHL:HBD	1.95	0.49
2:9:94:HIS:CD2	32:9:318:LUT:H15	2.47	0.49
2:q:177:VAL:HG23	30:q:310:CHL:HBB1	1.94	0.49
5:a:341:LEU:HB3	5:a:343:LEU:HD13	1.93	0.49
7:c:41:HIS:CD2	31:c:609:CLA:NA	2.81	0.49
7:c:364:ASP:HB2	7:c:367:LYS:HB2	1.95	0.49
11:h:76:ASP:N	11:h:76:ASP:OD1	2.40	0.49
3:n:233:LEU:O	3:n:237:LEU:HG	2.12	0.49
30:n:306:CHL:H18	30:n:306:CHL:H141	1.94	0.49
30:2:607:CHL:C2	35:2:614:RRX:H12	2.42	0.49
31:2:610:CLA:HBA1	38:6:301:SQD:H1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:162:ILE:HD11	36:3:319:NEX:C35	2.42	0.49
2:4:147:ILE:HA	30:4:605:CHL:C4D	2.43	0.49
34:4:620:LMG:H112	34:4:621:LMG:C12	2.43	0.49
3:5:221:GLN:C	3:5:225:THR:HG22	2.37	0.49
31:5:613:CLA:C2	31:5:613:CLA:HBA2	2.42	0.49
31:6:303:CLA:HED2	31:6:303:CLA:H2A	1.95	0.49
31:B:608:CLA:HBB1	31:B:608:CLA:HMB3	1.94	0.49
33:D:408:LHG:HC91	15:L:20:TRP:HZ2	1.78	0.49
30:G:623:CHL:H171	31:Y:304:CLA:CAC	2.43	0.49
30:N:302:CHL:HAA2	30:N:302:CHL:HBD	1.93	0.49
31:Y:312:CLA:HHC	31:Y:312:CLA:HBB1	1.94	0.49
4:0:228:GLY:HA3	2:q:261:PRO:HG3	1.93	0.49
1:7:134:TYR:HB3	1:7:140:LEU:HD12	1.94	0.49
3:8:251:PRO:HB3	2:9:133:PHE:CD2	2.48	0.49
2:9:146:LEU:HA	30:9:307:CHL:HED3	1.95	0.49
3:p:162:ILE:HD11	36:p:618:NEX:C34	2.42	0.49
2:q:130:ALA:CB	30:q:309:CHL:HED1	2.42	0.49
5:a:160:ILE:HG12	7:c:419:PHE:CZ	2.48	0.49
5:a:283:ILE:HG13	42:a:408:PHO:HBC3	1.94	0.49
2:g:257:PHE:CE1	31:n:316:CLA:H43	2.46	0.49
3:n:123:LYS:HA	30:n:308:CHL:HED3	1.94	0.49
18:r:183:ILE:HG22	48:r:302:LMU:H3'	1.95	0.49
48:r:302:LMU:H52	31:r:307:CLA:CAB	2.43	0.49
31:1:602:CLA:H43	31:1:602:CLA:HMB2	1.94	0.49
30:1:619:CHL:HHC	30:1:619:CHL:HBB1	1.95	0.49
2:2:125:TRP:CH2	2:2:224:PHE:HD1	2.30	0.49
2:2:182:ASP:OD2	2:2:185:TYR:HB2	2.12	0.49
30:4:605:CHL:HBD	30:4:605:CHL:HAA1	1.95	0.49
31:6:303:CLA:H52	32:6:318:LUT:H30	1.94	0.49
38:A:413:SQD:O9	49:A:501:HOH:O	2.20	0.49
6:B:348:ASP:OD1	6:B:349:LYS:N	2.46	0.49
6:B:469:HIS:HE1	31:B:611:CLA:NA	2.07	0.49
31:C:608:CLA:HBC3	31:C:610:CLA:H71	1.93	0.49
9:E:19:TYR:HE2	47:E:101:HEM:C3D	2.30	0.49
19:S:246:PHE:CE2	32:S:318:LUT:H10	2.46	0.49
31:0:614:CLA:CBA	34:p:620:LMG:H111	2.40	0.49
3:8:58:TYR:CD2	3:8:59:LEU:HD13	2.48	0.49
31:8:604:CLA:HMA3	30:8:606:CHL:C3C	2.43	0.49
2:9:205:LEU:HD13	31:9:312:CLA:H12	1.95	0.49
8:d:55:VAL:HG21	8:d:110:LEU:HD22	1.93	0.49
31:g:313:CLA:H201	24:y:156:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:o:204:ASP:OD1	17:o:208:ARG:N	2.46	0.49
2:2:130:ALA:H	30:3:302:CHL:CED	2.24	0.49
2:4:133:PHE:HZ	3:5:246:TRP:HB3	1.78	0.49
3:5:46:PRO:HB2	3:5:67:TYR:CE2	2.48	0.49
30:5:607:CHL:HBA1	30:5:607:CHL:CBD	2.43	0.49
6:B:33:TRP:HD1	43:t:101:BCR:H332	1.78	0.49
30:G:605:CHL:HBA1	30:G:605:CHL:CHA	2.42	0.49
3:N:224:ILE:HG23	3:N:258:TYR:CE2	2.47	0.49
17:O:125:MET:HE3	17:O:163:GLN:HB2	1.94	0.49
19:S:113:LEU:HB3	31:S:305:CLA:HAB	1.95	0.49
24:Y:95:ALA:HB1	24:Y:214:GLY:HA3	1.95	0.49
3:8:71:THR:CB	30:9:311:CHL:HAA2	2.43	0.49
31:8:603:CLA:CAD	30:8:608:CHL:H11	2.43	0.49
3:n:58:TYR:CD2	3:n:59:LEU:HD13	2.47	0.49
30:n:306:CHL:H201	31:s:313:CLA:HMC2	1.94	0.49
19:s:246:PHE:CZ	32:s:318:LUT:H10	2.48	0.49
31:s:303:CLA:H72	32:s:318:LUT:H30	1.94	0.49
22:w:73:ILE:HG13	34:w:204:LMG:HC61	1.93	0.49
22:w:84:ALA:HA	34:w:205:LMG:H341	1.94	0.49
1:1:198:LEU:HB3	31:1:610:CLA:HMA2	1.95	0.49
34:2:621:LMG:O7	34:2:621:LMG:HC1	2.13	0.49
3:3:104:THR:OG1	31:3:306:CLA:HBC3	2.13	0.49
3:3:118:GLU:CG	3:3:124:ALA:HA	2.42	0.49
31:4:610:CLA:HBA1	35:4:615:RRX:H7	1.95	0.49
3:5:171:PRO:HB3	36:5:618:NEX:H181	1.95	0.49
30:5:607:CHL:H2A	30:5:607:CHL:O2D	2.13	0.49
31:A:406:CLA:H141	31:A:406:CLA:H161	1.65	0.49
7:C:270:MET:HG2	31:C:601:CLA:H72	1.95	0.49
7:C:304:THR:HG21	7:C:384:MET:HE1	1.95	0.49
45:C:618:DGD:HBF1	34:D:409:LMG:H191	1.95	0.49
31:G:603:CLA:C2	31:G:603:CLA:HED2	2.42	0.49
31:R:305:CLA:HBC1	31:R:311:CLA:CBC	2.43	0.49
4:0:144:LEU:O	4:0:146:HIS:N	2.46	0.49
3:p:219:GLY:O	3:p:223:LEU:HG	2.13	0.49
30:q:309:CHL:H102	30:q:309:CHL:NB	2.28	0.49
10:f:12:TYR:OH	28:p1:71:THR:O	2.28	0.49
2:g:146:LEU:O	2:g:148:HIS:N	2.46	0.49
31:n:311:CLA:H8	32:n:317:LUT:C30	2.42	0.49
1:1:132:ILE:HD12	30:1:606:CHL:HMD3	1.95	0.48
30:1:605:CHL:CHA	34:6:321:LMG:H341	2.43	0.48
30:1:608:CHL:HBD	30:1:608:CHL:HAA1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:603:CLA:H72	31:3:305:CLA:H92	1.95	0.48
2:4:90:ILE:HG21	31:4:603:CLA:HAA2	1.94	0.48
2:4:175:GLY:N	2:4:176:PRO:HD2	2.27	0.48
31:5:603:CLA:H2	31:5:603:CLA:HMA3	1.95	0.48
44:A:416:PL9:H222	42:D:401:PHO:HMA2	1.95	0.48
6:B:29:LEU:HD11	43:B:617:BCR:H19C	1.95	0.48
6:B:487:ASP:O	6:B:491:GLU:HG3	2.12	0.48
7:C:194:PRO:HG3	31:Y:314:CLA:HMB1	1.94	0.48
8:D:223:PHE:HE2	8:D:242:GLU:HG3	1.77	0.48
43:D:405:BCR:H272	34:D:409:LMG:H241	1.95	0.48
2:G:258:LEU:HD23	2:G:259:PRO:HD2	1.94	0.48
34:G:622:LMG:H171	31:N:315:CLA:H92	1.95	0.48
17:O:162:VAL:HG23	17:O:170:VAL:HG13	1.95	0.48
4:0:199:LEU:HD11	4:0:203:LYS:HZ2	1.78	0.48
30:0:605:CHL:HAA1	31:r:315:CLA:HMD3	1.95	0.48
3:p:206:LYS:HE3	33:p:619:LHG:O8	2.12	0.48
31:c:613:CLA:H72	33:c:622:LHG:H281	1.95	0.48
2:g:77:LEU:HD13	31:g:303:CLA:H42	1.94	0.48
11:h:62:VAL:O	11:h:66:GLU:HG2	2.12	0.48
18:r:186:LEU:HD13	30:r:308:CHL:HMD1	1.94	0.48
19:s:236:ILE:HD12	19:s:237:LYS:HG3	1.95	0.48
34:w:205:LMG:H292	34:w:205:LMG:HC5	1.95	0.48
29:F1:170:ASP:HB2	29:F1:176:TYR:CE1	2.46	0.48
29:F1:200:THR:HB	29:F1:235:VAL:HG11	1.95	0.48
31:4:610:CLA:H72	35:4:615:RRX:C21	2.42	0.48
3:5:107:LEU:HD13	3:5:110:ARG:HD3	1.95	0.48
3:5:218:PHE:HZ	32:5:616:LUT:H8	1.77	0.48
31:5:614:CLA:CED	31:5:614:CLA:H2A	2.44	0.48
4:6:125:LYS:HA	30:6:308:CHL:HED2	1.94	0.48
5:A:308:ASP:OD1	5:A:312:ARG:N	2.47	0.48
31:A:409:CLA:H41	31:A:409:CLA:H62	1.55	0.48
6:B:216:HIS:HE1	31:B:609:CLA:CHA	2.26	0.48
8:D:239:GLN:HA	28:P1:56:TYR:CZ	2.48	0.48
31:G:612:CLA:CMA	35:G:614:RRX:H4	2.42	0.48
31:G:612:CLA:H112	37:G:620:XAT:H34	1.94	0.48
12:I:6:ILE:HG21	34:I:101:LMG:HC91	1.94	0.48
17:O:176:VAL:O	17:O:179:LEU:HB2	2.12	0.48
19:S:37:GLY:H	34:S:321:LMG:HC61	1.77	0.48
3:p:197:PHE:HE1	31:p:610:CLA:H2A	1.78	0.48
2:q:85:ALA:HA	2:q:88:ARG:NH1	2.28	0.48
30:q:309:CHL:H101	30:q:309:CHL:H61	1.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:121:LEU:HD23	31:a:409:CLA:HMB2	1.95	0.48
5:a:278:TRP:HB3	5:a:279:PRO:HD3	1.94	0.48
6:b:99:ALA:HB1	31:b:607:CLA:H62	1.94	0.48
6:b:156:PHE:CZ	33:b:628:LHG:H282	2.47	0.48
31:c:604:CLA:HAC2	14:k:26:PRO:O	2.13	0.48
8:d:91:PHE:CE1	31:d:405:CLA:HAA1	2.48	0.48
2:g:186:PRO:HG3	30:g:308:CHL:HBC2	1.95	0.48
24:y:193:PRO:HD2	32:y:616:LUT:H23	1.95	0.48
3:3:205:LEU:O	3:3:209:ARG:N	2.31	0.48
3:3:215:MET:HA	3:3:218:PHE:CD2	2.49	0.48
3:3:245:PHE:O	3:3:246:TRP:HB2	2.13	0.48
3:5:117:GLY:HA3	3:5:130:GLN:HE22	1.78	0.48
3:5:125:GLY:O	3:5:128:ILE:HG22	2.12	0.48
31:5:602:CLA:H92	31:5:602:CLA:H61	1.65	0.48
4:6:235:LEU:HB2	32:6:317:LUT:H22	1.94	0.48
30:6:307:CHL:H3A	36:6:319:NEX:C31	2.43	0.48
7:C:287:SER:OG	7:C:296:GLU:OE1	2.31	0.48
9:E:7:GLU:HB2	10:F:18:ARG:NH2	2.28	0.48
34:G:621:LMG:H411	34:G:621:LMG:H372	1.95	0.48
30:N:309:CHL:HAA1	30:N:309:CHL:HBD	1.96	0.48
18:R:165:GLN:HG2	37:R:318:XAT:H21	1.95	0.48
30:7:321:CHL:HED3	3:8:123:LYS:HA	1.94	0.48
3:p:221:GLN:HE22	32:p:616:LUT:H41	1.79	0.48
31:p:602:CLA:HED2	31:p:602:CLA:H2A	1.95	0.48
2:q:78:SER:OG	31:q:304:CLA:HAA2	2.12	0.48
31:b:613:CLA:HBB1	31:b:613:CLA:CMB	2.43	0.48
7:c:142:LYS:HE3	7:c:254:TRP:CD1	2.49	0.48
7:c:240:ILE:HG21	34:c:620:LMG:H121	1.94	0.48
7:c:334:THR:HG21	17:o:67:GLY:HA2	1.95	0.48
7:c:351:GLY:O	7:c:355:GLU:HG2	2.14	0.48
33:g:319:LHG:H142	33:g:319:LHG:H241	1.95	0.48
24:y:145:LEU:O	24:y:147:HIS:N	2.45	0.48
3:5:236:HIS:CG	31:5:613:CLA:HAA2	2.49	0.48
31:6:311:CLA:H51	32:6:317:LUT:C28	2.44	0.48
5:A:259:ILE:HG22	5:A:260:PHE:CD2	2.49	0.48
2:G:130:ALA:HA	2:G:133:PHE:CD1	2.48	0.48
2:G:259:PRO:HA	34:G:621:LMG:HC4	1.95	0.48
31:G:609:CLA:HBA1	35:G:614:RRX:C40	2.42	0.48
31:G:610:CLA:HAA2	38:G:617:SQD:C44	2.40	0.48
31:N:311:CLA:HBB1	31:N:311:CLA:CHC	2.19	0.48
31:S:314:CLA:H141	31:S:314:CLA:H202	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:110:ARG:NH2	3:p:230:ILE:HG21	2.29	0.48
6:b:464:PHE:HD2	31:b:612:CLA:HAC2	1.78	0.48
34:g:322:LMG:H322	31:y:615:CLA:ND	2.28	0.48
30:n:301:CHL:HBD	30:n:301:CHL:HAA1	1.95	0.48
24:y:100:LEU:HB3	31:y:604:CLA:HAB	1.95	0.48
34:q1:101:LMG:HC8	34:q1:101:LMG:HC1	1.50	0.48
1:1:117:ILE:CD1	1:1:122:ALA:HA	2.43	0.48
30:2:606:CHL:HBB1	30:2:608:CHL:HBC1	1.94	0.48
31:3:301:CLA:H72	31:3:316:CLA:CAC	2.43	0.48
45:C:620:DGD:HB32	31:Y:311:CLA:C1B	2.43	0.48
3:N:165:TYR:OH	19:S:39:TRP:O	2.26	0.48
18:R:223:ALA:HB1	18:R:230:THR:HG23	1.95	0.48
36:R:319:NEX:H181	36:R:319:NEX:H193	1.95	0.48
19:S:264:TRP:HB2	32:S:317:LUT:H22	1.96	0.48
31:7:303:CLA:H61	32:7:318:LUT:H28	1.95	0.48
3:8:70:ASP:OD2	3:8:75:SER:OG	2.30	0.48
5:a:118:HIS:CE1	31:a:409:CLA:C4D	2.96	0.48
5:a:140:ARG:HH22	33:a:415:LHG:HC41	1.78	0.48
6:b:224:ARG:HG2	11:h:44:TRP:CE2	2.49	0.48
7:c:306:LEU:HD12	7:c:328:TYR:HB3	1.95	0.48
30:g:307:CHL:HBB2	30:n:301:CHL:HBB1	1.95	0.48
1:1:89:GLU:HG3	1:1:177:VAL:HG22	1.95	0.48
1:1:131:GLY:HA3	1:1:144:LYS:HG2	1.96	0.48
1:1:184:ASP:HA	32:1:615:LUT:H24	1.95	0.48
2:2:72:TRP:CZ3	30:2:601:CHL:HBD	2.49	0.48
2:2:125:TRP:O	2:2:126:PHE:C	2.56	0.48
3:3:252:LYS:O	3:3:258:TYR:HB3	2.13	0.48
31:3:312:CLA:C3C	33:3:320:LHG:HC62	2.43	0.48
2:4:149:ALA:HA	30:4:605:CHL:C1C	2.44	0.48
3:5:41:TYR:CZ	3:5:202:VAL:HG23	2.48	0.48
33:5:619:LHG:O10	33:5:619:LHG:H291	2.13	0.48
30:6:306:CHL:HAA1	30:6:306:CHL:HBD	1.95	0.48
31:6:314:CLA:HMB1	31:6:315:CLA:CBC	2.43	0.48
34:6:321:LMG:HC71	18:R:273:PHE:CG	2.49	0.48
6:B:204:ALA:HB3	31:B:602:CLA:HAB	1.95	0.48
33:B:624:LHG:H321	33:B:624:LHG:H291	1.56	0.48
31:G:603:CLA:ND	30:G:608:CHL:H8	2.28	0.48
3:N:200:LEU:HD12	3:N:203:LYS:HD2	1.94	0.48
18:R:223:ALA:HB3	31:R:312:CLA:HAA2	1.94	0.48
31:R:306:CLA:C1C	36:R:319:NEX:H222	2.44	0.48
19:S:167:ALA:O	19:S:171:ILE:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:15:ILE:O	43:V:101:BCR:H14C	2.14	0.48
24:Y:252:TYR:CD1	31:Y:314:CLA:HED2	2.48	0.48
31:Y:305:CLA:HMA3	30:Y:307:CHL:C3C	2.44	0.48
31:0:610:CLA:H91	31:0:610:CLA:H111	1.60	0.48
3:8:214:SER:HB2	32:8:615:LUT:H8	1.95	0.48
2:9:111:LEU:HB2	2:9:119:PHE:HE1	1.79	0.48
5:a:304:GLN:HG2	5:a:313:VAL:HG21	1.94	0.48
31:a:409:CLA:H42	12:i:9:TYR:CE2	2.48	0.48
7:c:155:VAL:HG12	34:c:620:LMG:H371	1.95	0.48
8:d:157:PHE:CE2	8:d:171:PRO:HG2	2.49	0.48
30:g:302:CHL:H121	30:g:302:CHL:H93	1.95	0.48
33:g:319:LHG:H282	37:g:321:XAT:C32	2.43	0.48
34:g:322:LMG:H361	31:y:615:CLA:C1C	2.43	0.48
31:n:315:CLA:HMB1	31:n:315:CLA:HBB1	1.96	0.48
31:s:303:CLA:C6	32:s:318:LUT:H28	2.42	0.48
28:P1:53:ALA:O	28:P1:54:ASN:HB3	2.13	0.48
29:f1:136:PHE:CE1	29:f1:181:VAL:HG11	2.49	0.48
1:1:157:MET:HB3	30:1:609:CHL:CBB	2.43	0.48
1:1:198:LEU:CB	31:1:610:CLA:HMA2	2.44	0.48
31:2:602:CLA:H62	32:2:615:LUT:H28	1.96	0.48
3:3:246:TRP:HA	3:3:250:ALA:HB2	1.95	0.48
30:4:606:CHL:CBB	30:4:609:CHL:HBC1	2.43	0.48
3:5:61:GLY:HA2	3:5:66:ASP:HB3	1.94	0.48
3:5:253:SER:HA	3:5:258:TYR:HE1	1.79	0.48
6:B:149:LEU:HD11	34:B:622:LMG:H342	1.95	0.48
31:C:608:CLA:H161	45:C:618:DGD:HAH1	1.95	0.48
45:C:620:DGD:HA22	45:C:620:DGD:HG12	1.58	0.48
31:N:305:CLA:H112	31:S:306:CLA:CHB	2.43	0.48
36:R:301:NEX:H192	36:R:301:NEX:H183	1.95	0.48
31:R:303:CLA:HBD	33:R:320:LHG:HC82	1.96	0.48
31:p:615:CLA:CGA	34:q:302:LMG:HC2	2.44	0.48
31:b:612:CLA:H2	31:b:612:CLA:H61	1.62	0.48
7:c:225:HIS:HE1	31:c:601:CLA:NA	2.12	0.48
7:c:285:TYR:O	7:c:411:ARG:NH2	2.43	0.48
31:c:610:CLA:H161	31:c:610:CLA:H202	1.69	0.48
30:n:307:CHL:OMC	32:n:318:LUT:H163	2.13	0.48
31:s:303:CLA:H12	31:s:303:CLA:HBA2	1.56	0.48
30:y:607:CHL:HAA2	30:y:607:CHL:HBD	1.96	0.48
29:f1:196:LEU:HB3	29:f1:230:TRP:CG	2.49	0.48
30:1:601:CHL:CHD	33:1:617:LHG:HC82	2.44	0.48
2:4:119:PHE:CE2	2:4:141:LEU:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:607:CHL:CHD	3:5:246:TRP:HZ3	2.27	0.48
6:B:103:LEU:HD21	31:B:605:CLA:HMC3	1.95	0.48
31:B:603:CLA:H41	31:B:603:CLA:H61	1.46	0.48
38:B:620:SQD:H2	38:B:620:SQD:H441	1.46	0.48
38:B:623:SQD:H91	8:D:130:PHE:HB3	1.96	0.48
31:N:314:CLA:HBC1	32:N:316:LUT:C16	2.43	0.48
17:O:184:ASN:H	17:O:184:ASN:HD22	1.62	0.48
30:R:310:CHL:CBB	38:R:322:SQD:H91	2.43	0.48
30:S:302:CHL:HBB1	30:S:302:CHL:HMB3	1.96	0.48
1:7:165:VAL:CG1	2:9:57:SER:HB3	2.40	0.48
31:8:612:CLA:C1A	31:8:612:CLA:CGA	2.92	0.48
3:p:41:TYR:OH	3:p:64:PRO:HB3	2.13	0.48
34:q:302:LMG:H152	34:q:302:LMG:O9	2.13	0.48
6:b:6:TYR:O	31:b:612:CLA:HBD	2.14	0.48
6:b:216:HIS:HE1	31:b:610:CLA:CHA	2.26	0.48
43:d:406:BCR:H363	10:f:32:PHE:HB3	1.96	0.48
9:e:19:TYR:HE2	47:e:102:HEM:C3D	2.32	0.48
3:n:214:SER:HB2	32:n:317:LUT:H8	1.95	0.48
31:n:314:CLA:CGA	31:n:314:CLA:C1A	2.92	0.48
18:r:53:TRP:CE3	18:r:54:LEU:HD13	2.49	0.48
19:s:141:ALA:H	30:s:308:CHL:HED1	1.78	0.48
29:f1:66:PHE:HZ	29:f1:225:GLU:HA	1.78	0.48
29:f1:165:VAL:HG12	29:f1:179:TYR:HD1	1.79	0.48
31:3:315:CLA:HBA2	31:3:315:CLA:C2	2.43	0.48
2:4:207:VAL:C	2:4:209:GLU:N	2.71	0.48
3:5:200:LEU:HD23	3:5:203:LYS:CD	2.44	0.48
4:6:193:ALA:HB2	31:6:311:CLA:HAA2	1.96	0.48
9:E:27:ILE:HB	9:E:28:PRO:HD3	1.94	0.48
1:7:56:ASN:CG	3:8:168:ASN:OD1	2.57	0.48
31:p:615:CLA:HHC	31:p:615:CLA:HBB1	1.96	0.48
2:q:103:LEU:HD12	35:q:317:RRX:H30	1.95	0.48
2:q:208:LYS:HD3	31:q:314:CLA:HAA2	1.95	0.48
7:c:129:GLU:HA	7:c:136:GLY:HA3	1.96	0.48
45:c:617:DGD:HB61	45:c:617:DGD:HB92	1.71	0.48
8:d:153:PHE:CE1	42:d:402:PHO:H91	2.49	0.48
2:g:241:HIS:HB2	31:g:313:CLA:HAA2	1.95	0.48
31:n:314:CLA:H172	31:n:315:CLA:C4D	2.44	0.48
19:s:112:MET:HG3	19:s:239:GLY:HA2	1.94	0.48
30:1:608:CHL:O1A	31:1:610:CLA:HMD1	2.14	0.48
2:2:50:LEU:HB2	2:2:54:SER:HB3	1.96	0.48
31:3:306:CLA:C1C	36:3:319:NEX:H222	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:97:TRP:CD1	30:4:609:CHL:HMD2	2.49	0.48
3:5:104:THR:O	3:5:108:LEU:HG	2.14	0.48
3:5:199:GLU:HG3	3:5:200:LEU:N	2.29	0.48
6:B:466:HIS:HE1	31:B:608:CLA:C4D	2.27	0.48
2:G:238:LEU:HD21	34:G:619:LMG:H161	1.96	0.48
30:G:601:CHL:H62	30:G:601:CHL:H41	1.64	0.48
3:N:245:PHE:HB3	31:N:313:CLA:C1	2.42	0.48
31:R:306:CLA:CHC	36:R:319:NEX:H222	2.44	0.48
31:8:614:CLA:HED2	34:9:302:LMG:O4	2.14	0.48
2:9:72:TRP:O	32:9:318:LUT:H24	2.13	0.48
2:9:85:ALA:HA	2:9:88:ARG:NH1	2.29	0.48
2:9:222:GLY:O	2:9:226:GLN:HG3	2.13	0.48
31:9:305:CLA:H2	31:9:305:CLA:H61	1.68	0.48
32:p:617:LUT:H35	32:p:617:LUT:H401	1.40	0.48
2:q:208:LYS:HD3	31:q:314:CLA:HBD	1.96	0.48
47:e:102:HEM:HMC2	10:f:30:VAL:HG21	1.95	0.48
30:n:302:CHL:HAA2	30:n:302:CHL:HBD	1.95	0.48
31:y:610:CLA:H8	32:y:616:LUT:C30	2.44	0.48
31:2:604:CLA:O1A	31:2:604:CLA:H3A	2.14	0.47
31:2:609:CLA:H71	31:2:611:CLA:HMA2	1.96	0.47
31:3:314:CLA:H62	31:3:314:CLA:NC	2.28	0.47
31:4:603:CLA:HED3	32:5:617:LUT:H372	1.96	0.47
4:6:173:PRO:HB2	30:6:309:CHL:HBB2	1.96	0.47
31:B:601:CLA:C2B	34:X:202:LMG:H342	2.44	0.47
18:R:78:LEU:HD13	31:R:304:CLA:H42	1.96	0.47
19:S:191:GLY:HA3	31:S:316:CLA:C2D	2.44	0.47
31:Y:314:CLA:H2	31:Y:314:CLA:H62	1.63	0.47
31:0:614:CLA:H2	31:0:614:CLA:NA	2.29	0.47
3:8:191:ALA:HB2	31:8:609:CLA:HAA2	1.96	0.47
31:8:604:CLA:CHA	31:8:604:CLA:HBA1	2.41	0.47
30:9:303:CHL:HHD	33:9:320:LHG:HC41	1.96	0.47
31:9:304:CLA:H62	31:9:304:CLA:H41	1.67	0.47
31:9:312:CLA:H72	31:9:314:CLA:CMA	2.36	0.47
3:p:47:GLN:HB3	3:p:53:SER:OG	2.14	0.47
8:d:200:GLY:HA3	8:d:282:SER:OG	2.13	0.47
9:e:13:ILE:HD13	47:e:102:HEM:HBD1	1.96	0.47
31:n:316:CLA:HAC1	31:y:615:CLA:H62	1.96	0.47
17:o:106:VAL:HB	17:o:164:LEU:HD21	1.95	0.47
17:o:208:ARG:HD2	17:o:233:ASN:HA	1.96	0.47
3:3:139:ASN:HB3	3:3:142:LEU:HG	1.96	0.47
3:3:171:PRO:HG2	30:3:309:CHL:HBB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:301:CLA:H41	31:3:301:CLA:H93	1.96	0.47
2:4:220:MET:SD	2:4:223:PHE:HD2	2.37	0.47
34:4:620:LMG:C38	3:5:223:LEU:HD11	2.38	0.47
3:5:96:MET:HE3	31:5:610:CLA:HMC2	1.95	0.47
31:5:603:CLA:HED3	32:6:318:LUT:H372	1.95	0.47
38:B:620:SQD:H361	20:t:19:PHE:HE1	1.80	0.47
12:I:2:LEU:HD21	22:W:78:ASP:OD2	2.14	0.47
3:N:109:GLN:HE22	3:N:115:ASN:ND2	2.11	0.47
3:N:185:PHE:O	32:N:316:LUT:H24	2.14	0.47
4:0:255:LEU:CB	30:p:607:CHL:HBA2	2.44	0.47
2:9:226:GLN:HG2	31:9:315:CLA:C1D	2.43	0.47
3:p:158:LEU:HD11	30:p:606:CHL:HED3	1.95	0.47
31:c:606:CLA:H111	31:c:606:CLA:H152	1.54	0.47
31:n:303:CLA:H61	32:n:318:LUT:H28	1.95	0.47
31:n:316:CLA:C1	34:n:322:LMG:HC92	2.44	0.47
31:1:603:CLA:HAC1	30:1:607:CHL:CBB	2.40	0.47
2:2:109:GLU:OE2	2:2:235:LEU:HB2	2.14	0.47
30:3:303:CHL:HAC2	33:3:320:LHG:HC41	1.96	0.47
30:4:601:CHL:HED3	31:4:602:CLA:HBC1	1.96	0.47
31:4:602:CLA:H102	31:4:603:CLA:HMB1	1.95	0.47
3:5:109:GLN:HA	3:5:114:ALA:HB3	1.97	0.47
4:6:178:VAL:HG23	4:6:179:ASP:H	1.80	0.47
6:B:26:HIS:CE1	31:B:612:CLA:HMA2	2.49	0.47
7:C:151:ILE:HG23	34:C:621:LMG:H342	1.95	0.47
31:C:613:CLA:H72	33:C:623:LHG:H291	1.95	0.47
8:D:239:GLN:HG3	8:D:241:GLU:CD	2.39	0.47
18:R:38:ARG:HD2	18:R:38:ARG:N	2.29	0.47
34:Y:319:LMG:H321	18:r:181:PHE:CE1	2.49	0.47
1:7:223:THR:HG21	31:7:314:CLA:O1D	2.15	0.47
31:9:304:CLA:H2	32:9:318:LUT:H26	1.96	0.47
3:p:203:LYS:HD3	31:p:612:CLA:HAA2	1.96	0.47
2:q:99:MET:HG3	2:q:213:GLY:HA2	1.96	0.47
31:a:407:CLA:HMA2	44:d:407:PL9:H402	1.96	0.47
6:b:29:LEU:HD13	31:b:614:CLA:HMD2	1.96	0.47
6:b:462:PHE:HA	31:b:612:CLA:HMC2	1.96	0.47
2:g:47:ALA:HB1	30:g:302:CHL:HBC1	1.95	0.47
31:g:313:CLA:H171	37:g:321:XAT:H201	1.96	0.47
13:j:40:SER:C	13:j:42:LEU:H	2.22	0.47
31:n:305:CLA:HMA3	30:n:307:CHL:C3C	2.45	0.47
31:n:314:CLA:H151	31:n:315:CLA:C2D	2.43	0.47
31:r:305:CLA:HED2	31:r:305:CLA:H2A	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:y:606:CHL:CBB	32:y:617:LUT:H161	2.45	0.47
1:1:211:LEU:HD23	33:1:617:LHG:H291	1.95	0.47
31:1:602:CLA:H92	31:1:603:CLA:HMA1	1.95	0.47
31:3:312:CLA:C4C	33:3:320:LHG:HC62	2.43	0.47
3:5:38:VAL:HG22	3:5:41:TYR:HD2	1.78	0.47
31:6:305:CLA:HBA1	30:6:307:CHL:C1D	2.44	0.47
42:A:408:PHO:H112	42:A:408:PHO:H93	1.68	0.47
6:B:65:PHE:HE1	31:B:604:CLA:HED2	1.80	0.47
7:C:23:TRP:HD1	48:K:101:LMU:H6'1	1.80	0.47
7:C:401:GLU:OE1	49:C:701:HOH:O	2.20	0.47
38:G:624:SQD:H91	31:7:312:CLA:H42	1.96	0.47
19:S:122:GLU:HA	19:S:134:ALA:HB1	1.96	0.47
31:S:313:CLA:HBC1	31:S:314:CLA:H201	1.96	0.47
31:S:314:CLA:H143	33:S:320:LHG:H331	1.96	0.47
23:X:88:GLY:O	23:X:91:THR:HG22	2.15	0.47
4:0:58:PRO:HB2	4:0:61:LEU:HB2	1.97	0.47
4:0:165:GLU:HG3	30:0:609:CHL:C4B	2.43	0.47
4:0:252:ALA:N	4:0:255:LEU:HD13	2.29	0.47
36:0:618:NEX:H173	18:r:53:TRP:HH2	1.80	0.47
1:7:185:PRO:HD2	32:7:317:LUT:H23	1.96	0.47
31:7:316:CLA:H52	34:9:301:LMG:HC72	1.96	0.47
2:9:94:HIS:HD2	32:9:318:LUT:H15	1.79	0.47
2:9:124:VAL:HG11	2:9:127:LYS:HE3	1.95	0.47
2:9:143:ASN:HB3	2:9:146:LEU:HG	1.96	0.47
31:9:305:CLA:HED2	31:9:305:CLA:C1	2.40	0.47
2:q:101:GLY:HA2	32:q:318:LUT:H181	1.97	0.47
31:a:409:CLA:HMA3	45:c:616:DGD:HBW1	1.96	0.47
7:c:394:SER:HA	7:c:408:VAL:HG23	1.95	0.47
8:d:145:ALA:CB	8:d:272:LEU:HD11	2.44	0.47
18:r:45:ARG:HD2	18:r:47:TYR:OH	2.15	0.47
30:s:302:CHL:HBB1	30:s:302:CHL:HMB1	1.96	0.47
30:s:307:CHL:CMC	32:s:318:LUT:H163	2.44	0.47
24:y:257:ASN:N	24:y:257:ASN:OD1	2.47	0.47
29:F1:118:ASN:HB2	29:F1:121:GLU:HG3	1.95	0.47
2:2:47:ALA:HB1	30:2:601:CHL:CBC	2.44	0.47
2:2:125:TRP:HH2	2:2:224:PHE:HD1	1.61	0.47
3:3:233:LEU:HB2	32:3:317:LUT:H22	1.96	0.47
34:3:321:LMG:HC71	34:3:321:LMG:H312	1.97	0.47
2:4:94:HIS:HE1	31:4:603:CLA:C4D	2.28	0.47
2:4:223:PHE:CE1	35:4:615:RRX:H52	2.49	0.47
3:5:258:TYR:OH	31:5:615:CLA:HBC3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:314:CLA:C4B	31:6:314:CLA:H62	2.43	0.47
43:A:410:BCR:H351	43:A:410:BCR:H15C	1.65	0.47
6:B:36:SER:OG	43:B:618:BCR:H362	2.14	0.47
7:C:216:ASP:OD1	7:C:216:ASP:N	2.47	0.47
45:C:620:DGD:HBF1	45:C:620:DGD:HBG2	1.97	0.47
2:G:171:TYR:HE2	3:N:54:ASN:H	1.62	0.47
30:G:623:CHL:HAA2	30:G:623:CHL:HBD	1.95	0.47
31:S:303:CLA:H8	31:S:303:CLA:H122	1.35	0.47
31:8:604:CLA:NB	36:8:617:NEX:H242	2.30	0.47
3:p:245:PHE:CE1	3:p:249:TYR:HB2	2.49	0.47
2:q:130:ALA:HB2	30:q:309:CHL:HED1	1.97	0.47
2:q:130:ALA:O	2:q:134:ASN:N	2.47	0.47
6:b:385:ARG:NH1	17:o:213:GLY:O	2.38	0.47
8:d:20:ASP:O	8:d:24:ARG:HG3	2.15	0.47
19:s:140:GLY:HA3	30:s:308:CHL:C3D	2.44	0.47
33:s:322:LHG:H262	33:s:322:LHG:H161	1.96	0.47
34:x:202:LMG:H301	34:x:202:LMG:H332	1.62	0.47
26:u:153:GLU:OE1	26:u:197:LYS:NZ	2.47	0.47
29:F1:89:ASP:N	29:F1:89:ASP:OD1	2.47	0.47
2:2:234:PRO:HB3	35:2:614:RRX:H50	1.95	0.47
31:2:613:CLA:HMB1	31:2:613:CLA:HBB1	1.95	0.47
3:3:258:TYR:OH	31:3:316:CLA:HAC1	2.14	0.47
2:4:230:THR:HG21	31:4:613:CLA:O1D	2.15	0.47
31:4:604:CLA:C1C	36:4:617:NEX:H362	2.45	0.47
34:4:620:LMG:H141	30:6:308:CHL:C2	2.45	0.47
7:C:225:HIS:HE1	31:C:601:CLA:NA	2.12	0.47
2:G:223:PHE:HE1	35:G:614:RRX:C31	2.26	0.47
31:G:604:CLA:C1C	36:G:616:NEX:H222	2.44	0.47
13:J:6:THR:HG22	28:P1:82:GLY:HA2	1.96	0.47
34:W:201:LMG:H151	34:W:201:LMG:H122	1.56	0.47
1:7:157:MET:HG2	30:7:310:CHL:CMC	2.44	0.47
34:7:322:LMG:H341	34:7:322:LMG:H122	1.95	0.47
31:8:613:CLA:HBA1	31:8:613:CLA:HBD	1.95	0.47
3:p:253:SER:OG	30:q:309:CHL:HAA1	2.15	0.47
30:q:309:CHL:H102	30:q:309:CHL:CHC	2.45	0.47
6:b:237:VAL:HG22	31:b:611:CLA:HBC2	1.96	0.47
7:c:74:LEU:HD13	7:c:77:LEU:HD22	1.95	0.47
7:c:373:GLN:HG2	26:u:131:GLN:HA	1.97	0.47
8:d:351:ALA:N	29:f1:187:ASP:O	2.46	0.47
30:g:307:CHL:HAA2	30:g:307:CHL:HBD	1.97	0.47
34:r:321:LMG:H121	34:x:202:LMG:O7	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:178:PHE:CZ	38:y:621:SQD:H92	2.50	0.47
29:f1:54:ARG:HB3	29:f1:57:ALA:HB2	1.97	0.47
1:1:86:ARG:O	1:1:90:ILE:HG13	2.15	0.47
1:1:247:TYR:O	1:1:251:LEU:HD13	2.13	0.47
34:2:621:LMG:HC2	31:3:316:CLA:O2A	2.15	0.47
3:3:111:ASN:HB2	3:3:113:VAL:HG23	1.96	0.47
3:3:116:PHE:C	3:3:118:GLU:H	2.23	0.47
3:3:245:PHE:HB3	31:3:314:CLA:C1	2.43	0.47
2:4:222:GLY:O	2:4:226:GLN:HG3	2.15	0.47
31:4:614:CLA:H41	31:4:614:CLA:H61	1.68	0.47
3:5:47:GLN:NE2	3:5:55:PRO:HG3	2.29	0.47
31:5:603:CLA:HBC2	30:5:609:CHL:HHD	1.95	0.47
4:6:69:TYR:HE2	30:6:302:CHL:HBC2	1.79	0.47
4:6:115:ALA:HB2	34:6:322:LMG:O10	2.14	0.47
4:6:217:MET:CG	32:6:318:LUT:H12	2.29	0.47
31:6:304:CLA:HHC	31:6:304:CLA:CBB	2.44	0.47
7:C:358:ARG:O	26:U:126:ASN:ND2	2.47	0.47
45:C:620:DGD:HAF2	31:Y:311:CLA:HBB2	1.96	0.47
8:D:148:ALA:HB1	8:D:279:LEU:HB2	1.97	0.47
8:D:191:TRP:CE3	8:D:289:LEU:HD11	2.50	0.47
2:G:234:PRO:HB3	35:G:614:RRX:H50	1.97	0.47
30:G:606:CHL:HBD	30:G:606:CHL:HAA2	1.97	0.47
38:G:617:SQD:C32	33:7:319:LHG:C9	2.92	0.47
30:N:306:CHL:H122	32:S:317:LUT:C17	2.45	0.47
31:N:313:CLA:C1A	31:N:313:CLA:CGA	2.93	0.47
17:O:204:ASP:OD1	17:O:208:ARG:N	2.41	0.47
18:R:139:HIS:CE1	31:R:305:CLA:C4D	2.96	0.47
19:S:284:ASP:OD1	19:S:284:ASP:N	2.47	0.47
1:7:218:ILE:HD12	31:7:314:CLA:HAC2	1.96	0.47
31:8:603:CLA:HBA2	31:8:603:CLA:H12	1.59	0.47
31:8:609:CLA:H3A	31:8:609:CLA:HBA2	1.50	0.47
33:8:618:LHG:H271	33:8:618:LHG:H242	1.75	0.47
2:9:167:GLU:HG3	30:9:311:CHL:C4B	2.44	0.47
3:p:118:GLU:H	3:p:127:GLN:HE22	1.60	0.47
2:q:52:PRO:HD2	30:q:303:CHL:CBB	2.45	0.47
5:a:151:VAL:O	5:a:155:THR:HG23	2.15	0.47
5:a:312:ARG:NH1	29:f1:83:ASN:OD1	2.48	0.47
6:b:207:ILE:CD1	33:b:628:LHG:H201	2.45	0.47
31:b:603:CLA:H41	31:b:603:CLA:H61	1.41	0.47
31:b:609:CLA:H152	31:b:610:CLA:H172	1.97	0.47
7:c:14:ARG:HA	7:c:14:ARG:HE	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:404:CLA:H62	31:d:404:CLA:H41	1.47	0.47
14:k:17:PRO:HB2	33:z:102:LHG:HC61	1.96	0.47
15:l:30:VAL:HG22	20:t:9:LEU:HB3	1.97	0.47
3:n:177:ASP:HB3	3:n:180:TYR:O	2.15	0.47
17:o:106:VAL:HG22	17:o:280:VAL:HG22	1.95	0.47
31:s:316:CLA:CHA	31:s:316:CLA:HBA1	2.45	0.47
24:y:157:VAL:HG11	30:y:606:CHL:HED2	1.95	0.47
31:y:613:CLA:H18	31:y:614:CLA:CGA	2.44	0.47
28:P1:17:ASN:HD22	28:P1:20:VAL:HG23	1.80	0.47
1:1:198:LEU:HD23	1:1:201:LYS:HD2	1.97	0.47
2:2:92:VAL:HB	2:2:184:LEU:HD21	1.95	0.47
31:2:604:CLA:CHB	36:2:616:NEX:H383	2.45	0.47
31:3:301:CLA:H93	31:3:301:CLA:H62	1.65	0.47
2:4:129:GLY:HA3	30:4:607:CHL:CGD	2.45	0.47
4:6:106:THR:HG21	31:6:305:CLA:HAC2	1.96	0.47
6:B:123:PHE:O	6:B:131:PRO:HA	2.15	0.47
6:B:201:HIS:HE1	31:B:602:CLA:C1D	2.14	0.47
7:C:120:HIS:HE1	31:C:613:CLA:NA	2.11	0.47
34:D:409:LMG:H152	34:D:409:LMG:H181	1.78	0.47
3:N:162:ILE:HD11	36:N:318:NEX:C34	2.45	0.47
17:O:270:THR:HG22	17:O:277:PRO:HB3	1.97	0.47
4:0:189:PRO:HA	18:r:47:TYR:OH	2.14	0.47
31:0:610:CLA:H41	31:0:612:CLA:HMA2	1.97	0.47
31:8:610:CLA:HHC	31:8:610:CLA:HBB1	1.97	0.47
31:8:612:CLA:NC	31:8:612:CLA:H51	2.30	0.47
3:p:166:ARG:HG3	30:p:608:CHL:CHD	2.45	0.47
31:p:613:CLA:C3B	32:p:616:LUT:H183	2.45	0.47
2:q:226:GLN:HG2	31:q:315:CLA:C1D	2.45	0.47
30:q:309:CHL:HHC	30:q:309:CHL:HBB1	1.97	0.47
5:a:259:ILE:HD13	44:a:414:PL9:H18	1.96	0.47
6:b:112:ILE:HG12	43:b:618:BCR:H272	1.97	0.47
31:c:607:CLA:H112	43:c:615:BCR:H362	1.97	0.47
43:d:406:BCR:H19C	10:f:29:THR:HG23	1.96	0.47
31:g:313:CLA:H122	31:g:313:CLA:H8	1.63	0.47
11:h:56:LEU:HB3	43:h:101:BCR:H14C	1.97	0.47
3:n:224:ILE:HD12	3:n:258:TYR:OH	2.14	0.47
2:2:211:LYS:NZ	33:2:617:LHG:O5	2.48	0.47
2:2:258:LEU:HD22	2:2:260:LEU:HD12	1.96	0.47
3:3:69:TRP:CG	3:3:69:TRP:O	2.68	0.47
34:A:414:LMG:HC71	34:A:414:LMG:HC2	1.62	0.47
31:B:606:CLA:H193	43:B:619:BCR:H363	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:D:401:PHO:H71	42:D:401:PHO:H112	1.55	0.47
18:R:204:GLU:OE1	18:R:206:ASP:N	2.48	0.47
19:S:180:GLU:HG3	31:S:310:CLA:C4B	2.45	0.47
31:9:306:CLA:H8	31:9:306:CLA:H51	1.36	0.47
3:p:136:TYR:CE1	31:p:604:CLA:H2	2.49	0.47
3:p:227:LYS:HB2	3:p:232:ASN:OD1	2.15	0.47
6:b:36:SER:OG	43:b:619:BCR:H362	2.15	0.47
6:b:333:GLY:O	6:b:439:SER:HB3	2.15	0.47
31:b:614:CLA:H62	31:b:614:CLA:H41	1.56	0.47
7:c:36:LYS:NZ	7:c:121:SER:O	2.47	0.47
31:c:601:CLA:H203	31:c:607:CLA:H152	1.96	0.47
45:c:619:DGD:HE1	31:y:611:CLA:CMA	2.44	0.47
11:h:57:PHE:HB2	43:h:101:BCR:H12C	1.97	0.47
24:y:90:ILE:HG21	31:y:603:CLA:HAA2	1.97	0.47
31:1:611:CLA:HHC	31:1:611:CLA:CBB	2.44	0.47
30:1:619:CHL:HED3	3:3:123:LYS:HA	1.96	0.47
30:3:302:CHL:CGA	30:3:302:CHL:C1A	2.93	0.47
31:3:306:CLA:HMA2	30:3:308:CHL:C3C	2.45	0.47
31:5:602:CLA:HED2	31:5:602:CLA:H2A	1.95	0.47
4:6:93:HIS:CE1	31:6:304:CLA:C4D	2.97	0.47
4:6:246:ASN:HB2	31:6:314:CLA:O1A	2.15	0.47
30:6:307:CHL:O2D	30:6:307:CHL:HBA2	2.15	0.47
31:6:312:CLA:NB	33:6:320:LHG:O4	2.48	0.47
31:B:602:CLA:HBD	31:B:602:CLA:HBA2	1.97	0.47
31:B:610:CLA:C2	31:B:610:CLA:H72	2.45	0.47
38:B:623:SQD:H223	38:B:623:SQD:H341	1.95	0.47
8:D:157:PHE:CE2	8:D:171:PRO:HG2	2.50	0.47
2:G:218:PHE:CE1	31:G:612:CLA:HMC1	2.50	0.47
36:N:318:NEX:H161	36:N:318:NEX:H192	1.96	0.47
18:R:233:LEU:HB3	31:R:312:CLA:HMA2	1.97	0.47
31:R:305:CLA:HED2	31:R:305:CLA:H2A	1.97	0.47
4:0:72:ASP:HA	32:0:617:LUT:H24	1.97	0.47
3:p:54:ASN:N	2:q:171:TYR:HE2	2.06	0.47
3:p:75:SER:OG	31:p:602:CLA:O1A	2.21	0.47
5:a:101:SER:HA	34:a:413:LMG:HC61	1.97	0.47
7:c:36:LYS:HE2	7:c:126:GLU:HG3	1.97	0.47
7:c:101:VAL:HG21	38:s:301:SQD:H462	1.97	0.47
31:c:612:CLA:CBB	33:c:622:LHG:H102	2.45	0.47
3:n:134:LEU:HD21	31:n:305:CLA:HAA1	1.97	0.47
30:n:306:CHL:C2	19:s:120:ILE:HA	2.44	0.47
30:n:308:CHL:H122	30:n:310:CHL:CMC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:n:314:CLA:NC	31:n:314:CLA:H51	2.30	0.47
36:r:301:NEX:H161	36:r:301:NEX:H193	1.97	0.47
22:w:67:GLY:O	22:w:70:THR:OG1	2.26	0.47
25:z:61:VAL:HG13	25:z:62:VAL:HG23	1.97	0.47
1:1:90:ILE:HD13	31:1:603:CLA:HBA1	1.97	0.46
2:2:240:ASP:HB3	2:2:248:ASN:HD22	1.80	0.46
32:2:615:LUT:H35	32:2:615:LUT:H401	1.38	0.46
3:3:86:GLU:HA	3:3:179:LEU:HD11	1.97	0.46
3:3:221:GLN:HE21	3:3:232:ASN:HD22	1.63	0.46
2:4:118:ASP:HB3	34:Q1:101:LMG:C38	2.44	0.46
3:5:110:ARG:CZ	3:5:230:ILE:HB	2.45	0.46
5:A:106:LEU:HD11	43:A:410:BCR:H402	1.97	0.46
33:A:415:LHG:H162	34:A:418:LMG:H151	1.97	0.46
7:C:244:PRO:HA	31:C:606:CLA:HED3	1.96	0.46
34:G:622:LMG:H151	31:N:321:CLA:H11	1.97	0.46
11:H:74:LEU:HB2	11:H:77:VAL:HG22	1.97	0.46
34:J:101:LMG:H331	34:J:101:LMG:H161	1.97	0.46
48:R:302:LMU:O2'	48:R:302:LMU:H5'	2.15	0.46
1:7:132:ILE:HD12	30:7:307:CHL:HMD1	1.97	0.46
3:8:177:ASP:HB3	3:8:180:TYR:O	2.15	0.46
2:9:118:ASP:HB3	2:9:142:GLY:HA3	1.96	0.46
2:9:127:LYS:HA	30:9:309:CHL:HED3	1.96	0.46
2:9:218:PHE:CD1	33:9:320:LHG:H301	2.50	0.46
3:p:94:TRP:CE2	30:p:608:CHL:HED2	2.50	0.46
3:p:249:TYR:CD1	3:p:258:TYR:CD1	3.03	0.46
31:p:610:CLA:HMB1	31:p:610:CLA:HBB1	1.96	0.46
2:q:49:TRP:CD1	2:q:49:TRP:H	2.33	0.46
2:q:94:HIS:HE1	31:q:305:CLA:C4D	2.28	0.46
2:q:177:VAL:HG22	2:q:189:PHE:CD2	2.50	0.46
5:a:46:SER:O	5:a:50:ILE:HG12	2.15	0.46
6:b:315:ILE:HG12	6:b:321:LYS:HG3	1.97	0.46
31:b:614:CLA:HBB1	31:b:614:CLA:HMB1	1.96	0.46
34:b:626:LMG:H121	8:d:32:TRP:CD1	2.50	0.46
10:f:15:PHE:CD2	27:q1:27:LEU:HD13	2.49	0.46
31:n:312:CLA:HHC	31:n:312:CLA:HBB1	1.97	0.46
19:s:114:ALA:HA	32:s:318:LUT:C18	2.45	0.46
31:s:304:CLA:HED2	31:s:304:CLA:H2A	1.96	0.46
30:1:601:CHL:HHC	30:1:601:CHL:CBB	2.43	0.46
31:1:612:CLA:HBB1	31:1:612:CLA:HHC	1.98	0.46
33:1:617:LHG:H281	33:1:617:LHG:H242	1.97	0.46
2:2:256:LYS:HD3	2:2:257:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:172:SER:HA	3:5:54:ASN:OD1	2.15	0.46
3:5:115:ASN:N	3:5:115:ASN:ND2	2.63	0.46
3:5:241:ASP:OD1	3:5:241:ASP:N	2.47	0.46
31:5:602:CLA:CHA	31:5:602:CLA:HBA1	2.45	0.46
4:6:49:PHE:CE2	4:6:50:LEU:HD13	2.49	0.46
7:C:149:LEU:O	7:C:153:LEU:HB2	2.15	0.46
45:C:620:DGD:HD2	45:C:620:DGD:HG31	1.64	0.46
2:G:223:PHE:CZ	35:G:614:RRX:H48	2.48	0.46
31:G:603:CLA:HMC2	30:G:608:CHL:H13	1.97	0.46
17:O:179:LEU:HD23	17:O:192:PHE:HB3	1.98	0.46
32:S:318:LUT:H35	32:S:318:LUT:H401	1.76	0.46
20:T:29:ILE:HG22	20:T:30:VAL:HG22	1.97	0.46
4:0:47:VAL:HB	30:0:601:CHL:CBC	2.45	0.46
4:0:169:VAL:HG21	2:q:50:LEU:CD2	2.46	0.46
30:0:609:CHL:HMB3	30:q:303:CHL:HHB	1.96	0.46
2:9:170:ARG:HA	30:9:310:CHL:C3C	2.44	0.46
31:9:315:CLA:C1A	31:9:315:CLA:CGA	2.93	0.46
3:p:134:LEU:HD13	30:p:606:CHL:HHD	1.96	0.46
2:q:187:GLY:O	2:q:188:GLY:C	2.59	0.46
2:q:188:GLY:O	2:q:189:PHE:C	2.59	0.46
33:q:320:LHG:H291	33:q:320:LHG:H261	1.58	0.46
41:a:404:CL:CL	8:d:317:LYS:HE2	2.51	0.46
31:b:609:CLA:HBA2	31:b:609:CLA:H3A	1.60	0.46
45:c:616:DGD:HBV2	34:w:201:LMG:H122	1.96	0.46
2:g:146:LEU:HD23	30:g:306:CHL:HED2	1.97	0.46
33:g:319:LHG:C6	37:g:321:XAT:H382	2.46	0.46
3:n:38:VAL:HG12	3:n:42:GLY:HA3	1.97	0.46
3:n:104:THR:HB	3:n:105:PRO:HD3	1.97	0.46
31:n:305:CLA:H101	31:s:306:CLA:CMA	2.45	0.46
17:o:209:GLY:HA2	17:o:235:LYS:HD2	1.97	0.46
19:s:90:LEU:HD23	31:s:303:CLA:H42	1.98	0.46
31:s:305:CLA:H92	31:s:305:CLA:H61	1.69	0.46
34:Q1:101:LMG:H362	34:Q1:101:LMG:H151	1.97	0.46
31:2:610:CLA:C4D	31:2:611:CLA:HMD3	2.45	0.46
3:3:79:GLU:OE1	3:3:79:GLU:N	2.46	0.46
2:4:153:VAL:O	2:4:157:LEU:HD13	2.14	0.46
2:4:164:GLY:HA2	30:4:609:CHL:CAB	2.45	0.46
31:4:602:CLA:HAC2	33:4:618:LHG:H252	1.97	0.46
3:5:246:TRP:H	3:5:246:TRP:CD1	2.33	0.46
30:6:308:CHL:H41	30:6:308:CHL:H101	1.96	0.46
44:A:416:PL9:H451	44:A:416:PL9:H471	1.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:B:619:BCR:H382	34:a:401:LMG:H151	1.97	0.46
31:G:610:CLA:H61	31:G:610:CLA:H41	1.62	0.46
33:K:102:LHG:HC82	33:K:102:LHG:HC5	1.66	0.46
30:N:307:CHL:OMC	32:N:317:LUT:H163	2.15	0.46
1:7:168:GLY:HA2	18:r:44:TYR:CE1	2.50	0.46
31:7:305:CLA:HBB1	31:7:305:CLA:CMB	2.44	0.46
30:q:303:CHL:C1D	33:q:320:LHG:HC81	2.45	0.46
44:a:414:PL9:H321	10:f:25:LEU:HD21	1.97	0.46
6:b:53:ASN:OD1	6:b:58:GLN:NE2	2.48	0.46
6:b:243:ALA:HA	6:b:246:PHE:CD2	2.51	0.46
31:b:612:CLA:HBB1	31:b:612:CLA:CMB	2.45	0.46
45:c:619:DGD:CIA	31:y:614:CLA:H51	2.45	0.46
38:g:301:SQD:H462	38:g:301:SQD:H242	1.60	0.46
30:g:302:CHL:HED3	33:g:319:LHG:H292	1.96	0.46
33:j:102:LHG:HC31	29:f1:58:GLY:HA2	1.98	0.46
3:n:70:ASP:OD2	3:n:75:SER:OG	2.30	0.46
30:n:306:CHL:H142	32:s:317:LUT:H171	1.96	0.46
31:r:304:CLA:H93	31:r:304:CLA:H62	1.72	0.46
34:y:620:LMG:H332	34:y:620:LMG:H361	1.81	0.46
26:u:63:ALA:O	26:u:68:PHE:HB2	2.15	0.46
29:F1:118:ASN:HB3	29:F1:120:ASP:OD1	2.16	0.46
30:1:601:CHL:HHB	30:3:310:CHL:HMB3	1.96	0.46
2:4:74:THR:HG21	30:6:310:CHL:HBA1	1.98	0.46
34:4:621:LMG:H171	34:4:621:LMG:H142	1.69	0.46
36:6:319:NEX:H161	36:6:319:NEX:H193	1.97	0.46
7:C:406:ASN:HD21	45:C:617:DGD:HD4	1.81	0.46
7:C:412:SER:O	7:C:416:THR:HB	2.15	0.46
31:C:613:CLA:H11	43:C:614:BCR:H381	1.98	0.46
34:C:624:LMG:H322	34:C:624:LMG:H291	1.75	0.46
8:D:202:ALA:HB2	44:D:406:PL9:H353	1.98	0.46
10:F:15:PHE:CD2	27:Q1:27:LEU:HD13	2.51	0.46
3:N:180:TYR:HB3	31:N:310:CLA:HED3	1.96	0.46
31:N:305:CLA:CHA	31:N:305:CLA:HBA1	2.39	0.46
17:O:112:PHE:HZ	6:b:82:GLY:HA3	1.79	0.46
31:S:313:CLA:HBB1	31:S:313:CLA:HMB3	1.96	0.46
31:0:614:CLA:H92	31:0:614:CLA:H62	1.76	0.46
36:0:618:NEX:H161	36:0:618:NEX:H193	1.97	0.46
31:7:311:CLA:H41	31:7:311:CLA:H61	1.61	0.46
31:q:312:CLA:ND	35:q:317:RRX:H11	2.30	0.46
7:c:105:LEU:HD23	38:s:301:SQD:H141	1.97	0.46
2:2:124:VAL:O	2:2:125:TRP:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:132:ILE:HG13	2:2:152:ILE:HD13	1.96	0.46
2:2:195:LEU:HB2	31:2:609:CLA:O1A	2.16	0.46
31:2:609:CLA:H62	31:2:609:CLA:H41	1.75	0.46
36:2:616:NEX:H171	36:2:616:NEX:H193	1.97	0.46
37:2:619:XAT:H31	37:2:619:XAT:H391	1.77	0.46
2:4:49:TRP:CD1	2:4:49:TRP:H	2.34	0.46
2:4:139:ASN:CG	2:4:144:PRO:HA	2.41	0.46
30:4:606:CHL:HAA2	30:4:606:CHL:HBD	1.98	0.46
8:D:113:PHE:CZ	43:D:405:BCR:HC22	2.50	0.46
31:N:303:CLA:H72	32:N:317:LUT:H30	1.97	0.46
31:Y:310:CLA:H92	31:Y:310:CLA:H61	1.65	0.46
4:0:151:VAL:O	4:0:154:LEU:N	2.49	0.46
31:7:305:CLA:H61	31:7:305:CLA:H92	1.61	0.46
31:7:316:CLA:CHC	34:9:301:LMG:H361	2.45	0.46
3:p:118:GLU:N	3:p:127:GLN:HE22	2.14	0.46
3:p:142:LEU:O	3:p:144:HIS:N	2.49	0.46
31:p:610:CLA:H92	32:p:616:LUT:C28	2.46	0.46
2:q:110:LEU:HD23	2:q:110:LEU:C	2.40	0.46
38:b:627:SQD:H341	38:b:627:SQD:H202	1.98	0.46
33:b:628:LHG:H182	31:r:316:CLA:H202	1.96	0.46
7:c:40:ALA:HB2	31:c:611:CLA:HMA2	1.98	0.46
45:c:618:DGD:HA91	45:c:618:DGD:HA62	1.60	0.46
30:y:601:CHL:H41	30:y:601:CHL:H61	1.72	0.46
1:1:48:LYS:HG2	1:1:54:SER:OG	2.16	0.46
30:1:605:CHL:HAA2	30:1:605:CHL:HBD	1.97	0.46
34:1:618:LMG:H351	36:R:301:NEX:H402	1.98	0.46
31:2:609:CLA:HMB2	31:2:611:CLA:HBA2	1.96	0.46
3:3:66:ASP:HA	31:3:304:CLA:O1D	2.15	0.46
31:5:613:CLA:HBA1	31:5:614:CLA:C2D	2.46	0.46
34:5:620:LMG:C6	31:6:315:CLA:CMA	2.93	0.46
4:6:208:LYS:HE2	31:6:312:CLA:O1D	2.15	0.46
4:6:221:PHE:O	4:6:225:ILE:HG13	2.15	0.46
6:B:237:VAL:CG2	31:B:610:CLA:HBC2	2.45	0.46
6:B:464:PHE:CZ	33:D:407:LHG:H261	2.51	0.46
31:B:606:CLA:H91	31:B:606:CLA:H111	1.69	0.46
43:B:618:BCR:H363	43:t:101:BCR:H341	1.97	0.46
34:B:625:LMG:H342	30:R:309:CHL:C4	2.44	0.46
8:D:46:GLY:CA	43:D:405:BCR:H11C	2.45	0.46
31:G:604:CLA:H3A	31:G:604:CLA:HBA2	1.36	0.46
33:G:618:LHG:H362	37:G:620:XAT:C12	2.44	0.46
34:G:622:LMG:HC91	34:G:622:LMG:C13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:145:LEU:HD11	34:Y:319:LMG:H322	1.98	0.46
26:U:130:ARG:C	26:U:132:VAL:H	2.23	0.46
31:0:614:CLA:H71	31:0:614:CLA:C3B	2.45	0.46
3:8:38:VAL:HG12	3:8:42:GLY:HA3	1.98	0.46
2:q:101:GLY:HA2	32:q:318:LUT:C18	2.46	0.46
5:a:221:SER:HA	8:d:139:ARG:HB2	1.98	0.46
6:b:159:THR:O	6:b:180:ALA:HB1	2.15	0.46
31:b:605:CLA:HBA1	31:b:613:CLA:H152	1.98	0.46
31:b:612:CLA:O2A	33:b:625:LHG:H381	2.16	0.46
8:d:93:TRP:HB3	34:d:410:LMG:HC92	1.98	0.46
31:d:405:CLA:H43	23:x:76:VAL:HA	1.98	0.46
31:n:312:CLA:HHC	31:n:312:CLA:CBB	2.46	0.46
19:s:163:LEU:HD23	19:s:168:VAL:HG22	1.96	0.46
31:y:613:CLA:H93	31:y:613:CLA:H112	1.62	0.46
29:f1:120:ASP:HB3	29:f1:175:LYS:NZ	2.31	0.46
1:1:123:GLY:O	1:1:126:ILE:HG22	2.16	0.46
31:1:610:CLA:C2	32:1:615:LUT:H28	2.37	0.46
2:2:146:LEU:O	2:2:148:HIS:N	2.45	0.46
30:2:605:CHL:HHC	30:2:605:CHL:CBB	2.44	0.46
3:5:115:ASN:ND2	3:5:138:GLY:HA3	2.31	0.46
31:6:304:CLA:CMA	31:6:304:CLA:H2	2.46	0.46
33:A:415:LHG:H251	33:A:415:LHG:H142	1.98	0.46
6:B:186:ASP:OD1	6:B:186:ASP:N	2.49	0.46
31:C:613:CLA:HBB1	31:C:613:CLA:HMB3	1.97	0.46
2:G:147:ILE:HG23	30:G:605:CHL:C1D	2.46	0.46
31:G:603:CLA:H52	31:G:603:CLA:H8	1.47	0.46
30:G:605:CHL:HHC	30:G:605:CHL:CBB	2.44	0.46
18:R:245:MET:SD	31:R:304:CLA:HAB	2.56	0.46
19:S:121:PRO:HA	19:S:124:LEU:HD12	1.98	0.46
1:7:140:LEU:HD13	31:7:305:CLA:H91	1.97	0.46
1:7:244:TYR:HA	1:7:248:ALA:HB2	1.96	0.46
31:8:613:CLA:HBA1	31:8:613:CLA:CBD	2.46	0.46
3:p:104:THR:HB	3:p:105:PRO:HD3	1.98	0.46
31:p:613:CLA:C2	31:p:614:CLA:HMD2	2.45	0.46
2:q:50:LEU:HD12	2:q:50:LEU:HA	1.80	0.46
2:q:169:TYR:HB2	30:q:310:CHL:CHC	2.46	0.46
5:a:60:ILE:HD12	5:a:84:PRO:HD2	1.98	0.46
6:b:258:TYR:OH	8:d:162:LEU:O	2.24	0.46
2:g:259:PRO:HD3	30:y:607:CHL:C1	2.46	0.46
33:l:101:LHG:H122	33:l:101:LHG:HC92	1.53	0.46
3:n:143:ILE:HA	30:n:306:CHL:C4D	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:162:ILE:HD11	36:n:319:NEX:C34	2.45	0.46
31:n:313:CLA:HBB1	31:n:313:CLA:CMB	2.45	0.46
31:s:303:CLA:H112	31:s:303:CLA:H152	1.53	0.46
29:f1:107:LEU:C	29:f1:107:LEU:HD12	2.41	0.46
3:3:89:VAL:HG22	3:3:205:LEU:HD21	1.97	0.46
30:3:302:CHL:H71	30:3:302:CHL:CHC	2.46	0.46
32:3:318:LUT:H15	32:3:318:LUT:H201	1.71	0.46
3:5:49:LEU:HA	30:5:601:CHL:C4B	2.46	0.46
34:5:620:LMG:HC62	31:6:315:CLA:HMA2	1.95	0.46
31:6:316:CLA:HBB1	31:6:316:CLA:CMB	2.45	0.46
5:A:131:TRP:CH2	31:C:605:CLA:HAA2	2.51	0.46
31:A:406:CLA:H121	31:A:406:CLA:HMA3	1.98	0.46
6:B:311:PHE:O	6:B:317:ASN:ND2	2.47	0.46
6:B:385:ARG:NH1	17:O:213:GLY:O	2.43	0.46
7:C:374:PRO:O	7:C:378:ARG:HG3	2.16	0.46
9:E:13:ILE:HD13	47:E:101:HEM:HBD1	1.96	0.46
14:K:18:PHE:CD1	33:K:102:LHG:H261	2.51	0.46
31:N:313:CLA:H172	31:N:314:CLA:ND	2.31	0.46
32:R:317:LUT:H35	32:R:317:LUT:H401	1.41	0.46
36:S:319:NEX:H161	36:S:319:NEX:H193	1.98	0.46
24:Y:176:ASN:HB2	38:Y:320:SQD:O3	2.15	0.46
4:0:72:ASP:OD2	4:0:77:SER:OG	2.29	0.46
32:7:317:LUT:H11	32:7:317:LUT:H191	1.81	0.46
3:8:143:ILE:HA	30:8:605:CHL:C4D	2.46	0.46
3:8:239:ALA:O	3:8:243:THR:HG22	2.16	0.46
31:9:314:CLA:HMC3	35:9:317:RRX:H44	1.97	0.46
3:p:245:PHE:O	3:p:247:VAL:N	2.48	0.46
2:q:85:ALA:O	2:q:89:GLU:HG3	2.15	0.46
5:a:159:ILE:HG23	45:c:616:DGD:HB61	1.98	0.46
6:b:314:TYR:CE2	6:b:316:GLY:HA3	2.51	0.46
33:b:628:LHG:H321	33:b:628:LHG:H291	1.40	0.46
7:c:23:TRP:CD1	48:c:623:LMU:H6'1	2.50	0.46
7:c:270:MET:HG2	31:c:601:CLA:H72	1.98	0.46
44:d:407:PL9:H513	33:d:408:LHG:H221	1.96	0.46
3:n:239:ALA:O	3:n:243:THR:HG22	2.16	0.46
30:r:308:CHL:HMB2	31:r:311:CLA:HMC1	1.98	0.46
33:s:322:LHG:H311	33:s:322:LHG:H282	1.56	0.46
29:F1:174:LYS:HE3	29:F1:200:THR:HG21	1.97	0.46
1:1:215:GLY:O	1:1:219:GLN:HG3	2.15	0.46
3:3:118:GLU:HG2	3:3:123:LYS:O	2.16	0.46
3:5:239:ALA:HB1	3:5:242:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:C:617:DGD:HAF2	45:C:618:DGD:HAF2	1.97	0.46
11:H:75:ASP:OD1	11:H:75:ASP:N	2.48	0.46
3:N:126:ALA:HB2	30:Y:301:CHL:HED2	1.98	0.46
30:S:302:CHL:C1D	33:S:320:LHG:HC82	2.46	0.46
31:S:303:CLA:H92	31:S:303:CLA:H62	1.64	0.46
24:Y:192:ASP:OD1	32:Y:315:LUT:O23	2.23	0.46
31:0:603:CLA:H3A	31:0:603:CLA:HBA1	1.56	0.46
34:0:620:LMG:H142	34:7:301:LMG:H301	1.97	0.46
3:8:104:THR:HB	3:8:105:PRO:HD3	1.98	0.46
3:8:134:LEU:HD21	31:8:604:CLA:HAA1	1.97	0.46
3:8:219:GLY:HA3	34:9:301:LMG:H392	1.98	0.46
2:q:201:THR:O	2:q:205:LEU:HB2	2.15	0.46
34:a:416:LMG:H132	48:c:623:LMU:O2'	2.16	0.46
6:b:26:HIS:CE1	31:b:613:CLA:HMA2	2.51	0.46
33:b:628:LHG:H171	31:r:316:CLA:C20	2.45	0.46
8:d:117:HIS:CE1	31:d:405:CLA:C4D	2.99	0.46
8:d:237:PRO:HD3	28:p1:60:VAL:HG12	1.98	0.46
31:n:304:CLA:CAD	30:n:310:CHL:H11	2.46	0.46
31:n:305:CLA:H202	31:s:306:CLA:CHA	2.46	0.46
17:o:227:GLU:HA	17:o:230:LEU:HD12	1.97	0.46
31:r:304:CLA:H102	31:r:305:CLA:CMB	2.45	0.46
20:t:29:ILE:HG22	20:t:30:VAL:HG13	1.98	0.46
29:F1:165:VAL:HG13	29:F1:179:TYR:CE1	2.50	0.46
3:3:56:PRO:HG2	3:3:59:LEU:HB2	1.97	0.46
2:4:72:TRP:O	32:4:616:LUT:H24	2.16	0.46
3:5:190:LEU:HB2	31:5:610:CLA:O2A	2.16	0.46
3:5:239:ALA:CB	3:5:242:ALA:HB3	2.45	0.46
31:5:610:CLA:H12	31:5:610:CLA:C3A	2.45	0.46
33:5:619:LHG:HC62	33:5:619:LHG:P	2.56	0.46
5:A:307:VAL:HG23	10:F:44:ARG:HD2	1.97	0.46
31:B:605:CLA:H91	31:B:605:CLA:H111	1.72	0.46
38:B:623:SQD:H242	34:D:410:LMG:H311	1.98	0.46
7:C:304:THR:HG23	26:U:71:ILE:HG21	1.98	0.46
7:C:454:VAL:HG13	8:D:251:ARG:HD2	1.97	0.46
31:C:607:CLA:H3A	31:C:607:CLA:HBA1	1.74	0.46
47:E:101:HEM:CAC	10:F:26:ALA:HB1	2.46	0.46
34:G:621:LMG:H311	31:N:321:CLA:H42	1.98	0.46
16:M:16:ILE:HG23	38:M:102:SQD:H191	1.98	0.46
17:O:135:MET:HA	17:O:154:GLY:HA3	1.98	0.46
18:R:115:VAL:HG23	18:R:207:PRO:HG3	1.97	0.46
18:R:238:ILE:HD12	18:R:239:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S:306:CLA:O1D	31:S:306:CLA:H2A	2.16	0.46
30:Y:301:CHL:HBD	30:Y:301:CHL:HAA1	1.97	0.46
4:0:202:LEU:HB3	31:0:610:CLA:HMA1	1.96	0.46
3:p:122:PHE:O	30:p:607:CHL:HMA3	2.15	0.46
3:p:126:ALA:HA	3:p:129:PHE:HD2	1.81	0.46
3:p:220:VAL:CG1	31:p:613:CLA:HAC2	2.44	0.46
2:q:103:LEU:HD12	35:q:317:RRX:C36	2.45	0.46
45:c:619:DGD:HAN2	45:c:619:DGD:CBB	2.46	0.46
47:e:102:HEM:CMB	27:q1:19:VAL:HG21	2.46	0.46
31:g:305:CLA:HBA2	31:g:305:CLA:H3A	1.26	0.46
30:g:306:CHL:HHC	30:g:306:CHL:CBB	2.44	0.46
31:n:311:CLA:H171	31:s:306:CLA:HBB2	1.97	0.46
30:r:310:CHL:HBA1	38:r:322:SQD:H301	1.97	0.46
43:t:101:BCR:H361	43:t:101:BCR:H20C	1.62	0.46
31:2:602:CLA:CGA	32:2:615:LUT:H24	2.46	0.45
31:3:305:CLA:HMC3	32:3:318:LUT:H12	1.97	0.45
31:4:602:CLA:H122	31:4:602:CLA:H8	1.76	0.45
31:6:311:CLA:HBB1	31:6:311:CLA:HMB1	1.98	0.45
5:A:118:HIS:CE1	31:A:409:CLA:C4D	2.98	0.45
5:A:170:ASP:OD2	7:C:345:ARG:NH1	2.47	0.45
34:A:418:LMG:H321	34:A:418:LMG:H292	1.72	0.45
6:B:149:LEU:HD13	31:B:604:CLA:H202	1.98	0.45
6:B:202:HIS:HE1	31:B:603:CLA:NA	2.12	0.45
6:B:466:HIS:CE1	31:B:608:CLA:C4D	2.99	0.45
31:B:606:CLA:H161	31:B:616:CLA:H111	1.98	0.45
7:C:384:MET:HE1	26:U:75:ARG:HH11	1.81	0.45
31:G:602:CLA:H2	31:G:602:CLA:C1B	2.47	0.45
19:S:115:ALA:HB1	32:S:317:LUT:H12	1.98	0.45
19:S:241:LEU:HD21	31:S:313:CLA:CBC	2.46	0.45
31:S:311:CLA:O2A	32:S:317:LUT:H26	2.17	0.45
4:0:111:GLN:OE1	4:0:117:ASN:ND2	2.46	0.45
31:7:316:CLA:HBB1	31:7:316:CLA:HMB3	1.98	0.45
31:8:611:CLA:HBB1	31:8:611:CLA:CMB	2.45	0.45
36:8:617:NEX:H171	36:8:617:NEX:H192	1.98	0.45
2:9:66:PHE:HB3	2:9:67:PRO:HD2	1.99	0.45
31:9:306:CLA:C3B	32:9:318:LUT:H183	2.45	0.45
30:9:310:CHL:HAA1	30:9:310:CHL:HBD	1.97	0.45
2:q:46:ARG:NH2	2:q:62:LEU:O	2.50	0.45
2:q:177:VAL:HA	2:q:189:PHE:CG	2.51	0.45
2:q:211:LYS:HD3	31:q:313:CLA:O1D	2.16	0.45
31:q:313:CLA:CAC	33:q:320:LHG:HC61	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:132:GLU:O	5:a:136:ARG:HG2	2.16	0.45
6:b:341:LEU:HD22	6:b:429:ILE:HG22	1.97	0.45
8:d:148:ALA:HB2	8:d:276:VAL:HG13	1.97	0.45
8:d:261:PHE:CZ	33:d:408:LHG:HC81	2.51	0.45
8:d:261:PHE:CE2	33:d:408:LHG:HC81	2.51	0.45
31:g:305:CLA:O1A	36:g:317:NEX:H241	2.16	0.45
3:n:39:GLU:O	3:n:46:PRO:HD3	2.16	0.45
17:o:186:ASP:N	17:o:186:ASP:OD1	2.48	0.45
31:s:303:CLA:H12	31:s:303:CLA:H3A	1.98	0.45
34:x:202:LMG:HC8	34:x:202:LMG:H111	1.45	0.45
31:y:612:CLA:H2	31:y:612:CLA:HMA3	1.98	0.45
2:2:238:LEU:HD13	34:2:618:LMG:C9	2.46	0.45
2:4:157:LEU:HD11	31:5:614:CLA:O1A	2.16	0.45
2:4:171:TYR:HE2	3:5:54:ASN:N	2.12	0.45
3:5:108:LEU:HB2	3:5:116:PHE:HE2	1.81	0.45
31:5:611:CLA:HHC	31:5:611:CLA:HBB1	1.97	0.45
31:A:406:CLA:H52	44:D:406:PL9:H151	1.98	0.45
43:B:619:BCR:HC41	34:B:622:LMG:H141	1.97	0.45
31:C:604:CLA:H42	45:C:617:DGD:HB61	1.98	0.45
3:N:131:GLU:CD	3:N:132:GLY:H	2.23	0.45
31:N:304:CLA:H8	31:N:304:CLA:H51	1.38	0.45
31:N:305:CLA:H101	31:S:306:CLA:HMA2	1.98	0.45
18:R:79:SER:OG	31:R:304:CLA:O1A	2.21	0.45
36:R:319:NEX:H10	38:R:322:SQD:H132	1.97	0.45
23:X:86:ILE:O	23:X:90:ILE:HG12	2.16	0.45
30:Y:301:CHL:C1C	30:Y:301:CHL:H51	2.45	0.45
30:0:601:CHL:HAA2	30:0:601:CHL:HBD	1.98	0.45
30:7:307:CHL:HAA2	30:7:307:CHL:HBD	1.97	0.45
2:9:72:TRP:CD2	32:9:318:LUT:H383	2.51	0.45
2:9:86:ARG:HH22	30:9:311:CHL:HED1	1.81	0.45
30:9:308:CHL:HBB2	30:9:309:CHL:HBB1	1.97	0.45
3:p:105:PRO:HA	3:p:116:PHE:CE2	2.52	0.45
6:b:218:CYS:SG	31:r:316:CLA:HBA1	2.56	0.45
31:b:615:CLA:H151	31:b:615:CLA:H18	1.74	0.45
2:g:127:LYS:HA	30:n:301:CHL:HED2	1.98	0.45
3:n:121:TRP:CH2	31:y:615:CLA:HBB2	2.52	0.45
19:s:180:GLU:HG3	31:s:310:CLA:C4B	2.47	0.45
28:P1:11:GLY:HA2	28:P1:70:ASP:HB2	1.97	0.45
3:3:200:LEU:HD21	31:3:313:CLA:O1A	2.15	0.45
3:5:49:LEU:HB2	3:5:52:PHE:O	2.17	0.45
31:5:611:CLA:HHC	31:5:611:CLA:CBB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:445:THR:HG21	8:D:293:LEU:HD13	1.98	0.45
19:S:218:PRO:HD2	32:S:317:LUT:H23	1.97	0.45
32:S:318:LUT:H31	32:S:318:LUT:H391	1.74	0.45
30:Y:301:CHL:H122	30:Y:302:CHL:H61	1.99	0.45
30:0:606:CHL:HMB1	30:0:606:CHL:HBB1	1.98	0.45
1:7:191:ASP:OD2	1:7:194:THR:HG23	2.17	0.45
1:7:221:ILE:HD12	1:7:221:ILE:HA	1.80	0.45
31:7:312:CLA:H2	31:7:312:CLA:H62	1.72	0.45
3:p:74:LEU:HD21	31:q:305:CLA:H12	1.97	0.45
31:q:313:CLA:C2C	38:x:201:SQD:H142	2.46	0.45
31:q:315:CLA:C10	37:q:321:XAT:H34	2.41	0.45
6:b:450:TRP:NE1	31:b:608:CLA:HBA1	2.32	0.45
31:b:616:CLA:H52	31:b:617:CLA:HBB1	1.97	0.45
33:b:628:LHG:H132	33:b:628:LHG:C25	2.46	0.45
30:g:309:CHL:H41	31:n:303:CLA:H161	1.99	0.45
31:n:316:CLA:C1C	34:n:322:LMG:H331	2.47	0.45
19:s:234:LYS:HD3	31:s:313:CLA:HAA2	1.97	0.45
24:y:239:LEU:HB2	32:y:616:LUT:H22	1.98	0.45
1:1:137:ILE:HB	1:1:140:LEU:HD23	1.99	0.45
2:2:82:GLU:O	2:2:86:ARG:HG2	2.16	0.45
30:2:606:CHL:HAA2	30:2:606:CHL:HBD	1.98	0.45
31:3:312:CLA:H2	31:3:313:CLA:OBD	2.17	0.45
34:5:620:LMG:HC8	34:5:620:LMG:C36	2.47	0.45
30:6:309:CHL:HMA1	36:6:319:NEX:H402	1.98	0.45
32:6:317:LUT:H35	32:6:317:LUT:H401	1.81	0.45
31:B:603:CLA:HAB	31:B:605:CLA:H18	1.99	0.45
7:C:135:PHE:HA	31:C:612:CLA:HMC1	1.98	0.45
31:C:612:CLA:HBB1	33:C:623:LHG:H102	1.99	0.45
8:D:97:ALA:HB2	8:D:107:LEU:HD22	1.99	0.45
31:D:403:CLA:HBA2	31:D:403:CLA:H3A	1.78	0.45
2:G:46:ARG:HD3	2:G:64:GLY:HA3	1.98	0.45
31:R:316:CLA:C4B	31:R:316:CLA:H52	2.47	0.45
1:7:224:GLY:O	2:9:261:PRO:HG3	2.17	0.45
31:q:312:CLA:HBA1	35:q:317:RRX:H6	1.96	0.45
31:q:313:CLA:CMB	33:q:320:LHG:HC11	2.46	0.45
31:q:315:CLA:CGA	31:q:315:CLA:C1A	2.95	0.45
33:a:415:LHG:H251	33:a:415:LHG:H301	1.97	0.45
6:b:201:HIS:HE1	31:b:603:CLA:C1D	2.18	0.45
6:b:466:HIS:CE1	31:b:609:CLA:C4D	2.99	0.45
7:c:202:PHE:HZ	31:c:606:CLA:H13	1.80	0.45
31:g:313:CLA:H121	31:g:313:CLA:H162	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:102:LHG:H332	33:j:102:LHG:H362	1.83	0.45
31:n:315:CLA:HBA1	31:n:315:CLA:HBD	1.97	0.45
31:1:610:CLA:H62	31:1:612:CLA:HMA2	1.99	0.45
31:2:604:CLA:HED2	31:2:604:CLA:H2A	1.97	0.45
5:A:162:PRO:HB3	5:A:168:PHE:HA	1.98	0.45
5:A:262:TYR:HB3	33:A:415:LHG:HC92	1.99	0.45
5:A:288:LEU:O	5:A:292:THR:HG23	2.16	0.45
31:A:405:CLA:H3A	31:A:405:CLA:HBA1	1.71	0.45
6:B:6:TYR:O	31:B:611:CLA:HBD	2.17	0.45
31:C:602:CLA:H71	31:C:612:CLA:H42	1.98	0.45
31:C:606:CLA:H43	43:C:615:BCR:H332	1.97	0.45
8:D:126:MET:HE3	8:D:143:ALA:O	2.16	0.45
9:E:18:ARG:NH1	27:Q1:26:PRO:HG3	2.31	0.45
9:E:22:ILE:HG23	27:Q1:19:VAL:HG22	1.97	0.45
31:N:304:CLA:HBC1	30:N:309:CHL:HAC2	1.97	0.45
31:0:610:CLA:H92	32:0:616:LUT:H371	1.98	0.45
3:p:129:PHE:HE2	30:p:607:CHL:HMD1	1.81	0.45
43:a:410:BCR:H21C	43:a:410:BCR:H361	1.99	0.45
6:b:477:ASP:N	6:b:477:ASP:OD1	2.48	0.45
7:c:296:GLU:HG3	7:c:349:PHE:CZ	2.51	0.45
8:d:253:TRP:CG	44:d:407:PL9:HC71	2.52	0.45
42:d:402:PHO:H2	42:d:402:PHO:H61	1.61	0.45
18:r:140:GLY:HA3	18:r:241:ALA:HB1	1.97	0.45
19:s:164:PRO:HD2	19:s:167:ALA:HB3	1.97	0.45
2:2:90:ILE:HD13	31:2:603:CLA:HBA1	1.98	0.45
30:3:308:CHL:HMB2	30:3:310:CHL:OMC	2.17	0.45
3:5:48:PHE:N	3:5:67:TYR:HB3	2.32	0.45
3:5:215:MET:HE2	32:5:617:LUT:C10	2.35	0.45
3:5:237:LEU:HD22	31:5:614:CLA:HBB1	1.97	0.45
31:6:305:CLA:H3A	31:6:305:CLA:HBA2	1.47	0.45
5:A:118:HIS:HE1	31:A:409:CLA:ND	2.12	0.45
31:B:612:CLA:H61	31:B:612:CLA:H102	1.83	0.45
31:C:606:CLA:H112	31:C:606:CLA:H72	1.52	0.45
2:G:86:ARG:O	2:G:90:ILE:HG13	2.17	0.45
31:G:610:CLA:HBD	31:G:610:CLA:HBA1	1.98	0.45
3:N:117:GLY:O	3:N:118:GLU:HG3	2.16	0.45
17:O:256:GLY:O	17:O:290:LEU:N	2.50	0.45
22:W:93:TRP:CZ2	34:W:201:LMG:C11	3.00	0.45
24:Y:97:TRP:CE2	30:Y:308:CHL:HED3	2.52	0.45
1:7:176:ALA:HB2	18:r:38:ARG:NH2	2.29	0.45
1:7:219:GLN:HG2	31:7:314:CLA:C1D	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:q:305:CLA:HBC1	30:q:311:CHL:CBC	2.45	0.45
9:e:10:PHE:N	33:e:101:LHG:O5	2.44	0.45
2:g:196:ALA:HB1	2:g:202:LEU:HG	1.98	0.45
31:g:303:CLA:H2	31:g:303:CLA:O1A	2.16	0.45
31:n:316:CLA:H42	34:n:322:LMG:H121	1.99	0.45
18:r:238:ILE:HD12	18:r:239:LYS:N	2.31	0.45
19:s:138:GLU:HA	30:s:308:CHL:HED1	1.99	0.45
1:1:223:THR:HG21	31:1:613:CLA:O1D	2.16	0.45
3:3:245:PHE:HD2	3:3:246:TRP:CD1	2.34	0.45
30:3:307:CHL:C2C	34:3:321:LMG:H371	2.47	0.45
2:4:104:GLY:HA3	32:4:616:LUT:H183	1.98	0.45
31:4:604:CLA:HMA1	32:4:616:LUT:H3	1.98	0.45
30:5:606:CHL:HMC	32:5:617:LUT:H163	1.98	0.45
31:5:610:CLA:H52	32:5:616:LUT:H28	1.99	0.45
7:C:40:ALA:HB2	31:C:611:CLA:HMA2	1.98	0.45
31:G:603:CLA:HHC	31:G:603:CLA:CBB	2.46	0.45
30:Y:308:CHL:HMB3	38:Y:320:SQD:H262	1.99	0.45
31:8:612:CLA:H172	31:8:613:CLA:ND	2.32	0.45
34:a:416:LMG:H122	33:e:101:LHG:HC81	1.99	0.45
7:c:183:ASP:OD1	7:c:184:VAL:N	2.45	0.45
45:c:617:DGD:HB71	45:c:617:DGD:HB42	1.82	0.45
31:n:304:CLA:HBC2	30:n:310:CHL:HHD	1.97	0.45
22:w:89:PHE:CZ	34:w:202:LMG:H371	2.52	0.45
31:y:615:CLA:HBA2	31:y:615:CLA:H3A	1.41	0.45
30:2:606:CHL:HAB	32:2:615:LUT:H161	1.99	0.45
3:3:142:LEU:HA	30:3:307:CHL:HED2	1.99	0.45
30:4:607:CHL:H101	30:4:607:CHL:H61	1.50	0.45
30:4:607:CHL:CAA	3:5:253:SER:HB2	2.46	0.45
5:A:133:LEU:HD22	5:A:137:LEU:HG	1.99	0.45
8:D:239:GLN:OE1	8:D:241:GLU:HG2	2.16	0.45
2:G:97:TRP:CE2	30:G:607:CHL:HED2	2.52	0.45
30:N:307:CHL:HAA2	30:N:307:CHL:HBD	1.97	0.45
17:O:74:CYS:HB2	17:O:98:CYS:SG	2.57	0.45
18:R:71:ARG:NH2	18:R:235:GLU:OE2	2.22	0.45
36:R:319:NEX:C10	38:R:322:SQD:H132	2.47	0.45
20:T:21:ILE:HD12	43:T:101:BCR:H402	1.99	0.45
24:Y:70:TYR:HE2	30:Y:302:CHL:HBC2	1.81	0.45
30:0:607:CHL:H61	30:0:607:CHL:HMA3	1.99	0.45
1:7:103:LEU:HB3	31:7:305:CLA:HMC1	1.99	0.45
31:7:312:CLA:H8	31:7:313:CLA:C4D	2.47	0.45
43:a:410:BCR:H371	43:a:410:BCR:H24C	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:204:ALA:HB3	31:b:603:CLA:HAB	1.99	0.45
31:c:612:CLA:H61	31:c:612:CLA:H41	1.82	0.45
2:g:132:ILE:HG21	2:g:152:ILE:HG12	1.98	0.45
18:r:180:PRO:HG2	18:r:181:PHE:CE2	2.52	0.45
19:s:83:TYR:HB2	31:s:303:CLA:HMD1	1.99	0.45
33:s:322:LHG:H251	25:z:41:PHE:CD1	2.52	0.45
22:w:89:PHE:CE2	34:w:202:LMG:H422	2.52	0.45
1:1:40:GLN:O	1:1:46:ARG:HA	2.17	0.45
1:1:72:TRP:HD1	1:1:74:THR:HG23	1.81	0.45
1:1:204:LYS:HE3	33:1:617:LHG:HC61	1.98	0.45
30:1:609:CHL:HBD	30:1:609:CHL:HAA1	1.99	0.45
31:1:610:CLA:H62	31:1:612:CLA:CMA	2.47	0.45
2:2:147:ILE:HA	30:2:605:CHL:C4D	2.46	0.45
3:3:237:LEU:HD11	31:3:315:CLA:HMC3	1.99	0.45
2:4:138:LEU:HD13	30:4:606:CHL:CMD	2.47	0.45
2:4:166:ALA:HA	2:4:169:TYR:CD2	2.52	0.45
31:4:610:CLA:H41	31:4:610:CLA:H61	1.55	0.45
32:4:616:LUT:H35	32:4:616:LUT:H401	1.87	0.45
4:6:94:ALA:HB1	4:6:210:GLY:HA3	1.98	0.45
31:B:611:CLA:H152	31:B:613:CLA:O1D	2.17	0.45
45:C:620:DGD:HBV1	34:W:201:LMG:H142	1.99	0.45
8:D:51:GLY:HA2	8:D:55:VAL:HB	1.98	0.45
8:D:199:MET:HG2	44:D:406:PL9:H321	1.99	0.45
43:D:405:BCR:H321	43:D:405:BCR:HC8	1.98	0.45
43:D:405:BCR:H363	10:F:32:PHE:HB3	1.97	0.45
33:G:618:LHG:H281	37:G:620:XAT:C31	2.46	0.45
33:L:101:LHG:H101	33:L:101:LHG:H132	1.75	0.45
3:N:233:LEU:HD22	32:N:316:LUT:H163	1.99	0.45
30:N:306:CHL:H12	19:S:123:GLY:HA3	1.99	0.45
17:O:122:THR:HB	17:O:162:VAL:HB	1.99	0.45
36:R:301:NEX:H15	36:R:301:NEX:H201	1.88	0.45
30:R:308:CHL:HAA2	30:R:308:CHL:HBD	1.98	0.45
30:Y:307:CHL:HAA2	30:Y:307:CHL:HBD	1.98	0.45
31:0:610:CLA:H41	31:0:610:CLA:H61	1.54	0.45
31:0:610:CLA:H3A	31:0:610:CLA:HBA2	1.35	0.45
2:9:69:ASP:HA	31:9:304:CLA:O1D	2.16	0.45
30:9:308:CHL:C1C	30:9:309:CHL:HBC2	2.47	0.45
37:9:322:XAT:H31	37:9:322:XAT:H391	1.77	0.45
31:p:610:CLA:H12	31:p:610:CLA:C3A	2.47	0.45
2:q:198:ASP:HB3	2:q:201:THR:OG1	2.17	0.45
31:q:306:CLA:H92	31:q:306:CLA:H61	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:309:CHL:O1A	30:q:309:CHL:C2	2.64	0.45
5:a:201:GLY:HA3	5:a:286:THR:HB	1.99	0.45
38:a:412:SQD:H121	34:a:413:LMG:H291	1.99	0.45
6:b:270:PRO:HG3	6:b:312:TYR:CD1	2.52	0.45
33:b:625:LHG:H101	33:b:625:LHG:H352	1.99	0.45
33:b:625:LHG:H341	33:b:625:LHG:H311	1.54	0.45
7:c:156:LEU:HD11	31:c:609:CLA:H61	1.99	0.45
7:c:240:ILE:CG2	34:c:620:LMG:H121	2.46	0.45
7:c:326:GLY:HA2	17:o:157:TYR:OH	2.17	0.45
31:c:610:CLA:H12	31:c:610:CLA:HBA2	1.76	0.45
45:c:618:DGD:HB51	34:d:409:LMG:H121	1.98	0.45
2:g:95:ALA:HB1	2:g:213:GLY:HA3	1.98	0.45
30:n:310:CHL:HBD	30:n:310:CHL:HAA1	1.98	0.45
19:s:113:LEU:HB3	31:s:305:CLA:HAB	1.99	0.45
24:y:203:LEU:HD22	24:y:207:LYS:HE3	1.99	0.45
29:f1:170:ASP:HB2	29:f1:176:TYR:CE1	2.51	0.45
1:1:100:LEU:HB3	31:1:604:CLA:HAB	1.99	0.45
1:1:219:GLN:OE1	32:1:615:LUT:H42	2.17	0.45
31:1:604:CLA:HMA2	30:1:606:CHL:CBC	2.43	0.45
2:2:139:ASN:ND2	2:2:144:PRO:HA	2.32	0.45
31:2:613:CLA:HED2	37:2:619:XAT:C20	2.47	0.45
30:3:302:CHL:O1A	30:3:302:CHL:C2	2.65	0.45
3:5:69:TRP:CD1	32:5:617:LUT:H24	2.52	0.45
3:5:158:LEU:HA	36:5:618:NEX:C20	2.46	0.45
3:5:215:MET:HA	3:5:218:PHE:CD2	2.52	0.45
31:B:609:CLA:H2	31:B:609:CLA:H62	1.77	0.45
31:B:612:CLA:HBB1	31:B:612:CLA:CMB	2.44	0.45
8:D:126:MET:SD	8:D:150:ILE:HD12	2.57	0.45
9:E:8:ARG:HE	9:E:12:ASP:CG	2.24	0.45
3:N:122:PHE:CB	31:N:321:CLA:HAB	2.47	0.45
31:N:313:CLA:HHB	31:N:314:CLA:HBC3	1.98	0.45
17:O:86:ASP:OD1	17:O:86:ASP:N	2.49	0.45
34:7:322:LMG:H291	34:7:322:LMG:H111	1.98	0.45
31:8:610:CLA:HHC	31:8:610:CLA:CBB	2.46	0.45
2:9:197:ASP:N	2:9:197:ASP:OD1	2.49	0.45
31:9:312:CLA:C8	35:9:317:RRX:H25	2.47	0.45
3:p:177:ASP:HB3	3:p:180:TYR:O	2.17	0.45
3:p:233:LEU:O	3:p:237:LEU:HG	2.17	0.45
30:p:606:CHL:HBB1	30:p:609:CHL:HBC1	1.99	0.45
31:p:613:CLA:HED3	31:p:613:CLA:CHA	2.46	0.45
31:p:615:CLA:H3A	31:p:615:CLA:HBA2	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:89:GLU:HA	2:q:184:LEU:HD11	1.99	0.45
31:n:314:CLA:H152	31:n:314:CLA:H193	1.99	0.45
19:s:107:HIS:HE1	31:s:304:CLA:C4D	2.30	0.45
31:s:303:CLA:H61	32:s:318:LUT:H26	1.99	0.45
29:F1:174:LYS:NZ	29:F1:202:SER:HB2	2.32	0.45
33:2:617:LHG:HC82	37:2:619:XAT:H381	1.98	0.44
3:5:200:LEU:HD23	3:5:203:LYS:HD2	1.98	0.44
30:5:606:CHL:HBB1	30:5:609:CHL:HBC1	1.99	0.44
30:5:608:CHL:CMB	36:5:618:NEX:H14	2.47	0.44
30:6:310:CHL:HBD	30:6:310:CHL:HAA1	1.99	0.44
5:A:140:ARG:HB2	8:D:220:ASN:HA	2.00	0.44
6:B:486:LEU:O	6:B:490:VAL:HG23	2.17	0.44
7:C:30:LEU:HD21	31:C:611:CLA:H2A	1.98	0.44
7:C:183:ASP:OD1	7:C:184:VAL:N	2.47	0.44
31:C:605:CLA:CMD	31:C:607:CLA:HAB	2.47	0.44
34:C:621:LMG:HC71	34:C:621:LMG:HC2	1.73	0.44
34:G:622:LMG:C17	31:N:321:CLA:H43	2.43	0.44
31:N:321:CLA:HMC2	30:Y:301:CHL:HHB	1.99	0.44
31:S:312:CLA:H192	31:S:313:CLA:HBB2	1.98	0.44
4:0:93:HIS:CE1	31:0:603:CLA:C4D	2.98	0.44
4:0:144:LEU:HG	18:r:269:PHE:HE1	1.82	0.44
30:0:607:CHL:CAA	37:q:321:XAT:H41	2.46	0.44
34:9:302:LMG:HC2	34:9:302:LMG:HC72	1.72	0.44
31:p:602:CLA:H92	31:p:602:CLA:H61	1.68	0.44
2:q:149:ALA:HA	30:q:307:CHL:C1C	2.47	0.44
6:b:3:LEU:HD22	6:b:7:ARG:HB2	1.98	0.44
6:b:275:TRP:CD1	6:b:361:THR:HG23	2.52	0.44
31:b:610:CLA:H42	38:b:627:SQD:H261	1.98	0.44
34:b:622:LMG:H151	34:b:622:LMG:H182	1.76	0.44
31:c:602:CLA:H71	31:c:612:CLA:H42	1.99	0.44
2:g:76:GLY:CA	24:y:86:LYS:HD2	2.47	0.44
38:g:301:SQD:H442	31:g:311:CLA:HMB1	1.98	0.44
32:g:316:LUT:H31	32:g:316:LUT:H391	1.64	0.44
33:l:101:LHG:H331	16:m:21:PHE:CD2	2.52	0.44
3:n:87:LEU:CD1	31:n:304:CLA:HBA1	2.44	0.44
37:r:318:XAT:H15	37:r:318:XAT:H201	1.78	0.44
1:1:188:LEU:CD1	32:1:615:LUT:H221	2.47	0.44
2:2:96:ARG:HA	2:2:99:MET:HE3	2.00	0.44
2:2:134:ASN:O	2:2:135:GLU:C	2.60	0.44
2:2:138:LEU:HD11	30:2:606:CHL:HAC1	1.99	0.44
3:3:98:GLY:HA3	32:3:318:LUT:C10	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:185:PHE:HA	30:3:309:CHL:C2	2.46	0.44
31:3:315:CLA:HHC	31:3:315:CLA:CBB	2.47	0.44
2:4:75:ALA:HB3	2:4:77:LEU:HD22	1.99	0.44
34:4:621:LMG:HC92	34:4:621:LMG:HC2	2.00	0.44
31:6:305:CLA:HBB1	31:6:305:CLA:CMB	2.46	0.44
30:6:308:CHL:H41	30:6:308:CHL:H62	1.62	0.44
5:A:132:GLU:O	5:A:136:ARG:HG2	2.17	0.44
31:A:405:CLA:H72	31:A:405:CLA:H111	1.85	0.44
6:B:43:ALA:HA	34:m:102:LMG:HC2	1.99	0.44
31:B:608:CLA:H3A	31:B:608:CLA:HBA2	1.67	0.44
31:B:615:CLA:H122	31:B:615:CLA:H162	1.67	0.44
31:C:604:CLA:CAD	45:C:617:DGD:HB21	2.47	0.44
33:G:618:LHG:H301	37:G:620:XAT:C40	2.47	0.44
3:N:226:ARG:HH22	31:N:321:CLA:HBA1	1.83	0.44
17:O:78:ASP:OD1	17:O:79:SER:N	2.46	0.44
31:S:304:CLA:HBB1	31:S:304:CLA:CMB	2.47	0.44
22:W:107:SER:O	22:W:108:ASP:HB2	2.18	0.44
4:0:220:PHE:HE1	32:0:616:LUT:H41	1.82	0.44
31:p:615:CLA:HHC	31:p:615:CLA:CBB	2.47	0.44
2:q:163:MET:CE	30:q:308:CHL:HMA3	2.47	0.44
2:q:226:GLN:NE2	35:q:317:RRX:H50	2.33	0.44
30:q:311:CHL:HBD	30:q:311:CHL:HAA1	1.98	0.44
31:b:610:CLA:C4	38:b:627:SQD:H261	2.47	0.44
7:c:130:GLU:H	7:c:130:GLU:CD	2.25	0.44
7:c:452:GLU:OE2	8:d:245:SER:OG	2.34	0.44
30:g:309:CHL:HAA1	30:g:309:CHL:HBD	1.99	0.44
31:n:305:CLA:CHA	31:n:305:CLA:HBA1	2.40	0.44
34:n:322:LMG:O9	34:n:322:LMG:H142	2.17	0.44
26:u:73:GLU:OE2	26:u:89:GLN:NE2	2.51	0.44
31:2:609:CLA:H72	35:2:614:RRX:H25	1.99	0.44
2:4:167:GLU:HG3	30:4:609:CHL:C4B	2.47	0.44
2:4:253:SER:HB2	2:4:256:LYS:HZ2	1.83	0.44
31:5:613:CLA:H52	31:5:613:CLA:NC	2.31	0.44
31:6:311:CLA:H52	31:6:311:CLA:H8	1.47	0.44
31:D:404:CLA:H62	31:D:404:CLA:H41	1.41	0.44
2:G:259:PRO:HD3	30:G:623:CHL:H12	1.98	0.44
30:N:306:CHL:HAA2	30:N:306:CHL:HBD	1.98	0.44
31:S:303:CLA:H203	31:S:304:CLA:CBB	2.46	0.44
31:S:311:CLA:H161	31:S:311:CLA:H122	1.71	0.44
4:0:182:TYR:CE2	4:0:203:LYS:HE3	2.53	0.44
1:7:67:PRO:HG3	1:7:199:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:251:LEU:CD2	30:7:321:CHL:O1A	2.66	0.44
31:7:305:CLA:HMA2	30:7:307:CHL:C2C	2.47	0.44
30:9:303:CHL:C4D	33:9:320:LHG:HC91	2.48	0.44
31:b:602:CLA:HBA2	31:b:602:CLA:H3A	1.58	0.44
7:c:206:PHE:HZ	45:c:616:DGD:HBW2	1.81	0.44
43:c:615:BCR:H20C	43:c:615:BCR:H361	1.74	0.44
31:g:312:CLA:HBB1	31:g:312:CLA:CMB	2.44	0.44
15:l:25:ILE:HG22	16:m:15:ILE:HD13	1.99	0.44
31:s:312:CLA:C3C	33:s:320:LHG:HC62	2.48	0.44
34:w:202:LMG:H111	31:y:611:CLA:H11	1.98	0.44
30:y:606:CHL:HAA2	30:y:606:CHL:HBD	1.98	0.44
2:2:145:SER:O	30:2:605:CHL:H2A	2.18	0.44
31:2:603:CLA:HED3	32:3:318:LUT:H372	1.99	0.44
3:3:185:PHE:HA	30:3:309:CHL:H2	2.00	0.44
3:3:193:ASP:HB2	3:3:196:THR:OG1	2.18	0.44
2:4:169:TYR:CD1	2:4:174:GLU:HG3	2.53	0.44
3:5:48:PHE:HD2	30:5:601:CHL:HBA1	1.82	0.44
3:5:56:PRO:HD2	3:5:59:LEU:HB2	2.00	0.44
3:5:135:ASP:HB3	3:5:139:ASN:O	2.17	0.44
31:B:611:CLA:H193	31:B:611:CLA:H162	1.75	0.44
34:C:622:LMG:HC8	34:N:320:LMG:O10	2.17	0.44
2:G:168:ALA:HB1	3:N:52:PHE:CG	2.52	0.44
31:G:609:CLA:H122	35:G:614:RRX:H22	1.99	0.44
32:G:615:LUT:H28	32:G:615:LUT:H361	1.98	0.44
17:O:106:VAL:HB	17:O:164:LEU:HD21	1.99	0.44
19:S:39:TRP:HE1	34:S:321:LMG:HC3	1.82	0.44
22:W:110:GLU:O	22:W:112:ASP:N	2.45	0.44
1:7:178:TYR:CE2	1:7:199:LYS:HE3	2.52	0.44
31:7:305:CLA:HMA2	30:7:307:CHL:HBC3	1.99	0.44
3:8:100:LEU:HD13	31:8:611:CLA:HBB2	1.99	0.44
3:p:144:HIS:CE1	3:p:146:GLN:HE22	2.35	0.44
2:q:138:LEU:HD21	31:q:306:CLA:HAA1	1.99	0.44
33:q:320:LHG:HC5	37:q:321:XAT:C38	2.46	0.44
34:b:601:LMG:H311	34:b:601:LMG:H141	2.00	0.44
3:n:106:GLU:O	3:n:110:ARG:HG2	2.17	0.44
31:s:303:CLA:CAB	32:s:318:LUT:H32	2.47	0.44
34:w:202:LMG:H211	31:y:612:CLA:C14	2.43	0.44
30:y:606:CHL:HBB1	32:y:617:LUT:H161	1.99	0.44
29:f1:178:LYS:HB3	29:f1:230:TRP:CZ2	2.53	0.44
3:3:125:GLY:HA2	30:3:308:CHL:HAC2	1.99	0.44
2:4:93:ILE:HG22	2:4:97:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:158:THR:HG21	30:4:606:CHL:CED	2.47	0.44
2:4:179:THR:HB	2:4:188:GLY:CA	2.48	0.44
2:4:202:LEU:O	2:4:206:LYS:N	2.50	0.44
2:4:228:LEU:HD11	34:4:621:LMG:H361	1.98	0.44
3:5:110:ARG:HH22	3:5:231:GLU:HA	1.82	0.44
5:A:107:TYR:CG	17:O:125:MET:HG3	2.53	0.44
6:B:26:HIS:O	6:B:30:VAL:HG23	2.17	0.44
6:B:33:TRP:CD1	43:t:101:BCR:H332	2.52	0.44
2:G:107:THR:HB	2:G:108:PRO:HD3	1.99	0.44
2:G:221:PHE:CE2	31:G:612:CLA:HAC1	2.52	0.44
15:L:30:VAL:HG22	20:T:9:LEU:HB3	1.99	0.44
31:N:304:CLA:HAC1	30:Y:301:CHL:CBB	2.42	0.44
36:S:319:NEX:H35	36:S:319:NEX:H401	1.87	0.44
3:8:39:GLU:O	3:8:46:PRO:HD3	2.16	0.44
31:p:613:CLA:HAA1	31:p:613:CLA:HBD	1.99	0.44
2:q:100:LEU:HB3	31:q:306:CLA:HAB	1.99	0.44
7:c:274:ALA:HB2	31:c:602:CLA:HMD1	2.00	0.44
8:d:45:LEU:HD12	8:d:49:PHE:HE2	1.82	0.44
2:g:86:ARG:HG3	3:n:73:GLY:HA3	1.98	0.44
31:n:304:CLA:HBA2	31:n:304:CLA:H12	1.60	0.44
18:r:71:ARG:NH2	18:r:235:GLU:OE2	2.31	0.44
32:r:317:LUT:H15	32:r:317:LUT:H201	1.90	0.44
31:y:613:CLA:H62	31:y:613:CLA:C1C	2.48	0.44
27:q1:15:VAL:O	27:q1:19:VAL:HG23	2.18	0.44
2:2:235:LEU:HD13	34:2:618:LMG:HC72	2.00	0.44
30:2:608:CHL:HMB3	30:3:303:CHL:HHB	1.99	0.44
2:4:180:SER:O	2:4:182:ASP:N	2.51	0.44
3:5:105:PRO:HA	3:5:116:PHE:CE2	2.52	0.44
4:6:251:TYR:HB2	4:6:252:ALA:H	1.56	0.44
6:B:492:PHE:HB2	9:E:2:SER:O	2.17	0.44
31:B:611:CLA:H112	31:B:611:CLA:H72	1.64	0.44
33:B:624:LHG:H251	33:B:624:LHG:H132	1.98	0.44
8:D:67:TYR:O	34:D:409:LMG:O5	2.26	0.44
8:D:239:GLN:HG3	8:D:241:GLU:OE2	2.16	0.44
3:N:158:LEU:HG	36:N:318:NEX:H15	1.98	0.44
18:R:208:GLU:HA	18:R:211:CSU:OD2	2.18	0.44
31:R:305:CLA:HBC1	31:R:311:CLA:HBC2	1.99	0.44
31:0:610:CLA:H12	31:0:610:CLA:CHB	2.47	0.44
30:7:321:CHL:H122	30:8:608:CHL:CMC	2.47	0.44
3:8:246:TRP:O	2:9:133:PHE:CZ	2.71	0.44
3:p:250:ALA:C	3:p:252:LYS:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:49:ILE:HG21	34:m:102:LMG:H381	2.00	0.44
5:a:267:ASN:HD22	38:a:411:SQD:C3	2.29	0.44
6:b:328:GLY:HA3	34:b:622:LMG:HC5	1.98	0.44
33:d:408:LHG:H311	33:d:408:LHG:H341	1.76	0.44
2:g:251:PHE:HB3	24:y:132:PHE:HZ	1.81	0.44
12:i:27:ASP:N	12:i:28:PRO:CD	2.81	0.44
14:k:38:VAL:HG23	43:v:101:BCR:H21C	1.99	0.44
16:m:12:ALA:O	16:m:16:ILE:HG12	2.18	0.44
17:o:153:ASP:N	17:o:153:ASP:OD1	2.51	0.44
30:r:309:CHL:H62	30:r:309:CHL:H41	1.79	0.44
31:r:315:CLA:HBA2	31:r:315:CLA:H3A	1.36	0.44
19:s:251:VAL:HG21	31:s:314:CLA:HAC2	2.00	0.44
19:s:264:TRP:CD1	32:s:317:LUT:H163	2.53	0.44
20:t:21:ILE:HD12	43:t:101:BCR:H401	2.00	0.44
34:y:620:LMG:O9	34:y:620:LMG:H162	2.18	0.44
1:1:237:ASP:HB3	1:1:240:ALA:HB3	1.98	0.44
2:2:54:SER:O	2:2:58:VAL:HG23	2.18	0.44
2:2:90:ILE:HG23	30:2:608:CHL:OBD	2.18	0.44
2:2:132:ILE:HB	2:2:138:LEU:HD12	1.99	0.44
2:2:138:LEU:CD1	30:2:606:CHL:HHD	2.48	0.44
31:2:603:CLA:HBC1	30:2:608:CHL:CBC	2.48	0.44
3:3:236:HIS:CB	31:3:314:CLA:HAA2	2.44	0.44
31:3:306:CLA:H92	36:3:319:NEX:H403	1.99	0.44
2:4:186:PRO:HB2	2:4:190:PHE:CD1	2.53	0.44
3:5:98:GLY:HA2	32:5:617:LUT:H181	2.00	0.44
3:5:190:LEU:HB2	31:5:610:CLA:CGA	2.47	0.44
3:5:210:LEU:HA	33:5:619:LHG:H301	1.99	0.44
31:B:614:CLA:HBB1	31:B:614:CLA:CMB	2.48	0.44
38:B:623:SQD:H151	8:D:127:LEU:HD13	1.99	0.44
33:D:408:LHG:H362	43:T:101:BCR:H281	2.00	0.44
2:G:84:PHE:O	2:G:88:ARG:HG3	2.17	0.44
2:G:154:ALA:O	2:G:158:THR:OG1	2.30	0.44
31:G:610:CLA:H2	31:G:611:CLA:OBD	2.17	0.44
31:N:310:CLA:HBA2	31:N:310:CLA:H3A	1.41	0.44
32:N:317:LUT:H15	32:N:317:LUT:H201	1.85	0.44
19:S:149:LEU:HG	31:S:305:CLA:HED1	1.99	0.44
24:Y:107:PHE:HB3	24:Y:108:PRO:HD3	2.00	0.44
30:Y:307:CHL:CBB	32:Y:316:LUT:H161	2.48	0.44
31:8:612:CLA:H151	31:8:613:CLA:CMD	2.47	0.44
31:8:614:CLA:C4	34:9:302:LMG:H112	2.46	0.44
2:q:72:TRP:CE3	32:q:318:LUT:H383	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:401:LMG:H111	34:a:401:LMG:HC8	1.39	0.44
6:b:6:TYR:HB2	33:b:625:LHG:H382	2.00	0.44
8:d:51:GLY:HA2	8:d:55:VAL:HB	1.98	0.44
9:e:23:HIS:HA	9:e:26:THR:OG1	2.18	0.44
31:g:314:CLA:HAA2	31:g:314:CLA:H12	2.00	0.44
34:m:102:LMG:H311	34:m:102:LMG:H342	1.75	0.44
31:n:315:CLA:HBA1	31:n:315:CLA:CBD	2.47	0.44
34:n:321:LMG:O1	34:n:321:LMG:HC61	2.18	0.44
18:r:269:PHE:CD1	31:r:315:CLA:HAA2	2.53	0.44
31:s:305:CLA:CHC	36:s:319:NEX:H362	2.48	0.44
22:w:116:GLY:O	22:w:118:THR:HG23	2.18	0.44
1:1:86:ARG:HA	1:1:86:ARG:HE	1.83	0.44
3:3:186:ASP:HA	32:3:317:LUT:C24	2.36	0.44
2:4:96:ARG:HA	2:4:99:MET:HE3	2.00	0.44
2:4:195:LEU:HB2	31:4:610:CLA:CGA	2.47	0.44
2:4:253:SER:HB2	2:4:256:LYS:NZ	2.33	0.44
30:4:607:CHL:H42	3:5:245:PHE:CE2	2.53	0.44
31:5:610:CLA:C5	32:5:616:LUT:H30	2.45	0.44
4:6:244:THR:O	4:6:249:SER:HB2	2.18	0.44
30:6:308:CHL:H101	30:6:308:CHL:H62	1.75	0.44
45:C:618:DGD:HE4	13:J:42:LEU:HD11	1.99	0.44
34:C:621:LMG:HC8	34:C:621:LMG:H111	1.58	0.44
8:D:210:LEU:HA	8:D:213:ILE:HG22	2.00	0.44
14:K:27:VAL:O	14:K:30:VAL:HG12	2.18	0.44
3:N:235:ASP:O	3:N:243:THR:HG21	2.18	0.44
30:N:308:CHL:HAA1	30:N:308:CHL:HBD	2.00	0.44
31:N:313:CLA:H13	33:N:319:LHG:H321	1.99	0.44
18:R:174:TYR:HD2	31:R:306:CLA:CBA	2.30	0.44
31:R:305:CLA:H143	31:R:305:CLA:H111	1.78	0.44
30:R:309:CHL:HHC	30:R:309:CHL:CBB	2.46	0.44
32:R:317:LUT:H393	32:R:317:LUT:H27	1.84	0.44
19:S:264:TRP:CD1	32:S:317:LUT:H163	2.53	0.44
31:S:312:CLA:H92	31:S:312:CLA:H61	1.67	0.44
31:Y:303:CLA:H93	31:Y:304:CLA:HMB1	2.00	0.44
30:0:607:CHL:HAA1	37:q:321:XAT:C4	2.48	0.44
3:8:223:LEU:CD2	34:9:302:LMG:H172	2.47	0.44
3:p:131:GLU:H	3:p:131:GLU:CD	2.26	0.44
2:q:99:MET:HB2	31:q:312:CLA:HMC2	2.00	0.44
30:q:309:CHL:HBB2	30:q:311:CHL:HBC1	2.00	0.44
30:q:310:CHL:HHC	30:q:310:CHL:CBB	2.44	0.44
31:q:312:CLA:H2	35:q:317:RRX:H8	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:272:ARG:HA	6:b:318:ASN:ND2	2.33	0.44
6:b:458:PHE:HB3	31:b:605:CLA:HBC2	2.00	0.44
31:c:608:CLA:H152	31:c:608:CLA:H112	1.77	0.44
19:s:221:LEU:HD12	31:s:311:CLA:H12	2.00	0.44
1:1:94:HIS:CE1	31:1:603:CLA:C4D	3.00	0.44
1:1:246:LEU:H	1:1:246:LEU:HD22	1.83	0.44
2:2:139:ASN:OD1	2:2:148:HIS:HA	2.18	0.44
3:3:245:PHE:HB3	31:3:314:CLA:C2	2.48	0.44
31:3:304:CLA:H93	31:3:304:CLA:H111	1.64	0.44
2:4:146:LEU:HD13	30:4:605:CHL:O1D	2.18	0.44
3:5:91:HIS:HE1	31:5:603:CLA:C4D	2.30	0.44
3:5:121:TRP:CE2	3:5:122:PHE:HD1	2.36	0.44
3:5:161:LEU:HB3	3:5:165:TYR:CE2	2.52	0.44
32:5:617:LUT:H31	32:5:617:LUT:H391	1.87	0.44
32:5:617:LUT:H35	32:5:617:LUT:H401	1.91	0.44
4:6:45:ASP:OD1	4:6:45:ASP:N	2.47	0.44
7:C:132:PHE:HD1	33:C:623:LHG:HC11	1.82	0.44
31:N:310:CLA:H52	32:N:316:LUT:C30	2.48	0.44
31:0:611:CLA:C3C	33:0:619:LHG:HC62	2.48	0.44
1:7:251:LEU:HD23	30:7:321:CHL:O1A	2.17	0.44
30:7:306:CHL:CMA	18:r:270:ALA:HB2	2.47	0.44
2:9:90:ILE:HG23	30:9:311:CHL:OBD	2.17	0.44
2:9:241:HIS:CB	31:9:315:CLA:HAA2	2.48	0.44
2:q:200:ASP:OD1	2:q:201:THR:N	2.51	0.44
2:q:220:MET:HE2	32:q:318:LUT:H12	2.00	0.44
31:q:304:CLA:H92	31:q:305:CLA:HMA1	1.99	0.44
31:b:612:CLA:H151	31:b:614:CLA:C3D	2.48	0.44
43:b:618:BCR:H332	34:b:622:LMG:H111	1.99	0.44
7:c:267:ILE:HD11	31:c:603:CLA:H142	2.00	0.44
30:n:308:CHL:HMA2	31:y:615:CLA:CHC	2.48	0.44
32:n:318:LUT:H35	32:n:318:LUT:H401	1.87	0.44
18:r:174:TYR:HD1	31:r:306:CLA:HBA1	1.83	0.44
23:x:88:GLY:O	23:x:91:THR:HG22	2.18	0.44
26:u:157:ALA:HB2	26:u:197:LYS:HZ1	1.83	0.44
1:1:176:ALA:HB2	18:R:38:ARG:HH21	1.82	0.43
34:1:618:LMG:H151	31:R:313:CLA:NC	2.33	0.43
2:2:260:LEU:O	34:2:620:LMG:HC61	2.18	0.43
3:3:127:GLN:HE22	31:3:306:CLA:HED2	1.82	0.43
31:3:305:CLA:HBC2	30:3:310:CHL:HHD	1.99	0.43
2:4:147:ILE:HG23	30:4:605:CHL:CHD	2.48	0.43
34:4:620:LMG:HC91	34:4:621:LMG:C15	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:197:PHE:CE2	45:C:617:DGD:HBV2	2.53	0.43
5:A:299:GLY:O	7:C:391:SER:HB2	2.18	0.43
31:B:607:CLA:H141	31:B:607:CLA:H162	1.73	0.43
3:N:47:GLN:HG3	3:N:53:SER:CB	2.44	0.43
30:N:302:CHL:HED1	33:N:319:LHG:H292	2.00	0.43
30:N:307:CHL:HMB1	30:N:309:CHL:HAC1	2.00	0.43
2:9:230:THR:HG21	2:9:237:ASN:ND2	2.33	0.43
3:p:38:VAL:HA	3:p:41:TYR:O	2.18	0.43
2:q:138:LEU:O	2:q:138:LEU:HD23	2.18	0.43
2:q:254:ALA:O	37:q:321:XAT:H42	2.18	0.43
31:q:315:CLA:C2B	35:q:317:RRX:H53	2.47	0.43
31:q:315:CLA:H2	31:q:315:CLA:H61	1.61	0.43
33:a:415:LHG:HC92	7:c:24:TRP:CZ3	2.53	0.43
6:b:202:HIS:HE1	31:b:604:CLA:NA	2.13	0.43
7:c:117:GLY:O	7:c:121:SER:OG	2.28	0.43
7:c:120:HIS:HE1	31:c:613:CLA:C1A	2.30	0.43
7:c:219:GLU:HG3	26:u:173:ARG:NH1	2.33	0.43
7:c:392:LEU:HD22	7:c:392:LEU:HA	1.86	0.43
31:c:610:CLA:H152	31:c:610:CLA:H112	1.84	0.43
9:e:8:ARG:CD	9:e:13:ILE:HG12	2.48	0.43
2:g:72:TRP:CZ3	32:g:316:LUT:H383	2.53	0.43
2:g:107:THR:HB	2:g:108:PRO:HD3	2.00	0.43
38:g:301:SQD:H111	37:g:321:XAT:H222	1.99	0.43
31:n:303:CLA:HBA1	32:n:318:LUT:H382	1.99	0.43
36:r:301:NEX:H35	36:r:301:NEX:H401	1.84	0.43
34:w:202:LMG:H252	31:y:612:CLA:C16	2.47	0.43
31:y:603:CLA:HED2	31:y:603:CLA:H2A	2.00	0.43
1:1:246:LEU:HD23	1:1:247:TYR:CD2	2.52	0.43
2:2:62:LEU:HD13	2:2:71:GLY:HA2	2.00	0.43
2:2:139:ASN:CG	2:2:144:PRO:HA	2.43	0.43
3:3:169:GLY:HA2	30:3:309:CHL:HAC1	2.00	0.43
2:4:99:MET:HG3	2:4:213:GLY:HA2	2.00	0.43
3:5:206:LYS:HG2	33:5:619:LHG:H252	1.99	0.43
31:5:610:CLA:H2	32:5:616:LUT:C28	2.44	0.43
5:A:77:ILE:HD13	15:L:30:VAL:HG13	1.98	0.43
5:A:333:GLU:HB3	5:A:336:ALA:HB3	2.00	0.43
31:A:409:CLA:H122	34:A:412:LMG:H162	2.00	0.43
43:A:410:BCR:H24C	43:A:410:BCR:H371	1.89	0.43
6:B:75:TRP:CE2	38:a:412:SQD:H441	2.53	0.43
43:B:617:BCR:C2	34:B:621:LMG:H292	2.45	0.43
7:C:151:ILE:HG21	31:C:612:CLA:C3B	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:155:SER:HA	8:D:159:ILE:HB	1.98	0.43
8:D:201:VAL:HG22	31:D:403:CLA:C2B	2.48	0.43
18:R:44:TYR:HB2	36:R:301:NEX:O3	2.18	0.43
18:R:163:ALA:O	18:R:167:LEU:HG	2.17	0.43
31:S:303:CLA:CAB	32:S:318:LUT:H32	2.49	0.43
1:7:92:VAL:HG11	1:7:177:VAL:CG1	2.49	0.43
1:7:188:LEU:HB2	31:7:311:CLA:O1A	2.18	0.43
3:8:106:GLU:O	3:8:110:ARG:HG2	2.17	0.43
2:9:96:ARG:HA	2:9:99:MET:HE3	1.98	0.43
3:p:233:LEU:HA	31:p:613:CLA:HMA2	1.98	0.43
5:a:32:TRP:O	5:a:35:VAL:HG22	2.19	0.43
7:c:112:VAL:HG21	43:c:614:BCR:C17	2.48	0.43
45:c:619:DGD:O4E	33:y:619:LHG:HC12	2.18	0.43
38:g:318:SQD:H462	38:g:318:SQD:H2	2.00	0.43
31:r:306:CLA:HMA3	30:r:308:CHL:C3C	2.48	0.43
2:2:253:SER:HB2	2:2:256:LYS:HG2	2.00	0.43
2:4:96:ARG:HD2	30:4:608:CHL:OBD	2.17	0.43
4:6:110:LEU:HD21	34:6:322:LMG:C33	2.40	0.43
7:C:274:ALA:HB2	31:C:602:CLA:HMD1	1.99	0.43
34:D:410:LMG:H202	34:D:410:LMG:H172	1.82	0.43
31:R:316:CLA:HBA2	31:R:316:CLA:H3A	1.24	0.43
24:Y:145:LEU:HD11	34:Y:319:LMG:H301	1.99	0.43
30:Y:301:CHL:H51	30:Y:301:CHL:NC	2.34	0.43
26:U:93:ASN:O	26:U:96:VAL:HG22	2.18	0.43
4:0:255:LEU:O	4:0:256:ALA:C	2.61	0.43
1:7:100:LEU:HB3	31:7:305:CLA:HAB	1.99	0.43
31:8:612:CLA:H193	31:8:612:CLA:H152	1.99	0.43
2:9:205:LEU:HD22	31:9:312:CLA:H43	2.00	0.43
34:9:301:LMG:H161	34:9:301:LMG:H132	1.75	0.43
3:p:247:VAL:HG22	2:q:133:PHE:HD2	1.82	0.43
3:p:247:VAL:HG22	2:q:133:PHE:CE2	2.54	0.43
31:p:602:CLA:H62	31:p:603:CLA:H3A	1.99	0.43
31:p:613:CLA:C1	31:p:614:CLA:HMD2	2.48	0.43
2:q:190:PHE:HZ	30:q:310:CHL:NB	2.16	0.43
31:b:612:CLA:C4B	31:b:614:CLA:HMA2	2.48	0.43
31:b:614:CLA:H92	31:b:614:CLA:H61	1.60	0.43
31:c:608:CLA:HBC3	31:c:610:CLA:H71	2.01	0.43
2:g:162:ILE:HD12	30:g:307:CHL:HED2	2.00	0.43
3:n:252:LYS:HB2	3:n:258:TYR:HD2	1.83	0.43
31:n:314:CLA:H151	31:n:315:CLA:CMD	2.48	0.43
17:o:122:THR:HG22	17:o:164:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:TRP:H	2:2:49:TRP:CD1	2.36	0.43
2:2:112:GLN:HA	2:2:117:ALA:HA	2.00	0.43
3:3:91:HIS:HE1	31:3:305:CLA:ND	2.13	0.43
3:3:218:PHE:HD1	3:3:229:PRO:HB3	1.83	0.43
3:3:223:LEU:HD22	3:3:223:LEU:HA	1.87	0.43
3:3:233:LEU:C	3:3:233:LEU:HD13	2.43	0.43
3:3:246:TRP:HA	3:3:250:ALA:HB3	2.00	0.43
31:3:304:CLA:H93	31:3:305:CLA:HMB1	2.00	0.43
2:4:168:ALA:HB1	3:5:52:PHE:CG	2.52	0.43
31:4:611:CLA:CHD	33:4:618:LHG:HC62	2.49	0.43
3:5:96:MET:HG3	3:5:208:GLY:HA2	2.00	0.43
5:A:27:ARG:NH2	8:D:258:GLY:O	2.46	0.43
5:A:133:LEU:HD11	8:D:255:GLN:HB2	2.01	0.43
33:A:417:LHG:H292	33:A:417:LHG:H322	1.77	0.43
6:B:30:VAL:HG12	31:B:605:CLA:HHD	2.00	0.43
6:B:204:ALA:HA	34:B:625:LMG:H322	1.99	0.43
33:C:623:LHG:H331	33:C:623:LHG:H362	1.68	0.43
8:D:241:GLU:CD	8:D:241:GLU:H	2.26	0.43
31:G:612:CLA:HMA1	35:G:614:RRX:C4	2.48	0.43
16:M:4:ASN:C	16:M:6:LEU:N	2.76	0.43
31:N:305:CLA:H152	31:S:306:CLA:C4A	2.48	0.43
18:R:56:ASN:ND2	18:R:56:ASN:O	2.52	0.43
31:R:312:CLA:H3A	31:R:312:CLA:HBA2	1.25	0.43
24:Y:187:PRO:HD2	31:Y:310:CLA:OBD	2.18	0.43
1:7:96:ARG:HA	1:7:99:MET:HE3	2.00	0.43
1:7:183:PHE:HZ	30:7:309:CHL:C1C	2.32	0.43
34:9:301:LMG:H321	34:9:301:LMG:H352	1.83	0.43
3:p:245:PHE:HB2	31:p:613:CLA:OBD	2.19	0.43
31:b:611:CLA:C2	31:b:611:CLA:H72	2.48	0.43
7:c:203:ARG:HG3	7:c:211:TRP:HA	1.98	0.43
8:d:12:ARG:NH1	8:d:16:ASP:HB3	2.33	0.43
31:s:311:CLA:H11	32:s:317:LUT:H373	2.00	0.43
33:y:619:LHG:H331	33:y:619:LHG:H362	1.85	0.43
25:z:15:VAL:HG11	25:z:50:LEU:HD12	2.00	0.43
29:f1:216:LYS:NZ	29:f1:217:ARG:HH12	2.16	0.43
1:1:150:LEU:CD1	37:2:619:XAT:H202	2.49	0.43
31:3:314:CLA:H2	31:3:314:CLA:C4D	2.48	0.43
2:4:171:TYR:CD2	3:5:49:LEU:HD12	2.54	0.43
37:4:619:XAT:H31	37:4:619:XAT:H391	1.77	0.43
34:4:620:LMG:H111	34:4:620:LMG:H142	1.72	0.43
3:5:141:SER:O	30:5:605:CHL:H2A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:184:ALA:O	3:5:187:PRO:HD3	2.18	0.43
4:6:104:CYS:SG	4:6:217:MET:HE1	2.59	0.43
8:D:117:HIS:CE1	31:D:404:CLA:C4D	3.00	0.43
8:D:261:PHE:CE2	33:D:408:LHG:HC81	2.53	0.43
8:D:279:LEU:HD11	42:D:401:PHO:CMC	2.48	0.43
14:K:21:ILE:HD11	33:K:102:LHG:H271	2.00	0.43
32:N:316:LUT:H15	32:N:316:LUT:H201	1.82	0.43
22:W:87:ILE:O	22:W:91:ILE:HG13	2.18	0.43
1:7:99:MET:SD	31:7:311:CLA:HAB	2.59	0.43
1:7:244:TYR:CD1	31:7:315:CLA:HED3	2.53	0.43
31:8:602:CLA:H141	31:8:602:CLA:H162	1.82	0.43
31:8:604:CLA:HBB1	31:8:604:CLA:CMB	2.48	0.43
2:9:99:MET:HB3	35:9:317:RRX:C18	2.48	0.43
2:9:146:LEU:O	2:9:148:HIS:N	2.51	0.43
2:9:230:THR:HG23	2:9:232:LYS:N	2.27	0.43
2:q:96:ARG:HA	2:q:99:MET:HE3	1.99	0.43
2:q:124:VAL:HG13	2:q:126:PHE:CE1	2.54	0.43
2:q:127:LYS:HA	30:q:309:CHL:HED2	2.00	0.43
31:b:612:CLA:H93	31:b:612:CLA:H62	1.86	0.43
31:c:613:CLA:HMB1	31:c:613:CLA:HBB1	2.00	0.43
45:c:616:DGD:HBW2	45:c:616:DGD:HB92	1.63	0.43
31:g:313:CLA:HBB1	31:g:313:CLA:CMB	2.49	0.43
3:n:191:ALA:HB2	31:n:311:CLA:HAA2	1.99	0.43
19:s:59:LEU:HD13	19:s:71:ILE:HD11	1.99	0.43
31:s:305:CLA:H93	36:s:319:NEX:C37	2.48	0.43
23:x:82:VAL:O	23:x:86:ILE:HG13	2.18	0.43
24:y:194:LEU:HD12	32:y:616:LUT:H222	2.01	0.43
2:2:139:ASN:HB3	2:2:143:ASN:C	2.44	0.43
31:2:602:CLA:H72	32:2:615:LUT:H31	2.00	0.43
3:3:252:LYS:HA	3:3:256:ILE:CG2	2.37	0.43
2:4:89:GLU:O	2:4:93:ILE:HG12	2.19	0.43
2:4:110:LEU:O	2:4:114:ASN:N	2.52	0.43
2:4:122:ALA:HB1	31:4:604:CLA:HED3	2.00	0.43
31:4:612:CLA:HHC	31:4:612:CLA:CBB	2.48	0.43
3:5:181:PRO:HB3	30:5:608:CHL:HBC2	2.00	0.43
30:6:309:CHL:CMA	36:6:319:NEX:H30	2.46	0.43
31:C:605:CLA:H202	31:C:605:CLA:H162	1.77	0.43
2:G:133:PHE:CE1	30:N:301:CHL:HMD3	2.53	0.43
31:G:612:CLA:HMA1	35:G:614:RRX:H57	2.00	0.43
32:G:615:LUT:H361	32:G:615:LUT:C28	2.48	0.43
34:G:621:LMG:C41	30:N:309:CHL:H161	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:151:LYS:O	26:U:155:GLN:HG2	2.18	0.43
3:8:200:LEU:HB3	31:8:609:CLA:CMA	2.48	0.43
3:8:220:VAL:O	3:8:224:ILE:HG12	2.19	0.43
3:8:245:PHE:CD1	3:8:249:TYR:HB2	2.53	0.43
32:8:616:LUT:H31	32:8:616:LUT:H391	1.95	0.43
31:9:306:CLA:HMB1	31:9:306:CLA:HBB1	1.99	0.43
30:p:609:CHL:HBD	30:p:609:CHL:HAA1	2.00	0.43
2:q:54:SER:O	2:q:58:VAL:HG23	2.18	0.43
35:q:317:RRX:H26	35:q:317:RRX:H22	1.79	0.43
2:g:97:TRP:CE2	30:g:308:CHL:HED3	2.53	0.43
31:s:312:CLA:H3A	31:s:312:CLA:HBA2	1.50	0.43
24:y:59:PRO:HG2	24:y:73:ASP:HB3	2.00	0.43
31:y:610:CLA:H61	31:y:610:CLA:H92	1.61	0.43
34:Q1:101:LMG:HC8	34:Q1:101:LMG:H111	1.32	0.43
29:F1:181:VAL:HG13	29:F1:195:GLN:HB2	2.00	0.43
1:1:48:LYS:HD3	1:1:58:VAL:HG22	2.00	0.43
1:1:223:THR:HA	1:1:247:TYR:CZ	2.54	0.43
30:1:605:CHL:HED3	18:R:266:LEU:HD21	2.00	0.43
2:2:193:LEU:HB2	2:2:195:LEU:HG	2.00	0.43
2:2:258:LEU:HD23	2:2:259:PRO:N	2.34	0.43
31:2:609:CLA:HBA1	35:2:614:RRX:C40	2.48	0.43
31:2:613:CLA:HBB1	31:2:613:CLA:CMB	2.49	0.43
3:3:93:ARG:HA	3:3:96:MET:HE3	1.99	0.43
3:3:206:LYS:HE3	33:3:320:LHG:O10	2.18	0.43
3:3:258:TYR:CE2	31:3:316:CLA:CHD	3.00	0.43
2:4:93:ILE:HD12	2:4:170:ARG:HH21	1.84	0.43
2:4:164:GLY:HA2	30:4:609:CHL:HAB	2.01	0.43
2:4:207:VAL:HA	2:4:210:ILE:HG22	2.00	0.43
3:5:40:TRP:HE3	3:5:46:PRO:HG3	1.82	0.43
7:C:158:LEU:HD22	34:C:621:LMG:H371	2.01	0.43
7:C:187:ILE:HG21	7:C:222:ILE:HG12	2.01	0.43
7:C:348:ASP:OD1	7:C:348:ASP:N	2.40	0.43
31:G:612:CLA:HMA1	35:G:614:RRX:H4	2.00	0.43
17:O:153:ASP:CG	17:O:154:GLY:H	2.26	0.43
22:W:93:TRP:HZ2	34:W:201:LMG:C11	2.31	0.43
24:Y:175:PRO:HB2	36:Y:317:NEX:H183	2.01	0.43
24:Y:206:LEU:HB3	31:Y:310:CLA:CMA	2.48	0.43
43:Z:101:BCR:H24C	43:Z:101:BCR:H371	1.81	0.43
1:7:72:TRP:O	32:7:318:LUT:H24	2.18	0.43
34:7:320:LMG:HC1	31:r:313:CLA:CMA	2.47	0.43
2:9:99:MET:O	35:9:317:RRX:H28	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:219:SER:O	2:9:223:PHE:HD1	2.01	0.43
31:p:611:CLA:H92	31:p:612:CLA:CED	2.48	0.43
2:q:170:ARG:HA	30:q:310:CHL:C4C	2.49	0.43
32:q:318:LUT:H31	32:q:318:LUT:H391	1.91	0.43
5:a:51:ALA:HA	5:a:55:ALA:HB2	2.01	0.43
7:c:135:PHE:HA	31:c:612:CLA:HMC1	2.00	0.43
7:c:261:SER:HB2	7:c:433:ALA:HB2	2.01	0.43
43:c:615:BCR:H15C	34:w:201:LMG:H402	2.00	0.43
8:d:257:PHE:O	33:d:408:LHG:H341	2.18	0.43
3:n:100:LEU:HD13	31:n:313:CLA:HBB2	2.00	0.43
31:n:303:CLA:H141	31:n:303:CLA:H162	1.81	0.43
18:r:141:ARG:HA	18:r:144:MET:HE3	2.00	0.43
18:r:220:LEU:HD12	32:r:317:LUT:H222	2.01	0.43
19:s:236:ILE:HD12	19:s:237:LYS:N	2.33	0.43
26:u:130:ARG:C	26:u:132:VAL:H	2.25	0.43
2:2:138:LEU:HD13	30:2:606:CHL:HHD	2.01	0.43
2:4:126:PHE:CB	31:5:615:CLA:HMB3	2.49	0.43
31:4:604:CLA:NC	36:4:617:NEX:H222	2.33	0.43
3:5:162:ILE:HD11	36:5:618:NEX:C35	2.49	0.43
31:6:305:CLA:H42	36:6:319:NEX:H23	1.99	0.43
7:C:155:VAL:HG12	34:C:621:LMG:C36	2.42	0.43
31:D:403:CLA:H62	31:D:403:CLA:H41	1.61	0.43
2:G:160:LEU:HA	30:G:608:CHL:HBB2	2.01	0.43
38:G:624:SQD:H252	31:7:312:CLA:H43	2.00	0.43
22:W:117:LEU:HD23	22:W:117:LEU:HA	1.86	0.43
31:Y:310:CLA:C2	32:Y:315:LUT:H28	2.48	0.43
1:7:94:HIS:CE1	31:7:304:CLA:C4D	3.02	0.43
1:7:178:TYR:HA	31:7:311:CLA:O1D	2.19	0.43
3:8:85:ARG:HG3	31:8:602:CLA:HMA3	2.01	0.43
31:p:610:CLA:HBB1	31:p:610:CLA:CMB	2.49	0.43
2:q:153:VAL:O	2:q:157:LEU:HD13	2.19	0.43
2:q:163:MET:HE1	30:q:308:CHL:HMA3	2.00	0.43
31:q:312:CLA:NA	35:q:317:RRX:H7	2.33	0.43
5:a:286:THR:OG1	31:a:406:CLA:O1D	2.32	0.43
7:c:132:PHE:CE1	31:c:613:CLA:HAA1	2.53	0.43
8:d:148:ALA:HB1	8:d:279:LEU:HB2	2.01	0.43
10:f:44:ARG:NH1	29:f1:60:ILE:HG21	2.33	0.43
32:g:316:LUT:H11	32:g:316:LUT:H191	1.82	0.43
32:g:316:LUT:H8	32:g:316:LUT:H181	2.01	0.43
18:r:139:HIS:CE1	31:r:305:CLA:C4D	3.02	0.43
37:r:318:XAT:H35	37:r:318:XAT:H401	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:124:VAL:HG13	2:2:127:LYS:HB2	2.00	0.43
2:2:153:VAL:O	2:2:156:LEU:HB2	2.19	0.43
3:3:41:TYR:OH	3:3:198:ALA:O	2.33	0.43
3:3:145:ALA:HA	30:3:307:CHL:CHC	2.48	0.43
3:3:160:GLY:HA2	30:3:310:CHL:CBB	2.48	0.43
3:3:166:ARG:HG3	3:3:167:VAL:HG13	2.01	0.43
2:4:116:ALA:HA	34:Q1:101:LMG:H112	2.01	0.43
2:4:132:ILE:CG1	2:4:152:ILE:HG13	2.48	0.43
30:4:606:CHL:HMC	32:4:616:LUT:H163	2.00	0.43
4:6:248:TYR:CD1	31:6:315:CLA:HED2	2.54	0.43
31:C:609:CLA:H141	31:C:609:CLA:H161	1.75	0.43
32:G:615:LUT:H402	32:G:615:LUT:H31	1.18	0.43
30:N:306:CHL:H122	32:S:317:LUT:H171	2.01	0.43
38:R:322:SQD:H161	38:R:322:SQD:H131	1.92	0.43
26:U:130:ARG:O	26:U:131:GLN:HB3	2.18	0.43
30:0:605:CHL:HAA1	31:r:315:CLA:CMD	2.49	0.43
30:0:607:CHL:CAA	37:q:321:XAT:C4	2.97	0.43
31:7:311:CLA:H62	31:7:313:CLA:CMA	2.49	0.43
31:p:615:CLA:C4C	34:q:302:LMG:H301	2.48	0.43
38:a:411:SQD:H312	31:c:608:CLA:H62	2.00	0.43
6:b:74:SER:OG	6:b:94:GLU:OE2	2.23	0.43
6:b:112:ILE:HG22	43:b:620:BCR:H402	2.01	0.43
6:b:124:ARG:O	11:h:31:LYS:NZ	2.48	0.43
33:b:628:LHG:H252	30:r:309:CHL:CHD	2.49	0.43
34:c:624:LMG:C31	33:y:619:LHG:HC92	2.48	0.43
3:n:245:PHE:CD1	3:n:249:TYR:HB2	2.53	0.43
48:r:302:LMU:H12	48:r:302:LMU:H41	1.37	0.43
30:r:310:CHL:HBB2	38:r:322:SQD:H81	2.01	0.43
31:2:603:CLA:H11	3:3:74:LEU:HD11	2.01	0.43
31:2:611:CLA:HBB1	31:2:611:CLA:HMB3	2.00	0.43
3:3:46:PRO:HB2	30:3:303:CHL:CBC	2.49	0.43
3:3:75:SER:HB3	3:3:81:PHE:CD1	2.54	0.43
31:3:314:CLA:CGA	31:3:314:CLA:C1A	2.97	0.43
2:4:54:SER:O	2:4:58:VAL:HG23	2.18	0.43
31:4:604:CLA:C1B	36:4:617:NEX:H383	2.49	0.43
32:4:616:LUT:H15	32:4:616:LUT:H201	1.85	0.43
31:5:610:CLA:H52	32:5:616:LUT:C28	2.48	0.43
36:5:618:NEX:H35	36:5:618:NEX:H401	1.90	0.43
4:6:49:PHE:CD2	30:6:302:CHL:HAA1	2.54	0.43
31:6:315:CLA:H42	31:6:315:CLA:C2D	2.49	0.43
31:6:315:CLA:H62	31:6:315:CLA:H2	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:338:ILE:HG21	7:C:347:TRP:HB2	2.00	0.43
7:C:361:ASN:O	7:C:361:ASN:ND2	2.51	0.43
8:D:117:HIS:HE1	31:D:404:CLA:ND	2.14	0.43
43:H:101:BCR:H11C	43:H:101:BCR:H341	1.82	0.43
34:I:101:LMG:O9	34:I:101:LMG:HC71	2.18	0.43
14:K:46:ARG:NH2	21:V:33:LEU:O	2.51	0.43
30:N:301:CHL:HBD	30:N:301:CHL:HAA1	2.00	0.43
31:N:303:CLA:HED2	31:N:303:CLA:H2A	2.01	0.43
30:7:302:CHL:HHC	30:7:302:CHL:CBB	2.47	0.43
31:7:312:CLA:HHC	31:7:312:CLA:CBB	2.49	0.43
30:7:321:CHL:H42	30:7:321:CHL:C1D	2.49	0.43
2:9:95:ALA:HB1	2:9:213:GLY:HA3	2.01	0.43
32:9:318:LUT:H31	32:9:318:LUT:H391	1.72	0.43
31:p:604:CLA:HMA3	30:p:606:CHL:C2C	2.49	0.43
44:a:414:PL9:H303	33:e:101:LHG:H382	2.01	0.43
6:b:121:GLU:HG3	11:h:22:ILE:O	2.19	0.43
31:b:615:CLA:HBB1	31:b:615:CLA:CMB	2.49	0.43
7:c:426:PHE:CE1	31:c:605:CLA:HAB	2.54	0.43
33:j:102:LHG:C3	29:f1:58:GLY:HA2	2.49	0.43
31:n:305:CLA:HBB1	31:n:305:CLA:CMB	2.47	0.43
22:w:111:ASN:C	22:w:111:ASN:HD22	2.26	0.43
27:q1:31:LEU:HA	27:q1:34:MET:HG2	2.01	0.43
28:p1:25:MET:HB3	28:p1:27:LYS:HE2	2.00	0.43
31:1:603:CLA:CMC	30:1:607:CHL:H122	2.49	0.42
31:1:614:CLA:C8	31:1:614:CLA:H2	2.48	0.42
2:2:238:LEU:HD11	34:2:618:LMG:H162	2.00	0.42
3:3:95:ALA:HA	32:3:318:LUT:C11	2.46	0.42
3:3:157:VAL:O	3:3:161:LEU:HG	2.19	0.42
33:3:320:LHG:H281	33:3:320:LHG:C7	2.49	0.42
2:4:223:PHE:CE1	35:4:615:RRX:H51	2.53	0.42
31:4:602:CLA:HED2	31:4:602:CLA:H2A	2.00	0.42
31:4:603:CLA:HED2	31:4:603:CLA:H2A	2.00	0.42
3:5:143:ILE:O	3:5:144:HIS:C	2.62	0.42
31:B:604:CLA:H143	31:B:615:CLA:HMA3	2.01	0.42
31:B:613:CLA:H141	31:B:613:CLA:H162	1.86	0.42
7:C:299:GLN:OE1	7:C:343:THR:OG1	2.37	0.42
7:C:336:GLU:H	7:C:336:GLU:HG2	1.57	0.42
31:C:603:CLA:HMB1	31:C:603:CLA:HBB1	2.01	0.42
44:D:406:PL9:H101	33:D:408:LHG:H101	2.01	0.42
2:G:254:ALA:O	37:G:620:XAT:H42	2.18	0.42
30:N:306:CHL:H101	30:N:306:CHL:H61	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:168:TYR:CZ	24:Y:175:PRO:HD3	2.53	0.42
30:Y:301:CHL:C12	30:Y:302:CHL:H61	2.49	0.42
1:7:198:LEU:CB	31:7:311:CLA:HMA2	2.49	0.42
30:8:605:CHL:H101	30:8:605:CHL:H61	1.67	0.42
31:q:314:CLA:H2A	31:q:314:CLA:O1D	2.19	0.42
6:b:357:ARG:HD2	6:b:366:PHE:CE2	2.54	0.42
7:c:264:LEU:HD21	31:c:608:CLA:CAB	2.49	0.42
34:c:620:LMG:H331	34:c:620:LMG:H362	1.90	0.42
33:g:319:LHG:HC61	37:g:321:XAT:H382	2.01	0.42
30:n:308:CHL:H42	30:n:308:CHL:C1D	2.49	0.42
36:n:319:NEX:H201	36:n:319:NEX:H15	1.78	0.42
18:r:78:LEU:HD13	31:r:304:CLA:H42	2.01	0.42
36:r:301:NEX:H15	36:r:301:NEX:H201	1.90	0.42
19:s:236:ILE:H	19:s:236:ILE:HG13	1.64	0.42
24:y:90:ILE:HD13	31:y:603:CLA:HBA1	2.01	0.42
25:z:33:TRP:CE2	25:z:37:LYS:HE2	2.54	0.42
29:F1:99:ASP:HB3	29:F1:102:ASP:O	2.19	0.42
1:1:157:MET:HE1	36:R:301:NEX:H30	2.01	0.42
1:1:170:ALA:O	1:1:182:ASN:ND2	2.52	0.42
3:3:245:PHE:CG	3:3:246:TRP:N	2.86	0.42
30:3:309:CHL:HAA1	30:3:309:CHL:CBD	2.48	0.42
30:5:605:CHL:HHC	30:5:605:CHL:CBB	2.45	0.42
4:6:71:TRP:CZ2	30:6:302:CHL:HAA2	2.55	0.42
4:6:165:GLU:HG3	30:6:310:CHL:C4B	2.49	0.42
4:6:182:TYR:CE2	4:6:203:LYS:HE3	2.54	0.42
31:6:303:CLA:H52	32:6:318:LUT:H28	2.01	0.42
31:6:313:CLA:HHC	31:6:313:CLA:CBB	2.49	0.42
5:A:93:PHE:HZ	31:A:409:CLA:HAA1	1.83	0.42
30:G:601:CHL:H171	30:G:623:CHL:C4B	2.50	0.42
31:G:604:CLA:HBB1	31:G:604:CLA:CMB	2.49	0.42
38:G:617:SQD:O6	38:G:617:SQD:C6	2.67	0.42
34:I:101:LMG:HC8	34:I:101:LMG:HC1	1.79	0.42
16:M:30:ALA:HB3	38:M:102:SQD:H462	2.01	0.42
3:N:203:LYS:HD3	31:N:312:CLA:HAA2	2.00	0.42
32:N:317:LUT:H11	32:N:317:LUT:H191	1.81	0.42
17:O:65:VAL:HG13	17:O:70:ILE:HG13	2.00	0.42
17:O:75:PRO:HD2	17:O:98:CYS:SG	2.59	0.42
18:R:50:ASP:CG	18:R:59:ARG:HH21	2.26	0.42
43:T:101:BCR:C33	43:b:619:BCR:H14C	2.49	0.42
31:Y:304:CLA:HHC	31:Y:304:CLA:CBB	2.49	0.42
32:Y:315:LUT:H35	32:Y:315:LUT:H401	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:49:PHE:CG	4:0:71:TRP:HB2	2.54	0.42
31:0:615:CLA:HBB2	3:p:121:TRP:CH2	2.54	0.42
34:7:301:LMG:HC8	34:7:301:LMG:HC1	1.77	0.42
30:7:307:CHL:HMB2	30:7:310:CHL:OMC	2.19	0.42
3:8:222:GLY:O	3:8:226:ARG:HA	2.19	0.42
2:9:92:VAL:HB	2:9:184:LEU:HD21	1.99	0.42
35:q:317:RRX:H8	35:q:317:RRX:H21	2.00	0.42
5:a:141:PRO:HG3	7:c:434:GLY:C	2.45	0.42
6:b:469:HIS:HE1	31:b:612:CLA:NA	2.16	0.42
31:b:606:CLA:H142	31:b:611:CLA:C2	2.49	0.42
7:c:177:TRP:HZ3	7:c:355:GLU:HG3	1.83	0.42
10:f:14:ILE:HD13	27:q1:23:ILE:HD11	2.02	0.42
2:g:167:GLU:HG2	30:g:309:CHL:CHB	2.49	0.42
31:g:303:CLA:H13	31:g:303:CLA:H102	1.88	0.42
31:y:604:CLA:HBB1	31:y:604:CLA:CMB	2.48	0.42
27:Q1:3:ASN:HB2	34:Q1:101:LMG:O6	2.19	0.42
29:f1:170:ASP:OD1	29:f1:171:LYS:N	2.47	0.42
1:1:59:PRO:HB3	1:1:61:TYR:CZ	2.55	0.42
2:2:246:SER:O	2:2:249:ASN:ND2	2.52	0.42
2:4:169:TYR:CB	2:4:174:GLU:HG3	2.49	0.42
2:4:254:ALA:HA	37:4:619:XAT:H172	2.02	0.42
31:4:604:CLA:H11	30:4:606:CHL:C4D	2.49	0.42
3:5:98:GLY:HA2	32:5:617:LUT:C18	2.49	0.42
34:5:620:LMG:H331	34:5:620:LMG:H362	1.71	0.42
31:B:604:CLA:H12	31:B:605:CLA:C4D	2.49	0.42
11:H:78:THR:OG1	11:H:83:SER:HB3	2.19	0.42
3:N:51:PRO:O	3:N:53:SER:N	2.52	0.42
3:N:223:LEU:HD21	31:N:321:CLA:C4	2.48	0.42
17:O:173:LEU:HD12	17:O:197:TYR:HA	1.99	0.42
19:S:161:ASN:HD21	19:S:163:LEU:HD23	1.84	0.42
34:X:202:LMG:H322	34:X:202:LMG:H351	1.79	0.42
4:0:175:GLY:HA2	18:r:56:ASN:HB2	2.01	0.42
30:0:607:CHL:HAA2	37:q:321:XAT:H42	2.01	0.42
31:p:602:CLA:H42	32:p:617:LUT:C37	2.49	0.42
30:p:605:CHL:HHC	30:p:605:CHL:CBB	2.44	0.42
2:q:140:TYR:O	2:q:141:LEU:C	2.62	0.42
30:q:307:CHL:HHC	30:q:307:CHL:CBB	2.45	0.42
5:a:307:VAL:HG11	29:f1:81:LYS:HE3	2.01	0.42
6:b:115:TRP:CD2	43:b:618:BCR:H291	2.54	0.42
31:b:610:CLA:OBD	11:h:46:THR:OG1	2.36	0.42
7:c:113:LEU:HD12	7:c:113:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:449:ARG:NH2	8:d:241:GLU:HB3	2.35	0.42
31:s:305:CLA:HMA3	30:s:307:CHL:C3C	2.49	0.42
31:s:306:CLA:H3A	31:s:306:CLA:HBA1	1.72	0.42
33:s:322:LHG:H132	33:s:322:LHG:O10	2.19	0.42
30:y:609:CHL:HHC	30:y:609:CHL:CBB	2.48	0.42
27:q1:16:ILE:O	27:q1:20:LEU:HD13	2.19	0.42
29:F1:208:LEU:HD23	29:F1:208:LEU:C	2.44	0.42
29:f1:102:ASP:HB2	29:f1:217:ARG:HE	1.85	0.42
2:2:150:GLN:HB2	30:2:605:CHL:CBB	2.49	0.42
2:2:174:GLU:HA	2:2:179:THR:HG21	2.01	0.42
2:2:177:VAL:HB	2:2:189:PHE:CG	2.54	0.42
31:2:603:CLA:H93	31:2:603:CLA:H62	1.79	0.42
30:3:302:CHL:H61	30:3:302:CHL:H101	1.75	0.42
31:3:314:CLA:HHC	31:3:314:CLA:CBB	2.49	0.42
30:5:601:CHL:HHC	30:5:601:CHL:CBB	2.47	0.42
4:6:168:ARG:NH2	30:6:310:CHL:O1D	2.50	0.42
5:A:102:LEU:H	34:A:414:LMG:HC61	1.85	0.42
31:A:406:CLA:H92	31:A:406:CLA:H62	1.76	0.42
6:B:230:ARG:NH2	38:B:623:SQD:O4	2.52	0.42
31:C:604:CLA:O2A	45:C:617:DGD:HB31	2.19	0.42
31:C:605:CLA:H142	31:C:605:CLA:H111	1.84	0.42
33:G:618:LHG:HC62	37:G:620:XAT:C38	2.49	0.42
34:G:621:LMG:H111	34:G:621:LMG:H142	1.75	0.42
3:N:215:MET:HE2	32:N:317:LUT:H10	2.02	0.42
31:N:310:CLA:H92	31:N:310:CLA:H61	1.62	0.42
18:R:164:ALA:CB	31:R:306:CLA:HED1	2.45	0.42
43:T:101:BCR:H332	6:b:33:TRP:HD1	1.84	0.42
30:0:601:CHL:HED1	33:0:619:LHG:H281	2.01	0.42
30:0:607:CHL:H122	30:0:607:CHL:H93	2.01	0.42
31:8:613:CLA:H2A	31:8:613:CLA:HED3	2.02	0.42
5:a:191:ASN:HB2	7:c:399:ALA:HB1	2.01	0.42
7:c:104:VAL:HG22	43:z:101:BCR:HC41	2.01	0.42
7:c:134:PHE:HD1	34:c:620:LMG:HC4	1.84	0.42
7:c:205:PRO:O	45:c:616:DGD:HG12	2.19	0.42
7:c:310:GLN:HG3	7:c:316:VAL:CG1	2.49	0.42
8:d:191:TRP:CE3	8:d:289:LEU:HD11	2.54	0.42
8:d:197:HIS:HE1	31:d:404:CLA:C1C	2.32	0.42
33:d:408:LHG:H292	20:t:17:ILE:HG23	2.00	0.42
2:g:40:GLU:O	2:g:41:PHE:HB2	2.18	0.42
2:g:238:LEU:HD21	34:g:320:LMG:H162	2.00	0.42
14:k:15:TYR:CZ	25:z:5:PHE:HZ	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:s:318:LUT:H15	32:s:318:LUT:H201	1.93	0.42
24:y:95:ALA:HB1	24:y:214:GLY:HA3	2.01	0.42
24:y:139:TYR:HH	36:y:618:NEX:H1	1.55	0.42
33:z:102:LHG:HC82	33:z:102:LHG:HC5	1.90	0.42
31:1:604:CLA:CMA	30:1:606:CHL:HBC3	2.45	0.42
31:1:612:CLA:H3A	31:1:612:CLA:HBA1	1.63	0.42
34:2:621:LMG:HC2	31:3:316:CLA:CGA	2.50	0.42
3:3:87:LEU:HD13	31:3:305:CLA:CBA	2.48	0.42
30:3:307:CHL:HBB1	34:3:321:LMG:H351	2.02	0.42
2:4:94:HIS:CE1	31:4:603:CLA:C4D	3.02	0.42
31:4:611:CLA:C4D	31:4:612:CLA:HMD3	2.49	0.42
3:5:54:ASN:O	3:5:55:PRO:C	2.62	0.42
4:6:219:GLY:O	4:6:223:GLN:HG3	2.20	0.42
6:B:382:PRO:HG3	6:B:391:SER:HB3	2.01	0.42
45:C:618:DGD:HB51	45:C:618:DGD:HB21	1.89	0.42
31:D:404:CLA:H91	31:D:404:CLA:H112	1.74	0.42
9:E:64:PRO:HB3	9:E:79:LEU:HD13	2.01	0.42
30:G:601:CHL:H11	30:Y:309:CHL:C1B	2.49	0.42
31:G:602:CLA:H102	31:G:602:CLA:H13	1.78	0.42
30:R:309:CHL:HBD	30:R:309:CHL:HAA1	2.02	0.42
38:R:322:SQD:H311	38:R:322:SQD:H342	1.79	0.42
4:0:120:GLU:HB2	4:0:129:GLN:HG3	2.00	0.42
4:0:202:LEU:CB	31:0:610:CLA:HMA2	2.42	0.42
30:0:605:CHL:HBA1	30:0:605:CHL:CBD	2.45	0.42
30:0:608:CHL:HMB2	36:0:618:NEX:C35	2.49	0.42
31:8:614:CLA:H12	2:9:257:PHE:HE1	1.84	0.42
2:9:205:LEU:CD2	31:9:312:CLA:H43	2.50	0.42
3:p:118:GLU:HB2	3:p:123:LYS:O	2.19	0.42
3:p:217:GLY:O	3:p:221:GLN:HG2	2.20	0.42
3:p:218:PHE:HA	3:p:221:GLN:NE2	2.35	0.42
31:p:610:CLA:H2	32:p:616:LUT:C38	2.49	0.42
2:q:146:LEU:HD12	30:q:307:CHL:HED3	2.01	0.42
6:b:115:TRP:CG	43:b:618:BCR:H291	2.55	0.42
6:b:270:PRO:HG3	6:b:312:TYR:HD1	1.84	0.42
8:d:266:TRP:CZ3	33:l:101:LHG:HC42	2.54	0.42
33:e:101:LHG:HC62	34:k:102:LMG:H342	2.02	0.42
31:n:303:CLA:H161	31:n:303:CLA:H202	1.87	0.42
31:n:316:CLA:H61	31:n:316:CLA:H92	1.68	0.42
36:r:319:NEX:H15	36:r:319:NEX:H201	1.88	0.42
31:s:305:CLA:HMA3	30:s:307:CHL:C4C	2.49	0.42
34:Q1:101:LMG:H342	34:Q1:101:LMG:H311	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f1:110:LEU:HD12	29:f1:110:LEU:N	2.34	0.42
2:2:83:THR:HG22	2:2:87:TYR:CE2	2.54	0.42
31:2:611:CLA:HMC3	35:2:614:RRX:H44	2.01	0.42
3:3:252:LYS:HB3	3:3:256:ILE:HG23	2.01	0.42
2:4:111:LEU:HB3	2:4:117:ALA:HB3	2.01	0.42
2:4:173:GLY:HA2	30:4:608:CHL:HMC	2.02	0.42
3:5:107:LEU:O	3:5:110:ARG:HG2	2.20	0.42
3:5:166:ARG:HG3	30:5:608:CHL:C1D	2.48	0.42
3:5:190:LEU:HB2	31:5:610:CLA:O1A	2.20	0.42
3:5:209:ARG:HA	3:5:212:MET:HE3	2.01	0.42
3:5:225:THR:HG21	3:5:232:ASN:CG	2.45	0.42
31:A:405:CLA:H62	31:A:405:CLA:H2	1.79	0.42
31:C:601:CLA:H143	31:C:601:CLA:H112	1.79	0.42
34:C:624:LMG:H121	34:C:624:LMG:H152	1.78	0.42
8:D:56:THR:HG21	9:E:50:PRO:HD3	2.02	0.42
8:D:87:HIS:CD2	8:D:166:GLY:HA2	2.54	0.42
11:H:76:ASP:OD1	11:H:76:ASP:N	2.51	0.42
34:J:101:LMG:H151	33:F1:301:LHG:H281	2.02	0.42
3:N:249:TYR:C	3:N:251:PRO:HD2	2.44	0.42
18:R:123:TYR:OH	18:R:134:GLU:OE1	2.30	0.42
23:X:96:PHE:CE2	27:Q1:34:MET:HE2	2.55	0.42
2:9:223:PHE:CE1	35:9:317:RRX:H48	2.54	0.42
31:9:304:CLA:CHA	31:9:304:CLA:HBA1	2.40	0.42
30:p:608:CHL:HAA1	30:p:608:CHL:CBD	2.49	0.42
32:p:616:LUT:H35	32:p:616:LUT:H401	1.33	0.42
2:q:180:SER:O	2:q:181:GLY:C	2.62	0.42
2:q:256:LYS:HD3	2:q:257:PHE:CE1	2.55	0.42
31:a:409:CLA:CMA	45:c:616:DGD:HBW1	2.49	0.42
6:b:52:LEU:HD12	6:b:52:LEU:HA	1.81	0.42
7:c:61:ALA:HB2	14:k:11:LEU:HD13	2.01	0.42
7:c:104:VAL:HG11	43:c:614:BCR:HC42	2.01	0.42
7:c:361:ASN:O	7:c:361:ASN:ND2	2.50	0.42
45:c:617:DGD:HBV1	34:d:409:LMG:H152	2.01	0.42
2:g:92:VAL:HB	2:g:184:LEU:HD21	2.01	0.42
37:g:321:XAT:H202	24:y:155:LEU:HD21	2.01	0.42
3:n:243:THR:HA	3:n:248:ASP:OD2	2.19	0.42
19:s:154:VAL:HG11	31:s:306:CLA:CED	2.50	0.42
19:s:264:TRP:HE1	31:s:315:CLA:HMC2	1.85	0.42
1:1:89:GLU:O	1:1:93:ILE:HG12	2.20	0.42
1:1:251:LEU:O	1:1:252:ALA:HB2	2.19	0.42
3:3:180:TYR:CE2	3:3:201:LYS:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:197:PHE:CZ	31:5:610:CLA:HED3	2.55	0.42
31:B:610:CLA:H122	31:B:615:CLA:HAA1	2.00	0.42
31:C:604:CLA:H92	31:C:604:CLA:H62	1.76	0.42
33:D:407:LHG:H341	33:D:407:LHG:H101	2.02	0.42
9:E:25:ILE:C	9:E:28:PRO:HD2	2.45	0.42
34:I:101:LMG:H112	34:I:101:LMG:H141	1.80	0.42
17:O:150:LYS:HE3	17:O:150:LYS:HB3	1.90	0.42
31:S:312:CLA:H3A	31:S:312:CLA:HBA2	1.51	0.42
31:S:313:CLA:HED1	31:S:313:CLA:H2	2.01	0.42
31:Y:313:CLA:H2	31:Y:313:CLA:H61	1.77	0.42
3:8:252:LYS:HB2	3:8:258:TYR:HD2	1.83	0.42
2:9:205:LEU:HB3	31:9:312:CLA:CMA	2.50	0.42
2:9:205:LEU:HB3	31:9:312:CLA:HMA2	2.01	0.42
32:9:318:LUT:H15	32:9:318:LUT:H201	1.75	0.42
3:p:96:MET:HG3	3:p:208:GLY:HA2	2.00	0.42
3:p:190:LEU:HD22	32:p:616:LUT:H371	2.02	0.42
2:q:104:GLY:HA3	32:q:318:LUT:C18	2.50	0.42
5:a:266:ASN:HD21	34:a:416:LMG:HC62	1.84	0.42
31:a:409:CLA:H11	12:i:9:TYR:CZ	2.55	0.42
31:b:604:CLA:HBB1	31:b:604:CLA:HMB1	2.02	0.42
7:c:239:HIS:HE1	31:c:606:CLA:NA	2.14	0.42
31:c:601:CLA:H41	31:c:601:CLA:H61	1.84	0.42
45:c:619:DGD:HE62	24:y:40:VAL:HG11	2.02	0.42
32:g:316:LUT:H361	32:g:316:LUT:C28	2.50	0.42
19:s:108:ALA:HB1	19:s:239:GLY:HA3	2.02	0.42
43:t:101:BCR:H341	43:t:101:BCR:H11C	1.26	0.42
22:w:111:ASN:HA	22:w:115:PHE:CG	2.54	0.42
30:y:606:CHL:OMC	30:y:606:CHL:HAC2	2.18	0.42
36:y:618:NEX:H15	36:y:618:NEX:H201	1.90	0.42
1:1:61:TYR:OH	1:1:76:GLY:HA2	2.20	0.42
30:1:607:CHL:HAA2	37:2:619:XAT:H42	2.02	0.42
31:1:610:CLA:H61	31:1:610:CLA:H41	1.66	0.42
3:3:190:LEU:HB2	31:3:311:CLA:CGA	2.49	0.42
2:4:90:ILE:HD13	31:4:603:CLA:HBA1	2.01	0.42
30:4:606:CHL:OMC	30:4:606:CHL:HAC2	2.20	0.42
34:4:620:LMG:H351	3:5:223:LEU:HD21	2.01	0.42
3:5:106:GLU:HB3	3:5:230:ILE:HD12	1.99	0.42
4:6:146:HIS:O	4:6:148:GLN:NE2	2.50	0.42
31:6:311:CLA:H2	32:6:317:LUT:H28	2.02	0.42
36:6:319:NEX:H173	18:R:53:TRP:HH2	1.83	0.42
5:A:317:TRP:HZ3	8:D:180:ARG:HD2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:226:TYR:CD2	6:B:231:MET:HB2	2.55	0.42
6:B:477:ASP:HB2	18:R:100:LYS:NZ	2.35	0.42
7:C:418:HIS:CD2	31:C:602:CLA:ND	2.88	0.42
31:N:304:CLA:NC	30:N:309:CHL:H102	2.34	0.42
31:N:310:CLA:H62	31:N:310:CLA:H41	1.90	0.42
24:Y:145:LEU:O	24:Y:147:HIS:N	2.52	0.42
31:Y:305:CLA:HBB1	31:Y:305:CLA:CMB	2.49	0.42
43:Z:101:BCR:H15C	43:Z:101:BCR:H351	1.89	0.42
31:0:602:CLA:H61	31:0:602:CLA:H41	1.58	0.42
3:8:67:TYR:HE2	30:8:601:CHL:HBC2	1.85	0.42
30:8:606:CHL:H12	30:8:606:CHL:H51	1.72	0.42
31:9:306:CLA:NA	36:9:319:NEX:H242	2.34	0.42
31:p:611:CLA:H12	31:p:612:CLA:OBD	2.19	0.42
34:p:620:LMG:C28	34:p:620:LMG:HC72	2.49	0.42
31:b:608:CLA:C4A	31:b:608:CLA:HBA2	2.49	0.42
7:c:56:ASN:ND2	7:c:99:TYR:O	2.52	0.42
45:c:616:DGD:HBT1	45:c:616:DGD:HBN2	2.02	0.42
43:d:406:BCR:H15C	43:d:406:BCR:H351	1.25	0.42
31:n:305:CLA:H152	31:s:306:CLA:C1B	2.50	0.42
17:o:79:SER:O	17:o:250:LYS:HD3	2.19	0.42
18:r:127:PHE:HA	18:r:132:PHE:CZ	2.54	0.42
19:s:211:TYR:HB3	31:s:311:CLA:HED3	2.01	0.42
32:s:318:LUT:H31	32:s:318:LUT:H391	1.96	0.42
2:2:254:ALA:HA	37:2:619:XAT:H22	2.01	0.42
32:3:318:LUT:H31	32:3:318:LUT:H391	1.94	0.42
3:5:160:GLY:HA2	30:5:609:CHL:CAB	2.49	0.42
31:5:611:CLA:C2B	33:5:619:LHG:HC11	2.49	0.42
4:6:72:ASP:OD2	4:6:77:SER:OG	2.31	0.42
30:6:309:CHL:HHC	30:6:309:CHL:CBB	2.46	0.42
32:6:317:LUT:H15	32:6:317:LUT:H201	1.97	0.42
5:A:155:THR:HG22	5:A:160:ILE:HD13	2.02	0.42
31:B:609:CLA:HBA2	43:H:101:BCR:HC32	2.01	0.42
7:C:132:PHE:CD1	33:C:623:LHG:HC11	2.54	0.42
7:C:142:LYS:HE3	7:C:254:TRP:CG	2.55	0.42
17:O:272:LEU:HD12	17:O:272:LEU:HA	1.88	0.42
31:S:304:CLA:HBB1	31:S:304:CLA:HMB3	2.00	0.42
31:S:305:CLA:H203	31:S:316:CLA:H3A	2.02	0.42
22:W:62:ASP:N	22:W:62:ASP:OD1	2.53	0.42
26:U:128:LEU:HD12	26:U:128:LEU:HA	1.89	0.42
4:0:217:MET:HE2	32:0:617:LUT:H10	2.02	0.42
1:7:90:ILE:CD1	31:7:304:CLA:HBA1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:243:THR:HA	3:8:248:ASP:OD2	2.19	0.42
2:9:101:GLY:HA2	32:9:318:LUT:C18	2.50	0.42
31:9:306:CLA:H61	30:9:308:CHL:HAA1	2.01	0.42
3:p:48:PHE:HA	30:p:601:CHL:C1D	2.49	0.42
3:p:91:HIS:HE1	31:p:603:CLA:C4D	2.32	0.42
31:a:406:CLA:H72	31:a:406:CLA:H111	1.83	0.42
6:b:312:TYR:O	6:b:313:ASP:CB	2.67	0.42
34:c:624:LMG:H371	30:y:601:CHL:HMB3	2.00	0.42
38:g:301:SQD:C10	37:g:321:XAT:H222	2.49	0.42
34:j:101:LMG:H332	33:j:102:LHG:H322	2.01	0.42
31:r:306:CLA:C1C	36:r:319:NEX:H222	2.50	0.42
43:t:101:BCR:H351	43:t:101:BCR:H15C	1.28	0.42
29:F1:95:LEU:HD11	29:F1:97:TYR:HE1	1.85	0.42
1:1:52:PRO:HD2	30:1:601:CHL:CBB	2.48	0.42
2:2:168:ALA:HB1	3:3:52:PHE:CD2	2.55	0.42
37:2:619:XAT:H28	37:2:619:XAT:C36	2.30	0.42
3:3:139:ASN:OD1	3:3:141:SER:OG	2.28	0.42
30:3:307:CHL:HHC	30:3:307:CHL:CBB	2.45	0.42
2:4:119:PHE:HB3	2:4:122:ALA:HB3	2.02	0.42
2:4:138:LEU:HD13	30:4:606:CHL:HMD2	2.02	0.42
2:4:253:SER:HB2	2:4:256:LYS:CD	2.48	0.42
3:5:165:TYR:HA	3:5:169:GLY:O	2.19	0.42
3:5:177:ASP:HB3	3:5:180:TYR:C	2.45	0.42
3:5:250:ALA:N	3:5:251:PRO:CD	2.81	0.42
31:A:405:CLA:H92	31:A:405:CLA:H61	1.71	0.42
6:B:383:PHE:CZ	17:O:213:GLY:HA2	2.55	0.42
33:C:623:LHG:H312	33:S:320:LHG:HC81	2.02	0.42
8:D:15:PHE:HE1	34:D:410:LMG:H172	1.84	0.42
8:D:156:VAL:HG12	8:D:171:PRO:HG3	2.02	0.42
43:D:405:BCR:H372	34:D:409:LMG:H301	2.01	0.42
31:G:602:CLA:HMC2	32:G:615:LUT:H31	2.01	0.42
33:G:618:LHG:H261	37:G:620:XAT:C39	2.50	0.42
3:N:45:ARG:HD3	3:N:61:GLY:HA3	2.01	0.42
3:N:193:ASP:OD2	3:N:196:THR:HG23	2.20	0.42
3:N:233:LEU:O	3:N:237:LEU:HG	2.19	0.42
31:N:305:CLA:HMB3	31:N:305:CLA:HBB1	2.02	0.42
19:S:155:PRO:HG2	31:S:306:CLA:C4B	2.50	0.42
25:Z:26:VAL:HG21	25:Z:40:VAL:HG21	2.02	0.42
34:0:622:LMG:H351	34:0:622:LMG:H322	1.72	0.42
1:7:175:ASP:HB3	1:7:178:TYR:O	2.20	0.42
31:7:312:CLA:HHC	31:7:312:CLA:HBB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:66:ASP:HA	31:8:602:CLA:O1D	2.20	0.42
3:p:52:PHE:HE2	2:q:169:TYR:CE1	2.38	0.42
3:p:107:LEU:HA	3:p:110:ARG:HH21	1.85	0.42
2:q:96:ARG:HD3	31:q:312:CLA:CHD	2.49	0.42
2:q:146:LEU:HA	30:q:307:CHL:HED3	2.02	0.42
2:q:150:GLN:HB3	30:q:307:CHL:CBB	2.49	0.42
2:q:183:SER:HA	30:q:310:CHL:HBC1	2.02	0.42
5:a:227:THR:HG21	5:a:235:GLU:HB2	2.02	0.42
44:a:414:PL9:HC2	44:a:414:PL9:C10	2.46	0.42
31:b:603:CLA:H192	31:b:603:CLA:H161	1.79	0.42
3:n:67:TYR:HE2	30:n:302:CHL:HBC2	1.85	0.42
31:n:314:CLA:HHB	31:n:315:CLA:HBC3	2.01	0.42
17:o:65:VAL:HG13	17:o:70:ILE:HB	2.02	0.42
1:1:201:LYS:HD3	31:1:612:CLA:HAA2	2.01	0.41
2:2:178:GLU:OE2	2:2:180:SER:N	2.48	0.41
2:2:187:GLY:CA	31:2:609:CLA:HED2	2.48	0.41
2:2:256:LYS:HE2	2:2:256:LYS:HB2	1.55	0.41
3:3:206:LYS:NZ	33:3:320:LHG:O4	2.52	0.41
31:3:306:CLA:NB	36:3:319:NEX:H242	2.35	0.41
32:3:317:LUT:H15	32:3:317:LUT:H201	1.92	0.41
3:5:127:GLN:HG2	3:5:130:GLN:NE2	2.35	0.41
31:5:603:CLA:HMB3	31:5:603:CLA:HBB1	2.02	0.41
5:A:96:ILE:HG13	5:A:97:TRP:N	2.35	0.41
5:A:257:ARG:HG2	6:B:498:LEU:HD11	2.02	0.41
34:A:412:LMG:H331	7:C:205:PRO:HD3	2.02	0.41
31:B:604:CLA:H12	31:B:605:CLA:ND	2.35	0.41
2:G:226:GLN:HE22	35:G:614:RRX:H2	1.85	0.41
34:G:622:LMG:HC92	31:N:315:CLA:O2A	2.19	0.41
19:S:264:TRP:HE1	31:S:315:CLA:HMC2	1.85	0.41
24:Y:197:ALA:HB1	24:Y:203:LEU:HG	2.02	0.41
30:Y:301:CHL:H62	30:Y:302:CHL:H13	2.01	0.41
31:Y:304:CLA:HHC	31:Y:304:CLA:HBB1	2.01	0.41
4:0:197:ASP:N	4:0:197:ASP:OD1	2.51	0.41
30:0:608:CHL:HMA3	36:0:618:NEX:H30	2.01	0.41
31:0:610:CLA:H52	31:0:610:CLA:H8	1.65	0.41
2:9:163:MET:HE2	30:9:308:CHL:HMA1	2.02	0.41
2:9:195:LEU:HB2	31:9:312:CLA:CGA	2.49	0.41
37:9:322:XAT:H381	37:9:322:XAT:H27	1.83	0.41
2:q:146:LEU:O	2:q:147:ILE:C	2.63	0.41
2:q:232:LYS:HE2	2:q:232:LYS:HB2	1.73	0.41
30:q:309:CHL:H2A	30:q:309:CHL:O1D	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:409:CLA:H2	12:i:12:VAL:HG11	2.02	0.41
31:b:603:CLA:H91	31:b:610:CLA:H191	2.02	0.41
31:b:608:CLA:H92	31:b:608:CLA:H61	1.84	0.41
7:c:430:LEU:HD11	31:c:605:CLA:HMB2	2.01	0.41
31:c:606:CLA:H143	43:c:615:BCR:C18	2.50	0.41
8:d:274:VAL:N	8:d:275:PRO:HD2	2.34	0.41
14:k:12:PRO:HG3	19:s:288:VAL:HG11	2.02	0.41
3:n:66:ASP:HA	31:n:303:CLA:O1D	2.19	0.41
17:o:247:SER:O	17:o:260:GLY:HA3	2.20	0.41
18:r:154:GLU:HG2	18:r:159:ASP:O	2.20	0.41
19:s:191:GLY:HA3	31:s:316:CLA:C2D	2.49	0.41
32:s:317:LUT:H31	32:s:317:LUT:H391	1.92	0.41
43:z:101:BCR:H15C	43:z:101:BCR:H351	1.86	0.41
29:f1:171:LYS:HD3	29:f1:172:LYS:HZ3	1.85	0.41
30:1:606:CHL:HBB2	30:1:607:CHL:CAB	2.50	0.41
3:3:69:TRP:CZ2	30:3:303:CHL:HAA2	2.55	0.41
2:4:46:ARG:HD2	2:4:69:ASP:O	2.20	0.41
2:4:162:ILE:HG23	36:4:617:NEX:C15	2.51	0.41
2:4:170:ARG:NH2	30:4:608:CHL:O1D	2.53	0.41
2:4:198:ASP:HB3	2:4:201:THR:OG1	2.19	0.41
2:4:207:VAL:O	2:4:209:GLU:N	2.53	0.41
31:4:604:CLA:CGA	31:4:604:CLA:C3A	2.96	0.41
30:4:608:CHL:HBA1	31:4:610:CLA:HBC2	2.01	0.41
32:4:616:LUT:H31	32:4:616:LUT:H391	1.84	0.41
3:5:39:GLU:O	3:5:46:PRO:HD3	2.19	0.41
4:6:71:TRP:O	4:6:71:TRP:CD1	2.73	0.41
30:6:306:CHL:HHC	30:6:306:CHL:CBB	2.44	0.41
5:A:324:ALA:O	5:A:328:MET:HG3	2.19	0.41
43:B:619:BCR:H15C	43:B:619:BCR:H351	1.71	0.41
7:C:384:MET:HE2	7:C:384:MET:HB3	1.86	0.41
7:C:440:ALA:HB1	22:W:117:LEU:HD22	2.02	0.41
43:H:101:BCR:H15C	43:H:101:BCR:H351	1.88	0.41
36:R:319:NEX:H161	38:R:322:SQD:H112	2.01	0.41
24:Y:94:HIS:CE1	31:Y:304:CLA:C4D	3.01	0.41
31:Y:312:CLA:H92	31:Y:312:CLA:H62	1.75	0.41
31:0:602:CLA:H72	32:0:617:LUT:H30	2.01	0.41
31:0:603:CLA:H93	31:p:603:CLA:H93	2.01	0.41
34:0:620:LMG:H352	34:7:301:LMG:H172	2.03	0.41
1:7:103:LEU:HD13	31:7:305:CLA:HMC1	2.01	0.41
30:9:309:CHL:H43	30:9:309:CHL:CHC	2.51	0.41
30:9:309:CHL:C7	30:9:309:CHL:H41	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:197:PHE:O	3:p:201:LYS:HG3	2.20	0.41
2:q:148:HIS:HB3	30:q:307:CHL:C1B	2.51	0.41
6:b:159:THR:O	33:b:628:LHG:HC12	2.19	0.41
6:b:224:ARG:HG2	11:h:44:TRP:CZ2	2.55	0.41
6:b:440:ASP:OD1	6:b:440:ASP:N	2.52	0.41
31:b:606:CLA:H61	31:b:606:CLA:H41	1.74	0.41
33:b:628:LHG:H151	33:b:628:LHG:H192	2.01	0.41
7:c:388:PRO:HA	7:c:409:SER:HB2	2.02	0.41
9:e:12:ASP:OD1	13:j:9:ARG:NH1	2.49	0.41
9:e:25:ILE:C	9:e:28:PRO:HD2	2.45	0.41
31:g:314:CLA:HHC	31:g:314:CLA:CBB	2.49	0.41
33:l:101:LHG:H141	33:l:101:LHG:H111	1.79	0.41
30:n:308:CHL:H102	30:y:601:CHL:H102	2.00	0.41
18:r:198:GLU:HG3	31:r:311:CLA:C4B	2.51	0.41
19:s:153:ALA:CB	31:s:306:CLA:HBC3	2.51	0.41
22:w:94:GLY:O	22:w:98:VAL:HG23	2.19	0.41
24:y:107:PHE:HB3	24:y:108:PRO:HD3	2.02	0.41
24:y:111:LEU:HD21	34:y:620:LMG:H302	2.02	0.41
1:1:242:ASN:OD1	1:1:245:ALA:N	2.51	0.41
30:2:607:CHL:HHC	30:2:607:CHL:CBB	2.47	0.41
31:2:613:CLA:H2	31:2:613:CLA:H61	1.53	0.41
30:3:307:CHL:CHC	34:3:321:LMG:H371	2.51	0.41
33:4:618:LHG:HC92	37:4:619:XAT:C27	2.50	0.41
3:5:70:ASP:CB	31:5:602:CLA:HBA2	2.48	0.41
30:6:302:CHL:HHC	30:6:302:CHL:CBB	2.48	0.41
32:6:318:LUT:H35	32:6:318:LUT:H401	1.85	0.41
5:A:28:LEU:HD12	34:b:624:LMG:H311	2.03	0.41
5:A:160:ILE:HG12	7:C:419:PHE:CE2	2.56	0.41
6:B:297:SER:HB3	6:B:300:GLN:HG2	2.02	0.41
6:B:307:GLU:OE2	6:B:340:TRP:N	2.45	0.41
31:B:610:CLA:H72	31:B:610:CLA:H111	1.80	0.41
7:C:261:SER:HB2	7:C:433:ALA:HB2	2.01	0.41
31:C:613:CLA:H93	31:C:613:CLA:H61	1.88	0.41
33:G:618:LHG:H112	33:G:618:LHG:HC82	1.21	0.41
16:M:29:THR:O	16:M:32:GLN:HG2	2.19	0.41
31:N:304:CLA:HBC2	30:N:309:CHL:HHD	2.01	0.41
19:S:252:GLN:NE2	19:S:263:ASN:HD22	2.17	0.41
25:Z:5:PHE:HD1	25:Z:57:LEU:HB3	1.84	0.41
30:0:609:CHL:CMB	30:q:303:CHL:HHB	2.51	0.41
32:7:318:LUT:H31	32:7:318:LUT:H391	1.93	0.41
31:8:603:CLA:H2	31:8:603:CLA:H62	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:109:GLU:CD	2:9:235:LEU:HB2	2.45	0.41
34:9:321:LMG:HC1	34:9:321:LMG:HC8	1.71	0.41
3:p:239:ALA:O	3:p:243:THR:HG22	2.20	0.41
31:p:615:CLA:CAB	30:q:309:CHL:HMA2	2.49	0.41
2:q:140:TYR:C	2:q:142:GLY:N	2.75	0.41
2:q:218:PHE:CG	33:q:320:LHG:H281	2.56	0.41
36:q:319:NEX:H15	36:q:319:NEX:H201	1.87	0.41
5:a:18:CYS:SG	12:i:30:ARG:NH2	2.93	0.41
5:a:133:LEU:HD11	8:d:255:GLN:HB2	2.02	0.41
31:b:617:CLA:H11	31:b:617:CLA:H52	1.81	0.41
7:c:338:ILE:HG21	7:c:347:TRP:HB2	2.02	0.41
45:c:617:DGD:O1A	34:k:101:LMG:H302	2.20	0.41
3:n:93:ARG:HA	3:n:96:MET:HE3	2.02	0.41
31:n:314:CLA:H172	31:n:315:CLA:ND	2.35	0.41
34:r:321:LMG:HO2	34:r:321:LMG:C10	2.33	0.41
19:s:241:LEU:O	19:s:244:VAL:HG22	2.21	0.41
31:s:313:CLA:H12	34:s:321:LMG:O2	2.20	0.41
27:Q1:10:LEU:HG	34:Q1:101:LMG:O3	2.20	0.41
1:1:59:PRO:CG	1:1:62:LEU:HD12	2.49	0.41
2:2:224:PHE:CD1	31:3:316:CLA:HBB2	2.56	0.41
31:3:305:CLA:HMB3	31:3:305:CLA:HBB1	2.01	0.41
2:4:107:THR:N	2:4:108:PRO:HD2	2.34	0.41
3:5:106:GLU:HA	3:5:119:ALA:HB1	2.02	0.41
3:5:249:TYR:CB	3:5:258:TYR:CD2	3.02	0.41
31:5:603:CLA:H12	31:5:603:CLA:HBA2	1.85	0.41
31:6:305:CLA:H72	31:R:315:CLA:H92	2.01	0.41
31:6:314:CLA:H62	31:6:314:CLA:CHC	2.50	0.41
38:A:413:SQD:H5	6:b:75:TRP:HB3	2.02	0.41
6:B:148:LEU:HG	33:B:624:LHG:H361	2.02	0.41
6:B:161:LEU:HD12	33:B:624:LHG:H241	2.02	0.41
31:B:616:CLA:HMA3	43:B:619:BCR:C17	2.50	0.41
7:C:120:HIS:HE1	31:C:613:CLA:C1A	2.33	0.41
7:C:203:ARG:HG3	22:W:71:GLY:HA2	2.03	0.41
7:C:416:THR:HG22	45:C:617:DGD:HBF2	2.01	0.41
33:D:408:LHG:O2	15:L:14:ASN:ND2	2.54	0.41
47:E:101:HEM:HBC2	47:E:101:HEM:CHD	2.30	0.41
15:L:37:PHE:HD1	16:M:3:VAL:HG13	1.85	0.41
31:N:315:CLA:H61	31:N:315:CLA:H41	1.64	0.41
19:S:68:ARG:HA	19:S:71:ILE:HD13	2.02	0.41
22:W:76:ILE:HG23	22:W:81:LEU:HB2	2.01	0.41
30:Y:307:CHL:OMC	30:Y:307:CHL:HAC2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:93:HIS:HE1	31:0:603:CLA:ND	2.04	0.41
4:0:149:SER:CB	34:0:622:LMG:HC92	2.47	0.41
2:9:46:ARG:HG2	2:9:48:LYS:HE3	2.01	0.41
2:9:147:ILE:H	30:9:307:CHL:CGD	2.32	0.41
36:9:319:NEX:H15	36:9:319:NEX:H201	1.96	0.41
3:p:180:TYR:CE2	3:p:201:LYS:HE3	2.55	0.41
6:b:307:GLU:OE2	6:b:340:TRP:N	2.54	0.41
31:b:613:CLA:H161	31:b:613:CLA:H122	1.76	0.41
34:f:101:LMG:HC8	34:f:101:LMG:HC1	1.88	0.41
2:g:198:ASP:HB3	2:g:201:THR:HB	2.02	0.41
31:g:303:CLA:H93	31:g:304:CLA:HMA1	2.02	0.41
31:g:313:CLA:CGA	31:g:313:CLA:C1A	2.98	0.41
37:g:321:XAT:H201	37:g:321:XAT:H15	1.85	0.41
3:n:67:TYR:CE2	30:n:302:CHL:HBC2	2.55	0.41
31:r:303:CLA:CBD	33:r:320:LHG:HC82	2.50	0.41
31:r:315:CLA:HBB1	32:r:317:LUT:H192	2.01	0.41
31:s:311:CLA:H51	31:s:311:CLA:H11	1.85	0.41
31:y:604:CLA:H43	30:y:606:CHL:HBD	2.02	0.41
31:y:613:CLA:H61	31:y:613:CLA:H2	1.52	0.41
1:1:57:PHE:CE2	1:1:74:THR:HG22	2.56	0.41
31:1:610:CLA:H8	31:1:610:CLA:H52	1.33	0.41
2:2:186:PRO:O	2:2:190:PHE:HD1	2.04	0.41
31:3:315:CLA:HHC	31:3:315:CLA:HBB1	2.02	0.41
32:3:317:LUT:H31	32:3:317:LUT:H391	1.91	0.41
2:4:87:TYR:HB3	31:4:602:CLA:HMA1	2.02	0.41
2:4:215:LEU:HG	35:4:615:RRX:H36	2.02	0.41
3:5:38:VAL:HG23	3:5:40:TRP:N	2.36	0.41
36:6:319:NEX:H11	36:6:319:NEX:H191	1.90	0.41
5:A:228:THR:OG1	5:A:230:ASN:OD1	2.22	0.41
6:B:13:LEU:HD23	31:B:612:CLA:HBC1	2.02	0.41
6:B:94:GLU:H	6:B:94:GLU:HG2	1.49	0.41
31:B:607:CLA:H111	31:B:607:CLA:H143	1.73	0.41
31:C:610:CLA:HBA2	31:C:610:CLA:HBD	2.01	0.41
43:C:614:BCR:H15C	43:C:614:BCR:H351	1.79	0.41
45:C:620:DGD:HB42	45:C:620:DGD:HA92	2.01	0.41
45:C:620:DGD:O1A	34:W:201:LMG:O9	2.38	0.41
10:F:19:TRP:CE2	10:F:23:HIS:CE1	3.09	0.41
2:G:223:PHE:CE1	35:G:614:RRX:H52	2.54	0.41
16:M:-10:UNK:HA	6:b:46:ASP:OD2	2.21	0.41
3:N:143:ILE:HA	30:N:306:CHL:C4D	2.50	0.41
36:R:319:NEX:H11	36:R:319:NEX:H191	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S:305:CLA:H203	31:S:316:CLA:HBA1	2.03	0.41
31:0:611:CLA:C2C	33:0:619:LHG:HC62	2.50	0.41
1:7:177:VAL:C	1:7:179:PRO:HD3	2.46	0.41
31:7:311:CLA:H111	31:7:311:CLA:H93	1.61	0.41
31:7:311:CLA:O2A	32:7:317:LUT:H26	2.20	0.41
2:9:89:GLU:O	2:9:93:ILE:HG12	2.20	0.41
31:p:603:CLA:HBC2	30:p:609:CHL:HHD	2.03	0.41
44:a:414:PL9:H171	44:a:414:PL9:H151	1.82	0.41
31:b:602:CLA:HAC1	43:h:101:BCR:H383	2.01	0.41
34:b:629:LMG:H371	34:b:629:LMG:H341	1.87	0.41
31:c:605:CLA:H62	31:c:605:CLA:H2	1.81	0.41
45:c:619:DGD:HB41	45:c:619:DGD:HA51	2.03	0.41
8:d:92:LEU:HD13	34:d:410:LMG:H141	2.02	0.41
2:g:49:TRP:N	2:g:70:TYR:HB3	2.35	0.41
34:n:322:LMG:H151	31:y:615:CLA:H11	2.02	0.41
18:r:190:ASN:ND2	30:r:308:CHL:O1D	2.53	0.41
36:r:301:NEX:O3	36:r:301:NEX:H162	2.21	0.41
31:r:312:CLA:H3A	31:r:312:CLA:HBA2	1.23	0.41
31:r:313:CLA:NB	33:r:320:LHG:O4	2.54	0.41
19:s:115:ALA:HB1	32:s:317:LUT:H12	2.01	0.41
32:s:317:LUT:H35	32:s:317:LUT:H401	1.84	0.41
34:w:202:LMG:H453	34:w:202:LMG:H411	2.03	0.41
24:y:206:LEU:CB	31:y:610:CLA:HMA2	2.50	0.41
24:y:227:GLN:O	24:y:231:THR:OG1	2.34	0.41
30:y:608:CHL:H2	32:y:616:LUT:C38	2.50	0.41
25:z:33:TRP:O	25:z:37:LYS:HB2	2.20	0.41
43:z:101:BCR:HC8	43:z:101:BCR:H331	2.02	0.41
1:1:139:GLY:HA2	1:1:142:ASN:ND2	2.35	0.41
1:1:167:GLY:HA3	18:R:39:SER:O	2.20	0.41
2:2:179:THR:C	2:2:181:GLY:N	2.76	0.41
3:3:147:SER:O	3:3:151:ILE:HG13	2.20	0.41
3:3:225:THR:O	3:3:226:ARG:HB2	2.21	0.41
31:3:301:CLA:HHC	31:3:301:CLA:CBB	2.51	0.41
2:4:50:LEU:HD12	2:4:50:LEU:HA	1.80	0.41
32:5:616:LUT:H35	32:5:616:LUT:H401	1.82	0.41
4:6:72:ASP:HA	32:6:318:LUT:H24	2.02	0.41
4:6:139:LEU:HD13	4:6:139:LEU:HA	1.91	0.41
34:6:321:LMG:HC71	18:R:273:PHE:CD1	2.56	0.41
6:B:307:GLU:HG3	6:B:340:TRP:HB2	2.01	0.41
43:C:615:BCR:H351	43:C:615:BCR:H15C	1.17	0.41
8:D:53:THR:HG22	10:F:39:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:148:ALA:HB3	8:D:149:PRO:HD3	2.03	0.41
42:D:401:PHO:HMB1	42:D:401:PHO:HBB1	2.03	0.41
43:D:405:BCR:H311	43:D:405:BCR:C8	2.49	0.41
2:G:75:ALA:HB3	2:G:77:LEU:HG	2.03	0.41
2:G:259:PRO:HA	34:G:621:LMG:C4	2.50	0.41
31:G:604:CLA:H41	31:G:604:CLA:H61	1.79	0.41
30:G:606:CHL:OMC	30:G:606:CHL:HAC2	2.20	0.41
3:N:162:ILE:HD11	36:N:318:NEX:C35	2.51	0.41
31:N:313:CLA:H102	31:N:314:CLA:HMD3	2.02	0.41
18:R:222:LEU:HB2	31:R:312:CLA:HBA1	2.03	0.41
48:R:302:LMU:H3'	48:R:302:LMU:H1B	1.75	0.41
31:S:312:CLA:H141	31:S:312:CLA:H161	1.82	0.41
22:W:89:PHE:CZ	34:W:201:LMG:H371	2.56	0.41
43:Z:101:BCR:H11C	43:Z:101:BCR:H341	1.76	0.41
4:0:85:ARG:HH22	2:q:59:PRO:HA	1.86	0.41
4:0:199:LEU:HD11	4:0:203:LYS:NZ	2.34	0.41
1:7:218:ILE:HD12	31:7:314:CLA:CAC	2.50	0.41
3:8:67:TYR:CE2	30:8:601:CHL:HBC2	2.55	0.41
3:8:93:ARG:HA	3:8:96:MET:HE3	2.02	0.41
2:q:127:LYS:C	2:q:129:GLY:H	2.28	0.41
31:q:312:CLA:HED2	31:q:312:CLA:HBD	1.91	0.41
43:a:410:BCR:H15C	43:a:410:BCR:H351	1.94	0.41
31:b:608:CLA:OBD	34:b:622:LMG:O2	2.37	0.41
31:b:613:CLA:H62	31:b:613:CLA:H102	1.86	0.41
31:b:617:CLA:H152	31:b:617:CLA:H112	1.53	0.41
7:c:156:LEU:HD12	7:c:156:LEU:HA	1.89	0.41
43:c:615:BCR:H15C	43:c:615:BCR:H351	1.67	0.41
2:g:78:SER:HB3	2:g:84:PHE:CD1	2.56	0.41
2:g:147:ILE:N	30:g:306:CHL:O1D	2.49	0.41
30:g:308:CHL:HHC	30:g:308:CHL:CBB	2.47	0.41
31:g:311:CLA:C4D	31:g:312:CLA:HMD3	2.50	0.41
31:g:314:CLA:HHC	31:g:314:CLA:HBB1	2.03	0.41
3:n:102:CYS:SG	32:n:318:LUT:H41	2.61	0.41
19:s:133:GLY:O	19:s:139:THR:HG22	2.21	0.41
24:y:121:GLU:N	24:y:130:GLN:OE1	2.51	0.41
24:y:227:GLN:HE21	24:y:238:ASN:HD22	1.69	0.41
29:F1:60:ILE:N	29:F1:60:ILE:HD12	2.36	0.41
30:2:606:CHL:HAC2	30:2:606:CHL:OMC	2.20	0.41
2:4:132:ILE:HG21	2:4:152:ILE:HG23	2.01	0.41
2:4:175:GLY:O	2:4:176:PRO:C	2.63	0.41
31:4:604:CLA:CHC	36:4:617:NEX:H362	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:91:HIS:HD2	32:5:617:LUT:H15	1.85	0.41
3:5:134:LEU:HD21	31:5:604:CLA:HAA1	2.03	0.41
3:5:169:GLY:HA2	30:5:608:CHL:HMC	2.02	0.41
3:5:200:LEU:CA	3:5:203:LYS:HD2	2.40	0.41
3:5:251:PRO:HG2	3:5:252:LYS:CD	2.47	0.41
34:5:620:LMG:H361	34:5:620:LMG:HC8	2.03	0.41
4:6:50:LEU:HD12	4:6:50:LEU:HA	1.83	0.41
4:6:218:PHE:CE2	31:6:314:CLA:HAC1	2.56	0.41
31:B:609:CLA:H142	31:B:609:CLA:H112	1.86	0.41
7:C:211:TRP:CG	7:C:212:ILE:H	2.37	0.41
45:C:620:DGD:HG11	45:C:620:DGD:C2B	2.47	0.41
8:D:274:VAL:N	8:D:275:PRO:HD2	2.36	0.41
9:E:23:HIS:HA	9:E:26:THR:OG1	2.20	0.41
31:G:602:CLA:HBA1	32:G:615:LUT:H382	2.02	0.41
31:G:603:CLA:NC	30:G:608:CHL:H111	2.36	0.41
31:G:611:CLA:HED2	31:G:611:CLA:H2A	2.02	0.41
37:G:620:XAT:H41	30:G:623:CHL:HAA1	2.02	0.41
17:O:127:ARG:NH2	22:W:68:GLU:OE1	2.27	0.41
17:O:138:GLN:NE2	17:O:140:LYS:HD2	2.35	0.41
18:R:153:GLN:O	18:R:157:THR:OG1	2.37	0.41
19:S:57:ARG:HH12	19:S:84:GLY:N	2.18	0.41
19:S:108:ALA:HB1	19:S:239:GLY:HA3	2.01	0.41
24:Y:47:PRO:HB2	30:Y:302:CHL:CBC	2.51	0.41
31:Y:303:CLA:H93	31:Y:303:CLA:H111	1.78	0.41
4:0:111:GLN:HG2	4:0:118:PHE:HD1	1.85	0.41
1:7:185:PRO:HD2	32:7:317:LUT:C23	2.49	0.41
30:7:302:CHL:C2D	33:7:319:LHG:HC81	2.51	0.41
34:7:320:LMG:HC1	31:r:313:CLA:HMA3	2.03	0.41
3:8:224:ILE:HD12	3:8:258:TYR:OH	2.20	0.41
3:p:240:PRO:HG3	31:p:614:CLA:CMB	2.50	0.41
2:q:104:GLY:HA3	32:q:318:LUT:H183	2.03	0.41
2:q:186:PRO:HB2	2:q:190:PHE:CD2	2.56	0.41
5:a:307:VAL:HG23	10:f:44:ARG:CD	2.50	0.41
7:c:97:TYR:OH	25:z:58:ASN:ND2	2.54	0.41
7:c:105:LEU:HD12	7:c:105:LEU:HA	1.76	0.41
31:c:613:CLA:OBD	19:s:62:PRO:HB2	2.21	0.41
43:c:614:BCR:H10C	43:c:614:BCR:HC7	1.83	0.41
33:c:622:LHG:H242	31:s:312:CLA:CAB	2.47	0.41
33:c:622:LHG:H331	33:c:622:LHG:H301	1.96	0.41
8:d:279:LEU:HD11	42:d:402:PHO:HMC3	2.02	0.41
11:h:37:TYR:CE2	18:r:89:LEU:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:h:101:BCR:H21C	34:x:202:LMG:H311	2.03	0.41
34:k:101:LMG:H111	34:k:101:LMG:H142	1.85	0.41
31:r:305:CLA:H41	31:r:305:CLA:H62	1.85	0.41
19:s:110:TRP:CD2	31:s:310:CLA:HAC2	2.56	0.41
33:s:322:LHG:H271	33:s:322:LHG:H241	1.97	0.41
21:v:15:ILE:O	43:v:101:BCR:H14C	2.21	0.41
24:y:139:TYR:OH	36:y:618:NEX:O23	2.32	0.41
29:F1:105:ASN:ND2	29:F1:214:GLY:H	2.18	0.41
31:1:614:CLA:H2	31:1:614:CLA:H61	1.77	0.41
31:2:613:CLA:NC	31:2:613:CLA:H51	2.36	0.41
3:3:44:ASN:OD1	3:3:44:ASN:N	2.54	0.41
3:3:245:PHE:CD1	3:3:249:TYR:HB2	2.56	0.41
30:3:303:CHL:HHC	30:3:303:CHL:CBB	2.46	0.41
31:3:306:CLA:C1B	36:3:319:NEX:H383	2.51	0.41
2:4:175:GLY:N	2:4:176:PRO:CD	2.83	0.41
2:4:179:THR:H	2:4:188:GLY:CA	2.24	0.41
2:4:205:LEU:HD12	31:4:610:CLA:H12	2.03	0.41
2:4:207:VAL:O	2:4:208:LYS:C	2.63	0.41
30:4:607:CHL:HHB	31:5:615:CLA:HAB	2.03	0.41
30:4:609:CHL:HHC	30:4:609:CHL:CBB	2.46	0.41
3:5:69:TRP:CE2	30:5:601:CHL:HBA2	2.56	0.41
3:5:187:PRO:HD2	32:5:616:LUT:C23	2.50	0.41
3:5:197:PHE:CD1	31:5:610:CLA:HMA3	2.56	0.41
3:5:220:VAL:CG2	31:5:613:CLA:HAC2	2.48	0.41
3:5:252:LYS:CB	3:5:258:TYR:HA	2.51	0.41
31:5:611:CLA:H8	31:5:612:CLA:ND	2.35	0.41
5:A:250:ALA:HA	6:B:490:VAL:HG11	2.02	0.41
31:A:405:CLA:H192	31:A:405:CLA:H162	1.95	0.41
6:B:243:ALA:HA	6:B:246:PHE:CD2	2.55	0.41
7:C:385:THR:HG21	26:U:75:ARG:HB3	2.03	0.41
31:C:611:CLA:H91	31:C:611:CLA:H111	1.95	0.41
45:C:620:DGD:HBH2	31:Y:311:CLA:C5	2.50	0.41
8:D:134:ARG:HD2	8:D:134:ARG:HA	1.87	0.41
8:D:297:ASP:HB2	8:D:315:TYR:OH	2.21	0.41
2:G:140:TYR:O	2:G:146:LEU:HD12	2.20	0.41
2:G:169:TYR:CE1	3:N:52:PHE:HE2	2.38	0.41
2:G:259:PRO:HG3	30:G:623:CHL:H42	2.03	0.41
34:G:622:LMG:H151	31:N:321:CLA:H12	2.02	0.41
14:K:21:ILE:HG13	33:K:102:LHG:H292	2.03	0.41
31:N:313:CLA:H43	31:N:314:CLA:OBD	2.21	0.41
31:R:316:CLA:H143	31:R:316:CLA:H162	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:175:PRO:HD2	30:Y:308:CHL:CBB	2.50	0.41
4:0:161:MET:HE2	4:0:161:MET:HA	2.03	0.41
4:0:219:GLY:O	4:0:223:GLN:HG3	2.20	0.41
34:0:620:LMG:H311	34:0:620:LMG:H342	1.89	0.41
31:7:303:CLA:H61	31:7:303:CLA:H101	1.85	0.41
3:8:253:SER:HB2	30:9:309:CHL:HAA1	2.01	0.41
34:9:321:LMG:HC2	34:9:321:LMG:HC71	1.79	0.41
31:p:610:CLA:H2	32:p:616:LUT:C26	2.50	0.41
2:q:48:LYS:HB2	2:q:54:SER:OG	2.20	0.41
5:a:120:PHE:CD2	45:c:616:DGD:HBT2	2.56	0.41
6:b:39:PHE:CD1	34:b:601:LMG:HC92	2.55	0.41
31:b:610:CLA:H91	31:b:610:CLA:H111	1.82	0.41
7:c:35:GLY:HA3	7:c:125:PRO:O	2.20	0.41
7:c:95:ASP:OD1	7:c:96:THR:N	2.54	0.41
7:c:306:LEU:HD23	7:c:306:LEU:C	2.45	0.41
31:d:404:CLA:H162	31:d:404:CLA:H193	1.79	0.41
37:g:321:XAT:H31	37:g:321:XAT:H391	1.77	0.41
3:n:75:SER:HB2	3:n:81:PHE:CD1	2.56	0.41
3:n:206:LYS:HD3	31:n:312:CLA:O1D	2.21	0.41
30:n:308:CHL:HAA1	30:n:308:CHL:CBD	2.51	0.41
17:o:208:ARG:HB2	17:o:235:LYS:HE2	2.01	0.41
19:s:189:PRO:O	19:s:204:TYR:OH	2.32	0.41
30:s:307:CHL:HBB1	32:s:318:LUT:H161	2.02	0.41
24:y:94:HIS:CE1	31:y:603:CLA:C4D	3.00	0.41
29:f1:106:ASN:OD1	29:f1:212:GLN:HB3	2.21	0.41
1:1:90:ILE:HD11	2:2:75:ALA:HA	2.03	0.41
31:1:602:CLA:H92	31:1:602:CLA:H61	1.81	0.41
31:1:604:CLA:HMA2	30:1:606:CHL:C3C	2.50	0.41
30:1:607:CHL:HAA2	37:2:619:XAT:C4	2.51	0.41
31:2:604:CLA:C4A	36:2:616:NEX:H242	2.50	0.41
37:2:619:XAT:H381	37:2:619:XAT:H27	1.83	0.41
3:3:104:THR:O	3:3:108:LEU:HD13	2.20	0.41
3:3:215:MET:HA	3:3:218:PHE:HD2	1.85	0.41
30:4:607:CHL:H102	30:4:607:CHL:NB	2.35	0.41
3:5:58:TYR:OH	3:5:73:GLY:HA2	2.19	0.41
3:5:107:LEU:HA	3:5:110:ARG:HG2	2.03	0.41
3:5:203:LYS:HD3	31:5:612:CLA:HBA2	2.02	0.41
30:5:606:CHL:HAC2	30:5:606:CHL:OMC	2.21	0.41
32:5:616:LUT:H11	32:5:616:LUT:H191	1.98	0.41
4:6:136:LEU:HD21	31:6:305:CLA:HAA2	2.03	0.41
4:6:147:ALA:HA	30:6:306:CHL:C1C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:303:CLA:HMB1	31:6:303:CLA:HBB1	2.03	0.41
31:6:311:CLA:HBB1	31:6:311:CLA:CMB	2.51	0.41
5:A:96:ILE:HG22	5:A:105:TRP:CE2	2.56	0.41
6:B:24:LEU:HD21	31:B:616:CLA:CAB	2.51	0.41
31:B:601:CLA:C4B	34:X:202:LMG:H321	2.51	0.41
31:B:612:CLA:C17	31:B:613:CLA:HBB2	2.50	0.41
31:B:613:CLA:H62	31:B:613:CLA:H41	1.65	0.41
31:B:616:CLA:H11	31:B:616:CLA:H52	1.80	0.41
34:B:621:LMG:H151	34:B:621:LMG:H182	1.90	0.41
7:C:199:GLY:O	7:C:203:ARG:HB2	2.21	0.41
7:C:250:ARG:HH22	34:W:201:LMG:HC1	1.85	0.41
31:C:612:CLA:HBB1	31:C:612:CLA:HMB3	2.02	0.41
42:D:401:PHO:H2	42:D:401:PHO:H61	1.75	0.41
31:D:404:CLA:H143	31:D:404:CLA:H162	1.88	0.41
2:G:89:GLU:HA	2:G:184:LEU:HD11	2.02	0.41
14:K:23:ASP:OD2	21:V:8:GLN:NE2	2.54	0.41
3:N:86:GLU:HA	3:N:179:LEU:HD21	2.02	0.41
32:N:317:LUT:H35	32:N:317:LUT:H401	1.90	0.41
18:R:54:LEU:HD12	18:R:54:LEU:HA	1.89	0.41
18:R:180:PRO:HG2	18:R:181:PHE:CE1	2.56	0.41
19:S:70:GLU:HB3	33:S:322:LHG:HC12	2.03	0.41
38:S:301:SQD:H301	38:S:301:SQD:H332	1.93	0.41
23:X:82:VAL:O	23:X:86:ILE:HG13	2.20	0.41
38:X:201:SQD:H242	38:X:201:SQD:H462	1.86	0.41
31:Y:310:CLA:HMB3	31:Y:310:CLA:CBB	2.47	0.41
31:Y:310:CLA:H152	31:Y:310:CLA:H18	1.87	0.41
31:Y:312:CLA:H121	31:Y:312:CLA:H161	1.46	0.41
25:Z:5:PHE:HA	25:Z:57:LEU:HD23	2.03	0.41
4:0:71:TRP:O	32:0:617:LUT:H24	2.21	0.41
4:0:94:ALA:HB1	4:0:210:GLY:HA3	2.03	0.41
38:0:621:SQD:H1	31:9:313:CLA:O2A	2.21	0.41
3:8:75:SER:HB2	3:8:81:PHE:CD1	2.56	0.41
2:9:63:LYS:HB2	2:9:63:LYS:HZ3	1.85	0.41
2:9:101:GLY:HA2	32:9:318:LUT:H182	2.02	0.41
2:9:205:LEU:HD22	31:9:312:CLA:H12	2.03	0.41
30:9:303:CHL:HMD2	33:9:320:LHG:H251	2.03	0.41
31:9:315:CLA:H61	31:9:315:CLA:H2	1.70	0.41
3:p:96:MET:SD	31:p:610:CLA:HAB	2.61	0.41
3:p:173:GLY:O	30:p:608:CHL:HBC3	2.21	0.41
3:p:191:ALA:HB1	3:p:197:PHE:HB2	2.02	0.41
30:p:608:CHL:HHC	30:p:608:CHL:CBB	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:608:CHL:H11	31:p:610:CLA:HMD2	2.02	0.41
2:q:112:GLN:HB2	2:q:119:PHE:HD1	1.85	0.41
2:q:130:ALA:O	2:q:131:SER:C	2.64	0.41
2:q:132:ILE:HG13	2:q:149:ALA:C	2.46	0.41
2:q:144:PRO:C	2:q:146:LEU:H	2.29	0.41
31:a:409:CLA:H41	31:a:409:CLA:H62	1.55	0.41
6:b:55:MET:HE3	6:b:55:MET:HB2	1.84	0.41
6:b:238:LEU:N	31:b:613:CLA:HMD2	2.36	0.41
34:b:601:LMG:H332	34:b:601:LMG:H361	1.74	0.41
31:b:602:CLA:O1A	34:r:321:LMG:H112	2.21	0.41
31:b:606:CLA:H142	31:b:611:CLA:H2	2.02	0.41
31:b:611:CLA:H202	31:b:611:CLA:H161	1.81	0.41
31:b:614:CLA:HBB1	31:b:614:CLA:CMB	2.51	0.41
34:b:629:LMG:HC71	34:b:629:LMG:HC2	1.93	0.41
7:c:122:LEU:HD11	31:c:611:CLA:H92	2.03	0.41
7:c:153:LEU:HD13	31:c:607:CLA:HED1	2.03	0.41
7:c:265:GLY:C	31:c:605:CLA:HBC2	2.45	0.41
31:c:606:CLA:H91	43:c:615:BCR:H14C	2.02	0.41
45:c:619:DGD:HAN1	33:y:619:LHG:H341	2.03	0.41
33:g:319:LHG:H291	33:g:319:LHG:H261	1.48	0.41
14:k:12:PRO:HB2	14:k:15:TYR:HD1	1.86	0.41
15:l:23:LEU:HG	33:l:101:LHG:H181	2.02	0.41
3:n:51:PRO:HG2	3:n:52:PHE:CE1	2.56	0.41
3:n:85:ARG:HG3	31:n:303:CLA:HMA3	2.03	0.41
3:n:222:GLY:O	3:n:226:ARG:HA	2.19	0.41
30:n:306:CHL:H61	30:n:306:CHL:H101	1.67	0.41
31:n:311:CLA:HBA2	31:n:311:CLA:H3A	1.49	0.41
17:o:84:VAL:HA	17:o:251:VAL:HG11	2.03	0.41
18:r:75:PRO:HG2	37:r:318:XAT:H222	2.03	0.41
18:r:137:LEU:HD23	18:r:137:LEU:HA	1.92	0.41
18:r:182:ASP:OD1	18:r:182:ASP:N	2.54	0.41
34:r:321:LMG:O9	34:r:321:LMG:O2	2.37	0.41
19:s:153:ALA:HB1	31:s:306:CLA:HBC3	2.03	0.41
19:s:251:VAL:HG12	31:s:314:CLA:HMD3	2.03	0.41
34:s:321:LMG:H151	34:s:321:LMG:H182	1.85	0.41
25:z:23:VAL:O	25:z:27:LEU:HG	2.21	0.41
28:p1:50:TYR:CZ	28:p1:52:PHE:HB2	2.56	0.41
1:1:161:GLU:HG3	30:1:609:CHL:C4B	2.50	0.41
2:2:109:GLU:HA	2:2:123:ALA:HB1	2.03	0.41
3:3:197:PHE:CZ	3:3:201:LYS:HD2	2.55	0.41
2:4:124:VAL:HB	2:4:127:LYS:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:38:VAL:HG23	3:5:40:TRP:H	1.85	0.41
3:5:75:SER:HB3	3:5:81:PHE:HD1	1.81	0.41
3:5:141:SER:HA	30:5:605:CHL:HMA1	2.03	0.41
3:5:233:LEU:HD23	31:5:613:CLA:CMA	2.50	0.41
30:5:601:CHL:HED1	33:5:619:LHG:H292	2.03	0.41
31:5:610:CLA:H52	32:5:616:LUT:C30	2.48	0.41
4:6:113:ASN:HD22	34:6:322:LMG:H292	1.86	0.41
30:6:309:CHL:HMB2	36:6:319:NEX:C35	2.50	0.41
5:A:38:ILE:HB	5:A:39:PRO:HD3	2.02	0.41
6:B:65:PHE:CE1	31:B:604:CLA:HED2	2.56	0.41
31:B:611:CLA:HBB1	31:B:611:CLA:CMB	2.44	0.41
31:B:613:CLA:H61	31:B:613:CLA:H92	1.64	0.41
34:B:625:LMG:H371	34:B:625:LMG:H341	1.87	0.41
7:C:426:PHE:CE1	31:C:605:CLA:HAB	2.56	0.41
8:D:118:GLY:O	8:D:121:SER:OG	2.37	0.41
8:D:201:VAL:HG13	31:D:403:CLA:HMB1	2.03	0.41
31:G:610:CLA:O1A	38:G:617:SQD:H111	2.21	0.41
14:K:35:LEU:HA	14:K:38:VAL:HG12	2.02	0.41
33:L:101:LHG:H202	33:L:101:LHG:H171	1.88	0.41
3:N:94:TRP:CD1	30:N:309:CHL:HMD3	2.56	0.41
31:N:305:CLA:H152	31:N:305:CLA:H18	1.90	0.41
30:N:307:CHL:H62	31:S:313:CLA:H72	2.03	0.41
32:R:317:LUT:H191	32:R:317:LUT:H11	1.79	0.41
36:S:319:NEX:H15	36:S:319:NEX:H201	1.91	0.41
31:Y:303:CLA:H142	32:Y:316:LUT:H31	2.03	0.41
26:U:71:ILE:HG22	26:U:75:ARG:CZ	2.51	0.41
34:0:620:LMG:H332	34:0:620:LMG:H301	1.91	0.41
3:8:215:MET:HG3	32:8:616:LUT:H12	2.02	0.41
30:8:606:CHL:HBA1	36:8:617:NEX:C32	2.51	0.41
2:9:229:VAL:HA	2:9:257:PHE:HZ	1.86	0.41
31:9:306:CLA:NC	36:9:319:NEX:H222	2.35	0.41
3:p:160:GLY:HA2	30:p:609:CHL:HAB	2.03	0.41
3:p:245:PHE:HD1	3:p:249:TYR:HB2	1.82	0.41
2:q:139:ASN:HA	2:q:148:HIS:H	1.86	0.41
37:q:321:XAT:H15	37:q:321:XAT:H201	1.85	0.41
5:a:47:VAL:HG21	5:a:114:LEU:HD22	2.02	0.41
5:a:312:ARG:NH2	9:e:61:GLN:O	2.53	0.41
8:d:148:ALA:HB3	8:d:149:PRO:HD3	2.03	0.41
47:e:102:HEM:CAC	10:f:26:ALA:HB1	2.51	0.41
37:g:321:XAT:H11	37:g:321:XAT:H191	1.99	0.41
31:r:314:CLA:HBA1	31:r:314:CLA:H3A	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:241:LEU:HD21	31:s:313:CLA:CBC	2.46	0.41
31:s:312:CLA:H192	31:s:313:CLA:HBB2	2.02	0.41
24:y:187:PRO:HD2	31:y:610:CLA:OBD	2.21	0.41
31:y:610:CLA:H18	31:y:610:CLA:H152	1.88	0.41
26:u:190:LYS:O	26:u:194:VAL:HG23	2.21	0.41
29:f1:196:LEU:HD22	29:f1:196:LEU:N	2.36	0.41
2:2:204:GLU:HG2	2:2:208:LYS:HE2	2.03	0.40
3:3:136:TYR:O	3:3:142:LEU:HD12	2.21	0.40
3:3:245:PHE:CE1	3:3:249:TYR:HB2	2.56	0.40
2:4:151:SER:HB3	30:4:605:CHL:OMC	2.20	0.40
34:4:621:LMG:H301	31:5:615:CLA:CHD	2.51	0.40
31:5:602:CLA:H92	31:5:602:CLA:C4	2.51	0.40
31:5:610:CLA:C2	32:5:616:LUT:H26	2.47	0.40
5:A:136:ARG:NH2	12:I:27:ASP:OD1	2.52	0.40
5:A:174:LEU:HD22	42:A:408:PHO:H143	2.02	0.40
31:B:613:CLA:HED2	31:B:614:CLA:HMC2	2.02	0.40
38:B:623:SQD:H212	8:D:36:LEU:HB2	2.03	0.40
31:C:610:CLA:HBB1	31:C:610:CLA:HMB1	2.02	0.40
44:D:406:PL9:H422	44:D:406:PL9:H461	1.90	0.40
31:N:310:CLA:H192	31:S:306:CLA:HBB2	2.03	0.40
31:N:313:CLA:H122	31:N:314:CLA:CMD	2.51	0.40
18:R:180:PRO:HG2	18:R:181:PHE:CZ	2.55	0.40
31:R:306:CLA:HMA3	30:R:308:CHL:C3C	2.52	0.40
31:R:315:CLA:HBA1	31:R:315:CLA:H3A	1.73	0.40
19:S:112:MET:HG3	19:S:239:GLY:HA2	2.04	0.40
30:Y:309:CHL:HBD	30:Y:309:CHL:HAA1	2.03	0.40
26:U:147:PRO:O	26:U:151:LYS:N	2.47	0.40
34:9:301:LMG:HC2	34:9:301:LMG:HC71	1.71	0.40
2:q:241:HIS:HB2	31:q:315:CLA:HAA2	2.02	0.40
31:q:304:CLA:CHA	31:q:304:CLA:HBA1	2.48	0.40
6:b:451:PHE:CZ	31:b:605:CLA:HED2	2.56	0.40
24:y:155:LEU:HD13	30:y:607:CHL:HBC3	2.02	0.40
43:z:101:BCR:HC7	43:z:101:BCR:H321	1.91	0.40
30:1:606:CHL:HMB2	30:1:609:CHL:OMC	2.21	0.40
3:3:91:HIS:CE1	31:3:305:CLA:C4D	3.04	0.40
2:4:109:GLU:HA	2:4:123:ALA:HB1	2.01	0.40
2:4:159:GLN:HE21	2:4:159:GLN:HB2	1.66	0.40
3:5:160:GLY:HA2	30:5:609:CHL:HAB	2.03	0.40
31:5:610:CLA:HBA2	32:5:616:LUT:C24	2.52	0.40
4:6:144:LEU:HD23	4:6:144:LEU:HA	1.91	0.40
32:6:318:LUT:H31	32:6:318:LUT:H391	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:257:TRP:CZ2	6:B:272:ARG:HG2	2.56	0.40
31:B:607:CLA:H61	31:B:607:CLA:H92	1.76	0.40
31:B:610:CLA:H92	31:B:610:CLA:H61	1.86	0.40
34:B:621:LMG:H332	34:B:621:LMG:H361	1.54	0.40
7:C:201:LEU:HD21	43:C:615:BCR:C22	2.51	0.40
31:C:608:CLA:H111	31:C:608:CLA:H152	1.90	0.40
2:G:47:ALA:HB1	30:G:601:CHL:CBC	2.52	0.40
2:G:241:HIS:CD2	31:G:613:CLA:NC	2.88	0.40
31:N:311:CLA:C4D	31:N:312:CLA:HMD3	2.51	0.40
18:R:198:GLU:HG3	31:R:311:CLA:C4B	2.51	0.40
36:R:301:NEX:H35	36:R:301:NEX:H401	1.76	0.40
19:S:60:TYR:HB2	30:S:302:CHL:C4D	2.50	0.40
19:S:251:VAL:HG21	31:S:314:CLA:HAC2	2.03	0.40
33:S:322:LHG:H121	33:S:322:LHG:HC91	1.82	0.40
24:Y:62:LEU:HD23	24:Y:62:LEU:HA	1.92	0.40
3:8:206:LYS:HD3	31:8:610:CLA:O1D	2.21	0.40
2:q:88:ARG:O	2:q:92:VAL:HG23	2.21	0.40
2:q:163:MET:HE1	36:q:319:NEX:H30	2.03	0.40
2:q:251:PHE:CG	37:q:321:XAT:H192	2.56	0.40
5:a:324:ALA:O	5:a:328:MET:HG3	2.21	0.40
31:b:611:CLA:H142	31:b:613:CLA:H2	2.02	0.40
7:c:152:HIS:HE1	31:c:612:CLA:C1D	2.35	0.40
7:c:331:ARG:NH2	17:o:71:ALA:O	2.54	0.40
31:c:602:CLA:H62	31:c:603:CLA:C1B	2.52	0.40
31:g:305:CLA:NB	36:g:317:NEX:H242	2.36	0.40
19:s:284:ASP:OD1	19:s:284:ASP:N	2.47	0.40
31:s:305:CLA:H161	31:s:316:CLA:C2B	2.51	0.40
25:z:47:TRP:O	25:z:51:VAL:HG23	2.21	0.40
28:p1:86:LEU:HD12	28:p1:86:LEU:HA	1.89	0.40
29:F1:149:GLU:HG3	29:F1:157:VAL:HG12	2.03	0.40
31:1:602:CLA:H2	32:1:616:LUT:H26	2.02	0.40
2:2:202:LEU:CG	2:2:206:LYS:HE3	2.49	0.40
3:3:38:VAL:CA	3:3:42:GLY:H	2.33	0.40
3:3:236:HIS:O	3:3:240:PRO:N	2.55	0.40
30:3:302:CHL:HHC	30:3:302:CHL:CBB	2.48	0.40
2:4:99:MET:HG2	35:4:615:RRX:C16	2.51	0.40
2:4:152:ILE:HG22	2:4:156:LEU:HD21	2.02	0.40
2:4:221:PHE:CD2	31:4:613:CLA:HAC1	2.57	0.40
31:4:613:CLA:H2	31:4:614:CLA:HMD2	2.03	0.40
3:5:182:GLY:HA2	3:5:186:ASP:HB2	2.03	0.40
31:5:611:CLA:H62	31:5:611:CLA:H92	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:145:VAL:HG13	30:6:306:CHL:C1D	2.51	0.40
4:6:191:GLY:HA3	18:R:45:ARG:HB2	2.03	0.40
30:6:307:CHL:OMC	30:6:307:CHL:HAC2	2.21	0.40
34:A:418:LMG:H292	34:A:418:LMG:HC91	1.95	0.40
6:B:224:ARG:HG2	11:H:44:TRP:CZ2	2.56	0.40
31:B:610:CLA:H193	31:B:612:CLA:HMD2	2.04	0.40
7:C:201:LEU:HD13	7:C:201:LEU:HA	1.83	0.40
31:C:606:CLA:HBB2	31:C:607:CLA:H61	2.03	0.40
2:G:129:GLY:HA3	30:N:301:CHL:C3D	2.52	0.40
31:G:612:CLA:H101	31:G:612:CLA:H62	1.63	0.40
3:N:177:ASP:HB3	3:N:180:TYR:O	2.21	0.40
3:N:191:ALA:HB1	3:N:197:PHE:CD1	2.57	0.40
30:N:309:CHL:H101	30:N:309:CHL:H62	1.87	0.40
18:R:248:PHE:CZ	37:R:318:XAT:H8	2.57	0.40
31:R:306:CLA:C1B	36:R:319:NEX:H383	2.51	0.40
30:R:309:CHL:HAC2	30:R:309:CHL:OMC	2.22	0.40
19:S:110:TRP:CD2	31:S:310:CLA:HAC2	2.56	0.40
30:Y:309:CHL:HHC	30:Y:309:CHL:CBB	2.47	0.40
31:Y:312:CLA:H161	31:Y:312:CLA:H202	1.84	0.40
4:0:120:GLU:OE1	4:0:132:GLN:NE2	2.55	0.40
4:0:194:ASP:N	18:r:45:ARG:HH22	2.19	0.40
4:0:256:ALA:O	30:p:607:CHL:HMA2	2.22	0.40
30:0:606:CHL:HBA2	30:0:606:CHL:HBD	2.03	0.40
31:0:615:CLA:O2A	34:q:301:LMG:H292	2.21	0.40
3:8:71:THR:HG21	30:9:311:CHL:HAA2	2.03	0.40
31:8:602:CLA:HBA1	32:8:616:LUT:H382	2.02	0.40
32:8:616:LUT:H35	32:8:616:LUT:H401	1.87	0.40
34:9:302:LMG:H302	34:9:302:LMG:C9	2.52	0.40
3:p:96:MET:HB3	32:p:616:LUT:C34	2.51	0.40
31:p:615:CLA:C3B	30:q:309:CHL:HMA2	2.52	0.40
2:q:205:LEU:HD12	31:q:312:CLA:HHB	2.02	0.40
31:q:304:CLA:HBA1	32:q:318:LUT:H382	2.03	0.40
5:a:263:ALA:HA	33:e:101:LHG:H131	2.02	0.40
31:a:407:CLA:H52	44:d:407:PL9:H151	2.02	0.40
6:b:391:SER:O	6:b:395:VAL:HG23	2.21	0.40
31:b:605:CLA:H41	31:b:605:CLA:H61	1.76	0.40
31:b:608:CLA:H193	15:l:29:ALA:HA	2.02	0.40
7:c:418:HIS:CD2	31:c:602:CLA:ND	2.89	0.40
45:c:619:DGD:HBS1	31:y:614:CLA:HBC1	2.03	0.40
8:d:146:PHE:C	8:d:149:PRO:HD2	2.47	0.40
8:d:160:TYR:O	8:d:164:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:320:LEU:HD12	8:d:320:LEU:HA	1.90	0.40
9:e:37:PHE:CZ	9:e:47:PHE:HE2	2.39	0.40
10:f:35:ALA:O	10:f:39:MET:HG3	2.22	0.40
2:g:126:PHE:CD1	2:g:127:LYS:HG3	2.56	0.40
31:g:313:CLA:H61	31:g:313:CLA:H92	1.76	0.40
3:n:200:LEU:HB3	31:n:311:CLA:CMA	2.50	0.40
32:n:317:LUT:H35	32:n:317:LUT:H401	1.86	0.40
18:r:145:LEU:HD11	38:r:322:SQD:H372	2.03	0.40
19:s:191:GLY:HA3	31:s:316:CLA:C3D	2.51	0.40
32:y:617:LUT:H15	32:y:617:LUT:H201	1.89	0.40
32:y:617:LUT:H35	32:y:617:LUT:H401	1.88	0.40
30:2:607:CHL:HBA2	31:2:609:CLA:CMD	2.50	0.40
3:3:118:GLU:OE2	3:3:130:GLN:NE2	2.54	0.40
3:3:188:LEU:HB2	3:3:190:LEU:HG	2.03	0.40
2:4:152:ILE:O	2:4:153:VAL:C	2.64	0.40
30:4:606:CHL:HMB1	30:4:606:CHL:CBB	2.49	0.40
31:4:612:CLA:HHC	31:4:612:CLA:HBB1	2.03	0.40
34:4:620:LMG:HC72	34:4:620:LMG:O9	2.22	0.40
31:5:603:CLA:HBB1	31:5:603:CLA:CMB	2.52	0.40
4:6:139:LEU:HD11	34:6:321:LMG:O9	2.22	0.40
34:6:321:LMG:H132	34:6:321:LMG:H161	1.89	0.40
43:B:619:BCR:H371	43:B:619:BCR:H24C	1.90	0.40
7:C:14:ARG:HE	7:C:14:ARG:HA	1.86	0.40
2:G:89:GLU:O	2:G:93:ILE:HG12	2.22	0.40
2:G:121:GLU:HB2	2:G:127:LYS:HE2	2.04	0.40
2:G:146:LEU:O	2:G:147:ILE:C	2.65	0.40
2:G:167:GLU:HG3	30:G:608:CHL:C4B	2.50	0.40
14:K:15:TYR:CZ	25:Z:5:PHE:HZ	2.40	0.40
3:N:252:LYS:HA	3:N:256:ILE:CG2	2.48	0.40
17:O:100:GLU:HA	17:O:131:THR:HG22	2.03	0.40
17:O:116:ASP:O	17:O:118:GLU:HG3	2.22	0.40
31:R:304:CLA:H93	31:R:304:CLA:H62	1.90	0.40
19:S:114:ALA:O	19:S:118:ALA:N	2.53	0.40
19:S:155:PRO:HD3	31:S:306:CLA:ND	2.35	0.40
31:S:305:CLA:NC	36:S:319:NEX:H222	2.36	0.40
31:S:312:CLA:CHD	33:S:320:LHG:HC62	2.51	0.40
20:T:18:PHE:HA	43:T:101:BCR:H403	2.04	0.40
4:0:191:GLY:HA3	18:r:45:ARG:HB2	2.04	0.40
4:0:253:LYS:HE2	4:0:253:LYS:HB2	1.90	0.40
31:7:316:CLA:HBB1	3:8:222:GLY:HA3	2.03	0.40
3:8:51:PRO:HG2	3:8:52:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:8:602:CLA:C9	31:9:305:CLA:H52	2.52	0.40
31:8:614:CLA:C3D	34:9:302:LMG:H292	2.51	0.40
2:q:116:ALA:HA	34:q1:101:LMG:HC8	2.03	0.40
2:q:195:LEU:HB2	31:q:312:CLA:O1A	2.21	0.40
5:a:198:HIS:HE1	31:a:406:CLA:C4B	2.35	0.40
6:b:149:LEU:HD22	31:b:605:CLA:H162	2.04	0.40
31:c:606:CLA:H111	31:c:606:CLA:H93	1.84	0.40
45:c:619:DGD:HA61	45:c:619:DGD:HA92	1.91	0.40
30:n:306:CHL:H93	30:n:306:CHL:H111	1.85	0.40
48:r:302:LMU:H22	31:r:307:CLA:CBB	2.51	0.40
31:r:312:CLA:HBA2	31:r:312:CLA:H12	1.94	0.40
1:1:134:TYR:CE1	31:1:604:CLA:H2	2.57	0.40
1:1:246:LEU:HD23	1:1:247:TYR:CE2	2.57	0.40
30:1:606:CHL:HAC1	30:1:606:CHL:OMC	2.22	0.40
31:1:611:CLA:CHD	33:1:617:LHG:HC62	2.52	0.40
30:2:608:CHL:HHC	30:2:608:CHL:CBB	2.47	0.40
3:3:241:ASP:N	3:3:241:ASP:OD1	2.55	0.40
31:3:305:CLA:HBB1	31:3:305:CLA:CMB	2.51	0.40
31:3:311:CLA:H2	32:3:317:LUT:H28	2.03	0.40
31:3:312:CLA:H92	31:3:312:CLA:H62	1.82	0.40
2:4:77:LEU:HD23	31:4:602:CLA:H11	2.04	0.40
2:4:152:ILE:H	2:4:152:ILE:CD1	2.21	0.40
2:4:158:THR:O	2:4:162:ILE:HD13	2.21	0.40
3:5:91:HIS:CD2	32:5:617:LUT:H15	2.57	0.40
31:5:610:CLA:H51	31:5:610:CLA:C2B	2.51	0.40
34:5:620:LMG:H122	34:5:620:LMG:H152	1.79	0.40
4:6:235:LEU:C	4:6:235:LEU:HD13	2.47	0.40
30:6:307:CHL:H3A	36:6:319:NEX:H31	2.02	0.40
34:6:323:LMG:C28	34:6:323:LMG:HC72	2.51	0.40
34:6:323:LMG:C28	34:X:202:LMG:H121	2.52	0.40
6:B:225:LEU:HD12	6:B:225:LEU:HA	1.90	0.40
31:B:610:CLA:H202	31:B:610:CLA:H161	1.87	0.40
31:B:616:CLA:H161	31:B:616:CLA:H141	1.81	0.40
31:C:602:CLA:H141	31:C:602:CLA:H161	1.90	0.40
45:C:620:DGD:HB42	45:C:620:DGD:HB71	1.72	0.40
14:K:19:ASP:N	14:K:20:PRO:HD2	2.36	0.40
19:S:163:LEU:HD13	19:S:163:LEU:HA	1.94	0.40
31:S:315:CLA:HBA2	31:S:315:CLA:H3A	1.53	0.40
20:T:26:PRO:HA	20:T:27:PRO:HD3	1.93	0.40
31:Y:312:CLA:H143	31:Y:312:CLA:H111	1.65	0.40
4:0:61:LEU:HD23	4:0:70:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:0:602:CLA:H52	32:0:617:LUT:H28	2.02	0.40
3:8:87:LEU:CD1	31:8:603:CLA:HBA1	2.43	0.40
31:p:610:CLA:HBA2	32:p:616:LUT:H24	2.03	0.40
2:q:138:LEU:HD23	2:q:138:LEU:C	2.47	0.40
6:b:280:PHE:O	6:b:284:ILE:HG13	2.22	0.40
31:b:614:CLA:H112	31:b:614:CLA:H152	1.86	0.40
9:e:40:THR:HB	27:q1:4:ARG:HD2	2.03	0.40
2:g:185:TYR:CE2	2:g:206:LYS:HE3	2.56	0.40
31:g:304:CLA:H52	31:g:304:CLA:H8	1.50	0.40
31:g:313:CLA:H102	33:g:319:LHG:H281	2.02	0.40
3:n:226:ARG:NH1	31:y:615:CLA:HMA2	2.37	0.40
18:r:266:LEU:HD12	18:r:266:LEU:HA	1.92	0.40
31:s:315:CLA:H3A	31:s:315:CLA:HBA2	1.49	0.40
24:y:46:ARG:NH2	24:y:62:LEU:O	2.54	0.40
24:y:46:ARG:HD2	24:y:69:ASP:O	2.21	0.40
24:y:178:PHE:HD1	38:y:621:SQD:H2	1.86	0.40
24:y:251:PHE:HB2	31:y:613:CLA:CAD	2.52	0.40
31:y:610:CLA:C2	32:y:616:LUT:H28	2.48	0.40
27:q1:3:ASN:HB2	34:q1:101:LMG:C5	2.51	0.40
27:q1:23:ILE:HD12	27:q1:23:ILE:HA	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	212/214 (99%)	202 (95%)	10 (5%)	0	100 100
1	7	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	24 40
2	2	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	14 26
2	4	220/222 (99%)	200 (91%)	15 (7%)	5 (2%)	5 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	9	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
2	G	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
2	g	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
2	q	220/222 (99%)	196 (89%)	22 (10%)	2 (1%)	14	26
3	3	219/221 (99%)	198 (90%)	21 (10%)	0	100	100
3	5	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	14	26
3	8	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
3	N	219/221 (99%)	211 (96%)	7 (3%)	1 (0%)	24	40
3	n	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
3	p	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	9	15
4	0	215/217 (99%)	202 (94%)	12 (6%)	1 (0%)	24	40
4	6	215/217 (99%)	205 (95%)	9 (4%)	1 (0%)	24	40
5	A	334/336 (99%)	329 (98%)	5 (2%)	0	100	100
5	a	334/336 (99%)	329 (98%)	5 (2%)	0	100	100
6	B	502/504 (100%)	493 (98%)	9 (2%)	0	100	100
6	b	502/504 (100%)	491 (98%)	11 (2%)	0	100	100
7	C	446/448 (100%)	437 (98%)	9 (2%)	0	100	100
7	c	446/448 (100%)	438 (98%)	8 (2%)	0	100	100
8	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
8	d	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	54
9	E	79/81 (98%)	79 (100%)	0	0	100	100
9	e	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
10	F	35/37 (95%)	35 (100%)	0	0	100	100
10	f	35/37 (95%)	35 (100%)	0	0	100	100
11	H	65/67 (97%)	65 (100%)	0	0	100	100
11	h	65/67 (97%)	65 (100%)	0	0	100	100
12	I	32/34 (94%)	32 (100%)	0	0	100	100
12	i	32/34 (94%)	32 (100%)	0	0	100	100
13	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	j	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
14	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
15	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
15	l	35/37 (95%)	35 (100%)	0	0	100	100
16	M	31/57 (54%)	30 (97%)	0	1 (3%)	3	5
16	m	31/57 (54%)	31 (100%)	0	0	100	100
17	O	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
17	o	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
18	R	233/236 (99%)	227 (97%)	6 (3%)	0	100	100
18	r	233/236 (99%)	230 (99%)	3 (1%)	0	100	100
19	S	255/257 (99%)	249 (98%)	6 (2%)	0	100	100
19	s	255/257 (99%)	249 (98%)	6 (2%)	0	100	100
20	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
20	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
21	V	30/32 (94%)	30 (100%)	0	0	100	100
21	v	30/32 (94%)	30 (100%)	0	0	100	100
22	W	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
22	w	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
23	X	35/37 (95%)	35 (100%)	0	0	100	100
23	x	35/37 (95%)	35 (100%)	0	0	100	100
24	Y	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
24	y	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
25	Z	60/62 (97%)	60 (100%)	0	0	100	100
25	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	U	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	18	32
26	u	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
27	Q1	32/34 (94%)	32 (100%)	0	0	100	100
27	q1	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
28	P1	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
28	p1	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
29	F1	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
29	f1	186/188 (99%)	180 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	10672/10854 (98%)	10317 (97%)	334 (3%)	21 (0%)	44 62

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	181	GLY
2	4	188	GLY
2	4	191	ASP
3	N	52	PHE
4	0	252	ALA
2	q	191	ASP
2	4	186	PRO
26	U	110	ALA
2	q	188	GLY
2	2	125	TRP
2	2	257	PHE
3	5	248	ASP
4	6	251	TYR
1	7	140	LEU
3	p	39	GLU
3	p	246	TRP
2	4	146	LEU
16	M	5	ILE
3	5	256	ILE
3	p	51	PRO
8	d	140	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	165/165 (100%)	156 (94%)	9 (6%)	19 35
1	7	165/165 (100%)	158 (96%)	7 (4%)	26 47
2	2	171/171 (100%)	164 (96%)	7 (4%)	27 48
2	4	171/171 (100%)	161 (94%)	10 (6%)	18 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	9	171/171 (100%)	165 (96%)	6 (4%)	32	54
2	G	171/171 (100%)	164 (96%)	7 (4%)	27	48
2	g	171/171 (100%)	161 (94%)	10 (6%)	18	33
2	q	171/171 (100%)	164 (96%)	7 (4%)	27	48
3	3	168/168 (100%)	156 (93%)	12 (7%)	13	24
3	5	168/168 (100%)	156 (93%)	12 (7%)	13	24
3	8	168/168 (100%)	159 (95%)	9 (5%)	20	36
3	N	168/168 (100%)	158 (94%)	10 (6%)	17	31
3	n	168/168 (100%)	159 (95%)	9 (5%)	20	36
3	p	168/168 (100%)	161 (96%)	7 (4%)	26	47
4	0	169/169 (100%)	159 (94%)	10 (6%)	18	32
4	6	169/169 (100%)	161 (95%)	8 (5%)	23	43
5	A	274/274 (100%)	261 (95%)	13 (5%)	23	43
5	a	274/274 (100%)	265 (97%)	9 (3%)	33	55
6	B	402/402 (100%)	375 (93%)	27 (7%)	15	27
6	b	402/402 (100%)	377 (94%)	25 (6%)	16	30
7	C	350/350 (100%)	324 (93%)	26 (7%)	13	23
7	c	350/350 (100%)	332 (95%)	18 (5%)	21	39
8	D	277/277 (100%)	268 (97%)	9 (3%)	34	56
8	d	277/277 (100%)	260 (94%)	17 (6%)	17	30
9	E	72/72 (100%)	69 (96%)	3 (4%)	26	47
9	e	72/72 (100%)	69 (96%)	3 (4%)	26	47
10	F	31/31 (100%)	31 (100%)	0	100	100
10	f	31/31 (100%)	31 (100%)	0	100	100
11	H	57/57 (100%)	56 (98%)	1 (2%)	51	69
11	h	57/57 (100%)	55 (96%)	2 (4%)	32	54
12	I	31/31 (100%)	30 (97%)	1 (3%)	34	56
12	i	31/31 (100%)	30 (97%)	1 (3%)	34	56
13	J	27/27 (100%)	24 (89%)	3 (11%)	6	11
13	j	27/27 (100%)	25 (93%)	2 (7%)	13	23
14	K	33/33 (100%)	29 (88%)	4 (12%)	5	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	k	33/33 (100%)	28 (85%)	5 (15%)	3	3
15	L	34/34 (100%)	32 (94%)	2 (6%)	18	32
15	l	34/34 (100%)	32 (94%)	2 (6%)	18	32
16	M	28/28 (100%)	27 (96%)	1 (4%)	31	53
16	m	28/28 (100%)	27 (96%)	1 (4%)	31	53
17	O	189/189 (100%)	176 (93%)	13 (7%)	14	26
17	o	189/189 (100%)	181 (96%)	8 (4%)	26	47
18	R	184/184 (100%)	178 (97%)	6 (3%)	33	55
18	r	184/184 (100%)	177 (96%)	7 (4%)	29	51
19	S	192/192 (100%)	185 (96%)	7 (4%)	31	53
19	s	192/192 (100%)	186 (97%)	6 (3%)	35	57
20	T	26/26 (100%)	26 (100%)	0	100	100
20	t	26/26 (100%)	23 (88%)	3 (12%)	5	10
21	V	26/26 (100%)	24 (92%)	2 (8%)	12	21
21	v	26/26 (100%)	25 (96%)	1 (4%)	29	51
22	W	50/50 (100%)	49 (98%)	1 (2%)	48	67
22	w	50/50 (100%)	50 (100%)	0	100	100
23	X	25/25 (100%)	23 (92%)	2 (8%)	11	20
23	x	25/25 (100%)	25 (100%)	0	100	100
24	Y	170/170 (100%)	161 (95%)	9 (5%)	20	37
24	y	170/170 (100%)	160 (94%)	10 (6%)	18	32
25	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
25	z	52/52 (100%)	49 (94%)	3 (6%)	18	33
26	U	108/108 (100%)	106 (98%)	2 (2%)	50	68
26	u	108/108 (100%)	100 (93%)	8 (7%)	13	23
27	Q1	28/28 (100%)	28 (100%)	0	100	100
27	q1	28/28 (100%)	28 (100%)	0	100	100
28	P1	88/88 (100%)	88 (100%)	0	100	100
28	p1	88/88 (100%)	84 (96%)	4 (4%)	24	44
29	F1	147/147 (100%)	139 (95%)	8 (5%)	20	36
29	f1	147/147 (100%)	146 (99%)	1 (1%)	76	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8504/8504 (100%)	8086 (95%)	418 (5%)	24 41

All (418) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	40	GLN
1	1	48	LYS
1	1	77	LEU
1	1	103	LEU
1	1	146	ILE
1	1	150	LEU
1	1	231	LEU
1	1	246	LEU
1	1	249	LYS
2	2	77	LEU
2	2	124	VAL
2	2	127	LYS
2	2	152	ILE
2	2	184	LEU
2	2	189	PHE
2	2	256	LYS
3	3	86	GLU
3	3	118	GLU
3	3	153	LEU
3	3	166	ARG
3	3	168	ASN
3	3	200	LEU
3	3	202	VAL
3	3	223	LEU
3	3	241	ASP
3	3	252	LYS
3	3	256	ILE
3	3	258	TYR
2	4	50	LEU
2	4	77	LEU
2	4	113	ASN
2	4	146	LEU
2	4	152	ILE
2	4	155	VAL
2	4	159	GLN
2	4	170	ARG
2	4	202	LEU

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Mol	Chain	Res	Type
2	4	205	LEU
3	5	74	LEU
3	5	86	GLU
3	5	107	LEU
3	5	113	VAL
3	5	115	ASN
3	5	152	LEU
3	5	158	LEU
3	5	230	ILE
3	5	233	LEU
3	5	241	ASP
3	5	249	TYR
3	5	256	ILE
4	6	76	LEU
4	6	106	THR
4	6	139	LEU
4	6	148	GLN
4	6	177	VAL
4	6	178	VAL
4	6	251	TYR
4	6	253	LYS
5	A	35	VAL
5	A	36	LEU
5	A	96	ILE
5	A	121	LEU
5	A	133	LEU
5	A	194	MET
5	A	214	MET
5	A	218	LEU
5	A	275	LEU
5	A	313	VAL
5	A	326	LEU
5	A	334	ARG
5	A	343	LEU
6	B	10	THR
6	B	22	VAL
6	B	37	MET
6	B	51	VAL
6	B	52	LEU
6	B	57	ARG
6	B	94	GLU
6	B	159	THR

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Mol	Chain	Res	Type
6	B	161	LEU
6	B	181	VAL
6	B	214	LEU
6	B	236	THR
6	B	245	VAL
6	B	252	VAL
6	B	272	ARG
6	B	292	LEU
6	B	345	VAL
6	B	362	PHE
6	B	368	VAL
6	B	369	VAL
6	B	373	LYS
6	B	393	GLU
6	B	422	ARG
6	B	437	LEU
6	B	440	ASP
6	B	473	THR
6	B	486	LEU
7	C	56	ASN
7	C	101	VAL
7	C	105	LEU
7	C	112	VAL
7	C	113	LEU
7	C	123	VAL
7	C	155	VAL
7	C	156	LEU
7	C	158	LEU
7	C	164	VAL
7	C	173	ILE
7	C	201	LEU
7	C	222	ILE
7	C	228	ILE
7	C	243	LYS
7	C	302	THR
7	C	304	THR
7	C	308	ARG
7	C	309	ASP
7	C	336	GLU
7	C	357	LEU
7	C	361	ASN
7	C	369	LYS

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Mol	Chain	Res	Type
7	C	392	LEU
7	C	398	VAL
7	C	416	THR
8	D	28	VAL
8	D	35	LEU
8	D	74	LEU
8	D	90	LEU
8	D	92	LEU
8	D	107	LEU
8	D	131	GLU
8	D	178	ILE
8	D	264	LYS
9	E	7	GLU
9	E	62	GLU
9	E	67	THR
2	G	50	LEU
2	G	100	LEU
2	G	132	ILE
2	G	198	ASP
2	G	202	LEU
2	G	244	GLU
2	G	258	LEU
11	H	77	VAL
12	I	4	LEU
13	J	6	THR
13	J	12	LEU
13	J	42	LEU
14	K	25	LEU
14	K	33	LEU
14	K	35	LEU
14	K	37	LEU
15	L	12	GLU
15	L	16	THR
16	M	3	VAL
3	N	59	LEU
3	N	62	GLU
3	N	131	GLU
3	N	146	GLN
3	N	152	LEU
3	N	156	LEU
3	N	158	LEU
3	N	226	ARG

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Mol	Chain	Res	Type
3	N	241	ASP
3	N	256	ILE
17	O	60	LEU
17	O	86	ASP
17	O	87	LEU
17	O	148	GLU
17	O	151	GLU
17	O	170	VAL
17	O	173	LEU
17	O	179	LEU
17	O	184	ASN
17	O	250	LYS
17	O	251	VAL
17	O	255	THR
17	O	272	LEU
18	R	54	LEU
18	R	56	ASN
18	R	137	LEU
18	R	162	VAL
18	R	243	LEU
18	R	249	LEU
19	S	36	SER
19	S	51	LYS
19	S	92	LYS
19	S	149	LEU
19	S	196	VAL
19	S	201	GLU
19	S	209	ASN
21	V	2	ASN
21	V	7	LEU
22	W	119	LEU
23	X	72	LEU
23	X	100	ARG
24	Y	57	LEU
24	Y	77	LEU
24	Y	155	LEU
24	Y	167	ILE
24	Y	185	LEU
24	Y	203	LEU
24	Y	219	LEU
24	Y	222	LEU
24	Y	236	LEU

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Mol	Chain	Res	Type
25	Z	9	LEU
25	Z	53	LEU
26	U	89	GLN
26	U	92	GLU
4	0	76	LEU
4	0	106	THR
4	0	111	GLN
4	0	133	GLU
4	0	148	GLN
4	0	177	VAL
4	0	197	ASP
4	0	227	THR
4	0	235	LEU
4	0	250	LEU
1	7	50	LEU
1	7	61	TYR
1	7	103	LEU
1	7	140	LEU
1	7	150	LEU
1	7	221	ILE
1	7	251	LEU
3	8	38	VAL
3	8	52	PHE
3	8	59	LEU
3	8	62	GLU
3	8	131	GLU
3	8	146	GLN
3	8	152	LEU
3	8	158	LEU
3	8	256	ILE
2	9	63	LYS
2	9	119	PHE
2	9	124	VAL
2	9	184	LEU
2	9	238	LEU
2	9	258	LEU
3	p	74	LEU
3	p	100	LEU
3	p	128	ILE
3	p	179	LEU
3	p	232	ASN
3	p	233	LEU

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Mol	Chain	Res	Type
3	p	258	TYR
2	q	50	LEU
2	q	77	LEU
2	q	152	ILE
2	q	170	ARG
2	q	192	PRO
2	q	202	LEU
2	q	205	LEU
5	a	133	LEU
5	a	165	GLN
5	a	194	MET
5	a	257	ARG
5	a	266	ASN
5	a	275	LEU
5	a	313	VAL
5	a	334	ARG
5	a	343	LEU
6	b	10	THR
6	b	13	LEU
6	b	22	VAL
6	b	51	VAL
6	b	52	LEU
6	b	94	GLU
6	b	159	THR
6	b	181	VAL
6	b	214	LEU
6	b	224	ARG
6	b	225	LEU
6	b	236	THR
6	b	246	PHE
6	b	252	VAL
6	b	272	ARG
6	b	289	GLN
6	b	292	LEU
6	b	362	PHE
6	b	368	VAL
6	b	369	VAL
6	b	374	ASP
6	b	399	VAL
6	b	445	THR
6	b	489	GLN
6	b	498	LEU

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Mol	Chain	Res	Type
7	c	55	MET
7	c	56	ASN
7	c	101	VAL
7	c	105	LEU
7	c	155	VAL
7	c	156	LEU
7	c	164	VAL
7	c	166	LYS
7	c	173	ILE
7	c	267	ILE
7	c	275	CYS
7	c	302	THR
7	c	323	THR
7	c	361	ASN
7	c	392	LEU
7	c	398	VAL
7	c	430	LEU
7	c	458	ARG
8	d	28	VAL
8	d	45	LEU
8	d	74	LEU
8	d	90	LEU
8	d	92	LEU
8	d	102	THR
8	d	107	LEU
8	d	158	LEU
8	d	178	ILE
8	d	192	THR
8	d	213	ILE
8	d	279	LEU
8	d	320	LEU
8	d	323	GLU
8	d	340	VAL
8	d	345	VAL
8	d	352	LEU
9	e	49	SER
9	e	65	LEU
9	e	66	ILE
2	g	50	LEU
2	g	74	THR
2	g	100	LEU
2	g	152	ILE

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Mol	Chain	Res	Type
2	g	156	LEU
2	g	158	THR
2	g	167	GLU
2	g	184	LEU
2	g	202	LEU
2	g	204	GLU
11	h	74	LEU
11	h	77	VAL
12	i	4	LEU
13	j	12	LEU
13	j	42	LEU
14	k	11	LEU
14	k	25	LEU
14	k	33	LEU
14	k	35	LEU
14	k	37	LEU
15	l	3	LYS
15	l	16	THR
16	m	9	ILE
3	n	38	VAL
3	n	52	PHE
3	n	59	LEU
3	n	62	GLU
3	n	131	GLU
3	n	146	GLN
3	n	152	LEU
3	n	158	LEU
3	n	256	ILE
17	o	77	LEU
17	o	88	LYS
17	o	170	VAL
17	o	173	LEU
17	o	179	LEU
17	o	186	ASP
17	o	250	LYS
17	o	251	VAL
18	r	54	LEU
18	r	145	LEU
18	r	151	LEU
18	r	162	VAL
18	r	179	LEU
18	r	243	LEU

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Mol	Chain	Res	Type
18	r	249	LEU
19	s	45	GLN
19	s	90	LEU
19	s	92	LYS
19	s	149	LEU
19	s	196	VAL
19	s	236	ILE
20	t	1	MET
20	t	2	GLU
20	t	30	VAL
21	v	5	ILE
24	y	57	LEU
24	y	77	LEU
24	y	121	GLU
24	y	167	ILE
24	y	185	LEU
24	y	203	LEU
24	y	219	LEU
24	y	222	LEU
24	y	236	LEU
24	y	257	ASN
25	z	3	LEU
25	z	9	LEU
25	z	49	LEU
26	u	55	LEU
26	u	62	LYS
26	u	98	LYS
26	u	106	LYS
26	u	113	ASP
26	u	122	THR
26	u	152	LYS
26	u	153	GLU
28	p1	7	ILE
28	p1	28	SER
28	p1	60	VAL
28	p1	79	TYR
29	F1	63	LYS
29	F1	89	ASP
29	F1	120	ASP
29	F1	175	LYS
29	F1	181	VAL
29	F1	187	ASP

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Mol	Chain	Res	Type
29	F1	216	LYS
29	F1	235	VAL
29	f1	181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	182	ASN
3	3	115	ASN
3	3	221	GLN
2	4	113	ASN
2	4	114	ASN
3	5	47	GLN
3	5	115	ASN
3	5	130	GLN
3	5	146	GLN
3	5	155	GLN
5	A	181	ASN
5	A	247	ASN
5	A	322	ASN
6	B	394	GLN
7	C	62	HIS
7	C	143	ASN
2	G	150	GLN
2	G	237	ASN
12	I	26	ASN
14	K	40	GLN
3	N	54	ASN
3	N	115	ASN
17	O	58	GLN
18	R	46	GLN
18	R	130	GLN
18	R	267	ASN
19	S	103	ASN
19	S	160	ASN
22	W	111	ASN
24	Y	238	ASN
26	U	131	GLN
26	U	171	GLN
4	0	148	GLN
4	0	170	ASN
4	0	234	ASN

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Mol	Chain	Res	Type
2	9	143	ASN
3	p	127	GLN
3	p	146	GLN
3	p	221	GLN
3	p	232	ASN
3	p	244	ASN
5	a	108	ASN
5	a	165	GLN
5	a	241	GLN
5	a	266	ASN
5	a	267	ASN
5	a	337	HIS
6	b	331	ASN
7	c	315	ASN
7	c	376	GLN
8	d	142	ASN
8	d	332	GLN
2	g	148	HIS
2	g	237	ASN
16	m	4	ASN
17	o	56	GLN
17	o	243	GLN
19	s	45	GLN
19	s	158	ASN
26	u	171	GLN
28	P1	17	ASN
28	P1	54	ASN
29	F1	59	ASN
29	F1	105	ASN
29	F1	203	ASN
29	f1	59	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CSU	R	211	18	6,9,10	3.27	3 (50%)	3,12,14	2.40	2 (66%)
18	CSU	r	211	18	6,9,10	3.28	3 (50%)	3,12,14	2.38	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CSU	R	211	18	-	4/4/8/10	-
18	CSU	r	211	18	-	4/4/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	r	211	CSU	OD1-S	6.06	1.63	1.45
18	R	211	CSU	OD3-S	6.04	1.63	1.45
18	R	211	CSU	O-C	4.03	1.36	1.19
18	r	211	CSU	O-C	4.01	1.35	1.19
18	R	211	CSU	OD1-S	-2.73	1.37	1.45
18	r	211	CSU	OD3-S	-2.66	1.37	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	r	211	CSU	OD2-S-OD3	3.53	125.57	112.78
18	R	211	CSU	OD2-S-OD1	3.15	124.19	112.78
18	R	211	CSU	OD2-S-OD3	-2.70	102.99	112.78
18	r	211	CSU	OD2-S-OD1	-2.10	105.16	112.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	211	CSU	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
18	R	211	CSU	OD2-S-SG-CB
18	r	211	CSU	OD2-S-SG-CB
18	R	211	CSU	OD1-S-SG-CB
18	R	211	CSU	OD3-S-SG-CB
18	r	211	CSU	OD1-S-SG-CB
18	r	211	CSU	OD3-S-SG-CB
18	r	211	CSU	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	211	CSU	1	0
18	r	211	CSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 672 ligands modelled in this entry, 6 are monoatomic - leaving 666 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	BCR	b	619	-	41,41,41	4.78	26 (63%)	56,56,56	2.31	20 (35%)
33	LHG	9	320	31	32,32,48	0.46	0	35,38,54	1.25	3 (8%)
35	RRX	G	614	-	42,42,42	5.01	25 (59%)	57,58,58	2.49	22 (38%)
31	CLA	2	611	2	59,63,73	1.46	6 (10%)	71,101,113	2.02	18 (25%)
30	CHL	9	311	2	65,69,74	0.83	2 (3%)	74,108,114	1.33	13 (17%)
31	CLA	3	313	3	54,58,73	1.53	6 (11%)	65,95,113	2.15	20 (30%)
46	BCT	D	402	40	2,3,3	1.35	0	2,3,3	2.67	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CLA	C	607	49	69,73,73	1.37	7 (10%)	83,113,113	1.99	21 (25%)
38	SQD	a	412	-	44,45,54	0.90	1 (2%)	53,56,65	1.01	4 (7%)
32	LUT	Y	316	-	42,43,43	6.02	27 (64%)	51,60,60	2.08	18 (35%)
34	LMG	D	410	-	46,46,55	0.93	3 (6%)	54,54,63	1.07	4 (7%)
38	SQD	g	318	-	41,42,54	0.88	0	50,53,65	0.96	2 (4%)
30	CHL	4	606	31	55,59,74	0.88	2 (3%)	62,96,114	1.41	12 (19%)
31	CLA	B	610	49	69,73,73	1.35	6 (8%)	83,113,113	1.96	20 (24%)
31	CLA	y	610	24	69,73,73	1.35	7 (10%)	83,113,113	1.92	17 (20%)
31	CLA	3	306	49	59,63,73	1.47	7 (11%)	71,101,113	2.08	18 (25%)
32	LUT	5	617	-	42,43,43	6.08	27 (64%)	51,60,60	1.87	12 (23%)
30	CHL	3	308	-	51,55,74	0.95	2 (3%)	57,91,114	1.41	10 (17%)
31	CLA	r	311	18	62,66,73	1.44	6 (9%)	74,104,113	2.05	18 (24%)
31	CLA	s	315	19	52,56,73	1.56	6 (11%)	62,92,113	2.05	15 (24%)
30	CHL	Y	302	24	70,74,74	0.80	2 (2%)	80,114,114	1.30	14 (17%)
34	LMG	b	629	-	38,38,55	0.63	1 (2%)	46,46,63	1.12	2 (4%)
30	CHL	G	608	2	67,71,74	0.86	3 (4%)	76,110,114	1.41	14 (18%)
34	LMG	X	203	-	38,38,55	0.61	1 (2%)	46,46,63	1.12	2 (4%)
38	SQD	A	413	-	44,45,54	0.84	0	53,56,65	0.96	2 (3%)
31	CLA	9	313	33	51,55,73	1.59	7 (13%)	61,91,113	2.07	16 (26%)
31	CLA	c	613	7	69,73,73	1.36	7 (10%)	83,113,113	1.99	19 (22%)
34	LMG	3	321	-	38,38,55	0.63	1 (2%)	46,46,63	0.96	2 (4%)
43	BCR	d	406	-	41,41,41	4.70	26 (63%)	56,56,56	3.60	25 (44%)
34	LMG	C	619	-	51,51,55	1.07	6 (11%)	59,59,63	1.18	4 (6%)
31	CLA	s	314	19	69,73,73	1.38	7 (10%)	83,113,113	1.94	19 (22%)
31	CLA	C	604	49	60,64,73	1.47	6 (10%)	72,102,113	2.06	16 (22%)
32	LUT	p	616	-	42,43,43	6.09	27 (64%)	51,60,60	2.78	18 (35%)
31	CLA	N	312	3	49,53,73	1.59	7 (14%)	59,89,113	2.06	17 (28%)
31	CLA	c	609	7	69,73,73	1.38	6 (8%)	83,113,113	1.92	19 (22%)
38	SQD	g	301	-	37,38,54	0.91	0	46,49,65	1.01	2 (4%)
38	SQD	r	322	-	50,51,54	0.80	0	59,62,65	0.93	2 (3%)
31	CLA	G	603	2	59,63,73	1.45	6 (10%)	71,101,113	2.08	18 (25%)
31	CLA	p	603	3	59,63,73	1.47	7 (11%)	71,101,113	2.14	19 (26%)
38	SQD	M	102	-	49,50,54	0.81	0	58,61,65	0.95	2 (3%)
31	CLA	3	314	3	59,63,73	1.46	7 (11%)	71,101,113	2.06	20 (28%)
31	CLA	r	304	18	64,68,73	1.40	6 (9%)	77,107,113	1.99	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
38	SQD	G	617	-	41,42,54	0.86	0	50,53,65	0.98	2 (4%)
31	CLA	2	603	2	59,63,73	1.46	6 (10%)	71,101,113	2.05	19 (26%)
43	BCR	D	405	-	41,41,41	4.84	27 (65%)	56,56,56	2.69	22 (39%)
30	CHL	7	310	1	70,74,74	0.80	2 (2%)	80,114,114	1.29	14 (17%)
30	CHL	2	608	2	61,65,74	0.89	3 (4%)	69,103,114	1.42	14 (20%)
31	CLA	B	611	6	69,73,73	1.37	7 (10%)	83,113,113	1.93	18 (21%)
34	LMG	9	301	-	51,51,55	1.10	6 (11%)	59,59,63	1.68	8 (13%)
34	LMG	D	411	-	51,51,55	1.07	6 (11%)	59,59,63	1.08	3 (5%)
31	CLA	N	311	33	53,57,73	1.54	6 (11%)	62,93,113	2.18	17 (27%)
31	CLA	7	305	49	69,73,73	1.35	6 (8%)	83,113,113	1.97	17 (20%)
31	CLA	Y	310	24	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
37	XAT	r	318	-	39,47,47	0.65	0	54,74,74	1.94	12 (22%)
31	CLA	n	305	49	69,73,73	1.34	5 (7%)	83,113,113	1.95	18 (21%)
35	RRX	g	315	-	42,42,42	5.02	25 (59%)	57,58,58	2.63	23 (40%)
31	CLA	B	604	6	69,73,73	1.40	7 (10%)	83,113,113	2.05	16 (19%)
31	CLA	S	316	19	50,54,73	1.58	6 (12%)	60,90,113	2.07	16 (26%)
31	CLA	c	610	7	69,73,73	1.36	6 (8%)	83,113,113	2.02	18 (21%)
31	CLA	p	615	3	50,54,73	1.58	7 (14%)	60,90,113	2.06	15 (25%)
33	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.08	4 (7%)
30	CHL	7	302	1	70,74,74	0.81	2 (2%)	80,114,114	1.32	14 (17%)
32	LUT	S	318	-	42,43,43	6.09	28 (66%)	51,60,60	2.11	14 (27%)
31	CLA	5	613	3	58,62,73	1.48	7 (12%)	69,99,113	2.07	18 (26%)
30	CHL	R	309	18	60,64,74	0.85	2 (3%)	68,102,114	1.33	12 (17%)
30	CHL	0	607	49	70,74,74	0.77	1 (1%)	80,114,114	1.31	14 (17%)
31	CLA	r	312	18	61,65,73	1.46	6 (9%)	73,103,113	2.06	19 (26%)
30	CHL	5	608	-	54,58,74	0.89	2 (3%)	59,94,114	1.44	12 (20%)
34	LMG	c	620	-	38,38,55	0.62	1 (2%)	46,46,63	1.18	5 (10%)
31	CLA	R	314	18	53,57,73	1.55	6 (11%)	62,93,113	2.12	18 (29%)
34	LMG	d	410	-	51,51,55	1.07	6 (11%)	59,59,63	1.08	3 (5%)
31	CLA	6	311	4	69,73,73	1.35	7 (10%)	83,113,113	1.93	19 (22%)
34	LMG	W	203	-	38,38,55	0.64	1 (2%)	46,46,63	1.12	2 (4%)
44	PL9	A	416	-	55,55,55	1.16	7 (12%)	68,69,69	1.60	13 (19%)
30	CHL	6	307	49	55,59,74	0.86	2 (3%)	62,96,114	1.39	11 (17%)
30	CHL	n	309	49	54,58,74	0.91	2 (3%)	59,94,114	1.45	12 (20%)
31	CLA	s	310	19	64,68,73	1.41	7 (10%)	77,107,113	2.02	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	LHG	8	618	31	48,48,48	0.38	0	51,54,54	1.03	2 (3%)
34	LMG	w	203	-	38,38,55	0.61	1 (2%)	46,46,63	1.46	8 (17%)
31	CLA	S	304	19	46,50,73	1.70	6 (13%)	55,85,113	2.05	18 (32%)
31	CLA	n	314	3	69,73,73	1.35	7 (10%)	83,113,113	1.91	19 (22%)
31	CLA	Y	305	49	59,63,73	1.47	6 (10%)	71,101,113	2.08	18 (25%)
31	CLA	1	603	1	59,63,73	1.48	7 (11%)	71,101,113	2.03	17 (23%)
34	LMG	Y	319	-	38,38,55	0.64	1 (2%)	46,46,63	1.12	3 (6%)
34	LMG	9	302	-	40,40,55	0.68	2 (5%)	48,48,63	1.09	3 (6%)
30	CHL	3	309	-	54,58,74	1.06	3 (5%)	59,94,114	1.43	10 (16%)
31	CLA	4	603	2	59,63,73	1.46	6 (10%)	71,101,113	2.03	19 (26%)
43	BCR	B	617	-	41,41,41	4.69	26 (63%)	56,56,56	2.52	22 (39%)
30	CHL	0	605	4	56,60,74	1.19	5 (8%)	63,97,114	1.61	11 (17%)
31	CLA	C	603	7	69,73,73	1.38	7 (10%)	83,113,113	1.99	15 (18%)
36	NEX	p	618	31	38,46,46	3.38	10 (26%)	50,70,70	1.59	11 (22%)
30	CHL	s	302	19	50,54,74	0.99	2 (4%)	56,90,114	1.32	9 (16%)
31	CLA	r	306	49	52,56,73	1.57	7 (13%)	62,92,113	2.14	15 (24%)
30	CHL	1	606	49	70,74,74	0.81	1 (1%)	80,114,114	1.25	13 (16%)
30	CHL	7	321	49	67,71,74	0.82	2 (2%)	76,110,114	1.34	12 (15%)
34	LMG	Q1	101	-	38,38,55	0.64	1 (2%)	46,46,63	1.20	4 (8%)
38	SQD	6	301	-	41,42,54	0.87	0	50,53,65	1.00	2 (4%)
31	CLA	S	303	19	69,73,73	1.35	7 (10%)	83,113,113	1.97	20 (24%)
31	CLA	Y	314	24	58,62,73	1.48	6 (10%)	69,99,113	2.10	19 (27%)
31	CLA	q	313	33	46,51,73	1.54	5 (10%)	59,86,113	2.20	16 (27%)
31	CLA	5	614	3	55,59,73	1.51	7 (12%)	66,96,113	2.19	19 (28%)
31	CLA	q	306	49	59,63,73	1.49	6 (10%)	71,101,113	2.03	20 (28%)
34	LMG	g	320	-	38,38,55	0.62	1 (2%)	46,46,63	1.12	4 (8%)
37	XAT	2	619	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
31	CLA	c	612	7	59,63,73	1.48	7 (11%)	71,101,113	2.13	18 (25%)
33	LHG	K	102	-	35,35,48	0.45	0	38,41,54	1.21	2 (5%)
31	CLA	1	612	1	69,73,73	1.37	6 (8%)	83,113,113	1.88	18 (21%)
30	CHL	Y	309	24	70,74,74	0.80	2 (2%)	80,114,114	1.32	12 (15%)
34	LMG	N	320	-	38,38,55	0.63	1 (2%)	46,46,63	1.01	2 (4%)
31	CLA	b	614	6	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
34	LMG	B	621	-	51,51,55	1.08	6 (11%)	59,59,63	1.29	4 (6%)
43	BCR	z	101	-	41,41,41	4.77	26 (63%)	56,56,56	2.35	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
30	CHL	R	310	49	59,63,74	0.97	3 (5%)	66,100,114	1.38	12 (18%)
30	CHL	6	308	49	70,74,74	0.77	1 (1%)	80,114,114	1.24	13 (16%)
32	LUT	S	317	-	42,43,43	6.08	27 (64%)	51,60,60	1.94	13 (25%)
31	CLA	R	307	49	52,56,73	1.59	7 (13%)	62,92,113	2.08	16 (25%)
32	LUT	y	616	-	42,43,43	6.00	28 (66%)	51,60,60	2.00	20 (39%)
34	LMG	6	323	-	38,38,55	0.63	1 (2%)	46,46,63	1.16	4 (8%)
36	NEX	Y	317	-	38,46,46	3.37	11 (28%)	50,70,70	1.73	11 (22%)
30	CHL	3	310	3	65,69,74	0.85	3 (4%)	74,108,114	1.36	12 (16%)
31	CLA	G	613	2	53,57,73	1.56	6 (11%)	62,93,113	2.11	18 (29%)
34	LMG	b	622	-	51,51,55	1.09	6 (11%)	59,59,63	1.33	7 (11%)
31	CLA	N	304	3	59,63,73	1.46	6 (10%)	71,101,113	2.08	19 (26%)
34	LMG	0	622	-	38,38,55	0.65	1 (2%)	46,46,63	1.13	3 (6%)
33	LHG	d	408	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
43	BCR	c	614	-	41,41,41	4.75	26 (63%)	56,56,56	2.96	25 (44%)
37	XAT	q	321	-	39,47,47	0.65	0	54,74,74	1.91	13 (24%)
33	LHG	N	319	31	48,48,48	0.38	0	51,54,54	1.02	2 (3%)
31	CLA	2	604	49,36	58,62,73	1.49	7 (12%)	69,99,113	2.14	19 (27%)
43	BCR	Z	101	-	41,41,41	4.77	26 (63%)	56,56,56	2.36	18 (32%)
34	LMG	C	621	-	38,38,55	0.62	1 (2%)	46,46,63	1.11	3 (6%)
34	LMG	x	202	-	38,38,55	0.61	1 (2%)	46,46,63	1.14	4 (8%)
31	CLA	p	611	33	64,68,73	1.41	7 (10%)	77,107,113	1.97	17 (22%)
43	BCR	C	615	-	41,41,41	4.70	25 (60%)	56,56,56	4.03	31 (55%)
32	LUT	4	616	-	42,43,43	6.06	28 (66%)	51,60,60	2.18	13 (25%)
42	PHO	A	408	-	58,69,69	1.94	10 (17%)	56,99,99	1.49	7 (12%)
30	CHL	9	308	-	56,60,74	0.88	1 (1%)	63,97,114	1.43	13 (20%)
31	CLA	b	615	6	69,73,73	1.35	7 (10%)	83,113,113	1.97	18 (21%)
31	CLA	5	602	3	64,68,73	1.41	6 (9%)	77,107,113	2.00	19 (24%)
43	BCR	C	614	-	41,41,41	4.70	25 (60%)	56,56,56	2.59	23 (41%)
31	CLA	q	316	2	54,58,73	1.54	7 (12%)	65,95,113	2.16	18 (27%)
39	OEX	a	402	7,5	0,14,14	-	-	-		
45	DGD	c	619	-	67,67,67	1.16	7 (10%)	81,81,81	1.02	3 (3%)
31	CLA	b	613	6	69,73,73	1.35	7 (10%)	83,113,113	1.99	20 (24%)
30	CHL	N	307	49	62,66,74	0.88	2 (3%)	70,104,114	1.38	12 (17%)
31	CLA	b	611	49	69,73,73	1.36	7 (10%)	83,113,113	1.92	18 (21%)
34	LMG	p	620	-	38,38,55	0.62	1 (2%)	46,46,63	1.10	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
30	CHL	Y	307	49	63,67,74	0.87	3 (4%)	71,105,114	1.36	13 (18%)
42	PHO	d	402	-	58,69,69	0.79	3 (5%)	56,99,99	0.98	3 (5%)
31	CLA	B	602	6	69,73,73	1.37	7 (10%)	83,113,113	2.02	19 (22%)
31	CLA	8	614	3	58,62,73	1.48	7 (12%)	69,99,113	2.04	18 (26%)
36	NEX	R	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.61	9 (18%)
34	LMG	a	401	-	38,38,55	0.62	1 (2%)	46,46,63	1.04	3 (6%)
31	CLA	N	315	3	58,62,73	1.47	6 (10%)	69,99,113	2.10	19 (27%)
30	CHL	R	308	18	60,64,74	0.88	2 (3%)	68,102,114	1.40	13 (19%)
31	CLA	c	608	7	69,73,73	1.38	6 (8%)	83,113,113	1.82	19 (22%)
34	LMG	n	322	-	40,40,55	0.71	3 (7%)	48,48,63	1.39	5 (10%)
31	CLA	8	611	3	49,53,73	1.59	7 (14%)	59,89,113	2.07	14 (23%)
31	CLA	g	314	2	53,57,73	1.54	6 (11%)	62,93,113	2.18	19 (30%)
33	LHG	t	102	-	40,40,48	0.43	0	43,46,54	1.18	4 (9%)
32	LUT	N	317	-	42,43,43	6.07	28 (66%)	51,60,60	2.10	14 (27%)
32	LUT	6	318	-	42,43,43	6.06	28 (66%)	51,60,60	1.94	12 (23%)
33	LHG	y	619	31	45,45,48	0.43	0	48,51,54	1.05	3 (6%)
31	CLA	0	615	-	59,63,73	1.46	6 (10%)	71,101,113	2.06	18 (25%)
37	XAT	G	620	-	39,47,47	0.65	0	54,74,74	1.91	13 (24%)
30	CHL	s	309	49	53,57,74	0.98	2 (3%)	59,93,114	1.40	11 (18%)
30	CHL	p	606	-	55,59,74	0.86	2 (3%)	62,96,114	1.41	13 (20%)
36	NEX	y	618	-	38,46,46	3.41	11 (28%)	50,70,70	1.59	11 (22%)
34	LMG	w	204	-	38,38,55	0.65	1 (2%)	46,46,63	1.11	4 (8%)
31	CLA	6	315	4	58,62,73	1.46	6 (10%)	69,99,113	2.13	18 (26%)
30	CHL	G	607	49	55,59,74	0.93	2 (3%)	62,96,114	1.44	14 (22%)
30	CHL	g	302	2	70,74,74	0.80	2 (2%)	80,114,114	1.28	14 (17%)
34	LMG	n	321	-	38,38,55	0.66	1 (2%)	46,46,63	1.20	3 (6%)
36	NEX	g	317	31	38,46,46	3.36	11 (28%)	50,70,70	1.67	10 (20%)
30	CHL	q	307	2	50,54,74	0.93	2 (4%)	56,90,114	1.46	12 (21%)
31	CLA	A	405	5	69,73,73	1.36	6 (8%)	83,113,113	1.99	20 (24%)
31	CLA	5	610	3	64,68,73	1.40	6 (9%)	77,107,113	2.03	19 (24%)
30	CHL	7	309	49	54,58,74	0.91	1 (1%)	59,94,114	1.49	12 (20%)
33	LHG	S	320	31	40,40,48	0.43	0	43,46,54	1.17	4 (9%)
31	CLA	5	603	3	56,60,73	1.49	5 (8%)	67,97,113	2.17	19 (28%)
35	RRX	q	317	-	42,42,42	4.96	25 (59%)	57,58,58	2.57	19 (33%)
30	CHL	p	609	3	60,64,74	0.88	3 (5%)	68,102,114	1.39	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	LHG	C	623	-	39,39,48	0.42	0	42,45,54	1.21	4 (9%)
30	CHL	n	310	3	70,74,74	0.82	3 (4%)	80,114,114	1.38	12 (15%)
31	CLA	G	610	33	64,68,73	1.42	7 (10%)	77,107,113	1.94	17 (22%)
30	CHL	7	307	49	70,74,74	0.81	1 (1%)	80,114,114	1.34	14 (17%)
34	LMG	2	618	-	38,38,55	0.62	1 (2%)	46,46,63	1.11	3 (6%)
31	CLA	b	609	6	69,73,73	1.38	6 (8%)	83,113,113	1.91	16 (19%)
30	CHL	Y	308	49	54,58,74	0.93	2 (3%)	59,94,114	1.45	13 (22%)
34	LMG	2	621	-	40,40,55	0.67	2 (5%)	48,48,63	1.16	4 (8%)
33	LHG	6	320	31	36,36,48	0.44	0	39,42,54	1.19	3 (7%)
30	CHL	8	606	49	62,66,74	0.85	1 (1%)	70,104,114	1.36	12 (17%)
31	CLA	C	611	7	69,73,73	1.38	7 (10%)	83,113,113	2.00	19 (22%)
31	CLA	B	601	49	53,57,73	1.56	7 (13%)	62,93,113	2.15	18 (29%)
32	LUT	Y	315	-	42,43,43	6.00	28 (66%)	51,60,60	1.95	18 (35%)
33	LHG	G	618	31	43,43,48	0.40	0	46,49,54	1.10	3 (6%)
31	CLA	2	610	33	64,68,73	1.40	6 (9%)	77,107,113	2.01	17 (22%)
34	LMG	J	102	-	38,38,55	0.60	1 (2%)	46,46,63	1.10	2 (4%)
34	LMG	a	413	-	38,38,55	0.64	1 (2%)	46,46,63	1.49	6 (13%)
32	LUT	3	318	-	42,43,43	6.07	28 (66%)	51,60,60	2.00	13 (25%)
30	CHL	p	605	3	50,54,74	0.92	2 (4%)	56,90,114	1.46	12 (21%)
32	LUT	7	318	-	42,43,43	6.07	28 (66%)	51,60,60	1.88	12 (23%)
31	CLA	q	305	2	59,63,73	1.45	6 (10%)	71,101,113	2.08	18 (25%)
33	LHG	3	320	31	32,32,48	0.45	0	35,38,54	1.29	4 (11%)
31	CLA	g	310	2	69,73,73	1.37	7 (10%)	83,113,113	1.91	21 (25%)
31	CLA	c	605	7	69,73,73	1.38	6 (8%)	83,113,113	1.87	16 (19%)
30	CHL	N	309	3	70,74,74	0.81	3 (4%)	80,114,114	1.34	13 (16%)
30	CHL	9	310	49	54,58,74	0.89	2 (3%)	59,94,114	1.41	12 (20%)
38	SQD	X	201	-	37,38,54	0.91	0	46,49,65	1.02	2 (4%)
31	CLA	2	609	2	64,68,73	1.41	7 (10%)	77,107,113	2.02	21 (27%)
38	SQD	b	627	-	51,52,54	0.87	0	60,63,65	1.02	2 (3%)
31	CLA	6	313	4	64,68,73	1.41	7 (10%)	77,107,113	1.98	18 (23%)
33	LHG	A	417	-	38,38,48	0.45	0	41,44,54	1.09	3 (7%)
30	CHL	3	307	3	50,54,74	0.93	2 (4%)	56,90,114	1.46	12 (21%)
34	LMG	6	321	-	42,42,55	0.77	2 (4%)	50,50,63	1.24	5 (10%)
30	CHL	6	306	4	50,54,74	0.90	1 (2%)	56,90,114	1.47	12 (21%)
30	CHL	s	307	19	48,52,74	0.95	1 (2%)	53,87,114	1.47	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CLA	3	316	3	61,65,73	1.47	7 (11%)	73,103,113	2.08	21 (28%)
30	CHL	S	309	49	53,57,74	0.97	2 (3%)	59,93,114	1.44	13 (22%)
31	CLA	2	602	2	69,73,73	1.35	6 (8%)	83,113,113	1.94	17 (20%)
33	LHG	1	617	31	34,34,48	0.44	0	37,40,54	1.17	3 (8%)
31	CLA	s	313	19	60,64,73	1.46	6 (10%)	72,102,113	2.11	18 (25%)
33	LHG	S	322	-	43,43,48	0.41	0	46,49,54	1.08	3 (6%)
31	CLA	C	606	7	61,65,73	1.45	6 (9%)	73,103,113	2.05	18 (24%)
34	LMG	c	624	-	44,44,55	0.86	3 (6%)	52,52,63	1.05	3 (5%)
30	CHL	4	607	-	61,65,74	0.88	2 (3%)	69,103,114	1.38	12 (17%)
30	CHL	8	601	3	60,64,74	0.86	2 (3%)	68,102,114	1.42	14 (20%)
31	CLA	c	602	7	69,73,73	1.38	6 (8%)	83,113,113	1.94	16 (19%)
43	BCR	B	618	-	41,41,41	4.77	25 (60%)	56,56,56	2.19	20 (35%)
31	CLA	8	603	3	59,63,73	1.46	6 (10%)	71,101,113	2.09	18 (25%)
31	CLA	b	610	6	69,73,73	1.36	7 (10%)	83,113,113	1.98	18 (21%)
31	CLA	6	316	4	59,63,73	1.47	5 (8%)	71,101,113	2.07	18 (25%)
33	LHG	7	319	31	34,34,48	0.44	0	37,40,54	1.11	2 (5%)
31	CLA	G	602	2	69,73,73	1.36	7 (10%)	83,113,113	1.90	20 (24%)
34	LMG	k	101	-	48,48,55	0.99	5 (10%)	56,56,63	1.14	4 (7%)
38	SQD	s	301	-	50,51,54	0.79	0	59,62,65	0.94	3 (5%)
33	LHG	2	617	31	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
32	LUT	R	317	-	42,43,43	6.05	27 (64%)	51,60,60	2.98	15 (29%)
31	CLA	3	315	3	58,62,73	1.48	7 (12%)	69,99,113	2.10	19 (27%)
33	LHG	r	320	31	37,37,48	0.45	0	40,43,54	1.14	3 (7%)
31	CLA	0	613	4	60,64,73	1.46	7 (11%)	72,102,113	2.03	19 (26%)
31	CLA	5	604	-	54,58,73	1.53	7 (12%)	65,95,113	2.14	18 (27%)
31	CLA	C	605	7	69,73,73	1.46	8 (11%)	83,113,113	1.92	16 (19%)
31	CLA	Y	304	24	59,63,73	1.46	7 (11%)	71,101,113	2.06	20 (28%)
30	CHL	p	601	3	55,59,74	0.89	2 (3%)	62,96,114	1.39	14 (22%)
31	CLA	R	304	18	64,68,73	1.42	6 (9%)	77,107,113	1.95	17 (22%)
32	LUT	3	317	-	42,43,43	6.08	28 (66%)	51,60,60	1.88	12 (23%)
34	LMG	r	321	-	38,38,55	0.69	2 (5%)	46,46,63	1.27	4 (8%)
31	CLA	p	610	3	60,64,73	1.46	7 (11%)	72,102,113	2.03	20 (27%)
30	CHL	y	606	49	63,67,74	0.84	2 (3%)	71,105,114	1.34	14 (19%)
31	CLA	0	611	33	64,68,73	1.41	7 (10%)	77,107,113	1.93	16 (20%)
34	LMG	q	302	-	40,40,55	0.69	2 (5%)	48,48,63	1.13	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CLA	6	304	4	60,64,73	1.46	7 (11%)	72,102,113	2.08	21 (29%)
36	NEX	s	319	-	38,46,46	3.46	10 (26%)	50,70,70	1.56	10 (20%)
37	XAT	4	619	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
31	CLA	R	313	33	53,57,73	1.56	7 (13%)	62,93,113	2.12	17 (27%)
31	CLA	p	612	3	50,54,73	1.59	7 (14%)	60,90,113	2.08	17 (28%)
31	CLA	9	314	2	54,58,73	1.55	6 (11%)	65,95,113	2.12	17 (26%)
31	CLA	y	614	24	58,62,73	1.47	6 (10%)	69,99,113	2.08	20 (28%)
33	LHG	q	320	31	45,45,48	0.43	0	48,51,54	1.09	2 (4%)
30	CHL	3	302	49	61,65,74	1.02	4 (6%)	69,103,114	1.53	15 (21%)
33	LHG	B	624	-	48,48,48	0.37	0	51,54,54	0.98	2 (3%)
33	LHG	5	619	31	34,34,48	0.46	0	37,40,54	1.14	3 (8%)
31	CLA	8	610	33	53,57,73	1.54	7 (13%)	62,93,113	2.15	17 (27%)
30	CHL	4	601	2	70,74,74	0.81	2 (2%)	80,114,114	1.27	14 (17%)
32	LUT	G	615	-	42,43,43	6.12	28 (66%)	51,60,60	6.98	17 (33%)
30	CHL	N	301	-	54,58,74	0.92	2 (3%)	59,94,114	1.40	12 (20%)
33	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
34	LMG	B	622	-	38,38,55	0.64	1 (2%)	46,46,63	1.22	4 (8%)
34	LMG	s	321	-	41,41,55	0.85	2 (4%)	49,49,63	1.28	5 (10%)
32	LUT	r	317	-	42,43,43	6.02	28 (66%)	51,60,60	2.07	20 (39%)
31	CLA	b	606	6	69,73,73	1.37	6 (8%)	83,113,113	1.95	16 (19%)
37	XAT	R	318	-	39,47,47	0.64	0	54,74,74	1.94	14 (25%)
31	CLA	R	312	18	61,65,73	1.45	6 (9%)	73,103,113	2.05	18 (24%)
30	CHL	S	308	49	47,51,74	1.08	3 (6%)	52,86,114	1.56	12 (23%)
31	CLA	b	607	6	69,73,73	1.37	6 (8%)	83,113,113	1.98	17 (20%)
31	CLA	g	305	49,36	59,63,73	1.46	7 (11%)	71,101,113	2.08	17 (23%)
34	LMG	f	101	-	38,38,55	0.58	1 (2%)	46,46,63	1.13	2 (4%)
31	CLA	b	616	6	69,73,73	1.35	7 (10%)	83,113,113	1.97	16 (19%)
47	HEM	E	101	9,10	50,50,50	1.58	8 (16%)	66,82,82	1.70	13 (19%)
31	CLA	4	613	2	65,69,73	1.39	6 (9%)	78,108,113	1.96	20 (25%)
31	CLA	7	303	1	64,68,73	1.40	6 (9%)	77,107,113	1.97	19 (24%)
31	CLA	8	612	3	69,73,73	1.35	7 (10%)	83,113,113	1.91	19 (22%)
31	CLA	9	305	2	59,63,73	1.46	7 (11%)	71,101,113	2.10	20 (28%)
34	LMG	7	322	-	38,38,55	0.65	1 (2%)	46,46,63	1.06	4 (8%)
44	PL9	D	406	-	55,55,55	0.66	1 (1%)	68,69,69	0.62	1 (1%)
45	DGD	C	616	-	51,51,67	0.82	2 (3%)	65,65,81	1.00	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	LHG	b	625	-	43,43,48	0.41	0	46,49,54	1.07	3 (6%)
33	LHG	0	619	31	35,35,48	0.44	0	38,41,54	1.20	4 (10%)
31	CLA	b	608	49	69,73,73	1.37	7 (10%)	83,113,113	1.99	16 (19%)
31	CLA	r	316	18	69,73,73	1.37	6 (8%)	83,113,113	1.95	16 (19%)
36	NEX	S	319	-	38,46,46	3.44	10 (26%)	50,70,70	1.55	11 (22%)
30	CHL	G	605	2	52,56,74	0.92	2 (3%)	58,92,114	1.47	14 (24%)
34	LMG	C	622	-	32,32,55	0.48	0	40,40,63	1.08	2 (5%)
31	CLA	R	316	18	69,73,73	1.36	7 (10%)	83,113,113	2.00	19 (22%)
46	BCT	d	403	40	2,3,3	1.15	0	2,3,3	4.30	2 (100%)
32	LUT	q	318	-	42,43,43	6.07	28 (66%)	51,60,60	2.12	14 (27%)
31	CLA	y	611	33	69,73,73	1.36	7 (10%)	83,113,113	1.84	16 (19%)
31	CLA	4	604	30	55,59,73	1.51	6 (10%)	66,96,113	2.20	18 (27%)
31	CLA	d	405	8	69,73,73	1.35	7 (10%)	83,113,113	2.04	20 (24%)
36	NEX	0	618	-	38,46,46	3.37	10 (26%)	50,70,70	1.59	11 (22%)
36	NEX	r	301	-	38,46,46	3.37	9 (23%)	50,70,70	1.69	12 (24%)
30	CHL	g	309	2	67,71,74	0.84	3 (4%)	76,110,114	1.41	14 (18%)
31	CLA	b	603	6	69,73,73	1.36	7 (10%)	83,113,113	2.03	17 (20%)
31	CLA	S	314	19	69,73,73	1.37	7 (10%)	83,113,113	1.91	18 (21%)
30	CHL	9	309	-	57,61,74	0.92	2 (3%)	64,98,114	1.49	13 (20%)
45	DGD	C	618	-	67,67,67	1.16	7 (10%)	81,81,81	0.93	3 (3%)
31	CLA	C	601	7	69,73,73	1.37	7 (10%)	83,113,113	1.93	18 (21%)
32	LUT	5	616	-	42,43,43	6.10	27 (64%)	51,60,60	1.89	11 (21%)
34	LMG	G	621	-	51,51,55	1.07	6 (11%)	59,59,63	1.07	3 (5%)
33	LHG	c	622	-	46,46,48	0.40	0	49,52,54	1.01	2 (4%)
30	CHL	9	307	2	50,54,74	0.96	2 (4%)	56,90,114	1.42	10 (17%)
31	CLA	c	607	49	69,73,73	1.39	6 (8%)	83,113,113	1.91	19 (22%)
33	LHG	e	101	-	43,43,48	0.40	0	46,49,54	1.18	4 (8%)
30	CHL	p	608	-	54,58,74	0.88	2 (3%)	59,94,114	1.39	11 (18%)
34	LMG	A	414	-	38,38,55	0.64	1 (2%)	46,46,63	1.14	4 (8%)
31	CLA	Y	312	24	69,73,73	1.38	6 (8%)	83,113,113	1.93	19 (22%)
31	CLA	C	612	7	59,63,73	1.48	7 (11%)	71,101,113	2.14	16 (22%)
31	CLA	s	303	19	69,73,73	1.36	7 (10%)	83,113,113	1.96	21 (25%)
38	SQD	A	411	-	50,51,54	0.80	0	59,62,65	0.97	3 (5%)
34	LMG	b	626	-	46,46,55	0.92	3 (6%)	54,54,63	1.10	4 (7%)
31	CLA	6	312	33	64,68,73	1.42	8 (12%)	77,107,113	1.99	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
43	BCR	b	620	-	41,41,41	4.75	25 (60%)	56,56,56	2.33	20 (35%)
34	LMG	w	205	-	38,38,55	0.62	1 (2%)	46,46,63	1.13	2 (4%)
33	LHG	4	618	31	46,46,48	0.39	0	49,52,54	1.06	4 (8%)
30	CHL	2	601	2	70,74,74	0.80	2 (2%)	80,114,114	1.28	14 (17%)
31	CLA	4	612	2	50,54,73	1.58	6 (12%)	60,90,113	2.18	15 (25%)
33	LHG	Y	318	31	41,41,48	0.45	0	44,47,54	1.07	3 (6%)
34	LMG	W	202	-	38,38,55	0.64	1 (2%)	46,46,63	1.25	5 (10%)
34	LMG	4	620	-	51,51,55	1.06	5 (9%)	59,59,63	1.07	3 (5%)
38	SQD	Y	320	-	41,42,54	0.87	0	50,53,65	0.99	2 (4%)
31	CLA	d	401	49	53,57,73	1.55	6 (11%)	62,93,113	2.19	18 (29%)
31	CLA	G	609	2	69,73,73	1.37	6 (8%)	83,113,113	1.90	19 (22%)
34	LMG	7	301	-	39,39,55	0.62	1 (2%)	47,47,63	1.00	2 (4%)
30	CHL	7	308	49	70,74,74	0.77	2 (2%)	80,114,114	1.25	13 (16%)
31	CLA	B	607	49	69,73,73	1.43	6 (8%)	83,113,113	2.10	20 (24%)
30	CHL	y	601	24	70,74,74	0.79	2 (2%)	80,114,114	1.29	13 (16%)
31	CLA	B	612	6	69,73,73	1.35	7 (10%)	83,113,113	1.93	18 (21%)
30	CHL	q	310	-	54,58,74	1.02	3 (5%)	59,94,114	1.56	13 (22%)
34	LMG	S	321	-	41,41,55	0.83	2 (4%)	49,49,63	1.23	3 (6%)
34	LMG	G	622	-	40,40,55	0.69	2 (5%)	48,48,63	1.09	4 (8%)
31	CLA	G	604	49	59,63,73	1.46	6 (10%)	71,101,113	2.05	17 (23%)
31	CLA	7	315	1	58,62,73	1.46	5 (8%)	69,99,113	2.05	19 (27%)
31	CLA	q	315	2	69,73,73	1.38	6 (8%)	83,113,113	1.93	19 (22%)
31	CLA	3	311	-	58,62,73	1.49	7 (12%)	69,99,113	2.12	19 (27%)
31	CLA	y	615	24	58,62,73	1.47	7 (12%)	69,99,113	2.18	20 (28%)
31	CLA	S	310	19	64,68,73	1.41	7 (10%)	77,107,113	2.00	18 (23%)
30	CHL	5	605	3	50,54,74	0.92	2 (4%)	56,90,114	1.42	13 (23%)
32	LUT	n	318	-	42,43,43	6.07	28 (66%)	51,60,60	1.94	13 (25%)
31	CLA	4	610	2	64,68,73	1.44	6 (9%)	77,107,113	2.01	22 (28%)
43	BCR	t	101	-	41,41,41	4.71	25 (60%)	56,56,56	3.99	27 (48%)
33	LHG	a	415	-	38,38,48	0.45	0	41,44,54	1.24	3 (7%)
33	LHG	g	319	31	43,43,48	0.40	0	46,49,54	1.13	4 (8%)
33	LHG	b	628	-	48,48,48	0.40	0	51,54,54	1.11	3 (5%)
36	NEX	r	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.61	10 (20%)
32	LUT	1	616	-	42,43,43	6.03	27 (64%)	51,60,60	1.89	16 (31%)
31	CLA	N	313	3	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	CLA	R	305	18	64,68,73	1.42	6 (9%)	77,107,113	2.04	14 (18%)
33	LHG	l	101	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
30	CHL	s	308	49	47,51,74	0.93	2 (4%)	52,86,114	1.46	11 (21%)
36	NEX	5	618	-	38,46,46	3.36	10 (26%)	50,70,70	1.56	9 (18%)
32	LUT	0	617	-	42,43,43	6.02	28 (66%)	51,60,60	1.96	14 (27%)
31	CLA	B	606	6	69,73,73	1.38	6 (8%)	83,113,113	1.94	19 (22%)
31	CLA	r	303	18	53,57,73	1.60	6 (11%)	62,93,113	2.32	19 (30%)
34	LMG	W	201	-	55,55,55	1.18	6 (10%)	63,63,63	1.20	4 (6%)
30	CHL	8	608	3	70,74,74	0.79	3 (4%)	80,114,114	1.35	12 (15%)
38	SQD	a	411	-	47,48,54	0.82	0	56,59,65	0.97	2 (3%)
31	CLA	7	316	1	55,59,73	1.52	7 (12%)	66,96,113	2.14	19 (28%)
34	LMG	q1	101	-	38,38,55	0.64	1 (2%)	46,46,63	1.10	2 (4%)
43	BCR	T	101	-	41,41,41	4.76	27 (65%)	56,56,56	2.30	19 (33%)
36	NEX	4	617	-	38,46,46	3.38	11 (28%)	50,70,70	1.53	9 (18%)
31	CLA	p	614	3	55,59,73	1.52	7 (12%)	66,96,113	2.18	19 (28%)
31	CLA	c	611	7	69,73,73	1.37	7 (10%)	83,113,113	1.99	19 (22%)
33	LHG	M	101	-	40,40,48	0.42	0	43,46,54	1.10	3 (6%)
31	CLA	4	611	33	46,51,73	1.54	5 (10%)	59,86,113	2.12	15 (25%)
32	LUT	y	617	-	42,43,43	6.02	28 (66%)	51,60,60	2.00	17 (33%)
31	CLA	q	304	2	69,73,73	1.36	7 (10%)	83,113,113	1.95	19 (22%)
30	CHL	0	606	49	55,59,74	0.94	2 (3%)	62,96,114	1.38	9 (14%)
31	CLA	R	303	18	53,57,73	1.56	7 (13%)	62,93,113	2.30	17 (27%)
31	CLA	A	407	49	53,57,73	1.56	6 (11%)	62,93,113	2.17	19 (30%)
31	CLA	N	314	3	53,57,73	1.54	6 (11%)	62,93,113	2.15	17 (27%)
30	CHL	n	307	49	62,66,74	0.85	1 (1%)	70,104,114	1.36	12 (17%)
34	LMG	1	618	-	38,38,55	0.62	1 (2%)	46,46,63	1.04	2 (4%)
31	CLA	0	614	4	58,62,73	1.46	6 (10%)	69,99,113	2.10	20 (28%)
31	CLA	3	312	33	69,73,73	1.36	7 (10%)	83,113,113	1.90	17 (20%)
30	CHL	2	605	2	50,54,74	0.92	2 (4%)	56,90,114	1.46	13 (23%)
38	SQD	x	201	-	41,42,54	0.88	1 (2%)	50,53,65	0.98	4 (8%)
36	NEX	N	318	-	38,46,46	3.36	11 (28%)	50,70,70	1.79	14 (28%)
31	CLA	R	306	49	52,56,73	1.58	7 (13%)	62,92,113	2.32	18 (29%)
36	NEX	9	319	31	38,46,46	3.44	10 (26%)	50,70,70	1.63	9 (18%)
30	CHL	y	608	49	54,58,74	0.92	2 (3%)	59,94,114	1.49	13 (22%)
30	CHL	1	601	1	70,74,74	1.05	5 (7%)	80,114,114	1.39	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	CHL	1	619	-	65,69,74	1.10	4 (6%)	74,108,114	1.54	16 (21%)
30	CHL	q	303	2	70,74,74	0.79	2 (2%)	80,114,114	1.25	13 (16%)
32	LUT	7	317	-	42,43,43	6.01	27 (64%)	51,60,60	2.12	15 (29%)
31	CLA	g	303	2	69,73,73	1.33	6 (8%)	83,113,113	1.94	17 (20%)
35	RRX	2	614	-	42,42,42	5.00	25 (59%)	57,58,58	2.53	22 (38%)
30	CHL	q	311	2	60,64,74	0.84	2 (3%)	68,102,114	1.31	12 (17%)
31	CLA	a	406	5	69,73,73	1.37	6 (8%)	83,113,113	1.96	16 (19%)
31	CLA	s	316	19	50,54,73	1.58	7 (14%)	60,90,113	2.08	17 (28%)
30	CHL	9	303	2	70,74,74	0.78	2 (2%)	80,114,114	1.28	13 (16%)
31	CLA	y	603	24	59,63,73	1.47	7 (11%)	71,101,113	2.06	19 (26%)
32	LUT	8	615	-	42,43,43	6.09	28 (66%)	51,60,60	1.83	17 (33%)
31	CLA	3	301	1	58,62,73	1.51	6 (10%)	69,99,113	2.17	19 (27%)
31	CLA	6	314	4	69,73,73	1.35	5 (7%)	83,113,113	1.95	19 (22%)
30	CHL	1	607	-	70,74,74	0.78	2 (2%)	80,114,114	1.24	13 (16%)
31	CLA	S	313	19	60,64,73	1.49	6 (10%)	72,102,113	2.11	20 (27%)
31	CLA	c	606	7	69,73,73	1.39	6 (8%)	83,113,113	1.91	15 (18%)
42	PHO	D	401	-	58,69,69	1.94	9 (15%)	56,99,99	1.51	9 (16%)
32	LUT	6	317	-	42,43,43	6.05	28 (66%)	51,60,60	1.94	16 (31%)
30	CHL	r	310	49	59,63,74	0.93	2 (3%)	66,100,114	1.40	13 (19%)
45	DGD	C	620	-	67,67,67	1.18	7 (10%)	81,81,81	1.02	4 (4%)
30	CHL	2	607	49	54,58,74	0.91	2 (3%)	59,94,114	1.49	12 (20%)
30	CHL	6	309	49	54,58,74	0.92	3 (5%)	59,94,114	1.50	13 (22%)
43	BCR	h	101	-	41,41,41	4.72	25 (60%)	56,56,56	2.41	20 (35%)
30	CHL	1	605	1	70,74,74	0.82	2 (2%)	80,114,114	1.28	10 (12%)
31	CLA	2	612	2	69,73,73	1.34	8 (11%)	83,113,113	1.92	19 (22%)
32	LUT	s	318	-	42,43,43	6.04	28 (66%)	51,60,60	1.92	15 (29%)
30	CHL	4	605	2	50,54,74	0.92	2 (4%)	56,90,114	1.43	12 (21%)
30	CHL	0	609	4	65,69,74	0.86	3 (4%)	74,108,114	1.38	14 (18%)
31	CLA	S	305	49	69,73,73	1.35	5 (7%)	83,113,113	1.94	18 (21%)
34	LMG	j	101	-	43,43,55	0.82	2 (4%)	51,51,63	1.03	3 (5%)
31	CLA	3	304	3	64,68,73	1.41	6 (9%)	77,107,113	2.02	19 (24%)
34	LMG	5	620	-	38,38,55	0.63	1 (2%)	46,46,63	1.09	2 (4%)
31	CLA	p	604	36	54,58,73	1.53	8 (14%)	65,95,113	2.14	18 (27%)
32	LUT	g	316	-	42,43,43	6.09	28 (66%)	51,60,60	2.29	15 (29%)
34	LMG	D	409	-	46,46,55	0.94	4 (8%)	54,54,63	1.14	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	CLA	B	614	6	69,73,73	1.37	7 (10%)	83,113,113	1.91	18 (21%)
31	CLA	7	304	1	59,63,73	1.46	7 (11%)	71,101,113	2.08	20 (28%)
30	CHL	Y	306	24	50,54,74	1.01	3 (6%)	56,90,114	1.45	13 (23%)
36	NEX	3	319	-	38,46,46	3.45	9 (23%)	50,70,70	1.67	12 (24%)
32	LUT	N	316	-	42,43,43	6.09	28 (66%)	51,60,60	2.01	12 (23%)
34	LMG	R	321	-	38,38,55	0.63	1 (2%)	46,46,63	1.11	2 (4%)
31	CLA	7	313	1	69,73,73	1.36	6 (8%)	83,113,113	1.90	20 (24%)
43	BCR	H	101	-	41,41,41	4.74	26 (63%)	56,56,56	2.38	20 (35%)
31	CLA	B	615	6	69,73,73	1.36	7 (10%)	83,113,113	2.00	16 (19%)
30	CHL	5	607	-	55,59,74	0.96	3 (5%)	62,96,114	1.40	11 (17%)
37	XAT	g	321	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
31	CLA	0	604	49	59,63,73	1.46	6 (10%)	71,101,113	2.09	16 (22%)
34	LMG	c	621	-	38,38,55	0.63	1 (2%)	46,46,63	1.11	4 (8%)
30	CHL	3	303	3	54,58,74	0.91	2 (3%)	59,94,114	1.46	13 (22%)
31	CLA	1	610	1	69,73,73	1.35	7 (10%)	83,113,113	1.95	19 (22%)
30	CHL	4	609	2	61,65,74	0.86	2 (3%)	69,103,114	1.43	15 (21%)
33	LHG	s	322	-	43,43,48	0.40	0	46,49,54	1.14	3 (6%)
31	CLA	p	613	-	58,62,73	1.47	7 (12%)	69,99,113	2.07	15 (21%)
31	CLA	d	404	8	69,73,73	1.37	6 (8%)	83,113,113	1.90	16 (19%)
34	LMG	J	101	-	51,51,55	1.08	6 (11%)	59,59,63	1.08	3 (5%)
30	CHL	5	606	49	55,59,74	0.90	2 (3%)	62,96,114	1.44	12 (19%)
34	LMG	4	621	-	40,40,55	0.68	2 (5%)	48,48,63	1.04	2 (4%)
31	CLA	g	311	33	64,68,73	1.44	7 (10%)	77,107,113	1.97	18 (23%)
31	CLA	C	609	7	69,73,73	1.37	7 (10%)	83,113,113	1.91	15 (18%)
43	BCR	c	615	-	41,41,41	4.78	25 (60%)	56,56,56	2.74	24 (42%)
30	CHL	g	308	49	55,59,74	0.90	2 (3%)	62,96,114	1.46	14 (22%)
31	CLA	a	409	5	64,68,73	1.41	7 (10%)	77,107,113	2.09	18 (23%)
30	CHL	6	310	4	65,69,74	0.83	2 (3%)	74,108,114	1.34	15 (20%)
30	CHL	1	608	49	54,58,74	0.92	2 (3%)	59,94,114	1.45	10 (16%)
31	CLA	7	312	33	69,73,73	1.35	6 (8%)	83,113,113	1.95	18 (21%)
37	XAT	9	322	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
32	LUT	8	616	-	42,43,43	6.07	28 (66%)	51,60,60	1.93	14 (27%)
45	DGD	C	617	-	67,67,67	1.17	7 (10%)	81,81,81	0.92	3 (3%)
48	LMU	r	302	-	36,36,36	0.38	0	47,47,47	0.78	0
31	CLA	s	304	19	46,50,73	1.64	5 (10%)	55,85,113	2.17	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	LHG	R	320	31	37,37,48	0.46	0	40,43,54	1.21	3 (7%)
32	LUT	s	317	-	42,43,43	6.07	28 (66%)	51,60,60	1.89	16 (31%)
30	CHL	p	607	-	55,59,74	0.94	2 (3%)	62,96,114	1.42	11 (17%)
31	CLA	R	311	18	62,66,73	1.45	6 (9%)	74,104,113	2.00	18 (24%)
38	SQD	B	623	-	51,52,54	0.81	0	60,63,65	0.95	3 (5%)
30	CHL	0	601	4	60,64,74	0.87	2 (3%)	68,102,114	1.40	14 (20%)
34	LMG	A	412	-	41,41,55	0.75	2 (4%)	49,49,63	1.06	2 (4%)
30	CHL	7	306	1	70,74,74	0.83	3 (4%)	80,114,114	1.30	14 (17%)
31	CLA	8	613	3	53,57,73	1.54	6 (11%)	62,93,113	2.16	18 (29%)
34	LMG	d	409	-	41,41,55	0.72	2 (4%)	49,49,63	1.08	3 (6%)
30	CHL	6	302	4	60,64,74	0.86	2 (3%)	68,102,114	1.38	14 (20%)
38	SQD	R	322	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
43	BCR	a	410	-	41,41,41	4.73	25 (60%)	56,56,56	2.54	21 (37%)
33	LHG	n	320	31	48,48,48	0.38	0	51,54,54	1.03	2 (3%)
31	CLA	r	315	18	59,63,73	1.47	7 (11%)	71,101,113	2.16	20 (28%)
31	CLA	G	611	2	47,51,73	1.67	6 (12%)	56,86,113	2.09	15 (26%)
31	CLA	1	611	33	69,73,73	1.35	7 (10%)	83,113,113	1.90	19 (22%)
30	CHL	n	308	49	67,71,74	0.81	2 (2%)	76,110,114	1.34	12 (15%)
30	CHL	N	308	49	54,58,74	0.93	3 (5%)	59,94,114	1.43	11 (18%)
31	CLA	2	613	2	58,62,73	1.48	6 (10%)	69,99,113	2.12	19 (27%)
34	LMG	I	101	-	38,38,55	0.62	1 (2%)	46,46,63	1.10	2 (4%)
31	CLA	N	310	3	69,73,73	1.36	7 (10%)	83,113,113	1.96	20 (24%)
31	CLA	c	604	49	60,64,73	1.44	6 (10%)	72,102,113	2.08	19 (26%)
31	CLA	N	321	24	58,62,73	1.48	7 (12%)	69,99,113	2.09	18 (26%)
31	CLA	A	406	49	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
31	CLA	8	604	49,36	69,73,73	1.35	6 (8%)	83,113,113	1.96	18 (21%)
34	LMG	D	412	-	48,48,55	0.99	5 (10%)	56,56,63	1.11	2 (3%)
30	CHL	8	607	49	54,58,74	0.91	2 (3%)	59,94,114	1.45	12 (20%)
31	CLA	n	311	3	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
31	CLA	r	305	18	64,68,73	1.40	6 (9%)	77,107,113	2.01	18 (23%)
31	CLA	s	312	33	69,73,73	1.35	6 (8%)	83,113,113	1.94	15 (18%)
30	CHL	G	623	49	70,74,74	0.79	1 (1%)	80,114,114	1.31	14 (17%)
36	NEX	2	616	31	38,46,46	3.38	10 (26%)	50,70,70	1.60	10 (20%)
31	CLA	R	315	18	59,63,73	1.48	6 (10%)	71,101,113	2.08	18 (25%)
43	BCR	b	618	-	41,41,41	4.69	25 (60%)	56,56,56	2.52	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	HEM	e	102	9,10	50,50,50	1.57	8 (16%)	66,82,82	1.68	11 (16%)
31	CLA	A	409	5	64,68,73	1.42	7 (10%)	77,107,113	2.09	18 (23%)
31	CLA	c	601	7	69,73,73	1.36	7 (10%)	83,113,113	1.91	18 (21%)
30	CHL	y	609	24	70,74,74	0.80	2 (2%)	80,114,114	1.29	11 (13%)
31	CLA	n	315	3	53,57,73	1.54	6 (11%)	62,93,113	2.17	18 (29%)
31	CLA	b	612	6	69,73,73	1.35	6 (8%)	83,113,113	1.94	19 (22%)
30	CHL	r	309	18	60,64,74	0.84	2 (3%)	68,102,114	1.34	10 (14%)
34	LMG	a	416	-	38,38,55	0.61	1 (2%)	46,46,63	1.06	3 (6%)
30	CHL	5	609	3	60,64,74	0.89	3 (5%)	68,102,114	1.44	14 (20%)
32	LUT	n	317	-	42,43,43	6.09	28 (66%)	51,60,60	1.83	17 (33%)
31	CLA	Y	311	33	69,73,73	1.37	6 (8%)	83,113,113	1.88	16 (19%)
31	CLA	C	613	7	69,73,73	1.36	7 (10%)	83,113,113	2.06	21 (25%)
31	CLA	s	306	-	54,58,73	1.53	6 (11%)	65,95,113	2.23	19 (29%)
33	LHG	D	407	-	43,43,48	0.41	0	46,49,54	1.10	3 (6%)
30	CHL	4	608	-	54,58,74	0.88	2 (3%)	59,94,114	1.46	12 (20%)
31	CLA	S	306	-	54,58,73	1.53	6 (11%)	65,95,113	2.20	18 (27%)
31	CLA	N	305	49	69,73,73	1.35	5 (7%)	83,113,113	1.96	18 (21%)
30	CHL	n	302	3	60,64,74	0.86	2 (3%)	68,102,114	1.42	14 (20%)
31	CLA	S	315	19	52,56,73	1.57	6 (11%)	62,92,113	2.05	16 (25%)
31	CLA	r	314	18	53,57,73	1.56	6 (11%)	62,93,113	2.12	18 (29%)
48	LMU	R	302	-	36,36,36	0.44	0	47,47,47	0.95	2 (4%)
34	LMG	b	623	-	38,38,55	0.62	1 (2%)	46,46,63	1.09	2 (4%)
38	SQD	0	621	-	41,42,54	0.86	0	50,53,65	0.96	3 (6%)
30	CHL	2	606	-	55,59,74	0.87	2 (3%)	62,96,114	1.43	13 (20%)
31	CLA	y	602	24	64,68,73	1.41	7 (10%)	77,107,113	2.01	19 (24%)
34	LMG	g	322	-	49,49,55	1.03	5 (10%)	57,57,63	1.22	2 (3%)
38	SQD	S	301	-	50,51,54	0.80	0	59,62,65	0.94	2 (3%)
31	CLA	n	316	3	58,62,73	1.48	7 (12%)	69,99,113	2.07	19 (27%)
36	NEX	R	301	-	38,46,46	3.42	11 (28%)	50,70,70	1.56	9 (18%)
31	CLA	5	611	33	62,66,73	1.43	7 (11%)	74,104,113	2.03	18 (24%)
31	CLA	C	610	7	69,73,73	1.38	7 (10%)	83,113,113	1.97	17 (20%)
31	CLA	y	612	24	69,73,73	1.37	6 (8%)	83,113,113	1.94	18 (21%)
31	CLA	B	608	6	69,73,73	1.38	6 (8%)	83,113,113	1.89	16 (19%)
31	CLA	N	303	3	69,73,73	1.35	7 (10%)	83,113,113	1.93	21 (25%)
34	LMG	7	320	-	38,38,55	0.61	1 (2%)	46,46,63	1.17	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	NEX	8	617	31	38,46,46	3.38	11 (28%)	50,70,70	1.65	12 (24%)
31	CLA	Y	313	24	69,73,73	1.38	7 (10%)	83,113,113	1.92	17 (20%)
30	CHL	n	306	3	70,74,74	0.79	2 (2%)	80,114,114	1.30	14 (17%)
35	RRX	9	317	-	42,42,42	5.01	25 (59%)	57,58,58	2.49	22 (38%)
31	CLA	a	407	49	69,73,73	1.37	7 (10%)	83,113,113	1.96	17 (20%)
32	LUT	p	617	-	42,43,43	6.06	29 (69%)	51,60,60	2.82	20 (39%)
31	CLA	p	602	3	64,68,73	1.41	7 (10%)	77,107,113	1.96	18 (23%)
31	CLA	6	305	49	59,63,73	1.46	6 (10%)	71,101,113	2.10	18 (25%)
30	CHL	S	302	19	50,54,74	1.01	2 (4%)	56,90,114	1.35	10 (17%)
31	CLA	S	312	33	69,73,73	1.35	6 (8%)	83,113,113	1.95	16 (19%)
34	LMG	m	102	-	45,45,55	0.91	3 (6%)	53,53,63	1.25	5 (9%)
30	CHL	5	601	3	55,59,74	0.88	2 (3%)	62,96,114	1.47	13 (20%)
31	CLA	y	613	24	69,73,73	1.44	6 (8%)	83,113,113	1.97	20 (24%)
30	CHL	S	307	19	48,52,74	0.95	2 (4%)	53,87,114	1.46	10 (18%)
34	LMG	G	619	-	38,38,55	0.63	1 (2%)	46,46,63	1.10	3 (6%)
35	RRX	4	615	-	42,42,42	5.02	25 (59%)	57,58,58	2.49	22 (38%)
31	CLA	B	616	6	69,73,73	1.38	6 (8%)	83,113,113	1.95	14 (16%)
32	LUT	1	615	-	42,43,43	6.01	27 (64%)	51,60,60	2.01	18 (35%)
31	CLA	5	612	3	54,58,73	1.54	7 (12%)	65,95,113	2.16	20 (30%)
31	CLA	6	303	4	69,73,73	1.35	7 (10%)	83,113,113	1.95	19 (22%)
31	CLA	9	316	2	50,54,73	1.59	7 (14%)	60,90,113	2.05	16 (26%)
31	CLA	4	602	2	69,73,73	1.35	7 (10%)	83,113,113	1.97	20 (24%)
31	CLA	5	615	3	50,54,73	1.59	6 (12%)	60,90,113	2.20	16 (26%)
34	LMG	6	322	-	39,39,55	0.61	1 (2%)	47,47,63	1.18	3 (6%)
30	CHL	G	606	49	54,58,74	0.91	2 (3%)	59,94,114	1.41	13 (22%)
31	CLA	3	305	3	59,63,73	1.47	7 (11%)	71,101,113	2.03	18 (25%)
31	CLA	C	608	7	69,73,73	1.38	6 (8%)	83,113,113	1.85	18 (21%)
30	CHL	q	308	-	55,59,74	0.98	4 (7%)	62,96,114	1.51	10 (16%)
31	CLA	g	304	2	59,63,73	1.46	6 (10%)	71,101,113	2.09	18 (25%)
31	CLA	1	614	1	58,62,73	1.46	5 (8%)	69,99,113	2.07	19 (27%)
30	CHL	y	607	49	70,74,74	0.79	2 (2%)	80,114,114	1.29	14 (17%)
31	CLA	8	602	3	69,73,73	1.35	6 (8%)	83,113,113	1.92	20 (24%)
34	LMG	d	411	-	48,48,55	0.99	5 (10%)	56,56,63	1.15	3 (5%)
31	CLA	9	304	2	69,73,73	1.35	6 (8%)	83,113,113	2.00	20 (24%)
30	CHL	1	609	1	70,74,74	0.82	3 (4%)	80,114,114	1.33	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CLA	1	613	1	69,73,73	1.36	7 (10%)	83,113,113	1.89	17 (20%)
32	LUT	9	318	-	42,43,43	6.10	27 (64%)	51,60,60	2.23	17 (33%)
48	LMU	c	623	-	29,29,36	0.44	0	40,40,47	1.11	2 (5%)
30	CHL	0	608	49	54,58,74	0.91	1 (1%)	59,94,114	1.53	12 (20%)
31	CLA	r	307	49	52,56,73	1.59	6 (11%)	62,92,113	2.06	17 (27%)
31	CLA	c	603	7	69,73,73	1.38	7 (10%)	83,113,113	2.00	19 (22%)
34	LMG	A	418	-	38,38,55	0.61	1 (2%)	46,46,63	1.09	3 (6%)
31	CLA	0	612	4	50,54,73	1.61	7 (14%)	60,90,113	2.03	17 (28%)
33	LHG	A	415	-	43,43,48	0.40	0	46,49,54	1.15	5 (10%)
34	LMG	k	102	-	38,38,55	0.61	1 (2%)	46,46,63	1.10	3 (6%)
48	LMU	K	101	-	36,36,36	0.42	0	47,47,47	1.10	4 (8%)
34	LMG	X	202	-	38,38,55	0.62	1 (2%)	46,46,63	1.06	2 (4%)
34	LMG	0	620	-	42,42,55	0.81	2 (4%)	50,50,63	1.16	4 (8%)
33	LHG	s	320	31	40,40,48	0.43	0	43,46,54	1.11	3 (6%)
36	NEX	q	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.55	10 (20%)
31	CLA	s	311	19	69,73,73	1.36	6 (8%)	83,113,113	1.94	22 (26%)
30	CHL	y	605	24	50,54,74	1.01	2 (4%)	56,90,114	1.44	10 (17%)
31	CLA	g	312	2	47,51,73	1.63	7 (14%)	56,86,113	2.13	15 (26%)
31	CLA	n	304	3	59,63,73	1.46	6 (10%)	71,101,113	2.09	18 (25%)
34	LMG	q	301	-	51,51,55	1.07	5 (9%)	59,59,63	1.16	5 (8%)
30	CHL	q	309	-	61,65,74	1.06	3 (4%)	69,103,114	1.39	11 (15%)
34	LMG	C	624	-	44,44,55	0.88	3 (6%)	52,52,63	1.05	2 (3%)
31	CLA	9	312	2	58,62,73	1.48	6 (10%)	69,99,113	2.19	21 (30%)
44	PL9	d	407	-	55,55,55	0.72	1 (1%)	68,69,69	0.59	1 (1%)
30	CHL	G	601	2	70,74,74	0.80	2 (2%)	80,114,114	1.27	14 (17%)
31	CLA	s	305	49	69,73,73	1.35	7 (10%)	83,113,113	1.97	18 (21%)
31	CLA	q	314	2	50,54,73	1.59	6 (12%)	60,90,113	2.09	15 (25%)
31	CLA	C	602	7	69,73,73	1.37	6 (8%)	83,113,113	1.95	18 (21%)
31	CLA	n	313	3	49,53,73	1.59	6 (12%)	59,89,113	2.08	14 (23%)
31	CLA	0	603	4	60,64,73	1.47	7 (11%)	72,102,113	2.00	18 (25%)
36	NEX	n	319	-	38,46,46	3.30	9 (23%)	50,70,70	1.78	14 (28%)
43	BCR	B	619	-	41,41,41	4.74	25 (60%)	56,56,56	2.46	21 (37%)
31	CLA	1	602	1	64,68,73	1.42	7 (10%)	77,107,113	1.97	19 (24%)
38	SQD	y	621	-	41,42,54	0.87	0	50,53,65	1.00	2 (4%)
31	CLA	g	313	2	69,73,73	1.35	7 (10%)	83,113,113	1.90	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
30	CHL	g	306	2	52,56,74	0.94	2 (3%)	58,92,114	1.46	12 (20%)
31	CLA	D	403	8	69,73,73	1.39	6 (8%)	83,113,113	1.90	16 (19%)
31	CLA	9	306	49,36	69,73,73	1.35	6 (8%)	83,113,113	1.99	18 (21%)
31	CLA	7	314	1	69,73,73	1.37	7 (10%)	83,113,113	1.89	19 (22%)
30	CHL	N	306	3	70,74,74	0.81	2 (2%)	80,114,114	1.33	14 (17%)
31	CLA	0	610	4	69,73,73	1.41	6 (8%)	83,113,113	1.95	21 (25%)
31	CLA	n	303	3	69,73,73	1.35	7 (10%)	83,113,113	1.93	21 (25%)
32	LUT	0	616	-	42,43,43	6.02	27 (64%)	51,60,60	1.99	17 (33%)
34	LMG	B	625	-	38,38,55	0.62	1 (2%)	46,46,63	1.09	4 (8%)
38	SQD	B	620	-	53,54,54	0.77	0	62,65,65	0.91	2 (3%)
39	OEX	A	401	7,5	0,14,14	-	-	-		
45	DGD	c	616	-	67,67,67	1.16	7 (10%)	81,81,81	1.07	2 (2%)
33	LHG	z	102	-	35,35,48	0.43	0	38,41,54	1.20	3 (7%)
31	CLA	n	312	33	53,57,73	1.54	7 (13%)	62,93,113	2.15	16 (25%)
30	CHL	r	308	18	60,64,74	0.89	3 (5%)	68,102,114	1.39	14 (20%)
31	CLA	B	609	6	69,73,73	1.36	6 (8%)	83,113,113	1.96	19 (22%)
34	LMG	2	620	-	51,51,55	1.06	5 (9%)	59,59,63	1.06	3 (5%)
44	PL9	a	414	-	55,55,55	1.21	5 (9%)	68,69,69	1.51	15 (22%)
31	CLA	9	315	2	59,63,73	1.46	6 (10%)	71,101,113	2.02	18 (25%)
36	NEX	G	616	-	38,46,46	3.40	9 (23%)	50,70,70	1.68	10 (20%)
31	CLA	D	404	8	69,73,73	1.36	7 (10%)	83,113,113	2.04	19 (22%)
30	CHL	8	605	3	70,74,74	0.79	2 (2%)	80,114,114	1.31	15 (18%)
31	CLA	B	613	6	69,73,73	1.35	7 (10%)	83,113,113	1.86	18 (21%)
38	SQD	b	621	-	53,54,54	0.79	0	62,65,65	0.91	3 (4%)
30	CHL	n	301	49	54,58,74	0.93	2 (3%)	59,94,114	1.43	13 (22%)
31	CLA	b	617	6	69,73,73	1.39	6 (8%)	83,113,113	1.93	17 (20%)
33	LHG	j	102	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
31	CLA	S	311	19	69,73,73	1.37	6 (8%)	83,113,113	1.93	22 (26%)
30	CHL	N	302	3	60,64,74	0.86	2 (3%)	68,102,114	1.44	14 (20%)
34	LMG	9	321	-	38,38,55	0.65	1 (2%)	46,46,63	1.14	4 (8%)
33	LHG	p	619	31	34,34,48	0.44	0	37,40,54	1.18	3 (8%)
34	LMG	b	624	-	38,38,55	0.66	1 (2%)	46,46,63	1.33	7 (15%)
45	DGD	c	618	-	67,67,67	1.16	7 (10%)	81,81,81	1.02	2 (2%)
31	CLA	1	604	49	69,73,73	1.37	6 (8%)	83,113,113	1.98	18 (21%)
43	BCR	v	101	-	41,41,41	4.75	25 (60%)	56,56,56	2.24	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
30	CHL	g	307	49	54,58,74	0.93	1 (1%)	59,94,114	1.45	11 (18%)
31	CLA	b	602	49	53,57,73	1.54	6 (11%)	62,93,113	2.16	15 (24%)
42	PHO	a	408	-	58,69,69	0.78	2 (3%)	56,99,99	0.97	3 (5%)
31	CLA	B	603	6	69,73,73	1.39	6 (8%)	83,113,113	1.87	16 (19%)
34	LMG	w	202	-	55,55,55	1.14	6 (10%)	63,63,63	1.13	3 (4%)
38	SQD	m	101	-	49,50,54	0.82	0	58,61,65	0.96	2 (3%)
31	CLA	y	604	49	59,63,73	1.47	6 (10%)	71,101,113	2.11	19 (26%)
31	CLA	Y	303	24	64,68,73	1.40	7 (10%)	77,107,113	2.05	20 (25%)
36	NEX	6	319	-	38,46,46	3.37	11 (28%)	50,70,70	1.59	11 (22%)
30	CHL	Y	301	49	67,71,74	0.83	3 (4%)	76,110,114	1.32	12 (15%)
33	LHG	F1	301	-	34,34,48	0.44	0	37,40,54	1.09	2 (5%)
34	LMG	w	201	-	48,48,55	1.00	5 (10%)	56,56,63	1.08	3 (5%)
31	CLA	G	612	2	69,73,73	1.37	7 (10%)	83,113,113	1.93	17 (20%)
31	CLA	4	614	2	58,62,73	1.48	8 (13%)	69,99,113	2.13	20 (28%)
43	BCR	A	410	-	41,41,41	4.72	25 (60%)	56,56,56	2.56	20 (35%)
43	BCR	V	101	-	41,41,41	4.71	25 (60%)	56,56,56	2.39	22 (39%)
32	LUT	2	615	-	42,43,43	5.91	28 (66%)	51,60,60	3.00	18 (35%)
31	CLA	7	311	1	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
31	CLA	b	605	6	69,73,73	1.40	7 (10%)	83,113,113	1.96	17 (20%)
31	CLA	8	609	3	69,73,73	1.35	6 (8%)	83,113,113	1.95	19 (22%)
38	SQD	G	624	-	37,38,54	0.94	1 (2%)	46,49,65	1.04	2 (4%)
31	CLA	0	602	4	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
31	CLA	r	313	33	53,57,73	1.56	8 (15%)	62,93,113	2.14	17 (27%)
31	CLA	b	604	6	69,73,73	1.39	6 (8%)	83,113,113	1.88	17 (20%)
31	CLA	B	605	6	69,73,73	1.37	6 (8%)	83,113,113	1.95	16 (19%)
34	LMG	b	601	-	45,45,55	0.90	3 (6%)	53,53,63	1.07	3 (5%)
34	LMG	y	620	-	38,38,55	0.60	1 (2%)	46,46,63	1.13	3 (6%)
31	CLA	q	312	2	56,61,73	1.40	6 (10%)	71,98,113	2.21	19 (26%)
45	DGD	c	617	-	63,63,67	1.14	7 (11%)	77,77,81	1.29	9 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	BCR	b	619	-	-	15/29/63/63	0/2/2/2
33	LHG	9	320	31	-	24/37/37/53	-
35	RRX	G	614	-	-	15/29/65/65	0/2/2/2
31	CLA	2	611	2	-	10/27/103/115	-
30	CHL	9	311	2	-	14/35/111/117	-
31	CLA	3	313	3	-	11/21/97/115	-
31	CLA	C	607	49	-	15/39/115/115	-
38	SQD	a	412	-	-	18/40/60/69	0/1/1/1
32	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
34	LMG	D	410	-	-	12/41/61/70	0/1/1/1
38	SQD	g	318	-	-	3/37/57/69	0/1/1/1
30	CHL	4	606	31	-	6/23/99/117	-
31	CLA	B	610	49	-	14/39/115/115	-
31	CLA	y	610	24	-	11/39/115/115	-
31	CLA	3	306	49	-	17/27/103/115	-
32	LUT	5	617	-	-	7/29/67/67	0/2/2/2
30	CHL	3	308	-	-	3/19/95/117	-
31	CLA	r	311	18	-	17/31/107/115	-
31	CLA	s	315	19	-	8/19/95/115	-
30	CHL	Y	302	24	-	11/41/117/117	-
34	LMG	b	629	-	-	12/33/53/70	0/1/1/1
30	CHL	G	608	2	-	4/38/114/117	-
34	LMG	X	203	-	-	10/33/53/70	0/1/1/1
38	SQD	A	413	-	-	15/40/60/69	0/1/1/1
31	CLA	9	313	33	-	10/18/94/115	-
31	CLA	c	613	7	-	10/39/115/115	-
34	LMG	3	321	-	-	10/33/53/70	0/1/1/1
43	BCR	d	406	-	-	11/29/63/63	0/2/2/2
34	LMG	C	619	-	-	10/46/66/70	0/1/1/1
31	CLA	s	314	19	-	17/39/115/115	-
31	CLA	C	604	49	-	10/29/105/115	-
32	LUT	p	616	-	-	9/29/67/67	0/2/2/2
31	CLA	N	312	3	-	6/15/91/115	-
31	CLA	c	609	7	-	12/39/115/115	-
38	SQD	g	301	-	-	6/33/53/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SQD	r	322	-	-	15/46/66/69	0/1/1/1
31	CLA	G	603	2	-	11/27/103/115	-
31	CLA	p	603	3	-	13/27/103/115	-
38	SQD	M	102	-	-	16/45/65/69	0/1/1/1
31	CLA	3	314	3	-	6/27/103/115	-
31	CLA	r	304	18	-	11/33/109/115	-
38	SQD	G	617	-	-	11/37/57/69	0/1/1/1
31	CLA	2	603	2	-	13/27/103/115	-
43	BCR	D	405	-	-	13/29/63/63	0/2/2/2
30	CHL	7	310	1	-	9/41/117/117	-
30	CHL	2	608	2	-	7/31/107/117	-
31	CLA	B	611	6	-	13/39/115/115	-
34	LMG	9	301	-	-	11/46/66/70	0/1/1/1
34	LMG	D	411	-	-	15/46/66/70	0/1/1/1
31	CLA	N	311	33	-	9/20/96/115	-
31	CLA	7	305	49	-	14/39/115/115	-
31	CLA	Y	310	24	-	11/39/115/115	-
37	XAT	r	318	-	-	1/31/93/93	0/4/4/4
31	CLA	n	305	49	-	19/39/115/115	-
35	RRX	g	315	-	-	7/29/65/65	0/2/2/2
31	CLA	B	604	6	-	16/39/115/115	-
31	CLA	S	316	19	-	7/17/93/115	-
31	CLA	c	610	7	-	14/39/115/115	-
31	CLA	p	615	3	-	7/17/93/115	-
33	LHG	D	408	-	-	30/53/53/53	-
30	CHL	7	302	1	-	12/41/117/117	-
32	LUT	S	318	-	-	9/29/67/67	0/2/2/2
31	CLA	5	613	3	-	11/26/102/115	-
30	CHL	R	309	18	-	6/29/105/117	-
30	CHL	0	607	49	-	19/41/117/117	-
31	CLA	r	312	18	-	12/30/106/115	-
30	CHL	5	608	-	-	8/22/98/117	-
34	LMG	c	620	-	-	14/33/53/70	0/1/1/1
31	CLA	R	314	18	-	6/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	d	410	-	-	15/46/66/70	0/1/1/1
31	CLA	6	311	4	-	16/39/115/115	-
34	LMG	W	203	-	-	13/33/53/70	0/1/1/1
44	PL9	A	416	-	-	13/53/73/73	0/1/1/1
30	CHL	6	307	49	-	5/23/99/117	-
30	CHL	n	309	49	-	5/22/98/117	-
31	CLA	s	310	19	-	15/33/109/115	-
33	LHG	8	618	31	-	35/53/53/53	-
34	LMG	w	203	-	-	6/33/53/70	0/1/1/1
31	CLA	S	304	19	-	5/12/88/115	-
31	CLA	n	314	3	-	15/39/115/115	-
31	CLA	Y	305	49	-	13/27/103/115	-
31	CLA	1	603	1	-	10/27/103/115	-
34	LMG	Y	319	-	-	8/33/53/70	0/1/1/1
34	LMG	9	302	-	-	13/35/55/70	0/1/1/1
30	CHL	3	309	-	-	10/22/98/117	-
31	CLA	4	603	2	-	10/27/103/115	-
43	BCR	B	617	-	-	14/29/63/63	0/2/2/2
30	CHL	0	605	4	-	10/25/101/117	-
31	CLA	C	603	7	-	18/39/115/115	-
36	NEX	p	618	31	-	9/27/83/83	0/3/3/3
30	CHL	s	302	19	-	2/17/93/117	-
31	CLA	r	306	49	-	8/19/95/115	-
30	CHL	1	606	49	-	16/41/117/117	-
30	CHL	7	321	49	-	13/38/114/117	-
34	LMG	Q1	101	-	-	10/33/53/70	0/1/1/1
38	SQD	6	301	-	-	18/37/57/69	0/1/1/1
31	CLA	S	303	19	-	17/39/115/115	-
31	CLA	Y	314	24	-	11/26/102/115	-
31	CLA	q	313	33	-	7/13/89/115	-
31	CLA	5	614	3	-	8/23/99/115	-
31	CLA	q	306	49	-	12/27/103/115	-
34	LMG	g	320	-	-	11/33/53/70	0/1/1/1
37	XAT	2	619	-	-	9/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	612	7	-	12/27/103/115	-
33	LHG	K	102	-	-	24/40/40/53	-
31	CLA	1	612	1	-	19/39/115/115	-
30	CHL	Y	309	24	-	10/41/117/117	-
34	LMG	N	320	-	-	9/33/53/70	0/1/1/1
31	CLA	b	614	6	-	13/39/115/115	-
34	LMG	B	621	-	-	15/46/66/70	0/1/1/1
43	BCR	z	101	-	-	4/29/63/63	0/2/2/2
30	CHL	R	310	49	-	4/28/104/117	-
30	CHL	6	308	49	-	13/41/117/117	-
32	LUT	S	317	-	-	6/29/67/67	0/2/2/2
31	CLA	R	307	49	-	11/19/95/115	-
32	LUT	y	616	-	-	2/29/67/67	0/2/2/2
34	LMG	6	323	-	-	14/33/53/70	0/1/1/1
36	NEX	Y	317	-	-	2/27/83/83	0/3/3/3
30	CHL	3	310	3	-	8/35/111/117	-
31	CLA	G	613	2	-	10/20/96/115	-
34	LMG	b	622	-	-	16/46/66/70	0/1/1/1
31	CLA	N	304	3	-	12/27/103/115	-
34	LMG	0	622	-	-	15/33/53/70	0/1/1/1
33	LHG	d	408	-	-	29/53/53/53	-
43	BCR	c	614	-	-	16/29/63/63	0/2/2/2
37	XAT	q	321	-	-	9/31/93/93	0/4/4/4
33	LHG	N	319	31	-	32/53/53/53	-
31	CLA	2	604	49,36	-	11/26/102/115	-
43	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
34	LMG	C	621	-	-	9/33/53/70	0/1/1/1
34	LMG	x	202	-	-	19/33/53/70	0/1/1/1
31	CLA	p	611	33	-	19/33/109/115	-
43	BCR	C	615	-	-	8/29/63/63	0/2/2/2
32	LUT	4	616	-	-	6/29/67/67	0/2/2/2
42	PHO	A	408	-	-	13/37/103/103	0/5/6/6
30	CHL	9	308	-	-	6/25/101/117	-
31	CLA	b	615	6	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	5	602	3	-	14/33/109/115	-
43	BCR	C	614	-	-	12/29/63/63	0/2/2/2
31	CLA	q	316	2	-	10/21/97/115	-
45	DGD	c	619	-	-	16/55/95/95	0/2/2/2
31	CLA	b	613	6	-	18/39/115/115	-
30	CHL	N	307	49	-	6/32/108/117	-
31	CLA	b	611	49	-	12/39/115/115	-
34	LMG	p	620	-	-	7/33/53/70	0/1/1/1
30	CHL	Y	307	49	-	10/33/109/117	-
42	PHO	d	402	-	-	6/37/103/103	0/5/6/6
31	CLA	B	602	6	-	16/39/115/115	-
31	CLA	8	614	3	-	10/26/102/115	-
36	NEX	R	319	-	-	7/27/83/83	0/3/3/3
34	LMG	a	401	-	-	6/33/53/70	0/1/1/1
31	CLA	N	315	3	-	8/26/102/115	-
30	CHL	R	308	18	-	5/29/105/117	-
31	CLA	c	608	7	-	11/39/115/115	-
34	LMG	n	322	-	-	12/35/55/70	0/1/1/1
31	CLA	8	611	3	-	4/15/91/115	-
31	CLA	g	314	2	-	7/20/96/115	-
33	LHG	t	102	-	-	30/45/45/53	-
32	LUT	N	317	-	-	6/29/67/67	0/2/2/2
32	LUT	6	318	-	-	6/29/67/67	0/2/2/2
33	LHG	y	619	31	-	30/50/50/53	-
31	CLA	0	615	-	-	14/27/103/115	-
37	XAT	G	620	-	-	9/31/93/93	0/4/4/4
30	CHL	s	309	49	-	2/21/97/117	-
30	CHL	p	606	-	-	2/23/99/117	-
36	NEX	y	618	-	-	2/27/83/83	0/3/3/3
34	LMG	w	204	-	-	12/33/53/70	0/1/1/1
31	CLA	6	315	4	-	16/26/102/115	-
30	CHL	G	607	49	-	5/23/99/117	-
30	CHL	g	302	2	-	14/41/117/117	-
34	LMG	n	321	-	-	12/33/53/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEX	g	317	31	-	12/27/83/83	0/3/3/3
30	CHL	q	307	2	-	4/17/93/117	-
31	CLA	A	405	5	-	10/39/115/115	-
31	CLA	5	610	3	-	11/33/109/115	-
30	CHL	7	309	49	-	7/22/98/117	-
33	LHG	S	320	31	-	30/45/45/53	-
31	CLA	5	603	3	-	10/24/100/115	-
35	RRX	q	317	-	-	9/29/65/65	0/2/2/2
30	CHL	p	609	3	-	4/29/105/117	-
33	LHG	C	623	-	-	28/44/44/53	-
30	CHL	n	310	3	-	6/41/117/117	-
31	CLA	G	610	33	-	17/33/109/115	-
30	CHL	7	307	49	-	9/41/117/117	-
34	LMG	2	618	-	-	13/33/53/70	0/1/1/1
31	CLA	b	609	6	-	14/39/115/115	-
30	CHL	Y	308	49	-	7/22/98/117	-
34	LMG	2	621	-	-	9/35/55/70	0/1/1/1
33	LHG	6	320	31	-	24/41/41/53	-
30	CHL	8	606	49	-	3/32/108/117	-
31	CLA	C	611	7	-	15/39/115/115	-
31	CLA	B	601	49	-	10/20/96/115	-
32	LUT	Y	315	-	-	0/29/67/67	0/2/2/2
33	LHG	G	618	31	-	29/48/48/53	-
31	CLA	2	610	33	-	15/33/109/115	-
34	LMG	J	102	-	-	7/33/53/70	0/1/1/1
34	LMG	a	413	-	-	9/33/53/70	0/1/1/1
32	LUT	3	318	-	-	8/29/67/67	0/2/2/2
30	CHL	p	605	3	-	3/17/93/117	-
32	LUT	7	318	-	-	6/29/67/67	0/2/2/2
31	CLA	q	305	2	-	14/27/103/115	-
33	LHG	3	320	31	-	25/37/37/53	-
31	CLA	g	310	2	-	14/39/115/115	-
31	CLA	c	605	7	-	18/39/115/115	-
30	CHL	N	309	3	-	7/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	9	310	49	-	7/22/98/117	-
38	SQD	X	201	-	-	9/33/53/69	0/1/1/1
31	CLA	2	609	2	-	18/33/109/115	-
38	SQD	b	627	-	-	14/47/67/69	0/1/1/1
31	CLA	6	313	4	-	12/33/109/115	-
33	LHG	A	417	-	-	24/43/43/53	-
30	CHL	3	307	3	-	7/17/93/117	-
34	LMG	6	321	-	-	13/37/57/70	0/1/1/1
30	CHL	6	306	4	-	8/17/93/117	-
30	CHL	s	307	19	-	0/15/91/117	-
31	CLA	3	316	3	-	13/30/106/115	-
30	CHL	S	309	49	-	1/21/97/117	-
31	CLA	2	602	2	-	25/39/115/115	-
33	LHG	1	617	31	-	29/39/39/53	-
31	CLA	s	313	19	-	9/29/105/115	-
33	LHG	S	322	-	-	31/48/48/53	-
31	CLA	C	606	7	-	15/30/106/115	-
34	LMG	c	624	-	-	11/39/59/70	0/1/1/1
30	CHL	4	607	-	-	15/31/107/117	-
30	CHL	8	601	3	-	8/29/105/117	-
31	CLA	c	602	7	-	12/39/115/115	-
43	BCR	B	618	-	-	10/29/63/63	0/2/2/2
31	CLA	8	603	3	-	13/27/103/115	-
31	CLA	b	610	6	-	20/39/115/115	-
31	CLA	6	316	4	-	14/27/103/115	-
33	LHG	7	319	31	-	28/39/39/53	-
31	CLA	G	602	2	-	16/39/115/115	-
34	LMG	k	101	-	-	9/43/63/70	0/1/1/1
38	SQD	s	301	-	-	16/46/66/69	0/1/1/1
33	LHG	2	617	31	-	32/53/53/53	-
32	LUT	R	317	-	-	8/29/67/67	0/2/2/2
31	CLA	3	315	3	-	12/26/102/115	-
33	LHG	r	320	31	-	23/42/42/53	-
31	CLA	0	613	4	-	10/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	5	604	-	-	6/21/97/115	-
31	CLA	C	605	7	-	18/39/115/115	-
31	CLA	Y	304	24	-	13/27/103/115	-
30	CHL	p	601	3	-	8/23/99/117	-
31	CLA	R	304	18	-	14/33/109/115	-
32	LUT	3	317	-	-	2/29/67/67	0/2/2/2
34	LMG	r	321	-	-	15/33/53/70	0/1/1/1
31	CLA	p	610	3	-	15/29/105/115	-
30	CHL	y	606	49	-	9/33/109/117	-
31	CLA	0	611	33	-	12/33/109/115	-
34	LMG	q	302	-	-	9/35/55/70	0/1/1/1
31	CLA	6	304	4	-	18/29/105/115	-
36	NEX	s	319	-	-	3/27/83/83	0/3/3/3
37	XAT	4	619	-	-	9/31/93/93	0/4/4/4
31	CLA	R	313	33	-	8/20/96/115	-
31	CLA	p	612	3	-	8/17/93/115	-
31	CLA	9	314	2	-	5/21/97/115	-
31	CLA	y	614	24	-	10/26/102/115	-
33	LHG	q	320	31	-	31/50/50/53	-
30	CHL	3	302	49	-	13/31/107/117	-
33	LHG	B	624	-	-	35/53/53/53	-
33	LHG	5	619	31	-	27/39/39/53	-
31	CLA	8	610	33	-	7/20/96/115	-
30	CHL	4	601	2	-	12/41/117/117	-
32	LUT	G	615	-	-	10/29/67/67	0/2/2/2
30	CHL	N	301	-	-	6/22/98/117	-
33	LHG	L	101	-	-	31/53/53/53	-
34	LMG	B	622	-	-	8/33/53/70	0/1/1/1
34	LMG	s	321	-	-	11/36/56/70	0/1/1/1
32	LUT	r	317	-	-	5/29/67/67	0/2/2/2
31	CLA	b	606	6	-	16/39/115/115	-
37	XAT	R	318	-	-	6/31/93/93	0/4/4/4
31	CLA	R	312	18	-	12/30/106/115	-
30	CHL	S	308	49	-	1/14/90/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	607	6	-	16/39/115/115	-
31	CLA	g	305	49,36	-	13/27/103/115	-
34	LMG	f	101	-	-	11/33/53/70	0/1/1/1
31	CLA	b	616	6	-	17/39/115/115	-
47	HEM	E	101	9,10	-	5/14/54/54	-
31	CLA	4	613	2	-	15/35/111/115	-
31	CLA	7	303	1	-	11/33/109/115	-
31	CLA	8	612	3	-	15/39/115/115	-
31	CLA	9	305	2	-	12/27/103/115	-
34	LMG	7	322	-	-	13/33/53/70	0/1/1/1
44	PL9	D	406	-	-	9/53/73/73	0/1/1/1
45	DGD	C	616	-	-	9/39/79/95	0/2/2/2
33	LHG	b	625	-	-	30/48/48/53	-
33	LHG	0	619	31	-	29/40/40/53	-
31	CLA	b	608	49	-	24/39/115/115	-
31	CLA	r	316	18	-	20/39/115/115	-
36	NEX	S	319	-	-	2/27/83/83	0/3/3/3
30	CHL	G	605	2	-	5/20/96/117	-
34	LMG	C	622	-	-	6/27/47/70	0/1/1/1
31	CLA	R	316	18	-	22/39/115/115	-
32	LUT	q	318	-	-	6/29/67/67	0/2/2/2
31	CLA	y	611	33	-	17/39/115/115	-
31	CLA	4	604	30	-	12/23/99/115	-
31	CLA	d	405	8	-	13/39/115/115	-
36	NEX	0	618	-	-	9/27/83/83	0/3/3/3
36	NEX	r	301	-	-	2/27/83/83	0/3/3/3
30	CHL	g	309	2	-	7/38/114/117	-
31	CLA	b	603	6	-	19/39/115/115	-
31	CLA	S	314	19	-	16/39/115/115	-
30	CHL	9	309	-	-	11/26/102/117	-
45	DGD	C	618	-	-	16/55/95/95	0/2/2/2
31	CLA	C	601	7	-	20/39/115/115	-
32	LUT	5	616	-	-	7/29/67/67	0/2/2/2
34	LMG	G	621	-	-	13/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	c	622	-	-	32/51/51/53	-
30	CHL	9	307	2	-	7/17/93/117	-
31	CLA	c	607	49	-	12/39/115/115	-
33	LHG	e	101	-	-	31/48/48/53	-
30	CHL	p	608	-	-	10/22/98/117	-
34	LMG	A	414	-	-	10/33/53/70	0/1/1/1
31	CLA	Y	312	24	-	17/39/115/115	-
31	CLA	C	612	7	-	14/27/103/115	-
31	CLA	s	303	19	-	14/39/115/115	-
38	SQD	A	411	-	-	13/46/66/69	0/1/1/1
34	LMG	b	626	-	-	14/41/61/70	0/1/1/1
31	CLA	6	312	33	-	19/33/109/115	-
43	BCR	b	620	-	-	9/29/63/63	0/2/2/2
34	LMG	w	205	-	-	13/33/53/70	0/1/1/1
33	LHG	4	618	31	-	28/51/51/53	-
30	CHL	2	601	2	-	10/41/117/117	-
31	CLA	4	612	2	-	6/17/93/115	-
33	LHG	Y	318	31	-	30/46/46/53	-
34	LMG	W	202	-	-	11/33/53/70	0/1/1/1
34	LMG	4	620	-	-	15/46/66/70	0/1/1/1
38	SQD	Y	320	-	-	8/37/57/69	0/1/1/1
31	CLA	d	401	49	-	8/20/96/115	-
31	CLA	G	609	2	-	7/39/115/115	-
34	LMG	7	301	-	-	11/34/54/70	0/1/1/1
30	CHL	7	308	49	-	10/41/117/117	-
31	CLA	B	607	49	-	20/39/115/115	-
30	CHL	y	601	24	-	13/41/117/117	-
31	CLA	B	612	6	-	11/39/115/115	-
30	CHL	q	310	-	-	4/22/98/117	-
34	LMG	S	321	-	-	9/36/56/70	0/1/1/1
34	LMG	G	622	-	-	7/35/55/70	0/1/1/1
31	CLA	G	604	49	-	14/27/103/115	-
31	CLA	7	315	1	-	16/26/102/115	-
31	CLA	q	315	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	3	311	-	-	6/26/102/115	-
31	CLA	y	615	24	-	12/26/102/115	-
31	CLA	S	310	19	-	16/33/109/115	-
30	CHL	5	605	3	-	3/17/93/117	-
32	LUT	n	318	-	-	6/29/67/67	0/2/2/2
31	CLA	4	610	2	-	20/33/109/115	-
43	BCR	t	101	-	-	6/29/63/63	0/2/2/2
33	LHG	a	415	-	-	23/43/43/53	-
33	LHG	g	319	31	-	26/48/48/53	-
33	LHG	b	628	-	-	31/53/53/53	-
36	NEX	r	319	-	-	4/27/83/83	0/3/3/3
32	LUT	1	616	-	-	3/29/67/67	0/2/2/2
31	CLA	N	313	3	-	13/39/115/115	-
31	CLA	R	305	18	-	8/33/109/115	-
33	LHG	l	101	-	-	29/53/53/53	-
30	CHL	s	308	49	-	3/14/90/117	-
36	NEX	5	618	-	-	9/27/83/83	0/3/3/3
32	LUT	0	617	-	-	0/29/67/67	0/2/2/2
31	CLA	B	606	6	-	16/39/115/115	-
31	CLA	r	303	18	-	9/20/96/115	-
34	LMG	W	201	-	-	19/50/70/70	0/1/1/1
30	CHL	8	608	3	-	8/41/117/117	-
38	SQD	a	411	-	-	16/43/63/69	0/1/1/1
31	CLA	7	316	1	-	7/23/99/115	-
34	LMG	q1	101	-	-	7/33/53/70	0/1/1/1
43	BCR	T	101	-	-	14/29/63/63	0/2/2/2
36	NEX	4	617	-	-	6/27/83/83	0/3/3/3
31	CLA	p	614	3	-	11/23/99/115	-
31	CLA	c	611	7	-	15/39/115/115	-
33	LHG	M	101	-	-	25/45/45/53	-
31	CLA	4	611	33	-	5/13/89/115	-
32	LUT	y	617	-	-	2/29/67/67	0/2/2/2
31	CLA	q	304	2	-	12/39/115/115	-
30	CHL	0	606	49	-	3/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	R	303	18	-	11/20/96/115	-
31	CLA	A	407	49	-	6/20/96/115	-
31	CLA	N	314	3	-	9/20/96/115	-
30	CHL	n	307	49	-	3/32/108/117	-
34	LMG	1	618	-	-	8/33/53/70	0/1/1/1
31	CLA	0	614	4	-	12/26/102/115	-
31	CLA	3	312	33	-	15/39/115/115	-
30	CHL	2	605	2	-	4/17/93/117	-
38	SQD	x	201	-	-	14/37/57/69	0/1/1/1
36	NEX	N	318	-	-	15/27/83/83	0/3/3/3
31	CLA	R	306	49	-	7/19/95/115	-
36	NEX	9	319	31	-	6/27/83/83	0/3/3/3
30	CHL	y	608	49	-	3/22/98/117	-
30	CHL	1	601	1	-	12/41/117/117	-
30	CHL	1	619	-	-	11/35/111/117	-
30	CHL	q	303	2	-	9/41/117/117	-
32	LUT	7	317	-	-	6/29/67/67	0/2/2/2
31	CLA	g	303	2	-	11/39/115/115	-
35	RRX	2	614	-	-	15/29/65/65	0/2/2/2
30	CHL	q	311	2	-	3/29/105/117	-
31	CLA	a	406	5	-	15/39/115/115	-
31	CLA	s	316	19	-	6/17/93/115	-
30	CHL	9	303	2	-	11/41/117/117	-
31	CLA	y	603	24	-	12/27/103/115	-
32	LUT	8	615	-	-	6/29/67/67	0/2/2/2
31	CLA	3	301	1	-	13/26/102/115	-
31	CLA	6	314	4	-	13/39/115/115	-
30	CHL	1	607	-	-	14/41/117/117	-
31	CLA	S	313	19	-	9/29/105/115	-
31	CLA	c	606	7	-	20/39/115/115	-
42	PHO	D	401	-	-	12/37/103/103	0/5/6/6
32	LUT	6	317	-	-	6/29/67/67	0/2/2/2
30	CHL	r	310	49	-	3/28/104/117	-
45	DGD	C	620	-	-	17/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	2	607	49	-	6/22/98/117	-
30	CHL	6	309	49	-	2/22/98/117	-
43	BCR	h	101	-	-	9/29/63/63	0/2/2/2
30	CHL	1	605	1	-	13/41/117/117	-
31	CLA	2	612	2	-	17/39/115/115	-
32	LUT	s	318	-	-	5/29/67/67	0/2/2/2
30	CHL	4	605	2	-	4/17/93/117	-
30	CHL	0	609	4	-	4/35/111/117	-
31	CLA	S	305	49	-	11/39/115/115	-
34	LMG	j	101	-	-	12/38/58/70	0/1/1/1
31	CLA	3	304	3	-	14/33/109/115	-
34	LMG	5	620	-	-	14/33/53/70	0/1/1/1
31	CLA	p	604	36	-	8/21/97/115	-
32	LUT	g	316	-	-	10/29/67/67	0/2/2/2
34	LMG	D	409	-	-	12/41/61/70	0/1/1/1
31	CLA	B	614	6	-	19/39/115/115	-
31	CLA	7	304	1	-	12/27/103/115	-
30	CHL	Y	306	24	-	0/17/93/117	-
36	NEX	3	319	-	-	9/27/83/83	0/3/3/3
32	LUT	N	316	-	-	6/29/67/67	0/2/2/2
34	LMG	R	321	-	-	9/33/53/70	0/1/1/1
31	CLA	7	313	1	-	15/39/115/115	-
43	BCR	H	101	-	-	5/29/63/63	0/2/2/2
31	CLA	B	615	6	-	11/39/115/115	-
30	CHL	5	607	-	-	8/23/99/117	-
37	XAT	g	321	-	-	9/31/93/93	0/4/4/4
31	CLA	0	604	49	-	15/27/103/115	-
34	LMG	c	621	-	-	8/33/53/70	0/1/1/1
30	CHL	3	303	3	-	6/22/98/117	-
31	CLA	1	610	1	-	19/39/115/115	-
30	CHL	4	609	2	-	10/31/107/117	-
33	LHG	s	322	-	-	29/48/48/53	-
31	CLA	p	613	-	-	9/26/102/115	-
31	CLA	d	404	8	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	J	101	-	-	13/46/66/70	0/1/1/1
30	CHL	5	606	49	-	2/23/99/117	-
34	LMG	4	621	-	-	11/35/55/70	0/1/1/1
31	CLA	g	311	33	-	15/33/109/115	-
31	CLA	C	609	7	-	12/39/115/115	-
43	BCR	c	615	-	-	11/29/63/63	0/2/2/2
30	CHL	g	308	49	-	4/23/99/117	-
31	CLA	a	409	5	-	16/33/109/115	-
30	CHL	6	310	4	-	12/35/111/117	-
30	CHL	1	608	49	-	5/22/98/117	-
31	CLA	7	312	33	-	19/39/115/115	-
37	XAT	9	322	-	-	9/31/93/93	0/4/4/4
32	LUT	8	616	-	-	6/29/67/67	0/2/2/2
45	DGD	C	617	-	-	16/55/95/95	0/2/2/2
48	LMU	r	302	-	-	9/21/61/61	0/2/2/2
31	CLA	s	304	19	-	6/12/88/115	-
33	LHG	R	320	31	-	26/42/42/53	-
32	LUT	s	317	-	-	6/29/67/67	0/2/2/2
30	CHL	p	607	-	-	7/23/99/117	-
31	CLA	R	311	18	-	18/31/107/115	-
38	SQD	B	623	-	-	20/47/67/69	0/1/1/1
30	CHL	0	601	4	-	8/29/105/117	-
34	LMG	A	412	-	-	11/36/56/70	0/1/1/1
30	CHL	7	306	1	-	17/41/117/117	-
31	CLA	8	613	3	-	8/20/96/115	-
34	LMG	d	409	-	-	10/36/56/70	0/1/1/1
30	CHL	6	302	4	-	5/29/105/117	-
38	SQD	R	322	-	-	16/46/66/69	0/1/1/1
43	BCR	a	410	-	-	11/29/63/63	0/2/2/2
33	LHG	n	320	31	-	34/53/53/53	-
31	CLA	r	315	18	-	13/27/103/115	-
31	CLA	G	611	2	-	2/13/89/115	-
31	CLA	1	611	33	-	11/39/115/115	-
30	CHL	n	308	49	-	13/38/114/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	N	308	49	-	8/22/98/117	-
31	CLA	2	613	2	-	13/26/102/115	-
34	LMG	I	101	-	-	15/33/53/70	0/1/1/1
31	CLA	N	310	3	-	11/39/115/115	-
31	CLA	c	604	49	-	11/29/105/115	-
31	CLA	N	321	24	-	9/26/102/115	-
31	CLA	A	406	49	-	12/39/115/115	-
31	CLA	8	604	49,36	-	21/39/115/115	-
34	LMG	D	412	-	-	7/43/63/70	0/1/1/1
30	CHL	8	607	49	-	5/22/98/117	-
31	CLA	n	311	3	-	10/39/115/115	-
31	CLA	r	305	18	-	14/33/109/115	-
31	CLA	s	312	33	-	25/39/115/115	-
30	CHL	G	623	49	-	12/41/117/117	-
36	NEX	2	616	31	-	14/27/83/83	0/3/3/3
31	CLA	R	315	18	-	8/27/103/115	-
43	BCR	b	618	-	-	14/29/63/63	0/2/2/2
47	HEM	e	102	9,10	-	7/14/54/54	-
31	CLA	A	409	5	-	16/33/109/115	-
31	CLA	c	601	7	-	24/39/115/115	-
30	CHL	y	609	24	-	6/41/117/117	-
31	CLA	n	315	3	-	8/20/96/115	-
31	CLA	b	612	6	-	13/39/115/115	-
30	CHL	r	309	18	-	5/29/105/117	-
34	LMG	a	416	-	-	11/33/53/70	0/1/1/1
30	CHL	5	609	3	-	5/29/105/117	-
32	LUT	n	317	-	-	6/29/67/67	0/2/2/2
31	CLA	Y	311	33	-	16/39/115/115	-
31	CLA	C	613	7	-	13/39/115/115	-
31	CLA	s	306	-	-	5/21/97/115	-
33	LHG	D	407	-	-	31/48/48/53	-
30	CHL	4	608	-	-	5/22/98/117	-
31	CLA	S	306	-	-	4/21/97/115	-
31	CLA	N	305	49	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	n	302	3	-	8/29/105/117	-
31	CLA	S	315	19	-	5/19/95/115	-
31	CLA	r	314	18	-	8/20/96/115	-
48	LMU	R	302	-	-	12/21/61/61	0/2/2/2
34	LMG	b	623	-	-	7/33/53/70	0/1/1/1
38	SQD	0	621	-	-	9/37/57/69	0/1/1/1
30	CHL	2	606	-	-	6/23/99/117	-
31	CLA	y	602	24	-	10/33/109/115	-
34	LMG	g	322	-	-	15/44/64/70	0/1/1/1
38	SQD	S	301	-	-	14/46/66/69	0/1/1/1
31	CLA	n	316	3	-	10/26/102/115	-
36	NEX	R	301	-	-	3/27/83/83	0/3/3/3
31	CLA	5	611	33	-	15/31/107/115	-
31	CLA	C	610	7	-	14/39/115/115	-
31	CLA	y	612	24	-	18/39/115/115	-
31	CLA	B	608	6	-	12/39/115/115	-
31	CLA	N	303	3	-	19/39/115/115	-
34	LMG	7	320	-	-	7/33/53/70	0/1/1/1
36	NEX	8	617	31	-	11/27/83/83	0/3/3/3
31	CLA	Y	313	24	-	12/39/115/115	-
30	CHL	n	306	3	-	15/41/117/117	-
35	RRX	9	317	-	-	15/29/65/65	0/2/2/2
31	CLA	a	407	49	-	13/39/115/115	-
32	LUT	p	617	-	-	9/29/67/67	0/2/2/2
31	CLA	p	602	3	-	12/33/109/115	-
31	CLA	6	305	49	-	16/27/103/115	-
30	CHL	S	302	19	-	0/17/93/117	-
31	CLA	S	312	33	-	19/39/115/115	-
34	LMG	m	102	-	-	10/40/60/70	0/1/1/1
30	CHL	5	601	3	-	9/23/99/117	-
31	CLA	y	613	24	-	17/39/115/115	-
30	CHL	S	307	19	-	0/15/91/117	-
34	LMG	G	619	-	-	11/33/53/70	0/1/1/1
35	RRX	4	615	-	-	15/29/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	616	6	-	15/39/115/115	-
32	LUT	1	615	-	-	1/29/67/67	0/2/2/2
31	CLA	5	612	3	-	8/21/97/115	-
31	CLA	6	303	4	-	15/39/115/115	-
31	CLA	9	316	2	-	9/17/93/115	-
31	CLA	4	602	2	-	15/39/115/115	-
31	CLA	5	615	3	-	11/17/93/115	-
34	LMG	6	322	-	-	11/34/54/70	0/1/1/1
30	CHL	G	606	49	-	6/22/98/117	-
31	CLA	3	305	3	-	13/27/103/115	-
31	CLA	C	608	7	-	13/39/115/115	-
30	CHL	q	308	-	-	6/23/99/117	-
31	CLA	g	304	2	-	12/27/103/115	-
31	CLA	1	614	1	-	16/26/102/115	-
30	CHL	y	607	49	-	11/41/117/117	-
31	CLA	8	602	3	-	13/39/115/115	-
34	LMG	d	411	-	-	8/43/63/70	0/1/1/1
31	CLA	9	304	2	-	19/39/115/115	-
30	CHL	1	609	1	-	6/41/117/117	-
31	CLA	1	613	1	-	15/39/115/115	-
32	LUT	9	318	-	-	5/29/67/67	0/2/2/2
48	LMU	c	623	-	-	5/14/54/61	0/2/2/2
30	CHL	0	608	49	-	5/22/98/117	-
31	CLA	r	307	49	-	11/19/95/115	-
31	CLA	c	603	7	-	22/39/115/115	-
34	LMG	A	418	-	-	11/33/53/70	0/1/1/1
31	CLA	0	612	4	-	8/17/93/115	-
33	LHG	A	415	-	-	31/48/48/53	-
34	LMG	k	102	-	-	10/33/53/70	0/1/1/1
48	LMU	K	101	-	-	7/21/61/61	0/2/2/2
34	LMG	X	202	-	-	5/33/53/70	0/1/1/1
34	LMG	0	620	-	-	13/37/57/70	0/1/1/1
33	LHG	s	320	31	-	25/45/45/53	-
36	NEX	q	319	-	-	11/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	s	311	19	-	13/39/115/115	-
30	CHL	y	605	24	-	2/17/93/117	-
31	CLA	g	312	2	-	3/13/89/115	-
31	CLA	n	304	3	-	13/27/103/115	-
34	LMG	q	301	-	-	14/46/66/70	0/1/1/1
30	CHL	q	309	-	-	19/31/107/117	-
34	LMG	C	624	-	-	13/39/59/70	0/1/1/1
31	CLA	9	312	2	-	13/26/102/115	-
44	PL9	d	407	-	-	7/53/73/73	0/1/1/1
30	CHL	G	601	2	-	10/41/117/117	-
31	CLA	s	305	49	-	16/39/115/115	-
31	CLA	q	314	2	-	9/17/93/115	-
31	CLA	C	602	7	-	11/39/115/115	-
31	CLA	n	313	3	-	4/15/91/115	-
31	CLA	0	603	4	-	16/29/105/115	-
36	NEX	n	319	-	-	10/27/83/83	0/3/3/3
43	BCR	B	619	-	-	9/29/63/63	0/2/2/2
31	CLA	1	602	1	-	14/33/109/115	-
38	SQD	y	621	-	-	9/37/57/69	0/1/1/1
31	CLA	g	313	2	-	13/39/115/115	-
30	CHL	g	306	2	-	5/20/96/117	-
31	CLA	D	403	8	-	14/39/115/115	-
31	CLA	9	306	49,36	-	17/39/115/115	-
31	CLA	7	314	1	-	17/39/115/115	-
30	CHL	N	306	3	-	12/41/117/117	-
31	CLA	0	610	4	-	15/39/115/115	-
31	CLA	n	303	3	-	13/39/115/115	-
32	LUT	0	616	-	-	2/29/67/67	0/2/2/2
34	LMG	B	625	-	-	13/33/53/70	0/1/1/1
38	SQD	B	620	-	-	18/49/69/69	0/1/1/1
45	DGD	c	616	-	-	22/55/95/95	0/2/2/2
33	LHG	z	102	-	-	22/40/40/53	-
31	CLA	n	312	33	-	7/20/96/115	-
30	CHL	r	308	18	-	8/29/105/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	609	6	-	20/39/115/115	-
34	LMG	2	620	-	-	18/46/66/70	0/1/1/1
44	PL9	a	414	-	-	16/53/73/73	0/1/1/1
31	CLA	9	315	2	-	8/27/103/115	-
36	NEX	G	616	-	-	2/27/83/83	0/3/3/3
31	CLA	D	404	8	-	19/39/115/115	-
30	CHL	8	605	3	-	15/41/117/117	-
31	CLA	B	613	6	-	9/39/115/115	-
38	SQD	b	621	-	-	13/49/69/69	0/1/1/1
30	CHL	n	301	49	-	6/22/98/117	-
31	CLA	b	617	6	-	15/39/115/115	-
33	LHG	j	102	-	-	36/53/53/53	-
31	CLA	S	311	19	-	13/39/115/115	-
30	CHL	N	302	3	-	4/29/105/117	-
34	LMG	9	321	-	-	10/33/53/70	0/1/1/1
33	LHG	p	619	31	-	26/39/39/53	-
34	LMG	b	624	-	-	14/33/53/70	0/1/1/1
45	DGD	c	618	-	-	19/55/95/95	0/2/2/2
31	CLA	1	604	49	-	14/39/115/115	-
43	BCR	v	101	-	-	15/29/63/63	0/2/2/2
30	CHL	g	307	49	-	3/22/98/117	-
31	CLA	b	602	49	-	14/20/96/115	-
42	PHO	a	408	-	-	10/37/103/103	0/5/6/6
31	CLA	B	603	6	-	19/39/115/115	-
34	LMG	w	202	-	-	12/50/70/70	0/1/1/1
38	SQD	m	101	-	-	13/45/65/69	0/1/1/1
31	CLA	y	604	49	-	15/27/103/115	-
31	CLA	Y	303	24	-	10/33/109/115	-
36	NEX	6	319	-	-	9/27/83/83	0/3/3/3
30	CHL	Y	301	49	-	10/38/114/117	-
33	LHG	F1	301	-	-	26/39/39/53	-
34	LMG	w	201	-	-	13/43/63/70	0/1/1/1
31	CLA	G	612	2	-	19/39/115/115	-
31	CLA	4	614	2	-	8/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	BCR	A	410	-	-	6/29/63/63	0/2/2/2
43	BCR	V	101	-	-	15/29/63/63	0/2/2/2
32	LUT	2	615	-	-	5/29/67/67	0/2/2/2
31	CLA	7	311	1	-	17/39/115/115	-
31	CLA	b	605	6	-	25/39/115/115	-
31	CLA	8	609	3	-	10/39/115/115	-
38	SQD	G	624	-	-	12/33/53/69	0/1/1/1
31	CLA	0	602	4	-	18/39/115/115	-
31	CLA	r	313	33	-	8/20/96/115	-
31	CLA	b	604	6	-	16/39/115/115	-
31	CLA	B	605	6	-	19/39/115/115	-
34	LMG	b	601	-	-	10/40/60/70	0/1/1/1
34	LMG	y	620	-	-	10/33/53/70	0/1/1/1
31	CLA	q	312	2	-	11/25/101/115	-
45	DGD	c	617	-	-	23/51/91/95	0/2/2/2

All (4254) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	316	LUT	C24-C25	23.29	1.62	1.33
32	5	616	LUT	C24-C25	23.25	1.62	1.33
32	G	615	LUT	C24-C25	23.25	1.62	1.33
32	3	317	LUT	C24-C25	23.24	1.62	1.33
32	9	318	LUT	C24-C25	23.23	1.62	1.33
32	8	615	LUT	C24-C25	23.22	1.62	1.33
32	n	317	LUT	C24-C25	23.21	1.62	1.33
32	p	616	LUT	C24-C25	23.21	1.62	1.33
32	S	318	LUT	C24-C25	23.19	1.62	1.33
32	q	318	LUT	C24-C25	23.18	1.62	1.33
32	g	316	LUT	C24-C25	23.16	1.62	1.33
32	8	616	LUT	C24-C25	23.15	1.62	1.33
32	N	317	LUT	C24-C25	23.15	1.62	1.33
32	n	318	LUT	C24-C25	23.13	1.62	1.33
32	6	318	LUT	C24-C25	23.10	1.61	1.33
32	6	317	LUT	C24-C25	23.09	1.61	1.33
32	p	617	LUT	C24-C25	23.09	1.61	1.33
32	7	318	LUT	C24-C25	23.08	1.61	1.33
32	3	318	LUT	C24-C25	23.07	1.61	1.33
32	S	317	LUT	C24-C25	23.05	1.61	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	s	317	LUT	C24-C25	23.04	1.61	1.33
32	s	318	LUT	C24-C25	23.02	1.61	1.33
32	4	616	LUT	C24-C25	23.00	1.61	1.33
32	1	616	LUT	C24-C25	23.00	1.61	1.33
32	5	617	LUT	C24-C25	23.00	1.61	1.33
32	0	616	LUT	C24-C25	22.96	1.61	1.33
32	R	317	LUT	C24-C25	22.94	1.61	1.33
32	1	615	LUT	C24-C25	22.93	1.61	1.33
32	r	317	LUT	C24-C25	22.86	1.61	1.33
32	Y	315	LUT	C24-C25	22.80	1.61	1.33
32	7	317	LUT	C24-C25	22.80	1.61	1.33
32	0	617	LUT	C24-C25	22.76	1.61	1.33
32	y	617	LUT	C24-C25	22.76	1.61	1.33
32	y	616	LUT	C24-C25	22.71	1.61	1.33
32	Y	316	LUT	C24-C25	22.64	1.61	1.33
32	2	615	LUT	C24-C25	21.68	1.60	1.33
43	B	618	BCR	C26-C25	15.74	1.61	1.34
43	b	619	BCR	C26-C25	15.68	1.61	1.34
43	Z	101	BCR	C26-C25	15.46	1.61	1.34
43	z	101	BCR	C26-C25	15.43	1.61	1.34
43	D	405	BCR	C26-C25	15.38	1.61	1.34
35	9	317	RRX	C26-C25	15.35	1.61	1.34
35	4	615	RRX	C26-C25	15.35	1.61	1.34
35	G	614	RRX	C26-C25	15.32	1.61	1.34
32	8	615	LUT	C5-C6	15.32	1.61	1.34
32	n	317	LUT	C5-C6	15.32	1.61	1.34
35	2	614	RRX	C26-C25	15.32	1.61	1.34
43	b	620	BCR	C26-C25	15.29	1.60	1.34
35	g	315	RRX	C26-C25	15.27	1.60	1.34
32	G	615	LUT	C5-C6	15.25	1.60	1.34
43	t	101	BCR	C26-C25	15.25	1.60	1.34
43	c	615	BCR	C26-C25	15.25	1.60	1.34
32	s	317	LUT	C5-C6	15.25	1.60	1.34
32	5	617	LUT	C5-C6	15.25	1.60	1.34
32	S	317	LUT	C5-C6	15.23	1.60	1.34
35	q	317	RRX	C26-C25	15.23	1.60	1.34
43	H	101	BCR	C26-C25	15.23	1.60	1.34
32	6	318	LUT	C5-C6	15.23	1.60	1.34
32	7	318	LUT	C5-C6	15.23	1.60	1.34
32	5	616	LUT	C5-C6	15.21	1.60	1.34
32	9	318	LUT	C5-C6	15.21	1.60	1.34
43	T	101	BCR	C26-C25	15.21	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	8	616	LUT	C5-C6	15.20	1.60	1.34
32	n	318	LUT	C5-C6	15.19	1.60	1.34
43	c	614	BCR	C26-C25	15.19	1.60	1.34
43	v	101	BCR	C26-C25	15.18	1.60	1.34
43	a	410	BCR	C26-C25	15.18	1.60	1.34
43	C	615	BCR	C26-C25	15.16	1.60	1.34
43	B	619	BCR	C26-C25	15.15	1.60	1.34
32	p	616	LUT	C5-C6	15.15	1.60	1.34
32	4	616	LUT	C5-C6	15.14	1.60	1.34
43	h	101	BCR	C26-C25	15.13	1.60	1.34
32	3	317	LUT	C5-C6	15.12	1.60	1.34
32	0	617	LUT	C5-C6	15.10	1.60	1.34
32	N	316	LUT	C5-C6	15.08	1.60	1.34
32	g	316	LUT	C5-C6	15.08	1.60	1.34
32	r	317	LUT	C5-C6	15.07	1.60	1.34
32	S	318	LUT	C5-C6	15.07	1.60	1.34
43	d	406	BCR	C26-C25	15.07	1.60	1.34
32	y	617	LUT	C5-C6	15.03	1.60	1.34
32	Y	315	LUT	C5-C6	15.03	1.60	1.34
32	p	617	LUT	C5-C6	15.01	1.60	1.34
32	s	318	LUT	C5-C6	15.01	1.60	1.34
32	N	317	LUT	C5-C6	15.01	1.60	1.34
32	Y	316	LUT	C5-C6	15.01	1.60	1.34
43	A	410	BCR	C26-C25	15.00	1.60	1.34
32	1	616	LUT	C5-C6	14.98	1.60	1.34
32	3	318	LUT	C5-C6	14.98	1.60	1.34
32	6	317	LUT	C5-C6	14.96	1.60	1.34
32	R	317	LUT	C5-C6	14.95	1.60	1.34
32	q	318	LUT	C5-C6	14.94	1.60	1.34
32	y	616	LUT	C5-C6	14.93	1.60	1.34
43	B	617	BCR	C26-C25	14.91	1.60	1.34
32	0	616	LUT	C5-C6	14.90	1.60	1.34
32	1	615	LUT	C5-C6	14.82	1.60	1.34
32	7	317	LUT	C5-C6	14.82	1.60	1.34
32	2	615	LUT	C5-C6	14.81	1.60	1.34
43	b	618	BCR	C26-C25	14.79	1.60	1.34
43	C	614	BCR	C26-C25	14.74	1.60	1.34
43	V	101	BCR	C26-C25	14.70	1.59	1.34
35	g	315	RRX	C5-C6	14.30	1.59	1.34
35	4	615	RRX	C5-C6	14.25	1.59	1.34
43	D	405	BCR	C5-C6	14.24	1.59	1.34
35	9	317	RRX	C5-C6	14.23	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	G	614	RRX	C5-C6	14.20	1.59	1.34
35	2	614	RRX	C5-C6	14.18	1.59	1.34
43	z	101	BCR	C5-C6	14.16	1.59	1.34
43	Z	101	BCR	C5-C6	14.06	1.58	1.34
43	B	618	BCR	C5-C6	13.99	1.58	1.34
35	q	317	RRX	C5-C6	13.95	1.58	1.34
43	T	101	BCR	C5-C6	13.91	1.58	1.34
43	a	410	BCR	C5-C6	13.90	1.58	1.34
43	b	619	BCR	C5-C6	13.89	1.58	1.34
43	c	614	BCR	C5-C6	13.86	1.58	1.34
43	H	101	BCR	C5-C6	13.84	1.58	1.34
43	v	101	BCR	C5-C6	13.82	1.58	1.34
43	A	410	BCR	C5-C6	13.82	1.58	1.34
43	b	620	BCR	C5-C6	13.81	1.58	1.34
43	B	619	BCR	C5-C6	13.79	1.58	1.34
43	V	101	BCR	C5-C6	13.75	1.58	1.34
43	C	614	BCR	C5-C6	13.73	1.58	1.34
43	h	101	BCR	C5-C6	13.72	1.58	1.34
43	b	618	BCR	C5-C6	13.69	1.58	1.34
43	c	615	BCR	C5-C6	13.62	1.58	1.34
43	B	617	BCR	C5-C6	13.57	1.57	1.34
43	d	406	BCR	C5-C6	13.56	1.57	1.34
43	t	101	BCR	C5-C6	13.39	1.57	1.34
32	R	317	LUT	C22-C21	-13.33	1.38	1.54
32	y	617	LUT	C22-C21	-13.31	1.38	1.54
32	Y	315	LUT	C22-C21	-13.30	1.38	1.54
32	r	317	LUT	C22-C21	-13.29	1.38	1.54
32	y	616	LUT	C22-C21	-13.25	1.38	1.54
32	1	616	LUT	C22-C21	-13.24	1.38	1.54
32	Y	316	LUT	C22-C21	-13.18	1.38	1.54
32	1	615	LUT	C22-C21	-13.16	1.38	1.54
32	7	317	LUT	C22-C21	-13.14	1.38	1.54
32	0	616	LUT	C22-C21	-13.07	1.38	1.54
32	9	318	LUT	C22-C21	-13.06	1.38	1.54
32	S	317	LUT	C22-C21	-13.05	1.38	1.54
32	n	317	LUT	C22-C21	-13.02	1.38	1.54
32	6	317	LUT	C22-C21	-13.01	1.38	1.54
32	8	615	LUT	C22-C21	-13.00	1.38	1.54
43	C	615	BCR	C5-C6	12.98	1.56	1.34
32	N	316	LUT	C22-C21	-12.96	1.38	1.54
32	8	616	LUT	C22-C21	-12.96	1.38	1.54
32	5	616	LUT	C22-C21	-12.95	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	318	LUT	C22-C21	-12.95	1.38	1.54
32	G	615	LUT	C22-C21	-12.95	1.38	1.54
32	s	317	LUT	C22-C21	-12.93	1.38	1.54
32	3	317	LUT	C22-C21	-12.93	1.38	1.54
32	n	318	LUT	C22-C21	-12.89	1.38	1.54
32	q	318	LUT	C22-C21	-12.88	1.38	1.54
32	N	317	LUT	C22-C21	-12.87	1.38	1.54
32	7	318	LUT	C22-C21	-12.84	1.38	1.54
32	g	316	LUT	C22-C21	-12.84	1.38	1.54
32	3	318	LUT	C22-C21	-12.83	1.38	1.54
32	4	616	LUT	C22-C21	-12.82	1.38	1.54
32	s	318	LUT	C22-C21	-12.81	1.38	1.54
32	6	318	LUT	C22-C21	-12.78	1.38	1.54
32	0	617	LUT	C22-C21	-12.72	1.38	1.54
32	p	616	LUT	C22-C21	-12.70	1.38	1.54
32	5	617	LUT	C22-C21	-12.58	1.38	1.54
32	p	617	LUT	C22-C21	-12.49	1.39	1.54
32	2	615	LUT	C22-C21	-12.17	1.39	1.54
32	y	616	LUT	C2-C3	-11.58	1.35	1.52
32	r	317	LUT	C2-C3	-11.48	1.35	1.52
32	y	617	LUT	C2-C3	-11.45	1.35	1.52
32	Y	315	LUT	C2-C3	-11.40	1.35	1.52
32	Y	316	LUT	C2-C3	-11.40	1.35	1.52
32	8	615	LUT	C2-C3	-11.35	1.36	1.52
32	S	317	LUT	C2-C3	-11.31	1.36	1.52
32	n	317	LUT	C2-C3	-11.30	1.36	1.52
32	s	317	LUT	C2-C3	-11.29	1.36	1.52
32	1	615	LUT	C2-C3	-11.27	1.36	1.52
32	R	317	LUT	C2-C3	-11.26	1.36	1.52
32	7	317	LUT	C2-C3	-11.25	1.36	1.52
32	0	617	LUT	C2-C3	-11.24	1.36	1.52
32	1	616	LUT	C2-C3	-11.21	1.36	1.52
32	3	317	LUT	C2-C3	-11.16	1.36	1.52
32	5	616	LUT	C2-C3	-11.15	1.36	1.52
32	6	318	LUT	C2-C3	-11.13	1.36	1.52
32	N	316	LUT	C2-C3	-11.09	1.36	1.52
32	G	615	LUT	C2-C3	-11.08	1.36	1.52
32	0	616	LUT	C2-C3	-11.08	1.36	1.52
32	6	317	LUT	C2-C3	-11.08	1.36	1.52
32	4	616	LUT	C2-C3	-11.08	1.36	1.52
32	7	318	LUT	C2-C3	-11.07	1.36	1.52
32	n	318	LUT	C2-C3	-11.02	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	9	318	LUT	C2-C3	-11.01	1.36	1.52
32	S	318	LUT	C2-C3	-11.01	1.36	1.52
32	8	616	LUT	C2-C3	-10.99	1.36	1.52
32	5	617	LUT	C2-C3	-10.97	1.36	1.52
32	g	316	LUT	C2-C3	-10.96	1.36	1.52
32	N	317	LUT	C2-C3	-10.94	1.36	1.52
32	p	616	LUT	C2-C3	-10.92	1.36	1.52
32	s	318	LUT	C2-C3	-10.87	1.36	1.52
32	2	615	LUT	C2-C3	-10.86	1.36	1.52
32	3	318	LUT	C2-C3	-10.85	1.36	1.52
32	q	318	LUT	C2-C3	-10.83	1.36	1.52
32	p	617	LUT	C2-C3	-10.72	1.36	1.52
35	q	317	RRX	C29-C28	-10.36	1.37	1.52
35	G	614	RRX	C29-C28	-10.33	1.37	1.52
35	2	614	RRX	C29-C28	-10.32	1.37	1.52
35	9	317	RRX	C29-C28	-10.32	1.37	1.52
35	4	615	RRX	C29-C28	-10.29	1.37	1.52
35	g	315	RRX	C29-C28	-10.27	1.37	1.52
42	A	408	PHO	C1B-C2B	8.79	1.49	1.39
42	D	401	PHO	C1B-C2B	8.64	1.49	1.39
32	S	318	LUT	C22-C23	8.51	1.67	1.53
32	5	617	LUT	C22-C23	8.38	1.67	1.53
35	g	315	RRX	C27-C28	8.34	1.66	1.52
32	g	316	LUT	C22-C23	8.28	1.66	1.53
32	7	318	LUT	C22-C23	8.24	1.66	1.53
32	s	318	LUT	C22-C23	8.24	1.66	1.53
32	p	617	LUT	C22-C23	8.17	1.66	1.53
32	p	616	LUT	C22-C23	8.16	1.66	1.53
32	2	615	LUT	C22-C23	8.15	1.66	1.53
32	3	318	LUT	C4-C3	8.14	1.66	1.52
32	5	616	LUT	C22-C23	8.14	1.66	1.53
32	4	616	LUT	C22-C23	8.14	1.66	1.53
35	4	615	RRX	C27-C28	8.13	1.66	1.52
32	G	615	LUT	C22-C23	8.13	1.66	1.53
35	9	317	RRX	C27-C28	8.12	1.66	1.52
32	q	318	LUT	C22-C23	8.10	1.66	1.53
32	6	318	LUT	C22-C23	8.08	1.66	1.53
32	p	617	LUT	C4-C3	8.08	1.66	1.52
32	3	318	LUT	C22-C23	8.07	1.66	1.53
35	G	614	RRX	C27-C28	8.07	1.66	1.52
32	N	317	LUT	C4-C3	8.06	1.66	1.52
32	g	316	LUT	C4-C3	8.03	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	q	318	LUT	C4-C3	8.03	1.66	1.52
32	0	617	LUT	C22-C23	8.02	1.66	1.53
35	2	614	RRX	C27-C28	8.01	1.66	1.52
32	N	317	LUT	C22-C23	8.01	1.66	1.53
32	s	317	LUT	C22-C23	8.01	1.66	1.53
32	8	616	LUT	C22-C23	8.01	1.66	1.53
32	n	318	LUT	C22-C23	8.00	1.66	1.53
32	S	318	LUT	C4-C3	8.00	1.66	1.52
43	B	617	BCR	C30-C25	-7.99	1.42	1.53
32	5	617	LUT	C4-C3	7.99	1.66	1.52
32	2	615	LUT	C4-C3	7.98	1.66	1.52
32	S	317	LUT	C22-C23	7.97	1.66	1.53
32	1	615	LUT	C22-C23	7.96	1.66	1.53
32	6	317	LUT	C22-C23	7.96	1.66	1.53
32	8	616	LUT	C4-C3	7.95	1.66	1.52
32	n	318	LUT	C4-C3	7.93	1.66	1.52
36	S	319	NEX	C10-C9	-7.93	1.25	1.35
35	q	317	RRX	C27-C28	7.93	1.66	1.52
32	0	616	LUT	C22-C23	7.93	1.66	1.53
32	p	616	LUT	C4-C3	7.93	1.66	1.52
32	3	317	LUT	C22-C23	7.92	1.66	1.53
32	G	615	LUT	C32-C33	7.92	1.63	1.45
36	3	319	NEX	C14-C13	-7.91	1.25	1.35
36	3	319	NEX	C10-C9	-7.91	1.25	1.35
32	1	616	LUT	C22-C23	7.91	1.66	1.53
32	9	318	LUT	C22-C23	7.91	1.66	1.53
32	3	317	LUT	C4-C3	7.91	1.66	1.52
36	R	301	NEX	C34-C33	-7.90	1.25	1.35
36	9	319	NEX	C30-C29	-7.90	1.25	1.35
36	9	319	NEX	C34-C33	-7.89	1.25	1.35
36	R	301	NEX	C14-C13	-7.88	1.25	1.35
36	s	319	NEX	C34-C33	-7.88	1.25	1.35
32	n	317	LUT	C22-C23	7.88	1.66	1.53
32	N	316	LUT	C4-C3	7.88	1.65	1.52
32	Y	316	LUT	C22-C23	7.87	1.66	1.53
32	8	615	LUT	C22-C23	7.87	1.66	1.53
32	9	318	LUT	C4-C3	7.85	1.65	1.52
32	s	318	LUT	C4-C3	7.85	1.65	1.52
32	6	317	LUT	C4-C3	7.85	1.65	1.52
32	S	317	LUT	C4-C3	7.85	1.65	1.52
32	N	316	LUT	C22-C23	7.85	1.66	1.53
32	G	615	LUT	C4-C3	7.84	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	616	LUT	C22-C23	7.84	1.66	1.53
32	4	616	LUT	C4-C3	7.84	1.65	1.52
32	7	318	LUT	C4-C3	7.83	1.65	1.52
32	7	317	LUT	C22-C23	7.82	1.66	1.53
36	s	319	NEX	C30-C29	-7.81	1.25	1.35
32	0	616	LUT	C4-C3	7.80	1.65	1.52
36	s	319	NEX	C10-C9	-7.80	1.25	1.35
32	s	317	LUT	C4-C3	7.80	1.65	1.52
32	r	317	LUT	C22-C23	7.79	1.66	1.53
36	9	319	NEX	C10-C9	-7.78	1.25	1.35
32	y	617	LUT	C22-C23	7.78	1.66	1.53
32	5	616	LUT	C4-C3	7.78	1.65	1.52
36	3	319	NEX	C34-C33	-7.78	1.25	1.35
36	G	616	NEX	C34-C33	-7.78	1.25	1.35
32	0	617	LUT	C4-C3	7.77	1.65	1.52
36	G	616	NEX	C30-C29	-7.77	1.25	1.35
36	s	319	NEX	C14-C13	-7.77	1.25	1.35
32	6	318	LUT	C4-C3	7.75	1.65	1.52
36	G	616	NEX	C14-C13	-7.75	1.25	1.35
36	y	618	NEX	C34-C33	-7.75	1.25	1.35
32	Y	315	LUT	C22-C23	7.74	1.65	1.53
36	3	319	NEX	C30-C29	-7.73	1.25	1.35
32	R	317	LUT	C22-C23	7.72	1.65	1.53
32	8	615	LUT	C4-C3	7.71	1.65	1.52
36	S	319	NEX	C30-C29	-7.71	1.25	1.35
32	Y	316	LUT	C4-C3	7.71	1.65	1.52
36	N	318	NEX	C14-C13	-7.71	1.25	1.35
36	2	616	NEX	C10-C9	-7.69	1.25	1.35
32	n	317	LUT	C4-C3	7.68	1.65	1.52
36	4	617	NEX	C10-C9	-7.68	1.25	1.35
36	y	618	NEX	C10-C9	-7.68	1.25	1.35
32	p	616	LUT	C32-C33	7.68	1.62	1.45
36	R	301	NEX	C10-C9	-7.66	1.25	1.35
36	g	317	NEX	C10-C9	-7.65	1.25	1.35
32	1	615	LUT	C4-C3	7.65	1.65	1.52
36	y	618	NEX	C30-C29	-7.64	1.25	1.35
36	8	617	NEX	C34-C33	-7.64	1.25	1.35
36	S	319	NEX	C14-C13	-7.63	1.25	1.35
32	7	317	LUT	C4-C3	7.62	1.65	1.52
36	r	319	NEX	C30-C29	-7.62	1.25	1.35
36	6	319	NEX	C30-C29	-7.62	1.25	1.35
36	y	618	NEX	C14-C13	-7.62	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	319	NEX	C14-C13	-7.62	1.25	1.35
36	S	319	NEX	C34-C33	-7.61	1.25	1.35
32	y	617	LUT	C4-C3	7.61	1.65	1.52
36	R	319	NEX	C30-C29	-7.60	1.25	1.35
36	0	618	NEX	C30-C29	-7.60	1.25	1.35
36	R	319	NEX	C10-C9	-7.60	1.25	1.35
32	R	317	LUT	C4-C3	7.60	1.65	1.52
32	2	615	LUT	C32-C33	7.59	1.62	1.45
36	Y	317	NEX	C14-C13	-7.59	1.25	1.35
36	5	618	NEX	C14-C13	-7.59	1.25	1.35
36	r	301	NEX	C30-C29	-7.59	1.25	1.35
36	r	319	NEX	C34-C33	-7.59	1.25	1.35
43	C	615	BCR	C30-C25	-7.58	1.43	1.53
36	4	617	NEX	C14-C13	-7.58	1.25	1.35
36	p	618	NEX	C30-C29	-7.58	1.25	1.35
36	R	319	NEX	C34-C33	-7.57	1.25	1.35
36	q	319	NEX	C30-C29	-7.57	1.25	1.35
36	2	616	NEX	C34-C33	-7.57	1.25	1.35
36	9	319	NEX	C14-C13	-7.57	1.25	1.35
36	2	616	NEX	C14-C13	-7.57	1.25	1.35
36	q	319	NEX	C34-C33	-7.57	1.25	1.35
36	G	616	NEX	C10-C9	-7.56	1.25	1.35
36	Y	317	NEX	C34-C33	-7.56	1.25	1.35
32	g	316	LUT	C32-C33	7.56	1.62	1.45
43	b	618	BCR	C30-C25	-7.55	1.43	1.53
32	p	617	LUT	C32-C33	7.54	1.62	1.45
36	4	617	NEX	C30-C29	-7.54	1.25	1.35
36	8	617	NEX	C14-C13	-7.54	1.25	1.35
36	5	618	NEX	C30-C29	-7.54	1.25	1.35
36	q	319	NEX	C14-C13	-7.53	1.25	1.35
36	r	301	NEX	C10-C9	-7.53	1.25	1.35
36	p	618	NEX	C34-C33	-7.53	1.25	1.35
36	r	319	NEX	C14-C13	-7.53	1.25	1.35
32	9	318	LUT	C32-C33	7.52	1.62	1.45
32	1	616	LUT	C4-C3	7.52	1.65	1.52
36	r	301	NEX	C14-C13	-7.52	1.25	1.35
36	r	301	NEX	C34-C33	-7.52	1.25	1.35
36	Y	317	NEX	C10-C9	-7.52	1.25	1.35
32	5	617	LUT	C32-C33	7.52	1.62	1.45
36	8	617	NEX	C30-C29	-7.52	1.25	1.35
36	4	617	NEX	C34-C33	-7.52	1.25	1.35
36	5	618	NEX	C34-C33	-7.51	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	301	NEX	C30-C29	-7.51	1.25	1.35
36	p	618	NEX	C14-C13	-7.51	1.25	1.35
43	V	101	BCR	C30-C25	-7.50	1.43	1.53
36	g	317	NEX	C34-C33	-7.50	1.25	1.35
36	r	319	NEX	C10-C9	-7.50	1.25	1.35
32	Y	315	LUT	C4-C3	7.50	1.65	1.52
43	d	406	BCR	C30-C25	-7.50	1.43	1.53
32	3	318	LUT	C32-C33	7.50	1.62	1.45
36	2	616	NEX	C30-C29	-7.49	1.25	1.35
36	5	618	NEX	C10-C9	-7.49	1.25	1.35
36	8	617	NEX	C10-C9	-7.48	1.25	1.35
32	r	317	LUT	C4-C3	7.48	1.65	1.52
36	0	618	NEX	C34-C33	-7.48	1.25	1.35
32	5	616	LUT	C32-C33	7.48	1.62	1.45
32	q	318	LUT	C32-C33	7.47	1.62	1.45
36	6	319	NEX	C34-C33	-7.47	1.25	1.35
32	4	616	LUT	C32-C33	7.47	1.62	1.45
36	6	319	NEX	C14-C13	-7.47	1.25	1.35
36	0	618	NEX	C14-C13	-7.47	1.25	1.35
36	Y	317	NEX	C30-C29	-7.46	1.25	1.35
36	g	317	NEX	C14-C13	-7.46	1.25	1.35
36	q	319	NEX	C10-C9	-7.45	1.25	1.35
32	y	616	LUT	C4-C3	7.44	1.65	1.52
32	N	317	LUT	C32-C33	7.44	1.61	1.45
36	g	317	NEX	C30-C29	-7.44	1.25	1.35
32	S	318	LUT	C32-C33	7.42	1.61	1.45
36	N	318	NEX	C30-C29	-7.41	1.26	1.35
36	N	318	NEX	C34-C33	-7.41	1.26	1.35
32	3	317	LUT	C32-C33	7.41	1.61	1.45
32	6	318	LUT	C32-C33	7.39	1.61	1.45
36	p	618	NEX	C10-C9	-7.39	1.26	1.35
36	N	318	NEX	C10-C9	-7.39	1.26	1.35
32	N	316	LUT	C32-C33	7.39	1.61	1.45
43	C	614	BCR	C30-C25	-7.38	1.43	1.53
36	n	319	NEX	C14-C13	-7.37	1.26	1.35
36	6	319	NEX	C10-C9	-7.36	1.26	1.35
32	8	616	LUT	C32-C33	7.35	1.61	1.45
32	7	318	LUT	C32-C33	7.34	1.61	1.45
36	0	618	NEX	C10-C9	-7.33	1.26	1.35
32	n	318	LUT	C32-C33	7.33	1.61	1.45
43	c	615	BCR	C30-C25	-7.31	1.43	1.53
32	n	317	LUT	C32-C33	7.28	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	n	319	NEX	C10-C9	-7.27	1.26	1.35
32	8	615	LUT	C32-C33	7.27	1.61	1.45
32	s	317	LUT	C32-C33	7.27	1.61	1.45
32	S	317	LUT	C32-C33	7.26	1.61	1.45
32	6	317	LUT	C32-C33	7.25	1.61	1.45
32	s	318	LUT	C32-C33	7.25	1.61	1.45
36	n	319	NEX	C34-C33	-7.25	1.26	1.35
42	D	401	PHO	C3B-C4B	7.20	1.49	1.41
43	t	101	BCR	C2-C3	-7.19	1.34	1.52
32	0	617	LUT	C32-C33	7.19	1.61	1.45
32	R	317	LUT	C32-C33	7.19	1.61	1.45
36	n	319	NEX	C30-C29	-7.17	1.26	1.35
43	A	410	BCR	C30-C25	-7.15	1.43	1.53
43	h	101	BCR	C30-C25	-7.13	1.44	1.53
43	t	101	BCR	C30-C25	-7.11	1.44	1.53
43	B	619	BCR	C30-C25	-7.09	1.44	1.53
43	Z	101	BCR	C30-C25	-7.07	1.44	1.53
32	Y	316	LUT	C32-C33	7.06	1.61	1.45
32	1	616	LUT	C32-C33	7.06	1.61	1.45
43	B	617	BCR	C1-C6	-7.06	1.44	1.53
43	H	101	BCR	C30-C25	-7.05	1.44	1.53
43	b	620	BCR	C30-C25	-7.05	1.44	1.53
43	v	101	BCR	C30-C25	-7.05	1.44	1.53
32	0	616	LUT	C32-C33	7.05	1.61	1.45
43	c	615	BCR	C1-C6	-7.02	1.44	1.53
32	7	317	LUT	C32-C33	7.02	1.61	1.45
43	c	614	BCR	C30-C25	-7.00	1.44	1.53
43	T	101	BCR	C2-C3	-7.00	1.35	1.52
42	A	408	PHO	C3B-C4B	6.99	1.49	1.41
43	z	101	BCR	C1-C6	-6.98	1.44	1.53
32	y	617	LUT	C32-C33	6.98	1.60	1.45
36	3	319	NEX	C35-C15	-6.96	1.17	1.36
43	d	406	BCR	C2-C3	-6.96	1.35	1.52
43	D	405	BCR	C30-C25	-6.95	1.44	1.53
43	z	101	BCR	C30-C25	-6.95	1.44	1.53
43	C	615	BCR	C2-C3	-6.94	1.35	1.52
43	Z	101	BCR	C1-C6	-6.94	1.44	1.53
32	1	615	LUT	C32-C33	6.91	1.60	1.45
36	s	319	NEX	C35-C15	-6.91	1.18	1.36
36	9	319	NEX	C35-C15	-6.90	1.18	1.36
36	R	301	NEX	C35-C15	-6.90	1.18	1.36
43	B	618	BCR	C30-C25	-6.89	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	319	NEX	C35-C15	-6.88	1.18	1.36
43	Z	101	BCR	C2-C3	-6.87	1.35	1.52
43	T	101	BCR	C30-C25	-6.87	1.44	1.53
36	R	319	NEX	C35-C15	-6.86	1.18	1.36
43	C	614	BCR	C1-C6	-6.85	1.44	1.53
36	r	319	NEX	C35-C15	-6.85	1.18	1.36
32	Y	315	LUT	C32-C33	6.85	1.60	1.45
36	G	616	NEX	C35-C15	-6.85	1.18	1.36
43	C	615	BCR	C1-C6	-6.84	1.44	1.53
32	1	615	LUT	C1-C6	-6.83	1.44	1.53
43	B	619	BCR	C1-C6	-6.83	1.44	1.53
36	p	618	NEX	C35-C15	-6.83	1.18	1.36
43	z	101	BCR	C2-C3	-6.83	1.35	1.52
36	y	618	NEX	C35-C15	-6.82	1.18	1.36
32	y	616	LUT	C32-C33	6.82	1.60	1.45
36	6	319	NEX	C35-C15	-6.81	1.18	1.36
43	c	614	BCR	C2-C3	-6.81	1.35	1.52
43	V	101	BCR	C1-C6	-6.81	1.44	1.53
36	0	618	NEX	C35-C15	-6.81	1.18	1.36
32	Y	316	LUT	C1-C6	-6.81	1.44	1.53
43	h	101	BCR	C2-C3	-6.80	1.35	1.52
36	r	301	NEX	C35-C15	-6.80	1.18	1.36
43	B	617	BCR	C2-C3	-6.80	1.35	1.52
43	H	101	BCR	C2-C3	-6.79	1.35	1.52
35	g	315	RRX	C30-C25	-6.79	1.44	1.53
36	q	319	NEX	C35-C15	-6.79	1.18	1.36
32	r	317	LUT	C32-C33	6.79	1.60	1.45
36	8	617	NEX	C35-C15	-6.79	1.18	1.36
43	b	619	BCR	C1-C6	-6.79	1.44	1.53
36	2	616	NEX	C35-C15	-6.79	1.18	1.36
32	R	317	LUT	C1-C6	-6.79	1.44	1.53
43	b	619	BCR	C30-C25	-6.78	1.44	1.53
36	Y	317	NEX	C35-C15	-6.77	1.18	1.36
43	b	620	BCR	C2-C3	-6.77	1.35	1.52
36	5	618	NEX	C35-C15	-6.77	1.18	1.36
32	y	617	LUT	C1-C6	-6.76	1.44	1.53
43	b	620	BCR	C1-C6	-6.76	1.44	1.53
36	4	617	NEX	C35-C15	-6.76	1.18	1.36
43	B	619	BCR	C2-C3	-6.76	1.35	1.52
43	a	410	BCR	C2-C3	-6.76	1.35	1.52
43	v	101	BCR	C2-C3	-6.74	1.35	1.52
43	v	101	BCR	C1-C6	-6.74	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	b	618	BCR	C2-C3	-6.73	1.35	1.52
43	C	615	BCR	C29-C28	-6.73	1.35	1.52
43	A	410	BCR	C2-C3	-6.73	1.35	1.52
36	g	317	NEX	C35-C15	-6.72	1.18	1.36
43	a	410	BCR	C30-C25	-6.72	1.44	1.53
36	N	318	NEX	C35-C15	-6.72	1.18	1.36
43	V	101	BCR	C2-C3	-6.71	1.36	1.52
36	n	319	NEX	C35-C15	-6.70	1.18	1.36
32	0	617	LUT	C1-C6	-6.70	1.44	1.53
43	D	405	BCR	C2-C3	-6.69	1.36	1.52
43	C	614	BCR	C2-C3	-6.69	1.36	1.52
43	h	101	BCR	C1-C6	-6.67	1.44	1.53
32	7	317	LUT	C1-C6	-6.67	1.44	1.53
32	y	616	LUT	C1-C6	-6.67	1.44	1.53
43	a	410	BCR	C1-C6	-6.67	1.44	1.53
43	c	615	BCR	C2-C3	-6.63	1.36	1.52
35	q	317	RRX	C2-C3	-6.62	1.36	1.52
43	B	618	BCR	C2-C3	-6.62	1.36	1.52
32	2	615	LUT	C1-C6	-6.60	1.44	1.53
32	3	318	LUT	C1-C6	-6.60	1.44	1.53
32	8	616	LUT	C1-C6	-6.60	1.44	1.53
32	0	616	LUT	C1-C6	-6.60	1.44	1.53
32	r	317	LUT	C1-C6	-6.59	1.44	1.53
32	N	317	LUT	C1-C6	-6.59	1.44	1.53
32	Y	315	LUT	C1-C6	-6.59	1.44	1.53
43	B	617	BCR	C29-C28	-6.57	1.36	1.52
43	b	619	BCR	C2-C3	-6.57	1.36	1.52
43	H	101	BCR	C1-C6	-6.56	1.44	1.53
43	a	410	BCR	C29-C28	-6.56	1.36	1.52
43	d	406	BCR	C29-C28	-6.55	1.36	1.52
32	n	318	LUT	C1-C6	-6.54	1.44	1.53
43	z	101	BCR	C29-C28	-6.52	1.36	1.52
43	Z	101	BCR	C29-C28	-6.51	1.36	1.52
43	A	410	BCR	C1-C6	-6.50	1.44	1.53
35	2	614	RRX	C2-C3	-6.50	1.36	1.52
43	c	614	BCR	C29-C28	-6.50	1.36	1.52
35	G	614	RRX	C2-C3	-6.50	1.36	1.52
31	B	604	CLA	MG-NA	6.48	2.21	2.06
43	t	101	BCR	C1-C6	-6.48	1.44	1.53
36	9	319	NEX	C11-C12	-6.47	1.17	1.34
43	B	618	BCR	C29-C28	-6.47	1.36	1.52
36	s	319	NEX	C11-C12	-6.47	1.17	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	9	317	RRX	C2-C3	-6.46	1.36	1.52
32	1	616	LUT	C1-C6	-6.46	1.44	1.53
35	4	615	RRX	C2-C3	-6.46	1.36	1.52
32	g	316	LUT	C1-C6	-6.46	1.44	1.53
31	b	605	CLA	MG-NA	6.46	2.21	2.06
31	5	615	CLA	MG-NA	6.46	2.21	2.06
35	g	315	RRX	C2-C3	-6.45	1.36	1.52
32	q	318	LUT	C1-C6	-6.45	1.44	1.53
43	b	619	BCR	C29-C28	-6.45	1.36	1.52
36	9	319	NEX	C31-C32	-6.45	1.18	1.34
43	b	618	BCR	C1-C6	-6.44	1.44	1.53
43	B	619	BCR	C29-C28	-6.43	1.36	1.52
43	B	618	BCR	C1-C6	-6.43	1.44	1.53
32	p	617	LUT	C1-C6	-6.43	1.44	1.53
43	h	101	BCR	C29-C28	-6.42	1.36	1.52
36	3	319	NEX	C11-C12	-6.42	1.18	1.34
43	T	101	BCR	C1-C6	-6.42	1.45	1.53
36	S	319	NEX	C11-C12	-6.41	1.18	1.34
36	s	319	NEX	C31-C32	-6.41	1.18	1.34
35	2	614	RRX	C30-C25	-6.40	1.45	1.53
36	G	616	NEX	C31-C32	-6.40	1.18	1.34
36	R	301	NEX	C11-C12	-6.39	1.18	1.34
36	y	618	NEX	C11-C12	-6.39	1.18	1.34
36	p	618	NEX	C11-C12	-6.39	1.18	1.34
32	6	317	LUT	C1-C6	-6.39	1.45	1.53
43	H	101	BCR	C29-C28	-6.39	1.36	1.52
43	b	620	BCR	C29-C28	-6.39	1.36	1.52
32	s	318	LUT	C1-C6	-6.39	1.45	1.53
32	N	316	LUT	C1-C6	-6.38	1.45	1.53
31	G	610	CLA	MG-NA	6.38	2.21	2.06
36	4	617	NEX	C11-C12	-6.38	1.18	1.34
36	g	317	NEX	C11-C12	-6.38	1.18	1.34
32	6	318	LUT	C1-C6	-6.37	1.45	1.53
43	T	101	BCR	C29-C28	-6.37	1.36	1.52
31	g	311	CLA	MG-NA	6.37	2.21	2.06
36	S	319	NEX	C31-C32	-6.37	1.18	1.34
31	2	604	CLA	MG-NA	6.37	2.21	2.06
43	d	406	BCR	C1-C6	-6.37	1.45	1.53
32	S	317	LUT	C1-C6	-6.37	1.45	1.53
32	4	616	LUT	C1-C6	-6.36	1.45	1.53
36	2	616	NEX	C11-C12	-6.36	1.18	1.34
36	6	319	NEX	C11-C12	-6.36	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	t	101	BCR	C29-C28	-6.36	1.36	1.52
43	v	101	BCR	C29-C28	-6.36	1.36	1.52
36	R	319	NEX	C11-C12	-6.36	1.18	1.34
36	R	319	NEX	C31-C32	-6.35	1.18	1.34
32	7	318	LUT	C1-C6	-6.35	1.45	1.53
36	y	618	NEX	C31-C32	-6.35	1.18	1.34
31	6	304	CLA	MG-NA	6.35	2.21	2.06
36	0	618	NEX	C11-C12	-6.35	1.18	1.34
36	G	616	NEX	C11-C12	-6.35	1.18	1.34
32	S	318	LUT	C1-C6	-6.34	1.45	1.53
36	0	618	NEX	C31-C32	-6.34	1.18	1.34
36	3	319	NEX	C31-C32	-6.34	1.18	1.34
36	r	319	NEX	C31-C32	-6.34	1.18	1.34
36	6	319	NEX	C31-C32	-6.33	1.18	1.34
31	G	613	CLA	MG-NA	6.33	2.21	2.06
36	5	618	NEX	C11-C12	-6.33	1.18	1.34
32	5	617	LUT	C1-C6	-6.33	1.45	1.53
35	G	614	RRX	C30-C25	-6.33	1.45	1.53
43	A	410	BCR	C29-C28	-6.32	1.37	1.52
31	q	304	CLA	MG-NA	6.32	2.21	2.06
36	Y	317	NEX	C11-C12	-6.32	1.18	1.34
36	p	618	NEX	C31-C32	-6.32	1.18	1.34
31	6	312	CLA	MG-NA	6.32	2.21	2.06
36	r	319	NEX	C11-C12	-6.32	1.18	1.34
31	q	316	CLA	MG-NA	6.31	2.21	2.06
35	4	615	RRX	C30-C25	-6.31	1.45	1.53
31	2	609	CLA	MG-NA	6.31	2.21	2.06
31	Y	313	CLA	MG-NA	6.31	2.21	2.06
31	S	314	CLA	MG-NA	6.31	2.21	2.06
36	2	616	NEX	C31-C32	-6.31	1.18	1.34
35	q	317	RRX	C30-C25	-6.30	1.45	1.53
43	c	615	BCR	C29-C28	-6.30	1.37	1.52
31	b	607	CLA	MG-NA	6.30	2.21	2.06
36	Y	317	NEX	C31-C32	-6.30	1.18	1.34
32	s	317	LUT	C1-C6	-6.30	1.45	1.53
31	4	603	CLA	MG-NA	6.30	2.21	2.06
31	7	314	CLA	MG-NA	6.30	2.21	2.06
31	p	612	CLA	MG-NA	6.30	2.21	2.06
36	8	617	NEX	C31-C32	-6.30	1.18	1.34
31	0	603	CLA	MG-NA	6.30	2.21	2.06
31	9	315	CLA	MG-NA	6.29	2.21	2.06
31	5	612	CLA	MG-NA	6.29	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	b	618	BCR	C29-C28	-6.29	1.37	1.52
31	B	606	CLA	MG-NA	6.29	2.21	2.06
32	p	616	LUT	C1-C6	-6.29	1.45	1.53
43	D	405	BCR	C1-C6	-6.29	1.45	1.53
31	n	314	CLA	MG-NA	6.29	2.21	2.06
36	5	618	NEX	C31-C32	-6.29	1.18	1.34
31	N	311	CLA	MG-NA	6.29	2.21	2.06
32	9	318	LUT	C1-C6	-6.29	1.45	1.53
31	7	304	CLA	MG-NA	6.29	2.21	2.06
31	3	305	CLA	MG-NA	6.29	2.21	2.06
36	8	617	NEX	C11-C12	-6.28	1.18	1.34
31	9	305	CLA	MG-NA	6.28	2.21	2.06
36	N	318	NEX	C31-C32	-6.28	1.18	1.34
31	7	313	CLA	MG-NA	6.28	2.21	2.06
31	N	313	CLA	MG-NA	6.28	2.21	2.06
31	8	612	CLA	MG-NA	6.27	2.21	2.06
36	r	301	NEX	C31-C32	-6.27	1.18	1.34
31	3	315	CLA	MG-NA	6.27	2.21	2.06
31	5	603	CLA	MG-NA	6.27	2.21	2.06
31	9	313	CLA	MG-NA	6.27	2.21	2.06
32	G	615	LUT	C1-C6	-6.27	1.45	1.53
31	4	604	CLA	MG-NA	6.27	2.21	2.06
35	9	317	RRX	C30-C25	-6.27	1.45	1.53
43	c	614	BCR	C1-C6	-6.27	1.45	1.53
36	R	301	NEX	C31-C32	-6.27	1.18	1.34
31	Y	304	CLA	MG-NA	6.27	2.21	2.06
31	q	305	CLA	MG-NA	6.27	2.21	2.06
31	4	611	CLA	MG-NA	6.27	2.21	2.06
31	5	602	CLA	MG-NA	6.27	2.21	2.06
31	G	611	CLA	MG-NA	6.27	2.21	2.06
31	0	613	CLA	MG-NA	6.26	2.21	2.06
31	b	611	CLA	MG-NA	6.26	2.21	2.06
31	R	307	CLA	MG-NA	6.26	2.21	2.06
31	n	315	CLA	MG-NA	6.26	2.21	2.06
31	s	304	CLA	MG-NA	6.26	2.21	2.06
31	0	612	CLA	MG-NA	6.26	2.21	2.06
31	p	611	CLA	MG-NA	6.26	2.21	2.06
31	3	313	CLA	MG-NA	6.26	2.21	2.06
31	8	613	CLA	MG-NA	6.26	2.21	2.06
31	s	314	CLA	MG-NA	6.26	2.21	2.06
31	g	313	CLA	MG-NA	6.25	2.21	2.06
36	4	617	NEX	C31-C32	-6.25	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	614	CLA	MG-NA	6.25	2.21	2.06
31	c	601	CLA	MG-NA	6.25	2.21	2.06
31	0	614	CLA	MG-NA	6.25	2.21	2.06
31	1	613	CLA	MG-NA	6.25	2.21	2.06
43	D	405	BCR	C29-C28	-6.25	1.37	1.52
31	p	602	CLA	MG-NA	6.25	2.21	2.06
31	1	612	CLA	MG-NA	6.25	2.21	2.06
31	6	314	CLA	MG-NA	6.25	2.21	2.06
31	G	602	CLA	MG-NA	6.24	2.21	2.06
31	9	316	CLA	MG-NA	6.24	2.21	2.06
31	p	610	CLA	MG-NA	6.24	2.21	2.06
31	2	602	CLA	MG-NA	6.24	2.21	2.06
43	C	614	BCR	C29-C28	-6.24	1.37	1.52
31	3	312	CLA	MG-NA	6.24	2.21	2.06
31	S	316	CLA	MG-NA	6.24	2.21	2.06
31	0	611	CLA	MG-NA	6.24	2.21	2.06
31	3	304	CLA	MG-NA	6.23	2.21	2.06
31	y	603	CLA	MG-NA	6.23	2.21	2.06
31	2	603	CLA	MG-NA	6.23	2.21	2.06
31	S	310	CLA	MG-NA	6.23	2.21	2.06
31	1	603	CLA	MG-NA	6.23	2.21	2.06
31	7	303	CLA	MG-NA	6.23	2.21	2.06
31	n	312	CLA	MG-NA	6.23	2.21	2.06
31	B	611	CLA	MG-NA	6.23	2.21	2.06
31	5	613	CLA	MG-NA	6.23	2.21	2.06
31	g	305	CLA	MG-NA	6.23	2.21	2.06
31	8	603	CLA	MG-NA	6.23	2.21	2.06
31	y	614	CLA	MG-NA	6.23	2.21	2.06
31	4	610	CLA	MG-NA	6.23	2.21	2.06
31	8	602	CLA	MG-NA	6.23	2.21	2.06
31	4	602	CLA	MG-NA	6.23	2.21	2.06
36	g	317	NEX	C31-C32	-6.23	1.18	1.34
36	r	301	NEX	C11-C12	-6.23	1.18	1.34
31	s	312	CLA	MG-NA	6.23	2.21	2.06
31	3	314	CLA	MG-NA	6.23	2.21	2.06
31	G	612	CLA	MG-NA	6.22	2.21	2.06
31	r	307	CLA	MG-NA	6.22	2.21	2.06
31	Y	303	CLA	MG-NA	6.22	2.21	2.06
31	n	313	CLA	MG-NA	6.22	2.21	2.06
31	C	603	CLA	MG-NA	6.22	2.21	2.06
31	b	609	CLA	MG-NA	6.22	2.21	2.06
31	S	306	CLA	MG-NA	6.22	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	8	615	LUT	C1-C6	-6.22	1.45	1.53
31	8	609	CLA	MG-NA	6.22	2.21	2.06
31	Y	310	CLA	MG-NA	6.22	2.21	2.06
31	s	306	CLA	MG-NA	6.21	2.21	2.06
31	b	612	CLA	MG-NA	6.21	2.21	2.06
31	5	611	CLA	MG-NA	6.21	2.21	2.06
36	q	319	NEX	C31-C32	-6.21	1.18	1.34
31	N	314	CLA	MG-NA	6.21	2.21	2.06
31	Y	312	CLA	MG-NA	6.21	2.21	2.06
31	c	603	CLA	MG-NA	6.21	2.21	2.06
31	g	314	CLA	MG-NA	6.21	2.21	2.06
31	n	311	CLA	MG-NA	6.21	2.21	2.06
31	7	311	CLA	MG-NA	6.21	2.21	2.06
31	8	610	CLA	MG-NA	6.21	2.21	2.06
31	7	316	CLA	MG-NA	6.21	2.21	2.06
31	p	603	CLA	MG-NA	6.21	2.21	2.06
31	7	315	CLA	MG-NA	6.21	2.21	2.06
35	q	317	RRX	C1-C6	-6.21	1.45	1.53
36	q	319	NEX	C11-C12	-6.21	1.18	1.34
31	s	316	CLA	MG-NA	6.21	2.21	2.06
31	5	604	CLA	MG-NA	6.21	2.21	2.06
31	N	312	CLA	MG-NA	6.21	2.21	2.06
31	7	312	CLA	MG-NA	6.21	2.21	2.06
31	4	614	CLA	MG-NA	6.20	2.21	2.06
31	N	315	CLA	MG-NA	6.20	2.21	2.06
31	b	614	CLA	MG-NA	6.20	2.21	2.06
31	6	316	CLA	MG-NA	6.20	2.21	2.06
31	B	614	CLA	MG-NA	6.20	2.21	2.06
31	S	304	CLA	MG-NA	6.20	2.21	2.06
31	8	614	CLA	MG-NA	6.20	2.21	2.06
31	2	610	CLA	MG-NA	6.20	2.21	2.06
31	1	614	CLA	MG-NA	6.20	2.21	2.06
31	1	611	CLA	MG-NA	6.20	2.21	2.06
32	n	317	LUT	C1-C6	-6.20	1.45	1.53
31	g	312	CLA	MG-NA	6.20	2.21	2.06
31	8	604	CLA	MG-NA	6.20	2.21	2.06
31	r	313	CLA	MG-NA	6.20	2.21	2.06
31	s	303	CLA	MG-NA	6.20	2.21	2.06
31	C	611	CLA	MG-NA	6.19	2.21	2.06
31	9	306	CLA	MG-NA	6.19	2.21	2.06
31	3	311	CLA	MG-NA	6.19	2.21	2.06
31	N	304	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	303	CLA	MG-NA	6.19	2.21	2.06
31	b	603	CLA	MG-NA	6.19	2.21	2.06
31	y	602	CLA	MG-NA	6.19	2.21	2.06
31	S	305	CLA	MG-NA	6.19	2.21	2.06
32	3	317	LUT	C1-C6	-6.19	1.45	1.53
31	8	611	CLA	MG-NA	6.19	2.21	2.06
31	n	303	CLA	MG-NA	6.19	2.21	2.06
31	C	601	CLA	MG-NA	6.19	2.21	2.06
31	p	614	CLA	MG-NA	6.19	2.21	2.06
36	n	319	NEX	C11-C12	-6.18	1.18	1.34
31	B	610	CLA	MG-NA	6.18	2.21	2.06
31	p	604	CLA	MG-NA	6.18	2.21	2.06
31	N	321	CLA	MG-NA	6.18	2.21	2.06
31	y	610	CLA	MG-NA	6.18	2.21	2.06
31	3	306	CLA	MG-NA	6.18	2.21	2.06
31	N	310	CLA	MG-NA	6.18	2.20	2.06
31	q	312	CLA	MG-NA	6.18	2.20	2.06
31	2	613	CLA	MG-NA	6.18	2.20	2.06
31	2	612	CLA	MG-NA	6.18	2.20	2.06
31	a	407	CLA	MG-NA	6.18	2.20	2.06
31	6	313	CLA	MG-NA	6.18	2.20	2.06
31	G	603	CLA	MG-NA	6.17	2.20	2.06
35	2	614	RRX	C1-C6	-6.17	1.45	1.53
31	R	303	CLA	MG-NA	6.17	2.20	2.06
31	y	604	CLA	MG-NA	6.17	2.20	2.06
31	B	613	CLA	MG-NA	6.17	2.20	2.06
31	b	613	CLA	MG-NA	6.17	2.20	2.06
31	6	311	CLA	MG-NA	6.17	2.20	2.06
31	b	604	CLA	MG-NA	6.17	2.20	2.06
31	R	306	CLA	MG-NA	6.17	2.20	2.06
31	R	313	CLA	MG-NA	6.17	2.20	2.06
31	b	615	CLA	MG-NA	6.17	2.20	2.06
31	r	314	CLA	MG-NA	6.17	2.20	2.06
31	Y	314	CLA	MG-NA	6.17	2.20	2.06
31	c	602	CLA	MG-NA	6.17	2.20	2.06
31	s	310	CLA	MG-NA	6.17	2.20	2.06
31	6	303	CLA	MG-NA	6.17	2.20	2.06
31	S	313	CLA	MG-NA	6.17	2.20	2.06
31	n	305	CLA	MG-NA	6.17	2.20	2.06
31	4	613	CLA	MG-NA	6.16	2.20	2.06
31	g	304	CLA	MG-NA	6.16	2.20	2.06
31	s	305	CLA	MG-NA	6.16	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	303	CLA	MG-NA	6.16	2.20	2.06
31	0	615	CLA	MG-NA	6.16	2.20	2.06
31	1	602	CLA	MG-NA	6.16	2.20	2.06
31	n	316	CLA	MG-NA	6.15	2.20	2.06
31	Y	311	CLA	MG-NA	6.15	2.20	2.06
31	B	608	CLA	MG-NA	6.15	2.20	2.06
31	Y	305	CLA	MG-NA	6.14	2.20	2.06
31	5	610	CLA	MG-NA	6.14	2.20	2.06
31	G	604	CLA	MG-NA	6.14	2.20	2.06
31	N	305	CLA	MG-NA	6.14	2.20	2.06
31	r	305	CLA	MG-NA	6.14	2.20	2.06
31	s	313	CLA	MG-NA	6.14	2.20	2.06
31	y	615	CLA	MG-NA	6.14	2.20	2.06
36	n	319	NEX	C31-C32	-6.14	1.18	1.34
31	c	611	CLA	MG-NA	6.14	2.20	2.06
31	y	612	CLA	MG-NA	6.13	2.20	2.06
31	n	304	CLA	MG-NA	6.13	2.20	2.06
31	6	315	CLA	MG-NA	6.13	2.20	2.06
31	c	607	CLA	MG-NA	6.13	2.20	2.06
31	2	611	CLA	MG-NA	6.13	2.20	2.06
31	B	612	CLA	MG-NA	6.13	2.20	2.06
43	V	101	BCR	C29-C28	-6.13	1.37	1.52
31	b	617	CLA	MG-NA	6.12	2.20	2.06
35	9	317	RRX	C19-C18	6.12	1.59	1.45
31	r	316	CLA	MG-NA	6.12	2.20	2.06
31	B	601	CLA	MG-NA	6.12	2.20	2.06
31	S	315	CLA	MG-NA	6.12	2.20	2.06
31	p	615	CLA	MG-NA	6.12	2.20	2.06
31	6	305	CLA	MG-NA	6.12	2.20	2.06
31	C	602	CLA	MG-NA	6.11	2.20	2.06
31	7	305	CLA	MG-NA	6.11	2.20	2.06
35	4	615	RRX	C19-C18	6.11	1.59	1.45
31	C	612	CLA	MG-NA	6.11	2.20	2.06
31	C	607	CLA	MG-NA	6.11	2.20	2.06
31	0	602	CLA	MG-NA	6.11	2.20	2.06
31	S	312	CLA	MG-NA	6.11	2.20	2.06
35	4	615	RRX	C1-C6	-6.11	1.45	1.53
31	9	304	CLA	MG-NA	6.11	2.20	2.06
31	B	602	CLA	MG-NA	6.10	2.20	2.06
31	c	608	CLA	MG-NA	6.10	2.20	2.06
31	b	610	CLA	MG-NA	6.10	2.20	2.06
35	9	317	RRX	C1-C6	-6.10	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	609	CLA	MG-NA	6.10	2.20	2.06
31	q	306	CLA	MG-NA	6.10	2.20	2.06
31	r	304	CLA	MG-NA	6.10	2.20	2.06
31	r	306	CLA	MG-NA	6.10	2.20	2.06
31	p	613	CLA	MG-NA	6.09	2.20	2.06
31	d	405	CLA	MG-NA	6.09	2.20	2.06
31	C	606	CLA	MG-NA	6.09	2.20	2.06
31	C	613	CLA	MG-NA	6.09	2.20	2.06
31	b	616	CLA	MG-NA	6.09	2.20	2.06
31	B	603	CLA	MG-NA	6.09	2.20	2.06
31	R	314	CLA	MG-NA	6.09	2.20	2.06
36	N	318	NEX	C11-C12	-6.08	1.18	1.34
35	G	614	RRX	C1-C6	-6.08	1.45	1.53
31	s	315	CLA	MG-NA	6.08	2.20	2.06
31	B	616	CLA	MG-NA	6.08	2.20	2.06
31	1	610	CLA	MG-NA	6.08	2.20	2.06
31	B	615	CLA	MG-NA	6.08	2.20	2.06
31	S	311	CLA	MG-NA	6.08	2.20	2.06
31	R	305	CLA	MG-NA	6.07	2.20	2.06
31	y	611	CLA	MG-NA	6.07	2.20	2.06
31	s	311	CLA	MG-NA	6.07	2.20	2.06
31	C	610	CLA	MG-NA	6.07	2.20	2.06
31	c	613	CLA	MG-NA	6.07	2.20	2.06
31	c	612	CLA	MG-NA	6.07	2.20	2.06
35	G	614	RRX	C19-C18	6.06	1.59	1.45
31	B	609	CLA	MG-NA	6.06	2.20	2.06
31	R	304	CLA	MG-NA	6.06	2.20	2.06
31	c	605	CLA	MG-NA	6.06	2.20	2.06
31	q	314	CLA	MG-NA	6.05	2.20	2.06
31	C	609	CLA	MG-NA	6.05	2.20	2.06
31	B	605	CLA	MG-NA	6.05	2.20	2.06
31	C	604	CLA	MG-NA	6.05	2.20	2.06
31	D	403	CLA	MG-NA	6.04	2.20	2.06
31	R	312	CLA	MG-NA	6.04	2.20	2.06
31	d	401	CLA	MG-NA	6.04	2.20	2.06
31	R	316	CLA	MG-NA	6.04	2.20	2.06
31	c	606	CLA	MG-NA	6.04	2.20	2.06
35	2	614	RRX	C19-C18	6.04	1.58	1.45
31	g	310	CLA	MG-NA	6.03	2.20	2.06
32	5	616	LUT	C1-C6	-6.03	1.45	1.53
31	A	406	CLA	MG-NA	6.03	2.20	2.06
31	a	406	CLA	MG-NA	6.03	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	608	CLA	MG-NA	6.02	2.20	2.06
31	b	606	CLA	MG-NA	6.02	2.20	2.06
31	b	608	CLA	MG-NA	6.02	2.20	2.06
31	0	604	CLA	MG-NA	6.01	2.20	2.06
31	b	602	CLA	MG-NA	6.01	2.20	2.06
35	g	315	RRX	C19-C18	6.01	1.58	1.45
31	R	315	CLA	MG-NA	6.01	2.20	2.06
35	g	315	RRX	C1-C6	-6.00	1.45	1.53
31	c	610	CLA	MG-NA	6.00	2.20	2.06
31	D	404	CLA	MG-NA	6.00	2.20	2.06
31	d	404	CLA	MG-NA	6.00	2.20	2.06
31	R	311	CLA	MG-NA	5.99	2.20	2.06
31	G	609	CLA	MG-NA	5.99	2.20	2.06
31	0	610	CLA	MG-NA	5.99	2.20	2.06
31	A	405	CLA	MG-NA	5.98	2.20	2.06
31	A	407	CLA	MG-NA	5.96	2.20	2.06
31	r	312	CLA	MG-NA	5.96	2.20	2.06
31	1	604	CLA	MG-NA	5.96	2.20	2.06
31	y	613	CLA	MG-NA	5.95	2.20	2.06
31	c	604	CLA	MG-NA	5.95	2.20	2.06
31	r	315	CLA	MG-NA	5.93	2.20	2.06
31	3	301	CLA	MG-NA	5.92	2.20	2.06
31	g	303	CLA	MG-NA	5.90	2.20	2.06
31	A	409	CLA	MG-NA	5.88	2.20	2.06
31	9	314	CLA	MG-NA	5.88	2.20	2.06
31	3	316	CLA	MG-NA	5.88	2.20	2.06
31	r	311	CLA	MG-NA	5.88	2.20	2.06
31	q	313	CLA	MG-NA	5.88	2.20	2.06
31	a	409	CLA	MG-NA	5.86	2.20	2.06
31	4	612	CLA	MG-NA	5.86	2.20	2.06
31	r	303	CLA	MG-NA	5.84	2.20	2.06
43	c	614	BCR	C12-C13	5.82	1.58	1.45
43	D	405	BCR	C12-C13	5.82	1.58	1.45
31	B	607	CLA	MG-NA	5.82	2.20	2.06
31	q	315	CLA	MG-NA	5.81	2.20	2.06
31	9	312	CLA	MG-NA	5.80	2.20	2.06
43	T	101	BCR	C12-C13	5.74	1.58	1.45
31	C	605	CLA	MG-NA	5.69	2.19	2.06
35	q	317	RRX	C19-C18	5.67	1.58	1.45
43	c	615	BCR	C12-C13	5.66	1.58	1.45
36	p	618	NEX	C7-C8	5.56	1.41	1.32
43	v	101	BCR	C12-C13	5.56	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	y	618	NEX	C28-C29	-5.56	1.34	1.45
43	A	410	BCR	C12-C13	5.54	1.57	1.45
43	D	405	BCR	C8-C9	5.54	1.57	1.45
36	0	618	NEX	C28-C29	-5.54	1.34	1.45
36	r	319	NEX	C28-C29	-5.54	1.34	1.45
43	z	101	BCR	C12-C13	5.53	1.57	1.45
36	6	319	NEX	C28-C29	-5.53	1.34	1.45
36	N	318	NEX	C7-C8	5.53	1.41	1.32
43	B	619	BCR	C12-C13	5.53	1.57	1.45
36	R	319	NEX	C28-C29	-5.53	1.34	1.45
36	q	319	NEX	C28-C29	-5.52	1.34	1.45
36	s	319	NEX	C28-C29	-5.52	1.34	1.45
36	S	319	NEX	C28-C29	-5.52	1.34	1.45
43	C	614	BCR	C12-C13	5.52	1.57	1.45
43	H	101	BCR	C12-C13	5.50	1.57	1.45
36	9	319	NEX	C28-C29	-5.49	1.34	1.45
43	b	618	BCR	C12-C13	5.48	1.57	1.45
36	2	616	NEX	C28-C29	-5.48	1.34	1.45
43	V	101	BCR	C12-C13	5.47	1.57	1.45
36	r	301	NEX	C28-C29	-5.47	1.34	1.45
43	Z	101	BCR	C12-C13	5.47	1.57	1.45
36	4	617	NEX	C28-C29	-5.47	1.34	1.45
36	3	319	NEX	C28-C29	-5.45	1.34	1.45
36	5	618	NEX	C28-C29	-5.45	1.34	1.45
43	b	620	BCR	C12-C13	5.44	1.57	1.45
36	n	319	NEX	C7-C8	5.44	1.41	1.32
36	G	616	NEX	C28-C29	-5.44	1.34	1.45
36	8	617	NEX	C28-C29	-5.44	1.34	1.45
43	C	615	BCR	C12-C13	5.42	1.57	1.45
36	R	301	NEX	C28-C29	-5.41	1.34	1.45
36	Y	317	NEX	C28-C29	-5.41	1.34	1.45
43	h	101	BCR	C12-C13	5.40	1.57	1.45
36	q	319	NEX	C7-C8	5.40	1.41	1.32
36	p	618	NEX	C28-C29	-5.39	1.34	1.45
43	t	101	BCR	C12-C13	5.39	1.57	1.45
36	g	317	NEX	C28-C29	-5.38	1.34	1.45
36	N	318	NEX	C28-C29	-5.38	1.34	1.45
43	b	619	BCR	C12-C13	5.37	1.57	1.45
43	B	618	BCR	C12-C13	5.35	1.57	1.45
36	S	319	NEX	C7-C8	5.33	1.40	1.32
43	c	614	BCR	C8-C9	5.33	1.57	1.45
43	c	615	BCR	C8-C9	5.33	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	D	405	BCR	C23-C22	5.32	1.57	1.45
43	a	410	BCR	C12-C13	5.31	1.57	1.45
36	r	301	NEX	C7-C8	5.31	1.40	1.32
36	Y	317	NEX	C7-C8	5.31	1.40	1.32
36	s	319	NEX	C7-C8	5.30	1.40	1.32
43	t	101	BCR	C29-C30	5.30	1.66	1.54
43	v	101	BCR	C8-C9	5.29	1.57	1.45
36	3	319	NEX	C7-C8	5.28	1.40	1.32
43	T	101	BCR	C8-C9	5.28	1.57	1.45
47	E	101	HEM	FE-NB	5.27	2.11	1.94
36	n	319	NEX	C28-C29	-5.27	1.34	1.45
36	8	617	NEX	C7-C8	5.25	1.40	1.32
36	r	319	NEX	C7-C8	5.24	1.40	1.32
43	d	406	BCR	C12-C13	5.24	1.57	1.45
43	V	101	BCR	C8-C9	5.24	1.57	1.45
36	0	618	NEX	C7-C8	5.24	1.40	1.32
36	6	319	NEX	C7-C8	5.23	1.40	1.32
43	V	101	BCR	C29-C30	5.23	1.66	1.54
43	B	617	BCR	C12-C13	5.22	1.57	1.45
47	e	102	HEM	FE-NB	5.21	2.11	1.94
36	y	618	NEX	C7-C8	5.20	1.40	1.32
36	5	618	NEX	C7-C8	5.19	1.40	1.32
43	b	619	BCR	C23-C22	5.19	1.57	1.45
43	b	618	BCR	C8-C9	5.18	1.57	1.45
43	b	619	BCR	C8-C9	5.18	1.57	1.45
43	A	410	BCR	C8-C9	5.18	1.57	1.45
36	R	319	NEX	C7-C8	5.16	1.40	1.32
43	D	405	BCR	C29-C30	5.16	1.66	1.54
43	T	101	BCR	C29-C30	5.15	1.66	1.54
43	B	618	BCR	C8-C9	5.15	1.57	1.45
43	B	619	BCR	C8-C9	5.15	1.57	1.45
36	g	317	NEX	C7-C8	5.14	1.40	1.32
43	b	620	BCR	C23-C22	5.13	1.57	1.45
36	4	617	NEX	C7-C8	5.11	1.40	1.32
43	z	101	BCR	C8-C9	5.10	1.56	1.45
36	2	616	NEX	C7-C8	5.10	1.40	1.32
43	c	615	BCR	C23-C22	5.10	1.56	1.45
43	H	101	BCR	C29-C30	5.09	1.65	1.54
43	v	101	BCR	C23-C22	5.09	1.56	1.45
35	q	317	RRX	C8-C9	5.09	1.56	1.45
43	h	101	BCR	C29-C30	5.09	1.65	1.54
32	p	616	LUT	C8-C9	5.08	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	G	614	RRX	C8-C9	5.07	1.56	1.45
35	4	615	RRX	C8-C9	5.07	1.56	1.45
32	5	617	LUT	C8-C9	5.07	1.56	1.45
35	9	317	RRX	C8-C9	5.06	1.56	1.45
43	v	101	BCR	C29-C30	5.06	1.65	1.54
32	5	616	LUT	C8-C9	5.05	1.56	1.45
35	g	315	RRX	C8-C9	5.05	1.56	1.45
43	a	410	BCR	C8-C9	5.04	1.56	1.45
43	C	614	BCR	C8-C9	5.04	1.56	1.45
43	H	101	BCR	C8-C9	5.04	1.56	1.45
43	C	614	BCR	C29-C30	5.03	1.65	1.54
43	B	618	BCR	C23-C22	5.03	1.56	1.45
32	9	318	LUT	C8-C9	5.02	1.56	1.45
43	B	619	BCR	C23-C22	5.01	1.56	1.45
43	T	101	BCR	C23-C22	5.01	1.56	1.45
43	b	620	BCR	C8-C9	5.01	1.56	1.45
43	B	618	BCR	C29-C30	5.01	1.65	1.54
43	H	101	BCR	C23-C22	5.00	1.56	1.45
43	A	410	BCR	C23-C22	5.00	1.56	1.45
43	A	410	BCR	C29-C30	4.99	1.65	1.54
43	c	615	BCR	C29-C30	4.99	1.65	1.54
43	d	406	BCR	C8-C9	4.99	1.56	1.45
32	3	318	LUT	C8-C9	4.98	1.56	1.45
32	G	615	LUT	C8-C9	4.98	1.56	1.45
43	b	620	BCR	C29-C30	4.98	1.65	1.54
35	2	614	RRX	C8-C9	4.98	1.56	1.45
43	b	619	BCR	C29-C30	4.98	1.65	1.54
36	9	319	NEX	C7-C8	4.97	1.40	1.32
43	b	618	BCR	C29-C30	4.97	1.65	1.54
36	R	301	NEX	C7-C8	4.97	1.40	1.32
43	B	619	BCR	C29-C30	4.97	1.65	1.54
43	a	410	BCR	C29-C30	4.97	1.65	1.54
32	g	316	LUT	C8-C9	4.97	1.56	1.45
32	2	615	LUT	C8-C9	4.96	1.56	1.45
43	B	617	BCR	C8-C9	4.96	1.56	1.45
32	q	318	LUT	C8-C9	4.96	1.56	1.45
32	p	617	LUT	C8-C9	4.95	1.56	1.45
43	h	101	BCR	C8-C9	4.94	1.56	1.45
43	t	101	BCR	C8-C9	4.94	1.56	1.45
43	a	410	BCR	C23-C22	4.93	1.56	1.45
43	d	406	BCR	C29-C30	4.93	1.65	1.54
32	3	317	LUT	C8-C9	4.93	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	616	LUT	C4-C5	-4.93	1.43	1.51
36	G	616	NEX	C7-C8	4.93	1.40	1.32
35	g	315	RRX	C2-C1	4.91	1.65	1.54
43	z	101	BCR	C29-C30	4.91	1.65	1.54
32	Y	315	LUT	C4-C5	-4.91	1.43	1.51
43	h	101	BCR	C23-C22	4.91	1.56	1.45
35	4	615	RRX	C23-C22	4.90	1.56	1.45
43	Z	101	BCR	C8-C9	4.88	1.56	1.45
35	9	317	RRX	C23-C22	4.88	1.56	1.45
43	D	405	BCR	C15-C14	4.88	1.58	1.43
32	S	318	LUT	C8-C9	4.88	1.56	1.45
35	2	614	RRX	C23-C22	4.88	1.56	1.45
43	C	615	BCR	C23-C22	4.87	1.56	1.45
43	Z	101	BCR	C29-C30	4.86	1.65	1.54
32	7	317	LUT	C4-C5	-4.86	1.43	1.51
32	7	318	LUT	C8-C9	4.86	1.56	1.45
32	N	316	LUT	C8-C9	4.86	1.56	1.45
35	G	614	RRX	C23-C22	4.86	1.56	1.45
32	N	317	LUT	C8-C9	4.86	1.56	1.45
35	g	315	RRX	C23-C22	4.85	1.56	1.45
43	C	615	BCR	C15-C14	4.85	1.58	1.43
43	t	101	BCR	C23-C22	4.85	1.56	1.45
43	Z	101	BCR	C23-C22	4.84	1.56	1.45
32	n	318	LUT	C8-C9	4.82	1.56	1.45
43	c	615	BCR	C15-C14	4.82	1.58	1.43
32	p	616	LUT	C12-C13	4.82	1.56	1.45
32	4	616	LUT	C8-C9	4.81	1.56	1.45
32	n	317	LUT	C8-C9	4.81	1.56	1.45
43	c	614	BCR	C29-C30	4.81	1.65	1.54
32	6	317	LUT	C8-C9	4.81	1.56	1.45
32	8	616	LUT	C8-C9	4.81	1.56	1.45
43	V	101	BCR	C23-C22	4.81	1.56	1.45
35	4	615	RRX	C12-C13	4.80	1.56	1.45
43	c	614	BCR	C15-C14	4.80	1.58	1.43
32	6	318	LUT	C8-C9	4.80	1.56	1.45
35	G	614	RRX	C2-C1	4.79	1.65	1.54
32	s	318	LUT	C8-C9	4.79	1.56	1.45
32	Y	316	LUT	C4-C5	-4.79	1.43	1.51
32	s	317	LUT	C8-C9	4.79	1.56	1.45
43	c	614	BCR	C23-C22	4.79	1.56	1.45
43	C	614	BCR	C23-C22	4.78	1.56	1.45
32	8	615	LUT	C8-C9	4.78	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	a	410	BCR	C19-C18	4.78	1.56	1.45
32	r	317	LUT	C4-C5	-4.78	1.43	1.51
32	S	317	LUT	C8-C9	4.78	1.56	1.45
35	9	317	RRX	C12-C13	4.77	1.56	1.45
35	4	615	RRX	C2-C1	4.77	1.65	1.54
32	1	616	LUT	C4-C5	-4.77	1.43	1.51
35	G	614	RRX	C12-C13	4.77	1.56	1.45
35	g	315	RRX	C12-C13	4.76	1.56	1.45
43	C	615	BCR	C29-C30	4.76	1.65	1.54
43	T	101	BCR	C15-C14	4.75	1.58	1.43
35	9	317	RRX	C2-C1	4.74	1.65	1.54
43	z	101	BCR	C23-C22	4.73	1.56	1.45
35	2	614	RRX	C2-C1	4.73	1.65	1.54
43	d	406	BCR	C23-C22	4.73	1.56	1.45
43	D	405	BCR	C19-C18	4.73	1.56	1.45
32	R	317	LUT	C4-C5	-4.71	1.43	1.51
32	y	617	LUT	C4-C5	-4.71	1.43	1.51
35	2	614	RRX	C12-C13	4.70	1.56	1.45
43	b	618	BCR	C23-C22	4.70	1.56	1.45
43	C	615	BCR	C8-C9	4.69	1.56	1.45
43	A	410	BCR	C15-C14	4.69	1.58	1.43
44	d	407	PL9	C3-C4	-4.68	1.41	1.49
32	p	617	LUT	C12-C13	4.68	1.56	1.45
32	1	615	LUT	C4-C5	-4.68	1.43	1.51
35	q	317	RRX	C12-C13	4.67	1.56	1.45
43	D	405	BCR	C2-C1	4.67	1.64	1.54
43	c	615	BCR	C19-C18	4.67	1.56	1.45
43	B	617	BCR	C29-C30	4.67	1.64	1.54
32	G	615	LUT	C12-C13	4.65	1.55	1.45
32	5	616	LUT	C12-C13	4.64	1.55	1.45
32	0	616	LUT	C8-C9	4.64	1.55	1.45
35	q	317	RRX	C23-C22	4.64	1.55	1.45
32	g	316	LUT	C12-C13	4.63	1.55	1.45
32	1	616	LUT	C8-C9	4.63	1.55	1.45
32	s	318	LUT	C4-C5	-4.63	1.43	1.51
43	Z	101	BCR	C15-C14	4.63	1.57	1.43
32	0	617	LUT	C8-C9	4.62	1.55	1.45
32	5	617	LUT	C12-C13	4.61	1.55	1.45
43	v	101	BCR	C15-C14	4.61	1.57	1.43
35	4	615	RRX	C24-C25	4.60	1.61	1.45
32	9	318	LUT	C12-C13	4.59	1.55	1.45
35	g	315	RRX	C24-C25	4.58	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	317	LUT	C8-C9	4.58	1.55	1.45
43	V	101	BCR	C15-C14	4.58	1.57	1.43
35	9	317	RRX	C24-C25	4.58	1.61	1.45
32	4	616	LUT	C12-C13	4.57	1.55	1.45
32	q	318	LUT	C12-C13	4.57	1.55	1.45
32	N	317	LUT	C12-C13	4.57	1.55	1.45
35	G	614	RRX	C24-C25	4.57	1.61	1.45
35	2	614	RRX	C24-C25	4.56	1.61	1.45
43	d	406	BCR	C15-C14	4.56	1.57	1.43
32	Y	316	LUT	C8-C9	4.56	1.55	1.45
32	S	318	LUT	C12-C13	4.56	1.55	1.45
43	t	101	BCR	C15-C14	4.55	1.57	1.43
32	3	318	LUT	C12-C13	4.55	1.55	1.45
32	3	317	LUT	C12-C13	4.54	1.55	1.45
32	N	316	LUT	C12-C13	4.54	1.55	1.45
32	R	317	LUT	C8-C9	4.54	1.55	1.45
43	B	618	BCR	C15-C14	4.54	1.57	1.43
43	H	101	BCR	C15-C14	4.54	1.57	1.43
43	C	614	BCR	C15-C14	4.54	1.57	1.43
43	C	615	BCR	C19-C18	4.54	1.55	1.45
35	q	317	RRX	C24-C25	4.53	1.61	1.45
43	b	620	BCR	C15-C14	4.53	1.57	1.43
32	0	617	LUT	C4-C5	-4.52	1.44	1.51
32	p	616	LUT	C15-C14	4.52	1.57	1.43
43	z	101	BCR	C15-C14	4.50	1.57	1.43
43	h	101	BCR	C15-C14	4.50	1.57	1.43
32	R	317	LUT	C12-C13	4.49	1.55	1.45
32	2	615	LUT	C12-C13	4.49	1.55	1.45
43	a	410	BCR	C15-C14	4.49	1.57	1.43
32	7	318	LUT	C12-C13	4.49	1.55	1.45
35	G	614	RRX	C3-C4	4.48	1.66	1.52
32	n	317	LUT	C4-C5	-4.47	1.44	1.51
43	b	619	BCR	C15-C14	4.47	1.57	1.43
35	4	615	RRX	C3-C4	4.47	1.66	1.52
32	0	616	LUT	C4-C5	-4.46	1.44	1.51
35	2	614	RRX	C3-C4	4.46	1.66	1.52
43	b	618	BCR	C15-C14	4.45	1.57	1.43
32	8	615	LUT	C4-C5	-4.45	1.44	1.51
32	S	317	LUT	C4-C5	-4.45	1.44	1.51
32	S	318	LUT	C4-C5	-4.45	1.44	1.51
30	1	619	CHL	C3A-C2A	-4.45	1.42	1.54
32	2	615	LUT	C15-C14	4.45	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	9	317	RRX	C3-C4	4.45	1.66	1.52
32	6	318	LUT	C4-C5	-4.45	1.44	1.51
32	p	616	LUT	C31-C30	4.45	1.57	1.43
43	B	619	BCR	C15-C14	4.44	1.57	1.43
32	2	615	LUT	C35-C34	4.44	1.57	1.43
32	N	316	LUT	C4-C5	-4.44	1.44	1.51
32	r	317	LUT	C8-C9	4.44	1.55	1.45
32	7	318	LUT	C4-C5	-4.44	1.44	1.51
31	C	605	CLA	MG-ND	-4.44	1.97	2.05
32	n	317	LUT	C12-C13	4.43	1.55	1.45
32	4	616	LUT	C4-C5	-4.43	1.44	1.51
43	T	101	BCR	C19-C18	4.43	1.55	1.45
32	p	616	LUT	C35-C34	4.43	1.57	1.43
32	2	615	LUT	C31-C30	4.43	1.57	1.43
32	6	317	LUT	C4-C5	-4.42	1.44	1.51
32	p	617	LUT	C15-C14	4.42	1.57	1.43
43	b	619	BCR	C2-C1	4.41	1.64	1.54
35	q	317	RRX	C11-C10	4.41	1.57	1.43
32	q	318	LUT	C4-C5	-4.41	1.44	1.51
32	2	615	LUT	C4-C5	-4.41	1.44	1.51
43	B	619	BCR	C2-C1	4.41	1.64	1.54
43	B	618	BCR	C2-C1	4.41	1.64	1.54
32	n	318	LUT	C12-C13	4.41	1.55	1.45
32	s	318	LUT	C12-C13	4.41	1.55	1.45
32	G	615	LUT	C15-C14	4.40	1.57	1.43
32	N	317	LUT	C4-C5	-4.40	1.44	1.51
35	q	317	RRX	C2-C1	4.40	1.64	1.54
32	6	318	LUT	C12-C13	4.40	1.55	1.45
32	9	318	LUT	C4-C5	-4.40	1.44	1.51
32	p	617	LUT	C31-C30	4.40	1.57	1.43
32	8	615	LUT	C12-C13	4.39	1.55	1.45
32	6	317	LUT	C12-C13	4.39	1.55	1.45
43	c	614	BCR	C2-C1	4.39	1.64	1.54
32	8	616	LUT	C12-C13	4.39	1.55	1.45
32	1	615	LUT	C8-C9	4.39	1.55	1.45
43	c	614	BCR	C19-C18	4.39	1.55	1.45
32	3	317	LUT	C4-C5	-4.38	1.44	1.51
43	A	410	BCR	C19-C18	4.38	1.55	1.45
43	a	410	BCR	C2-C1	4.38	1.64	1.54
43	d	406	BCR	C2-C1	4.38	1.64	1.54
35	g	315	RRX	C11-C10	4.38	1.57	1.43
32	y	616	LUT	C8-C9	4.38	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	D	405	BCR	C20-C21	4.38	1.57	1.43
32	s	317	LUT	C4-C5	-4.37	1.44	1.51
43	B	617	BCR	C15-C14	4.37	1.57	1.43
43	b	618	BCR	C2-C1	4.37	1.64	1.54
43	A	410	BCR	C2-C1	4.37	1.64	1.54
43	H	101	BCR	C2-C1	4.37	1.64	1.54
32	3	318	LUT	C15-C14	4.37	1.57	1.43
43	v	101	BCR	C19-C18	4.36	1.55	1.45
32	9	318	LUT	C15-C14	4.36	1.57	1.43
31	S	304	CLA	CBB-CAB	4.36	1.51	1.30
32	5	617	LUT	C15-C14	4.36	1.57	1.43
32	s	317	LUT	C12-C13	4.36	1.55	1.45
43	c	615	BCR	C20-C21	4.36	1.57	1.43
43	c	615	BCR	C2-C1	4.36	1.64	1.54
43	b	619	BCR	C19-C18	4.36	1.55	1.45
32	n	318	LUT	C4-C5	-4.36	1.44	1.51
32	g	316	LUT	C31-C30	4.36	1.57	1.43
35	4	615	RRX	C11-C10	4.36	1.56	1.43
32	G	615	LUT	C4-C5	-4.36	1.44	1.51
32	q	318	LUT	C31-C30	4.35	1.56	1.43
35	9	317	RRX	C11-C10	4.35	1.56	1.43
32	G	615	LUT	C31-C30	4.35	1.56	1.43
32	S	317	LUT	C12-C13	4.35	1.55	1.45
32	q	318	LUT	C15-C14	4.34	1.56	1.43
35	g	315	RRX	C3-C4	4.34	1.66	1.52
32	5	617	LUT	C31-C30	4.34	1.56	1.43
32	7	317	LUT	C12-C13	4.34	1.55	1.45
32	5	616	LUT	C15-C14	4.34	1.56	1.43
32	g	316	LUT	C15-C14	4.34	1.56	1.43
35	G	614	RRX	C11-C10	4.34	1.56	1.43
43	h	101	BCR	C2-C1	4.34	1.64	1.54
43	C	614	BCR	C2-C1	4.34	1.64	1.54
32	g	316	LUT	C4-C5	-4.33	1.44	1.51
31	y	613	CLA	C4B-NB	-4.33	1.32	1.37
32	8	616	LUT	C4-C5	-4.33	1.44	1.51
32	p	617	LUT	C35-C34	4.33	1.56	1.43
32	0	617	LUT	C12-C13	4.33	1.55	1.45
32	5	616	LUT	C31-C30	4.33	1.56	1.43
32	9	318	LUT	C31-C30	4.33	1.56	1.43
43	b	620	BCR	C2-C1	4.33	1.64	1.54
35	q	317	RRX	C3-C4	4.33	1.66	1.52
32	p	617	LUT	C4-C5	-4.32	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	3	318	LUT	C31-C30	4.32	1.56	1.43
32	4	616	LUT	C15-C14	4.32	1.56	1.43
32	S	318	LUT	C15-C14	4.32	1.56	1.43
31	p	604	CLA	CBB-CAB	4.32	1.51	1.30
32	5	616	LUT	C4-C5	-4.32	1.44	1.51
32	p	616	LUT	C4-C5	-4.32	1.44	1.51
35	2	614	RRX	C11-C10	4.31	1.56	1.43
30	p	608	CHL	CBB-CAB	4.31	1.51	1.30
32	R	317	LUT	C15-C14	4.30	1.56	1.43
30	9	307	CHL	CBB-CAB	4.30	1.51	1.30
31	s	316	CLA	CBB-CAB	4.30	1.51	1.30
32	N	317	LUT	C31-C30	4.30	1.56	1.43
44	a	414	PL9	C7-C3	-4.30	1.46	1.51
32	N	316	LUT	C15-C14	4.30	1.56	1.43
31	4	614	CLA	CBB-CAB	4.30	1.51	1.30
30	4	609	CHL	CBB-CAB	4.30	1.51	1.30
32	g	316	LUT	C35-C34	4.29	1.56	1.43
31	3	304	CLA	CBB-CAB	4.29	1.51	1.30
35	2	614	RRX	C29-C30	4.29	1.68	1.54
30	5	605	CHL	CBB-CAB	4.29	1.51	1.30
32	S	318	LUT	C31-C30	4.29	1.56	1.43
32	G	615	LUT	C35-C34	4.29	1.56	1.43
32	4	616	LUT	C31-C30	4.29	1.56	1.43
30	3	307	CHL	CBB-CAB	4.29	1.51	1.30
31	8	602	CLA	CBB-CAB	4.29	1.51	1.30
32	5	617	LUT	C4-C5	-4.29	1.44	1.51
32	3	318	LUT	C35-C34	4.29	1.56	1.43
30	p	605	CHL	CBB-CAB	4.29	1.51	1.30
31	3	312	CLA	CBB-CAB	4.28	1.51	1.30
31	3	314	CLA	CBB-CAB	4.28	1.51	1.30
31	9	306	CLA	CBB-CAB	4.28	1.51	1.30
32	Y	315	LUT	C8-C9	4.28	1.55	1.45
30	g	306	CHL	CBB-CAB	4.28	1.51	1.30
31	3	315	CLA	CBB-CAB	4.28	1.51	1.30
30	p	601	CHL	CBB-CAB	4.28	1.51	1.30
35	G	614	RRX	C29-C30	4.28	1.68	1.54
31	5	603	CLA	CBB-CAB	4.28	1.51	1.30
31	5	613	CLA	CBB-CAB	4.28	1.51	1.30
31	3	313	CLA	CBB-CAB	4.28	1.51	1.30
30	G	605	CHL	CBB-CAB	4.28	1.51	1.30
31	5	612	CLA	CBB-CAB	4.28	1.51	1.30
31	6	315	CLA	CBB-CAB	4.28	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	V	101	BCR	C2-C1	4.28	1.64	1.54
31	5	610	CLA	CBB-CAB	4.28	1.51	1.30
31	0	611	CLA	CBB-CAB	4.28	1.51	1.30
31	p	612	CLA	CBB-CAB	4.28	1.51	1.30
31	7	303	CLA	CBB-CAB	4.28	1.51	1.30
31	b	615	CLA	CBB-CAB	4.28	1.51	1.30
32	3	317	LUT	C15-C14	4.27	1.56	1.43
32	3	317	LUT	C31-C30	4.27	1.56	1.43
31	9	304	CLA	CBB-CAB	4.27	1.51	1.30
31	q	304	CLA	CBB-CAB	4.27	1.51	1.30
31	6	313	CLA	CBB-CAB	4.27	1.51	1.30
35	4	615	RRX	C29-C30	4.27	1.68	1.54
31	8	614	CLA	CBB-CAB	4.27	1.51	1.30
32	N	317	LUT	C15-C14	4.27	1.56	1.43
30	2	605	CHL	CBB-CAB	4.27	1.51	1.30
31	n	303	CLA	CBB-CAB	4.27	1.51	1.30
31	s	305	CLA	CBB-CAB	4.27	1.51	1.30
30	G	607	CHL	CBB-CAB	4.27	1.51	1.30
31	5	611	CLA	CBB-CAB	4.27	1.51	1.30
31	s	303	CLA	CBB-CAB	4.27	1.51	1.30
31	5	602	CLA	CBB-CAB	4.27	1.51	1.30
31	7	311	CLA	CBB-CAB	4.27	1.51	1.30
31	N	312	CLA	CBB-CAB	4.27	1.51	1.30
31	7	315	CLA	CBB-CAB	4.27	1.51	1.30
31	3	306	CLA	CBB-CAB	4.27	1.51	1.30
31	S	303	CLA	CBB-CAB	4.27	1.51	1.30
31	8	603	CLA	CBB-CAB	4.27	1.51	1.30
31	y	610	CLA	CBB-CAB	4.27	1.51	1.30
31	6	304	CLA	CBB-CAB	4.27	1.51	1.30
35	9	317	RRX	C29-C30	4.27	1.68	1.54
31	8	610	CLA	CBB-CAB	4.27	1.51	1.30
35	q	317	RRX	C29-C30	4.27	1.68	1.54
43	V	101	BCR	C28-C27	4.27	1.65	1.52
31	6	312	CLA	CBB-CAB	4.27	1.51	1.30
31	Y	310	CLA	CBB-CAB	4.27	1.51	1.30
32	5	616	LUT	C35-C34	4.27	1.56	1.43
31	0	612	CLA	CBB-CAB	4.27	1.51	1.30
43	B	617	BCR	C23-C22	4.27	1.55	1.45
32	5	617	LUT	C35-C34	4.27	1.56	1.43
31	9	316	CLA	CBB-CAB	4.27	1.51	1.30
30	2	608	CHL	CBB-CAB	4.27	1.51	1.30
31	4	604	CLA	CBB-CAB	4.27	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	607	CLA	CBB-CAB	4.27	1.51	1.30
31	n	305	CLA	CBB-CAB	4.27	1.51	1.30
31	5	604	CLA	CBB-CAB	4.27	1.51	1.30
31	2	604	CLA	CBB-CAB	4.27	1.51	1.30
31	3	305	CLA	CBB-CAB	4.27	1.51	1.30
31	N	303	CLA	CBB-CAB	4.27	1.51	1.30
31	N	314	CLA	CBB-CAB	4.27	1.51	1.30
31	p	610	CLA	CBB-CAB	4.27	1.51	1.30
31	7	312	CLA	CBB-CAB	4.26	1.51	1.30
31	n	313	CLA	CBB-CAB	4.26	1.51	1.30
32	6	318	LUT	C31-C30	4.26	1.56	1.43
43	V	101	BCR	C19-C18	4.26	1.55	1.45
31	6	303	CLA	CBB-CAB	4.26	1.51	1.30
31	S	305	CLA	CBB-CAB	4.26	1.51	1.30
31	B	611	CLA	CBB-CAB	4.26	1.51	1.30
31	N	305	CLA	CBB-CAB	4.26	1.51	1.30
31	p	614	CLA	CBB-CAB	4.26	1.51	1.30
31	y	603	CLA	CBB-CAB	4.26	1.51	1.30
31	1	614	CLA	CBB-CAB	4.26	1.51	1.30
31	5	614	CLA	CBB-CAB	4.26	1.51	1.30
32	q	318	LUT	C35-C34	4.26	1.56	1.43
31	3	311	CLA	CBB-CAB	4.26	1.51	1.30
31	4	603	CLA	CBB-CAB	4.26	1.51	1.30
31	r	305	CLA	CBB-CAB	4.26	1.51	1.30
31	g	314	CLA	CBB-CAB	4.26	1.51	1.30
31	2	610	CLA	CBB-CAB	4.26	1.51	1.30
31	4	602	CLA	CBB-CAB	4.26	1.51	1.30
31	N	304	CLA	CBB-CAB	4.26	1.51	1.30
31	0	614	CLA	CBB-CAB	4.26	1.51	1.30
31	G	602	CLA	CBB-CAB	4.26	1.51	1.30
31	s	304	CLA	CBB-CAB	4.26	1.51	1.30
30	9	311	CHL	CBB-CAB	4.26	1.51	1.30
31	6	311	CLA	CBB-CAB	4.26	1.51	1.30
31	n	312	CLA	CBB-CAB	4.26	1.51	1.30
31	y	612	CLA	CBB-CAB	4.26	1.51	1.30
31	9	305	CLA	CBB-CAB	4.26	1.51	1.30
30	2	607	CHL	CBB-CAB	4.26	1.51	1.30
31	n	315	CLA	CBB-CAB	4.26	1.51	1.30
32	3	318	LUT	C4-C5	-4.26	1.44	1.51
31	g	305	CLA	CBB-CAB	4.26	1.51	1.30
31	9	315	CLA	CBB-CAB	4.26	1.51	1.30
31	B	614	CLA	CBB-CAB	4.26	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	p	609	CHL	CBB-CAB	4.26	1.51	1.30
31	N	313	CLA	CBB-CAB	4.26	1.51	1.30
31	S	304	CLA	MG-ND	-4.26	1.97	2.05
30	Y	302	CHL	CBB-CAB	4.26	1.51	1.30
31	8	604	CLA	CBB-CAB	4.26	1.51	1.30
30	4	605	CHL	CBB-CAB	4.26	1.51	1.30
31	1	611	CLA	CBB-CAB	4.26	1.51	1.30
31	Y	303	CLA	CBB-CAB	4.26	1.51	1.30
31	8	609	CLA	CBB-CAB	4.26	1.51	1.30
31	9	312	CLA	CBB-CAB	4.26	1.51	1.30
31	6	314	CLA	CBB-CAB	4.26	1.51	1.30
30	6	306	CHL	CBB-CAB	4.26	1.51	1.30
30	q	307	CHL	CBB-CAB	4.26	1.51	1.30
31	N	310	CLA	CBB-CAB	4.26	1.51	1.30
31	s	306	CLA	CBB-CAB	4.26	1.51	1.30
31	R	313	CLA	CBB-CAB	4.26	1.51	1.30
31	Y	305	CLA	CBB-CAB	4.26	1.51	1.30
31	q	316	CLA	CBB-CAB	4.26	1.51	1.30
31	0	603	CLA	CBB-CAB	4.26	1.51	1.30
31	9	313	CLA	CBB-CAB	4.26	1.51	1.30
31	b	613	CLA	CBB-CAB	4.26	1.51	1.30
31	G	610	CLA	CBB-CAB	4.26	1.51	1.30
31	q	306	CLA	CBB-CAB	4.26	1.51	1.30
31	r	304	CLA	CBB-CAB	4.26	1.51	1.30
43	b	620	BCR	C19-C18	4.26	1.55	1.45
31	8	611	CLA	CBB-CAB	4.26	1.51	1.30
31	p	611	CLA	CBB-CAB	4.26	1.51	1.30
43	Z	101	BCR	C2-C1	4.26	1.63	1.54
31	b	614	CLA	CBB-CAB	4.26	1.51	1.30
31	n	316	CLA	CBB-CAB	4.26	1.51	1.30
30	g	309	CHL	CBB-CAB	4.26	1.51	1.30
31	g	303	CLA	CBB-CAB	4.26	1.51	1.30
31	N	315	CLA	CBB-CAB	4.25	1.51	1.30
43	Z	101	BCR	C19-C18	4.25	1.55	1.45
30	8	607	CHL	CBB-CAB	4.25	1.51	1.30
31	B	610	CLA	CBB-CAB	4.25	1.51	1.30
31	0	602	CLA	CBB-CAB	4.25	1.51	1.30
43	C	615	BCR	C20-C21	4.25	1.56	1.43
30	1	605	CHL	CBB-CAB	4.25	1.51	1.30
32	N	316	LUT	C31-C30	4.25	1.56	1.43
31	6	305	CLA	CBB-CAB	4.25	1.51	1.30
31	2	609	CLA	CBB-CAB	4.25	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	G	608	CHL	CBB-CAB	4.25	1.51	1.30
31	c	607	CLA	MG-ND	-4.25	1.97	2.05
31	8	613	CLA	CBB-CAB	4.25	1.51	1.30
31	n	314	CLA	CBB-CAB	4.25	1.51	1.30
30	3	303	CHL	CBB-CAB	4.25	1.51	1.30
30	8	601	CHL	CBB-CAB	4.25	1.51	1.30
31	S	306	CLA	CBB-CAB	4.25	1.51	1.30
31	q	305	CLA	CBB-CAB	4.25	1.51	1.30
30	n	302	CHL	CBB-CAB	4.25	1.51	1.30
43	T	101	BCR	C2-C1	4.25	1.63	1.54
31	b	612	CLA	CBB-CAB	4.25	1.51	1.30
30	7	309	CHL	CBB-CAB	4.25	1.51	1.30
31	g	311	CLA	CBB-CAB	4.25	1.51	1.30
35	q	317	RRX	C27-C26	-4.25	1.44	1.51
30	7	306	CHL	CBB-CAB	4.25	1.51	1.30
31	p	602	CLA	CBB-CAB	4.25	1.51	1.30
32	1	616	LUT	C12-C13	4.25	1.55	1.45
31	R	316	CLA	CBB-CAB	4.25	1.51	1.30
31	n	304	CLA	CBB-CAB	4.25	1.51	1.30
31	b	617	CLA	MG-ND	-4.25	1.97	2.05
31	7	305	CLA	CBB-CAB	4.25	1.51	1.30
31	p	603	CLA	CBB-CAB	4.25	1.51	1.30
31	y	602	CLA	CBB-CAB	4.25	1.51	1.30
31	8	612	CLA	CBB-CAB	4.25	1.51	1.30
31	0	613	CLA	CBB-CAB	4.25	1.51	1.30
30	q	311	CHL	CBB-CAB	4.25	1.51	1.30
31	y	604	CLA	CBB-CAB	4.25	1.51	1.30
31	G	604	CLA	CBB-CAB	4.25	1.51	1.30
31	7	316	CLA	CBB-CAB	4.25	1.51	1.30
31	s	315	CLA	CBB-CAB	4.25	1.51	1.30
31	2	613	CLA	CBB-CAB	4.24	1.51	1.30
31	r	313	CLA	CBB-CAB	4.24	1.51	1.30
30	g	308	CHL	CBB-CAB	4.24	1.51	1.30
31	1	610	CLA	CBB-CAB	4.24	1.51	1.30
31	G	613	CLA	CBB-CAB	4.24	1.51	1.30
31	7	304	CLA	CBB-CAB	4.24	1.51	1.30
30	0	609	CHL	CBB-CAB	4.24	1.51	1.30
31	y	615	CLA	CBB-CAB	4.24	1.51	1.30
32	Y	316	LUT	C12-C13	4.24	1.55	1.45
31	b	611	CLA	CBB-CAB	4.24	1.51	1.30
31	g	304	CLA	CBB-CAB	4.24	1.51	1.30
31	N	311	CLA	CBB-CAB	4.24	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	311	CLA	CBB-CAB	4.24	1.51	1.30
43	b	619	BCR	C20-C21	4.24	1.56	1.43
30	5	609	CHL	CBB-CAB	4.24	1.51	1.30
31	N	321	CLA	CBB-CAB	4.24	1.51	1.30
30	N	302	CHL	CBB-CAB	4.24	1.51	1.30
31	G	603	CLA	CBB-CAB	4.24	1.51	1.30
43	H	101	BCR	C19-C18	4.24	1.55	1.45
43	h	101	BCR	C19-C18	4.24	1.55	1.45
31	g	313	CLA	CBB-CAB	4.24	1.51	1.30
31	2	611	CLA	CBB-CAB	4.24	1.51	1.30
31	Y	314	CLA	CBB-CAB	4.24	1.51	1.30
32	7	318	LUT	C15-C14	4.24	1.56	1.43
43	D	405	BCR	C28-C27	4.24	1.65	1.52
30	Y	309	CHL	CBB-CAB	4.24	1.51	1.30
31	0	615	CLA	CBB-CAB	4.24	1.51	1.30
30	r	309	CHL	CBB-CAB	4.24	1.51	1.30
31	g	312	CLA	CBB-CAB	4.24	1.51	1.30
32	y	617	LUT	C8-C9	4.24	1.55	1.45
30	9	310	CHL	CBB-CAB	4.24	1.51	1.30
31	5	615	CLA	CBB-CAB	4.24	1.51	1.30
31	G	612	CLA	CBB-CAB	4.24	1.51	1.30
30	3	310	CHL	CBB-CAB	4.24	1.51	1.30
30	n	309	CHL	CBB-CAB	4.24	1.51	1.30
31	b	609	CLA	CBB-CAB	4.24	1.51	1.30
43	B	617	BCR	C2-C1	4.24	1.63	1.54
30	1	608	CHL	CBB-CAB	4.24	1.51	1.30
31	B	608	CLA	CBB-CAB	4.24	1.51	1.30
30	y	601	CHL	CBB-CAB	4.24	1.51	1.30
31	2	603	CLA	CBB-CAB	4.24	1.51	1.30
31	B	613	CLA	CBB-CAB	4.23	1.51	1.30
44	D	406	PL9	C3-C4	-4.23	1.42	1.49
30	7	310	CHL	CBB-CAB	4.23	1.51	1.30
31	S	316	CLA	CBB-CAB	4.23	1.51	1.30
30	g	302	CHL	CBB-CAB	4.23	1.51	1.30
31	R	314	CLA	CBB-CAB	4.23	1.51	1.30
30	y	609	CHL	CBB-CAB	4.23	1.51	1.30
31	B	612	CLA	CBB-CAB	4.23	1.51	1.30
43	v	101	BCR	C2-C1	4.23	1.63	1.54
31	C	610	CLA	CBB-CAB	4.23	1.51	1.30
31	9	314	CLA	CBB-CAB	4.23	1.51	1.30
31	R	307	CLA	CBB-CAB	4.23	1.51	1.30
31	D	404	CLA	CBB-CAB	4.23	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	303	CLA	CBB-CAB	4.23	1.51	1.30
30	N	308	CHL	CBB-CAB	4.23	1.51	1.30
30	9	303	CHL	CBB-CAB	4.23	1.51	1.30
31	Y	304	CLA	CBB-CAB	4.23	1.51	1.30
31	7	314	CLA	CBB-CAB	4.23	1.51	1.30
30	n	310	CHL	CBB-CAB	4.23	1.51	1.30
30	s	308	CHL	CBB-CAB	4.23	1.51	1.30
31	n	311	CLA	CBB-CAB	4.23	1.51	1.30
31	2	612	CLA	CBB-CAB	4.23	1.51	1.30
30	R	309	CHL	CBB-CAB	4.23	1.51	1.30
31	C	603	CLA	MG-ND	-4.23	1.97	2.05
31	7	313	CLA	CBB-CAB	4.22	1.51	1.30
31	1	612	CLA	CBB-CAB	4.22	1.51	1.30
31	p	615	CLA	CBB-CAB	4.22	1.51	1.30
31	1	613	CLA	CBB-CAB	4.22	1.51	1.30
31	4	612	CLA	CBB-CAB	4.22	1.51	1.30
30	4	606	CHL	CBB-CAB	4.22	1.51	1.30
43	B	618	BCR	C19-C18	4.22	1.55	1.45
43	z	101	BCR	C2-C1	4.22	1.63	1.54
31	s	310	CLA	CBB-CAB	4.22	1.51	1.30
32	7	318	LUT	C31-C30	4.22	1.56	1.43
30	5	608	CHL	CBB-CAB	4.22	1.51	1.30
31	S	310	CLA	CBB-CAB	4.22	1.51	1.30
31	1	602	CLA	CBB-CAB	4.22	1.51	1.30
31	s	312	CLA	CBB-CAB	4.22	1.51	1.30
31	S	312	CLA	CBB-CAB	4.22	1.51	1.30
31	S	315	CLA	CBB-CAB	4.22	1.51	1.30
32	6	318	LUT	C15-C14	4.22	1.56	1.43
30	5	601	CHL	CBB-CAB	4.22	1.51	1.30
31	4	610	CLA	CBB-CAB	4.22	1.51	1.30
31	p	613	CLA	CBB-CAB	4.22	1.51	1.30
30	8	608	CHL	CBB-CAB	4.22	1.51	1.30
30	N	309	CHL	CBB-CAB	4.22	1.51	1.30
30	9	309	CHL	CBB-CAB	4.22	1.51	1.30
31	R	311	CLA	CBB-CAB	4.22	1.51	1.30
32	R	317	LUT	C35-C34	4.22	1.56	1.43
30	7	308	CHL	CBB-CAB	4.22	1.51	1.30
31	6	316	CLA	CBB-CAB	4.22	1.51	1.30
31	r	311	CLA	CBB-CAB	4.22	1.51	1.30
31	s	313	CLA	CBB-CAB	4.22	1.51	1.30
30	y	608	CHL	CBB-CAB	4.22	1.51	1.30
30	S	302	CHL	CBB-CAB	4.22	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	313	CLA	CBB-CAB	4.22	1.51	1.30
31	B	615	CLA	CBB-CAB	4.22	1.51	1.30
30	q	303	CHL	CBB-CAB	4.22	1.51	1.30
32	N	316	LUT	C35-C34	4.22	1.56	1.43
31	2	602	CLA	CBB-CAB	4.22	1.51	1.30
32	s	317	LUT	C31-C30	4.22	1.56	1.43
31	b	606	CLA	CBB-CAB	4.21	1.51	1.30
31	c	604	CLA	CBB-CAB	4.21	1.51	1.30
31	3	301	CLA	CBB-CAB	4.21	1.51	1.30
31	r	303	CLA	CBB-CAB	4.21	1.51	1.30
31	1	603	CLA	CBB-CAB	4.21	1.51	1.30
31	Y	313	CLA	CBB-CAB	4.21	1.51	1.30
31	r	314	CLA	CBB-CAB	4.21	1.51	1.30
31	0	604	CLA	CBB-CAB	4.21	1.51	1.30
32	n	318	LUT	C15-C14	4.21	1.56	1.43
30	6	302	CHL	CBB-CAB	4.21	1.51	1.30
31	B	609	CLA	CBB-CAB	4.21	1.51	1.30
31	B	604	CLA	CBB-CAB	4.21	1.51	1.30
31	B	602	CLA	CBB-CAB	4.21	1.51	1.30
30	2	601	CHL	CBB-CAB	4.21	1.51	1.30
30	0	601	CHL	CBB-CAB	4.21	1.51	1.30
31	r	307	CLA	CBB-CAB	4.21	1.51	1.30
30	3	309	CHL	CBB-CAB	4.21	1.51	1.30
30	G	601	CHL	CBB-CAB	4.21	1.51	1.30
31	r	316	CLA	CBB-CAB	4.21	1.51	1.30
31	R	306	CLA	CBB-CAB	4.21	1.51	1.30
32	S	317	LUT	C31-C30	4.21	1.56	1.43
31	b	608	CLA	CBB-CAB	4.21	1.51	1.30
31	C	601	CLA	CBB-CAB	4.21	1.51	1.30
31	S	314	CLA	CBB-CAB	4.21	1.51	1.30
30	Y	301	CHL	CBB-CAB	4.21	1.51	1.30
31	S	311	CLA	CBB-CAB	4.21	1.51	1.30
31	c	606	CLA	CBB-CAB	4.21	1.51	1.30
30	1	607	CHL	CBB-CAB	4.21	1.51	1.30
31	G	609	CLA	CBB-CAB	4.21	1.51	1.30
30	7	302	CHL	CBB-CAB	4.21	1.51	1.30
31	b	604	CLA	CBB-CAB	4.21	1.51	1.30
31	y	614	CLA	CBB-CAB	4.21	1.51	1.30
31	G	611	CLA	CBB-CAB	4.21	1.51	1.30
30	s	302	CHL	CBB-CAB	4.20	1.51	1.30
31	R	305	CLA	CBB-CAB	4.20	1.51	1.30
31	r	315	CLA	CBB-CAB	4.20	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	n	306	CHL	CBB-CAB	4.20	1.51	1.30
31	A	406	CLA	CBB-CAB	4.20	1.51	1.30
30	4	608	CHL	CBB-CAB	4.20	1.51	1.30
30	Y	308	CHL	CBB-CAB	4.20	1.51	1.30
31	R	315	CLA	CBB-CAB	4.20	1.51	1.30
31	q	315	CLA	CBB-CAB	4.20	1.51	1.30
31	c	610	CLA	CBB-CAB	4.20	1.51	1.30
30	4	601	CHL	CBB-CAB	4.20	1.51	1.30
31	C	608	CLA	CBB-CAB	4.20	1.51	1.30
43	T	101	BCR	C20-C21	4.20	1.56	1.43
31	G	611	CLA	MG-ND	-4.20	1.97	2.05
30	1	609	CHL	CBB-CAB	4.20	1.51	1.30
31	q	314	CLA	CBB-CAB	4.20	1.51	1.30
31	b	605	CLA	CBB-CAB	4.20	1.51	1.30
43	C	614	BCR	C19-C18	4.20	1.55	1.45
32	8	616	LUT	C15-C14	4.20	1.56	1.43
31	Y	312	CLA	CBB-CAB	4.20	1.51	1.30
31	c	601	CLA	CBB-CAB	4.20	1.51	1.30
43	v	101	BCR	C28-C27	4.20	1.65	1.52
32	8	616	LUT	C31-C30	4.20	1.56	1.43
30	n	301	CHL	CBB-CAB	4.20	1.51	1.30
30	5	606	CHL	CBB-CAB	4.20	1.51	1.30
30	0	608	CHL	CBB-CAB	4.20	1.51	1.30
32	S	318	LUT	C35-C34	4.20	1.56	1.43
31	b	603	CLA	CBB-CAB	4.20	1.51	1.30
31	b	610	CLA	CBB-CAB	4.20	1.51	1.30
31	s	314	CLA	CBB-CAB	4.20	1.51	1.30
32	6	318	LUT	C35-C34	4.20	1.56	1.43
31	c	603	CLA	MG-ND	-4.20	1.97	2.05
30	p	607	CHL	CBB-CAB	4.20	1.51	1.30
31	R	312	CLA	CBB-CAB	4.20	1.51	1.30
31	c	603	CLA	CBB-CAB	4.20	1.51	1.30
32	n	318	LUT	C31-C30	4.20	1.56	1.43
31	c	602	CLA	CBB-CAB	4.20	1.51	1.30
32	4	616	LUT	C35-C34	4.19	1.56	1.43
31	c	605	CLA	CBB-CAB	4.19	1.51	1.30
32	s	317	LUT	C15-C14	4.19	1.56	1.43
32	s	318	LUT	C15-C14	4.19	1.56	1.43
30	Y	306	CHL	CBB-CAB	4.19	1.51	1.30
45	C	620	DGD	O1G-C1A	4.19	1.45	1.33
30	0	607	CHL	CBB-CAB	4.19	1.51	1.30
30	S	309	CHL	CBB-CAB	4.19	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	310	CHL	CBB-CAB	4.19	1.51	1.30
31	b	607	CLA	CBB-CAB	4.19	1.51	1.30
31	g	310	CLA	CBB-CAB	4.19	1.51	1.30
31	y	611	CLA	CBB-CAB	4.19	1.51	1.30
31	R	304	CLA	CBB-CAB	4.19	1.51	1.30
30	s	309	CHL	CBB-CAB	4.19	1.51	1.30
31	C	607	CLA	CBB-CAB	4.19	1.51	1.30
32	3	317	LUT	C35-C34	4.19	1.56	1.43
30	p	606	CHL	CBB-CAB	4.19	1.51	1.30
43	c	615	BCR	C28-C27	4.19	1.65	1.52
30	8	605	CHL	CBB-CAB	4.19	1.51	1.30
31	C	612	CLA	CBB-CAB	4.19	1.51	1.30
32	9	318	LUT	C35-C34	4.19	1.56	1.43
30	5	607	CHL	CBB-CAB	4.19	1.51	1.30
31	C	603	CLA	CBB-CAB	4.19	1.51	1.30
31	c	611	CLA	CBB-CAB	4.19	1.51	1.30
30	N	306	CHL	CBB-CAB	4.18	1.51	1.30
32	6	317	LUT	C31-C30	4.18	1.56	1.43
31	r	312	CLA	CBB-CAB	4.18	1.51	1.30
31	r	306	CLA	CBB-CAB	4.18	1.51	1.30
30	9	308	CHL	CBB-CAB	4.18	1.51	1.30
31	C	613	CLA	CBB-CAB	4.18	1.51	1.30
31	B	606	CLA	CBB-CAB	4.18	1.51	1.30
32	N	317	LUT	C35-C34	4.18	1.56	1.43
30	N	301	CHL	CBB-CAB	4.18	1.51	1.30
30	n	308	CHL	CBB-CAB	4.18	1.51	1.30
32	s	318	LUT	C31-C30	4.18	1.56	1.43
30	7	321	CHL	CBB-CAB	4.18	1.51	1.30
30	6	308	CHL	CBB-CAB	4.18	1.51	1.30
31	b	617	CLA	CBB-CAB	4.18	1.51	1.30
32	0	617	LUT	C31-C30	4.18	1.56	1.43
31	4	613	CLA	CBB-CAB	4.18	1.51	1.30
31	C	605	CLA	C4B-NB	-4.18	1.32	1.37
31	1	604	CLA	CBB-CAB	4.18	1.51	1.30
31	a	406	CLA	CBB-CAB	4.18	1.51	1.30
32	8	615	LUT	C15-C14	4.18	1.56	1.43
30	G	623	CHL	CBB-CAB	4.18	1.51	1.30
31	b	616	CLA	CBB-CAB	4.18	1.51	1.30
30	1	606	CHL	CBB-CAB	4.17	1.51	1.30
31	A	405	CLA	CBB-CAB	4.17	1.51	1.30
47	E	101	HEM	FE-NC	4.17	2.09	1.95
32	n	317	LUT	C15-C14	4.17	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	307	CHL	CBB-CAB	4.17	1.51	1.30
31	C	611	CLA	CBB-CAB	4.17	1.51	1.30
31	d	401	CLA	CBB-CAB	4.17	1.51	1.30
31	a	409	CLA	CBB-CAB	4.17	1.51	1.30
31	B	603	CLA	MG-ND	-4.17	1.97	2.05
31	A	407	CLA	CBB-CAB	4.17	1.51	1.30
31	a	407	CLA	CBB-CAB	4.17	1.51	1.30
30	y	605	CHL	CBB-CAB	4.17	1.51	1.30
31	d	404	CLA	CBB-CAB	4.17	1.51	1.30
31	c	608	CLA	CBB-CAB	4.17	1.51	1.30
31	c	609	CLA	MG-ND	-4.17	1.97	2.05
32	0	616	LUT	C12-C13	4.17	1.54	1.45
31	B	603	CLA	CBB-CAB	4.17	1.50	1.30
31	B	605	CLA	CBB-CAB	4.17	1.50	1.30
31	d	405	CLA	CBB-CAB	4.17	1.50	1.30
32	6	317	LUT	C15-C14	4.17	1.56	1.43
32	S	317	LUT	C15-C14	4.16	1.56	1.43
31	A	409	CLA	CBB-CAB	4.16	1.50	1.30
31	B	616	CLA	CBB-CAB	4.16	1.50	1.30
31	C	604	CLA	CBB-CAB	4.16	1.50	1.30
31	C	602	CLA	CBB-CAB	4.16	1.50	1.30
43	C	614	BCR	C28-C27	4.16	1.65	1.52
30	6	307	CHL	CBB-CAB	4.16	1.50	1.30
30	Y	307	CHL	CBB-CAB	4.16	1.50	1.30
31	3	316	CLA	CBB-CAB	4.16	1.50	1.30
32	7	317	LUT	C15-C14	4.16	1.56	1.43
31	B	616	CLA	MG-ND	-4.16	1.97	2.05
43	B	619	BCR	C19-C18	4.16	1.54	1.45
32	R	317	LUT	C31-C30	4.16	1.56	1.43
31	c	613	CLA	CBB-CAB	4.15	1.50	1.30
31	C	610	CLA	MG-ND	-4.15	1.97	2.05
30	y	607	CHL	CBB-CAB	4.15	1.50	1.30
30	2	606	CHL	CBB-CAB	4.15	1.50	1.30
32	2	615	LUT	C21-C26	4.15	1.67	1.56
30	6	309	CHL	CBB-CAB	4.15	1.50	1.30
43	T	101	BCR	C28-C27	4.15	1.65	1.52
31	C	607	CLA	MG-ND	-4.15	1.97	2.05
45	c	619	DGD	O1G-C1A	4.15	1.45	1.33
31	D	403	CLA	CBB-CAB	4.15	1.50	1.30
32	n	317	LUT	C31-C30	4.15	1.56	1.43
43	b	620	BCR	C20-C21	4.14	1.56	1.43
30	y	606	CHL	CBB-CAB	4.14	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	8	615	LUT	C31-C30	4.14	1.56	1.43
43	v	101	BCR	C20-C21	4.14	1.56	1.43
31	C	609	CLA	CBB-CAB	4.14	1.50	1.30
31	b	605	CLA	MG-ND	-4.14	1.97	2.05
32	0	617	LUT	C15-C14	4.14	1.56	1.43
31	c	612	CLA	CBB-CAB	4.14	1.50	1.30
30	g	307	CHL	CBB-CAB	4.14	1.50	1.30
43	b	618	BCR	C28-C27	4.14	1.65	1.52
45	C	618	DGD	O1G-C1A	4.14	1.45	1.33
30	8	606	CHL	CBB-CAB	4.13	1.50	1.30
30	s	307	CHL	CBB-CAB	4.13	1.50	1.30
30	q	310	CHL	CBB-CAB	4.13	1.50	1.30
31	0	610	CLA	CBB-CAB	4.13	1.50	1.30
31	c	609	CLA	CBB-CAB	4.13	1.50	1.30
31	c	612	CLA	MG-ND	-4.13	1.97	2.05
30	G	606	CHL	CBB-CAB	4.13	1.50	1.30
32	5	616	LUT	C28-C29	4.13	1.54	1.45
47	e	102	HEM	FE-NC	4.13	2.09	1.95
35	g	315	RRX	C29-C30	4.12	1.67	1.54
32	7	318	LUT	C35-C34	4.12	1.56	1.43
30	n	307	CHL	CBB-CAB	4.12	1.50	1.30
32	2	615	LUT	C23-C24	-4.12	1.44	1.50
32	0	617	LUT	C35-C34	4.12	1.56	1.43
31	B	607	CLA	CBB-CAB	4.12	1.50	1.30
43	A	410	BCR	C28-C27	4.12	1.65	1.52
31	Y	311	CLA	CBB-CAB	4.12	1.50	1.30
32	1	615	LUT	C12-C13	4.12	1.54	1.45
32	8	616	LUT	C35-C34	4.12	1.56	1.43
30	S	307	CHL	CBB-CAB	4.12	1.50	1.30
31	B	601	CLA	CBB-CAB	4.12	1.50	1.30
30	q	308	CHL	CBB-CAB	4.11	1.50	1.30
43	d	406	BCR	C28-C27	4.11	1.65	1.52
31	C	612	CLA	MG-ND	-4.11	1.97	2.05
43	Z	101	BCR	C28-C27	4.11	1.65	1.52
32	n	318	LUT	C35-C34	4.11	1.56	1.43
43	a	410	BCR	C28-C27	4.11	1.65	1.52
32	p	616	LUT	C7-C6	4.11	1.59	1.45
31	C	609	CLA	MG-ND	-4.11	1.97	2.05
32	8	615	LUT	C35-C34	4.11	1.56	1.43
32	n	317	LUT	C35-C34	4.11	1.56	1.43
31	D	403	CLA	MG-ND	-4.11	1.97	2.05
31	c	606	CLA	MG-ND	-4.11	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	617	LUT	C12-C13	4.11	1.54	1.45
43	H	101	BCR	C28-C27	4.10	1.65	1.52
43	b	620	BCR	C28-C27	4.10	1.65	1.52
32	0	616	LUT	C15-C14	4.10	1.56	1.43
31	r	303	CLA	MG-ND	-4.10	1.97	2.05
32	Y	316	LUT	C15-C14	4.10	1.56	1.43
31	B	604	CLA	MG-ND	-4.10	1.97	2.05
43	A	410	BCR	C20-C21	4.10	1.56	1.43
30	R	308	CHL	CBB-CAB	4.10	1.50	1.30
31	b	604	CLA	MG-ND	-4.10	1.97	2.05
32	g	316	LUT	C28-C29	4.10	1.54	1.45
35	2	614	RRX	C27-C26	-4.10	1.44	1.51
30	N	307	CHL	CBB-CAB	4.09	1.50	1.30
43	z	101	BCR	C19-C18	4.09	1.54	1.45
31	b	602	CLA	CBB-CAB	4.09	1.50	1.30
43	b	619	BCR	C28-C27	4.09	1.65	1.52
43	t	101	BCR	C28-C27	4.09	1.65	1.52
43	t	101	BCR	C19-C18	4.09	1.54	1.45
32	S	317	LUT	C35-C34	4.09	1.56	1.43
31	C	606	CLA	CBB-CAB	4.09	1.50	1.30
32	5	616	LUT	C7-C6	4.09	1.59	1.45
43	Z	101	BCR	C20-C21	4.09	1.56	1.43
32	5	617	LUT	C28-C29	4.08	1.54	1.45
31	C	605	CLA	CBB-CAB	4.08	1.50	1.30
32	s	318	LUT	C35-C34	4.08	1.56	1.43
43	B	618	BCR	C28-C27	4.08	1.65	1.52
31	S	313	CLA	MG-ND	-4.08	1.97	2.05
43	t	101	BCR	C4-C5	-4.08	1.43	1.51
32	6	317	LUT	C35-C34	4.08	1.56	1.43
43	H	101	BCR	C20-C21	4.08	1.56	1.43
32	Y	316	LUT	C31-C30	4.08	1.56	1.43
43	t	101	BCR	C2-C1	4.07	1.63	1.54
43	B	619	BCR	C28-C27	4.07	1.65	1.52
43	B	618	BCR	C20-C21	4.07	1.56	1.43
43	c	614	BCR	C20-C21	4.07	1.56	1.43
32	s	317	LUT	C35-C34	4.07	1.56	1.43
32	p	617	LUT	C21-C26	4.07	1.67	1.56
31	r	307	CLA	MG-ND	-4.07	1.97	2.05
31	q	315	CLA	MG-ND	-4.07	1.97	2.05
30	4	607	CHL	CBB-CAB	4.07	1.50	1.30
30	0	606	CHL	CBB-CAB	4.07	1.50	1.30
32	Y	316	LUT	C35-C34	4.07	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	616	LUT	C31-C30	4.07	1.56	1.43
35	4	615	RRX	C15-C14	4.07	1.56	1.43
31	y	613	CLA	MG-ND	-4.07	1.97	2.05
45	C	617	DGD	O1G-C1A	4.07	1.45	1.33
31	1	604	CLA	MG-ND	-4.06	1.97	2.05
45	C	616	DGD	O1G-C1A	4.06	1.45	1.33
35	g	315	RRX	C15-C14	4.06	1.56	1.43
30	r	310	CHL	CBB-CAB	4.06	1.50	1.30
31	B	607	CLA	C1C-NC	-4.06	1.31	1.37
30	r	308	CHL	CBB-CAB	4.06	1.50	1.30
43	h	101	BCR	C28-C27	4.06	1.65	1.52
43	c	614	BCR	C28-C27	4.06	1.65	1.52
32	1	616	LUT	C15-C14	4.06	1.56	1.43
45	c	616	DGD	O1G-C1A	4.06	1.45	1.33
31	r	314	CLA	MG-ND	-4.06	1.97	2.05
30	3	302	CHL	CBB-CAB	4.05	1.50	1.30
43	B	619	BCR	C20-C21	4.05	1.56	1.43
43	V	101	BCR	C20-C21	4.05	1.56	1.43
35	4	615	RRX	C27-C26	-4.05	1.44	1.51
32	3	318	LUT	C28-C29	4.05	1.54	1.45
32	N	317	LUT	C28-C29	4.05	1.54	1.45
32	q	318	LUT	C28-C29	4.05	1.54	1.45
45	c	618	DGD	O1G-C1A	4.05	1.45	1.33
31	R	305	CLA	MG-ND	-4.05	1.97	2.05
31	c	602	CLA	MG-ND	-4.05	1.97	2.05
35	9	317	RRX	C15-C14	4.05	1.56	1.43
45	c	617	DGD	O1G-C1A	4.05	1.45	1.33
31	0	610	CLA	MG-ND	-4.05	1.97	2.05
32	9	318	LUT	C7-C6	4.05	1.59	1.45
43	h	101	BCR	C20-C21	4.04	1.56	1.43
35	G	614	RRX	C27-C26	-4.04	1.44	1.51
32	5	617	LUT	C7-C6	4.04	1.59	1.45
32	g	316	LUT	C7-C6	4.04	1.59	1.45
32	1	615	LUT	C31-C30	4.04	1.56	1.43
31	1	603	CLA	MG-ND	-4.04	1.97	2.05
35	G	614	RRX	C15-C14	4.04	1.56	1.43
35	9	317	RRX	C27-C26	-4.04	1.44	1.51
32	3	317	LUT	C28-C29	4.04	1.54	1.45
31	R	307	CLA	MG-ND	-4.04	1.97	2.05
32	G	615	LUT	C7-C6	4.04	1.59	1.45
31	y	613	CLA	CBB-CAB	4.04	1.50	1.30
32	N	316	LUT	C28-C29	4.03	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	605	CHL	CBB-CAB	4.03	1.50	1.30
30	3	308	CHL	CBB-CAB	4.03	1.50	1.30
31	c	613	CLA	MG-ND	-4.03	1.97	2.05
35	2	614	RRX	C15-C14	4.03	1.55	1.43
31	C	605	CLA	C1C-NC	-4.03	1.31	1.37
31	Y	312	CLA	MG-ND	-4.02	1.97	2.05
31	0	603	CLA	MG-ND	-4.02	1.97	2.05
31	p	603	CLA	MG-ND	-4.02	1.97	2.05
31	c	610	CLA	MG-ND	-4.02	1.97	2.05
43	b	618	BCR	C19-C18	4.02	1.54	1.45
31	R	306	CLA	MG-ND	-4.02	1.97	2.05
30	S	308	CHL	CBB-CAB	4.02	1.50	1.30
31	7	314	CLA	MG-ND	-4.02	1.97	2.05
31	0	612	CLA	MG-ND	-4.02	1.97	2.05
31	c	608	CLA	MG-ND	-4.02	1.97	2.05
32	p	617	LUT	C7-C6	4.02	1.59	1.45
32	q	318	LUT	C7-C6	4.02	1.59	1.45
31	1	613	CLA	MG-ND	-4.01	1.97	2.05
30	1	601	CHL	CBB-CAB	4.01	1.50	1.30
31	S	314	CLA	MG-ND	-4.01	1.97	2.05
43	C	614	BCR	C20-C21	4.01	1.55	1.43
31	g	311	CLA	MG-ND	-4.01	1.97	2.05
43	z	101	BCR	C28-C27	4.01	1.65	1.52
31	r	316	CLA	MG-ND	-4.00	1.97	2.05
32	1	616	LUT	C35-C34	4.00	1.55	1.43
31	R	313	CLA	MG-ND	-4.00	1.97	2.05
31	G	610	CLA	MG-ND	-4.00	1.97	2.05
35	q	317	RRX	C15-C14	4.00	1.55	1.43
31	b	608	CLA	MG-ND	-4.00	1.97	2.05
31	Y	311	CLA	MG-ND	-4.00	1.97	2.05
32	y	617	LUT	C15-C14	4.00	1.55	1.43
32	1	615	LUT	C15-C14	4.00	1.55	1.43
32	3	318	LUT	C7-C6	4.00	1.59	1.45
32	0	616	LUT	C31-C30	3.99	1.55	1.43
31	s	314	CLA	MG-ND	-3.99	1.97	2.05
30	R	310	CHL	CBB-CAB	3.99	1.50	1.30
32	7	317	LUT	C31-C30	3.99	1.55	1.43
31	Y	313	CLA	MG-ND	-3.99	1.97	2.05
32	2	615	LUT	C7-C6	3.99	1.59	1.45
43	c	614	BCR	C11-C10	3.99	1.55	1.43
31	C	602	CLA	MG-ND	-3.99	1.97	2.05
32	7	317	LUT	C35-C34	3.99	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	616	LUT	C12-C13	3.99	1.54	1.45
31	B	608	CLA	MG-ND	-3.99	1.97	2.05
32	7	318	LUT	C7-C6	3.98	1.59	1.45
31	R	314	CLA	MG-ND	-3.98	1.97	2.05
32	N	317	LUT	C7-C6	3.98	1.59	1.45
31	b	609	CLA	MG-ND	-3.98	1.97	2.05
32	S	318	LUT	C28-C29	3.98	1.54	1.45
32	9	318	LUT	C28-C29	3.98	1.54	1.45
32	6	318	LUT	C28-C29	3.98	1.54	1.45
31	q	315	CLA	C1C-NC	-3.98	1.31	1.37
32	4	616	LUT	C7-C6	3.98	1.59	1.45
32	6	317	LUT	C28-C29	3.98	1.54	1.45
31	d	404	CLA	MG-ND	-3.98	1.97	2.05
32	0	617	LUT	C21-C26	3.98	1.67	1.56
31	y	613	CLA	C1C-NC	-3.98	1.31	1.37
31	s	313	CLA	MG-ND	-3.98	1.97	2.05
31	1	612	CLA	MG-ND	-3.97	1.97	2.05
31	y	612	CLA	MG-ND	-3.97	1.97	2.05
32	G	615	LUT	C28-C29	3.97	1.54	1.45
43	d	406	BCR	C20-C21	3.97	1.55	1.43
32	4	616	LUT	C28-C29	3.97	1.54	1.45
43	z	101	BCR	C20-C21	3.96	1.55	1.43
32	3	317	LUT	C7-C6	3.96	1.59	1.45
32	y	616	LUT	C15-C14	3.96	1.55	1.43
31	C	604	CLA	MG-ND	-3.96	1.97	2.05
31	a	406	CLA	MG-ND	-3.96	1.97	2.05
43	t	101	BCR	C20-C21	3.96	1.55	1.43
31	c	605	CLA	MG-ND	-3.96	1.97	2.05
31	4	612	CLA	MG-ND	-3.95	1.98	2.05
31	R	303	CLA	MG-ND	-3.95	1.98	2.05
31	C	606	CLA	MG-ND	-3.95	1.98	2.05
32	0	616	LUT	C35-C34	3.95	1.55	1.43
31	C	608	CLA	MG-ND	-3.95	1.98	2.05
43	a	410	BCR	C20-C21	3.95	1.55	1.43
31	R	316	CLA	MG-ND	-3.95	1.98	2.05
31	3	301	CLA	MG-ND	-3.95	1.98	2.05
31	q	306	CLA	MG-ND	-3.95	1.98	2.05
32	s	317	LUT	C7-C6	3.95	1.59	1.45
32	n	317	LUT	C28-C29	3.94	1.54	1.45
32	6	318	LUT	C7-C6	3.94	1.59	1.45
32	N	316	LUT	C7-C6	3.94	1.59	1.45
32	S	318	LUT	C7-C6	3.94	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	316	CLA	MG-ND	-3.94	1.98	2.05
32	r	317	LUT	C12-C13	3.94	1.54	1.45
43	B	617	BCR	C28-C27	3.94	1.64	1.52
31	B	615	CLA	MG-ND	-3.94	1.98	2.05
31	b	606	CLA	MG-ND	-3.94	1.98	2.05
32	n	318	LUT	C7-C6	3.94	1.59	1.45
43	C	615	BCR	C2-C1	3.94	1.63	1.54
31	S	315	CLA	MG-ND	-3.94	1.98	2.05
32	1	615	LUT	C35-C34	3.94	1.55	1.43
32	8	615	LUT	C28-C29	3.94	1.54	1.45
31	B	605	CLA	MG-ND	-3.94	1.98	2.05
31	r	312	CLA	MG-ND	-3.94	1.98	2.05
32	n	317	LUT	C7-C6	3.94	1.59	1.45
32	Y	315	LUT	C12-C13	3.94	1.54	1.45
31	c	611	CLA	MG-ND	-3.94	1.98	2.05
31	r	313	CLA	MG-ND	-3.94	1.98	2.05
31	y	611	CLA	MG-ND	-3.94	1.98	2.05
31	G	612	CLA	MG-ND	-3.94	1.98	2.05
32	3	317	LUT	C21-C26	3.93	1.67	1.56
32	s	317	LUT	C28-C29	3.93	1.54	1.45
31	r	311	CLA	MG-ND	-3.93	1.98	2.05
32	8	615	LUT	C7-C6	3.93	1.59	1.45
31	R	315	CLA	MG-ND	-3.93	1.98	2.05
43	d	406	BCR	C19-C18	3.93	1.54	1.45
32	8	616	LUT	C7-C6	3.93	1.59	1.45
31	B	601	CLA	MG-ND	-3.93	1.98	2.05
31	6	312	CLA	MG-ND	-3.93	1.98	2.05
31	R	312	CLA	MG-ND	-3.93	1.98	2.05
32	y	617	LUT	C31-C30	3.93	1.55	1.43
32	p	617	LUT	C28-C29	3.93	1.54	1.45
31	C	611	CLA	MG-ND	-3.93	1.98	2.05
31	C	613	CLA	MG-ND	-3.93	1.98	2.05
32	p	616	LUT	C21-C26	3.92	1.67	1.56
31	p	602	CLA	MG-ND	-3.92	1.98	2.05
32	7	318	LUT	C28-C29	3.92	1.54	1.45
32	Y	315	LUT	C15-C14	3.92	1.55	1.43
31	b	617	CLA	C1C-NC	-3.92	1.31	1.37
32	G	615	LUT	C21-C26	3.92	1.67	1.56
30	q	309	CHL	CBB-CAB	3.92	1.49	1.30
31	3	311	CLA	MG-ND	-3.92	1.98	2.05
31	B	606	CLA	MG-ND	-3.91	1.98	2.05
32	S	317	LUT	C7-C6	3.91	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	318	LUT	C28-C29	3.91	1.54	1.45
32	y	617	LUT	C35-C34	3.91	1.55	1.43
32	8	616	LUT	C28-C29	3.91	1.54	1.45
31	0	613	CLA	MG-ND	-3.91	1.98	2.05
43	C	615	BCR	C28-C27	3.91	1.64	1.52
32	5	617	LUT	C11-C10	3.91	1.55	1.43
32	r	317	LUT	C31-C30	3.90	1.55	1.43
31	g	310	CLA	MG-ND	-3.90	1.98	2.05
32	p	616	LUT	C28-C29	3.90	1.54	1.45
32	S	317	LUT	C28-C29	3.90	1.54	1.45
31	A	405	CLA	MG-ND	-3.90	1.98	2.05
31	B	616	CLA	C1C-NC	-3.90	1.32	1.37
31	R	311	CLA	MG-ND	-3.90	1.98	2.05
32	y	616	LUT	C31-C30	3.90	1.55	1.43
43	b	619	BCR	C3-C4	3.90	1.64	1.52
32	s	318	LUT	C7-C6	3.90	1.58	1.45
31	4	610	CLA	MG-ND	-3.90	1.98	2.05
32	p	616	LUT	C11-C10	3.89	1.55	1.43
32	R	317	LUT	C7-C6	3.89	1.58	1.45
32	6	317	LUT	C7-C6	3.89	1.58	1.45
31	S	312	CLA	MG-ND	-3.89	1.98	2.05
43	B	617	BCR	C4-C5	-3.89	1.43	1.51
32	Y	315	LUT	C35-C34	3.89	1.55	1.43
31	9	314	CLA	MG-ND	-3.89	1.98	2.05
31	4	613	CLA	MG-ND	-3.89	1.98	2.05
32	R	317	LUT	C21-C26	3.89	1.67	1.56
31	0	611	CLA	MG-ND	-3.89	1.98	2.05
31	3	312	CLA	MG-ND	-3.89	1.98	2.05
43	V	101	BCR	C3-C4	3.88	1.64	1.52
32	2	615	LUT	C28-C29	3.88	1.54	1.45
32	5	617	LUT	C21-C26	3.88	1.67	1.56
31	s	312	CLA	MG-ND	-3.88	1.98	2.05
43	D	405	BCR	C16-C17	3.88	1.55	1.43
30	1	619	CHL	CBB-CAB	3.88	1.49	1.30
43	c	615	BCR	C3-C4	3.88	1.64	1.52
31	a	407	CLA	MG-ND	-3.88	1.98	2.05
31	B	607	CLA	C4B-NB	-3.88	1.33	1.37
31	R	304	CLA	MG-ND	-3.87	1.98	2.05
31	0	604	CLA	MG-ND	-3.87	1.98	2.05
32	s	318	LUT	C28-C29	3.87	1.54	1.45
32	g	316	LUT	C21-C26	3.87	1.67	1.56
32	Y	316	LUT	C7-C6	3.87	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	313	CLA	MG-ND	-3.87	1.98	2.05
31	A	406	CLA	MG-ND	-3.87	1.98	2.05
32	Y	315	LUT	C31-C30	3.87	1.55	1.43
43	C	615	BCR	C3-C4	3.87	1.64	1.52
35	2	614	RRX	C16-C17	3.87	1.55	1.43
32	0	616	LUT	C7-C6	3.87	1.58	1.45
31	b	602	CLA	MG-ND	-3.87	1.98	2.05
43	C	615	BCR	C27-C26	-3.87	1.43	1.51
31	b	607	CLA	MG-ND	-3.87	1.98	2.05
35	G	614	RRX	C16-C17	3.87	1.55	1.43
32	9	318	LUT	C21-C26	3.87	1.67	1.56
31	1	602	CLA	MG-ND	-3.87	1.98	2.05
31	A	407	CLA	MG-ND	-3.86	1.98	2.05
31	d	401	CLA	MG-ND	-3.86	1.98	2.05
43	B	618	BCR	C3-C4	3.86	1.64	1.52
31	r	306	CLA	MG-ND	-3.86	1.98	2.05
35	9	317	RRX	C16-C17	3.86	1.55	1.43
31	S	311	CLA	MG-ND	-3.86	1.98	2.05
43	b	618	BCR	C20-C21	3.85	1.55	1.43
31	S	316	CLA	MG-ND	-3.85	1.98	2.05
32	q	318	LUT	C21-C26	3.85	1.67	1.56
31	0	602	CLA	MG-ND	-3.85	1.98	2.05
31	q	316	CLA	MG-ND	-3.85	1.98	2.05
32	S	318	LUT	C21-C26	3.85	1.67	1.56
35	4	615	RRX	C16-C17	3.85	1.55	1.43
35	g	315	RRX	C27-C26	-3.85	1.45	1.51
31	b	610	CLA	MG-ND	-3.85	1.98	2.05
31	s	310	CLA	MG-ND	-3.85	1.98	2.05
32	4	616	LUT	C21-C26	3.85	1.67	1.56
31	G	609	CLA	MG-ND	-3.85	1.98	2.05
32	y	616	LUT	C35-C34	3.85	1.55	1.43
32	s	317	LUT	C21-C26	3.85	1.67	1.56
32	N	317	LUT	C21-C26	3.85	1.67	1.56
31	C	608	CLA	C1C-NC	-3.85	1.32	1.37
32	0	617	LUT	C7-C6	3.85	1.58	1.45
31	s	311	CLA	MG-ND	-3.84	1.98	2.05
32	r	317	LUT	C15-C14	3.84	1.55	1.43
32	6	318	LUT	C21-C26	3.84	1.67	1.56
32	N	316	LUT	C21-C26	3.84	1.67	1.56
32	3	318	LUT	C11-C10	3.84	1.55	1.43
31	B	602	CLA	MG-ND	-3.84	1.98	2.05
32	S	317	LUT	C21-C26	3.84	1.67	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	613	CLA	MG-ND	-3.84	1.98	2.05
32	0	617	LUT	C28-C29	3.84	1.54	1.45
31	s	315	CLA	MG-ND	-3.83	1.98	2.05
35	G	614	RRX	C20-C21	3.83	1.55	1.43
31	c	604	CLA	MG-ND	-3.83	1.98	2.05
31	C	602	CLA	C1C-NC	-3.83	1.32	1.37
31	b	616	CLA	MG-ND	-3.83	1.98	2.05
43	v	101	BCR	C3-C4	3.83	1.64	1.52
35	g	315	RRX	C16-C17	3.82	1.55	1.43
32	3	318	LUT	C21-C26	3.82	1.67	1.56
32	1	616	LUT	C7-C6	3.82	1.58	1.45
32	5	616	LUT	C21-C26	3.82	1.67	1.56
32	7	317	LUT	C7-C6	3.82	1.58	1.45
32	8	615	LUT	C21-C26	3.82	1.67	1.56
31	r	303	CLA	C1C-NC	-3.82	1.32	1.37
31	r	315	CLA	MG-ND	-3.82	1.98	2.05
31	q	314	CLA	MG-ND	-3.82	1.98	2.05
31	S	310	CLA	MG-ND	-3.82	1.98	2.05
31	C	601	CLA	MG-ND	-3.81	1.98	2.05
31	B	609	CLA	MG-ND	-3.81	1.98	2.05
32	n	317	LUT	C21-C26	3.81	1.67	1.56
35	q	317	RRX	C16-C17	3.81	1.55	1.43
35	g	315	RRX	C20-C21	3.81	1.55	1.43
35	4	615	RRX	C20-C21	3.81	1.55	1.43
31	A	407	CLA	C1C-NC	-3.81	1.32	1.37
32	8	616	LUT	C21-C26	3.81	1.67	1.56
31	b	608	CLA	C1C-NC	-3.81	1.32	1.37
31	B	607	CLA	MG-ND	-3.80	1.98	2.05
31	0	615	CLA	MG-ND	-3.80	1.98	2.05
31	4	614	CLA	MG-ND	-3.80	1.98	2.05
32	7	318	LUT	C21-C26	3.80	1.67	1.56
35	9	317	RRX	C20-C21	3.80	1.55	1.43
32	6	317	LUT	C21-C26	3.79	1.67	1.56
31	b	603	CLA	MG-ND	-3.79	1.98	2.05
32	p	617	LUT	C11-C10	3.79	1.55	1.43
43	B	617	BCR	C19-C18	3.79	1.54	1.45
43	z	101	BCR	C3-C4	3.79	1.64	1.52
31	d	405	CLA	MG-ND	-3.79	1.98	2.05
32	n	318	LUT	C21-C26	3.78	1.66	1.56
32	Y	316	LUT	C28-C29	3.78	1.54	1.45
31	s	316	CLA	MG-ND	-3.78	1.98	2.05
31	a	409	CLA	MG-ND	-3.78	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	313	CLA	MG-ND	-3.77	1.98	2.05
32	1	615	LUT	C7-C6	3.77	1.58	1.45
43	C	614	BCR	C3-C4	3.77	1.64	1.52
32	G	615	LUT	C11-C10	3.77	1.55	1.43
32	g	316	LUT	C11-C10	3.77	1.55	1.43
32	7	317	LUT	C28-C29	3.77	1.54	1.45
35	2	614	RRX	C20-C21	3.77	1.55	1.43
32	y	616	LUT	C7-C6	3.76	1.58	1.45
31	c	601	CLA	MG-ND	-3.76	1.98	2.05
31	5	615	CLA	MG-ND	-3.76	1.98	2.05
43	B	619	BCR	C3-C4	3.76	1.64	1.52
31	A	409	CLA	MG-ND	-3.76	1.98	2.05
31	c	602	CLA	C1C-NC	-3.76	1.32	1.37
31	c	606	CLA	C1C-NC	-3.76	1.32	1.37
32	s	318	LUT	C21-C26	3.76	1.66	1.56
31	a	406	CLA	C1C-NC	-3.76	1.32	1.37
43	D	405	BCR	C11-C10	3.76	1.55	1.43
32	r	317	LUT	C35-C34	3.75	1.55	1.43
32	y	617	LUT	C7-C6	3.75	1.58	1.45
43	b	620	BCR	C3-C4	3.75	1.64	1.52
31	3	301	CLA	C1C-NC	-3.75	1.32	1.37
32	1	616	LUT	C28-C29	3.75	1.54	1.45
32	r	317	LUT	C7-C6	3.75	1.58	1.45
32	5	616	LUT	C11-C10	3.75	1.55	1.43
43	c	614	BCR	C3-C4	3.74	1.64	1.52
32	0	616	LUT	C28-C29	3.74	1.54	1.45
31	p	604	CLA	MG-ND	-3.74	1.98	2.05
31	R	311	CLA	C1C-NC	-3.74	1.32	1.37
31	r	312	CLA	C1C-NC	-3.73	1.32	1.37
31	n	315	CLA	MG-ND	-3.73	1.98	2.05
43	b	618	BCR	C3-C4	3.73	1.64	1.52
43	A	410	BCR	C3-C4	3.73	1.64	1.52
43	c	614	BCR	C16-C17	3.73	1.55	1.43
43	a	410	BCR	C3-C4	3.73	1.64	1.52
31	8	613	CLA	MG-ND	-3.72	1.98	2.05
43	D	405	BCR	C3-C4	3.72	1.64	1.52
31	c	609	CLA	C1C-NC	-3.72	1.32	1.37
31	d	401	CLA	C1C-NC	-3.72	1.32	1.37
32	0	616	LUT	C21-C26	3.72	1.66	1.56
31	N	314	CLA	MG-ND	-3.72	1.98	2.05
43	C	614	BCR	C27-C26	-3.72	1.43	1.51
43	Z	101	BCR	C3-C4	3.71	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	T	101	BCR	C16-C17	3.71	1.55	1.43
32	y	617	LUT	C21-C26	3.71	1.66	1.56
31	0	610	CLA	C4B-NB	-3.71	1.33	1.37
31	p	612	CLA	MG-ND	-3.71	1.98	2.05
31	0	610	CLA	C1C-NC	-3.71	1.32	1.37
43	h	101	BCR	C3-C4	3.71	1.64	1.52
31	r	311	CLA	C1C-NC	-3.71	1.32	1.37
32	q	318	LUT	C11-C10	3.71	1.54	1.43
32	2	615	LUT	C11-C10	3.71	1.54	1.43
43	b	618	BCR	C27-C26	-3.71	1.43	1.51
31	D	404	CLA	MG-ND	-3.70	1.98	2.05
31	A	405	CLA	C1C-NC	-3.70	1.32	1.37
31	c	608	CLA	C1C-NC	-3.70	1.32	1.37
43	B	617	BCR	C3-C4	3.70	1.64	1.52
32	Y	315	LUT	C21-C26	3.70	1.66	1.56
32	9	318	LUT	C11-C10	3.70	1.54	1.43
31	7	316	CLA	MG-ND	-3.70	1.98	2.05
32	7	317	LUT	C21-C26	3.69	1.66	1.56
31	6	316	CLA	MG-ND	-3.69	1.98	2.05
43	H	101	BCR	C3-C4	3.69	1.64	1.52
31	5	612	CLA	MG-ND	-3.69	1.98	2.05
31	2	611	CLA	MG-ND	-3.69	1.98	2.05
32	1	616	LUT	C21-C26	3.69	1.66	1.56
31	c	603	CLA	C1C-NC	-3.69	1.32	1.37
32	1	615	LUT	C21-C26	3.69	1.66	1.56
43	d	406	BCR	C4-C5	-3.69	1.43	1.51
31	5	611	CLA	MG-ND	-3.69	1.98	2.05
31	C	607	CLA	C1C-NC	-3.69	1.32	1.37
32	4	616	LUT	C11-C10	3.69	1.54	1.43
31	B	605	CLA	C1C-NC	-3.69	1.32	1.37
31	c	604	CLA	C1C-NC	-3.69	1.32	1.37
31	B	604	CLA	C1C-NC	-3.69	1.32	1.37
31	g	310	CLA	C1C-NC	-3.69	1.32	1.37
31	G	609	CLA	C1C-NC	-3.68	1.32	1.37
31	c	607	CLA	C1C-NC	-3.68	1.32	1.37
32	N	317	LUT	C11-C10	3.68	1.54	1.43
31	C	604	CLA	C1C-NC	-3.68	1.32	1.37
31	9	312	CLA	MG-ND	-3.68	1.98	2.05
32	S	318	LUT	C11-C10	3.68	1.54	1.43
32	3	317	LUT	C11-C10	3.68	1.54	1.43
31	2	612	CLA	MG-ND	-3.68	1.98	2.05
32	S	317	LUT	C38-C25	3.68	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	p	613	CLA	MG-ND	-3.67	1.98	2.05
31	3	316	CLA	C1C-NC	-3.67	1.32	1.37
32	Y	315	LUT	C7-C6	3.67	1.58	1.45
31	N	313	CLA	MG-ND	-3.67	1.98	2.05
32	N	316	LUT	C11-C10	3.67	1.54	1.43
32	s	317	LUT	C38-C25	3.67	1.57	1.50
31	b	606	CLA	C1C-NC	-3.67	1.32	1.37
30	q	309	CHL	C3A-C2A	-3.67	1.44	1.54
31	B	614	CLA	MG-ND	-3.66	1.98	2.05
32	R	317	LUT	C11-C10	3.66	1.54	1.43
31	b	605	CLA	C1C-NC	-3.66	1.32	1.37
31	R	315	CLA	C1C-NC	-3.66	1.32	1.37
31	8	610	CLA	MG-ND	-3.66	1.98	2.05
32	5	617	LUT	C19-C9	3.66	1.58	1.50
43	B	617	BCR	C27-C26	-3.66	1.43	1.51
31	3	314	CLA	MG-ND	-3.66	1.98	2.05
32	R	317	LUT	C28-C29	3.66	1.53	1.45
43	v	101	BCR	C16-C17	3.65	1.54	1.43
31	C	611	CLA	C1C-NC	-3.65	1.32	1.37
43	H	101	BCR	C4-C5	-3.65	1.43	1.51
43	d	406	BCR	C3-C4	3.65	1.63	1.52
31	s	305	CLA	MG-ND	-3.65	1.98	2.05
43	b	619	BCR	C16-C17	3.65	1.54	1.43
31	1	604	CLA	C1C-NC	-3.65	1.32	1.37
32	y	616	LUT	C21-C26	3.65	1.66	1.56
31	g	313	CLA	MG-ND	-3.65	1.98	2.05
43	t	101	BCR	C11-C10	3.65	1.54	1.43
31	N	321	CLA	MG-ND	-3.65	1.98	2.05
31	p	611	CLA	MG-ND	-3.65	1.98	2.05
31	q	313	CLA	MG-ND	-3.65	1.98	2.05
32	6	317	LUT	C38-C25	3.65	1.57	1.50
31	N	305	CLA	MG-ND	-3.65	1.98	2.05
43	T	101	BCR	C11-C10	3.65	1.54	1.43
31	A	409	CLA	C1C-NC	-3.65	1.32	1.37
32	1	615	LUT	C28-C29	3.65	1.53	1.45
31	9	312	CLA	C1C-NC	-3.65	1.32	1.37
32	7	318	LUT	C11-C10	3.64	1.54	1.43
31	y	604	CLA	MG-ND	-3.64	1.98	2.05
31	B	612	CLA	MG-ND	-3.64	1.98	2.05
35	q	317	RRX	C20-C21	3.64	1.54	1.43
43	c	615	BCR	C11-C10	3.64	1.54	1.43
32	4	616	LUT	C38-C25	3.64	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	312	CLA	MG-ND	-3.64	1.98	2.05
32	p	617	LUT	C38-C25	3.64	1.57	1.50
32	8	615	LUT	C11-C10	3.64	1.54	1.43
31	C	612	CLA	C1C-NC	-3.64	1.32	1.37
32	n	317	LUT	C11-C10	3.64	1.54	1.43
32	Y	316	LUT	C21-C26	3.64	1.66	1.56
31	D	403	CLA	C1C-NC	-3.64	1.32	1.37
31	5	614	CLA	MG-ND	-3.64	1.98	2.05
31	5	604	CLA	MG-ND	-3.64	1.98	2.05
31	B	603	CLA	C1C-NC	-3.64	1.32	1.37
31	a	409	CLA	C1C-NC	-3.63	1.32	1.37
32	g	316	LUT	C38-C25	3.63	1.57	1.50
31	2	604	CLA	MG-ND	-3.63	1.98	2.05
31	8	614	CLA	MG-ND	-3.63	1.98	2.05
31	R	304	CLA	C1C-NC	-3.63	1.32	1.37
32	Y	315	LUT	C28-C29	3.63	1.53	1.45
31	B	611	CLA	MG-ND	-3.63	1.98	2.05
31	n	312	CLA	MG-ND	-3.63	1.98	2.05
30	0	605	CHL	C3A-C2A	-3.63	1.44	1.54
31	6	313	CLA	MG-ND	-3.63	1.98	2.05
31	A	406	CLA	C1C-NC	-3.62	1.32	1.37
31	3	313	CLA	MG-ND	-3.62	1.98	2.05
43	T	101	BCR	C4-C5	-3.62	1.43	1.51
31	r	304	CLA	MG-ND	-3.62	1.98	2.05
32	8	616	LUT	C11-C10	3.62	1.54	1.43
31	p	614	CLA	MG-ND	-3.62	1.98	2.05
31	7	312	CLA	MG-ND	-3.62	1.98	2.05
31	Y	314	CLA	MG-ND	-3.62	1.98	2.05
31	C	603	CLA	C1C-NC	-3.62	1.32	1.37
31	4	611	CLA	MG-ND	-3.62	1.98	2.05
31	G	602	CLA	MG-ND	-3.62	1.98	2.05
32	n	318	LUT	C11-C10	3.62	1.54	1.43
31	2	613	CLA	MG-ND	-3.61	1.98	2.05
32	8	615	LUT	C38-C25	3.61	1.57	1.50
32	s	318	LUT	C11-C10	3.61	1.54	1.43
31	q	313	CLA	C1C-NC	-3.61	1.32	1.37
31	g	314	CLA	MG-ND	-3.61	1.98	2.05
43	B	617	BCR	C20-C21	3.61	1.54	1.43
43	t	101	BCR	C27-C26	-3.61	1.43	1.51
43	c	615	BCR	C16-C17	3.61	1.54	1.43
32	y	617	LUT	C28-C29	3.61	1.53	1.45
31	B	610	CLA	MG-ND	-3.61	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	T	101	BCR	C3-C4	3.61	1.63	1.52
31	p	610	CLA	MG-ND	-3.61	1.98	2.05
32	5	617	LUT	C38-C25	3.61	1.57	1.50
31	Y	311	CLA	C1C-NC	-3.61	1.32	1.37
32	6	317	LUT	C11-C10	3.61	1.54	1.43
32	q	318	LUT	C19-C9	3.61	1.58	1.50
31	c	613	CLA	C1C-NC	-3.61	1.32	1.37
43	C	614	BCR	C4-C5	-3.61	1.43	1.51
31	S	313	CLA	C1C-NC	-3.61	1.32	1.37
31	y	615	CLA	MG-ND	-3.61	1.98	2.05
31	S	311	CLA	C1C-NC	-3.61	1.32	1.37
43	V	101	BCR	C16-C17	3.60	1.54	1.43
31	9	316	CLA	MG-ND	-3.60	1.98	2.05
32	3	317	LUT	C38-C25	3.60	1.57	1.50
31	n	316	CLA	MG-ND	-3.60	1.98	2.05
31	G	604	CLA	MG-ND	-3.60	1.98	2.05
31	8	611	CLA	MG-ND	-3.60	1.98	2.05
31	p	615	CLA	MG-ND	-3.60	1.98	2.05
32	s	317	LUT	C11-C10	3.60	1.54	1.43
43	C	615	BCR	C11-C10	3.60	1.54	1.43
32	9	318	LUT	C19-C9	3.60	1.58	1.50
31	r	307	CLA	C1C-NC	-3.60	1.32	1.37
32	0	616	LUT	C38-C25	3.60	1.57	1.50
32	8	616	LUT	C19-C9	3.60	1.58	1.50
31	N	315	CLA	MG-ND	-3.60	1.98	2.05
32	7	318	LUT	C38-C25	3.60	1.57	1.50
32	n	317	LUT	C38-C25	3.60	1.57	1.50
31	R	312	CLA	C1C-NC	-3.60	1.32	1.37
31	3	315	CLA	MG-ND	-3.60	1.98	2.05
31	8	603	CLA	MG-ND	-3.60	1.98	2.05
31	R	314	CLA	C1C-NC	-3.60	1.32	1.37
31	N	312	CLA	MG-ND	-3.60	1.98	2.05
31	S	305	CLA	MG-ND	-3.60	1.98	2.05
31	7	315	CLA	MG-ND	-3.60	1.98	2.05
31	8	602	CLA	MG-ND	-3.60	1.98	2.05
31	7	305	CLA	MG-ND	-3.60	1.98	2.05
31	8	612	CLA	MG-ND	-3.60	1.98	2.05
31	Y	313	CLA	C1C-NC	-3.60	1.32	1.37
31	n	314	CLA	MG-ND	-3.59	1.98	2.05
31	n	313	CLA	MG-ND	-3.59	1.98	2.05
31	6	314	CLA	MG-ND	-3.59	1.98	2.05
32	6	318	LUT	C11-C10	3.59	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	A	410	BCR	C27-C26	-3.59	1.43	1.51
30	0	605	CHL	C1B-NB	-3.59	1.33	1.37
32	3	318	LUT	C19-C9	3.59	1.58	1.50
31	5	613	CLA	MG-ND	-3.59	1.98	2.05
31	n	304	CLA	MG-ND	-3.59	1.98	2.05
43	h	101	BCR	C4-C5	-3.59	1.43	1.51
32	n	318	LUT	C19-C9	3.59	1.58	1.50
43	B	618	BCR	C16-C17	3.59	1.54	1.43
31	B	613	CLA	MG-ND	-3.58	1.98	2.05
32	3	317	LUT	C19-C9	3.58	1.58	1.50
31	B	609	CLA	C1C-NC	-3.58	1.32	1.37
31	7	313	CLA	C1C-NC	-3.58	1.32	1.37
43	a	410	BCR	C27-C26	-3.58	1.43	1.51
35	g	315	RRX	C7-C6	3.58	1.57	1.45
32	S	317	LUT	C11-C10	3.58	1.54	1.43
31	c	605	CLA	C1C-NC	-3.58	1.32	1.37
31	a	407	CLA	C1C-NC	-3.58	1.32	1.37
31	N	304	CLA	MG-ND	-3.58	1.98	2.05
31	y	614	CLA	MG-ND	-3.58	1.98	2.05
32	6	317	LUT	C19-C9	3.58	1.58	1.50
32	N	316	LUT	C19-C9	3.58	1.58	1.50
31	g	305	CLA	MG-ND	-3.58	1.98	2.05
32	s	318	LUT	C38-C25	3.58	1.57	1.50
43	c	614	BCR	C4-C5	-3.58	1.43	1.51
32	6	318	LUT	C38-C25	3.58	1.57	1.50
31	1	614	CLA	MG-ND	-3.58	1.98	2.05
31	7	303	CLA	MG-ND	-3.58	1.98	2.05
43	C	615	BCR	C4-C5	-3.58	1.43	1.51
31	0	614	CLA	MG-ND	-3.58	1.98	2.05
32	Y	316	LUT	C23-C24	-3.58	1.45	1.50
32	S	317	LUT	C19-C9	3.58	1.58	1.50
32	s	317	LUT	C19-C9	3.58	1.58	1.50
31	6	303	CLA	MG-ND	-3.58	1.98	2.05
31	8	604	CLA	MG-ND	-3.58	1.98	2.05
43	Z	101	BCR	C16-C17	3.58	1.54	1.43
31	9	312	CLA	C4B-NB	-3.58	1.33	1.37
43	B	619	BCR	C4-C5	-3.57	1.43	1.51
32	9	318	LUT	C38-C25	3.57	1.57	1.50
31	c	611	CLA	C1C-NC	-3.57	1.32	1.37
31	y	602	CLA	MG-ND	-3.57	1.98	2.05
31	g	304	CLA	MG-ND	-3.57	1.98	2.05
31	5	602	CLA	MG-ND	-3.57	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	316	CLA	C1C-NC	-3.57	1.32	1.37
31	2	603	CLA	MG-ND	-3.57	1.98	2.05
31	b	611	CLA	MG-ND	-3.57	1.98	2.05
31	r	316	CLA	C1C-NC	-3.57	1.32	1.37
31	4	602	CLA	MG-ND	-3.57	1.98	2.05
31	Y	310	CLA	MG-ND	-3.57	1.98	2.05
43	A	410	BCR	C11-C10	3.57	1.54	1.43
31	n	305	CLA	MG-ND	-3.57	1.98	2.05
32	r	317	LUT	C21-C26	3.56	1.66	1.56
31	9	315	CLA	MG-ND	-3.56	1.98	2.05
32	5	616	LUT	C19-C9	3.56	1.58	1.50
32	G	615	LUT	C19-C9	3.56	1.58	1.50
32	n	317	LUT	C19-C9	3.56	1.58	1.50
31	6	304	CLA	MG-ND	-3.56	1.98	2.05
32	g	316	LUT	C19-C9	3.56	1.58	1.50
43	c	614	BCR	C27-C26	-3.56	1.44	1.51
43	B	619	BCR	C11-C10	3.56	1.54	1.43
43	b	618	BCR	C11-C10	3.56	1.54	1.43
31	B	606	CLA	C1C-NC	-3.56	1.32	1.37
31	3	306	CLA	MG-ND	-3.56	1.98	2.05
31	6	305	CLA	MG-ND	-3.56	1.98	2.05
31	Y	303	CLA	MG-ND	-3.56	1.98	2.05
31	B	602	CLA	C1C-NC	-3.56	1.32	1.37
32	7	318	LUT	C19-C9	3.56	1.58	1.50
31	N	311	CLA	MG-ND	-3.56	1.98	2.05
43	c	615	BCR	C27-C26	-3.55	1.44	1.51
31	1	603	CLA	C1C-NC	-3.55	1.32	1.37
31	9	306	CLA	MG-ND	-3.55	1.98	2.05
43	v	101	BCR	C11-C10	3.55	1.54	1.43
32	s	318	LUT	C19-C9	3.55	1.58	1.50
31	1	611	CLA	MG-ND	-3.55	1.98	2.05
32	S	318	LUT	C19-C9	3.55	1.58	1.50
43	V	101	BCR	C11-C10	3.55	1.54	1.43
31	Y	305	CLA	MG-ND	-3.55	1.98	2.05
31	B	615	CLA	C1C-NC	-3.55	1.32	1.37
31	6	311	CLA	MG-ND	-3.55	1.98	2.05
31	q	315	CLA	C4B-NB	-3.55	1.33	1.37
31	2	610	CLA	MG-ND	-3.55	1.98	2.05
31	C	601	CLA	C1C-NC	-3.55	1.32	1.37
31	S	303	CLA	MG-ND	-3.54	1.98	2.05
31	q	312	CLA	MG-ND	-3.54	1.98	2.05
32	8	615	LUT	C19-C9	3.54	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	614	BCR	C11-C10	3.54	1.54	1.43
31	b	613	CLA	MG-ND	-3.54	1.98	2.05
31	n	303	CLA	MG-ND	-3.54	1.98	2.05
32	G	615	LUT	C38-C25	3.54	1.57	1.50
31	N	310	CLA	MG-ND	-3.54	1.98	2.05
32	7	317	LUT	C11-C10	3.54	1.54	1.43
31	9	305	CLA	MG-ND	-3.54	1.98	2.05
32	Y	316	LUT	C11-C10	3.54	1.54	1.43
31	9	314	CLA	C1C-NC	-3.54	1.32	1.37
43	d	406	BCR	C27-C26	-3.54	1.44	1.51
43	z	101	BCR	C27-C26	-3.54	1.44	1.51
43	D	405	BCR	C24-C25	3.54	1.57	1.45
32	n	318	LUT	C38-C25	3.54	1.57	1.50
31	C	606	CLA	C1C-NC	-3.54	1.32	1.37
43	B	618	BCR	C24-C25	3.54	1.57	1.45
31	9	304	CLA	MG-ND	-3.54	1.98	2.05
43	z	101	BCR	C11-C10	3.54	1.54	1.43
32	y	617	LUT	C23-C24	-3.54	1.45	1.50
31	b	615	CLA	MG-ND	-3.54	1.98	2.05
35	9	317	RRX	C7-C6	3.54	1.57	1.45
31	s	310	CLA	C1C-NC	-3.54	1.32	1.37
42	D	401	PHO	C1D-C2D	3.53	1.43	1.39
31	R	306	CLA	C1C-NC	-3.53	1.32	1.37
32	p	617	LUT	C19-C9	3.53	1.58	1.50
31	G	603	CLA	MG-ND	-3.53	1.98	2.05
31	7	311	CLA	MG-ND	-3.53	1.98	2.05
31	r	306	CLA	C1C-NC	-3.53	1.32	1.37
31	q	306	CLA	C4B-NB	-3.53	1.33	1.37
31	R	307	CLA	C1C-NC	-3.53	1.32	1.37
35	G	614	RRX	C7-C6	3.53	1.57	1.45
32	4	616	LUT	C19-C9	3.53	1.58	1.50
32	q	318	LUT	C38-C25	3.53	1.57	1.50
43	A	410	BCR	C16-C17	3.53	1.54	1.43
32	N	317	LUT	C19-C9	3.53	1.58	1.50
31	3	301	CLA	C4B-NB	-3.53	1.33	1.37
31	G	612	CLA	C1C-NC	-3.53	1.32	1.37
31	3	316	CLA	C4B-NB	-3.53	1.33	1.37
31	S	313	CLA	C4B-NB	-3.53	1.33	1.37
31	1	602	CLA	C1C-NC	-3.53	1.32	1.37
32	2	615	LUT	C19-C9	3.53	1.58	1.50
32	6	318	LUT	C19-C9	3.53	1.58	1.50
31	2	602	CLA	MG-ND	-3.53	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	303	CLA	MG-ND	-3.53	1.98	2.05
43	h	101	BCR	C27-C26	-3.53	1.44	1.51
32	7	317	LUT	C38-C25	3.52	1.57	1.50
32	8	616	LUT	C38-C25	3.52	1.57	1.50
31	1	610	CLA	MG-ND	-3.52	1.98	2.05
31	B	601	CLA	C1C-NC	-3.52	1.32	1.37
31	r	303	CLA	C4B-NB	-3.52	1.33	1.37
31	d	405	CLA	C1C-NC	-3.52	1.32	1.37
43	h	101	BCR	C16-C17	3.52	1.54	1.43
31	3	304	CLA	MG-ND	-3.52	1.98	2.05
43	b	619	BCR	C24-C25	3.52	1.57	1.45
43	h	101	BCR	C11-C10	3.52	1.54	1.43
32	r	317	LUT	C28-C29	3.52	1.53	1.45
31	n	311	CLA	MG-ND	-3.52	1.98	2.05
32	0	617	LUT	C11-C10	3.52	1.54	1.43
31	A	407	CLA	C4B-NB	-3.52	1.33	1.37
31	2	609	CLA	MG-ND	-3.52	1.98	2.05
31	4	604	CLA	MG-ND	-3.52	1.98	2.05
32	3	318	LUT	C38-C25	3.52	1.57	1.50
43	Z	101	BCR	C11-C10	3.52	1.54	1.43
31	q	304	CLA	MG-ND	-3.52	1.98	2.05
31	b	602	CLA	C1C-NC	-3.52	1.32	1.37
31	c	612	CLA	C1C-NC	-3.52	1.32	1.37
31	C	613	CLA	C1C-NC	-3.52	1.32	1.37
32	1	616	LUT	C38-C25	3.52	1.57	1.50
31	s	303	CLA	MG-ND	-3.52	1.98	2.05
35	4	615	RRX	C7-C6	3.52	1.57	1.45
32	5	616	LUT	C38-C25	3.52	1.57	1.50
31	3	305	CLA	MG-ND	-3.51	1.98	2.05
31	s	316	CLA	C1C-NC	-3.51	1.32	1.37
31	b	612	CLA	MG-ND	-3.51	1.98	2.05
32	N	316	LUT	C38-C25	3.51	1.57	1.50
32	S	318	LUT	C38-C25	3.51	1.57	1.50
31	B	608	CLA	C1C-NC	-3.51	1.32	1.37
43	a	410	BCR	C16-C17	3.51	1.54	1.43
31	y	611	CLA	C1C-NC	-3.51	1.32	1.37
31	5	610	CLA	MG-ND	-3.51	1.98	2.05
43	B	619	BCR	C27-C26	-3.51	1.44	1.51
43	b	620	BCR	C11-C10	3.51	1.54	1.43
32	p	616	LUT	C19-C9	3.51	1.58	1.50
32	0	616	LUT	C11-C10	3.51	1.54	1.43
31	S	314	CLA	C1C-NC	-3.51	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	b	620	BCR	C16-C17	3.50	1.54	1.43
31	R	313	CLA	C1C-NC	-3.50	1.32	1.37
43	b	619	BCR	C11-C10	3.50	1.54	1.43
31	Y	312	CLA	C1C-NC	-3.50	1.32	1.37
31	s	311	CLA	C1C-NC	-3.50	1.32	1.37
31	4	612	CLA	C1C-NC	-3.50	1.32	1.37
31	r	315	CLA	C1C-NC	-3.50	1.32	1.37
32	y	616	LUT	C28-C29	3.50	1.53	1.45
43	b	620	BCR	C27-C26	-3.50	1.44	1.51
32	1	615	LUT	C38-C25	3.50	1.57	1.50
31	g	303	CLA	C1C-NC	-3.50	1.32	1.37
32	1	616	LUT	C11-C10	3.50	1.54	1.43
31	R	303	CLA	C1C-NC	-3.49	1.32	1.37
32	N	317	LUT	C38-C25	3.49	1.57	1.50
31	r	314	CLA	C1C-NC	-3.49	1.32	1.37
31	C	609	CLA	C1C-NC	-3.49	1.32	1.37
31	b	614	CLA	MG-ND	-3.49	1.98	2.05
43	C	614	BCR	C16-C17	3.49	1.54	1.43
43	b	620	BCR	C4-C5	-3.49	1.44	1.51
31	0	602	CLA	C1C-NC	-3.49	1.32	1.37
43	v	101	BCR	C24-C25	3.49	1.57	1.45
31	s	314	CLA	C1C-NC	-3.49	1.32	1.37
32	1	616	LUT	C19-C9	3.49	1.58	1.50
31	8	609	CLA	MG-ND	-3.49	1.98	2.05
43	H	101	BCR	C16-C17	3.49	1.54	1.43
43	H	101	BCR	C11-C10	3.49	1.54	1.43
31	6	315	CLA	MG-ND	-3.49	1.98	2.05
32	r	317	LUT	C38-C25	3.49	1.57	1.50
31	b	604	CLA	C1C-NC	-3.49	1.32	1.37
32	0	616	LUT	C19-C9	3.49	1.58	1.50
35	q	317	RRX	C7-C6	3.48	1.57	1.45
32	R	317	LUT	C23-C24	-3.48	1.45	1.50
31	D	404	CLA	C1C-NC	-3.48	1.32	1.37
31	s	313	CLA	C1C-NC	-3.48	1.32	1.37
43	A	410	BCR	C4-C5	-3.48	1.44	1.51
31	y	612	CLA	C1C-NC	-3.47	1.32	1.37
31	y	610	CLA	MG-ND	-3.47	1.98	2.05
31	s	304	CLA	MG-ND	-3.47	1.98	2.05
43	z	101	BCR	C16-C17	3.47	1.54	1.43
31	0	604	CLA	C1C-NC	-3.47	1.32	1.37
31	b	610	CLA	C1C-NC	-3.47	1.32	1.37
31	Y	304	CLA	MG-ND	-3.47	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	603	CLA	MG-ND	-3.47	1.98	2.05
31	4	613	CLA	C1C-NC	-3.47	1.32	1.37
43	Z	101	BCR	C27-C26	-3.47	1.44	1.51
43	T	101	BCR	C24-C25	3.47	1.57	1.45
43	a	410	BCR	C4-C5	-3.47	1.44	1.51
43	b	618	BCR	C4-C5	-3.47	1.44	1.51
31	3	311	CLA	C1C-NC	-3.46	1.32	1.37
43	B	619	BCR	C16-C17	3.46	1.54	1.43
31	C	604	CLA	C4B-NB	-3.46	1.33	1.37
31	R	305	CLA	C1C-NC	-3.46	1.32	1.37
35	2	614	RRX	C7-C6	3.46	1.57	1.45
43	c	615	BCR	C24-C25	3.46	1.57	1.45
31	r	305	CLA	MG-ND	-3.46	1.98	2.05
31	S	315	CLA	C1C-NC	-3.46	1.32	1.37
32	0	617	LUT	C38-C25	3.46	1.57	1.50
43	B	618	BCR	C11-C10	3.46	1.54	1.43
32	Y	315	LUT	C38-C25	3.46	1.57	1.50
43	T	101	BCR	C27-C26	-3.45	1.44	1.51
31	B	603	CLA	C4B-NB	-3.45	1.33	1.37
31	b	607	CLA	C1C-NC	-3.45	1.32	1.37
31	5	603	CLA	MG-ND	-3.45	1.98	2.05
31	1	613	CLA	C1C-NC	-3.45	1.32	1.37
47	E	101	HEM	C1B-NB	-3.44	1.34	1.40
43	H	101	BCR	C24-C25	3.44	1.57	1.45
43	t	101	BCR	C24-C25	3.44	1.57	1.45
31	s	315	CLA	C1C-NC	-3.44	1.32	1.37
32	y	616	LUT	C38-C25	3.44	1.57	1.50
31	A	409	CLA	C4B-NB	-3.44	1.33	1.37
43	b	620	BCR	C24-C25	3.44	1.57	1.45
43	a	410	BCR	C11-C10	3.44	1.54	1.43
31	s	306	CLA	MG-ND	-3.44	1.99	2.05
31	c	607	CLA	C4B-NB	-3.44	1.33	1.37
32	p	616	LUT	C38-C25	3.44	1.57	1.50
43	a	410	BCR	C24-C25	3.43	1.57	1.45
43	b	618	BCR	C16-C17	3.43	1.54	1.43
32	0	617	LUT	C19-C9	3.43	1.58	1.50
43	D	405	BCR	C4-C5	-3.43	1.44	1.51
43	c	615	BCR	C4-C5	-3.43	1.44	1.51
43	t	101	BCR	C16-C17	3.43	1.54	1.43
31	g	303	CLA	MG-ND	-3.43	1.99	2.05
31	G	613	CLA	C1C-NC	-3.43	1.32	1.37
32	p	616	LUT	C2-C1	3.43	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	q	314	CLA	C1C-NC	-3.43	1.32	1.37
31	0	615	CLA	C4B-NB	-3.43	1.33	1.37
30	1	601	CHL	C1B-NB	-3.43	1.33	1.37
31	D	403	CLA	C4B-NB	-3.42	1.33	1.37
31	C	610	CLA	C1C-NC	-3.42	1.32	1.37
31	1	612	CLA	C1C-NC	-3.42	1.32	1.37
31	7	304	CLA	MG-ND	-3.42	1.99	2.05
31	b	616	CLA	C1C-NC	-3.42	1.32	1.37
31	c	612	CLA	C4B-NB	-3.42	1.33	1.37
32	y	617	LUT	C19-C9	3.42	1.57	1.50
47	E	101	HEM	C4D-ND	-3.42	1.34	1.40
43	d	406	BCR	C16-C17	3.42	1.54	1.43
32	y	616	LUT	C19-C9	3.41	1.57	1.50
31	c	610	CLA	C1C-NC	-3.41	1.32	1.37
43	H	101	BCR	C27-C26	-3.41	1.44	1.51
43	B	617	BCR	C11-C10	3.41	1.54	1.43
43	h	101	BCR	C24-C25	3.41	1.57	1.45
31	c	602	CLA	C4B-NB	-3.41	1.33	1.37
31	d	404	CLA	C1C-NC	-3.41	1.32	1.37
43	t	101	BCR	C3-C4	3.41	1.63	1.52
31	B	616	CLA	C4B-NB	-3.41	1.33	1.37
32	1	615	LUT	C19-C9	3.41	1.57	1.50
31	4	603	CLA	MG-ND	-3.40	1.99	2.05
32	p	617	LUT	C2-C1	3.40	1.65	1.54
31	q	306	CLA	C1C-NC	-3.40	1.32	1.37
43	B	618	BCR	C27-C26	-3.40	1.44	1.51
43	V	101	BCR	C27-C26	-3.40	1.44	1.51
31	S	312	CLA	C1C-NC	-3.40	1.32	1.37
31	9	313	CLA	C1C-NC	-3.40	1.32	1.37
43	Z	101	BCR	C4-C5	-3.40	1.44	1.51
31	6	312	CLA	C1C-NC	-3.40	1.32	1.37
31	C	613	CLA	C4B-NB	-3.40	1.33	1.37
31	c	601	CLA	C1C-NC	-3.40	1.32	1.37
32	q	318	LUT	C2-C1	3.40	1.65	1.54
32	7	317	LUT	C19-C9	3.39	1.57	1.50
31	0	613	CLA	C1C-NC	-3.39	1.32	1.37
43	c	614	BCR	C24-C25	3.39	1.57	1.45
32	9	318	LUT	C2-C1	3.39	1.65	1.54
32	R	317	LUT	C38-C25	3.39	1.56	1.50
31	S	310	CLA	C1C-NC	-3.39	1.32	1.37
32	r	317	LUT	C19-C9	3.39	1.57	1.50
47	e	102	HEM	C1B-NB	-3.39	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	615	BCR	C24-C25	3.39	1.57	1.45
31	4	614	CLA	C1C-NC	-3.38	1.32	1.37
31	b	609	CLA	C1C-NC	-3.38	1.32	1.37
31	r	313	CLA	C1C-NC	-3.38	1.32	1.37
31	A	406	CLA	C4B-NB	-3.38	1.33	1.37
32	N	316	LUT	C2-C1	3.38	1.65	1.54
31	a	409	CLA	C4B-NB	-3.38	1.33	1.37
43	V	101	BCR	C24-C25	3.38	1.57	1.45
31	R	304	CLA	C4B-NB	-3.38	1.33	1.37
43	Z	101	BCR	C24-C25	3.38	1.57	1.45
31	c	609	CLA	C4B-NB	-3.38	1.33	1.37
43	A	410	BCR	C24-C25	3.38	1.57	1.45
31	C	607	CLA	C4B-NB	-3.38	1.33	1.37
31	4	610	CLA	C4B-NB	-3.38	1.33	1.37
31	g	311	CLA	C1C-NC	-3.38	1.32	1.37
31	0	612	CLA	C1C-NC	-3.37	1.32	1.37
31	b	603	CLA	C1C-NC	-3.37	1.32	1.37
43	z	101	BCR	C24-C25	3.37	1.57	1.45
32	5	616	LUT	C40-C33	3.37	1.57	1.50
43	d	406	BCR	C24-C25	3.37	1.57	1.45
32	1	615	LUT	C11-C10	3.37	1.53	1.43
31	G	611	CLA	C1C-NC	-3.37	1.32	1.37
31	7	314	CLA	C1C-NC	-3.37	1.32	1.37
31	R	315	CLA	C4B-NB	-3.37	1.33	1.37
31	r	311	CLA	C4B-NB	-3.37	1.33	1.37
43	v	101	BCR	C27-C26	-3.37	1.44	1.51
32	Y	315	LUT	C19-C9	3.37	1.57	1.50
31	B	604	CLA	C4B-NB	-3.37	1.33	1.37
32	8	615	LUT	C40-C33	3.36	1.57	1.50
32	5	616	LUT	C2-C1	3.36	1.65	1.54
32	6	317	LUT	C2-C1	3.36	1.65	1.54
45	c	616	DGD	CAB-C9B	-3.36	1.32	1.51
32	q	318	LUT	C40-C33	3.36	1.57	1.50
31	c	613	CLA	C4B-NB	-3.36	1.33	1.37
32	5	617	LUT	C2-C1	3.36	1.65	1.54
32	Y	316	LUT	C19-C9	3.36	1.57	1.50
47	e	102	HEM	C4D-ND	-3.36	1.34	1.40
32	s	318	LUT	C2-C1	3.36	1.65	1.54
31	0	603	CLA	C1C-NC	-3.36	1.32	1.37
31	s	312	CLA	C1C-NC	-3.36	1.32	1.37
31	C	602	CLA	C4B-NB	-3.36	1.33	1.37
31	p	602	CLA	C1C-NC	-3.35	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	605	CLA	C4B-NB	-3.35	1.33	1.37
43	B	619	BCR	C24-C25	3.35	1.57	1.45
31	q	305	CLA	MG-ND	-3.35	1.99	2.05
31	B	610	CLA	C1C-NC	-3.35	1.32	1.37
32	4	616	LUT	C40-C33	3.35	1.57	1.50
32	6	317	LUT	C40-C33	3.35	1.57	1.50
31	a	407	CLA	C4B-NB	-3.35	1.33	1.37
43	v	101	BCR	C4-C5	-3.35	1.44	1.51
32	S	317	LUT	C40-C33	3.35	1.57	1.50
31	S	306	CLA	MG-ND	-3.35	1.99	2.05
32	6	318	LUT	C2-C1	3.35	1.65	1.54
43	V	101	BCR	C4-C5	-3.35	1.44	1.51
43	C	615	BCR	C16-C17	3.35	1.53	1.43
43	d	406	BCR	C11-C10	3.35	1.53	1.43
32	y	617	LUT	C11-C10	3.35	1.53	1.43
32	6	318	LUT	C40-C33	3.35	1.57	1.50
34	B	621	LMG	C37-C36	-3.34	1.32	1.51
31	p	615	CLA	C1C-NC	-3.34	1.32	1.37
32	4	616	LUT	C2-C1	3.34	1.65	1.54
31	B	615	CLA	C4B-NB	-3.34	1.33	1.37
31	0	615	CLA	C1C-NC	-3.34	1.32	1.37
32	7	318	LUT	C2-C1	3.34	1.65	1.54
31	2	611	CLA	C1C-NC	-3.34	1.32	1.37
35	q	317	RRX	C4-C5	-3.34	1.44	1.51
32	5	617	LUT	C40-C33	3.34	1.57	1.50
32	2	615	LUT	C2-C1	3.34	1.65	1.54
32	S	318	LUT	C40-C33	3.34	1.57	1.50
31	B	605	CLA	C4B-NB	-3.34	1.33	1.37
32	Y	315	LUT	C11-C10	3.34	1.53	1.43
43	b	619	BCR	C27-C26	-3.34	1.44	1.51
31	b	617	CLA	C4B-NB	-3.34	1.33	1.37
34	g	322	LMG	C37-C36	-3.34	1.32	1.51
32	G	615	LUT	C2-C1	3.34	1.65	1.54
31	4	610	CLA	C1C-NC	-3.34	1.32	1.37
32	0	617	LUT	C23-C24	-3.34	1.45	1.50
32	3	317	LUT	C2-C1	3.33	1.65	1.54
32	G	615	LUT	C40-C33	3.33	1.57	1.50
43	z	101	BCR	C4-C5	-3.33	1.44	1.51
34	9	301	LMG	C19-C18	-3.33	1.32	1.51
32	1	616	LUT	C2-C1	3.33	1.65	1.54
32	p	616	LUT	C40-C33	3.33	1.57	1.50
32	n	317	LUT	C40-C33	3.33	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	c	617	DGD	CGB-CFB	-3.33	1.32	1.51
31	G	609	CLA	C4B-NB	-3.33	1.33	1.37
34	m	102	LMG	C37-C36	-3.32	1.32	1.51
32	8	615	LUT	C2-C1	3.32	1.65	1.54
31	C	611	CLA	C4B-NB	-3.32	1.33	1.37
31	B	602	CLA	C4B-NB	-3.32	1.33	1.37
32	n	317	LUT	C2-C1	3.32	1.65	1.54
32	g	316	LUT	C2-C1	3.32	1.65	1.54
32	N	316	LUT	C40-C33	3.32	1.57	1.50
31	B	611	CLA	C1C-NC	-3.32	1.32	1.37
32	r	317	LUT	C11-C10	3.32	1.53	1.43
32	7	318	LUT	C40-C33	3.32	1.57	1.50
45	c	618	DGD	CAA-C9A	-3.32	1.33	1.51
32	N	317	LUT	C40-C33	3.32	1.57	1.50
32	y	617	LUT	C38-C25	3.32	1.56	1.50
32	s	318	LUT	C40-C33	3.31	1.57	1.50
32	y	616	LUT	C30-C29	-3.31	1.31	1.35
32	S	318	LUT	C2-C1	3.31	1.65	1.54
34	d	410	LMG	C40-C39	-3.31	1.33	1.51
32	9	318	LUT	C40-C33	3.31	1.57	1.50
34	D	411	LMG	C40-C39	-3.31	1.33	1.51
31	3	313	CLA	C1C-NC	-3.31	1.32	1.37
32	0	616	LUT	C2-C1	3.31	1.65	1.54
31	g	310	CLA	C4B-NB	-3.31	1.33	1.37
32	7	317	LUT	C2-C1	3.30	1.65	1.54
32	s	317	LUT	C40-C33	3.30	1.57	1.50
34	b	601	LMG	C37-C36	-3.30	1.33	1.51
45	c	616	DGD	CGA-CFA	-3.30	1.33	1.51
31	q	316	CLA	C1C-NC	-3.30	1.32	1.37
32	n	318	LUT	C40-C33	3.30	1.57	1.50
43	C	614	BCR	C24-C25	3.30	1.56	1.45
32	3	318	LUT	C40-C33	3.30	1.57	1.50
31	R	311	CLA	C4B-NB	-3.30	1.33	1.37
45	c	617	DGD	CAB-C9B	-3.30	1.33	1.51
34	D	409	LMG	C19-C18	-3.30	1.33	1.51
31	q	312	CLA	C1C-NC	-3.30	1.32	1.37
34	D	410	LMG	C37-C36	-3.30	1.33	1.51
45	c	617	DGD	CAA-C9A	-3.30	1.33	1.51
32	N	317	LUT	C2-C1	3.30	1.65	1.54
34	m	102	LMG	C40-C39	-3.30	1.33	1.51
32	3	317	LUT	C40-C33	3.30	1.57	1.50
45	C	617	DGD	CGB-CFB	-3.30	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	617	DGD	CAB-C9B	-3.30	1.33	1.51
31	A	405	CLA	C4B-NB	-3.29	1.33	1.37
34	s	321	LMG	C19-C18	-3.29	1.33	1.51
34	W	201	LMG	C19-C18	-3.29	1.33	1.51
31	r	312	CLA	C4B-NB	-3.29	1.33	1.37
32	8	616	LUT	C40-C33	3.29	1.57	1.50
31	Y	314	CLA	C1C-NC	-3.29	1.32	1.37
31	p	614	CLA	C1C-NC	-3.29	1.32	1.37
34	b	601	LMG	C40-C39	-3.29	1.33	1.51
32	y	616	LUT	C11-C10	3.29	1.53	1.43
34	w	201	LMG	C19-C18	-3.29	1.33	1.51
43	B	618	BCR	C4-C5	-3.29	1.44	1.51
32	0	616	LUT	C23-C24	-3.29	1.45	1.50
31	G	612	CLA	C4B-NB	-3.29	1.33	1.37
34	b	622	LMG	C37-C36	-3.29	1.33	1.51
30	3	309	CHL	C1B-NB	-3.29	1.33	1.37
31	d	401	CLA	C4B-NB	-3.29	1.33	1.37
45	C	617	DGD	CDB-CCB	-3.29	1.33	1.51
31	n	316	CLA	C1C-NC	-3.29	1.32	1.37
31	r	305	CLA	C1C-NC	-3.29	1.32	1.37
34	W	201	LMG	C37-C36	-3.28	1.33	1.51
45	c	618	DGD	CAB-C9B	-3.28	1.33	1.51
45	c	619	DGD	CDA-CCA	-3.28	1.33	1.51
32	n	318	LUT	C2-C1	3.28	1.65	1.54
31	c	606	CLA	C4B-NB	-3.28	1.33	1.37
31	r	306	CLA	C4B-NB	-3.28	1.33	1.37
31	5	615	CLA	C1C-NC	-3.28	1.32	1.37
32	g	316	LUT	C40-C33	3.28	1.57	1.50
31	q	314	CLA	C4B-NB	-3.28	1.33	1.37
32	7	317	LUT	C23-C24	-3.28	1.45	1.50
31	b	605	CLA	C4B-NB	-3.28	1.33	1.37
34	W	201	LMG	C25-C24	-3.28	1.33	1.51
32	3	318	LUT	C2-C1	3.28	1.65	1.54
31	2	613	CLA	C1C-NC	-3.28	1.32	1.37
45	c	616	DGD	CGB-CFB	-3.28	1.33	1.51
34	W	201	LMG	C22-C21	-3.28	1.33	1.51
35	g	315	RRX	C4-C5	-3.28	1.44	1.51
31	6	314	CLA	C1C-NC	-3.28	1.32	1.37
31	p	603	CLA	C1C-NC	-3.28	1.32	1.37
34	w	201	LMG	C40-C39	-3.28	1.33	1.51
45	c	619	DGD	CAB-C9B	-3.28	1.33	1.51
31	S	316	CLA	C1C-NC	-3.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	J	101	LMG	C37-C36	-3.28	1.33	1.51
31	S	311	CLA	C4B-NB	-3.28	1.33	1.37
31	b	608	CLA	C4B-NB	-3.28	1.33	1.37
31	Y	305	CLA	C1C-NC	-3.28	1.32	1.37
30	1	601	CHL	C3A-C2A	-3.28	1.45	1.54
31	6	305	CLA	C1C-NC	-3.28	1.32	1.37
34	D	411	LMG	C37-C36	-3.27	1.33	1.51
31	r	304	CLA	C1C-NC	-3.27	1.32	1.37
43	b	618	BCR	C24-C25	3.27	1.56	1.45
34	b	622	LMG	C22-C21	-3.27	1.33	1.51
34	B	621	LMG	C22-C21	-3.27	1.33	1.51
31	1	610	CLA	C1C-NC	-3.27	1.32	1.37
34	D	409	LMG	C22-C21	-3.27	1.33	1.51
45	C	617	DGD	CAA-C9A	-3.27	1.33	1.51
31	C	612	CLA	C4B-NB	-3.27	1.33	1.37
31	a	406	CLA	C4B-NB	-3.27	1.33	1.37
34	J	101	LMG	C19-C18	-3.27	1.33	1.51
31	N	310	CLA	C1C-NC	-3.27	1.32	1.37
34	2	620	LMG	C40-C39	-3.27	1.33	1.51
32	8	616	LUT	C2-C1	3.27	1.65	1.54
32	y	616	LUT	C2-C1	3.27	1.65	1.54
43	b	619	BCR	C4-C5	-3.27	1.44	1.51
34	d	410	LMG	C37-C36	-3.27	1.33	1.51
34	C	619	LMG	C40-C39	-3.27	1.33	1.51
34	J	101	LMG	C40-C39	-3.27	1.33	1.51
34	B	621	LMG	C19-C18	-3.27	1.33	1.51
34	D	412	LMG	C37-C36	-3.27	1.33	1.51
45	c	616	DGD	CDA-CCA	-3.27	1.33	1.51
34	9	301	LMG	C37-C36	-3.27	1.33	1.51
31	Y	313	CLA	C4B-NB	-3.27	1.33	1.37
34	C	624	LMG	C19-C18	-3.27	1.33	1.51
31	C	609	CLA	C4B-NB	-3.26	1.33	1.37
34	b	626	LMG	C37-C36	-3.26	1.33	1.51
34	C	619	LMG	C19-C18	-3.26	1.33	1.51
31	q	312	CLA	C3B-C4B	3.26	1.46	1.39
34	c	624	LMG	C40-C39	-3.26	1.33	1.51
31	7	316	CLA	C1C-NC	-3.26	1.32	1.37
31	y	604	CLA	C1C-NC	-3.26	1.32	1.37
45	C	620	DGD	CAA-C9A	-3.26	1.33	1.51
45	c	616	DGD	CDB-CCB	-3.26	1.33	1.51
32	Y	315	LUT	C23-C24	-3.26	1.45	1.50
34	0	620	LMG	C19-C18	-3.26	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	304	CLA	C1C-NC	-3.26	1.32	1.37
34	A	412	LMG	C19-C18	-3.26	1.33	1.51
32	p	617	LUT	C40-C33	3.26	1.57	1.50
34	w	202	LMG	C37-C36	-3.26	1.33	1.51
34	j	101	LMG	C19-C18	-3.26	1.33	1.51
32	0	616	LUT	C40-C33	3.26	1.57	1.50
34	g	322	LMG	C19-C18	-3.26	1.33	1.51
31	N	312	CLA	C1C-NC	-3.26	1.32	1.37
45	c	618	DGD	CDA-CCA	-3.26	1.33	1.51
34	C	624	LMG	C22-C21	-3.26	1.33	1.51
45	C	618	DGD	CAA-C9A	-3.26	1.33	1.51
34	J	101	LMG	C22-C21	-3.26	1.33	1.51
34	w	202	LMG	C25-C24	-3.26	1.33	1.51
31	0	611	CLA	C1C-NC	-3.25	1.32	1.37
31	n	304	CLA	C1C-NC	-3.25	1.32	1.37
31	s	305	CLA	C1C-NC	-3.25	1.32	1.37
31	4	611	CLA	C3B-C4B	3.25	1.46	1.39
45	C	620	DGD	CGA-CFA	-3.25	1.33	1.51
31	b	610	CLA	C4B-NB	-3.25	1.33	1.37
45	C	620	DGD	CDB-CCB	-3.25	1.33	1.51
31	B	614	CLA	C1C-NC	-3.25	1.33	1.37
31	q	305	CLA	C1C-NC	-3.25	1.33	1.37
31	b	612	CLA	C1C-NC	-3.25	1.33	1.37
32	p	617	LUT	C23-C24	-3.25	1.45	1.50
34	b	622	LMG	C19-C18	-3.25	1.33	1.51
34	s	321	LMG	C22-C21	-3.25	1.33	1.51
31	3	314	CLA	C1C-NC	-3.25	1.33	1.37
34	G	621	LMG	C22-C21	-3.25	1.33	1.51
32	R	317	LUT	C2-C1	3.25	1.65	1.54
45	c	617	DGD	CDB-CCB	-3.25	1.33	1.51
31	N	314	CLA	C1C-NC	-3.25	1.33	1.37
31	7	304	CLA	C1C-NC	-3.25	1.33	1.37
32	S	317	LUT	C2-C1	3.25	1.65	1.54
31	N	321	CLA	C1C-NC	-3.25	1.33	1.37
31	p	612	CLA	C1C-NC	-3.25	1.33	1.37
34	D	412	LMG	C19-C18	-3.25	1.33	1.51
34	w	202	LMG	C22-C21	-3.25	1.33	1.51
32	0	617	LUT	C40-C33	3.25	1.57	1.50
34	D	412	LMG	C40-C39	-3.25	1.33	1.51
31	8	612	CLA	C1C-NC	-3.25	1.33	1.37
34	4	620	LMG	C40-C39	-3.24	1.33	1.51
34	d	410	LMG	C22-C21	-3.24	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	411	LMG	C19-C18	-3.24	1.33	1.51
34	w	202	LMG	C19-C18	-3.24	1.33	1.51
31	2	603	CLA	C1C-NC	-3.24	1.33	1.37
45	C	617	DGD	CGA-CFA	-3.24	1.33	1.51
31	3	305	CLA	C1C-NC	-3.24	1.33	1.37
31	g	304	CLA	C1C-NC	-3.24	1.33	1.37
34	j	101	LMG	C37-C36	-3.24	1.33	1.51
34	c	624	LMG	C37-C36	-3.24	1.33	1.51
34	C	619	LMG	C22-C21	-3.24	1.33	1.51
34	W	201	LMG	C43-C42	-3.24	1.33	1.51
32	y	616	LUT	C23-C24	-3.24	1.45	1.50
32	s	317	LUT	C2-C1	3.24	1.65	1.54
43	B	617	BCR	C16-C17	3.24	1.53	1.43
45	C	617	DGD	CDA-CCA	-3.24	1.33	1.51
34	k	101	LMG	C19-C18	-3.24	1.33	1.51
34	D	410	LMG	C19-C18	-3.24	1.33	1.51
34	9	301	LMG	C22-C21	-3.24	1.33	1.51
45	C	620	DGD	CDA-CCA	-3.24	1.33	1.51
32	8	615	LUT	C23-C24	-3.24	1.45	1.50
34	D	411	LMG	C22-C21	-3.24	1.33	1.51
31	G	610	CLA	C1C-NC	-3.24	1.33	1.37
32	8	616	LUT	C23-C24	-3.24	1.45	1.50
45	c	618	DGD	CDB-CCB	-3.24	1.33	1.51
31	r	315	CLA	C4B-NB	-3.24	1.33	1.37
32	R	317	LUT	C19-C9	3.24	1.57	1.50
34	C	619	LMG	C37-C36	-3.24	1.33	1.51
31	N	303	CLA	C1C-NC	-3.24	1.33	1.37
34	2	620	LMG	C22-C21	-3.23	1.33	1.51
34	k	101	LMG	C40-C39	-3.23	1.33	1.51
45	C	620	DGD	CAB-C9B	-3.23	1.33	1.51
31	7	305	CLA	C1C-NC	-3.23	1.33	1.37
34	4	620	LMG	C37-C36	-3.23	1.33	1.51
34	G	621	LMG	C19-C18	-3.23	1.33	1.51
45	c	619	DGD	CGA-CFA	-3.23	1.33	1.51
34	4	620	LMG	C22-C21	-3.23	1.33	1.51
34	w	202	LMG	C40-C39	-3.23	1.33	1.51
43	D	405	BCR	C27-C26	-3.23	1.44	1.51
31	b	611	CLA	C1C-NC	-3.23	1.33	1.37
45	C	618	DGD	CDA-CCA	-3.23	1.33	1.51
45	c	618	DGD	CGB-CFB	-3.23	1.33	1.51
31	Y	311	CLA	C4B-NB	-3.23	1.33	1.37
45	c	619	DGD	CAA-C9A	-3.23	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	604	CLA	C4B-NB	-3.23	1.33	1.37
31	D	404	CLA	C4B-NB	-3.23	1.33	1.37
34	d	411	LMG	C37-C36	-3.23	1.33	1.51
31	g	313	CLA	C1C-NC	-3.23	1.33	1.37
31	b	604	CLA	C4B-NB	-3.23	1.33	1.37
31	4	603	CLA	C1C-NC	-3.23	1.33	1.37
34	k	101	LMG	C37-C36	-3.23	1.33	1.51
31	g	312	CLA	C1C-NC	-3.23	1.33	1.37
31	s	306	CLA	C1C-NC	-3.23	1.33	1.37
31	G	604	CLA	C1C-NC	-3.23	1.33	1.37
34	S	321	LMG	C22-C21	-3.23	1.33	1.51
34	q	301	LMG	C22-C21	-3.23	1.33	1.51
31	C	608	CLA	C4B-NB	-3.23	1.33	1.37
31	S	304	CLA	C4B-NB	-3.23	1.33	1.37
34	B	621	LMG	C40-C39	-3.23	1.33	1.51
31	y	603	CLA	C1C-NC	-3.23	1.33	1.37
34	b	622	LMG	C40-C39	-3.23	1.33	1.51
32	9	318	LUT	C23-C24	-3.23	1.45	1.50
34	d	410	LMG	C19-C18	-3.23	1.33	1.51
31	2	610	CLA	C1C-NC	-3.22	1.33	1.37
34	2	620	LMG	C37-C36	-3.22	1.33	1.51
32	r	317	LUT	C2-C1	3.22	1.64	1.54
31	6	304	CLA	C1C-NC	-3.22	1.33	1.37
45	C	618	DGD	CAB-C9B	-3.22	1.33	1.51
34	D	411	LMG	C19-C18	-3.22	1.33	1.51
45	C	618	DGD	CGB-CFB	-3.22	1.33	1.51
31	3	315	CLA	C1C-NC	-3.22	1.33	1.37
31	5	612	CLA	C1C-NC	-3.22	1.33	1.37
31	d	404	CLA	C4B-NB	-3.22	1.33	1.37
31	g	314	CLA	C1C-NC	-3.22	1.33	1.37
34	G	621	LMG	C37-C36	-3.22	1.33	1.51
32	n	317	LUT	C23-C24	-3.22	1.45	1.50
31	Y	304	CLA	C1C-NC	-3.22	1.33	1.37
31	9	304	CLA	C1C-NC	-3.22	1.33	1.37
34	6	321	LMG	C19-C18	-3.22	1.33	1.51
31	6	303	CLA	C1C-NC	-3.22	1.33	1.37
34	d	411	LMG	C40-C39	-3.22	1.33	1.51
31	5	613	CLA	C1C-NC	-3.21	1.33	1.37
31	1	602	CLA	C4B-NB	-3.21	1.33	1.37
32	1	615	LUT	C2-C1	3.21	1.64	1.54
31	S	305	CLA	C1C-NC	-3.21	1.33	1.37
31	y	602	CLA	C1C-NC	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	q	301	LMG	C37-C36	-3.21	1.33	1.51
32	n	318	LUT	C23-C24	-3.21	1.45	1.50
31	s	311	CLA	C4B-NB	-3.21	1.33	1.37
34	S	321	LMG	C19-C18	-3.21	1.33	1.51
31	n	311	CLA	C1C-NC	-3.21	1.33	1.37
45	c	618	DGD	CGA-CFA	-3.21	1.33	1.51
31	8	610	CLA	C1C-NC	-3.21	1.33	1.37
31	R	306	CLA	C4B-NB	-3.21	1.33	1.37
31	2	613	CLA	C4B-NB	-3.21	1.33	1.37
45	C	618	DGD	CGA-CFA	-3.21	1.33	1.51
31	d	405	CLA	C4B-NB	-3.21	1.33	1.37
31	9	305	CLA	C1C-NC	-3.21	1.33	1.37
31	y	614	CLA	C1C-NC	-3.21	1.33	1.37
31	5	611	CLA	C1C-NC	-3.21	1.33	1.37
31	B	608	CLA	C4B-NB	-3.21	1.33	1.37
45	c	619	DGD	CDB-CCB	-3.21	1.33	1.51
32	7	317	LUT	C40-C33	3.21	1.57	1.50
34	w	202	LMG	C43-C42	-3.21	1.33	1.51
31	G	602	CLA	C1C-NC	-3.21	1.33	1.37
31	7	312	CLA	C1C-NC	-3.21	1.33	1.37
31	n	315	CLA	C1C-NC	-3.21	1.33	1.37
34	4	620	LMG	C19-C18	-3.21	1.33	1.51
31	N	305	CLA	C1C-NC	-3.20	1.33	1.37
31	n	305	CLA	C1C-NC	-3.20	1.33	1.37
44	A	416	PL9	C7-C3	-3.20	1.48	1.51
31	N	304	CLA	C1C-NC	-3.20	1.33	1.37
31	7	311	CLA	C1C-NC	-3.20	1.33	1.37
31	n	312	CLA	C1C-NC	-3.20	1.33	1.37
34	2	620	LMG	C19-C18	-3.20	1.33	1.51
34	q	301	LMG	C19-C18	-3.20	1.33	1.51
45	C	618	DGD	CDB-CCB	-3.20	1.33	1.51
31	p	611	CLA	C1C-NC	-3.20	1.33	1.37
31	n	314	CLA	C1C-NC	-3.20	1.33	1.37
31	5	604	CLA	C1C-NC	-3.20	1.33	1.37
31	y	610	CLA	C1C-NC	-3.20	1.33	1.37
31	Y	303	CLA	C1C-NC	-3.20	1.33	1.37
31	y	615	CLA	C1C-NC	-3.20	1.33	1.37
31	6	313	CLA	C1C-NC	-3.20	1.33	1.37
34	G	621	LMG	C40-C39	-3.20	1.33	1.51
44	a	414	PL9	C3-C4	-3.20	1.44	1.49
31	p	604	CLA	C1C-NC	-3.19	1.33	1.37
34	g	322	LMG	C40-C39	-3.19	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	606	CLA	C4B-NB	-3.19	1.33	1.37
31	8	614	CLA	C1C-NC	-3.19	1.33	1.37
32	1	616	LUT	C40-C33	3.19	1.57	1.50
32	Y	315	LUT	C2-C1	3.19	1.64	1.54
32	Y	316	LUT	C2-C1	3.19	1.64	1.54
31	Y	310	CLA	C1C-NC	-3.19	1.33	1.37
34	W	201	LMG	C40-C39	-3.19	1.33	1.51
45	c	619	DGD	CGB-CFB	-3.19	1.33	1.51
31	1	611	CLA	C1C-NC	-3.19	1.33	1.37
31	S	306	CLA	C1C-NC	-3.19	1.33	1.37
31	s	303	CLA	C1C-NC	-3.19	1.33	1.37
31	2	612	CLA	C1C-NC	-3.19	1.33	1.37
34	9	301	LMG	C40-C39	-3.19	1.33	1.51
31	2	609	CLA	C1C-NC	-3.19	1.33	1.37
31	1	614	CLA	C1C-NC	-3.18	1.33	1.37
31	8	604	CLA	C1C-NC	-3.18	1.33	1.37
31	6	316	CLA	C4B-NB	-3.18	1.33	1.37
32	N	316	LUT	C23-C24	-3.18	1.45	1.50
31	b	603	CLA	C4B-NB	-3.18	1.33	1.37
31	p	613	CLA	C1C-NC	-3.18	1.33	1.37
31	r	307	CLA	C4B-NB	-3.18	1.33	1.37
31	3	306	CLA	C1C-NC	-3.18	1.33	1.37
34	w	201	LMG	C37-C36	-3.18	1.33	1.51
31	S	303	CLA	C1C-NC	-3.18	1.33	1.37
32	0	617	LUT	C2-C1	3.18	1.64	1.54
31	R	312	CLA	C4B-NB	-3.18	1.33	1.37
32	y	617	LUT	C2-C1	3.18	1.64	1.54
31	9	306	CLA	C1C-NC	-3.18	1.33	1.37
34	q	301	LMG	C40-C39	-3.18	1.33	1.51
31	y	604	CLA	C4B-NB	-3.17	1.33	1.37
31	5	603	CLA	C1C-NC	-3.17	1.33	1.37
31	3	304	CLA	C1C-NC	-3.17	1.33	1.37
31	9	316	CLA	C1C-NC	-3.17	1.33	1.37
31	b	614	CLA	C1C-NC	-3.17	1.33	1.37
31	S	306	CLA	C4B-NB	-3.17	1.33	1.37
31	S	315	CLA	C4B-NB	-3.17	1.33	1.37
34	b	626	LMG	C19-C18	-3.17	1.33	1.51
42	A	408	PHO	C1D-C2D	3.17	1.43	1.39
31	4	602	CLA	C1C-NC	-3.17	1.33	1.37
31	B	611	CLA	C4B-NB	-3.17	1.33	1.37
31	n	303	CLA	C1C-NC	-3.17	1.33	1.37
31	n	313	CLA	C1C-NC	-3.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	608	CLA	C4B-NB	-3.16	1.33	1.37
31	r	316	CLA	C4B-NB	-3.16	1.33	1.37
31	3	312	CLA	C1C-NC	-3.16	1.33	1.37
31	9	315	CLA	C1C-NC	-3.16	1.33	1.37
31	g	305	CLA	C1C-NC	-3.16	1.33	1.37
32	1	615	LUT	C23-C24	-3.16	1.45	1.50
32	r	317	LUT	C23-C24	-3.16	1.45	1.50
31	8	609	CLA	C1C-NC	-3.16	1.33	1.37
31	N	315	CLA	C1C-NC	-3.16	1.33	1.37
31	b	606	CLA	C4B-NB	-3.16	1.33	1.37
31	2	602	CLA	C1C-NC	-3.16	1.33	1.37
31	2	604	CLA	C1C-NC	-3.16	1.33	1.37
31	5	614	CLA	C1C-NC	-3.16	1.33	1.37
31	B	609	CLA	C4B-NB	-3.16	1.33	1.37
31	Y	314	CLA	C4B-NB	-3.16	1.33	1.37
32	Y	316	LUT	C38-C25	3.16	1.56	1.50
31	b	616	CLA	C4B-NB	-3.16	1.33	1.37
31	y	602	CLA	C4B-NB	-3.16	1.33	1.37
31	8	611	CLA	C1C-NC	-3.16	1.33	1.37
32	Y	315	LUT	C40-C33	3.16	1.57	1.50
31	b	613	CLA	C1C-NC	-3.16	1.33	1.37
31	p	613	CLA	C4B-NB	-3.16	1.33	1.37
32	1	615	LUT	C40-C33	3.15	1.57	1.50
31	R	305	CLA	C4B-NB	-3.15	1.33	1.37
31	B	613	CLA	C1C-NC	-3.15	1.33	1.37
31	b	615	CLA	C1C-NC	-3.15	1.33	1.37
31	7	315	CLA	C1C-NC	-3.15	1.33	1.37
31	c	610	CLA	C4B-NB	-3.15	1.33	1.37
31	N	311	CLA	C1C-NC	-3.15	1.33	1.37
32	4	616	LUT	C23-C24	-3.15	1.45	1.50
31	5	610	CLA	C1C-NC	-3.15	1.33	1.37
31	6	315	CLA	C1C-NC	-3.15	1.33	1.37
45	C	620	DGD	CGB-CFB	-3.15	1.33	1.51
31	6	316	CLA	C1C-NC	-3.15	1.33	1.37
31	G	603	CLA	C1C-NC	-3.15	1.33	1.37
31	8	603	CLA	C1C-NC	-3.15	1.33	1.37
31	c	611	CLA	C4B-NB	-3.15	1.33	1.37
32	q	318	LUT	C23-C24	-3.15	1.45	1.50
31	5	602	CLA	C1C-NC	-3.14	1.33	1.37
31	Y	305	CLA	C4B-NB	-3.14	1.33	1.37
34	b	626	LMG	C22-C21	-3.14	1.33	1.51
31	6	311	CLA	C1C-NC	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	314	CLA	C4B-NB	-3.14	1.33	1.37
32	r	317	LUT	C40-C33	3.14	1.57	1.50
31	s	303	CLA	C4B-NB	-3.14	1.33	1.37
31	N	313	CLA	C1C-NC	-3.14	1.33	1.37
31	2	611	CLA	C4B-NB	-3.14	1.33	1.37
34	D	410	LMG	C22-C21	-3.14	1.34	1.51
31	b	607	CLA	C4B-NB	-3.14	1.33	1.37
32	6	317	LUT	C23-C24	-3.14	1.45	1.50
31	9	304	CLA	C4B-NB	-3.14	1.33	1.37
31	8	613	CLA	C1C-NC	-3.14	1.33	1.37
31	s	310	CLA	C4B-NB	-3.13	1.33	1.37
31	7	303	CLA	C1C-NC	-3.13	1.33	1.37
31	9	316	CLA	C4B-NB	-3.13	1.33	1.37
32	r	317	LUT	C30-C29	-3.13	1.31	1.35
32	N	317	LUT	C23-C24	-3.13	1.45	1.50
31	0	614	CLA	C1C-NC	-3.13	1.33	1.37
31	S	304	CLA	C1C-NC	-3.13	1.33	1.37
31	G	611	CLA	C4B-NB	-3.13	1.33	1.37
31	8	602	CLA	C1C-NC	-3.12	1.33	1.37
31	R	316	CLA	C4B-NB	-3.12	1.33	1.37
31	7	305	CLA	C4B-NB	-3.12	1.33	1.37
31	q	313	CLA	C3B-C4B	3.12	1.46	1.39
31	0	602	CLA	C4B-NB	-3.12	1.33	1.37
31	b	613	CLA	C4B-NB	-3.12	1.33	1.37
31	3	304	CLA	C4B-NB	-3.12	1.33	1.37
31	4	612	CLA	C4B-NB	-3.12	1.33	1.37
45	c	616	DGD	CAA-C9A	-3.12	1.34	1.51
31	3	311	CLA	C4B-NB	-3.12	1.34	1.37
31	c	603	CLA	C4B-NB	-3.12	1.34	1.37
31	b	612	CLA	C4B-NB	-3.12	1.34	1.37
31	B	612	CLA	C1C-NC	-3.12	1.33	1.37
31	4	614	CLA	C4B-NB	-3.11	1.34	1.37
31	N	310	CLA	C4B-NB	-3.11	1.34	1.37
31	7	315	CLA	C4B-NB	-3.11	1.34	1.37
31	r	304	CLA	C4B-NB	-3.11	1.34	1.37
32	2	615	LUT	C40-C33	3.11	1.57	1.50
32	R	317	LUT	C40-C33	3.11	1.57	1.50
31	p	610	CLA	C1C-NC	-3.11	1.33	1.37
32	y	616	LUT	C40-C33	3.11	1.57	1.50
31	G	604	CLA	C4B-NB	-3.11	1.34	1.37
31	b	609	CLA	C4B-NB	-3.11	1.34	1.37
31	S	303	CLA	C4B-NB	-3.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	313	CLA	C4B-NB	-3.11	1.34	1.37
31	s	305	CLA	C4B-NB	-3.10	1.34	1.37
32	Y	316	LUT	C40-C33	3.10	1.57	1.50
31	0	613	CLA	C4B-NB	-3.10	1.34	1.37
31	1	610	CLA	C4B-NB	-3.10	1.34	1.37
32	y	617	LUT	C40-C33	3.10	1.57	1.50
31	4	604	CLA	C1C-NC	-3.10	1.33	1.37
32	S	317	LUT	C23-C24	-3.10	1.45	1.50
31	B	601	CLA	C4B-NB	-3.10	1.34	1.37
31	7	316	CLA	C4B-NB	-3.09	1.34	1.37
31	6	305	CLA	C4B-NB	-3.09	1.34	1.37
31	4	611	CLA	C1C-NC	-3.09	1.33	1.37
31	1	613	CLA	C4B-NB	-3.09	1.34	1.37
31	n	311	CLA	C4B-NB	-3.09	1.34	1.37
31	3	306	CLA	C4B-NB	-3.09	1.34	1.37
43	B	617	BCR	C24-C25	3.09	1.56	1.45
31	y	603	CLA	C4B-NB	-3.09	1.34	1.37
31	b	602	CLA	C4B-NB	-3.09	1.34	1.37
31	B	612	CLA	C4B-NB	-3.09	1.34	1.37
31	C	610	CLA	C4B-NB	-3.09	1.34	1.37
31	n	304	CLA	C4B-NB	-3.09	1.34	1.37
31	p	603	CLA	C4B-NB	-3.08	1.34	1.37
31	B	614	CLA	C4B-NB	-3.08	1.34	1.37
31	C	603	CLA	C4B-NB	-3.08	1.34	1.37
31	r	305	CLA	C4B-NB	-3.08	1.34	1.37
31	N	314	CLA	C4B-NB	-3.08	1.34	1.37
31	C	601	CLA	C4B-NB	-3.08	1.34	1.37
31	N	303	CLA	C4B-NB	-3.08	1.34	1.37
31	s	315	CLA	C4B-NB	-3.08	1.34	1.37
31	q	304	CLA	C1C-NC	-3.08	1.33	1.37
35	2	614	RRX	C4-C5	-3.08	1.44	1.51
31	N	313	CLA	C4B-NB	-3.07	1.34	1.37
32	3	317	LUT	C23-C24	-3.07	1.45	1.50
31	4	602	CLA	C4B-NB	-3.07	1.34	1.37
31	Y	310	CLA	C4B-NB	-3.07	1.34	1.37
31	8	609	CLA	C4B-NB	-3.07	1.34	1.37
31	Y	303	CLA	C4B-NB	-3.07	1.34	1.37
31	7	314	CLA	C4B-NB	-3.07	1.34	1.37
31	8	611	CLA	C4B-NB	-3.07	1.34	1.37
31	n	303	CLA	C4B-NB	-3.07	1.34	1.37
31	S	310	CLA	C4B-NB	-3.07	1.34	1.37
35	4	615	RRX	C4-C5	-3.07	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	G	614	RRX	C4-C5	-3.07	1.45	1.51
31	9	314	CLA	C4B-NB	-3.07	1.34	1.37
31	G	602	CLA	C4B-NB	-3.06	1.34	1.37
31	8	603	CLA	C4B-NB	-3.06	1.34	1.37
32	1	616	LUT	C23-C24	-3.06	1.45	1.50
31	7	311	CLA	C4B-NB	-3.06	1.34	1.37
31	n	315	CLA	C4B-NB	-3.06	1.34	1.37
31	5	602	CLA	C4B-NB	-3.06	1.34	1.37
31	6	303	CLA	C4B-NB	-3.06	1.34	1.37
31	N	315	CLA	C4B-NB	-3.06	1.34	1.37
30	1	619	CHL	C1B-NB	-3.06	1.34	1.37
31	2	609	CLA	C4B-NB	-3.06	1.34	1.37
31	3	305	CLA	C4B-NB	-3.06	1.34	1.37
31	R	307	CLA	C4B-NB	-3.06	1.34	1.37
31	g	305	CLA	C4B-NB	-3.05	1.34	1.37
31	N	305	CLA	C4B-NB	-3.05	1.34	1.37
31	0	604	CLA	C4B-NB	-3.05	1.34	1.37
31	6	314	CLA	C4B-NB	-3.04	1.34	1.37
31	s	306	CLA	C4B-NB	-3.04	1.34	1.37
31	5	612	CLA	C4B-NB	-3.04	1.34	1.37
31	n	305	CLA	C4B-NB	-3.04	1.34	1.37
31	g	313	CLA	C4B-NB	-3.04	1.34	1.37
32	s	317	LUT	C23-C24	-3.04	1.45	1.50
35	9	317	RRX	C4-C5	-3.04	1.45	1.51
31	8	612	CLA	C4B-NB	-3.04	1.34	1.37
31	n	313	CLA	C4B-NB	-3.04	1.34	1.37
31	6	315	CLA	C4B-NB	-3.04	1.34	1.37
31	8	613	CLA	C4B-NB	-3.03	1.34	1.37
31	p	615	CLA	C4B-NB	-3.03	1.34	1.37
31	g	312	CLA	C4B-NB	-3.03	1.34	1.37
32	6	318	LUT	C23-C24	-3.03	1.45	1.50
31	n	314	CLA	C4B-NB	-3.03	1.34	1.37
32	r	317	LUT	C34-C33	-3.03	1.31	1.35
32	3	318	LUT	C23-C24	-3.03	1.45	1.50
31	n	316	CLA	C4B-NB	-3.03	1.34	1.37
32	y	617	LUT	C30-C29	-3.02	1.31	1.35
31	b	615	CLA	C4B-NB	-3.02	1.34	1.37
31	8	614	CLA	C4B-NB	-3.02	1.34	1.37
31	N	304	CLA	C4B-NB	-3.02	1.34	1.37
31	6	311	CLA	C4B-NB	-3.02	1.34	1.37
31	S	314	CLA	C4B-NB	-3.02	1.34	1.37
31	b	614	CLA	C4B-NB	-3.02	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S	302	CHL	C1B-NB	-3.02	1.34	1.37
31	p	602	CLA	C4B-NB	-3.02	1.34	1.37
31	S	305	CLA	C4B-NB	-3.02	1.34	1.37
31	y	610	CLA	C4B-NB	-3.02	1.34	1.37
31	2	602	CLA	C4B-NB	-3.01	1.34	1.37
31	0	614	CLA	C4B-NB	-3.01	1.34	1.37
31	N	321	CLA	C4B-NB	-3.01	1.34	1.37
31	8	602	CLA	C4B-NB	-3.01	1.34	1.37
31	9	315	CLA	C4B-NB	-3.01	1.34	1.37
31	B	610	CLA	C4B-NB	-3.01	1.34	1.37
31	1	614	CLA	C4B-NB	-3.00	1.34	1.37
31	7	303	CLA	C4B-NB	-3.00	1.34	1.37
31	B	613	CLA	C4B-NB	-3.00	1.34	1.37
31	r	313	CLA	C4B-NB	-3.00	1.34	1.37
31	y	615	CLA	C4B-NB	-3.00	1.34	1.37
31	5	615	CLA	C4B-NB	-3.00	1.34	1.37
31	5	603	CLA	C4B-NB	-3.00	1.34	1.37
31	8	604	CLA	C4B-NB	-3.00	1.34	1.37
32	1	615	LUT	C30-C29	-2.99	1.31	1.35
31	5	610	CLA	C4B-NB	-2.99	1.34	1.37
31	s	312	CLA	C4B-NB	-2.99	1.34	1.37
30	s	302	CHL	C1B-NB	-2.99	1.34	1.37
31	S	316	CLA	C4B-NB	-2.99	1.34	1.37
42	D	401	PHO	C4D-CHA	2.98	1.44	1.39
31	2	604	CLA	C4B-NB	-2.98	1.34	1.37
32	Y	315	LUT	C30-C29	-2.98	1.31	1.35
32	5	617	LUT	C23-C24	-2.98	1.45	1.50
31	R	303	CLA	C4B-NB	-2.97	1.34	1.37
31	9	306	CLA	C4B-NB	-2.97	1.34	1.37
32	7	318	LUT	C23-C24	-2.97	1.46	1.50
31	g	304	CLA	C4B-NB	-2.97	1.34	1.37
31	5	604	CLA	C4B-NB	-2.97	1.34	1.37
31	p	610	CLA	C4B-NB	-2.96	1.34	1.37
32	p	616	LUT	C23-C24	-2.96	1.46	1.50
31	c	604	CLA	C4B-NB	-2.96	1.34	1.37
31	4	604	CLA	C4B-NB	-2.96	1.34	1.37
31	3	315	CLA	C4B-NB	-2.96	1.34	1.37
31	3	313	CLA	C4B-NB	-2.96	1.34	1.37
31	5	611	CLA	C4B-NB	-2.95	1.34	1.37
31	g	311	CLA	C4B-NB	-2.95	1.34	1.37
31	p	614	CLA	C4B-NB	-2.95	1.34	1.37
31	g	303	CLA	C4B-NB	-2.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	312	CLA	C4B-NB	-2.94	1.34	1.37
31	2	612	CLA	C4B-NB	-2.93	1.34	1.37
31	r	314	CLA	C4B-NB	-2.93	1.34	1.37
31	y	614	CLA	C4B-NB	-2.93	1.34	1.37
32	s	318	LUT	C23-C24	-2.93	1.46	1.50
31	2	610	CLA	C4B-NB	-2.93	1.34	1.37
31	R	313	CLA	C4B-NB	-2.93	1.34	1.37
31	7	312	CLA	C4B-NB	-2.93	1.34	1.37
31	Y	304	CLA	C4B-NB	-2.92	1.34	1.37
31	y	611	CLA	C4B-NB	-2.91	1.34	1.37
31	q	304	CLA	C4B-NB	-2.91	1.34	1.37
31	3	314	CLA	C4B-NB	-2.90	1.34	1.37
42	A	408	PHO	C4D-CHA	2.90	1.44	1.39
31	n	312	CLA	C4B-NB	-2.90	1.34	1.37
42	a	408	PHO	C4D-CHA	2.90	1.44	1.39
32	5	616	LUT	C23-C24	-2.89	1.46	1.50
31	C	606	CLA	C4B-NB	-2.89	1.34	1.37
31	5	613	CLA	C4B-NB	-2.89	1.34	1.37
31	q	316	CLA	C4B-NB	-2.89	1.34	1.37
31	N	311	CLA	C4B-NB	-2.88	1.34	1.37
31	g	314	CLA	C4B-NB	-2.88	1.34	1.37
31	9	313	CLA	C4B-NB	-2.88	1.34	1.37
32	G	615	LUT	C23-C24	-2.88	1.46	1.50
31	p	611	CLA	C4B-NB	-2.87	1.34	1.37
31	6	313	CLA	C4B-NB	-2.87	1.34	1.37
31	5	614	CLA	C4B-NB	-2.87	1.34	1.37
31	b	611	CLA	C4B-NB	-2.86	1.34	1.37
31	8	610	CLA	C4B-NB	-2.86	1.34	1.37
31	6	304	CLA	C4B-NB	-2.86	1.34	1.37
35	q	317	RRX	C17-C18	-2.86	1.32	1.35
31	1	603	CLA	C4B-NB	-2.85	1.34	1.37
31	S	312	CLA	C4B-NB	-2.84	1.34	1.37
31	G	613	CLA	C4B-NB	-2.84	1.34	1.37
31	s	304	CLA	C4B-NB	-2.84	1.34	1.37
31	1	611	CLA	C4B-NB	-2.84	1.34	1.37
30	3	302	CHL	C1B-NB	-2.83	1.34	1.37
31	c	601	CLA	C4B-NB	-2.83	1.34	1.37
30	Y	306	CHL	C1B-NB	-2.82	1.34	1.37
31	0	611	CLA	C4B-NB	-2.82	1.34	1.37
31	p	612	CLA	C4B-NB	-2.81	1.34	1.37
31	G	603	CLA	C4B-NB	-2.81	1.34	1.37
32	y	617	LUT	C34-C33	-2.81	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	615	LUT	C38-C25	2.81	1.55	1.50
43	D	405	BCR	C34-C9	2.81	1.56	1.50
43	D	405	BCR	C7-C6	2.81	1.55	1.45
31	R	314	CLA	C4B-NB	-2.80	1.34	1.37
32	1	616	LUT	C30-C29	-2.80	1.32	1.35
30	q	310	CHL	C3A-C2A	-2.80	1.46	1.54
31	y	612	CLA	C4B-NB	-2.79	1.34	1.37
32	y	617	LUT	O23-C23	-2.79	1.38	1.43
31	7	304	CLA	C4B-NB	-2.79	1.34	1.37
31	Y	312	CLA	C4B-NB	-2.78	1.34	1.37
31	7	313	CLA	C4B-NB	-2.78	1.34	1.37
31	4	603	CLA	C4B-NB	-2.78	1.34	1.37
32	0	616	LUT	C30-C29	-2.77	1.32	1.35
31	9	305	CLA	C4B-NB	-2.77	1.34	1.37
32	y	616	LUT	C34-C33	-2.77	1.32	1.35
32	g	316	LUT	C23-C24	-2.77	1.46	1.50
31	0	603	CLA	C4B-NB	-2.76	1.34	1.37
32	7	317	LUT	C30-C29	-2.76	1.32	1.35
43	c	614	BCR	C7-C6	2.76	1.54	1.45
31	N	312	CLA	C4B-NB	-2.76	1.34	1.37
35	2	614	RRX	C17-C18	-2.76	1.32	1.35
31	2	603	CLA	C4B-NB	-2.76	1.34	1.37
31	G	610	CLA	C4B-NB	-2.76	1.34	1.37
43	V	101	BCR	C34-C9	2.75	1.56	1.50
30	q	309	CHL	C1B-NB	-2.75	1.34	1.37
30	3	302	CHL	C3A-C2A	-2.75	1.46	1.54
30	S	308	CHL	C1B-NB	-2.74	1.34	1.37
42	D	401	PHO	CMC-C2C	-2.73	1.46	1.50
32	Y	315	LUT	C34-C33	-2.73	1.32	1.35
35	4	615	RRX	C17-C18	-2.73	1.32	1.35
35	G	614	RRX	C17-C18	-2.72	1.32	1.35
43	v	101	BCR	C34-C9	2.72	1.56	1.50
42	A	408	PHO	CMC-C2C	-2.71	1.46	1.50
31	s	316	CLA	C4B-NB	-2.71	1.34	1.37
32	r	317	LUT	O23-C23	-2.71	1.38	1.43
31	0	612	CLA	C4B-NB	-2.71	1.34	1.37
32	R	317	LUT	C30-C29	-2.71	1.32	1.35
32	R	317	LUT	O23-C23	-2.71	1.38	1.43
43	b	619	BCR	C34-C9	2.70	1.56	1.50
30	0	606	CHL	C1B-NB	-2.70	1.34	1.37
43	A	410	BCR	C34-C9	2.70	1.56	1.50
43	b	618	BCR	C34-C9	2.70	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	612	CLA	C4B-NB	-2.70	1.34	1.37
35	9	317	RRX	C17-C18	-2.70	1.32	1.35
42	d	402	PHO	C1B-C2B	2.70	1.42	1.39
31	C	605	CLA	C3D-C4D	-2.69	1.38	1.44
43	b	620	BCR	C34-C9	2.69	1.56	1.50
31	4	613	CLA	C4B-NB	-2.69	1.34	1.37
43	v	101	BCR	C7-C6	2.69	1.54	1.45
32	2	615	LUT	O23-C23	-2.69	1.38	1.43
43	B	617	BCR	C39-C30	-2.69	1.48	1.53
34	y	620	LMG	C37-C36	-2.68	1.32	1.51
32	S	317	LUT	C18-C5	2.68	1.55	1.50
43	c	614	BCR	C34-C9	2.68	1.56	1.50
30	G	608	CHL	C3A-C2A	-2.68	1.47	1.54
32	Y	315	LUT	O23-C23	-2.68	1.38	1.43
34	0	622	LMG	C37-C36	-2.68	1.32	1.51
31	q	305	CLA	C4B-NB	-2.68	1.34	1.37
32	5	616	LUT	C18-C5	2.67	1.55	1.50
32	6	318	LUT	C18-C5	2.66	1.55	1.50
43	B	618	BCR	C7-C6	2.66	1.54	1.45
32	0	616	LUT	O23-C23	-2.66	1.38	1.43
47	E	101	HEM	C1C-C2C	-2.66	1.40	1.45
31	p	604	CLA	C4B-NB	-2.66	1.34	1.37
32	s	317	LUT	O23-C23	-2.66	1.38	1.43
32	n	317	LUT	C18-C5	2.66	1.55	1.50
32	3	317	LUT	C18-C5	2.66	1.55	1.50
43	c	615	BCR	C7-C6	2.65	1.54	1.45
32	s	317	LUT	C18-C5	2.65	1.55	1.50
42	A	408	PHO	CMB-C2B	-2.65	1.46	1.51
32	6	317	LUT	C18-C5	2.64	1.55	1.50
30	5	607	CHL	C3A-C2A	-2.64	1.47	1.54
43	c	615	BCR	C34-C9	2.64	1.56	1.50
42	D	401	PHO	C4D-ND	-2.64	1.34	1.38
32	8	615	LUT	C18-C5	2.64	1.55	1.50
32	N	317	LUT	O23-C23	-2.64	1.38	1.43
32	1	615	LUT	C34-C33	-2.64	1.32	1.35
32	Y	316	LUT	O23-C23	-2.64	1.38	1.43
43	B	618	BCR	C34-C9	2.64	1.56	1.50
43	a	410	BCR	C34-C9	2.63	1.56	1.50
47	e	102	HEM	C1C-C2C	-2.63	1.40	1.45
43	V	101	BCR	C7-C6	2.63	1.54	1.45
34	w	205	LMG	C37-C36	-2.63	1.33	1.51
32	Y	316	LUT	C30-C29	-2.63	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	a	408	PHO	C1B-C2B	2.62	1.42	1.39
30	q	310	CHL	C1B-NB	-2.62	1.34	1.37
42	D	401	PHO	CMD-C2D	-2.62	1.46	1.51
32	R	317	LUT	C34-C33	-2.62	1.32	1.35
30	R	310	CHL	C1B-NB	-2.62	1.34	1.37
34	b	624	LMG	C37-C36	-2.62	1.33	1.51
32	S	317	LUT	O23-C23	-2.62	1.38	1.43
31	3	312	CLA	C4B-NB	-2.62	1.34	1.37
34	r	321	LMG	C37-C36	-2.62	1.33	1.51
32	N	316	LUT	C18-C5	2.61	1.55	1.50
30	n	310	CHL	C3A-C2A	-2.61	1.47	1.54
42	A	408	PHO	CMD-C2D	-2.61	1.46	1.51
32	8	615	LUT	C30-C29	-2.61	1.32	1.35
43	b	619	BCR	C7-C6	2.61	1.54	1.45
31	B	607	CLA	C3D-C4D	-2.61	1.38	1.44
32	8	616	LUT	O23-C23	-2.61	1.38	1.43
32	0	617	LUT	O23-C23	-2.61	1.38	1.43
34	n	321	LMG	C37-C36	-2.61	1.33	1.51
34	R	321	LMG	C37-C36	-2.61	1.33	1.51
32	y	616	LUT	O23-C23	-2.60	1.38	1.43
32	7	317	LUT	C34-C33	-2.60	1.32	1.35
34	6	321	LMG	C37-C36	-2.60	1.33	1.51
32	7	318	LUT	C18-C5	2.60	1.55	1.50
45	c	617	DGD	CDA-CCA	-2.60	1.33	1.51
43	T	101	BCR	C34-C9	2.60	1.56	1.50
34	C	621	LMG	C37-C36	-2.60	1.33	1.51
43	C	615	BCR	C39-C30	-2.60	1.48	1.53
45	C	616	DGD	CAB-C9B	-2.60	1.33	1.51
43	T	101	BCR	C7-C6	2.60	1.54	1.45
32	5	617	LUT	C18-C5	2.60	1.55	1.50
34	Q1	101	LMG	C37-C36	-2.60	1.33	1.51
34	b	623	LMG	C37-C36	-2.60	1.33	1.51
32	p	616	LUT	C18-C5	2.60	1.55	1.50
32	6	318	LUT	O23-C23	-2.59	1.38	1.43
34	w	203	LMG	C37-C36	-2.59	1.33	1.51
32	n	317	LUT	O23-C23	-2.59	1.38	1.43
32	n	318	LUT	O23-C23	-2.59	1.38	1.43
34	A	418	LMG	C37-C36	-2.59	1.33	1.51
34	B	625	LMG	C37-C36	-2.59	1.33	1.51
34	A	414	LMG	C37-C36	-2.59	1.33	1.51
34	Y	319	LMG	C37-C36	-2.59	1.33	1.51
34	d	409	LMG	C19-C18	-2.58	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	4	621	LMG	C19-C18	-2.58	1.33	1.51
34	G	619	LMG	C37-C36	-2.58	1.33	1.51
42	A	408	PHO	C4D-ND	-2.58	1.35	1.38
34	7	322	LMG	C37-C36	-2.58	1.33	1.51
34	f	101	LMG	C37-C36	-2.58	1.33	1.51
34	m	102	LMG	C19-C18	-2.58	1.33	1.51
32	6	317	LUT	C30-C29	-2.58	1.32	1.35
32	g	316	LUT	C18-C5	2.58	1.55	1.50
34	3	321	LMG	C37-C36	-2.58	1.33	1.51
32	S	318	LUT	C18-C5	2.58	1.55	1.50
34	6	322	LMG	C19-C18	-2.58	1.33	1.51
32	9	318	LUT	O23-C23	-2.58	1.38	1.43
34	X	203	LMG	C37-C36	-2.58	1.33	1.51
43	z	101	BCR	C34-C9	2.58	1.56	1.50
34	d	409	LMG	C37-C36	-2.58	1.33	1.51
32	1	616	LUT	O23-C23	-2.57	1.38	1.43
43	h	101	BCR	C34-C9	2.57	1.56	1.50
34	N	320	LMG	C37-C36	-2.57	1.33	1.51
34	9	321	LMG	C37-C36	-2.57	1.33	1.51
34	7	320	LMG	C37-C36	-2.57	1.33	1.51
32	1	615	LUT	O23-C23	-2.57	1.38	1.43
32	g	316	LUT	C26-C27	2.57	1.54	1.50
32	6	317	LUT	O23-C23	-2.57	1.38	1.43
34	2	618	LMG	C37-C36	-2.57	1.33	1.51
34	5	620	LMG	C37-C36	-2.57	1.33	1.51
34	9	302	LMG	C19-C18	-2.57	1.33	1.51
32	N	317	LUT	C18-C5	2.57	1.55	1.50
34	g	320	LMG	C37-C36	-2.57	1.33	1.51
34	p	620	LMG	C37-C36	-2.57	1.33	1.51
32	8	615	LUT	O23-C23	-2.57	1.39	1.43
34	X	202	LMG	C37-C36	-2.57	1.33	1.51
34	1	618	LMG	C37-C36	-2.57	1.33	1.51
34	b	629	LMG	C37-C36	-2.57	1.33	1.51
32	n	317	LUT	C30-C29	-2.57	1.32	1.35
34	q1	101	LMG	C37-C36	-2.57	1.33	1.51
34	k	102	LMG	C37-C36	-2.57	1.33	1.51
30	7	306	CHL	C3A-C2A	-2.57	1.47	1.54
34	2	621	LMG	C19-C18	-2.57	1.33	1.51
32	3	317	LUT	O23-C23	-2.57	1.39	1.43
34	W	203	LMG	C37-C36	-2.57	1.33	1.51
34	c	621	LMG	C37-C36	-2.57	1.33	1.51
34	B	622	LMG	C37-C36	-2.56	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	B	619	BCR	C7-C6	2.56	1.54	1.45
34	I	101	LMG	C37-C36	-2.56	1.33	1.51
35	g	315	RRX	C17-C18	-2.56	1.32	1.35
34	q	302	LMG	C19-C18	-2.56	1.33	1.51
34	6	323	LMG	C37-C36	-2.56	1.33	1.51
32	7	317	LUT	C18-C5	2.56	1.55	1.50
34	b	601	LMG	C19-C18	-2.56	1.33	1.51
34	g	322	LMG	C22-C21	-2.56	1.33	1.51
34	0	620	LMG	C37-C36	-2.56	1.33	1.51
32	0	617	LUT	C18-C5	2.56	1.55	1.50
34	7	301	LMG	C19-C18	-2.56	1.33	1.51
34	n	322	LMG	C19-C18	-2.56	1.33	1.51
32	9	318	LUT	C18-C5	2.56	1.55	1.50
34	a	401	LMG	C37-C36	-2.56	1.33	1.51
32	G	615	LUT	C18-C5	2.55	1.55	1.50
34	J	102	LMG	C37-C36	-2.55	1.33	1.51
34	c	620	LMG	C37-C36	-2.55	1.33	1.51
34	D	409	LMG	C37-C36	-2.55	1.33	1.51
34	W	202	LMG	C37-C36	-2.55	1.33	1.51
34	a	416	LMG	C37-C36	-2.55	1.33	1.51
32	Y	315	LUT	C18-C5	2.55	1.55	1.50
43	B	619	BCR	C34-C9	2.55	1.56	1.50
34	G	622	LMG	C19-C18	-2.55	1.33	1.51
43	C	614	BCR	C34-C9	2.55	1.56	1.50
34	w	204	LMG	C37-C36	-2.55	1.33	1.51
32	0	616	LUT	C18-C5	2.54	1.55	1.50
43	A	410	BCR	C7-C6	2.54	1.54	1.45
32	q	318	LUT	O23-C23	-2.54	1.39	1.43
30	3	308	CHL	C1B-NB	-2.54	1.34	1.37
34	a	413	LMG	C37-C36	-2.54	1.33	1.51
32	p	617	LUT	C18-C5	2.54	1.55	1.50
32	G	615	LUT	O23-C23	-2.54	1.39	1.43
32	7	317	LUT	O23-C23	-2.53	1.39	1.43
32	r	317	LUT	C18-C5	2.53	1.55	1.50
34	x	202	LMG	C37-C36	-2.53	1.33	1.51
32	S	317	LUT	C30-C29	-2.53	1.32	1.35
32	5	617	LUT	O23-C23	-2.53	1.39	1.43
32	S	318	LUT	C23-C24	-2.53	1.46	1.50
43	H	101	BCR	C34-C9	2.53	1.56	1.50
43	C	614	BCR	C7-C6	2.53	1.54	1.45
43	b	618	BCR	C7-C6	2.53	1.54	1.45
32	N	316	LUT	O23-C23	-2.53	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S	309	CHL	C1B-NB	-2.52	1.34	1.37
32	s	318	LUT	C18-C5	2.52	1.55	1.50
32	3	318	LUT	O23-C23	-2.52	1.39	1.43
32	q	318	LUT	C18-C5	2.52	1.55	1.50
32	4	616	LUT	O23-C23	-2.52	1.39	1.43
32	8	616	LUT	C18-C5	2.52	1.55	1.50
32	4	616	LUT	C18-C5	2.52	1.55	1.50
32	0	617	LUT	C30-C29	-2.51	1.32	1.35
31	y	613	CLA	C3D-C4D	-2.51	1.38	1.44
32	n	318	LUT	C18-C5	2.51	1.55	1.50
30	r	310	CHL	C1B-NB	-2.51	1.34	1.37
32	1	616	LUT	C34-C33	-2.50	1.32	1.35
32	3	318	LUT	C18-C5	2.50	1.55	1.50
32	s	317	LUT	C30-C29	-2.49	1.32	1.35
44	a	414	PL9	C6-C1	-2.49	1.44	1.48
43	Z	101	BCR	C34-C9	2.49	1.56	1.50
43	d	406	BCR	C34-C9	2.49	1.56	1.50
32	y	616	LUT	C18-C5	2.48	1.55	1.50
32	g	316	LUT	O23-C23	-2.48	1.39	1.43
32	1	616	LUT	C18-C5	2.48	1.55	1.50
32	0	616	LUT	C34-C33	-2.47	1.32	1.35
30	y	605	CHL	C1B-NB	-2.47	1.34	1.37
43	B	617	BCR	C34-C9	2.47	1.56	1.50
31	0	610	CLA	C3D-C4D	-2.47	1.38	1.44
32	1	615	LUT	C18-C5	2.47	1.55	1.50
32	7	318	LUT	O23-C23	-2.47	1.39	1.43
43	b	620	BCR	C7-C6	2.46	1.53	1.45
43	d	406	BCR	C7-C6	2.46	1.53	1.45
43	a	410	BCR	C7-C6	2.46	1.53	1.45
32	G	615	LUT	C26-C27	2.46	1.53	1.50
36	q	319	NEX	O24-C25	-2.45	1.42	1.46
31	r	303	CLA	C3D-C4D	-2.45	1.38	1.44
43	z	101	BCR	C7-C6	2.45	1.53	1.45
43	C	615	BCR	C7-C6	2.45	1.53	1.45
42	D	401	PHO	CMB-C2B	-2.45	1.46	1.51
32	s	318	LUT	C30-C29	-2.45	1.32	1.35
30	s	309	CHL	C1B-NB	-2.44	1.34	1.37
32	5	616	LUT	O23-C23	-2.44	1.39	1.43
43	b	618	BCR	C39-C30	-2.44	1.49	1.53
32	Y	316	LUT	C18-C5	2.44	1.54	1.50
32	s	318	LUT	O23-C23	-2.44	1.39	1.43
32	2	615	LUT	C18-C5	2.44	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	9	317	RRX	C34-C9	2.44	1.55	1.50
32	7	318	LUT	C30-C29	-2.43	1.32	1.35
44	a	414	PL9	C53-C6	-2.43	1.45	1.50
43	H	101	BCR	C7-C6	2.43	1.53	1.45
32	p	617	LUT	O23-C23	-2.43	1.39	1.43
35	4	615	RRX	C34-C9	2.42	1.55	1.50
30	5	609	CHL	C3A-C2A	-2.42	1.47	1.54
47	e	102	HEM	FE-ND	-2.41	1.87	1.94
32	y	617	LUT	C18-C5	2.40	1.54	1.50
43	T	101	BCR	C36-C18	2.40	1.55	1.50
31	3	301	CLA	C3D-C4D	-2.40	1.38	1.44
42	d	402	PHO	C4D-CHA	2.40	1.43	1.39
32	8	616	LUT	C30-C29	-2.40	1.32	1.35
32	p	616	LUT	O23-C23	-2.40	1.39	1.43
35	G	614	RRX	C34-C9	2.40	1.55	1.50
32	S	318	LUT	O23-C23	-2.40	1.39	1.43
31	A	409	CLA	C3D-C4D	-2.40	1.38	1.44
30	2	608	CHL	C3A-C2A	-2.39	1.47	1.54
30	9	309	CHL	C3A-C2A	-2.39	1.47	1.54
43	C	615	BCR	C34-C9	2.39	1.55	1.50
32	n	318	LUT	C30-C29	-2.39	1.32	1.35
44	A	416	PL9	C3-C4	-2.39	1.45	1.49
43	t	101	BCR	C34-C9	2.39	1.55	1.50
31	c	608	CLA	C3D-C4D	-2.38	1.38	1.44
43	H	101	BCR	C39-C30	-2.38	1.49	1.53
42	A	408	PHO	CAC-C3C	-2.38	1.47	1.51
30	p	607	CHL	C3A-C2A	-2.38	1.47	1.54
31	a	409	CLA	C3D-C4D	-2.38	1.38	1.44
43	h	101	BCR	C7-C6	2.37	1.53	1.45
43	c	615	BCR	C39-C30	-2.37	1.49	1.53
30	q	308	CHL	C1B-NB	-2.37	1.34	1.37
42	D	401	PHO	CAC-C3C	-2.37	1.47	1.51
30	9	311	CHL	C1B-NB	-2.37	1.34	1.37
30	y	601	CHL	C1B-NB	-2.37	1.34	1.37
35	g	315	RRX	C34-C9	2.37	1.55	1.50
47	E	101	HEM	FE-ND	-2.36	1.87	1.94
31	C	605	CLA	C1D-ND	-2.36	1.34	1.37
43	Z	101	BCR	C7-C6	2.36	1.53	1.45
43	a	410	BCR	C36-C18	2.36	1.55	1.50
43	h	101	BCR	C39-C30	-2.36	1.49	1.53
43	d	406	BCR	C39-C30	-2.36	1.49	1.53
32	S	318	LUT	C26-C27	2.35	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	610	CLA	C3D-C4D	-2.35	1.38	1.44
30	R	310	CHL	C3A-C2A	-2.35	1.47	1.54
31	c	605	CLA	C3D-C4D	-2.35	1.38	1.44
32	0	617	LUT	C34-C33	-2.35	1.32	1.35
43	b	620	BCR	C39-C30	-2.35	1.49	1.53
31	B	603	CLA	C3D-C4D	-2.35	1.38	1.44
36	S	319	NEX	C1-C6	-2.35	1.50	1.54
43	C	614	BCR	C39-C30	-2.35	1.49	1.53
31	b	604	CLA	C3D-C4D	-2.35	1.38	1.44
36	R	301	NEX	C1-C6	-2.35	1.50	1.54
43	A	410	BCR	C39-C30	-2.35	1.49	1.53
43	c	614	BCR	C39-C30	-2.35	1.49	1.53
45	c	617	DGD	O5D-C1E	2.35	1.44	1.40
43	V	101	BCR	C39-C30	-2.35	1.49	1.53
32	R	317	LUT	C18-C5	2.34	1.54	1.50
32	N	316	LUT	C30-C29	-2.34	1.32	1.35
30	Y	302	CHL	C1B-NB	-2.34	1.34	1.37
31	Y	312	CLA	C3D-C4D	-2.34	1.38	1.44
31	b	607	CLA	C3D-C4D	-2.33	1.38	1.44
31	C	608	CLA	C3D-C4D	-2.33	1.38	1.44
31	b	609	CLA	C3D-C4D	-2.33	1.38	1.44
30	g	302	CHL	C1B-NB	-2.33	1.34	1.37
31	R	305	CLA	C3D-C4D	-2.33	1.38	1.44
35	2	614	RRX	C34-C9	2.33	1.55	1.50
32	S	317	LUT	C34-C33	-2.32	1.32	1.35
43	a	410	BCR	C39-C30	-2.32	1.49	1.53
30	1	601	CHL	C1D-ND	-2.32	1.34	1.37
30	q	303	CHL	C1B-NB	-2.32	1.34	1.37
43	z	101	BCR	C39-C30	-2.32	1.49	1.53
30	p	601	CHL	C1B-NB	-2.32	1.34	1.37
30	q	311	CHL	C1B-NB	-2.32	1.34	1.37
30	N	306	CHL	C1B-NB	-2.32	1.34	1.37
43	Z	101	BCR	C39-C30	-2.31	1.49	1.53
30	N	308	CHL	C3A-C2A	-2.31	1.48	1.54
30	g	309	CHL	C3A-C2A	-2.31	1.48	1.54
30	2	601	CHL	C1B-NB	-2.31	1.34	1.37
30	1	609	CHL	C3A-C2A	-2.31	1.48	1.54
30	3	310	CHL	C3A-C2A	-2.31	1.48	1.54
31	B	605	CLA	C3D-C4D	-2.31	1.39	1.44
43	t	101	BCR	C7-C6	2.31	1.53	1.45
30	6	302	CHL	C1B-NB	-2.30	1.35	1.37
30	0	609	CHL	C3A-C2A	-2.30	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	D	405	BCR	C36-C18	2.30	1.55	1.50
30	7	321	CHL	C1B-NB	-2.30	1.35	1.37
31	B	615	CLA	C3D-C4D	-2.30	1.39	1.44
30	6	307	CHL	C1B-NB	-2.30	1.35	1.37
32	s	318	LUT	C34-C33	-2.30	1.32	1.35
43	b	619	BCR	C39-C30	-2.29	1.49	1.53
31	4	612	CLA	C3D-C4D	-2.29	1.39	1.44
31	y	612	CLA	C3D-C4D	-2.29	1.39	1.44
32	6	317	LUT	C34-C33	-2.29	1.32	1.35
43	B	619	BCR	C39-C30	-2.29	1.49	1.53
30	Y	301	CHL	C1B-NB	-2.29	1.35	1.37
31	9	312	CLA	C3D-C4D	-2.29	1.39	1.44
32	5	617	LUT	C26-C27	2.29	1.53	1.50
31	D	403	CLA	C3D-C4D	-2.29	1.39	1.44
30	G	607	CHL	C1B-NB	-2.29	1.35	1.37
31	A	407	CLA	C3D-C4D	-2.29	1.39	1.44
31	d	404	CLA	C3D-C4D	-2.29	1.39	1.44
32	9	318	LUT	C26-C27	2.28	1.53	1.50
31	B	608	CLA	C3D-C4D	-2.28	1.39	1.44
44	A	416	PL9	C6-C1	-2.28	1.44	1.48
43	v	101	BCR	C39-C30	-2.28	1.49	1.53
31	a	406	CLA	C3D-C4D	-2.28	1.39	1.44
31	C	606	CLA	C3D-C4D	-2.28	1.39	1.44
31	q	315	CLA	C3D-C4D	-2.28	1.39	1.44
43	b	620	BCR	C36-C18	2.27	1.55	1.50
31	9	314	CLA	C3D-C4D	-2.27	1.39	1.44
31	s	313	CLA	C3D-C4D	-2.27	1.39	1.44
31	R	304	CLA	C3D-C4D	-2.27	1.39	1.44
31	B	604	CLA	C3D-C4D	-2.27	1.39	1.44
31	G	611	CLA	C3D-C4D	-2.27	1.39	1.44
31	B	606	CLA	C3D-C4D	-2.27	1.39	1.44
31	b	616	CLA	C3D-C4D	-2.27	1.39	1.44
43	B	618	BCR	C39-C30	-2.27	1.49	1.53
30	N	309	CHL	C3A-C2A	-2.27	1.48	1.54
43	t	101	BCR	C39-C30	-2.27	1.49	1.53
31	D	404	CLA	C3D-C4D	-2.26	1.39	1.44
31	b	606	CLA	C3D-C4D	-2.26	1.39	1.44
30	R	309	CHL	C1B-NB	-2.26	1.35	1.37
43	c	614	BCR	C36-C18	2.26	1.55	1.50
43	B	617	BCR	C7-C6	2.26	1.53	1.45
31	C	603	CLA	C3D-C4D	-2.26	1.39	1.44
31	d	401	CLA	C3D-C4D	-2.26	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	312	CLA	C3D-C4D	-2.26	1.39	1.44
31	c	607	CLA	C3D-C4D	-2.26	1.39	1.44
30	7	302	CHL	C1B-NB	-2.26	1.35	1.37
30	9	307	CHL	C1B-NB	-2.26	1.35	1.37
31	B	609	CLA	C3D-C4D	-2.26	1.39	1.44
30	n	308	CHL	C1B-NB	-2.25	1.35	1.37
31	c	602	CLA	C3D-C4D	-2.25	1.39	1.44
30	1	619	CHL	C1D-ND	-2.25	1.35	1.37
43	H	101	BCR	C36-C18	2.25	1.55	1.50
36	2	616	NEX	C1-C6	-2.25	1.50	1.54
30	3	310	CHL	C1B-NB	-2.25	1.35	1.37
30	4	609	CHL	C1B-NB	-2.25	1.35	1.37
31	A	405	CLA	C3D-C4D	-2.25	1.39	1.44
31	A	406	CLA	C3D-C4D	-2.25	1.39	1.44
43	v	101	BCR	C36-C18	2.25	1.55	1.50
30	1	607	CHL	C1B-NB	-2.24	1.35	1.37
32	3	317	LUT	C30-C29	-2.24	1.32	1.35
36	r	319	NEX	O24-C25	-2.24	1.43	1.46
32	6	318	LUT	C30-C29	-2.24	1.32	1.35
30	9	303	CHL	C1B-NB	-2.24	1.35	1.37
32	n	318	LUT	C34-C33	-2.24	1.32	1.35
32	3	317	LUT	C26-C27	2.24	1.53	1.50
30	5	607	CHL	C1B-NB	-2.24	1.35	1.37
30	g	308	CHL	C1B-NB	-2.24	1.35	1.37
32	r	317	LUT	C14-C13	-2.24	1.32	1.35
31	s	315	CLA	C3D-C4D	-2.24	1.39	1.44
31	c	606	CLA	C3D-C4D	-2.24	1.39	1.44
31	a	407	CLA	C3D-C4D	-2.24	1.39	1.44
30	5	601	CHL	C1B-NB	-2.24	1.35	1.37
31	R	314	CLA	C3D-C4D	-2.24	1.39	1.44
32	5	616	LUT	C30-C29	-2.24	1.32	1.35
31	R	311	CLA	C3D-C4D	-2.24	1.39	1.44
31	b	617	CLA	C3D-C4D	-2.24	1.39	1.44
32	5	616	LUT	C26-C27	2.24	1.53	1.50
32	N	316	LUT	C26-C27	2.24	1.53	1.50
32	N	317	LUT	C26-C27	2.24	1.53	1.50
32	8	616	LUT	C34-C33	-2.23	1.32	1.35
31	C	604	CLA	C3D-C4D	-2.23	1.39	1.44
31	B	612	CLA	C1C-C2C	2.23	1.48	1.44
31	q	314	CLA	C3D-C4D	-2.23	1.39	1.44
31	C	602	CLA	C3D-C4D	-2.23	1.39	1.44
36	9	319	NEX	C1-C6	-2.23	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	310	CHL	C1B-NB	-2.23	1.35	1.37
31	c	609	CLA	C3D-C4D	-2.23	1.39	1.44
32	8	615	LUT	C34-C33	-2.23	1.32	1.35
35	q	317	RRX	C34-C9	2.23	1.55	1.50
30	0	609	CHL	C1B-NB	-2.23	1.35	1.37
31	r	311	CLA	C3D-C4D	-2.23	1.39	1.44
30	n	301	CHL	C1B-NB	-2.23	1.35	1.37
43	V	101	BCR	C36-C18	2.23	1.55	1.50
30	Y	301	CHL	C3A-C2A	-2.23	1.48	1.54
36	N	318	NEX	C1-C6	-2.22	1.50	1.54
31	S	304	CLA	C3D-C4D	-2.22	1.39	1.44
31	0	615	CLA	C3D-C4D	-2.22	1.39	1.44
31	b	605	CLA	C3D-C4D	-2.22	1.39	1.44
32	S	318	LUT	C30-C29	-2.22	1.32	1.35
30	q	307	CHL	C1B-NB	-2.22	1.35	1.37
32	7	318	LUT	C34-C33	-2.22	1.32	1.35
32	N	317	LUT	C30-C29	-2.22	1.32	1.35
32	Y	316	LUT	C34-C33	-2.22	1.32	1.35
31	0	612	CLA	C3D-C4D	-2.22	1.39	1.44
31	R	307	CLA	C3D-C4D	-2.22	1.39	1.44
42	A	408	PHO	C3B-C2B	-2.22	1.37	1.40
30	2	606	CHL	C1B-NB	-2.22	1.35	1.37
30	r	309	CHL	C1B-NB	-2.22	1.35	1.37
31	b	613	CLA	C1C-C2C	2.22	1.48	1.44
36	r	319	NEX	C1-C6	-2.22	1.50	1.54
31	C	610	CLA	C3D-C4D	-2.22	1.39	1.44
31	2	602	CLA	C1C-C2C	2.21	1.48	1.44
43	B	619	BCR	C36-C18	2.21	1.55	1.50
30	y	609	CHL	C1B-NB	-2.21	1.35	1.37
35	4	615	RRX	C33-C5	2.21	1.54	1.50
43	Z	101	BCR	C36-C18	2.21	1.55	1.50
31	R	315	CLA	C3D-C4D	-2.21	1.39	1.44
35	G	614	RRX	C33-C5	2.21	1.54	1.50
44	A	416	PL9	C36-C34	-2.21	1.46	1.51
32	n	317	LUT	C34-C33	-2.21	1.32	1.35
31	C	609	CLA	C3D-C4D	-2.21	1.39	1.44
32	s	317	LUT	C34-C33	-2.21	1.32	1.35
30	2	608	CHL	C1B-NB	-2.21	1.35	1.37
31	B	602	CLA	C3D-C4D	-2.21	1.39	1.44
31	1	612	CLA	C3D-C4D	-2.21	1.39	1.44
30	4	601	CHL	C1B-NB	-2.21	1.35	1.37
43	h	101	BCR	C36-C18	2.20	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	610	CLA	C3D-C4D	-2.20	1.39	1.44
38	a	412	SQD	O47-C45	-2.20	1.41	1.46
32	4	616	LUT	C30-C29	-2.20	1.32	1.35
31	p	610	CLA	C1C-C2C	2.20	1.48	1.44
31	c	610	CLA	C3D-C4D	-2.20	1.39	1.44
36	8	617	NEX	O24-C25	-2.20	1.43	1.46
30	G	601	CHL	C1B-NB	-2.20	1.35	1.37
31	r	312	CLA	C3D-C4D	-2.20	1.39	1.44
31	b	602	CLA	C3D-C4D	-2.20	1.39	1.44
36	4	617	NEX	O24-C25	-2.20	1.43	1.46
44	A	416	PL9	C31-C29	-2.20	1.46	1.51
32	q	318	LUT	C26-C27	2.20	1.53	1.50
30	7	308	CHL	C1B-NB	-2.20	1.35	1.37
30	7	310	CHL	C1B-NB	-2.20	1.35	1.37
31	g	303	CLA	C3D-C4D	-2.19	1.39	1.44
32	2	615	LUT	C26-C27	2.19	1.53	1.50
35	9	317	RRX	C33-C5	2.19	1.54	1.50
31	1	603	CLA	C3D-C4D	-2.19	1.39	1.44
30	3	309	CHL	C1D-ND	-2.19	1.35	1.37
36	g	317	NEX	O24-C25	-2.19	1.43	1.46
31	b	608	CLA	C3D-C4D	-2.19	1.39	1.44
30	Y	307	CHL	C3A-C2A	-2.19	1.48	1.54
31	3	316	CLA	C3D-C4D	-2.19	1.39	1.44
31	c	603	CLA	C3D-C4D	-2.19	1.39	1.44
30	n	310	CHL	C1B-NB	-2.19	1.35	1.37
43	T	101	BCR	C39-C30	-2.19	1.49	1.53
31	r	315	CLA	C3D-C4D	-2.19	1.39	1.44
44	a	414	PL9	C52-C5	-2.19	1.46	1.50
31	Y	311	CLA	C3D-C4D	-2.19	1.39	1.44
30	6	309	CHL	C3A-C2A	-2.18	1.48	1.54
43	c	615	BCR	C36-C18	2.18	1.55	1.50
30	8	605	CHL	C1B-NB	-2.18	1.35	1.37
31	q	306	CLA	C3D-C4D	-2.18	1.39	1.44
31	0	603	CLA	C3D-C4D	-2.18	1.39	1.44
30	5	605	CHL	C1B-NB	-2.18	1.35	1.37
31	S	313	CLA	C3D-C4D	-2.18	1.39	1.44
30	N	308	CHL	C1B-NB	-2.18	1.35	1.37
31	G	613	CLA	C3D-C4D	-2.18	1.39	1.44
43	C	614	BCR	C36-C18	2.18	1.55	1.50
31	B	616	CLA	C3D-C4D	-2.18	1.39	1.44
31	y	611	CLA	C3D-C4D	-2.18	1.39	1.44
31	q	304	CLA	C1C-C2C	2.18	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	315	CLA	C3D-C4D	-2.18	1.39	1.44
30	8	601	CHL	C1B-NB	-2.18	1.35	1.37
31	q	313	CLA	C3D-C4D	-2.18	1.39	1.44
32	3	318	LUT	C26-C27	2.17	1.53	1.50
31	r	314	CLA	C3D-C4D	-2.17	1.39	1.44
31	B	601	CLA	C3D-C4D	-2.17	1.39	1.44
30	N	309	CHL	C1B-NB	-2.17	1.35	1.37
30	5	609	CHL	C1B-NB	-2.17	1.35	1.37
31	C	607	CLA	C3D-C4D	-2.17	1.39	1.44
31	1	602	CLA	C3D-C4D	-2.17	1.39	1.44
31	7	313	CLA	C3D-C4D	-2.17	1.39	1.44
31	b	603	CLA	C3D-C4D	-2.17	1.39	1.44
30	9	310	CHL	C1B-NB	-2.17	1.35	1.37
32	p	616	LUT	C28-C27	2.17	1.37	1.32
31	r	316	CLA	C3D-C4D	-2.17	1.39	1.44
32	6	318	LUT	C34-C33	-2.17	1.32	1.35
31	c	611	CLA	C3D-C4D	-2.17	1.39	1.44
36	8	617	NEX	C1-C6	-2.17	1.50	1.54
30	n	302	CHL	C1B-NB	-2.17	1.35	1.37
44	A	416	PL9	C53-C6	-2.16	1.46	1.50
36	0	618	NEX	O24-C25	-2.16	1.43	1.46
31	s	314	CLA	C3D-C4D	-2.16	1.39	1.44
31	r	306	CLA	C3D-C4D	-2.16	1.39	1.44
30	3	303	CHL	C1B-NB	-2.16	1.35	1.37
30	n	306	CHL	C1B-NB	-2.16	1.35	1.37
30	2	607	CHL	C1B-NB	-2.16	1.35	1.37
32	q	318	LUT	C30-C29	-2.16	1.32	1.35
32	6	318	LUT	C26-C27	2.16	1.53	1.50
32	N	317	LUT	C34-C33	-2.16	1.32	1.35
31	C	612	CLA	C3D-C4D	-2.16	1.39	1.44
30	g	306	CHL	C1B-NB	-2.16	1.35	1.37
31	C	613	CLA	C3D-C4D	-2.16	1.39	1.44
31	c	612	CLA	C3D-C4D	-2.16	1.39	1.44
31	S	303	CLA	C1C-C2C	2.16	1.48	1.44
30	8	608	CHL	C1B-NB	-2.16	1.35	1.37
30	G	608	CHL	C1B-NB	-2.15	1.35	1.37
31	Y	313	CLA	C3D-C4D	-2.15	1.39	1.44
30	Y	309	CHL	C1B-NB	-2.15	1.35	1.37
32	2	615	LUT	C34-C33	-2.15	1.32	1.35
32	4	616	LUT	C34-C33	-2.15	1.32	1.35
43	b	619	BCR	C36-C18	2.15	1.55	1.50
31	p	611	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	b	618	BCR	C36-C18	2.15	1.55	1.50
30	0	601	CHL	C1B-NB	-2.15	1.35	1.37
31	6	304	CLA	C3D-C4D	-2.15	1.39	1.44
32	2	615	LUT	C28-C27	2.15	1.37	1.32
31	9	304	CLA	C1C-C2C	2.15	1.48	1.44
32	G	615	LUT	C34-C33	-2.15	1.32	1.35
31	5	612	CLA	C1C-C2C	2.15	1.48	1.44
35	2	614	RRX	C33-C5	2.15	1.54	1.50
31	d	405	CLA	C3D-C4D	-2.15	1.39	1.44
31	R	306	CLA	C3D-C4D	-2.15	1.39	1.44
31	N	314	CLA	C1C-C2C	2.15	1.48	1.44
43	z	101	BCR	C36-C18	2.15	1.55	1.50
31	8	613	CLA	C1C-C2C	2.15	1.48	1.44
36	g	317	NEX	C1-C6	-2.15	1.51	1.54
31	C	601	CLA	C3D-C4D	-2.15	1.39	1.44
31	S	312	CLA	C3D-C4D	-2.15	1.39	1.44
36	R	319	NEX	O24-C25	-2.14	1.43	1.46
31	R	316	CLA	C3D-C4D	-2.14	1.39	1.44
31	8	602	CLA	C1C-C2C	2.14	1.48	1.44
43	D	405	BCR	C39-C30	-2.14	1.49	1.53
30	1	608	CHL	C3A-C2A	-2.14	1.48	1.54
31	n	315	CLA	C1C-C2C	2.14	1.48	1.44
30	5	606	CHL	C1B-NB	-2.14	1.35	1.37
30	R	308	CHL	C1B-NB	-2.14	1.35	1.37
30	1	601	CHL	C1A-CHA	-2.14	1.34	1.43
31	R	306	CLA	C1A-CHA	2.14	1.52	1.43
47	e	102	HEM	C1D-ND	-2.14	1.34	1.38
31	2	609	CLA	C1C-C2C	2.14	1.48	1.44
31	q	312	CLA	C1C-C2C	2.14	1.48	1.44
30	2	605	CHL	C1B-NB	-2.14	1.35	1.37
30	7	306	CHL	C1B-NB	-2.14	1.35	1.37
43	A	410	BCR	C36-C18	2.14	1.55	1.50
31	p	615	CLA	C1C-C2C	2.14	1.48	1.44
32	y	617	LUT	C14-C13	-2.14	1.32	1.35
36	4	617	NEX	C1-C6	-2.14	1.51	1.54
31	s	306	CLA	C1C-C2C	2.14	1.48	1.44
31	0	604	CLA	C3D-C4D	-2.14	1.39	1.44
32	3	318	LUT	C30-C29	-2.14	1.32	1.35
30	y	607	CHL	C1B-NB	-2.14	1.35	1.37
31	s	312	CLA	C3D-C4D	-2.14	1.39	1.44
31	C	611	CLA	C3D-C4D	-2.14	1.39	1.44
31	c	604	CLA	C3D-C4D	-2.14	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	603	CLA	C3D-C4D	-2.13	1.39	1.44
31	4	602	CLA	C1C-C2C	2.13	1.48	1.44
31	3	305	CLA	C3D-C4D	-2.13	1.39	1.44
31	0	611	CLA	C3D-C4D	-2.13	1.39	1.44
32	9	318	LUT	C34-C33	-2.13	1.33	1.35
31	1	604	CLA	C3D-C4D	-2.13	1.39	1.44
30	8	607	CHL	C1B-NB	-2.13	1.35	1.37
31	r	307	CLA	C3D-C4D	-2.13	1.39	1.44
32	N	316	LUT	C34-C33	-2.13	1.33	1.35
31	r	313	CLA	C3D-C4D	-2.13	1.39	1.44
30	3	307	CHL	C1B-NB	-2.13	1.35	1.37
31	7	304	CLA	C3D-C4D	-2.13	1.39	1.44
31	G	612	CLA	C3D-C4D	-2.13	1.39	1.44
36	q	319	NEX	C1-C6	-2.13	1.51	1.54
35	g	315	RRX	C33-C5	2.13	1.54	1.50
30	N	302	CHL	C1B-NB	-2.13	1.35	1.37
31	c	601	CLA	C3D-C4D	-2.13	1.39	1.44
31	p	603	CLA	C3D-C4D	-2.13	1.39	1.44
36	6	319	NEX	O24-C25	-2.12	1.43	1.46
36	p	618	NEX	C1-C6	-2.12	1.51	1.54
31	p	615	CLA	C3D-C4D	-2.12	1.39	1.44
30	n	309	CHL	C1B-NB	-2.12	1.35	1.37
31	g	310	CLA	C3D-C4D	-2.12	1.39	1.44
30	0	605	CHL	C3D-C4D	-2.12	1.39	1.44
32	4	616	LUT	C26-C27	2.12	1.53	1.50
31	G	610	CLA	C1A-CHA	2.12	1.51	1.43
36	5	618	NEX	C1-C6	-2.12	1.51	1.54
31	7	314	CLA	C3D-C4D	-2.12	1.39	1.44
30	1	609	CHL	C1B-NB	-2.12	1.35	1.37
31	q	316	CLA	C3D-C4D	-2.12	1.39	1.44
31	N	311	CLA	C1C-C2C	2.12	1.48	1.44
31	0	613	CLA	C3D-C4D	-2.12	1.39	1.44
31	b	605	CLA	C1A-CHA	2.12	1.51	1.43
31	0	602	CLA	C3D-C4D	-2.12	1.39	1.44
31	p	604	CLA	C1C-C2C	2.12	1.48	1.44
31	y	603	CLA	C3D-C4D	-2.12	1.39	1.44
31	g	314	CLA	C1C-C2C	2.12	1.48	1.44
30	r	308	CHL	C1B-NB	-2.11	1.35	1.37
31	3	315	CLA	C1C-C2C	2.11	1.48	1.44
31	c	613	CLA	C3D-C4D	-2.11	1.39	1.44
32	8	615	LUT	C26-C27	2.11	1.53	1.50
31	s	311	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	605	CHL	C1D-ND	-2.11	1.35	1.37
31	S	306	CLA	C1C-C2C	2.11	1.48	1.44
31	G	609	CLA	C3D-C4D	-2.11	1.39	1.44
32	S	318	LUT	C34-C33	-2.11	1.33	1.35
31	8	609	CLA	C1C-C2C	2.11	1.48	1.44
31	S	310	CLA	C3D-C4D	-2.11	1.39	1.44
42	d	402	PHO	C1D-C2D	2.11	1.41	1.39
31	3	312	CLA	C1C-C2C	2.11	1.48	1.44
31	p	613	CLA	C3D-C4D	-2.11	1.39	1.44
31	1	603	CLA	C1A-CHA	2.11	1.51	1.43
31	4	604	CLA	C1C-C2C	2.10	1.48	1.44
31	r	305	CLA	C3D-C4D	-2.10	1.39	1.44
30	4	605	CHL	C1B-NB	-2.10	1.35	1.37
30	s	308	CHL	C1B-NB	-2.10	1.35	1.37
31	y	602	CLA	C1C-C2C	2.10	1.48	1.44
30	G	605	CHL	C1B-NB	-2.10	1.35	1.37
31	s	303	CLA	C1C-C2C	2.10	1.48	1.44
30	5	608	CHL	C1B-NB	-2.10	1.35	1.37
31	N	310	CLA	C1C-C2C	2.10	1.48	1.44
31	N	321	CLA	C1C-C2C	2.10	1.48	1.44
31	7	311	CLA	C1C-C2C	2.10	1.48	1.44
32	7	318	LUT	C26-C27	2.10	1.53	1.50
31	7	303	CLA	C1C-C2C	2.10	1.48	1.44
31	n	311	CLA	C1C-C2C	2.10	1.48	1.44
36	Y	317	NEX	C1-C6	-2.10	1.51	1.54
43	t	101	BCR	C36-C18	2.10	1.55	1.50
31	y	615	CLA	C1C-C2C	2.10	1.48	1.44
31	5	602	CLA	C1C-C2C	2.10	1.48	1.44
31	B	612	CLA	C3D-C4D	-2.10	1.39	1.44
30	1	605	CHL	C1B-NB	-2.10	1.35	1.37
31	n	312	CLA	C1C-C2C	2.09	1.48	1.44
32	8	616	LUT	C26-C27	2.09	1.53	1.50
32	s	318	LUT	C26-C27	2.09	1.53	1.50
38	G	624	SQD	O47-C45	-2.09	1.41	1.46
31	N	312	CLA	C1C-C2C	2.09	1.48	1.44
43	d	406	BCR	C14-C13	-2.09	1.33	1.35
30	3	302	CHL	C1D-ND	-2.09	1.35	1.37
31	4	603	CLA	C3D-C4D	-2.09	1.39	1.44
31	S	314	CLA	C3D-C4D	-2.09	1.39	1.44
31	q	312	CLA	C3D-C4D	-2.09	1.39	1.44
31	4	614	CLA	C3D-C4D	-2.09	1.39	1.44
31	9	313	CLA	C3D-C4D	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	602	CLA	C3D-C4D	-2.09	1.39	1.44
30	6	309	CHL	C1B-NB	-2.09	1.35	1.37
31	b	612	CLA	C1C-C2C	2.09	1.48	1.44
30	y	606	CHL	C1B-NB	-2.09	1.35	1.37
47	E	101	HEM	C1D-ND	-2.09	1.34	1.38
32	n	317	LUT	C26-C27	2.09	1.53	1.50
30	p	605	CHL	C1B-NB	-2.09	1.35	1.37
31	g	311	CLA	C1A-CHA	2.09	1.51	1.43
31	N	312	CLA	C3D-C4D	-2.09	1.39	1.44
30	4	608	CHL	C1B-NB	-2.09	1.35	1.37
30	Y	308	CHL	C1B-NB	-2.09	1.35	1.37
31	b	615	CLA	C1C-C2C	2.09	1.48	1.44
31	S	316	CLA	C3D-C4D	-2.09	1.39	1.44
31	A	406	CLA	C1A-CHA	2.09	1.51	1.43
32	g	316	LUT	C30-C29	-2.09	1.33	1.35
43	z	101	BCR	C38-C26	2.09	1.54	1.50
31	d	405	CLA	C1A-CHA	2.09	1.51	1.43
30	r	308	CHL	C3A-C2A	-2.08	1.48	1.54
31	B	604	CLA	C1A-CHA	2.08	1.51	1.43
36	Y	317	NEX	O24-C25	-2.08	1.43	1.46
31	1	611	CLA	C1C-C2C	2.08	1.48	1.44
31	6	313	CLA	C1C-C2C	2.08	1.48	1.44
31	g	312	CLA	C3D-C4D	-2.08	1.39	1.44
30	G	606	CHL	C1B-NB	-2.08	1.35	1.37
43	D	405	BCR	C38-C26	2.08	1.54	1.50
31	B	613	CLA	C3D-C4D	-2.08	1.39	1.44
30	N	301	CHL	C1B-NB	-2.08	1.35	1.37
31	1	613	CLA	C3D-C4D	-2.08	1.39	1.44
30	y	608	CHL	C1B-NB	-2.08	1.35	1.37
43	Z	101	BCR	C38-C26	2.08	1.54	1.50
31	6	313	CLA	C3D-C4D	-2.08	1.39	1.44
31	S	311	CLA	C3D-C4D	-2.08	1.39	1.44
31	G	602	CLA	C1C-C2C	2.08	1.48	1.44
31	C	613	CLA	C1A-CHA	2.08	1.51	1.43
30	S	308	CHL	C1D-ND	-2.08	1.35	1.37
31	6	312	CLA	C3D-C4D	-2.08	1.39	1.44
31	D	404	CLA	C1A-CHA	2.08	1.51	1.43
31	a	407	CLA	C1A-CHA	2.08	1.51	1.43
31	3	304	CLA	C1C-C2C	2.08	1.48	1.44
31	B	614	CLA	C1C-C2C	2.08	1.48	1.44
31	C	610	CLA	C1A-CHA	2.08	1.51	1.43
32	0	617	LUT	C26-C27	2.08	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	312	CLA	C1A-CHA	2.08	1.51	1.43
31	G	604	CLA	C3D-C4D	-2.07	1.39	1.44
31	c	613	CLA	C1A-CHA	2.07	1.51	1.43
31	6	304	CLA	C1C-C2C	2.07	1.48	1.44
31	n	303	CLA	C1C-C2C	2.07	1.48	1.44
43	B	617	BCR	C10-C9	-2.07	1.33	1.35
31	5	610	CLA	C1C-C2C	2.07	1.48	1.44
31	g	304	CLA	C3D-C4D	-2.07	1.39	1.44
31	B	602	CLA	C1A-CHA	2.07	1.51	1.43
31	B	613	CLA	C1C-C2C	2.07	1.48	1.44
31	p	614	CLA	C1C-C2C	2.07	1.48	1.44
31	s	310	CLA	C3D-C4D	-2.07	1.39	1.44
31	4	611	CLA	C1C-C2C	2.07	1.48	1.44
31	y	610	CLA	C1C-C2C	2.07	1.48	1.44
43	D	405	BCR	C37-C22	2.07	1.55	1.50
32	p	616	LUT	C26-C27	2.07	1.53	1.50
31	Y	310	CLA	C1C-C2C	2.07	1.48	1.44
30	N	307	CHL	C3A-C2A	-2.07	1.48	1.54
31	G	602	CLA	C3D-C4D	-2.07	1.39	1.44
31	g	311	CLA	C3D-C4D	-2.07	1.39	1.44
31	8	611	CLA	C1C-C2C	2.07	1.48	1.44
30	Y	307	CHL	C1B-NB	-2.07	1.35	1.37
31	2	613	CLA	C3D-C4D	-2.07	1.39	1.44
31	p	602	CLA	C1A-CHA	2.07	1.51	1.43
31	G	603	CLA	C3D-C4D	-2.07	1.39	1.44
31	7	304	CLA	C1C-C2C	2.07	1.48	1.44
31	9	305	CLA	C3D-C4D	-2.07	1.39	1.44
31	s	316	CLA	C3D-C4D	-2.07	1.39	1.44
31	B	615	CLA	C1A-CHA	2.07	1.51	1.43
31	5	611	CLA	C3D-C4D	-2.07	1.39	1.44
31	8	610	CLA	C1C-C2C	2.07	1.48	1.44
31	3	306	CLA	C3D-C4D	-2.07	1.39	1.44
31	n	304	CLA	C3D-C4D	-2.07	1.39	1.44
31	1	610	CLA	C3D-C4D	-2.06	1.39	1.44
31	3	312	CLA	C3D-C4D	-2.06	1.39	1.44
31	p	614	CLA	C3D-C4D	-2.06	1.39	1.44
31	2	611	CLA	C3D-C4D	-2.06	1.39	1.44
31	q	305	CLA	C3D-C4D	-2.06	1.39	1.44
31	R	303	CLA	C1A-CHA	2.06	1.51	1.43
31	7	314	CLA	C1A-CHA	2.06	1.51	1.43
31	8	614	CLA	C1C-C2C	2.06	1.48	1.44
31	8	612	CLA	C1C-C2C	2.06	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	612	CLA	C3D-C4D	-2.06	1.39	1.44
31	N	304	CLA	C3D-C4D	-2.06	1.39	1.44
32	3	317	LUT	C34-C33	-2.06	1.33	1.35
31	b	613	CLA	C3D-C4D	-2.06	1.39	1.44
31	b	614	CLA	C3D-C4D	-2.06	1.39	1.44
31	n	316	CLA	C3D-C4D	-2.06	1.39	1.44
31	7	316	CLA	C1C-C2C	2.06	1.48	1.44
32	n	318	LUT	C26-C27	2.06	1.53	1.50
31	B	614	CLA	C3D-C4D	-2.06	1.39	1.44
30	8	608	CHL	C3A-C2A	-2.06	1.48	1.54
47	e	102	HEM	C4B-NB	-2.06	1.34	1.38
31	N	321	CLA	C3D-C4D	-2.06	1.39	1.44
31	p	610	CLA	C3D-C4D	-2.06	1.39	1.44
31	B	611	CLA	C1C-C2C	2.06	1.48	1.44
32	p	617	LUT	C28-C27	2.06	1.37	1.32
31	n	316	CLA	C1C-C2C	2.06	1.48	1.44
36	y	618	NEX	O24-C25	-2.06	1.43	1.46
30	p	609	CHL	C1B-NB	-2.06	1.35	1.37
43	C	615	BCR	C36-C18	2.06	1.55	1.50
30	p	609	CHL	C3A-C2A	-2.05	1.48	1.54
30	q	308	CHL	C3A-C2A	-2.05	1.48	1.54
31	b	608	CLA	C1A-CHA	2.05	1.51	1.43
31	Y	304	CLA	C3D-C4D	-2.05	1.39	1.44
31	2	610	CLA	C1C-C2C	2.05	1.48	1.44
31	C	601	CLA	C1C-C2C	2.05	1.48	1.44
31	g	313	CLA	C1C-C2C	2.05	1.48	1.44
31	5	614	CLA	C1C-C2C	2.05	1.48	1.44
31	p	612	CLA	C1C-C2C	2.05	1.48	1.44
31	S	310	CLA	C1A-CHA	2.05	1.51	1.43
31	n	313	CLA	C1C-C2C	2.05	1.48	1.44
31	n	314	CLA	C1C-C2C	2.05	1.48	1.44
31	N	303	CLA	C3D-C4D	-2.05	1.39	1.44
31	2	604	CLA	C1C-C2C	2.05	1.48	1.44
31	9	306	CLA	C1C-C2C	2.05	1.48	1.44
31	Y	313	CLA	C1A-CHA	2.05	1.51	1.43
32	p	617	LUT	C30-C29	-2.05	1.33	1.35
31	4	614	CLA	C1C-C2C	2.05	1.48	1.44
31	R	313	CLA	C3D-C4D	-2.05	1.39	1.44
36	R	319	NEX	C1-C6	-2.05	1.51	1.54
31	6	312	CLA	C1C-C2C	2.05	1.48	1.44
31	3	314	CLA	C3D-C4D	-2.05	1.39	1.44
34	g	322	LMG	C43-C42	-2.05	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	316	CLA	C3D-C4D	-2.05	1.39	1.44
43	T	101	BCR	C38-C26	2.05	1.54	1.50
31	N	303	CLA	C1C-C2C	2.05	1.48	1.44
32	p	617	LUT	C34-C33	-2.05	1.33	1.35
32	y	616	LUT	C14-C13	-2.05	1.33	1.35
31	2	604	CLA	C3D-C4D	-2.05	1.39	1.44
31	y	615	CLA	C3D-C4D	-2.05	1.39	1.44
31	0	612	CLA	C1C-C2C	2.05	1.48	1.44
31	p	604	CLA	C3D-C4D	-2.05	1.39	1.44
31	R	313	CLA	C1A-CHA	2.05	1.51	1.43
30	g	309	CHL	C1B-NB	-2.05	1.35	1.37
31	2	612	CLA	C1C-C2C	2.05	1.48	1.44
31	9	316	CLA	C1C-C2C	2.05	1.48	1.44
31	b	603	CLA	C1A-CHA	2.05	1.51	1.43
31	5	604	CLA	C1C-C2C	2.04	1.48	1.44
31	Y	303	CLA	C1C-C2C	2.04	1.48	1.44
31	8	604	CLA	C1C-C2C	2.04	1.48	1.44
31	r	306	CLA	C1A-CHA	2.04	1.51	1.43
31	1	613	CLA	C1A-CHA	2.04	1.51	1.43
31	c	603	CLA	C1A-CHA	2.04	1.51	1.43
31	4	613	CLA	C3D-C4D	-2.04	1.39	1.44
31	6	305	CLA	C3D-C4D	-2.04	1.39	1.44
31	C	605	CLA	C1B-NB	-2.04	1.35	1.37
34	C	624	LMG	C25-C24	-2.04	1.33	1.49
31	3	311	CLA	C1A-CHA	2.04	1.51	1.43
31	N	310	CLA	C3D-C4D	-2.04	1.39	1.44
31	R	303	CLA	C3D-C4D	-2.04	1.39	1.44
31	b	616	CLA	C1A-CHA	2.04	1.51	1.43
31	Y	310	CLA	C3D-C4D	-2.04	1.39	1.44
43	T	101	BCR	C37-C22	2.04	1.55	1.50
31	b	611	CLA	C1C-C2C	2.04	1.48	1.44
31	N	313	CLA	C3D-C4D	-2.04	1.39	1.44
31	7	311	CLA	C3D-C4D	-2.04	1.39	1.44
31	9	316	CLA	C3D-C4D	-2.04	1.39	1.44
34	n	322	LMG	C37-C36	-2.04	1.33	1.49
30	4	607	CHL	C3A-C2A	-2.04	1.48	1.54
36	6	319	NEX	C1-C6	-2.04	1.51	1.54
31	6	311	CLA	C1C-C2C	2.04	1.48	1.44
31	S	314	CLA	C1A-CHA	2.04	1.51	1.43
31	Y	303	CLA	C3D-C4D	-2.04	1.39	1.44
31	n	314	CLA	C3D-C4D	-2.04	1.39	1.44
31	6	303	CLA	C1C-C2C	2.04	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	315	CLA	C1C-C2C	2.04	1.48	1.44
31	0	603	CLA	C1A-CHA	2.04	1.51	1.43
31	n	312	CLA	C3D-C4D	-2.04	1.39	1.44
36	N	318	NEX	O24-C25	-2.03	1.43	1.46
31	y	610	CLA	C3D-C4D	-2.03	1.39	1.44
31	5	611	CLA	C1C-C2C	2.03	1.48	1.44
31	3	311	CLA	C3D-C4D	-2.03	1.39	1.44
36	R	301	NEX	O24-C25	-2.03	1.43	1.46
31	3	314	CLA	C1C-C2C	2.03	1.48	1.44
31	p	612	CLA	C3D-C4D	-2.03	1.39	1.44
32	5	617	LUT	C30-C29	-2.03	1.33	1.35
43	B	617	BCR	C17-C18	-2.03	1.33	1.35
31	2	612	CLA	C3D-C4D	-2.03	1.39	1.44
34	n	322	LMG	O1-C1	2.03	1.43	1.40
43	b	619	BCR	C38-C26	2.03	1.54	1.50
34	d	410	LMG	C25-C24	-2.03	1.33	1.49
35	q	317	RRX	C14-C13	-2.03	1.33	1.35
31	5	613	CLA	C1C-C2C	2.03	1.48	1.44
31	G	612	CLA	C1A-CHA	2.03	1.51	1.43
31	s	314	CLA	C1A-CHA	2.03	1.51	1.43
31	p	603	CLA	C1A-CHA	2.03	1.51	1.43
32	g	316	LUT	C34-C33	-2.03	1.33	1.35
34	w	201	LMG	C22-C21	-2.03	1.33	1.49
31	y	603	CLA	C1C-C2C	2.03	1.48	1.44
34	J	101	LMG	C25-C24	-2.03	1.33	1.49
31	y	614	CLA	C1C-C2C	2.03	1.48	1.44
31	8	610	CLA	C3D-C4D	-2.03	1.39	1.44
34	d	411	LMG	C22-C21	-2.03	1.33	1.49
31	C	612	CLA	C1A-CHA	2.03	1.51	1.43
43	B	618	BCR	C36-C18	2.03	1.55	1.50
43	H	101	BCR	C38-C26	2.03	1.54	1.50
31	9	315	CLA	C3D-C4D	-2.03	1.39	1.44
34	k	101	LMG	C43-C42	-2.03	1.33	1.49
31	y	611	CLA	C1C-C2C	2.03	1.48	1.44
31	A	409	CLA	C1A-CHA	2.03	1.51	1.43
31	5	613	CLA	C3D-C4D	-2.03	1.39	1.44
31	5	614	CLA	C1A-CHA	2.03	1.51	1.43
34	r	321	LMG	O7-C8	-2.03	1.41	1.46
31	s	305	CLA	C1C-C2C	2.03	1.48	1.44
34	D	411	LMG	C43-C42	-2.03	1.33	1.49
32	3	318	LUT	C34-C33	-2.03	1.33	1.35
31	p	602	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	406	BCR	C36-C18	2.03	1.55	1.50
31	7	312	CLA	C1C-C2C	2.03	1.48	1.44
34	D	411	LMG	C25-C24	-2.03	1.33	1.49
30	p	606	CHL	C1B-NB	-2.03	1.35	1.37
31	0	611	CLA	C1C-C2C	2.03	1.48	1.44
31	3	306	CLA	C1C-C2C	2.03	1.48	1.44
34	d	410	LMG	C43-C42	-2.03	1.33	1.49
32	Y	315	LUT	C14-C13	-2.03	1.33	1.35
34	B	621	LMG	C25-C24	-2.03	1.33	1.49
34	A	412	LMG	C22-C21	-2.03	1.33	1.49
31	Y	305	CLA	C3D-C4D	-2.03	1.39	1.44
38	x	201	SQD	O47-C45	-2.03	1.41	1.46
31	a	409	CLA	C1A-CHA	2.03	1.51	1.43
34	w	201	LMG	C43-C42	-2.02	1.33	1.49
30	Y	306	CHL	C3A-C2A	-2.02	1.48	1.54
31	b	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	6	303	CLA	C3D-C4D	-2.02	1.39	1.44
34	D	412	LMG	C22-C21	-2.02	1.33	1.49
32	G	615	LUT	C30-C29	-2.02	1.33	1.35
31	3	316	CLA	C1C-C2C	2.02	1.48	1.44
30	S	307	CHL	C1B-NB	-2.02	1.35	1.37
31	C	609	CLA	C1A-CHA	2.02	1.51	1.43
31	n	311	CLA	C3D-C4D	-2.02	1.39	1.44
34	C	619	LMG	C43-C42	-2.02	1.33	1.49
34	c	624	LMG	C43-C42	-2.02	1.33	1.49
47	E	101	HEM	C4B-NB	-2.02	1.34	1.38
31	1	610	CLA	C1C-C2C	2.02	1.48	1.44
31	b	615	CLA	C3D-C4D	-2.02	1.39	1.44
31	9	313	CLA	C1A-CHA	2.02	1.51	1.43
31	N	315	CLA	C1C-C2C	2.02	1.48	1.44
31	p	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	2	612	CLA	C1A-CHA	2.02	1.51	1.43
34	D	409	LMG	C25-C24	-2.02	1.33	1.49
31	B	610	CLA	C3D-C4D	-2.02	1.39	1.44
34	9	301	LMG	C43-C42	-2.02	1.33	1.49
36	s	319	NEX	O24-C25	-2.02	1.43	1.46
31	R	316	CLA	C1A-CHA	2.02	1.51	1.43
34	D	412	LMG	C43-C42	-2.02	1.33	1.49
31	6	311	CLA	C3D-C4D	-2.02	1.39	1.44
36	y	618	NEX	C1-C6	-2.02	1.51	1.54
31	g	310	CLA	C1A-CHA	2.02	1.51	1.43
31	G	610	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	305	CLA	C1C-C2C	2.02	1.48	1.44
31	B	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	Y	314	CLA	C3D-C4D	-2.02	1.39	1.44
34	q	302	LMG	C37-C36	-2.01	1.33	1.49
34	b	622	LMG	C25-C24	-2.01	1.33	1.49
31	c	612	CLA	C1A-CHA	2.01	1.51	1.43
31	s	310	CLA	C1A-CHA	2.01	1.51	1.43
34	9	302	LMG	C37-C36	-2.01	1.33	1.49
31	4	602	CLA	C3D-C4D	-2.01	1.39	1.44
32	p	617	LUT	C26-C27	2.01	1.53	1.50
31	5	604	CLA	C3D-C4D	-2.01	1.39	1.44
31	7	305	CLA	C3D-C4D	-2.01	1.39	1.44
34	9	301	LMG	C25-C24	-2.01	1.33	1.49
31	c	601	CLA	C1C-C2C	2.01	1.48	1.44
34	2	621	LMG	C37-C36	-2.01	1.33	1.49
44	A	416	PL9	C52-C5	-2.01	1.46	1.50
34	J	101	LMG	C43-C42	-2.01	1.33	1.49
30	4	606	CHL	C1B-NB	-2.01	1.35	1.37
31	0	613	CLA	C1A-CHA	2.01	1.51	1.43
34	b	622	LMG	C43-C42	-2.01	1.33	1.49
32	6	317	LUT	C26-C27	2.01	1.53	1.50
43	c	614	BCR	C37-C22	2.01	1.55	1.50
31	S	303	CLA	C3D-C4D	-2.01	1.39	1.44
31	g	313	CLA	C3D-C4D	-2.01	1.39	1.44
31	q	304	CLA	C1A-CHA	2.01	1.51	1.43
31	r	313	CLA	C1A-CHA	2.01	1.51	1.43
34	4	620	LMG	C43-C42	-2.01	1.33	1.49
31	n	303	CLA	C3D-C4D	-2.01	1.39	1.44
31	3	305	CLA	C1C-C2C	2.01	1.48	1.44
31	C	607	CLA	C1A-CHA	2.01	1.51	1.43
31	C	603	CLA	C1A-CHA	2.01	1.51	1.43
34	4	621	LMG	C37-C36	-2.01	1.33	1.49
31	s	316	CLA	C1A-CHA	2.01	1.51	1.43
31	1	611	CLA	C3D-C4D	-2.01	1.39	1.44
31	g	312	CLA	C1C-C2C	2.01	1.48	1.44
32	s	317	LUT	C26-C27	2.01	1.53	1.50
31	2	609	CLA	C3D-C4D	-2.01	1.39	1.44
31	y	604	CLA	C3D-C4D	-2.01	1.39	1.44
31	g	305	CLA	C3D-C4D	-2.01	1.39	1.44
34	d	411	LMG	C43-C42	-2.01	1.33	1.49
34	C	619	LMG	C25-C24	-2.01	1.33	1.49
31	5	612	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	307	CLA	C1A-CHA	2.01	1.51	1.43
32	q	318	LUT	C34-C33	-2.01	1.33	1.35
31	1	602	CLA	C1C-C2C	2.01	1.48	1.44
31	2	603	CLA	C1C-C2C	2.01	1.48	1.44
31	b	610	CLA	C1A-CHA	2.01	1.51	1.43
31	0	614	CLA	C3D-C4D	-2.00	1.39	1.44
31	p	604	CLA	C1A-CHA	2.00	1.51	1.43
31	p	613	CLA	C1C-C2C	2.00	1.48	1.44
34	2	620	LMG	C25-C24	-2.00	1.33	1.49
31	c	611	CLA	C1A-CHA	2.00	1.51	1.43
34	k	101	LMG	C22-C21	-2.00	1.33	1.49
31	9	305	CLA	C1C-C2C	2.00	1.48	1.44
31	3	315	CLA	C3D-C4D	-2.00	1.39	1.44
31	5	615	CLA	C3D-C4D	-2.00	1.39	1.44
34	B	621	LMG	C43-C42	-2.00	1.33	1.49
31	Y	304	CLA	C1C-C2C	2.00	1.48	1.44
31	q	316	CLA	C1C-C2C	2.00	1.48	1.44
34	q	301	LMG	C43-C42	-2.00	1.33	1.49
31	r	313	CLA	C1C-C2C	2.00	1.48	1.44
34	G	621	LMG	C43-C42	-2.00	1.33	1.49
31	3	313	CLA	C1C-C2C	2.00	1.48	1.44
31	B	601	CLA	C1C-C2C	2.00	1.48	1.44
34	G	621	LMG	C25-C24	-2.00	1.33	1.49
31	8	614	CLA	C3D-C4D	-2.00	1.39	1.44
31	s	303	CLA	C3D-C4D	-2.00	1.39	1.44
31	4	614	CLA	C1A-CHA	2.00	1.51	1.43
31	8	611	CLA	C3D-C4D	-2.00	1.39	1.44
30	p	608	CHL	C1B-NB	-2.00	1.35	1.37
34	G	622	LMG	C37-C36	-2.00	1.33	1.49
31	r	315	CLA	C1A-CHA	2.00	1.51	1.43
31	C	611	CLA	C1A-CHA	2.00	1.51	1.43
31	r	304	CLA	C3D-C4D	-2.00	1.39	1.44
31	s	305	CLA	C3D-C4D	-2.00	1.39	1.44
30	q	308	CHL	C1D-ND	-2.00	1.35	1.37

All (8510) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	G	615	LUT	C40-C33-C34	-33.47	76.04	122.92
32	G	615	LUT	C32-C33-C34	25.38	157.89	118.94
32	G	615	LUT	C40-C33-C32	-22.99	81.85	118.08
43	C	615	BCR	C15-C14-C13	-12.84	108.99	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	t	101	BCR	C11-C10-C9	-11.88	110.35	127.31
43	d	406	BCR	C15-C14-C13	-11.80	110.48	127.31
43	d	406	BCR	C7-C8-C9	-11.71	108.55	126.23
43	t	101	BCR	C15-C14-C13	-11.67	110.65	127.31
43	C	615	BCR	C7-C8-C9	-11.50	108.85	126.23
32	R	317	LUT	C35-C34-C33	-10.67	112.09	127.31
32	p	617	LUT	C35-C34-C33	-10.40	112.47	127.31
43	t	101	BCR	C7-C8-C9	-10.37	110.56	126.23
32	p	616	LUT	C35-C34-C33	-10.37	112.52	127.31
31	B	607	CLA	C4A-NA-C1A	10.23	111.31	106.71
43	c	614	BCR	C20-C21-C22	-10.11	112.88	127.31
31	b	608	CLA	C4A-NA-C1A	9.96	111.19	106.71
31	d	405	CLA	C4A-NA-C1A	9.94	111.18	106.71
31	B	615	CLA	C4A-NA-C1A	9.82	111.12	106.71
31	c	613	CLA	C4A-NA-C1A	9.78	111.11	106.71
31	R	306	CLA	C4A-NA-C1A	9.67	111.06	106.71
31	a	409	CLA	C4A-NA-C1A	9.64	111.04	106.71
31	A	409	CLA	C4A-NA-C1A	9.62	111.03	106.71
31	b	610	CLA	C4A-NA-C1A	9.60	111.02	106.71
31	g	305	CLA	C4A-NA-C1A	9.60	111.02	106.71
32	2	615	LUT	C35-C34-C33	-9.57	113.64	127.31
31	b	616	CLA	C4A-NA-C1A	9.57	111.01	106.71
31	D	404	CLA	C4A-NA-C1A	9.57	111.01	106.71
31	q	315	CLA	C4A-NA-C1A	9.55	111.00	106.71
31	C	612	CLA	C4A-NA-C1A	9.50	110.98	106.71
31	C	607	CLA	C4A-NA-C1A	9.48	110.97	106.71
31	c	606	CLA	C4A-NA-C1A	9.48	110.97	106.71
31	c	612	CLA	C4A-NA-C1A	9.45	110.95	106.71
31	R	316	CLA	C4A-NA-C1A	9.43	110.95	106.71
31	A	406	CLA	C4A-NA-C1A	9.42	110.94	106.71
31	b	609	CLA	C4A-NA-C1A	9.42	110.94	106.71
31	r	315	CLA	C4A-NA-C1A	9.40	110.93	106.71
31	A	405	CLA	C4A-NA-C1A	9.40	110.93	106.71
31	q	313	CLA	C4A-NA-C1A	9.40	110.93	106.71
31	C	609	CLA	C4A-NA-C1A	9.39	110.93	106.71
31	2	604	CLA	C4A-NA-C1A	9.38	110.92	106.71
31	9	312	CLA	C4A-NA-C1A	9.38	110.92	106.71
31	r	312	CLA	C4A-NA-C1A	9.37	110.92	106.71
31	4	612	CLA	C4A-NA-C1A	9.35	110.91	106.71
31	b	613	CLA	C4A-NA-C1A	9.34	110.90	106.71
31	s	310	CLA	C4A-NA-C1A	9.33	110.90	106.71
31	C	613	CLA	C4A-NA-C1A	9.33	110.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	609	CLA	C4A-NA-C1A	9.32	110.89	106.71
31	y	604	CLA	C4A-NA-C1A	9.29	110.88	106.71
31	c	610	CLA	C4A-NA-C1A	9.28	110.88	106.71
31	p	613	CLA	C4A-NA-C1A	9.28	110.88	106.71
31	7	305	CLA	C4A-NA-C1A	9.25	110.86	106.71
31	c	611	CLA	C4A-NA-C1A	9.20	110.84	106.71
31	y	613	CLA	C4A-NA-C1A	9.19	110.84	106.71
31	6	305	CLA	C4A-NA-C1A	9.17	110.83	106.71
31	a	406	CLA	C4A-NA-C1A	9.16	110.82	106.71
31	2	602	CLA	C4A-NA-C1A	9.15	110.82	106.71
31	4	604	CLA	C4A-NA-C1A	9.13	110.81	106.71
31	c	609	CLA	C4A-NA-C1A	9.13	110.81	106.71
31	G	604	CLA	C4A-NA-C1A	9.12	110.81	106.71
31	a	407	CLA	C4A-NA-C1A	9.12	110.80	106.71
31	0	604	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	n	315	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	R	312	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	r	306	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	4	610	CLA	C4A-NA-C1A	9.10	110.80	106.71
31	B	616	CLA	C4A-NA-C1A	9.09	110.79	106.71
31	S	306	CLA	C4A-NA-C1A	9.07	110.78	106.71
31	8	613	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	9	306	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	C	611	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	1	613	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	0	615	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	0	610	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	D	403	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	N	314	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	R	315	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	S	310	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	S	314	CLA	C4A-NA-C1A	9.01	110.76	106.71
31	s	312	CLA	C4A-NA-C1A	9.01	110.76	106.71
31	2	610	CLA	C4A-NA-C1A	9.00	110.75	106.71
31	q	304	CLA	C4A-NA-C1A	9.00	110.75	106.71
31	Y	305	CLA	C4A-NA-C1A	8.99	110.75	106.71
31	B	604	CLA	C4A-NA-C1A	8.98	110.75	106.71
31	y	615	CLA	C4A-NA-C1A	8.98	110.74	106.71
31	r	311	CLA	C4A-NA-C1A	8.98	110.74	106.71
31	q	312	CLA	C4A-NA-C1A	8.97	110.74	106.71
31	b	606	CLA	C4A-NA-C1A	8.96	110.74	106.71
31	R	303	CLA	C4A-NA-C1A	8.95	110.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	313	CLA	C4A-NA-C1A	8.95	110.73	106.71
31	Y	311	CLA	C4A-NA-C1A	8.95	110.73	106.71
31	N	304	CLA	C4A-NA-C1A	8.94	110.73	106.71
31	2	612	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	9	314	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	N	305	CLA	C4A-NA-C1A	8.92	110.72	106.71
31	N	311	CLA	C4A-NA-C1A	8.91	110.71	106.71
43	D	405	BCR	C7-C8-C9	-8.90	112.78	126.23
31	G	610	CLA	C4A-NA-C1A	8.90	110.71	106.71
31	c	605	CLA	C4A-NA-C1A	8.90	110.71	106.71
31	g	310	CLA	C4A-NA-C1A	8.90	110.71	106.71
31	1	603	CLA	C4A-NA-C1A	8.89	110.70	106.71
31	n	304	CLA	C4A-NA-C1A	8.89	110.70	106.71
31	b	614	CLA	C4A-NA-C1A	8.89	110.70	106.71
31	G	612	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	b	605	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	s	313	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	2	611	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	5	615	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	6	314	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	B	608	CLA	C4A-NA-C1A	8.86	110.69	106.71
31	5	603	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	1	604	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	1	614	CLA	C4A-NA-C1A	8.85	110.68	106.71
31	S	305	CLA	C4A-NA-C1A	8.85	110.68	106.71
31	0	602	CLA	C4A-NA-C1A	8.84	110.68	106.71
31	r	316	CLA	C4A-NA-C1A	8.84	110.68	106.71
31	8	604	CLA	C4A-NA-C1A	8.83	110.68	106.71
31	g	303	CLA	C4A-NA-C1A	8.83	110.68	106.71
31	s	305	CLA	C4A-NA-C1A	8.83	110.68	106.71
31	s	304	CLA	C4A-NA-C1A	8.83	110.67	106.71
31	G	611	CLA	C4A-NA-C1A	8.82	110.67	106.71
31	B	612	CLA	C4A-NA-C1A	8.82	110.67	106.71
31	n	305	CLA	C4A-NA-C1A	8.81	110.67	106.71
31	r	303	CLA	C4A-NA-C1A	8.81	110.67	106.71
31	3	306	CLA	C4A-NA-C1A	8.80	110.66	106.71
31	3	311	CLA	C4A-NA-C1A	8.80	110.66	106.71
31	b	602	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	C	610	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	Y	313	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	c	604	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	s	303	CLA	C4A-NA-C1A	8.78	110.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	303	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	y	612	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	R	305	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	p	602	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	c	607	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	6	311	CLA	C4A-NA-C1A	8.76	110.64	106.71
31	0	614	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	2	613	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	3	313	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	7	314	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	5	604	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	0	613	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	s	316	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	A	407	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	d	401	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	G	609	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	R	313	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	9	304	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	n	314	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	C	602	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	5	602	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	C	608	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	2	609	CLA	C4A-NA-C1A	8.72	110.62	106.71
31	y	611	CLA	C4A-NA-C1A	8.72	110.62	106.71
31	g	312	CLA	C4A-NA-C1A	8.71	110.62	106.71
31	g	313	CLA	C4A-NA-C1A	8.71	110.62	106.71
31	r	313	CLA	C4A-NA-C1A	8.71	110.62	106.71
31	5	611	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	8	603	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	9	305	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	n	312	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	r	305	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	q	316	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	n	303	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	s	306	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	c	603	CLA	C4A-NA-C1A	8.67	110.61	106.71
31	q	314	CLA	C4A-NA-C1A	8.67	110.61	106.71
31	s	314	CLA	C4A-NA-C1A	8.67	110.61	106.71
31	6	313	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	5	614	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	3	312	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	5	610	CLA	C4A-NA-C1A	8.67	110.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	610	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	B	603	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	6	315	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	b	615	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	4	614	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	S	311	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	Y	303	CLA	C4A-NA-C1A	8.65	110.60	106.71
31	8	612	CLA	C4A-NA-C1A	8.65	110.60	106.71
31	1	602	CLA	C4A-NA-C1A	8.65	110.59	106.71
31	7	315	CLA	C4A-NA-C1A	8.65	110.59	106.71
31	8	610	CLA	C4A-NA-C1A	8.64	110.59	106.71
31	c	602	CLA	C4A-NA-C1A	8.64	110.59	106.71
31	G	603	CLA	C4A-NA-C1A	8.63	110.58	106.71
31	N	313	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	S	312	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	8	609	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	3	316	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	B	605	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	g	304	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	N	303	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	b	612	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	r	304	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	7	303	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	9	315	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	n	311	CLA	C4A-NA-C1A	8.60	110.57	106.71
31	b	607	CLA	C4A-NA-C1A	8.60	110.57	106.71
31	R	307	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	6	316	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	y	603	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	b	617	CLA	C4A-NA-C1A	8.58	110.56	106.71
31	N	315	CLA	C4A-NA-C1A	8.58	110.56	106.71
31	Y	312	CLA	C4A-NA-C1A	8.57	110.56	106.71
31	7	312	CLA	C4A-NA-C1A	8.57	110.56	106.71
31	n	313	CLA	C4A-NA-C1A	8.57	110.56	106.71
31	S	316	CLA	C4A-NA-C1A	8.56	110.55	106.71
31	N	310	CLA	C4A-NA-C1A	8.55	110.55	106.71
31	p	611	CLA	C4A-NA-C1A	8.55	110.55	106.71
31	8	611	CLA	C4A-NA-C1A	8.54	110.54	106.71
31	Y	314	CLA	C4A-NA-C1A	8.53	110.54	106.71
31	d	404	CLA	C4A-NA-C1A	8.53	110.54	106.71
31	5	612	CLA	C4A-NA-C1A	8.52	110.54	106.71
31	3	314	CLA	C4A-NA-C1A	8.51	110.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	606	CLA	C4A-NA-C1A	8.51	110.53	106.71
31	C	601	CLA	C4A-NA-C1A	8.51	110.53	106.71
31	4	602	CLA	C4A-NA-C1A	8.50	110.53	106.71
31	6	303	CLA	C4A-NA-C1A	8.49	110.53	106.71
31	C	604	CLA	C4A-NA-C1A	8.49	110.52	106.71
31	p	603	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	y	602	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	4	611	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	g	314	CLA	C4A-NA-C1A	8.47	110.52	106.71
31	Y	304	CLA	C4A-NA-C1A	8.47	110.52	106.71
31	1	612	CLA	C4A-NA-C1A	8.47	110.51	106.71
31	8	602	CLA	C4A-NA-C1A	8.47	110.51	106.71
31	3	301	CLA	C4A-NA-C1A	8.46	110.51	106.71
31	p	612	CLA	C4A-NA-C1A	8.45	110.51	106.71
31	7	304	CLA	C4A-NA-C1A	8.45	110.50	106.71
31	y	610	CLA	C4A-NA-C1A	8.44	110.50	106.71
31	3	305	CLA	C4A-NA-C1A	8.44	110.50	106.71
31	7	316	CLA	C4A-NA-C1A	8.44	110.50	106.71
31	q	305	CLA	C4A-NA-C1A	8.43	110.50	106.71
31	R	304	CLA	C4A-NA-C1A	8.43	110.50	106.71
31	6	304	CLA	C4A-NA-C1A	8.42	110.49	106.71
31	2	603	CLA	C4A-NA-C1A	8.42	110.49	106.71
31	3	304	CLA	C4A-NA-C1A	8.41	110.49	106.71
31	B	601	CLA	C4A-NA-C1A	8.41	110.49	106.71
31	7	311	CLA	C4A-NA-C1A	8.41	110.49	106.71
31	g	311	CLA	C4A-NA-C1A	8.40	110.48	106.71
31	6	312	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	B	602	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	4	613	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	R	314	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	3	315	CLA	C4A-NA-C1A	8.36	110.46	106.71
31	5	613	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	R	311	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	r	314	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	B	611	CLA	C4A-NA-C1A	8.34	110.46	106.71
31	G	602	CLA	C4A-NA-C1A	8.34	110.46	106.71
31	n	316	CLA	C4A-NA-C1A	8.34	110.46	106.71
31	p	604	CLA	C4A-NA-C1A	8.33	110.45	106.71
31	C	605	CLA	C4A-NA-C1A	8.32	110.45	106.71
31	s	311	CLA	C4A-NA-C1A	8.32	110.45	106.71
31	N	321	CLA	C4A-NA-C1A	8.32	110.45	106.71
31	b	604	CLA	C4A-NA-C1A	8.31	110.44	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	310	CLA	C4A-NA-C1A	8.31	110.44	106.71
31	C	606	CLA	C4A-NA-C1A	8.29	110.43	106.71
31	b	611	CLA	C4A-NA-C1A	8.29	110.43	106.71
31	9	313	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	p	610	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	9	316	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	0	611	CLA	C4A-NA-C1A	8.26	110.42	106.71
31	4	603	CLA	C4A-NA-C1A	8.26	110.42	106.71
31	0	612	CLA	C4A-NA-C1A	8.25	110.42	106.71
31	r	307	CLA	C4A-NA-C1A	8.25	110.41	106.71
31	q	306	CLA	C4A-NA-C1A	8.24	110.41	106.71
31	1	611	CLA	C4A-NA-C1A	8.23	110.41	106.71
31	p	614	CLA	C4A-NA-C1A	8.23	110.41	106.71
31	c	608	CLA	C4A-NA-C1A	8.22	110.40	106.71
31	B	614	CLA	C4A-NA-C1A	8.22	110.40	106.71
31	c	601	CLA	C4A-NA-C1A	8.20	110.39	106.71
31	s	315	CLA	C4A-NA-C1A	8.20	110.39	106.71
31	0	603	CLA	C4A-NA-C1A	8.19	110.39	106.71
31	N	312	CLA	C4A-NA-C1A	8.17	110.38	106.71
31	b	603	CLA	C4A-NA-C1A	8.17	110.38	106.71
31	y	614	CLA	C4A-NA-C1A	8.17	110.38	106.71
31	1	610	CLA	C4A-NA-C1A	8.16	110.38	106.71
31	C	603	CLA	C4A-NA-C1A	8.13	110.36	106.71
31	8	614	CLA	C4A-NA-C1A	8.07	110.34	106.71
31	B	613	CLA	C4A-NA-C1A	8.07	110.33	106.71
43	D	405	BCR	C15-C14-C13	-8.03	115.85	127.31
31	S	315	CLA	C4A-NA-C1A	8.02	110.31	106.71
43	C	615	BCR	C20-C21-C22	-7.95	115.96	127.31
31	p	615	CLA	C4A-NA-C1A	7.95	110.28	106.71
31	7	313	CLA	C4A-NA-C1A	7.81	110.22	106.71
31	G	613	CLA	C4A-NA-C1A	7.67	110.16	106.71
31	r	303	CLA	O2D-CGD-CBD	7.59	124.75	111.27
43	c	614	BCR	C24-C23-C22	-7.58	114.78	126.23
43	c	615	BCR	C20-C21-C22	-7.40	116.76	127.31
43	C	615	BCR	C8-C9-C10	7.35	130.21	118.94
43	A	410	BCR	C15-C14-C13	-7.24	116.97	127.31
43	t	101	BCR	C33-C5-C6	-7.23	116.40	124.53
43	t	101	BCR	C15-C16-C17	-7.22	108.68	123.47
31	R	303	CLA	O2D-CGD-CBD	7.17	124.01	111.27
32	G	615	LUT	C31-C30-C29	-7.16	117.09	127.31
43	z	101	BCR	C11-C10-C9	-7.16	117.10	127.31
43	C	615	BCR	C12-C13-C14	6.99	129.66	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	306	CLA	O2D-CGD-CBD	6.88	123.49	111.27
43	c	615	BCR	C15-C14-C13	-6.71	117.73	127.31
43	d	406	BCR	C8-C9-C10	6.60	129.07	118.94
35	g	315	RRX	C11-C10-C9	-6.58	117.92	127.31
32	g	316	LUT	C31-C30-C29	-6.56	117.94	127.31
43	H	101	BCR	C11-C10-C9	-6.56	117.95	127.31
43	c	614	BCR	C16-C17-C18	-6.55	117.97	127.31
31	S	312	CLA	O2A-C1-C2	6.54	125.81	108.64
43	B	619	BCR	C11-C10-C9	-6.52	118.00	127.31
35	g	315	RRX	C15-C14-C13	-6.51	118.02	127.31
32	Y	316	LUT	C11-C10-C9	-6.51	118.03	127.31
43	a	410	BCR	C24-C23-C22	-6.44	116.50	126.23
43	C	615	BCR	C10-C11-C12	-6.43	103.16	123.22
43	d	406	BCR	C10-C11-C12	-6.43	103.16	123.22
43	a	410	BCR	C20-C21-C22	-6.42	118.15	127.31
43	Z	101	BCR	C7-C8-C9	-6.34	116.65	126.23
31	3	316	CLA	CMD-C2D-C1D	6.34	135.88	124.71
43	c	615	BCR	C1-C6-C5	-6.33	113.70	122.61
31	p	614	CLA	CMD-C2D-C1D	6.27	135.77	124.71
32	4	616	LUT	C11-C10-C9	-6.26	118.38	127.31
43	t	101	BCR	C20-C21-C22	-6.25	118.39	127.31
35	q	317	RRX	C15-C14-C13	-6.24	118.40	127.31
31	r	315	CLA	O2A-C1-C2	6.23	125.00	108.64
31	5	615	CLA	CMD-C2D-C1D	6.23	135.68	124.71
32	3	318	LUT	C15-C14-C13	-6.22	118.43	127.31
43	Z	101	BCR	C11-C10-C9	-6.22	118.44	127.31
43	C	615	BCR	C11-C10-C9	6.21	136.17	127.31
43	T	101	BCR	C33-C5-C6	-6.21	117.56	124.53
31	B	604	CLA	O2D-CGD-CBD	6.18	122.26	111.27
43	B	618	BCR	C15-C14-C13	-6.13	118.56	127.31
35	4	615	RRX	C20-C21-C22	-6.12	118.58	127.31
32	R	317	LUT	C30-C31-C32	-6.11	104.15	123.22
43	B	619	BCR	C15-C14-C13	-6.10	118.60	127.31
31	s	306	CLA	O2D-CGD-CBD	6.10	122.11	111.27
43	V	101	BCR	C16-C17-C18	-6.10	118.61	127.31
32	2	615	LUT	C38-C25-C24	-6.09	110.53	123.56
43	C	615	BCR	C1-C6-C5	-6.09	114.04	122.61
35	9	317	RRX	C20-C21-C22	-6.08	118.64	127.31
35	G	614	RRX	C20-C21-C22	-6.08	118.64	127.31
35	q	317	RRX	C1-C6-C5	-6.06	114.07	122.61
43	b	620	BCR	C7-C8-C9	-6.05	117.09	126.23
31	C	605	CLA	O2D-CGD-CBD	6.04	122.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	r	318	XAT	C31-C30-C29	-6.02	118.71	127.31
43	b	618	BCR	C38-C26-C25	-6.01	117.78	124.53
31	R	312	CLA	CMD-C2D-C1D	6.00	135.29	124.71
35	2	614	RRX	C20-C21-C22	-6.00	118.74	127.31
32	2	615	LUT	C28-C29-C30	5.99	128.13	118.94
43	C	614	BCR	C38-C26-C25	-5.98	117.81	124.53
31	5	614	CLA	O2D-CGD-CBD	5.97	121.87	111.27
31	B	606	CLA	O2D-CGD-CBD	5.97	121.87	111.27
31	1	604	CLA	O2D-CGD-CBD	5.96	121.86	111.27
31	S	313	CLA	O2D-CGD-CBD	5.95	121.84	111.27
32	2	615	LUT	C30-C31-C32	-5.94	104.67	123.22
31	c	612	CLA	O2D-CGD-CBD	5.94	121.83	111.27
31	S	304	CLA	C4A-NA-C1A	5.94	109.38	106.71
43	A	410	BCR	C38-C26-C25	-5.93	117.87	124.53
31	q	312	CLA	CMD-C2D-C1D	5.92	135.15	124.71
43	t	101	BCR	C27-C26-C25	-5.92	114.14	122.73
31	9	312	CLA	O2A-C1-C2	5.91	124.18	108.64
31	D	404	CLA	O2A-C1-C2	5.91	124.17	108.64
31	8	603	CLA	CMD-C2D-C1D	5.89	135.09	124.71
31	1	610	CLA	CMD-C2D-C1D	5.88	135.07	124.71
43	C	614	BCR	C11-C10-C9	-5.86	118.94	127.31
31	7	305	CLA	CMD-C2D-C1D	5.86	135.04	124.71
43	v	101	BCR	C16-C17-C18	-5.84	118.98	127.31
44	A	416	PL9	C7-C3-C4	5.83	121.62	116.88
43	b	618	BCR	C33-C5-C6	-5.82	117.99	124.53
31	r	311	CLA	O2A-C1-C2	5.82	123.94	108.64
31	C	613	CLA	O2A-C1-C2	5.82	123.94	108.64
35	q	317	RRX	C20-C21-C22	-5.82	119.01	127.31
43	d	406	BCR	C38-C26-C25	-5.82	118.00	124.53
32	S	318	LUT	C35-C34-C33	-5.81	119.02	127.31
31	R	306	CLA	CMD-C2D-C1D	5.80	134.94	124.71
43	h	101	BCR	C11-C10-C9	-5.80	119.04	127.31
31	S	315	CLA	CMD-C2D-C1D	5.79	134.92	124.71
43	T	101	BCR	C7-C8-C9	-5.78	117.51	126.23
31	d	401	CLA	CMD-C2D-C1D	5.77	134.88	124.71
31	2	613	CLA	CMD-C2D-C1D	5.77	134.88	124.71
31	r	313	CLA	O2A-C1-C2	5.77	122.45	108.97
32	9	318	LUT	C31-C30-C29	-5.77	119.08	127.31
43	C	615	BCR	C33-C5-C6	-5.76	118.06	124.53
31	7	313	CLA	O2D-CGD-CBD	5.76	121.50	111.27
31	D	404	CLA	O2D-CGD-CBD	5.76	121.50	111.27
31	C	603	CLA	CMD-C2D-C1D	5.76	134.86	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	g	316	LUT	C11-C10-C9	-5.76	119.09	127.31
31	7	304	CLA	CMD-C2D-C1D	5.75	134.85	124.71
31	b	607	CLA	CMD-C2D-C1D	5.75	134.85	124.71
31	4	614	CLA	CMD-C2D-C1D	5.75	134.84	124.71
31	r	316	CLA	CMD-C2D-C1D	5.75	134.84	124.71
43	t	101	BCR	C11-C12-C13	-5.74	110.28	126.42
31	7	313	CLA	CMD-C2D-C1D	5.73	134.82	124.71
31	0	612	CLA	CMD-C2D-C1D	5.73	134.81	124.71
31	y	610	CLA	CMD-C2D-C1D	5.72	134.80	124.71
31	9	304	CLA	O2A-C1-C2	5.72	123.67	108.64
31	p	604	CLA	CMD-C2D-C1D	5.72	134.79	124.71
31	N	310	CLA	CMD-C2D-C1D	5.71	134.78	124.71
31	c	607	CLA	O2D-CGD-CBD	5.71	121.41	111.27
31	R	314	CLA	CMD-C2D-C1D	5.70	134.76	124.71
31	q	316	CLA	CMD-C2D-C1D	5.70	134.76	124.71
31	d	404	CLA	O2A-C1-C2	5.70	123.61	108.64
32	p	617	LUT	C21-C26-C27	-5.69	105.50	112.70
43	d	406	BCR	C24-C23-C22	-5.69	117.64	126.23
31	s	315	CLA	CMD-C2D-C1D	5.69	134.74	124.71
43	b	619	BCR	C20-C21-C22	-5.69	119.19	127.31
31	B	605	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	5	610	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	p	610	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	g	304	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	g	303	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	s	303	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	G	602	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	b	603	CLA	CAA-C2A-C3A	-5.66	97.27	112.78
43	B	617	BCR	C4-C5-C6	-5.66	114.51	122.73
43	b	620	BCR	C11-C10-C9	-5.66	119.23	127.31
31	C	607	CLA	O2D-CGD-CBD	5.66	121.32	111.27
31	G	603	CLA	CMD-C2D-C1D	5.66	134.68	124.71
31	p	603	CLA	O2A-C1-C2	5.65	123.48	108.64
31	G	613	CLA	CMD-C2D-C1D	5.65	134.66	124.71
43	v	101	BCR	C38-C26-C25	-5.65	118.19	124.53
37	R	318	XAT	C31-C30-C29	-5.64	119.25	127.31
31	9	316	CLA	CMD-C2D-C1D	5.64	134.66	124.71
31	B	616	CLA	O2D-CGD-CBD	5.64	121.29	111.27
31	N	315	CLA	CMD-C2D-C1D	5.64	134.65	124.71
31	R	304	CLA	CMD-C2D-C1D	5.64	134.65	124.71
31	6	312	CLA	O2A-C1-C2	5.64	123.45	108.64
31	7	311	CLA	CMD-C2D-C1D	5.64	134.65	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	A	408	PHO	C4D-CHA-CBD	-5.63	105.97	108.52
31	y	612	CLA	O2D-CGD-CBD	5.63	121.28	111.27
32	7	317	LUT	C7-C8-C9	-5.63	117.73	126.23
31	0	604	CLA	O2D-CGD-CBD	5.63	121.27	111.27
31	R	316	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	6	304	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	q	304	CLA	CMD-C2D-C1D	5.62	134.62	124.71
32	9	318	LUT	C15-C14-C13	-5.62	119.29	127.31
31	B	605	CLA	O2D-CGD-CBD	5.62	121.25	111.27
31	r	304	CLA	CMD-C2D-C1D	5.62	134.61	124.71
31	s	306	CLA	CMD-C2D-C1D	5.62	134.61	124.71
31	9	312	CLA	CMD-C2D-C1D	5.62	134.61	124.71
31	B	604	CLA	CMD-C2D-C1D	5.62	134.61	124.71
31	7	305	CLA	O2D-CGD-CBD	5.61	121.24	111.27
31	9	305	CLA	CMD-C2D-C1D	5.61	134.60	124.71
31	2	603	CLA	CMD-C2D-C1D	5.61	134.60	124.71
31	6	303	CLA	CMD-C2D-C1D	5.61	134.59	124.71
31	B	601	CLA	O2D-CGD-CBD	5.60	121.22	111.27
31	4	610	CLA	CMD-C2D-C1D	5.60	134.59	124.71
31	C	612	CLA	O2D-CGD-CBD	5.60	121.22	111.27
31	b	603	CLA	O2A-C1-C2	5.60	123.35	108.64
31	2	609	CLA	CMD-C2D-C1D	5.60	134.58	124.71
31	6	311	CLA	CMD-C2D-C1D	5.60	134.58	124.71
31	y	615	CLA	CMD-C2D-C1D	5.60	134.58	124.71
43	V	101	BCR	C33-C5-C6	-5.59	118.25	124.53
31	g	312	CLA	CMD-C2D-C1D	5.59	134.56	124.71
31	B	606	CLA	CMD-C2D-C1D	5.58	134.56	124.71
31	1	602	CLA	O2D-CGD-CBD	5.58	121.19	111.27
35	4	615	RRX	C24-C23-C22	-5.58	117.80	126.23
31	B	615	CLA	O2D-CGD-CBD	5.58	121.19	111.27
31	3	304	CLA	CMD-C2D-C1D	5.58	134.55	124.71
31	c	601	CLA	CMD-C2D-C1D	5.58	134.55	124.71
31	6	315	CLA	CMD-C2D-C1D	5.58	134.54	124.71
31	b	605	CLA	O2D-CGD-CBD	5.58	121.18	111.27
31	R	303	CLA	O2A-C1-C2	5.58	122.01	108.97
31	r	312	CLA	CMD-C2D-C1D	5.57	134.54	124.71
35	9	317	RRX	C24-C23-C22	-5.57	117.81	126.23
42	D	401	PHO	C4D-CHA-CBD	-5.57	106.00	108.52
31	p	603	CLA	CMD-C2D-C1D	5.57	134.53	124.71
31	n	316	CLA	CMD-C2D-C1D	5.57	134.53	124.71
31	4	602	CLA	CMD-C2D-C1D	5.57	134.52	124.71
31	q	314	CLA	CMD-C2D-C1D	5.56	134.52	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	607	CLA	O2D-CGD-CBD	5.56	121.15	111.27
31	1	614	CLA	CMD-C2D-C1D	5.56	134.52	124.71
31	p	615	CLA	CMD-C2D-C1D	5.56	134.52	124.71
35	G	614	RRX	C24-C23-C22	-5.56	117.84	126.23
31	2	602	CLA	CMD-C2D-C1D	5.56	134.51	124.71
31	b	602	CLA	CMD-C2D-C1D	5.56	134.51	124.71
31	R	315	CLA	CMD-C2D-C1D	5.56	134.51	124.71
31	6	305	CLA	CMD-C2D-C1D	5.56	134.50	124.71
31	N	303	CLA	CMD-C2D-C1D	5.55	134.50	124.71
31	q	312	CLA	O2D-CGD-CBD	5.55	121.13	111.27
32	g	316	LUT	C35-C34-C33	-5.55	119.39	127.31
43	c	615	BCR	C11-C10-C9	-5.55	119.39	127.31
31	C	610	CLA	O2D-CGD-CBD	5.55	121.13	111.27
31	G	604	CLA	CMD-C2D-C1D	5.55	134.49	124.71
31	g	314	CLA	CMD-C2D-C1D	5.54	134.49	124.71
31	8	614	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	A	406	CLA	CMD-C2D-C1D	5.54	134.48	124.71
43	h	101	BCR	C15-C14-C13	-5.54	119.40	127.31
43	b	619	BCR	C16-C17-C18	-5.54	119.40	127.31
31	3	313	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	S	303	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	C	611	CLA	O2D-CGD-CBD	5.54	121.11	111.27
43	b	618	BCR	C27-C26-C25	-5.54	114.69	122.73
31	R	305	CLA	O2D-CGD-CBD	5.54	121.11	111.27
31	S	306	CLA	CMD-C2D-C1D	5.54	134.47	124.71
31	b	608	CLA	CMD-C2D-C1D	5.54	134.47	124.71
31	p	612	CLA	CMD-C2D-C1D	5.54	134.47	124.71
31	y	615	CLA	O2D-CGD-CBD	5.53	121.10	111.27
31	6	314	CLA	CMD-C2D-C1D	5.53	134.47	124.71
31	5	603	CLA	CMD-C2D-C1D	5.53	134.47	124.71
31	B	602	CLA	O2D-CGD-CBD	5.53	121.10	111.27
31	q	305	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	n	303	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	b	615	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	c	603	CLA	CMD-C2D-C1D	5.53	134.46	124.71
43	d	406	BCR	C34-C9-C10	-5.53	115.18	122.92
31	Y	310	CLA	CMD-C2D-C1D	5.53	134.46	124.71
35	2	614	RRX	C24-C23-C22	-5.53	117.88	126.23
31	N	321	CLA	CMD-C2D-C1D	5.53	134.45	124.71
31	C	604	CLA	CMD-C2D-C1D	5.52	134.45	124.71
31	A	409	CLA	O2D-CGD-CBD	5.52	121.08	111.27
35	g	315	RRX	C20-C21-C22	-5.52	119.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	306	CLA	CMD-C2D-C1D	5.52	134.45	124.71
31	6	313	CLA	CMD-C2D-C1D	5.52	134.44	124.71
31	R	313	CLA	O2A-C1-C2	5.52	121.88	108.97
31	2	604	CLA	CMD-C2D-C1D	5.52	134.44	124.71
31	Y	304	CLA	CMD-C2D-C1D	5.52	134.44	124.71
31	9	306	CLA	CMD-C2D-C1D	5.52	134.44	124.71
31	8	609	CLA	CMD-C2D-C1D	5.51	134.43	124.71
31	a	406	CLA	C1-C2-C3	-5.51	116.51	126.04
31	Y	305	CLA	CMD-C2D-C1D	5.51	134.43	124.71
31	4	604	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	0	614	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	Y	303	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	y	614	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	7	303	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	S	316	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	y	603	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	C	602	CLA	O2D-CGD-CBD	5.50	121.04	111.27
31	r	314	CLA	O2A-C1-C2	5.50	121.83	108.97
31	5	602	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	8	602	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	s	304	CLA	CMD-C2D-C1D	5.50	134.40	124.71
31	s	313	CLA	O2D-CGD-CBD	5.50	121.04	111.27
31	N	313	CLA	CMD-C2D-C1D	5.50	134.40	124.71
31	1	604	CLA	CMD-C2D-C1D	5.49	134.40	124.71
31	a	409	CLA	O2D-CGD-CBD	5.49	121.03	111.27
31	1	612	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	c	604	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	n	304	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	R	311	CLA	O2A-C1-C2	5.49	123.07	108.64
31	r	315	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	N	304	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	Y	312	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	b	612	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	n	313	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	7	316	CLA	CMD-C2D-C1D	5.49	134.38	124.71
31	d	405	CLA	O2D-CGD-CBD	5.49	121.02	111.27
31	s	313	CLA	CMD-C2D-C1D	5.49	134.38	124.71
31	9	304	CLA	CMD-C2D-C1D	5.48	134.38	124.71
31	5	614	CLA	CMD-C2D-C1D	5.48	134.38	124.71
31	B	615	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	G	612	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	7	315	CLA	CMD-C2D-C1D	5.48	134.37	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	607	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	c	602	CLA	O2A-C1-C2	5.48	123.03	108.64
31	8	611	CLA	CMD-C2D-C1D	5.47	134.36	124.71
31	n	311	CLA	CMD-C2D-C1D	5.47	134.36	124.71
31	N	312	CLA	CMD-C2D-C1D	5.47	134.36	124.71
32	R	317	LUT	C11-C10-C9	-5.47	119.50	127.31
31	r	306	CLA	O2D-CGD-CBD	5.47	120.99	111.27
32	S	318	LUT	C31-C30-C29	-5.47	119.50	127.31
31	c	609	CLA	CMD-C2D-C1D	5.47	134.35	124.71
37	R	318	XAT	C38-C25-C24	5.47	120.43	114.28
37	r	318	XAT	C38-C25-C24	5.47	120.43	114.28
43	v	101	BCR	C33-C5-C6	-5.47	118.39	124.53
31	5	612	CLA	CMD-C2D-C1D	5.46	134.34	124.71
31	5	604	CLA	CMD-C2D-C1D	5.46	134.34	124.71
31	0	602	CLA	CMD-C2D-C1D	5.46	134.34	124.71
31	3	315	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	3	311	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	r	305	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	y	602	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	c	610	CLA	CMD-C2D-C1D	5.45	134.32	124.71
32	7	317	LUT	C11-C10-C9	-5.45	119.53	127.31
31	9	315	CLA	CMD-C2D-C1D	5.45	134.32	124.71
47	e	102	HEM	CHC-C4B-NB	5.45	130.34	124.42
31	b	606	CLA	CMD-C2D-C1D	5.45	134.31	124.71
31	0	603	CLA	CMD-C2D-C1D	5.45	134.31	124.71
31	0	615	CLA	CMD-C2D-C1D	5.45	134.31	124.71
32	N	317	LUT	C11-C10-C9	-5.45	119.54	127.31
31	B	614	CLA	CMD-C2D-C1D	5.44	134.30	124.71
31	0	613	CLA	CMD-C2D-C1D	5.44	134.30	124.71
31	A	405	CLA	CMD-C2D-C1D	5.44	134.30	124.71
31	b	603	CLA	O2D-CGD-CBD	5.44	120.93	111.27
31	g	313	CLA	CMD-C2D-C1D	5.44	134.29	124.71
31	4	603	CLA	CMD-C2D-C1D	5.43	134.29	124.71
31	r	314	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	p	603	CLA	O2D-CGD-CBD	5.43	120.92	111.27
43	H	101	BCR	C7-C8-C9	-5.43	118.03	126.23
31	b	604	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	b	602	CLA	O2D-CGD-CBD	5.43	120.92	111.27
31	S	304	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	c	609	CLA	O2D-CGD-CBD	5.43	120.91	111.27
31	g	305	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	C	603	CLA	C1-C2-C3	-5.43	116.66	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	613	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	b	614	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	c	607	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	Y	314	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	s	310	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	p	613	CLA	O2D-CGD-CBD	5.42	120.90	111.27
31	S	305	CLA	CMD-C2D-C1D	5.42	134.26	124.71
31	S	310	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	B	602	CLA	CAA-C2A-C3A	-5.41	97.96	112.78
31	R	316	CLA	O2D-CGD-CBD	5.41	120.89	111.27
31	N	305	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	0	610	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	r	315	CLA	O2D-CGD-CBD	5.41	120.88	111.27
32	R	317	LUT	C28-C29-C30	5.40	127.23	118.94
31	a	406	CLA	O2A-C1-C2	5.40	122.84	108.64
31	B	601	CLA	CMD-C2D-C1D	5.40	134.24	124.71
31	b	611	CLA	CMD-C2D-C1D	5.40	134.24	124.71
31	y	604	CLA	CMD-C2D-C1D	5.40	134.23	124.71
43	C	614	BCR	C7-C8-C9	-5.40	118.08	126.23
31	B	612	CLA	O2D-CGD-CBD	5.40	120.86	111.27
31	8	604	CLA	CMD-C2D-C1D	5.40	134.23	124.71
31	3	314	CLA	CMD-C2D-C1D	5.40	134.23	124.71
31	G	611	CLA	O2D-CGD-CBD	5.40	120.86	111.27
31	n	305	CLA	CMD-C2D-C1D	5.40	134.23	124.71
31	S	313	CLA	CMD-C2D-C1D	5.40	134.22	124.71
31	s	316	CLA	CMD-C2D-C1D	5.40	134.22	124.71
31	r	316	CLA	O2D-CGD-CBD	5.39	120.85	111.27
31	A	409	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	a	409	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	B	610	CLA	O2D-CGD-CBD	5.39	120.85	111.27
32	N	316	LUT	C7-C8-C9	-5.39	118.09	126.23
31	C	610	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	B	613	CLA	CMD-C2D-C1D	5.39	134.21	124.71
32	5	616	LUT	C18-C5-C6	-5.39	118.48	124.53
31	b	607	CLA	O2A-C1-C2	5.39	122.79	108.64
31	A	407	CLA	CMD-C2D-C1D	5.39	134.21	124.71
31	A	407	CLA	O2A-C1-C2	5.39	121.56	108.97
31	a	406	CLA	CMD-C2D-C1D	5.39	134.21	124.71
31	7	316	CLA	O2D-CGD-CBD	5.38	120.84	111.27
31	s	311	CLA	CMD-C2D-C1D	5.38	134.20	124.71
31	R	307	CLA	O2D-CGD-CBD	5.38	120.84	111.27
31	b	617	CLA	O2D-CGD-CBD	5.38	120.83	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	q	317	RRX	C33-C5-C6	-5.38	118.49	124.53
31	3	301	CLA	O2A-C1-C2	5.38	122.77	108.64
31	B	604	CLA	O2A-C1-C2	5.38	122.76	108.64
31	C	606	CLA	O2D-CGD-CBD	5.38	120.82	111.27
31	B	610	CLA	CMD-C2D-C1D	5.37	134.19	124.71
35	2	614	RRX	C11-C10-C9	-5.37	119.64	127.31
43	d	406	BCR	C33-C5-C6	-5.37	118.50	124.53
31	S	310	CLA	O2A-C1-C2	5.37	122.75	108.64
31	5	615	CLA	O2D-CGD-CBD	5.37	120.81	111.27
31	y	613	CLA	O2D-CGD-CBD	5.37	120.81	111.27
31	C	604	CLA	O2D-CGD-CBD	5.37	120.81	111.27
31	6	316	CLA	CMD-C2D-C1D	5.37	134.17	124.71
32	2	615	LUT	C39-C29-C30	-5.36	115.41	122.92
31	B	611	CLA	CMD-C2D-C1D	5.36	134.17	124.71
31	C	611	CLA	CMD-C2D-C1D	5.36	134.17	124.71
31	3	305	CLA	CMD-C2D-C1D	5.36	134.16	124.71
31	B	602	CLA	O2A-C1-C2	5.36	122.71	108.64
31	6	315	CLA	O2A-C1-C2	5.36	122.71	108.64
31	S	311	CLA	CMD-C2D-C1D	5.35	134.15	124.71
31	1	611	CLA	CMD-C2D-C1D	5.35	134.15	124.71
31	s	305	CLA	CMD-C2D-C1D	5.35	134.15	124.71
31	b	616	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	0	604	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	8	612	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	n	314	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	1	604	CLA	O2A-C1-C2	5.35	122.69	108.64
31	c	604	CLA	O2D-CGD-CBD	5.35	120.77	111.27
31	c	605	CLA	O2D-CGD-CBD	5.35	120.77	111.27
31	b	605	CLA	O2A-C1-C2	5.35	122.69	108.64
43	z	101	BCR	C24-C23-C22	-5.34	118.16	126.23
31	9	313	CLA	O2D-CGD-CBD	5.34	120.76	111.27
31	2	611	CLA	CMD-C2D-C1D	5.34	134.13	124.71
31	B	609	CLA	CMD-C2D-C1D	5.34	134.12	124.71
31	G	613	CLA	O2D-CGD-CBD	5.34	120.76	111.27
31	R	315	CLA	O2D-CGD-CBD	5.34	120.76	111.27
31	8	610	CLA	O2A-C1-C2	5.34	121.45	108.97
31	n	312	CLA	O2A-C1-C2	5.34	121.45	108.97
47	E	101	HEM	CHC-C4B-NB	5.34	130.22	124.42
32	p	616	LUT	C32-C33-C34	5.33	127.13	118.94
31	p	604	CLA	O2D-CGD-CBD	5.33	120.75	111.27
31	c	610	CLA	O2A-C1-C2	5.33	122.65	108.64
36	2	616	NEX	C38-C25-C24	5.33	120.28	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	312	CLA	O2A-C1-C2	5.33	122.64	108.64
31	s	314	CLA	CMD-C2D-C1D	5.32	134.09	124.71
31	b	606	CLA	O2D-CGD-CBD	5.32	120.72	111.27
31	c	611	CLA	CMD-C2D-C1D	5.32	134.09	124.71
31	s	310	CLA	O2A-C1-C2	5.32	122.62	108.64
31	C	601	CLA	CMD-C2D-C1D	5.32	134.09	124.71
31	C	602	CLA	CMD-C2D-C1D	5.32	134.09	124.71
31	9	313	CLA	CMD-C2D-C1D	5.32	134.09	124.71
32	R	317	LUT	C21-C26-C27	-5.32	105.98	112.70
32	R	317	LUT	C32-C33-C34	5.32	127.10	118.94
31	d	405	CLA	CMD-C2D-C1D	5.32	134.08	124.71
31	b	616	CLA	O2D-CGD-CBD	5.31	120.71	111.27
31	4	612	CLA	CMD-C2D-C1D	5.31	134.08	124.71
31	D	404	CLA	CMD-C2D-C1D	5.31	134.08	124.71
31	B	607	CLA	O2A-C1-C2	5.31	122.60	108.64
31	4	611	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	G	609	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	g	310	CLA	CMD-C2D-C1D	5.31	134.07	124.71
43	D	405	BCR	C8-C9-C10	5.31	127.09	118.94
31	d	404	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	C	606	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	r	305	CLA	O2D-CGD-CBD	5.30	120.69	111.27
31	4	612	CLA	O2D-CGD-CBD	5.30	120.69	111.27
43	B	617	BCR	C38-C26-C25	-5.30	118.58	124.53
31	c	603	CLA	O2D-CGD-CBD	5.30	120.68	111.27
31	r	306	CLA	CMD-C2D-C1D	5.30	134.05	124.71
31	4	614	CLA	O2A-C1-C2	5.30	122.56	108.64
31	c	602	CLA	O2D-CGD-CBD	5.30	120.68	111.27
35	q	317	RRX	C38-C26-C25	-5.29	118.58	124.53
31	n	315	CLA	CMD-C2D-C1D	5.29	134.04	124.71
43	A	410	BCR	C16-C17-C18	-5.29	119.76	127.31
31	2	610	CLA	CMD-C2D-C1D	5.29	134.04	124.71
31	Y	312	CLA	O2A-C1-C2	5.29	122.53	108.64
31	8	613	CLA	CMD-C2D-C1D	5.29	134.03	124.71
31	g	314	CLA	O2A-C1-C2	5.29	121.34	108.97
31	B	614	CLA	O2A-C1-C2	5.29	122.53	108.64
31	C	612	CLA	O2A-C1-C2	5.29	122.53	108.64
31	N	311	CLA	O2A-C1-C2	5.29	121.33	108.97
31	b	603	CLA	CMD-C2D-C1D	5.28	134.03	124.71
31	s	313	CLA	O2A-C1-C2	5.28	122.52	108.64
31	2	612	CLA	CMD-C2D-C1D	5.28	134.02	124.71
31	5	613	CLA	CMD-C2D-C1D	5.28	134.02	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	314	CLA	O2D-CGD-CBD	5.28	120.65	111.27
31	Y	312	CLA	O2D-CGD-CBD	5.28	120.64	111.27
31	G	611	CLA	CMD-C2D-C1D	5.27	134.01	124.71
31	c	604	CLA	O2A-C1-C2	5.27	122.50	108.64
31	S	314	CLA	CMD-C2D-C1D	5.27	134.01	124.71
31	7	314	CLA	CMD-C2D-C1D	5.27	134.00	124.71
31	s	311	CLA	O2D-CGD-CBD	5.27	120.63	111.27
31	p	615	CLA	O2D-CGD-CBD	5.27	120.63	111.27
31	d	401	CLA	O2A-C1-C2	5.27	121.28	108.97
31	q	306	CLA	CMD-C2D-C1D	5.26	133.99	124.71
31	3	311	CLA	O2D-CGD-CBD	5.26	120.62	111.27
43	B	619	BCR	C16-C17-C18	-5.26	119.80	127.31
31	7	312	CLA	CMD-C2D-C1D	5.26	133.99	124.71
31	B	602	CLA	CMD-C2D-C1D	5.26	133.99	124.71
35	G	614	RRX	C15-C14-C13	-5.26	119.80	127.31
43	Z	101	BCR	C24-C23-C22	-5.26	118.29	126.23
31	c	605	CLA	CMD-C2D-C1D	5.26	133.98	124.71
43	c	614	BCR	C15-C14-C13	-5.26	119.81	127.31
32	2	615	LUT	C31-C30-C29	5.25	134.81	127.31
31	R	305	CLA	O2A-C1-C2	5.25	122.44	108.64
35	4	615	RRX	C15-C14-C13	-5.25	119.81	127.31
43	C	615	BCR	C34-C9-C10	-5.25	115.56	122.92
31	g	311	CLA	O2A-C1-C2	5.25	122.44	108.64
31	r	311	CLA	CMD-C2D-C1D	5.25	133.97	124.71
31	g	311	CLA	O2D-CGD-CBD	5.24	120.59	111.27
31	R	303	CLA	CMD-C2D-C1D	5.24	133.95	124.71
31	s	312	CLA	O2D-CGD-CBD	5.24	120.58	111.27
43	C	615	BCR	C4-C5-C6	-5.24	115.12	122.73
31	d	401	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	S	315	CLA	O2D-CGD-CBD	5.24	120.58	111.27
36	5	618	NEX	C38-C25-C24	5.24	120.18	114.28
31	q	313	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	b	610	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	R	311	CLA	CMD-C2D-C1D	5.24	133.95	124.71
31	B	603	CLA	CMD-C2D-C1D	5.24	133.94	124.71
31	b	617	CLA	CMD-C2D-C1D	5.24	133.94	124.71
31	B	616	CLA	O2A-C1-C2	5.23	122.38	108.64
31	q	315	CLA	O2D-CGD-CBD	5.23	120.56	111.27
32	5	617	LUT	C15-C14-C13	-5.23	119.85	127.31
31	D	403	CLA	CMD-C2D-C1D	5.23	133.93	124.71
35	9	317	RRX	C15-C14-C13	-5.23	119.85	127.31
31	N	311	CLA	CMD-C2D-C1D	5.23	133.92	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	603	CLA	O2D-CGD-CBD	5.23	120.55	111.27
31	N	311	CLA	O2D-CGD-CBD	5.22	120.55	111.27
31	6	305	CLA	O2D-CGD-CBD	5.22	120.55	111.27
31	2	609	CLA	O2D-CGD-CBD	5.22	120.55	111.27
31	9	314	CLA	CMD-C2D-C1D	5.22	133.91	124.71
43	d	406	BCR	C12-C13-C14	5.22	126.95	118.94
31	A	407	CLA	O2D-CGD-CBD	5.22	120.54	111.27
31	C	601	CLA	O2D-CGD-CBD	5.22	120.53	111.27
31	N	305	CLA	O2D-CGD-CBD	5.21	120.53	111.27
31	S	304	CLA	O2D-CGD-CBD	5.21	120.53	111.27
35	g	315	RRX	C30-C25-C26	-5.21	115.27	122.61
43	z	101	BCR	C7-C8-C9	-5.21	118.36	126.23
36	q	319	NEX	C27-C28-C29	-5.21	117.44	125.53
31	3	314	CLA	O2D-CGD-CBD	5.21	120.53	111.27
31	p	612	CLA	O2D-CGD-CBD	5.21	120.53	111.27
31	C	603	CLA	O2D-CGD-CBD	5.21	120.52	111.27
31	6	304	CLA	O2D-CGD-CBD	5.21	120.52	111.27
46	d	403	BCT	O2-C-O1	5.20	133.04	119.55
32	4	616	LUT	C15-C14-C13	-5.20	119.89	127.31
43	b	619	BCR	C15-C14-C13	-5.20	119.89	127.31
31	B	611	CLA	O2A-C1-C2	5.20	122.29	108.64
43	C	614	BCR	C27-C26-C25	-5.20	115.19	122.73
31	8	611	CLA	O2D-CGD-CBD	5.20	120.50	111.27
31	r	307	CLA	O2D-CGD-CBD	5.20	120.50	111.27
31	Y	313	CLA	CMD-C2D-C1D	5.20	133.87	124.71
32	G	615	LUT	C35-C15-C14	-5.20	112.83	123.47
31	8	604	CLA	O2D-CGD-CBD	5.20	120.50	111.27
31	1	602	CLA	CMD-C2D-C1D	5.19	133.87	124.71
31	b	613	CLA	O2D-CGD-CBD	5.19	120.48	111.27
31	b	613	CLA	CMD-C2D-C1D	5.18	133.85	124.71
31	2	613	CLA	O2D-CGD-CBD	5.18	120.48	111.27
31	r	307	CLA	CMD-C2D-C1D	5.18	133.85	124.71
43	C	614	BCR	C15-C14-C13	-5.18	119.92	127.31
31	d	405	CLA	O2A-C1-C2	5.18	122.25	108.64
31	c	613	CLA	O2D-CGD-CBD	5.18	120.47	111.27
32	N	317	LUT	C7-C8-C9	-5.18	118.41	126.23
31	B	607	CLA	O2D-CGD-CBD	5.18	120.47	111.27
31	c	603	CLA	C1-C2-C3	-5.18	117.09	126.04
31	0	613	CLA	O2D-CGD-CBD	5.18	120.47	111.27
31	0	612	CLA	O2D-CGD-CBD	5.18	120.46	111.27
31	C	602	CLA	O2A-C1-C2	5.17	122.23	108.64
31	6	312	CLA	O2D-CGD-CBD	5.17	120.46	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	615	CLA	O2A-C1-C2	5.17	122.23	108.64
32	s	317	LUT	C35-C34-C33	-5.17	119.93	127.31
31	s	315	CLA	O2D-CGD-CBD	5.17	120.46	111.27
31	5	611	CLA	CMD-C2D-C1D	5.17	133.82	124.71
31	B	609	CLA	O2D-CGD-CBD	5.17	120.45	111.27
31	n	313	CLA	O2D-CGD-CBD	5.17	120.45	111.27
31	B	601	CLA	O2A-C1-C2	5.17	121.06	108.97
37	2	619	XAT	C15-C14-C13	-5.17	119.94	127.31
31	Y	303	CLA	O2D-CGD-CBD	5.17	120.45	111.27
31	5	610	CLA	O2D-CGD-CBD	5.16	120.44	111.27
35	2	614	RRX	C15-C14-C13	-5.16	119.94	127.31
31	5	612	CLA	O2D-CGD-CBD	5.16	120.44	111.27
31	q	316	CLA	O2A-C1-C2	5.16	122.20	108.64
31	b	602	CLA	O2A-C1-C2	5.16	121.04	108.97
31	3	301	CLA	CMD-C2D-C1D	5.16	133.81	124.71
31	r	303	CLA	CMD-C2D-C1D	5.16	133.81	124.71
31	y	612	CLA	CMD-C2D-C1D	5.16	133.81	124.71
31	c	606	CLA	O2D-CGD-CBD	5.16	120.43	111.27
31	s	312	CLA	O2A-C1-C2	5.16	122.19	108.64
31	9	306	CLA	O2D-CGD-CBD	5.16	120.43	111.27
31	b	617	CLA	O2A-C1-C2	5.16	122.18	108.64
31	3	312	CLA	O2D-CGD-CBD	5.15	120.43	111.27
37	4	619	XAT	C15-C14-C13	-5.15	119.95	127.31
36	R	319	NEX	C38-C25-C24	5.15	120.08	114.28
31	b	605	CLA	CMD-C2D-C1D	5.15	133.79	124.71
31	q	305	CLA	O2D-CGD-CBD	5.15	120.42	111.27
31	S	316	CLA	O2D-CGD-CBD	5.15	120.42	111.27
37	G	620	XAT	C15-C14-C13	-5.15	119.96	127.31
31	b	611	CLA	O2D-CGD-CBD	5.15	120.42	111.27
31	p	602	CLA	CMD-C2D-C1D	5.15	133.78	124.71
31	s	311	CLA	O2A-C1-C2	5.15	122.16	108.64
31	C	604	CLA	O2A-C1-C2	5.15	122.16	108.64
31	B	608	CLA	O2D-CGD-CBD	5.14	120.41	111.27
32	6	317	LUT	C35-C34-C33	-5.14	119.97	127.31
37	g	321	XAT	C15-C14-C13	-5.14	119.97	127.31
31	C	609	CLA	O2D-CGD-CBD	5.14	120.41	111.27
31	C	611	CLA	O2A-C1-C2	5.14	122.15	108.64
31	a	407	CLA	CMD-C2D-C1D	5.14	133.78	124.71
37	q	321	XAT	C15-C14-C13	-5.14	119.97	127.31
31	Y	311	CLA	O2D-CGD-CBD	5.14	120.40	111.27
31	q	313	CLA	CMD-C2D-C1D	5.14	133.77	124.71
35	G	614	RRX	C11-C10-C9	-5.13	119.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	t	101	BCR	C38-C26-C25	-5.13	118.76	124.53
31	3	306	CLA	O2D-CGD-CBD	5.13	120.39	111.27
31	r	303	CLA	O2A-C1-C2	5.13	120.97	108.97
31	3	315	CLA	O2D-CGD-CBD	5.13	120.39	111.27
31	S	313	CLA	O2A-C1-C2	5.13	122.11	108.64
31	1	610	CLA	O2A-C1-C2	5.13	122.11	108.64
31	c	603	CLA	O2A-C1-C2	5.13	122.11	108.64
31	c	608	CLA	CMD-C2D-C1D	5.13	133.75	124.71
31	c	613	CLA	CMD-C2D-C1D	5.13	133.75	124.71
31	n	305	CLA	O2D-CGD-CBD	5.13	120.38	111.27
31	0	604	CLA	O2A-C1-C2	5.12	122.10	108.64
31	n	312	CLA	O2D-CGD-CBD	5.12	120.37	111.27
31	c	611	CLA	O2A-C1-C2	5.12	122.10	108.64
31	1	612	CLA	O2D-CGD-CBD	5.12	120.37	111.27
35	9	317	RRX	C11-C10-C9	-5.12	120.00	127.31
37	9	322	XAT	C15-C14-C13	-5.12	120.00	127.31
32	2	615	LUT	C32-C33-C34	5.12	126.80	118.94
31	c	610	CLA	O2D-CGD-CBD	5.12	120.36	111.27
31	1	603	CLA	CMD-C2D-C1D	5.12	133.73	124.71
31	8	610	CLA	O2D-CGD-CBD	5.11	120.36	111.27
44	a	414	PL9	C7-C3-C4	5.11	121.03	116.88
31	C	609	CLA	CMD-C2D-C1D	5.11	133.72	124.71
31	y	603	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	G	613	CLA	O2A-C1-C2	5.11	120.92	108.97
43	C	615	BCR	C16-C17-C18	-5.11	120.02	127.31
31	Y	304	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	c	601	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	y	614	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	Y	313	CLA	O2D-CGD-CBD	5.11	120.35	111.27
32	p	616	LUT	C11-C10-C9	-5.11	120.02	127.31
31	y	604	CLA	O2D-CGD-CBD	5.11	120.34	111.27
32	9	318	LUT	C35-C34-C33	-5.11	120.02	127.31
32	p	616	LUT	C28-C29-C30	5.11	126.78	118.94
31	G	609	CLA	O2D-CGD-CBD	5.11	120.34	111.27
36	8	617	NEX	C38-C25-C24	5.11	120.02	114.28
31	8	610	CLA	CMD-C2D-C1D	5.10	133.71	124.71
31	B	603	CLA	O2D-CGD-CBD	5.10	120.33	111.27
31	0	611	CLA	O2D-CGD-CBD	5.10	120.33	111.27
43	c	614	BCR	C33-C5-C6	-5.10	118.80	124.53
31	B	612	CLA	CMD-C2D-C1D	5.10	133.70	124.71
31	b	612	CLA	O2D-CGD-CBD	5.10	120.33	111.27
31	5	611	CLA	O2D-CGD-CBD	5.10	120.33	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	603	CLA	O2A-C1-C2	5.10	122.03	108.64
31	S	312	CLA	O2D-CGD-CBD	5.10	120.33	111.27
35	4	615	RRX	C11-C10-C9	-5.10	120.04	127.31
31	p	611	CLA	CMD-C2D-C1D	5.09	133.69	124.71
31	C	613	CLA	CMD-C2D-C1D	5.09	133.69	124.71
31	S	312	CLA	CMD-C2D-C1D	5.09	133.69	124.71
31	N	312	CLA	O2D-CGD-CBD	5.09	120.31	111.27
31	n	312	CLA	CMD-C2D-C1D	5.09	133.68	124.71
31	6	311	CLA	O2D-CGD-CBD	5.08	120.30	111.27
31	Y	305	CLA	O2D-CGD-CBD	5.08	120.30	111.27
36	r	301	NEX	C38-C25-C24	5.08	120.00	114.28
31	Y	303	CLA	O2A-C1-C2	5.08	121.98	108.64
31	y	612	CLA	O2A-C1-C2	5.08	121.98	108.64
32	q	318	LUT	C11-C10-C9	-5.08	120.07	127.31
31	b	610	CLA	CMD-C2D-C1D	5.08	133.66	124.71
43	z	101	BCR	C33-C5-C6	-5.08	118.83	124.53
43	h	101	BCR	C7-C8-C9	-5.07	118.57	126.23
31	7	314	CLA	O2D-CGD-CBD	5.07	120.28	111.27
31	A	405	CLA	O2A-C1-C2	5.07	121.96	108.64
31	4	604	CLA	O2D-CGD-CBD	5.07	120.28	111.27
31	s	303	CLA	O2D-CGD-CBD	5.07	120.27	111.27
36	r	319	NEX	C38-C25-C24	5.07	119.98	114.28
31	n	315	CLA	O2A-C1-C2	5.07	120.82	108.97
31	4	614	CLA	O2D-CGD-CBD	5.06	120.27	111.27
31	N	314	CLA	CMD-C2D-C1D	5.06	133.64	124.71
31	C	608	CLA	CMD-C2D-C1D	5.06	133.64	124.71
32	R	317	LUT	C39-C29-C30	-5.06	115.83	122.92
31	1	603	CLA	O2D-CGD-CBD	5.06	120.27	111.27
31	G	602	CLA	O2D-CGD-CBD	5.06	120.27	111.27
31	0	602	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	4	603	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	y	611	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	R	305	CLA	CMD-C2D-C1D	5.06	133.63	124.71
31	S	311	CLA	O2A-C1-C2	5.06	121.93	108.64
31	c	602	CLA	CMD-C2D-C1D	5.06	133.63	124.71
31	y	602	CLA	O2D-CGD-CBD	5.06	120.25	111.27
31	b	604	CLA	O2D-CGD-CBD	5.06	120.25	111.27
31	2	604	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	6	315	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	3	304	CLA	O2A-C1-C2	5.05	121.92	108.64
31	1	611	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	B	611	CLA	O2D-CGD-CBD	5.05	120.24	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	313	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	9	306	CLA	O2A-C1-C2	5.05	121.90	108.64
32	q	318	LUT	C7-C8-C9	-5.05	118.61	126.23
31	5	604	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	5	614	CLA	O2A-C1-C2	5.05	121.90	108.64
43	B	617	BCR	C33-C5-C6	-5.04	118.86	124.53
31	8	613	CLA	O2A-C1-C2	5.04	120.76	108.97
31	s	312	CLA	CMD-C2D-C1D	5.04	133.60	124.71
32	0	617	LUT	C7-C8-C9	-5.04	118.62	126.23
31	q	306	CLA	O2D-CGD-CBD	5.04	120.22	111.27
31	7	303	CLA	O2D-CGD-CBD	5.04	120.22	111.27
31	N	314	CLA	O2A-C1-C2	5.04	120.75	108.97
31	0	611	CLA	CMD-C2D-C1D	5.04	133.59	124.71
31	N	303	CLA	O2D-CGD-CBD	5.03	120.21	111.27
31	y	611	CLA	CMD-C2D-C1D	5.03	133.58	124.71
32	6	318	LUT	C7-C8-C9	-5.03	118.63	126.23
31	1	613	CLA	O2D-CGD-CBD	5.03	120.21	111.27
31	S	305	CLA	O2D-CGD-CBD	5.03	120.20	111.27
43	A	410	BCR	C20-C21-C22	-5.03	120.13	127.31
31	r	304	CLA	O2D-CGD-CBD	5.03	120.20	111.27
31	p	602	CLA	O2D-CGD-CBD	5.03	120.20	111.27
31	N	315	CLA	O2D-CGD-CBD	5.03	120.20	111.27
31	5	613	CLA	O2D-CGD-CBD	5.03	120.20	111.27
31	p	613	CLA	CMD-C2D-C1D	5.02	133.57	124.71
31	R	304	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	S	311	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	c	611	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	y	602	CLA	O2A-C1-C2	5.02	121.83	108.64
31	n	303	CLA	O2D-CGD-CBD	5.02	120.19	111.27
43	c	615	BCR	C33-C5-C6	-5.02	118.89	124.53
31	3	301	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	8	612	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	B	607	CLA	CMD-C2D-C1D	5.02	133.56	124.71
31	R	314	CLA	O2A-C1-C2	5.02	120.70	108.97
31	B	614	CLA	O2D-CGD-CBD	5.01	120.18	111.27
31	s	316	CLA	O2D-CGD-CBD	5.01	120.17	111.27
31	n	314	CLA	O2D-CGD-CBD	5.01	120.17	111.27
43	t	101	BCR	C20-C19-C18	-5.00	112.36	126.42
31	b	608	CLA	O2D-CGD-CBD	5.00	120.16	111.27
37	9	322	XAT	C38-C25-C24	5.00	119.91	114.28
37	g	321	XAT	C38-C25-C24	5.00	119.90	114.28
43	C	614	BCR	C33-C5-C6	-5.00	118.92	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	609	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	7	304	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	R	311	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	3	315	CLA	O2A-C1-C2	4.99	121.75	108.64
31	b	608	CLA	O2A-C1-C2	4.99	121.75	108.64
31	6	303	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	4	610	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	s	305	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	1	610	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	p	611	CLA	O2D-CGD-CBD	4.99	120.13	111.27
37	2	619	XAT	C38-C25-C24	4.99	119.89	114.28
37	G	620	XAT	C38-C25-C24	4.99	119.89	114.28
31	G	609	CLA	O2A-C1-C2	4.98	121.74	108.64
43	b	618	BCR	C16-C17-C18	-4.98	120.20	127.31
31	9	316	CLA	O2D-CGD-CBD	4.98	120.12	111.27
31	g	304	CLA	O2D-CGD-CBD	4.98	120.12	111.27
31	6	312	CLA	CMD-C2D-C1D	4.98	133.49	124.71
43	h	101	BCR	C24-C23-C22	-4.98	118.71	126.23
31	S	303	CLA	O2D-CGD-CBD	4.98	120.12	111.27
43	Z	101	BCR	C33-C5-C6	-4.98	118.94	124.53
31	p	614	CLA	O2D-CGD-CBD	4.98	120.11	111.27
32	S	317	LUT	C35-C34-C33	-4.98	120.21	127.31
31	s	304	CLA	O2D-CGD-CBD	4.98	120.11	111.27
31	b	612	CLA	O2A-C1-C2	4.98	121.71	108.64
31	D	403	CLA	O2D-CGD-CBD	4.98	120.11	111.27
37	4	619	XAT	C38-C25-C24	4.97	119.88	114.28
31	N	310	CLA	O2A-C1-C2	4.97	121.70	108.64
31	7	312	CLA	O2D-CGD-CBD	4.97	120.10	111.27
31	Y	314	CLA	O2A-C1-C2	4.97	121.70	108.64
43	c	615	BCR	C38-C26-C25	-4.96	118.95	124.53
31	0	610	CLA	O2D-CGD-CBD	4.96	120.09	111.27
31	C	601	CLA	O2A-C1-C2	4.96	121.68	108.64
31	6	316	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	S	306	CLA	O2A-C1-C2	4.96	121.67	108.64
35	g	315	RRX	C38-C26-C25	-4.96	118.96	124.53
31	8	604	CLA	O2A-C1-C2	4.96	121.67	108.64
37	q	321	XAT	C38-C25-C24	4.96	119.86	114.28
31	g	310	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	n	316	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	9	305	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	1	612	CLA	O2A-C1-C2	4.96	121.66	108.64
31	5	613	CLA	O2A-C1-C2	4.96	121.66	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	q	318	LUT	C15-C14-C13	-4.95	120.24	127.31
35	q	317	RRX	C16-C17-C18	-4.95	120.24	127.31
31	r	313	CLA	CMD-C2D-C1D	4.95	133.44	124.71
36	g	317	NEX	C38-C25-C24	4.95	119.85	114.28
32	5	616	LUT	C35-C34-C33	-4.95	120.24	127.31
31	1	613	CLA	CMD-C2D-C1D	4.95	133.43	124.71
31	8	602	CLA	O2D-CGD-CBD	4.95	120.06	111.27
31	p	610	CLA	O2D-CGD-CBD	4.94	120.05	111.27
31	c	612	CLA	O2A-C1-C2	4.94	121.62	108.64
32	g	316	LUT	C15-C14-C13	-4.94	120.26	127.31
31	0	611	CLA	O2A-C1-C2	4.94	121.61	108.64
31	4	611	CLA	O2D-CGD-CBD	4.94	120.04	111.27
32	0	616	LUT	C35-C34-C33	-4.94	120.26	127.31
31	G	604	CLA	O2D-CGD-CBD	4.94	120.04	111.27
31	4	604	CLA	C1-C2-C3	-4.94	117.51	126.04
31	G	610	CLA	O2D-CGD-CBD	4.94	120.04	111.27
32	4	616	LUT	C7-C8-C9	-4.94	118.78	126.23
31	C	608	CLA	O2D-CGD-CBD	4.93	120.04	111.27
32	y	616	LUT	C21-C26-C27	-4.93	106.46	112.70
31	p	614	CLA	O2A-C1-C2	4.93	121.60	108.64
31	n	304	CLA	O2D-CGD-CBD	4.93	120.03	111.27
31	G	612	CLA	O2D-CGD-CBD	4.93	120.02	111.27
31	R	313	CLA	CMD-C2D-C1D	4.93	133.40	124.71
36	r	319	NEX	C27-C28-C29	-4.93	117.89	125.53
31	N	304	CLA	O2D-CGD-CBD	4.93	120.02	111.27
31	n	305	CLA	O2A-C1-C2	4.93	121.58	108.64
31	N	315	CLA	O2A-C1-C2	4.92	121.57	108.64
31	A	405	CLA	C1-C2-C3	-4.92	117.53	126.04
31	B	616	CLA	CMD-C2D-C1D	4.92	133.38	124.71
31	N	305	CLA	O2A-C1-C2	4.92	121.56	108.64
43	a	410	BCR	C38-C26-C25	-4.92	119.01	124.53
32	3	317	LUT	C35-C34-C33	-4.91	120.30	127.31
31	9	304	CLA	O2D-CGD-CBD	4.91	120.00	111.27
36	6	319	NEX	C38-C25-C24	4.91	119.81	114.28
31	9	305	CLA	O2A-C1-C2	4.91	121.54	108.64
31	G	610	CLA	CMD-C2D-C1D	4.91	133.37	124.71
31	g	311	CLA	CMD-C2D-C1D	4.91	133.37	124.71
36	4	617	NEX	C38-C25-C24	4.91	119.80	114.28
31	A	406	CLA	O2A-C1-C2	4.91	121.53	108.64
31	5	603	CLA	O2D-CGD-CBD	4.91	119.99	111.27
31	S	306	CLA	O2D-CGD-CBD	4.91	119.99	111.27
31	b	616	CLA	O2A-C1-C2	4.91	121.53	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	V	101	BCR	C38-C26-C25	-4.90	119.02	124.53
31	D	403	CLA	O2A-C1-C2	4.90	121.52	108.64
31	N	310	CLA	O2D-CGD-CBD	4.90	119.98	111.27
31	r	312	CLA	O2D-CGD-CBD	4.90	119.98	111.27
31	C	613	CLA	O2D-CGD-CBD	4.90	119.98	111.27
31	R	307	CLA	CMD-C2D-C1D	4.90	133.34	124.71
31	2	610	CLA	O2D-CGD-CBD	4.90	119.97	111.27
31	8	609	CLA	O2D-CGD-CBD	4.89	119.97	111.27
31	g	305	CLA	O2D-CGD-CBD	4.89	119.97	111.27
32	s	318	LUT	C35-C34-C33	-4.89	120.33	127.31
31	g	313	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	3	313	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	d	404	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	0	603	CLA	O2A-C1-C2	4.89	121.49	108.64
31	g	312	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	3	312	CLA	CMD-C2D-C1D	4.89	133.33	124.71
31	9	315	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	0	615	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	3	304	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	b	606	CLA	O2A-C1-C2	4.89	121.47	108.64
31	b	610	CLA	O2A-C1-C2	4.88	121.47	108.64
31	2	613	CLA	O2A-C1-C2	4.88	121.47	108.64
31	4	613	CLA	O2D-CGD-CBD	4.88	119.94	111.27
43	B	619	BCR	C38-C26-C25	-4.88	119.05	124.53
31	5	612	CLA	O2A-C1-C2	4.88	121.46	108.64
31	q	316	CLA	O2D-CGD-CBD	4.88	119.94	111.27
36	0	618	NEX	C38-C25-C24	4.88	119.77	114.28
31	4	613	CLA	O2A-C1-C2	4.88	121.45	108.64
31	b	615	CLA	O2D-CGD-CBD	4.88	119.93	111.27
31	N	321	CLA	O2A-C1-C2	4.88	121.45	108.64
31	s	305	CLA	O2A-C1-C2	4.88	121.45	108.64
31	p	604	CLA	O2A-C1-C2	4.88	121.45	108.64
31	s	310	CLA	O2D-CGD-CBD	4.88	119.93	111.27
31	7	312	CLA	O2A-C1-C2	4.87	121.44	108.64
31	b	609	CLA	CMD-C2D-C1D	4.87	133.30	124.71
31	R	315	CLA	O2A-C1-C2	4.87	121.44	108.64
43	b	620	BCR	C15-C14-C13	-4.87	120.36	127.31
31	a	407	CLA	O2D-CGD-CBD	4.87	119.92	111.27
31	B	610	CLA	O2A-C1-C2	4.87	121.42	108.64
31	c	601	CLA	O2A-C1-C2	4.86	121.42	108.64
31	y	615	CLA	O2A-C1-C2	4.86	121.41	108.64
31	s	313	CLA	C1-C2-C3	-4.86	117.64	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	314	CLA	O2A-C1-C2	4.86	121.40	108.64
43	A	410	BCR	C33-C5-C6	-4.86	119.07	124.53
31	R	312	CLA	O2D-CGD-CBD	4.86	119.90	111.27
31	3	301	CLA	C1-C2-C3	-4.85	117.65	126.04
31	8	614	CLA	O2D-CGD-CBD	4.85	119.89	111.27
31	0	614	CLA	O2D-CGD-CBD	4.85	119.89	111.27
31	y	613	CLA	CMD-C2D-C1D	4.85	133.26	124.71
31	R	314	CLA	O2D-CGD-CBD	4.85	119.88	111.27
31	6	314	CLA	O2D-CGD-CBD	4.84	119.87	111.27
31	n	311	CLA	O2A-C1-C2	4.84	121.36	108.64
31	y	604	CLA	O2A-C1-C2	4.84	121.36	108.64
31	r	313	CLA	O2D-CGD-CBD	4.84	119.87	111.27
31	3	305	CLA	O2D-CGD-CBD	4.84	119.87	111.27
43	a	410	BCR	C15-C14-C13	-4.84	120.40	127.31
32	4	616	LUT	C35-C34-C33	-4.84	120.40	127.31
31	7	315	CLA	O2D-CGD-CBD	4.84	119.86	111.27
32	6	318	LUT	C35-C34-C33	-4.83	120.41	127.31
32	N	317	LUT	C15-C14-C13	-4.83	120.41	127.31
31	C	606	CLA	O2A-C1-C2	4.83	121.33	108.64
31	4	602	CLA	O2D-CGD-CBD	4.83	119.85	111.27
37	g	321	XAT	C31-C30-C29	-4.83	120.42	127.31
31	S	310	CLA	O2D-CGD-CBD	4.83	119.85	111.27
36	8	617	NEX	C27-C28-C29	-4.83	118.04	125.53
31	B	605	CLA	O2A-C1-C2	4.83	121.32	108.64
31	n	311	CLA	O2D-CGD-CBD	4.82	119.84	111.27
31	1	614	CLA	O2D-CGD-CBD	4.82	119.84	111.27
31	c	608	CLA	O2D-CGD-CBD	4.82	119.84	111.27
37	G	620	XAT	C31-C30-C29	-4.82	120.43	127.31
32	9	318	LUT	C11-C10-C9	-4.82	120.44	127.31
34	m	102	LMG	O7-C10-C11	4.82	121.88	111.50
31	8	603	CLA	O2D-CGD-CBD	4.81	119.82	111.27
31	Y	311	CLA	CMD-C2D-C1D	4.81	133.20	124.71
31	g	310	CLA	O2A-C1-C2	4.81	121.28	108.64
37	q	321	XAT	C31-C30-C29	-4.81	120.44	127.31
37	2	619	XAT	C31-C30-C29	-4.81	120.45	127.31
37	4	619	XAT	C31-C30-C29	-4.80	120.45	127.31
43	V	101	BCR	C27-C26-C25	-4.80	115.76	122.73
31	q	304	CLA	O2D-CGD-CBD	4.80	119.80	111.27
31	B	608	CLA	O2A-C1-C2	4.80	121.25	108.64
31	B	608	CLA	CMD-C2D-C1D	4.80	133.17	124.71
31	1	603	CLA	O2A-C1-C2	4.80	121.24	108.64
31	A	406	CLA	O2D-CGD-CBD	4.79	119.79	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	314	CLA	O2D-CGD-CBD	4.79	119.78	111.27
31	6	303	CLA	O2A-C1-C2	4.79	121.22	108.64
37	9	322	XAT	C31-C30-C29	-4.79	120.48	127.31
31	s	306	CLA	O2A-C1-C2	4.79	121.21	108.64
43	c	615	BCR	C4-C5-C6	-4.79	115.78	122.73
31	B	604	CLA	C1-C2-C3	-4.79	117.77	126.04
31	q	314	CLA	O2D-CGD-CBD	4.78	119.77	111.27
31	Y	305	CLA	O2A-C1-C2	4.78	121.20	108.64
31	q	315	CLA	CMD-C2D-C1D	4.78	133.14	124.71
31	y	610	CLA	O2A-C1-C2	4.78	121.20	108.64
34	9	301	LMG	C1-O6-C5	-4.78	104.30	113.69
31	C	610	CLA	O2A-C1-C2	4.78	121.20	108.64
43	C	614	BCR	C20-C21-C22	-4.78	120.49	127.31
31	Y	314	CLA	O2D-CGD-CBD	4.78	119.76	111.27
31	p	602	CLA	O2A-C1-C2	4.78	121.20	108.64
31	5	602	CLA	O2D-CGD-CBD	4.78	119.76	111.27
43	h	101	BCR	C33-C5-C6	-4.77	119.17	124.53
31	N	321	CLA	O2D-CGD-CBD	4.77	119.75	111.27
31	C	605	CLA	CMD-C2D-C1D	4.77	133.12	124.71
31	b	609	CLA	O2A-C1-C2	4.77	121.17	108.64
31	6	316	CLA	O2A-C1-C2	4.76	121.15	108.64
36	9	319	NEX	C27-C28-C29	-4.76	118.15	125.53
30	4	607	CHL	CHD-C1D-ND	-4.76	120.08	124.45
31	6	313	CLA	O2D-CGD-CBD	4.76	119.72	111.27
36	9	319	NEX	C38-C25-C24	4.76	119.63	114.28
36	g	317	NEX	C27-C28-C29	-4.76	118.15	125.53
31	n	316	CLA	O2A-C1-C2	4.76	121.14	108.64
31	a	407	CLA	O2A-C1-C2	4.75	121.13	108.64
31	q	305	CLA	O2A-C1-C2	4.75	121.12	108.64
36	R	319	NEX	C27-C28-C29	-4.75	118.16	125.53
34	w	203	LMG	O7-C10-C11	4.75	121.74	111.50
31	Y	310	CLA	O2D-CGD-CBD	4.75	119.70	111.27
31	2	603	CLA	O2D-CGD-CBD	4.75	119.70	111.27
31	s	314	CLA	O2D-CGD-CBD	4.74	119.70	111.27
43	H	101	BCR	C16-C17-C18	-4.74	120.54	127.31
43	B	617	BCR	C15-C14-C13	-4.74	120.55	127.31
31	Y	310	CLA	O2A-C1-C2	4.74	121.09	108.64
30	1	601	CHL	CHD-C1D-ND	-4.74	120.10	124.45
31	0	610	CLA	O2A-C1-C2	4.74	121.08	108.64
43	T	101	BCR	C38-C26-C25	-4.74	119.21	124.53
31	5	611	CLA	O2A-C1-C2	4.73	121.07	108.64
31	S	305	CLA	O2A-C1-C2	4.73	121.07	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	c	614	BCR	C38-C26-C25	-4.73	119.22	124.53
43	H	101	BCR	C24-C23-C22	-4.73	119.09	126.23
31	a	409	CLA	O2A-C1-C2	4.73	121.06	108.64
31	A	409	CLA	O2A-C1-C2	4.73	121.06	108.64
31	q	312	CLA	O2A-C1-C2	4.73	121.06	108.64
32	4	616	LUT	C18-C5-C6	-4.73	119.22	124.53
43	a	410	BCR	C11-C10-C9	-4.72	120.57	127.31
31	6	304	CLA	O2A-C1-C2	4.72	121.05	108.64
31	7	316	CLA	O2A-C1-C2	4.72	121.04	108.64
32	1	615	LUT	C18-C5-C6	-4.72	119.23	124.53
31	5	602	CLA	O2A-C1-C2	4.72	121.03	108.64
31	G	603	CLA	O2A-C1-C2	4.71	121.02	108.64
31	n	314	CLA	O2A-C1-C2	4.71	121.02	108.64
31	A	405	CLA	O2D-CGD-CBD	4.71	119.64	111.27
43	a	410	BCR	C33-C5-C6	-4.71	119.24	124.53
32	N	316	LUT	C18-C5-C6	-4.70	119.25	124.53
43	c	615	BCR	C27-C26-C25	-4.70	115.90	122.73
31	5	603	CLA	O2A-C1-C2	4.70	120.99	108.64
31	8	612	CLA	O2A-C1-C2	4.70	120.99	108.64
31	C	612	CLA	CMD-C2D-C1D	4.70	133.00	124.71
34	n	322	LMG	O7-C10-C11	4.70	121.63	111.50
31	c	612	CLA	CMD-C2D-C1D	4.70	133.00	124.71
31	b	604	CLA	O2A-C1-C2	4.70	120.99	108.64
31	R	313	CLA	O2D-CGD-CBD	4.70	119.61	111.27
31	b	614	CLA	O2D-CGD-CBD	4.69	119.61	111.27
31	7	311	CLA	O2D-CGD-CBD	4.69	119.61	111.27
31	n	315	CLA	O2D-CGD-CBD	4.69	119.61	111.27
35	g	315	RRX	C24-C23-C22	-4.69	119.15	126.23
31	r	314	CLA	O2D-CGD-CBD	4.69	119.60	111.27
34	b	622	LMG	O7-C10-C11	4.69	121.60	111.50
31	0	614	CLA	O2A-C1-C2	4.68	120.94	108.64
31	8	614	CLA	O2A-C1-C2	4.68	120.94	108.64
30	Y	309	CHL	CHD-C1D-ND	-4.68	120.15	124.45
31	8	609	CLA	O2A-C1-C2	4.68	120.93	108.64
31	C	606	CLA	C1-C2-C3	-4.68	117.95	126.04
31	2	612	CLA	O2D-CGD-CBD	4.67	119.57	111.27
31	3	305	CLA	O2A-C1-C2	4.67	120.91	108.64
36	g	317	NEX	C5-C4-C3	-4.67	106.22	111.75
31	4	602	CLA	O2A-C1-C2	4.67	120.91	108.64
31	r	305	CLA	O2A-C1-C2	4.67	120.91	108.64
31	2	602	CLA	O2D-CGD-CBD	4.67	119.56	111.27
32	n	317	LUT	C35-C34-C33	-4.67	120.65	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	303	CLA	O2A-C1-C2	4.67	120.90	108.64
31	y	614	CLA	O2A-C1-C2	4.67	120.90	108.64
31	p	611	CLA	O2A-C1-C2	4.66	120.89	108.64
34	w	205	LMG	O7-C10-C11	4.66	121.55	111.50
36	n	319	NEX	C27-C28-C29	-4.66	118.30	125.53
43	D	405	BCR	C33-C5-C6	-4.66	119.30	124.53
37	r	318	XAT	C15-C14-C13	-4.66	120.66	127.31
35	4	615	RRX	C1-C6-C5	-4.66	116.05	122.61
35	9	317	RRX	C1-C6-C5	-4.66	116.06	122.61
31	G	603	CLA	O2D-CGD-CBD	4.66	119.54	111.27
43	A	410	BCR	C11-C10-C9	-4.66	120.67	127.31
31	3	311	CLA	O2A-C1-C2	4.65	120.87	108.64
32	p	616	LUT	C30-C31-C32	-4.65	108.69	123.22
32	8	615	LUT	C35-C34-C33	-4.65	120.67	127.31
35	G	614	RRX	C1-C6-C5	-4.65	116.06	122.61
32	p	617	LUT	C35-C15-C14	-4.65	113.96	123.47
31	g	304	CLA	O2A-C1-C2	4.65	120.85	108.64
31	C	613	CLA	CAA-C2A-C3A	-4.64	100.06	112.78
37	R	318	XAT	C15-C14-C13	-4.64	120.68	127.31
31	G	610	CLA	O2A-C1-C2	4.64	120.84	108.64
36	r	301	NEX	C27-C28-C29	-4.64	118.33	125.53
31	B	613	CLA	O2A-C1-C2	4.64	120.83	108.64
31	q	304	CLA	O2A-C1-C2	4.64	120.83	108.64
43	B	618	BCR	C11-C10-C9	-4.64	120.69	127.31
31	9	312	CLA	O2D-CGD-CBD	4.64	119.51	111.27
31	7	311	CLA	O2A-C1-C2	4.63	120.81	108.64
31	8	602	CLA	O2A-C1-C2	4.63	120.81	108.64
43	b	619	BCR	C33-C5-C6	-4.63	119.33	124.53
30	6	306	CHL	CHD-C1D-ND	-4.63	120.20	124.45
30	n	310	CHL	CHD-C1D-ND	-4.63	120.20	124.45
32	8	616	LUT	C35-C34-C33	-4.63	120.70	127.31
31	3	313	CLA	O2A-C1-C2	4.63	120.80	108.64
33	z	102	LHG	O7-C7-C8	4.63	121.47	111.50
31	B	609	CLA	O2A-C1-C2	4.62	120.79	108.64
36	2	616	NEX	C27-C28-C29	-4.62	118.35	125.53
43	T	101	BCR	C20-C21-C22	-4.62	120.72	127.31
30	q	308	CHL	CHD-C1D-ND	-4.62	120.21	124.45
34	W	201	LMG	O7-C10-C11	4.62	121.46	111.50
31	B	613	CLA	O2D-CGD-CBD	4.62	119.47	111.27
32	N	316	LUT	C15-C14-C13	-4.61	120.72	127.31
35	2	614	RRX	C16-C17-C18	-4.61	120.73	127.31
31	a	406	CLA	O2D-CGD-CBD	4.61	119.46	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	n	318	LUT	C35-C34-C33	-4.61	120.73	127.31
43	C	615	BCR	C35-C13-C14	-4.61	116.47	122.92
31	4	604	CLA	O2A-C1-C2	4.61	120.75	108.64
35	q	317	RRX	C24-C23-C22	-4.61	119.27	126.23
32	6	317	LUT	C18-C5-C6	-4.61	119.36	124.53
43	B	618	BCR	C33-C5-C6	-4.60	119.36	124.53
35	g	315	RRX	C16-C17-C18	-4.60	120.74	127.31
43	D	405	BCR	C34-C9-C10	-4.60	116.48	122.92
36	y	618	NEX	C38-C25-C24	4.60	119.45	114.28
31	2	611	CLA	O2D-CGD-CBD	4.60	119.44	111.27
31	0	602	CLA	O2A-C1-C2	4.60	120.71	108.64
31	3	316	CLA	O2D-CGD-CBD	4.60	119.43	111.27
37	r	318	XAT	C18-C5-C4	4.59	119.45	114.28
34	c	620	LMG	O7-C10-C11	4.59	121.40	111.50
31	B	607	CLA	C1-C2-C3	-4.59	118.10	126.04
31	8	613	CLA	O2D-CGD-CBD	4.59	119.42	111.27
36	G	616	NEX	C38-C25-C24	4.59	119.44	114.28
31	2	610	CLA	O2A-C1-C2	4.59	120.70	108.64
31	b	611	CLA	O2A-C1-C2	4.59	120.69	108.64
31	y	610	CLA	O2D-CGD-CBD	4.59	119.42	111.27
32	2	615	LUT	C1-C6-C5	-4.59	116.15	122.61
30	0	608	CHL	CHD-C1D-ND	-4.58	120.24	124.45
32	Y	316	LUT	C7-C8-C9	-4.58	119.31	126.23
32	R	317	LUT	C18-C5-C6	-4.58	119.39	124.53
36	Y	317	NEX	C2-C1-C6	4.58	113.66	109.21
32	p	617	LUT	C32-C33-C34	4.58	125.96	118.94
31	N	313	CLA	O2A-C1-C2	4.58	120.66	108.64
31	1	611	CLA	O2A-C1-C2	4.58	120.66	108.64
35	2	614	RRX	C1-C6-C5	-4.57	116.17	122.61
32	0	617	LUT	C35-C34-C33	-4.57	120.79	127.31
31	2	604	CLA	O2A-C1-C2	4.57	120.64	108.64
33	C	623	LHG	O7-C7-C8	4.56	121.34	111.50
30	y	608	CHL	CHD-C1D-ND	-4.56	120.27	124.45
36	R	301	NEX	C27-C28-C29	-4.56	118.46	125.53
36	s	319	NEX	C38-C25-C24	4.56	119.41	114.28
30	3	302	CHL	C1-C2-C3	-4.56	118.16	126.04
34	B	621	LMG	O7-C10-C11	4.56	121.32	111.50
31	r	311	CLA	O2D-CGD-CBD	4.55	119.36	111.27
31	2	612	CLA	O2A-C1-C2	4.55	120.60	108.64
32	3	318	LUT	C1-C6-C5	-4.55	116.20	122.61
43	V	101	BCR	C24-C23-C22	-4.55	119.36	126.23
33	K	102	LHG	O7-C7-C8	4.55	121.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	605	CHL	CHD-C1D-ND	-4.54	120.28	124.45
37	g	321	XAT	C18-C5-C4	4.54	119.39	114.28
32	p	617	LUT	C28-C29-C30	4.54	125.91	118.94
30	g	307	CHL	CHD-C1D-ND	-4.54	120.28	124.45
32	7	318	LUT	C7-C8-C9	-4.54	119.37	126.23
43	t	101	BCR	C4-C5-C6	-4.54	116.14	122.73
31	8	603	CLA	O2A-C1-C2	4.54	120.56	108.64
31	n	304	CLA	O2A-C1-C2	4.54	120.56	108.64
32	7	317	LUT	C15-C14-C13	-4.53	120.84	127.31
35	G	614	RRX	C16-C17-C18	-4.53	120.84	127.31
43	D	405	BCR	C24-C23-C22	-4.53	119.39	126.23
33	a	415	LHG	O7-C7-C8	4.53	121.26	111.50
32	p	616	LUT	C18-C5-C6	-4.52	119.45	124.53
31	b	614	CLA	O2A-C1-C2	4.52	120.53	108.64
31	5	610	CLA	O2A-C1-C2	4.52	120.53	108.64
32	p	617	LUT	C11-C10-C9	-4.52	120.86	127.31
30	0	605	CHL	C1-O2A-CGA	4.52	128.30	116.44
31	6	316	CLA	C1-C2-C3	-4.52	118.22	126.04
37	G	620	XAT	C18-C5-C4	4.52	119.36	114.28
37	R	318	XAT	C18-C5-C4	4.52	119.36	114.28
37	4	619	XAT	C18-C5-C4	4.52	119.36	114.28
31	S	314	CLA	O2D-CGD-CBD	4.52	119.30	111.27
43	b	618	BCR	C7-C8-C9	-4.52	119.41	126.23
31	1	614	CLA	O2A-C1-C2	4.52	120.51	108.64
43	d	406	BCR	C11-C10-C9	4.52	133.76	127.31
43	C	614	BCR	C4-C5-C6	-4.52	116.17	122.73
35	4	615	RRX	C16-C17-C18	-4.51	120.87	127.31
31	c	606	CLA	CMD-C2D-C1D	4.51	132.66	124.71
43	t	101	BCR	C8-C9-C10	4.51	125.86	118.94
43	z	101	BCR	C20-C21-C22	-4.51	120.88	127.31
36	y	618	NEX	C27-C28-C29	-4.50	118.54	125.53
31	N	314	CLA	O2D-CGD-CBD	4.50	119.27	111.27
31	1	602	CLA	O2A-C1-C2	4.50	120.47	108.64
31	G	604	CLA	O2A-C1-C2	4.50	120.47	108.64
43	d	406	BCR	C35-C13-C14	-4.50	116.62	122.92
31	B	615	CLA	O2A-C1-C2	4.50	120.47	108.64
37	q	321	XAT	C18-C5-C4	4.50	119.34	114.28
35	g	315	RRX	C29-C28-C27	4.50	116.47	110.30
43	B	617	BCR	C7-C8-C9	-4.50	119.44	126.23
43	c	614	BCR	C7-C8-C9	-4.50	119.44	126.23
43	b	618	BCR	C15-C14-C13	-4.50	120.89	127.31
32	3	317	LUT	C18-C5-C6	-4.49	119.48	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n	303	CLA	O2A-C1-C2	4.49	120.44	108.64
36	3	319	NEX	C38-C25-C24	4.49	119.33	114.28
37	9	322	XAT	C18-C5-C4	4.49	119.33	114.28
31	y	603	CLA	O2A-C1-C2	4.49	120.44	108.64
45	c	618	DGD	O2G-C1B-C2B	4.49	121.17	111.50
31	6	314	CLA	O2A-C1-C2	4.49	120.43	108.64
35	9	317	RRX	C16-C17-C18	-4.49	120.91	127.31
32	N	316	LUT	C11-C10-C9	-4.48	120.91	127.31
31	2	603	CLA	O2A-C1-C2	4.48	120.41	108.64
31	N	303	CLA	O2A-C1-C2	4.48	120.41	108.64
32	S	317	LUT	C18-C5-C6	-4.48	119.50	124.53
34	6	321	LMG	O7-C10-C11	4.48	121.15	111.50
31	4	603	CLA	O2A-C1-C2	4.48	120.40	108.64
36	p	618	NEX	C38-C25-C24	4.47	119.31	114.28
32	q	318	LUT	C35-C34-C33	-4.47	120.93	127.31
43	C	614	BCR	C16-C17-C18	-4.47	120.93	127.31
37	2	619	XAT	C18-C5-C4	4.47	119.31	114.28
31	7	304	CLA	O2A-C1-C2	4.47	120.37	108.64
34	g	320	LMG	O7-C10-C11	4.47	121.12	111.50
30	1	608	CHL	CHD-C1D-ND	-4.46	120.35	124.45
36	Y	317	NEX	C27-C28-C29	-4.46	118.60	125.53
31	N	304	CLA	O2A-C1-C2	4.46	120.37	108.64
31	R	316	CLA	O2A-C1-C2	4.46	120.35	108.64
31	p	610	CLA	O2A-C1-C2	4.46	120.35	108.64
32	p	617	LUT	C1-C6-C5	-4.46	116.34	122.61
35	g	315	RRX	C1-C6-C5	-4.46	116.34	122.61
31	b	613	CLA	O2A-C1-C2	4.45	120.34	108.64
31	6	311	CLA	O2A-C1-C2	4.45	120.33	108.64
31	9	314	CLA	O2A-C1-C2	4.45	120.32	108.64
32	9	318	LUT	C18-C5-C6	-4.45	119.53	124.53
30	7	309	CHL	CHD-C1D-ND	-4.45	120.37	124.45
47	E	101	HEM	CHD-C1D-ND	4.45	129.25	124.42
32	4	616	LUT	C31-C30-C29	-4.43	120.98	127.31
34	d	411	LMG	O7-C10-C11	4.43	121.06	111.50
33	t	102	LHG	O7-C7-C8	4.43	121.05	111.50
43	a	410	BCR	C36-C18-C19	4.43	125.06	118.08
34	B	622	LMG	O7-C10-C11	4.43	121.05	111.50
31	3	306	CLA	O2A-C1-C2	4.43	120.28	108.64
31	7	313	CLA	O2A-C1-C2	4.43	120.27	108.64
43	B	617	BCR	C11-C10-C9	-4.42	121.00	127.31
43	z	101	BCR	C15-C14-C13	-4.42	121.00	127.31
36	S	319	NEX	C27-C28-C29	-4.42	118.67	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	305	CLA	C1-C2-C3	-4.42	118.40	126.04
30	7	307	CHL	CHD-C1D-ND	-4.42	120.39	124.45
36	R	301	NEX	C38-C25-C24	4.42	119.25	114.28
31	2	602	CLA	O2A-C1-C2	4.41	120.24	108.64
31	q	306	CLA	O2A-C1-C2	4.41	120.24	108.64
31	R	304	CLA	O2A-C1-C2	4.41	120.23	108.64
32	7	318	LUT	C35-C34-C33	-4.41	121.01	127.31
34	C	621	LMG	O7-C10-C11	4.41	121.01	111.50
30	7	302	CHL	CHD-C1D-ND	-4.41	120.40	124.45
36	n	319	NEX	C38-C25-C24	4.41	119.24	114.28
32	1	616	LUT	C35-C34-C33	-4.41	121.02	127.31
31	0	613	CLA	O2A-C1-C2	4.41	120.21	108.64
31	G	612	CLA	O2A-C1-C2	4.40	120.21	108.64
36	Y	317	NEX	C38-C25-C24	4.40	119.23	114.28
30	Y	307	CHL	CHD-C1D-ND	-4.40	120.41	124.45
31	Y	304	CLA	O2A-C1-C2	4.40	120.20	108.64
34	G	622	LMG	O7-C10-C11	4.40	120.98	111.50
32	S	318	LUT	C22-C23-C24	4.40	116.75	111.74
32	y	617	LUT	C18-C5-C6	-4.40	119.59	124.53
30	9	309	CHL	CHD-C1D-ND	-4.40	120.42	124.45
30	0	601	CHL	CHD-C1D-ND	-4.39	120.42	124.45
31	7	315	CLA	O2A-C1-C2	4.39	120.18	108.64
31	q	312	CLA	C1B-NB-C4B	4.39	109.45	106.33
31	c	608	CLA	O2A-C1-C2	4.39	120.17	108.64
32	p	616	LUT	C40-C33-C34	-4.38	116.78	122.92
31	c	606	CLA	O2A-C1-C2	4.38	120.15	108.64
43	h	101	BCR	C20-C21-C22	-4.38	121.06	127.31
32	9	318	LUT	C7-C8-C9	-4.38	119.62	126.23
34	9	301	LMG	C8-O7-C10	-4.38	107.01	117.79
36	N	318	NEX	C38-C25-C24	4.38	119.20	114.28
30	s	307	CHL	CHD-C1D-ND	-4.38	120.43	124.45
35	2	614	RRX	C38-C26-C25	-4.38	119.61	124.53
47	e	102	HEM	CHD-C1D-ND	4.37	129.17	124.42
30	g	309	CHL	CHD-C1D-ND	-4.37	120.44	124.45
31	s	303	CLA	O2A-C1-C2	4.37	120.13	108.64
33	3	320	LHG	O7-C7-C8	4.37	120.92	111.50
43	B	619	BCR	C24-C23-C22	-4.37	119.63	126.23
31	g	303	CLA	O2D-CGD-CBD	4.37	119.03	111.27
30	3	303	CHL	CHD-C1D-ND	-4.37	120.44	124.45
31	6	305	CLA	O2A-C1-C2	4.37	120.11	108.64
32	2	615	LUT	C40-C33-C34	-4.36	116.81	122.92
30	N	309	CHL	CHD-C1D-ND	-4.36	120.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	s	317	LUT	C18-C5-C6	-4.36	119.64	124.53
43	V	101	BCR	C20-C21-C22	-4.36	121.09	127.31
43	h	101	BCR	C16-C17-C18	-4.35	121.09	127.31
35	g	315	RRX	C4-C5-C6	-4.35	116.41	122.73
31	5	604	CLA	O2A-C1-C2	4.35	120.08	108.64
31	B	612	CLA	O2A-C1-C2	4.35	120.07	108.64
31	Y	311	CLA	O2A-C1-C2	4.35	120.07	108.64
30	2	607	CHL	CHD-C1D-ND	-4.35	120.46	124.45
30	9	308	CHL	CHD-C1D-ND	-4.35	120.46	124.45
30	8	608	CHL	CHD-C1D-ND	-4.35	120.46	124.45
35	G	614	RRX	C38-C26-C25	-4.34	119.65	124.53
31	R	305	CLA	C1-C2-C3	-4.34	118.54	126.04
32	p	617	LUT	C30-C31-C32	-4.34	109.67	123.22
30	p	609	CHL	CHD-C1D-ND	-4.34	120.47	124.45
35	9	317	RRX	C38-C26-C25	-4.34	119.66	124.53
30	y	609	CHL	CHD-C1D-ND	-4.34	120.47	124.45
31	S	313	CLA	C1-C2-C3	-4.34	118.55	126.04
35	4	615	RRX	C38-C26-C25	-4.33	119.67	124.53
34	b	624	LMG	O7-C10-C11	4.33	120.83	111.50
30	0	605	CHL	CHD-C1D-ND	-4.33	120.47	124.45
43	b	620	BCR	C16-C17-C18	-4.33	121.13	127.31
30	p	607	CHL	CHD-C1D-ND	-4.32	120.48	124.45
32	n	318	LUT	C7-C8-C9	-4.32	119.70	126.23
30	r	308	CHL	CHD-C1D-ND	-4.32	120.48	124.45
31	7	303	CLA	O2A-C1-C2	4.32	119.98	108.64
31	g	303	CLA	O2A-C1-C2	4.32	119.98	108.64
36	N	318	NEX	C27-C28-C29	-4.32	118.83	125.53
31	3	316	CLA	O2A-C1-C2	4.31	119.97	108.64
32	q	318	LUT	C1-C6-C5	-4.31	116.54	122.61
31	g	305	CLA	O2A-C1-C2	4.31	119.96	108.64
31	1	613	CLA	O2A-C1-C2	4.31	119.95	108.64
32	5	617	LUT	C18-C5-C6	-4.30	119.69	124.53
34	9	301	LMG	O1-C7-C8	-4.30	100.51	110.90
36	s	319	NEX	C17-C1-C6	-4.30	106.62	110.47
34	a	413	LMG	O7-C10-C11	4.30	120.77	111.50
34	W	203	LMG	O7-C10-C11	4.30	120.77	111.50
43	b	620	BCR	C33-C5-C6	-4.30	119.70	124.53
30	S	307	CHL	CHD-C1D-ND	-4.30	120.50	124.45
35	2	614	RRX	C33-C5-C6	-4.30	119.70	124.53
32	y	617	LUT	C35-C34-C33	-4.30	121.17	127.31
30	5	606	CHL	CHD-C1D-ND	-4.30	120.50	124.45
30	4	608	CHL	CHD-C1D-ND	-4.30	120.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	609	CHL	CHD-C1D-ND	-4.29	120.51	124.45
43	A	410	BCR	C27-C26-C25	-4.29	116.50	122.73
36	G	616	NEX	C27-C28-C29	-4.29	118.87	125.53
30	N	307	CHL	CHD-C1D-ND	-4.29	120.51	124.45
31	S	314	CLA	O2A-C1-C2	4.29	119.91	108.64
32	Y	316	LUT	C15-C14-C13	-4.29	121.19	127.31
35	2	614	RRX	C4-C5-C6	-4.29	116.50	122.73
30	n	309	CHL	CHD-C1D-ND	-4.29	120.52	124.45
32	8	616	LUT	C7-C8-C9	-4.29	119.76	126.23
34	q	302	LMG	O7-C10-C11	4.28	120.73	111.50
43	Z	101	BCR	C20-C21-C22	-4.28	121.20	127.31
32	3	318	LUT	C18-C5-C6	-4.28	119.72	124.53
31	2	611	CLA	O2A-C1-C2	4.28	119.88	108.64
30	Y	308	CHL	CHD-C1D-ND	-4.28	120.52	124.45
30	5	609	CHL	CHD-C1D-ND	-4.28	120.52	124.45
32	G	615	LUT	C18-C5-C6	-4.28	119.73	124.53
45	c	619	DGD	O2G-C1B-C2B	4.27	120.71	111.50
30	7	310	CHL	CHD-C1D-ND	-4.27	120.53	124.45
30	n	307	CHL	CHD-C1D-ND	-4.27	120.53	124.45
31	6	313	CLA	O2A-C1-C2	4.27	119.85	108.64
33	9	320	LHG	O7-C7-C8	4.27	120.70	111.50
30	0	609	CHL	CHD-C1D-ND	-4.27	120.53	124.45
30	8	607	CHL	CHD-C1D-ND	-4.26	120.54	124.45
30	R	308	CHL	CHD-C1D-ND	-4.26	120.54	124.45
30	N	302	CHL	CHD-C1D-ND	-4.26	120.54	124.45
43	C	615	BCR	C16-C15-C14	4.26	132.20	123.47
34	S	321	LMG	O7-C10-C11	4.26	120.68	111.50
32	3	318	LUT	C7-C8-C9	-4.26	119.80	126.23
33	R	320	LHG	O7-C7-C8	4.26	120.67	111.50
34	w	202	LMG	O7-C10-C11	4.25	120.67	111.50
36	S	319	NEX	C38-C25-C24	4.25	119.06	114.28
31	Y	313	CLA	O2A-C1-C2	4.25	119.80	108.64
33	s	322	LHG	O7-C7-C8	4.25	120.66	111.50
34	b	601	LMG	O7-C10-C11	4.25	120.65	111.50
34	2	618	LMG	O7-C10-C11	4.24	120.65	111.50
31	Y	303	CLA	C1-C2-C3	-4.24	118.70	126.04
30	5	601	CHL	CHD-C1D-ND	-4.24	120.56	124.45
35	q	317	RRX	C4-C5-C6	-4.24	116.57	122.73
43	c	615	BCR	C16-C17-C18	-4.24	121.26	127.31
30	1	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
32	7	317	LUT	C35-C34-C33	-4.24	121.26	127.31
30	2	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	608	CHL	CHD-C1D-ND	-4.24	120.56	124.45
43	B	617	BCR	C23-C24-C25	-4.24	115.30	127.20
30	p	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
30	6	308	CHL	CHD-C1D-ND	-4.24	120.56	124.45
31	r	304	CLA	O2A-C1-C2	4.23	119.76	108.64
30	8	606	CHL	CHD-C1D-ND	-4.23	120.56	124.45
31	c	613	CLA	O2A-C1-C2	4.23	119.76	108.64
31	3	314	CLA	O2A-C1-C2	4.23	119.75	108.64
32	p	617	LUT	C40-C33-C34	-4.22	117.00	122.92
32	p	616	LUT	C35-C15-C14	-4.22	114.82	123.47
34	f	101	LMG	O7-C10-C11	4.22	120.60	111.50
36	s	319	NEX	C27-C28-C29	-4.22	118.99	125.53
31	0	615	CLA	O2A-C1-C2	4.22	119.72	108.64
42	a	408	PHO	C4D-CHA-CBD	-4.21	106.61	108.52
30	4	609	CHL	CHD-C1D-ND	-4.21	120.58	124.45
30	5	608	CHL	CHD-C1D-ND	-4.21	120.58	124.45
30	6	309	CHL	CHD-C1D-ND	-4.21	120.58	124.45
34	I	101	LMG	O7-C10-C11	4.21	120.57	111.50
31	2	609	CLA	O2A-C1-C2	4.21	119.69	108.64
43	V	101	BCR	C30-C25-C26	-4.21	116.69	122.61
32	p	616	LUT	C39-C29-C30	-4.21	117.03	122.92
30	8	605	CHL	CHD-C1D-ND	-4.20	120.59	124.45
32	1	616	LUT	C7-C8-C9	-4.20	119.89	126.23
31	7	312	CLA	C1-C2-C3	-4.20	118.78	126.04
30	2	608	CHL	CHD-C1D-ND	-4.20	120.60	124.45
30	G	606	CHL	CHD-C1D-ND	-4.19	120.60	124.45
30	g	308	CHL	CHD-C1D-ND	-4.19	120.60	124.45
30	6	310	CHL	CHD-C1D-ND	-4.19	120.60	124.45
36	3	319	NEX	C2-C1-C6	4.19	113.28	109.21
43	H	101	BCR	C15-C14-C13	-4.19	121.33	127.31
32	8	615	LUT	C18-C5-C6	-4.19	119.83	124.53
32	g	316	LUT	C7-C8-C9	-4.18	119.91	126.23
34	Y	319	LMG	O7-C10-C11	4.18	120.51	111.50
32	n	317	LUT	C18-C5-C6	-4.18	119.83	124.53
38	b	627	SQD	O7-S-C6	-4.18	101.97	106.94
43	t	101	BCR	C34-C9-C10	-4.18	117.07	122.92
30	n	306	CHL	CHD-C1D-ND	-4.18	120.61	124.45
43	C	615	BCR	C20-C19-C18	-4.18	114.67	126.42
32	S	317	LUT	C7-C8-C9	-4.18	119.92	126.23
31	7	314	CLA	O2A-C1-C2	4.17	119.61	108.64
31	b	605	CLA	C1-C2-C3	-4.17	118.83	126.04
31	C	607	CLA	O2A-C1-C2	4.17	119.60	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	N	316	LUT	C35-C34-C33	-4.17	121.36	127.31
43	B	619	BCR	C20-C21-C22	-4.17	121.36	127.31
31	B	611	CLA	C1-C2-C3	-4.17	118.83	126.04
45	C	620	DGD	O2G-C1B-C2B	4.17	120.49	111.50
34	7	320	LMG	O7-C10-C11	4.16	120.48	111.50
31	8	604	CLA	C1-C2-C3	-4.16	118.84	126.04
30	3	307	CHL	CHD-C1D-ND	-4.16	120.63	124.45
32	Y	315	LUT	C18-C5-C6	-4.16	119.86	124.53
30	q	307	CHL	CHD-C1D-ND	-4.16	120.63	124.45
31	y	615	CLA	C1-C2-C3	-4.16	118.85	126.04
30	N	308	CHL	CHD-C1D-ND	-4.16	120.63	124.45
33	p	619	LHG	O7-C7-C8	4.16	120.46	111.50
34	J	102	LMG	O7-C10-C11	4.16	120.46	111.50
32	r	317	LUT	C18-C5-C6	-4.16	119.86	124.53
30	0	607	CHL	CHD-C1D-ND	-4.16	120.63	124.45
34	6	322	LMG	O7-C10-C11	4.16	120.46	111.50
34	2	621	LMG	O7-C10-C11	4.16	120.46	111.50
30	6	307	CHL	CHD-C1D-ND	-4.15	120.64	124.45
33	A	415	LHG	O7-C7-C8	4.15	120.45	111.50
34	Q1	101	LMG	O7-C10-C11	4.15	120.44	111.50
30	3	309	CHL	CHD-C1D-ND	-4.15	120.64	124.45
31	b	615	CLA	C1-C2-C3	-4.15	118.87	126.04
31	g	313	CLA	O2A-C1-C2	4.15	119.53	108.64
33	D	407	LHG	O7-C7-C8	4.15	120.44	111.50
36	q	319	NEX	C38-C25-C24	4.15	118.94	114.28
34	G	619	LMG	O7-C10-C11	4.15	120.44	111.50
31	B	603	CLA	O2A-C1-C2	4.15	119.53	108.64
36	4	617	NEX	C27-C28-C29	-4.15	119.10	125.53
32	R	317	LUT	C35-C15-C14	-4.15	114.98	123.47
32	r	317	LUT	C35-C34-C33	-4.14	121.40	127.31
43	A	410	BCR	C24-C23-C22	-4.14	119.98	126.23
32	N	317	LUT	C35-C34-C33	-4.14	121.40	127.31
43	a	410	BCR	C15-C16-C17	-4.14	115.00	123.47
43	c	614	BCR	C11-C12-C13	-4.13	114.80	126.42
30	y	605	CHL	CHD-C1D-ND	-4.13	120.66	124.45
30	N	306	CHL	CHD-C1D-ND	-4.12	120.66	124.45
32	6	318	LUT	C15-C14-C13	-4.12	121.43	127.31
34	b	629	LMG	O7-C10-C11	4.12	120.38	111.50
30	n	301	CHL	CHD-C1D-ND	-4.12	120.67	124.45
31	C	604	CLA	C1-C2-C3	-4.12	118.92	126.04
31	S	306	CLA	C1-C2-C3	-4.12	120.09	126.75
32	0	616	LUT	C18-C5-C6	-4.11	119.91	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	7	322	LMG	O7-C10-C11	4.11	120.37	111.50
31	9	315	CLA	O2A-C1-C2	4.11	119.44	108.64
31	9	306	CLA	C1-C2-C3	-4.11	118.93	126.04
43	t	101	BCR	C30-C25-C26	-4.11	116.82	122.61
30	r	309	CHL	CHD-C1D-ND	-4.11	120.67	124.45
43	Z	101	BCR	C15-C14-C13	-4.11	121.44	127.31
34	b	623	LMG	O7-C10-C11	4.11	120.36	111.50
31	C	605	CLA	O2A-C1-C2	4.11	119.44	108.64
34	A	412	LMG	O7-C10-C11	4.11	120.36	111.50
43	t	101	BCR	C36-C18-C17	-4.11	117.17	122.92
34	D	412	LMG	O7-C10-C11	4.11	120.35	111.50
32	0	616	LUT	C21-C26-C27	-4.10	107.51	112.70
30	y	606	CHL	CHD-C1D-ND	-4.10	120.68	124.45
33	S	320	LHG	O7-C7-C8	4.10	120.34	111.50
30	n	308	CHL	CHD-C1D-ND	-4.10	120.68	124.45
31	B	606	CLA	O2A-C1-C2	4.10	119.42	108.64
31	q	313	CLA	C1B-NB-C4B	4.10	109.25	106.33
43	d	406	BCR	C2-C1-C6	4.10	116.80	110.48
30	2	605	CHL	CHD-C1D-ND	-4.10	120.69	124.45
30	7	321	CHL	CHD-C1D-ND	-4.10	120.69	124.45
31	4	611	CLA	C1B-NB-C4B	4.10	109.25	106.33
30	p	608	CHL	CHD-C1D-ND	-4.10	120.69	124.45
31	q	316	CLA	C1-C2-C3	-4.09	120.13	126.75
30	9	303	CHL	CHD-C1D-ND	-4.09	120.69	124.45
36	5	618	NEX	C27-C28-C29	-4.09	119.18	125.53
32	n	318	LUT	C15-C14-C13	-4.09	121.47	127.31
30	G	601	CHL	CHD-C1D-ND	-4.09	120.70	124.45
32	8	616	LUT	C15-C14-C13	-4.09	121.48	127.31
34	w	204	LMG	O7-C10-C11	4.09	120.31	111.50
43	d	406	BCR	C27-C26-C25	-4.08	116.81	122.73
43	b	619	BCR	C11-C10-C9	-4.08	121.49	127.31
43	B	617	BCR	C16-C17-C18	-4.08	121.49	127.31
34	X	203	LMG	O7-C10-C11	4.08	120.29	111.50
30	n	302	CHL	CHD-C1D-ND	-4.08	120.71	124.45
43	B	618	BCR	C20-C21-C22	-4.08	121.49	127.31
31	5	615	CLA	C2C-C1C-NC	4.08	113.79	109.97
30	3	310	CHL	CHD-C1D-ND	-4.08	120.71	124.45
30	7	308	CHL	CHD-C1D-ND	-4.07	120.71	124.45
34	J	101	LMG	O7-C10-C11	4.07	120.27	111.50
45	c	617	DGD	O2G-C1B-C2B	4.07	120.27	111.50
30	p	605	CHL	CHD-C1D-ND	-4.07	120.72	124.45
30	R	309	CHL	CHD-C1D-ND	-4.07	120.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	302	CHL	CHD-C1D-ND	-4.07	120.72	124.45
31	c	609	CLA	O2A-C1-C2	4.06	119.32	108.64
34	k	102	LMG	O7-C10-C11	4.06	120.26	111.50
30	q	308	CHL	C4D-CHA-C1A	4.06	126.19	121.25
43	b	619	BCR	C4-C5-C6	-4.06	116.83	122.73
34	y	620	LMG	O7-C10-C11	4.06	120.25	111.50
30	8	601	CHL	CHD-C1D-ND	-4.06	120.72	124.45
32	y	617	LUT	C15-C14-C13	-4.06	121.52	127.31
33	b	625	LHG	O7-C7-C8	4.06	120.25	111.50
31	4	602	CLA	C1-C2-C3	-4.06	119.03	126.04
43	b	620	BCR	C24-C23-C22	-4.05	120.11	126.23
31	6	305	CLA	C1-C2-C3	-4.05	119.03	126.04
34	a	413	LMG	C1-O6-C5	-4.05	105.73	113.69
30	G	623	CHL	CHD-C1D-ND	-4.05	120.73	124.45
30	4	605	CHL	CHD-C1D-ND	-4.05	120.73	124.45
30	g	306	CHL	CHD-C1D-ND	-4.05	120.74	124.45
30	9	310	CHL	CHD-C1D-ND	-4.04	120.74	124.45
36	3	319	NEX	C27-C28-C29	-4.04	119.25	125.53
31	y	604	CLA	C1-C2-C3	-4.04	119.05	126.04
30	G	605	CHL	CHD-C1D-ND	-4.04	120.74	124.45
30	q	309	CHL	C3B-C4B-NB	-4.04	106.76	110.52
34	s	321	LMG	O7-C10-C11	4.04	120.21	111.50
30	r	310	CHL	CHD-C1D-ND	-4.04	120.74	124.45
30	y	607	CHL	CHD-C1D-ND	-4.04	120.74	124.45
43	H	101	BCR	C33-C5-C6	-4.04	119.99	124.53
32	2	615	LUT	C31-C32-C33	4.04	137.75	126.42
31	C	610	CLA	CAA-C2A-C3A	-4.03	101.73	112.78
32	p	617	LUT	C39-C29-C30	-4.03	117.27	122.92
31	N	321	CLA	C1-C2-C3	-4.03	119.07	126.04
33	c	622	LHG	O7-C7-C8	4.03	120.18	111.50
31	S	314	CLA	C1-C2-C3	-4.03	119.08	126.04
33	j	102	LHG	O7-C7-C8	4.02	120.17	111.50
31	C	612	CLA	C1-C2-C3	-4.02	119.09	126.04
31	c	605	CLA	O2A-C1-C2	4.02	119.19	108.64
33	0	619	LHG	O7-C7-C8	4.02	120.16	111.50
34	c	621	LMG	O7-C10-C11	4.02	120.16	111.50
32	2	615	LUT	C18-C5-C6	-4.01	120.02	124.53
31	C	608	CLA	O2A-C1-C2	4.01	119.18	108.64
32	R	317	LUT	C31-C30-C29	4.01	133.04	127.31
34	W	202	LMG	O7-C10-C11	4.01	120.15	111.50
48	c	623	LMU	C1B-O1B-C4'	-4.01	108.05	117.96
31	5	612	CLA	C1-C2-C3	-4.01	120.27	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	L	101	LHG	O7-C7-C8	4.00	120.12	111.50
43	t	101	BCR	C19-C18-C17	4.00	125.08	118.94
43	c	614	BCR	C15-C16-C17	-4.00	115.28	123.47
34	b	626	LMG	O7-C10-C11	4.00	120.12	111.50
32	N	317	LUT	C1-C6-C5	-4.00	116.98	122.61
32	g	316	LUT	C1-C6-C5	-4.00	116.98	122.61
43	t	101	BCR	C35-C13-C14	-4.00	117.32	122.92
35	9	317	RRX	C4-C5-C6	-4.00	116.93	122.73
33	1	617	LHG	O7-C7-C8	3.99	120.11	111.50
43	B	619	BCR	C4-C5-C6	-3.99	116.93	122.73
33	6	320	LHG	O7-C7-C8	3.99	120.11	111.50
30	G	607	CHL	CHD-C1D-ND	-3.99	120.78	124.45
32	Y	315	LUT	C35-C34-C33	-3.99	121.61	127.31
30	3	308	CHL	CHD-C1D-ND	-3.99	120.79	124.45
43	Z	101	BCR	C38-C26-C25	-3.99	120.05	124.53
35	4	615	RRX	C33-C5-C6	-3.99	120.05	124.53
32	Y	316	LUT	C35-C34-C33	-3.99	121.62	127.31
33	D	408	LHG	O7-C7-C8	3.99	120.09	111.50
43	b	618	BCR	C4-C5-C6	-3.99	116.94	122.73
33	d	408	LHG	O7-C7-C8	3.99	120.09	111.50
31	9	314	CLA	C1-C2-C3	-3.98	120.31	126.75
34	R	321	LMG	O7-C10-C11	3.98	120.08	111.50
34	B	625	LMG	O7-C10-C11	3.98	120.08	111.50
36	r	301	NEX	C5-C4-C3	3.98	116.46	111.75
43	A	410	BCR	C7-C8-C9	-3.98	120.22	126.23
32	Y	315	LUT	C21-C26-C27	-3.98	107.67	112.70
34	j	101	LMG	O7-C10-C11	3.98	120.07	111.50
30	N	301	CHL	CHD-C1D-ND	-3.98	120.80	124.45
30	4	601	CHL	CHD-C1D-ND	-3.97	120.80	124.45
30	y	601	CHL	CHD-C1D-ND	-3.97	120.80	124.45
34	d	409	LMG	O7-C10-C11	3.97	120.06	111.50
30	0	606	CHL	CHD-C1D-ND	-3.97	120.80	124.45
31	y	602	CLA	C1-C2-C3	-3.97	119.17	126.04
30	0	605	CHL	C3C-C4C-NC	-3.97	106.12	110.57
34	A	414	LMG	O7-C10-C11	3.97	120.06	111.50
35	G	614	RRX	C4-C5-C6	-3.97	116.97	122.73
34	9	302	LMG	O7-C10-C11	3.97	120.05	111.50
31	r	306	CLA	O2A-C1-C2	3.97	122.91	109.49
30	1	619	CHL	CMA-C3A-C4A	3.97	122.44	111.77
31	3	304	CLA	C1-C2-C3	-3.97	119.18	126.04
30	4	606	CHL	CHD-C1D-ND	-3.97	120.81	124.45
31	5	604	CLA	C1-C2-C3	-3.96	120.34	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1	616	LUT	C15-C14-C13	-3.96	121.65	127.31
34	q	301	LMG	O7-C10-C11	3.96	120.04	111.50
35	4	615	RRX	C4-C5-C6	-3.96	116.98	122.73
32	7	317	LUT	C21-C26-C27	-3.96	107.69	112.70
35	G	614	RRX	C33-C5-C6	-3.96	120.08	124.53
30	Y	301	CHL	CHD-C1D-ND	-3.96	120.82	124.45
30	q	311	CHL	CHD-C1D-ND	-3.96	120.82	124.45
35	2	614	RRX	C7-C8-C9	-3.95	120.26	126.23
43	b	619	BCR	C1-C6-C5	-3.95	117.05	122.61
32	5	617	LUT	C35-C34-C33	-3.95	121.67	127.31
30	1	607	CHL	CHD-C1D-ND	-3.95	120.83	124.45
31	C	605	CLA	C1-C2-C3	-3.95	119.22	126.04
35	9	317	RRX	C33-C5-C6	-3.94	120.10	124.53
31	N	305	CLA	C1-C2-C3	-3.94	119.22	126.04
34	C	619	LMG	O7-C10-C11	3.94	119.99	111.50
32	r	317	LUT	C21-C26-C27	-3.94	107.72	112.70
43	d	406	BCR	C15-C16-C17	-3.94	115.41	123.47
31	R	306	CLA	O2A-C1-C2	3.93	122.79	109.49
30	5	607	CHL	CHD-C1D-ND	-3.93	120.84	124.45
32	r	317	LUT	C15-C14-C13	-3.93	121.70	127.31
30	9	311	CHL	CHD-C1D-ND	-3.93	120.84	124.45
43	Z	101	BCR	C16-C17-C18	-3.93	121.70	127.31
33	M	101	LHG	O7-C7-C8	3.93	119.97	111.50
33	e	101	LHG	O7-C7-C8	3.92	119.96	111.50
33	5	619	LHG	O7-C7-C8	3.92	119.95	111.50
34	r	321	LMG	O7-C10-C11	3.92	119.94	111.50
43	b	620	BCR	C4-C5-C6	-3.92	117.05	122.73
31	C	603	CLA	CHD-C1D-ND	-3.92	120.86	124.45
31	c	612	CLA	C1-C2-C3	-3.91	119.28	126.04
30	S	309	CHL	CHD-C1D-ND	-3.91	120.86	124.45
30	5	605	CHL	CHD-C1D-ND	-3.91	120.86	124.45
34	n	321	LMG	O7-C10-C11	3.91	119.92	111.50
30	q	303	CHL	CHD-C1D-ND	-3.90	120.87	124.45
43	b	618	BCR	C11-C10-C9	-3.90	121.74	127.31
32	0	617	LUT	C15-C14-C13	-3.90	121.74	127.31
43	B	618	BCR	C1-C6-C5	-3.90	117.12	122.61
34	D	411	LMG	O7-C10-C11	3.90	119.91	111.50
31	n	305	CLA	C1-C2-C3	-3.90	119.30	126.04
43	H	101	BCR	C27-C26-C25	-3.90	117.07	122.73
43	H	101	BCR	C4-C5-C6	-3.90	117.07	122.73
43	B	618	BCR	C4-C5-C6	-3.90	117.07	122.73
30	g	302	CHL	CHD-C1D-ND	-3.90	120.87	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	d	410	LMG	O7-C10-C11	3.89	119.89	111.50
32	6	318	LUT	C11-C10-C9	-3.89	121.75	127.31
30	Y	306	CHL	CHD-C1D-ND	-3.89	120.88	124.45
33	G	618	LHG	O7-C7-C8	3.89	119.89	111.50
31	C	609	CLA	O2A-C1-C2	3.89	118.86	108.64
43	H	101	BCR	C38-C26-C25	-3.89	120.16	124.53
31	g	303	CLA	C1D-ND-C4D	-3.89	103.57	106.33
30	2	601	CHL	CHD-C1D-ND	-3.89	120.88	124.45
30	6	302	CHL	CHD-C1D-ND	-3.89	120.88	124.45
32	2	615	LUT	C21-C26-C27	-3.88	107.79	112.70
31	3	313	CLA	C1-C2-C3	-3.88	120.47	126.75
31	Y	305	CLA	C1-C2-C3	-3.88	119.33	126.04
33	r	320	LHG	O7-C7-C8	3.88	119.87	111.50
31	B	615	CLA	C2C-C1C-NC	3.88	113.61	109.97
31	B	608	CLA	C1-C2-C3	-3.88	119.33	126.04
32	y	616	LUT	C18-C5-C6	-3.88	120.17	124.53
31	R	312	CLA	O2A-C1-C2	3.88	118.83	108.64
32	y	616	LUT	C35-C34-C33	-3.88	121.77	127.31
32	1	615	LUT	C21-C26-C27	-3.88	107.80	112.70
30	s	308	CHL	CHD-C1D-ND	-3.88	120.89	124.45
43	B	617	BCR	C1-C6-C5	-3.88	117.15	122.61
33	2	617	LHG	O7-C7-C8	3.87	119.85	111.50
31	r	312	CLA	O2A-C1-C2	3.87	118.81	108.64
34	X	202	LMG	O7-C10-C11	3.87	119.84	111.50
30	1	619	CHL	C1-C2-C3	-3.87	119.35	126.04
43	c	614	BCR	C4-C5-C6	-3.87	117.11	122.73
48	K	101	LMU	C1B-O1B-C4'	-3.87	108.40	117.96
34	C	622	LMG	O7-C10-C11	3.86	119.82	111.50
32	s	318	LUT	C15-C14-C13	-3.86	121.81	127.31
30	s	309	CHL	CHD-C1D-ND	-3.85	120.91	124.45
34	6	323	LMG	O7-C10-C11	3.85	119.80	111.50
43	t	101	BCR	C24-C23-C22	-3.85	120.42	126.23
31	Y	313	CLA	C1-C2-C3	-3.85	119.38	126.04
45	C	616	DGD	O2G-C1B-C2B	3.85	119.79	111.50
33	S	322	LHG	O7-C7-C8	3.84	119.78	111.50
33	s	320	LHG	O7-C7-C8	3.84	119.78	111.50
30	q	309	CHL	C1-O2A-CGA	3.84	126.53	116.44
34	5	620	LMG	O7-C10-C11	3.84	119.78	111.50
34	0	620	LMG	O7-C10-C11	3.84	119.78	111.50
43	v	101	BCR	C27-C26-C25	-3.84	117.16	122.73
31	r	316	CLA	CHD-C1D-ND	-3.84	120.93	124.45
43	t	101	BCR	C12-C13-C14	3.83	124.83	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	601	CHL	CMA-C3A-C4A	3.83	122.08	111.77
34	k	101	LMG	O7-C10-C11	3.83	119.76	111.50
30	3	302	CHL	C1-O2A-CGA	3.83	126.50	116.44
34	7	301	LMG	O7-C10-C11	3.83	119.76	111.50
31	y	612	CLA	C1-C2-C3	-3.83	119.42	126.04
33	g	319	LHG	O7-C7-C8	3.83	119.75	111.50
33	A	417	LHG	O7-C7-C8	3.83	119.75	111.50
34	4	621	LMG	O7-C10-C11	3.83	119.75	111.50
34	p	620	LMG	O7-C10-C11	3.82	119.74	111.50
31	s	314	CLA	C1-C2-C3	-3.82	119.43	126.04
43	h	101	BCR	C27-C26-C25	-3.82	117.18	122.73
31	0	614	CLA	C1-C2-C3	-3.82	119.43	126.04
32	S	318	LUT	C1-C6-C5	-3.82	117.23	122.61
43	V	101	BCR	C38-C26-C27	3.82	120.95	113.62
30	n	310	CHL	CMA-C3A-C4A	3.82	122.04	111.77
31	c	613	CLA	CAA-C2A-C3A	-3.82	102.32	112.78
31	s	306	CLA	C1-C2-C3	-3.82	120.58	126.75
32	n	317	LUT	C15-C14-C13	-3.82	121.86	127.31
34	G	621	LMG	O7-C10-C11	3.82	119.72	111.50
43	c	614	BCR	C30-C25-C26	-3.81	117.24	122.61
30	p	601	CHL	CHD-C1D-ND	-3.81	120.95	124.45
31	c	606	CLA	C1-C2-C3	-3.81	119.45	126.04
34	D	409	LMG	O7-C10-C11	3.81	119.71	111.50
34	g	322	LMG	O7-C10-C11	3.81	119.71	111.50
31	0	604	CLA	C1-C2-C3	-3.81	119.46	126.04
32	y	617	LUT	C21-C26-C27	-3.81	107.89	112.70
32	q	318	LUT	C18-C5-C6	-3.81	120.25	124.53
33	N	319	LHG	O7-C7-C8	3.81	119.70	111.50
31	G	612	CLA	C1-C2-C3	-3.81	119.46	126.04
30	7	306	CHL	CHD-C1D-ND	-3.81	120.96	124.45
30	9	303	CHL	C1-C2-C3	-3.80	119.46	126.04
34	x	202	LMG	O7-C10-C11	3.80	119.69	111.50
34	9	321	LMG	O7-C10-C11	3.80	119.69	111.50
32	7	318	LUT	C18-C5-C6	-3.80	120.26	124.53
31	B	605	CLA	C1-C2-C3	-3.80	119.47	126.04
32	y	617	LUT	C7-C8-C9	-3.80	120.50	126.23
32	p	616	LUT	C1-C6-C5	-3.80	117.27	122.61
31	0	602	CLA	C1-C2-C3	-3.80	119.48	126.04
31	R	312	CLA	CHD-C1D-ND	-3.80	120.97	124.45
35	q	317	RRX	C20-C19-C18	-3.79	115.76	126.42
31	R	316	CLA	CHD-C1D-ND	-3.79	120.97	124.45
30	3	309	CHL	C3C-C4C-NC	-3.79	106.32	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	318	LUT	C15-C14-C13	-3.79	121.90	127.31
31	c	604	CLA	C1-C2-C3	-3.79	119.48	126.04
43	v	101	BCR	C20-C21-C22	-3.79	121.90	127.31
34	0	622	LMG	O7-C10-C11	3.79	119.67	111.50
31	a	407	CLA	C1-C2-C3	-3.79	119.49	126.04
43	v	101	BCR	C1-C6-C5	-3.79	117.28	122.61
32	8	615	LUT	C15-C14-C13	-3.79	121.91	127.31
30	9	307	CHL	CHD-C1D-ND	-3.79	120.97	124.45
31	0	613	CLA	C1-C2-C3	-3.79	119.49	126.04
35	q	317	RRX	C27-C26-C25	-3.79	112.41	120.85
45	c	616	DGD	O2G-C1B-C2B	3.78	119.66	111.50
36	p	618	NEX	C27-C28-C29	-3.78	119.66	125.53
31	G	602	CLA	O2A-C1-C2	3.78	118.56	108.64
33	F1	301	LHG	O7-C7-C8	3.77	119.63	111.50
31	1	610	CLA	C1-C2-C3	-3.77	119.52	126.04
30	R	310	CHL	CHD-C1D-ND	-3.77	120.99	124.45
30	1	619	CHL	CHD-C1D-ND	-3.77	120.99	124.45
31	4	614	CLA	C1-C2-C3	-3.77	119.53	126.04
34	w	201	LMG	O7-C10-C11	3.77	119.62	111.50
36	N	318	NEX	C20-C13-C14	-3.76	117.65	122.92
30	q	310	CHL	CHD-C1D-ND	-3.76	121.00	124.45
31	y	611	CLA	O2A-C1-C2	3.76	118.53	108.64
31	y	614	CLA	C1-C2-C3	-3.76	119.53	126.04
31	Y	314	CLA	C1-C2-C3	-3.76	119.54	126.04
31	s	312	CLA	C1-C2-C3	-3.76	119.54	126.04
32	p	617	LUT	C7-C8-C9	-3.76	120.56	126.23
31	4	610	CLA	O2A-C1-C2	3.76	118.51	108.64
47	e	102	HEM	C1B-NB-C4B	3.76	108.95	105.07
31	b	609	CLA	C1-C2-C3	-3.76	119.55	126.04
31	S	305	CLA	C1-C2-C3	-3.75	119.55	126.04
33	l	101	LHG	O7-C7-C8	3.75	119.59	111.50
43	T	101	BCR	C27-C26-C25	-3.75	117.28	122.73
31	b	612	CLA	C1-C2-C3	-3.75	119.55	126.04
31	g	303	CLA	C2D-C1D-ND	3.75	112.87	110.10
34	2	620	LMG	O7-C10-C11	3.75	119.58	111.50
33	n	320	LHG	O7-C7-C8	3.75	119.58	111.50
33	8	618	LHG	O7-C7-C8	3.74	119.57	111.50
34	n	322	LMG	C8-O7-C10	-3.74	108.58	117.79
32	5	617	LUT	C7-C8-C9	-3.74	120.58	126.23
31	R	314	CLA	CHD-C1D-ND	-3.74	121.02	124.45
43	B	619	BCR	C27-C26-C25	-3.74	117.30	122.73
31	7	305	CLA	O2A-C1-C2	3.74	118.46	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	T	101	BCR	C16-C15-C14	-3.74	115.82	123.47
31	1	613	CLA	C1-C2-C3	-3.74	119.58	126.04
30	G	608	CHL	CMA-C3A-C4A	3.74	121.81	111.77
31	2	604	CLA	C1-C2-C3	-3.73	119.58	126.04
43	t	101	BCR	C7-C6-C5	-3.73	112.42	121.46
31	R	307	CLA	O2A-C1-C2	3.73	122.11	109.49
31	b	617	CLA	CHD-C1D-ND	-3.73	121.03	124.45
36	n	319	NEX	C2-C1-C6	3.73	112.84	109.21
38	G	624	SQD	O7-S-C6	-3.73	102.51	106.94
43	h	101	BCR	C4-C5-C6	-3.73	117.32	122.73
31	2	612	CLA	C1-C2-C3	-3.72	119.60	126.04
31	b	606	CLA	C1-C2-C3	-3.72	119.60	126.04
31	C	613	CLA	C1-O2A-CGA	3.72	126.21	116.44
44	A	416	PL9	C7-C3-C2	-3.72	118.41	123.30
43	z	101	BCR	C16-C17-C18	-3.72	122.00	127.31
31	r	311	CLA	C1-C2-C3	-3.72	119.61	126.04
33	q	320	LHG	O7-C7-C8	3.72	119.52	111.50
32	5	616	LUT	C15-C14-C13	-3.72	122.00	127.31
32	2	615	LUT	C35-C15-C14	-3.72	115.86	123.47
31	N	315	CLA	C1-C2-C3	-3.72	119.61	126.04
34	c	624	LMG	O7-C10-C11	3.72	119.51	111.50
32	s	318	LUT	C1-C6-C5	-3.72	117.38	122.61
32	p	617	LUT	C18-C5-C6	-3.72	120.36	124.53
35	g	315	RRX	C33-C5-C6	-3.71	120.36	124.53
34	a	401	LMG	O7-C10-C11	3.71	119.50	111.50
33	7	319	LHG	O7-C7-C8	3.71	119.50	111.50
43	d	406	BCR	C4-C5-C6	-3.71	117.35	122.73
43	V	101	BCR	C1-C6-C5	-3.70	117.39	122.61
31	c	610	CLA	C1-C2-C3	-3.70	119.64	126.04
43	b	620	BCR	C20-C21-C22	-3.70	122.02	127.31
33	y	619	LHG	O7-C7-C8	3.70	119.48	111.50
34	q1	101	LMG	O7-C10-C11	3.70	119.48	111.50
31	C	613	CLA	C1-C2-C3	-3.70	119.64	126.04
36	N	318	NEX	C12-C13-C14	3.70	124.61	118.94
30	r	309	CHL	C1-C2-C3	-3.70	119.65	126.04
31	r	316	CLA	O2A-C1-C2	3.70	118.35	108.64
30	S	302	CHL	CHD-C1D-ND	-3.69	121.06	124.45
43	C	614	BCR	C30-C25-C26	-3.69	117.41	122.61
30	S	308	CHL	CHD-C1D-ND	-3.69	121.06	124.45
31	7	314	CLA	C1-C2-C3	-3.69	119.67	126.04
32	S	317	LUT	C31-C30-C29	-3.69	122.05	127.31
31	c	607	CLA	O2A-C1-C2	3.68	118.32	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	628	LHG	O7-C7-C8	3.68	119.44	111.50
43	b	619	BCR	C38-C26-C25	-3.68	120.39	124.53
31	B	616	CLA	C1-C2-C3	-3.68	119.67	126.04
32	5	617	LUT	C31-C30-C29	-3.68	122.05	127.31
31	y	613	CLA	O2A-C1-C2	3.68	118.31	108.64
31	r	307	CLA	O2A-C1-C2	3.68	121.92	109.49
31	c	606	CLA	C2C-C1C-NC	3.68	113.42	109.97
32	3	318	LUT	C35-C34-C33	-3.67	122.07	127.31
32	Y	315	LUT	C15-C14-C13	-3.67	122.07	127.31
31	8	609	CLA	C1-C2-C3	-3.67	119.69	126.04
32	q	318	LUT	C31-C30-C29	-3.67	122.07	127.31
31	C	601	CLA	C1-C2-C3	-3.67	119.70	126.04
31	9	304	CLA	C1-C2-C3	-3.67	119.70	126.04
31	b	603	CLA	C1-C2-C3	-3.66	119.71	126.04
32	0	617	LUT	C18-C5-C6	-3.66	120.42	124.53
31	9	313	CLA	O2A-C1-C2	3.66	121.87	108.42
31	p	604	CLA	CHD-C1D-ND	-3.66	121.09	124.45
38	X	201	SQD	O7-S-C6	-3.66	102.59	106.94
34	a	413	LMG	O1-C7-C8	-3.66	102.08	110.90
30	1	601	CHL	C4D-CHA-C1A	3.65	125.70	121.25
43	b	618	BCR	C30-C25-C26	-3.65	117.47	122.61
31	A	406	CLA	C1-C2-C3	-3.65	119.72	126.04
32	7	318	LUT	C31-C30-C29	-3.65	122.10	127.31
42	D	401	PHO	CMB-C2B-C3B	3.65	131.51	124.68
32	r	317	LUT	C8-C7-C6	-3.65	116.95	127.20
32	0	617	LUT	C11-C10-C9	-3.65	122.10	127.31
31	5	602	CLA	C1-C2-C3	-3.65	119.73	126.04
44	D	406	PL9	C7-C3-C4	3.65	119.84	116.88
43	Z	101	BCR	C27-C26-C25	-3.65	117.44	122.73
31	b	616	CLA	C2C-C1C-NC	3.64	113.39	109.97
31	B	613	CLA	C1-C2-C3	-3.64	119.75	126.04
43	a	410	BCR	C4-C5-C6	-3.64	117.45	122.73
34	4	620	LMG	O7-C10-C11	3.64	119.34	111.50
31	r	314	CLA	CHD-C1D-ND	-3.63	121.11	124.45
33	Y	318	LHG	O7-C7-C8	3.63	119.33	111.50
43	C	615	BCR	C11-C12-C13	3.63	136.62	126.42
31	g	305	CLA	C1-C2-C3	-3.63	119.76	126.04
30	3	310	CHL	C1-O2A-CGA	3.63	125.97	116.44
34	D	410	LMG	O7-C10-C11	3.63	119.32	111.50
30	S	308	CHL	C3C-C4C-NC	-3.63	106.50	110.57
43	d	406	BCR	C16-C17-C18	-3.63	122.14	127.31
31	d	405	CLA	C1-C2-C3	-3.62	119.77	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	601	CHL	C3C-C4C-NC	-3.62	106.51	110.57
30	7	302	CHL	C4D-CHA-C1A	3.62	125.66	121.25
31	1	610	CLA	CHD-C1D-ND	-3.62	121.12	124.45
43	B	617	BCR	C20-C21-C22	-3.62	122.14	127.31
32	1	615	LUT	C35-C34-C33	-3.62	122.14	127.31
31	c	601	CLA	C1-C2-C3	-3.62	119.78	126.04
32	R	317	LUT	C40-C33-C34	-3.62	117.85	122.92
38	6	301	SQD	O7-S-C6	-3.62	102.64	106.94
31	n	316	CLA	C1-C2-C3	-3.62	119.79	126.04
30	1	605	CHL	C4D-CHA-C1A	3.62	125.65	121.25
31	C	609	CLA	C2C-C1C-NC	3.62	113.36	109.97
31	D	404	CLA	C1-C2-C3	-3.61	119.80	126.04
30	9	309	CHL	C1-O2A-CGA	3.61	125.92	116.44
32	3	317	LUT	C15-C14-C13	-3.61	122.16	127.31
31	g	303	CLA	CHD-C1D-ND	-3.61	121.14	124.45
34	9	301	LMG	C3-C4-C5	3.61	116.68	110.24
38	a	411	SQD	O7-S-C6	-3.61	102.65	106.94
43	C	614	BCR	C23-C24-C25	-3.61	117.08	127.20
31	R	305	CLA	CHD-C1D-ND	-3.61	121.14	124.45
30	3	302	CHL	C3C-C4C-NC	-3.60	106.53	110.57
38	s	301	SQD	O7-S-C6	-3.60	102.66	106.94
31	8	603	CLA	C1-C2-C3	-3.60	119.82	126.04
31	s	311	CLA	CHD-C1D-ND	-3.60	121.15	124.45
32	S	317	LUT	C15-C14-C13	-3.60	122.18	127.31
33	4	618	LHG	O7-C7-C8	3.60	119.25	111.50
31	q	306	CLA	C1-C2-C3	-3.60	119.83	126.04
30	8	608	CHL	C1-O2A-CGA	3.59	125.88	116.44
34	w	203	LMG	O8-C28-C29	3.59	123.18	111.91
43	C	615	BCR	C33-C5-C4	3.59	120.52	113.62
34	a	416	LMG	O7-C10-C11	3.59	119.24	111.50
47	e	102	HEM	CHA-C4D-ND	3.59	128.80	124.37
31	N	310	CLA	C1-C2-C3	-3.59	119.84	126.04
30	1	619	CHL	C3C-C4C-NC	-3.58	106.55	110.57
31	c	603	CLA	CHD-C1D-ND	-3.58	121.16	124.45
38	R	322	SQD	O7-S-C6	-3.58	102.69	106.94
38	r	322	SQD	O7-S-C6	-3.58	102.69	106.94
30	3	302	CHL	CHD-C1D-ND	-3.58	121.17	124.45
31	3	311	CLA	C1-C2-C3	-3.58	119.86	126.04
32	1	616	LUT	C18-C5-C6	-3.57	120.52	124.53
30	Y	309	CHL	CMA-C3A-C4A	3.57	121.37	111.77
36	6	319	NEX	C27-C28-C29	-3.57	119.99	125.53
31	p	604	CLA	C1-C2-C3	-3.57	120.98	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	a	410	BCR	C30-C25-C26	-3.57	117.59	122.61
43	B	617	BCR	C27-C26-C25	-3.57	117.55	122.73
38	G	617	SQD	O7-S-C6	-3.57	102.70	106.94
31	B	614	CLA	C1-C2-C3	-3.57	119.87	126.04
35	q	317	RRX	C30-C25-C26	-3.57	117.59	122.61
34	1	618	LMG	O7-C10-C11	3.57	119.19	111.50
43	b	618	BCR	C24-C23-C22	-3.57	120.85	126.23
36	0	618	NEX	C27-C28-C29	-3.57	120.00	125.53
31	p	603	CLA	CHD-C1D-ND	-3.57	121.18	124.45
32	9	318	LUT	C1-C6-C5	-3.56	117.59	122.61
38	A	411	SQD	O7-S-C6	-3.56	102.70	106.94
47	E	101	HEM	C1B-NB-C4B	3.56	108.75	105.07
31	q	315	CLA	O2A-C1-C2	3.56	117.99	108.64
31	S	304	CLA	CAA-C2A-C3A	-3.56	105.37	114.26
43	B	617	BCR	C24-C23-C22	-3.56	120.86	126.23
31	5	615	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
31	4	612	CLA	C2D-C1D-ND	3.55	112.72	110.10
34	A	418	LMG	O7-C10-C11	3.55	119.16	111.50
31	p	602	CLA	C1-C2-C3	-3.55	119.90	126.04
30	Y	302	CHL	C3C-C4C-NC	-3.55	106.59	110.57
32	1	615	LUT	C8-C7-C6	-3.55	117.24	127.20
30	s	307	CHL	C4D-CHA-C1A	3.55	125.57	121.25
38	g	301	SQD	O7-S-C6	-3.55	102.72	106.94
31	6	314	CLA	C1-C2-C3	-3.54	119.91	126.04
30	n	302	CHL	C3C-C4C-NC	-3.54	106.60	110.57
31	0	603	CLA	CHD-C1D-ND	-3.54	121.20	124.45
35	G	614	RRX	C7-C8-C9	-3.54	120.89	126.23
38	m	101	SQD	O7-S-C6	-3.54	102.73	106.94
31	p	615	CLA	CHD-C1D-ND	-3.54	121.20	124.45
38	M	102	SQD	O7-S-C6	-3.54	102.74	106.94
30	8	601	CHL	C3C-C4C-NC	-3.53	106.61	110.57
30	G	608	CHL	C3C-C4C-NC	-3.53	106.61	110.57
30	9	309	CHL	C4D-CHA-C1A	3.53	125.55	121.25
30	2	608	CHL	CMA-C3A-C4A	3.53	121.26	111.77
30	y	609	CHL	CMA-C3A-C4A	3.53	121.26	111.77
30	8	608	CHL	CMA-C3A-C4A	3.53	121.26	111.77
30	S	307	CHL	C4D-CHA-C1A	3.53	125.54	121.25
43	A	410	BCR	C30-C25-C26	-3.53	117.65	122.61
31	r	306	CLA	CHD-C1D-ND	-3.52	121.22	124.45
31	R	304	CLA	CHD-C1D-ND	-3.52	121.22	124.45
30	g	309	CHL	C3C-C4C-NC	-3.52	106.62	110.57
31	S	311	CLA	CHD-C1D-ND	-3.52	121.22	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	b	620	BCR	C27-C26-C25	-3.52	117.62	122.73
32	Y	315	LUT	C7-C8-C9	-3.52	120.92	126.23
32	Y	316	LUT	C21-C26-C27	-3.52	108.25	112.70
38	B	620	SQD	O7-S-C6	-3.52	102.76	106.94
31	s	315	CLA	O2A-C1-C2	3.52	121.38	109.49
30	4	601	CHL	C1-C2-C3	-3.51	119.97	126.04
31	R	305	CLA	CBC-CAC-C3C	-3.51	102.74	112.43
38	y	621	SQD	O7-S-C6	-3.51	102.76	106.94
30	7	307	CHL	C1-C2-C3	-3.51	119.97	126.04
30	R	310	CHL	C3C-C4C-NC	-3.51	106.63	110.57
30	g	309	CHL	CMA-C3A-C4A	3.51	121.21	111.77
43	B	619	BCR	C7-C8-C9	-3.51	120.93	126.23
31	b	617	CLA	C1-C2-C3	-3.51	119.97	126.04
32	N	317	LUT	C18-C5-C4	3.51	120.86	114.36
31	B	601	CLA	CHD-C1D-ND	-3.51	121.23	124.45
35	4	615	RRX	C7-C8-C9	-3.51	120.93	126.23
30	N	309	CHL	C3C-C4C-NC	-3.51	106.64	110.57
35	9	317	RRX	C7-C8-C9	-3.51	120.93	126.23
31	3	306	CLA	C1-C2-C3	-3.51	119.97	126.04
37	R	318	XAT	C7-C8-C9	-3.51	120.09	125.53
31	r	307	CLA	C2C-C1C-NC	3.51	113.26	109.97
30	N	307	CHL	C3B-C4B-NB	-3.51	107.26	110.52
32	6	318	LUT	C18-C5-C6	-3.51	120.59	124.53
30	3	310	CHL	CMA-C3A-C4A	3.51	121.20	111.77
36	3	319	NEX	C16-C1-C6	-3.51	107.33	110.47
31	d	401	CLA	CHD-C1D-ND	-3.51	121.23	124.45
43	b	618	BCR	C23-C24-C25	-3.51	117.36	127.20
31	B	610	CLA	C1-C2-C3	-3.50	119.98	126.04
31	Y	312	CLA	C1-C2-C3	-3.50	119.98	126.04
31	b	607	CLA	CHD-C1D-ND	-3.50	121.23	124.45
31	S	303	CLA	C1-C2-C3	-3.50	119.98	126.04
31	7	316	CLA	C1-C2-C3	-3.50	119.98	126.04
31	c	611	CLA	C1-C2-C3	-3.50	119.99	126.04
34	C	624	LMG	O7-C10-C11	3.50	119.03	111.50
35	2	614	RRX	C30-C25-C26	-3.49	117.69	122.61
30	5	609	CHL	CMA-C3A-C4A	3.49	121.16	111.77
31	c	610	CLA	CHD-C1D-ND	-3.49	121.24	124.45
30	n	310	CHL	C3C-C4C-NC	-3.49	106.66	110.57
43	b	620	BCR	C38-C26-C25	-3.49	120.61	124.53
43	T	101	BCR	C4-C5-C6	-3.49	117.66	122.73
38	b	621	SQD	O7-S-C6	-3.49	102.79	106.94
31	c	604	CLA	CHD-C1D-ND	-3.49	121.25	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	307	CLA	C2C-C1C-NC	3.49	113.24	109.97
43	D	405	BCR	C38-C26-C27	3.49	120.31	113.62
32	y	616	LUT	C8-C7-C6	-3.48	117.42	127.20
30	N	309	CHL	CMA-C3A-C4A	3.48	121.14	111.77
31	b	610	CLA	C1-C2-C3	-3.48	120.02	126.04
31	p	613	CLA	C1-O2A-CGA	3.48	125.58	116.44
30	7	309	CHL	C3C-C4C-NC	-3.48	106.67	110.57
32	n	318	LUT	C18-C5-C6	-3.48	120.62	124.53
38	B	623	SQD	O7-S-C6	-3.48	102.80	106.94
31	A	409	CLA	C1-C2-C3	-3.48	120.02	126.04
31	p	614	CLA	CHD-C1D-ND	-3.48	121.26	124.45
30	y	605	CHL	C3C-C4C-NC	-3.48	106.67	110.57
43	z	101	BCR	C27-C26-C25	-3.48	117.68	122.73
32	g	316	LUT	C18-C5-C6	-3.48	120.62	124.53
43	t	101	BCR	C2-C1-C6	3.48	115.83	110.48
32	S	318	LUT	C18-C5-C4	3.48	120.80	114.36
38	S	301	SQD	O7-S-C6	-3.47	102.81	106.94
31	N	310	CLA	CHD-C1D-ND	-3.47	121.26	124.45
30	0	609	CHL	CMA-C3A-C4A	3.47	121.10	111.77
30	5	601	CHL	C1-C2-C3	-3.47	121.14	126.75
47	e	102	HEM	CHB-C1B-NB	3.47	128.65	124.37
32	y	616	LUT	C30-C31-C32	-3.47	112.39	123.22
32	6	317	LUT	C21-C26-C27	-3.47	108.32	112.70
32	3	317	LUT	C11-C10-C9	-3.47	122.36	127.31
31	q	305	CLA	C1-C2-C3	-3.47	120.05	126.04
42	A	408	PHO	C2B-C1B-NB	-3.47	107.13	109.53
38	g	318	SQD	O7-S-C6	-3.47	102.82	106.94
43	T	101	BCR	C20-C19-C18	-3.47	116.68	126.42
38	Y	320	SQD	O7-S-C6	-3.46	102.82	106.94
31	a	409	CLA	C1-C2-C3	-3.46	120.05	126.04
31	S	315	CLA	O2A-C1-C2	3.46	121.20	109.49
30	4	607	CHL	C3C-C4C-NC	-3.46	106.69	110.57
32	Y	315	LUT	C8-C7-C6	-3.46	117.48	127.20
31	C	610	CLA	CHD-C1D-ND	-3.46	121.27	124.45
31	2	613	CLA	C1-C2-C3	-3.46	120.06	126.04
45	c	617	DGD	C1E-O6E-C5E	3.46	120.48	113.69
32	8	616	LUT	C18-C5-C6	-3.46	120.64	124.53
30	6	309	CHL	C3C-C4C-NC	-3.46	106.69	110.57
30	s	302	CHL	CHD-C1D-ND	-3.46	121.28	124.45
44	a	414	PL9	C7-C3-C2	-3.46	118.75	123.30
43	B	618	BCR	C8-C7-C6	-3.46	117.49	127.20
31	9	312	CLA	C1-C2-C3	-3.46	120.06	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	604	CLA	C2C-C1C-NC	3.46	113.21	109.97
31	q	312	CLA	C2D-C1D-ND	3.46	112.65	110.10
32	1	615	LUT	C7-C8-C9	-3.45	121.02	126.23
31	8	614	CLA	C1-C2-C3	-3.45	120.07	126.04
31	b	613	CLA	C2D-C1D-ND	3.45	112.65	110.10
31	s	306	CLA	C2D-C1D-ND	3.45	112.65	110.10
34	N	320	LMG	O7-C10-C11	3.45	118.94	111.50
32	N	317	LUT	C31-C30-C29	-3.45	122.38	127.31
32	1	615	LUT	C11-C10-C9	-3.45	122.39	127.31
31	S	315	CLA	CHD-C1D-ND	-3.45	121.28	124.45
43	a	410	BCR	C27-C26-C25	-3.45	117.72	122.73
30	7	306	CHL	CMA-C3A-C4A	3.45	121.04	111.77
30	Y	309	CHL	C4D-CHA-C1A	3.45	125.44	121.25
43	v	101	BCR	C24-C23-C22	-3.45	121.03	126.23
36	G	616	NEX	C2-C1-C6	3.44	112.56	109.21
31	0	615	CLA	C1-C2-C3	-3.44	120.09	126.04
47	E	101	HEM	CHA-C4D-ND	3.44	128.62	124.37
31	6	303	CLA	C1-C2-C3	-3.44	120.09	126.04
30	7	321	CHL	C1-C2-C3	-3.44	120.09	126.04
31	y	613	CLA	C1-C2-C3	-3.44	120.10	126.04
32	8	616	LUT	C1-C6-C5	-3.44	117.77	122.61
30	4	607	CHL	C3B-C4B-NB	-3.44	107.33	110.52
30	r	310	CHL	C3C-C4C-NC	-3.44	106.72	110.57
32	S	318	LUT	C15-C14-C13	-3.44	122.41	127.31
32	5	617	LUT	C1-C6-C5	-3.44	117.78	122.61
32	s	317	LUT	C15-C14-C13	-3.43	122.41	127.31
30	R	310	CHL	C3B-C4B-NB	-3.43	107.33	110.52
31	C	612	CLA	C2C-C1C-NC	3.43	113.19	109.97
32	3	317	LUT	C7-C8-C9	-3.43	121.05	126.23
32	n	318	LUT	C1-C6-C5	-3.43	117.78	122.61
31	3	314	CLA	C1-C2-C3	-3.43	120.11	126.04
31	s	313	CLA	C2C-C1C-NC	3.43	113.18	109.97
30	R	308	CHL	C4D-CHA-C1A	3.42	125.42	121.25
36	y	618	NEX	C17-C1-C6	-3.42	107.41	110.47
31	6	315	CLA	CHD-C1D-ND	-3.42	121.31	124.45
30	1	609	CHL	CMA-C3A-C4A	3.42	120.97	111.77
31	r	303	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
31	C	604	CLA	CHD-C1D-ND	-3.42	121.31	124.45
34	3	321	LMG	O7-C10-C11	3.42	118.87	111.50
30	S	308	CHL	C2B-C1B-NB	-3.42	107.94	110.23
30	n	308	CHL	C1-C2-C3	-3.42	120.13	126.04
31	r	312	CLA	CHD-C1D-ND	-3.42	121.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	R	308	CHL	C1-C2-C3	-3.42	120.13	126.04
31	c	612	CLA	C2C-C1C-NC	3.42	113.17	109.97
30	7	309	CHL	C2C-C3C-C4C	3.42	108.92	106.49
32	R	317	LUT	C7-C8-C9	-3.41	121.08	126.23
30	Y	301	CHL	C3C-C4C-NC	-3.41	106.74	110.57
31	s	313	CLA	CHD-C1D-ND	-3.41	121.32	124.45
38	A	413	SQD	O7-S-C6	-3.41	102.89	106.94
31	n	311	CLA	C1-C2-C3	-3.41	120.15	126.04
32	0	617	LUT	C21-C26-C27	-3.41	108.39	112.70
43	D	405	BCR	C38-C26-C25	-3.41	120.70	124.53
31	2	603	CLA	C1-C2-C3	-3.40	120.15	126.04
30	3	303	CHL	C4D-CHA-C1A	3.40	125.39	121.25
30	4	608	CHL	C3C-C4C-NC	-3.40	106.75	110.57
42	a	408	PHO	C2B-C1B-NB	-3.40	107.18	109.53
31	7	304	CLA	C1-C2-C3	-3.40	120.17	126.04
30	3	302	CHL	CMA-C3A-C4A	3.40	120.91	111.77
30	y	609	CHL	C4D-CHA-C1A	3.40	125.38	121.25
30	G	607	CHL	C1-C2-C3	-3.40	121.26	126.75
43	c	614	BCR	C21-C20-C19	3.40	133.81	123.22
31	A	406	CLA	CHD-C1D-ND	-3.39	121.34	124.45
31	A	407	CLA	CHD-C1D-ND	-3.39	121.34	124.45
31	B	609	CLA	C1-C2-C3	-3.39	120.18	126.04
31	R	316	CLA	C1-C2-C3	-3.39	120.18	126.04
31	B	616	CLA	CHD-C1D-ND	-3.39	121.34	124.45
30	9	309	CHL	CMA-C3A-C4A	3.39	120.88	111.77
42	d	402	PHO	C2B-C1B-NB	-3.39	107.19	109.53
30	0	608	CHL	C3C-C4C-NC	-3.39	106.77	110.57
31	s	310	CLA	C1-C2-C3	-3.39	120.19	126.04
32	s	317	LUT	C7-C8-C9	-3.38	121.12	126.23
31	r	315	CLA	CHD-C1D-ND	-3.38	121.34	124.45
32	Y	315	LUT	C10-C11-C12	-3.38	112.66	123.22
31	A	406	CLA	C2C-C1C-NC	3.38	113.14	109.97
31	4	613	CLA	C1-C2-C3	-3.38	120.19	126.04
30	Y	306	CHL	C3C-C4C-NC	-3.38	106.78	110.57
31	G	609	CLA	CHD-C1D-ND	-3.38	121.35	124.45
31	B	616	CLA	C2C-C1C-NC	3.38	113.14	109.97
30	r	310	CHL	C3B-C4B-NB	-3.38	107.38	110.52
37	9	322	XAT	C6-C7-C8	-3.38	118.85	125.99
37	q	321	XAT	C6-C7-C8	-3.38	118.85	125.99
43	V	101	BCR	C4-C5-C6	-3.38	117.83	122.73
31	Y	310	CLA	C1-C2-C3	-3.38	120.20	126.04
31	q	315	CLA	C2C-C1C-NC	3.38	113.14	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	H	101	BCR	C2-C1-C6	3.37	115.68	110.48
31	R	311	CLA	CHD-C1D-ND	-3.37	121.35	124.45
37	4	619	XAT	C6-C7-C8	-3.37	118.86	125.99
31	y	610	CLA	CHD-C1D-ND	-3.37	121.36	124.45
31	S	313	CLA	C2C-C1C-NC	3.37	113.13	109.97
33	B	624	LHG	O7-C7-C8	3.37	118.77	111.50
43	D	405	BCR	C30-C25-C26	-3.37	117.87	122.61
31	b	605	CLA	C2C-C1C-NC	3.37	113.13	109.97
43	c	615	BCR	C20-C19-C18	-3.37	116.95	126.42
31	5	610	CLA	C1-C2-C3	-3.37	120.22	126.04
38	x	201	SQD	O7-S-C6	-3.37	102.94	106.94
32	6	318	LUT	C31-C30-C29	-3.37	122.50	127.31
31	S	306	CLA	C2D-C1D-ND	3.37	112.59	110.10
31	b	602	CLA	CHD-C1D-ND	-3.37	121.36	124.45
37	2	619	XAT	C6-C7-C8	-3.37	118.87	125.99
31	s	310	CLA	C2C-C1C-NC	3.37	113.13	109.97
37	g	321	XAT	C6-C7-C8	-3.37	118.88	125.99
38	a	412	SQD	O7-S-C6	-3.37	102.94	106.94
43	A	410	BCR	C20-C19-C18	-3.36	116.96	126.42
37	G	620	XAT	C6-C7-C8	-3.36	118.88	125.99
31	b	611	CLA	C1-C2-C3	-3.36	120.22	126.04
31	c	602	CLA	C2C-C1C-NC	3.36	113.12	109.97
31	n	304	CLA	C1-C2-C3	-3.36	120.23	126.04
44	d	407	PL9	C7-C3-C4	3.36	119.61	116.88
35	9	317	RRX	C30-C25-C26	-3.36	117.88	122.61
31	9	304	CLA	C2D-C1D-ND	3.36	112.58	110.10
31	C	609	CLA	CHD-C1D-ND	-3.36	121.37	124.45
30	q	308	CHL	C1-C2-C3	-3.36	121.32	126.75
34	9	301	LMG	O8-C28-C29	3.36	122.45	111.91
32	n	318	LUT	C11-C10-C9	-3.36	122.52	127.31
43	D	405	BCR	C27-C26-C25	-3.36	117.86	122.73
47	E	101	HEM	CHB-C1B-NB	3.36	128.51	124.37
33	e	101	LHG	O8-C23-C24	3.36	122.44	111.91
31	S	312	CLA	C1-O2A-CGA	3.36	125.25	116.44
32	5	616	LUT	C11-C10-C9	-3.36	122.52	127.31
30	G	623	CHL	C3C-C4C-NC	-3.36	106.81	110.57
35	G	614	RRX	C30-C25-C26	-3.35	117.89	122.61
31	8	609	CLA	CHD-C1D-ND	-3.35	121.37	124.45
31	r	316	CLA	C2C-C1C-NC	3.35	113.11	109.97
30	S	309	CHL	C3C-C4C-NC	-3.35	106.81	110.57
31	R	306	CLA	C2C-C1C-NC	3.35	113.11	109.97
43	v	101	BCR	C15-C14-C13	-3.35	122.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	603	CLA	CHD-C1D-ND	-3.35	121.38	124.45
30	N	308	CHL	CMA-C3A-C4A	3.35	120.78	111.77
43	D	405	BCR	C10-C11-C12	-3.35	112.77	123.22
30	3	309	CHL	C2C-C3C-C4C	3.35	108.88	106.49
30	0	607	CHL	C4D-CHA-C1A	3.35	125.32	121.25
30	2	601	CHL	C3C-C4C-NC	-3.35	106.82	110.57
32	G	615	LUT	C7-C8-C9	-3.35	121.18	126.23
30	7	307	CHL	C4D-CHA-C1A	3.35	125.32	121.25
31	D	404	CLA	C2D-C1D-ND	3.34	112.57	110.10
31	3	311	CLA	C2C-C1C-NC	3.34	113.11	109.97
31	9	304	CLA	CHD-C1D-ND	-3.34	121.38	124.45
32	s	317	LUT	C31-C30-C29	-3.34	122.54	127.31
31	g	304	CLA	C1-C2-C3	-3.34	120.26	126.04
31	3	316	CLA	CHD-C1D-ND	-3.34	121.38	124.45
31	s	303	CLA	CHD-C1D-ND	-3.34	121.38	124.45
31	N	304	CLA	C1-C2-C3	-3.34	120.27	126.04
30	n	307	CHL	C3B-C4B-NB	-3.34	107.42	110.52
35	4	615	RRX	C30-C25-C26	-3.34	117.91	122.61
36	p	618	NEX	C38-C25-C26	-3.34	116.67	122.26
30	5	607	CHL	C1-C2-C3	-3.34	121.35	126.75
30	8	608	CHL	C3C-C4C-NC	-3.34	106.83	110.57
32	8	616	LUT	C11-C10-C9	-3.33	122.55	127.31
31	6	311	CLA	CHD-C1D-ND	-3.33	121.39	124.45
32	s	318	LUT	C8-C7-C6	-3.33	117.84	127.20
30	N	302	CHL	C4D-CHA-C1A	3.33	125.31	121.25
31	n	311	CLA	CHD-C1D-ND	-3.33	121.39	124.45
31	s	315	CLA	CHD-C1D-ND	-3.33	121.39	124.45
32	3	317	LUT	C31-C30-C29	-3.33	122.56	127.31
42	d	402	PHO	C4D-CHA-CBD	-3.33	107.01	108.52
30	n	301	CHL	C4D-CHA-C1A	3.33	125.30	121.25
31	7	311	CLA	CHD-C1D-ND	-3.33	121.39	124.45
30	8	606	CHL	C3B-C4B-NB	-3.33	107.43	110.52
31	r	303	CLA	C2D-C1D-ND	3.33	112.56	110.10
36	G	616	NEX	C17-C1-C6	-3.33	107.49	110.47
30	p	607	CHL	C1-C2-C3	-3.33	121.37	126.75
30	q	309	CHL	CMA-C3A-C4A	3.33	120.71	111.77
30	7	308	CHL	C3C-C4C-NC	-3.32	106.84	110.57
32	0	616	LUT	C8-C7-C6	-3.32	117.87	127.20
31	R	315	CLA	C1-C2-C3	-3.32	120.30	126.04
32	S	318	LUT	C11-C10-C9	-3.32	122.57	127.31
32	y	617	LUT	C31-C30-C29	-3.32	122.57	127.31
43	h	101	BCR	C38-C26-C25	-3.32	120.80	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	310	CHL	C1-O2A-CGA	3.32	125.16	116.44
30	1	619	CHL	C2C-C3C-C4C	3.32	108.86	106.49
31	2	604	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	q	306	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	c	609	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	1	603	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	q	312	CLA	C1-C2-C3	-3.32	120.30	126.04
30	7	321	CHL	C3C-C4C-NC	-3.32	106.85	110.57
31	3	306	CLA	CHD-C1D-ND	-3.32	121.41	124.45
30	p	609	CHL	CMA-C3A-C4A	3.32	120.69	111.77
30	N	307	CHL	C3C-C4C-NC	-3.32	106.85	110.57
31	6	303	CLA	CHD-C1D-ND	-3.32	121.41	124.45
30	R	309	CHL	C1-C2-C3	-3.31	120.31	126.04
43	B	619	BCR	C33-C5-C4	3.31	119.98	113.62
31	R	316	CLA	C2C-C1C-NC	3.31	113.08	109.97
31	b	614	CLA	C1-C2-C3	-3.31	120.31	126.04
31	6	316	CLA	C2C-C1C-NC	3.31	113.07	109.97
30	N	308	CHL	C3C-C4C-NC	-3.31	106.86	110.57
31	0	604	CLA	CHD-C1D-ND	-3.31	121.41	124.45
31	1	604	CLA	C1-C2-C3	-3.31	120.32	126.04
30	q	308	CHL	CMA-C3A-C4A	3.31	120.66	111.77
30	7	310	CHL	C4D-CHA-C1A	3.31	125.27	121.25
30	5	607	CHL	C3C-C4C-NC	-3.30	106.86	110.57
31	1	604	CLA	CHD-C1D-ND	-3.30	121.42	124.45
30	N	302	CHL	C3C-C4C-NC	-3.30	106.87	110.57
30	g	302	CHL	C3C-C4C-NC	-3.30	106.87	110.57
31	b	608	CLA	C1-C2-C3	-3.30	120.33	126.04
30	y	608	CHL	C3C-C4C-NC	-3.30	106.87	110.57
30	q	310	CHL	C3C-C4C-NC	-3.30	106.87	110.57
31	B	615	CLA	CHD-C1D-ND	-3.30	121.42	124.45
30	n	308	CHL	C3C-C4C-NC	-3.30	106.87	110.57
30	9	309	CHL	C4B-CHC-C1C	3.30	134.16	126.34
31	B	604	CLA	CMA-C3A-C4A	3.30	120.64	111.77
31	1	603	CLA	CHD-C1D-ND	-3.30	121.42	124.45
43	b	618	BCR	C20-C21-C22	-3.30	122.61	127.31
31	3	313	CLA	C2C-C1C-NC	3.30	113.06	109.97
30	2	607	CHL	C3C-C4C-NC	-3.29	106.88	110.57
30	1	608	CHL	CMA-C3A-C4A	3.29	120.62	111.77
30	N	306	CHL	C1-O2A-CGA	3.29	125.08	116.44
31	n	315	CLA	C2D-C1D-ND	3.29	112.53	110.10
31	Y	310	CLA	CHD-C1D-ND	-3.29	121.43	124.45
43	D	405	BCR	C12-C13-C14	3.29	123.99	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	307	CHL	CMA-C3A-C4A	3.29	120.62	111.77
31	s	306	CLA	C1D-ND-C4D	-3.29	104.00	106.33
36	r	319	NEX	C17-C1-C6	-3.29	107.53	110.47
31	S	316	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	y	610	CLA	C1-C2-C3	-3.29	120.35	126.04
31	9	315	CLA	C2C-C1C-NC	3.29	113.05	109.97
32	s	318	LUT	C18-C5-C4	3.29	120.45	114.36
30	q	307	CHL	C4D-CHA-C1A	3.29	125.25	121.25
31	p	611	CLA	C1-C2-C3	-3.29	120.36	126.04
31	3	305	CLA	C1-C2-C3	-3.29	120.36	126.04
31	c	601	CLA	CHD-C1D-ND	-3.29	121.43	124.45
32	Y	316	LUT	C1-C6-C5	-3.29	117.98	122.61
31	5	602	CLA	CHD-C1D-ND	-3.29	121.43	124.45
43	Z	101	BCR	C4-C5-C6	-3.29	117.96	122.73
43	B	618	BCR	C30-C25-C26	-3.29	117.98	122.61
37	R	318	XAT	C38-C25-C26	-3.29	116.75	122.26
30	N	306	CHL	C1-C2-C3	-3.28	120.36	126.04
31	B	607	CLA	C2C-C1C-NC	3.28	113.05	109.97
30	r	308	CHL	C3B-C4B-NB	-3.28	107.47	110.52
31	4	614	CLA	CHD-C1D-ND	-3.28	121.44	124.45
43	T	101	BCR	C23-C24-C25	-3.28	117.99	127.20
30	7	321	CHL	C4D-CHA-C1A	3.28	125.24	121.25
30	1	605	CHL	CMA-C3A-C4A	3.28	120.59	111.77
30	1	607	CHL	C3C-C4C-NC	-3.28	106.89	110.57
30	0	606	CHL	C1-C2-C3	-3.28	121.45	126.75
30	9	308	CHL	C4D-CHA-C1A	3.28	125.24	121.25
31	N	314	CLA	C2D-C1D-ND	3.28	112.52	110.10
31	5	603	CLA	C6-C5-C3	-3.28	109.26	114.62
30	y	608	CHL	C4D-CHA-C1A	3.28	125.24	121.25
31	2	602	CLA	C2D-C1D-ND	3.28	112.52	110.10
31	R	305	CLA	C2C-C1C-NC	3.27	113.04	109.97
30	S	308	CHL	C3B-C4B-NB	-3.27	107.48	110.52
31	q	304	CLA	C1-C2-C3	-3.27	120.38	126.04
32	r	317	LUT	C31-C30-C29	-3.27	122.64	127.31
30	0	601	CHL	C4D-CHA-C1A	3.27	125.23	121.25
30	7	306	CHL	C1-C2-C3	-3.27	120.39	126.04
31	c	609	CLA	CHD-C1D-ND	-3.27	121.45	124.45
30	8	605	CHL	C3C-C4C-NC	-3.27	106.91	110.57
30	5	601	CHL	C4D-CHA-C1A	3.27	125.23	121.25
31	G	603	CLA	C1-C2-C3	-3.27	120.39	126.04
30	y	601	CHL	C3C-C4C-NC	-3.27	106.91	110.57
43	c	615	BCR	C8-C7-C6	-3.27	118.03	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	303	CLA	CHD-C1D-ND	-3.27	121.45	124.45
31	b	616	CLA	CHD-C1D-ND	-3.27	121.45	124.45
31	C	605	CLA	C2C-C1C-NC	3.27	113.03	109.97
32	3	317	LUT	C21-C26-C27	-3.27	108.57	112.70
31	2	602	CLA	C1-C2-C3	-3.27	120.39	126.04
30	q	309	CHL	CHD-C1D-ND	-3.27	121.45	124.45
30	n	306	CHL	C3C-C4C-NC	-3.27	106.91	110.57
31	N	303	CLA	CHD-C1D-ND	-3.26	121.45	124.45
30	6	310	CHL	C3C-C4C-NC	-3.26	106.91	110.57
30	p	607	CHL	C3C-C4C-NC	-3.26	106.91	110.57
30	g	307	CHL	C3B-C4B-NB	-3.26	107.49	110.52
31	5	615	CLA	CHD-C1D-ND	-3.26	121.46	124.45
31	Y	313	CLA	C2C-C1C-NC	3.26	113.03	109.97
31	G	602	CLA	CHD-C1D-ND	-3.26	121.46	124.45
31	5	610	CLA	CHD-C1D-ND	-3.26	121.46	124.45
30	7	308	CHL	C2C-C3C-C4C	3.26	108.81	106.49
30	g	306	CHL	C4D-CHA-C1A	3.26	125.21	121.25
31	S	310	CLA	CHD-C1D-ND	-3.26	121.46	124.45
30	8	607	CHL	C3C-C4C-NC	-3.26	106.92	110.57
32	6	317	LUT	C7-C8-C9	-3.26	121.31	126.23
31	q	312	CLA	C1D-ND-C4D	-3.26	104.02	106.33
30	6	306	CHL	C4D-CHA-C1A	3.26	125.21	121.25
30	S	302	CHL	C3C-C4C-NC	-3.26	106.92	110.57
30	n	310	CHL	C4D-CHA-C1A	3.25	125.21	121.25
31	C	607	CLA	CHD-C1D-ND	-3.25	121.46	124.45
31	7	305	CLA	C1-C2-C3	-3.25	120.41	126.04
31	b	605	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
43	h	101	BCR	C38-C26-C27	3.25	119.86	113.62
31	R	305	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
30	5	606	CHL	C4D-CHA-C1A	3.25	125.21	121.25
30	6	309	CHL	CMA-C3A-C4A	3.25	120.51	111.77
31	R	306	CLA	CHD-C1D-ND	-3.25	121.47	124.45
30	n	308	CHL	C4D-CHA-C1A	3.25	125.20	121.25
43	D	405	BCR	C2-C1-C6	3.25	115.48	110.48
30	8	608	CHL	C4D-CHA-C1A	3.25	125.20	121.25
31	G	603	CLA	CHD-C1D-ND	-3.25	121.47	124.45
30	0	605	CHL	C3B-C4B-NB	-3.25	107.50	110.52
30	g	307	CHL	C3C-C4C-NC	-3.25	106.93	110.57
43	b	618	BCR	C16-C15-C14	-3.25	116.82	123.47
31	1	613	CLA	C2C-C1C-NC	3.25	113.01	109.97
31	p	613	CLA	C2C-C1C-NC	3.25	113.01	109.97
30	1	609	CHL	C1-C2-C3	-3.25	120.43	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	608	CHL	C3C-C4C-NC	-3.25	106.93	110.57
35	q	317	RRX	C8-C7-C6	-3.25	118.09	127.20
31	r	311	CLA	CHD-C1D-ND	-3.24	121.47	124.45
31	p	610	CLA	CHD-C1D-ND	-3.24	121.47	124.45
30	3	302	CHL	C3B-C4B-NB	-3.24	107.51	110.52
32	2	615	LUT	C7-C8-C9	-3.24	121.33	126.23
34	9	301	LMG	O7-C10-C11	3.24	118.49	111.50
43	B	617	BCR	C16-C15-C14	-3.24	116.83	123.47
31	S	310	CLA	C2C-C1C-NC	3.24	113.01	109.97
43	C	615	BCR	C19-C18-C17	3.24	123.92	118.94
32	7	317	LUT	C18-C5-C6	-3.24	120.89	124.53
31	B	602	CLA	C1-C2-C3	-3.24	120.44	126.04
31	g	305	CLA	C2C-C1C-NC	3.24	113.01	109.97
31	y	613	CLA	C2C-C1C-NC	3.24	113.01	109.97
31	C	606	CLA	CHD-C1D-ND	-3.24	121.47	124.45
31	9	305	CLA	C1-C2-C3	-3.24	120.44	126.04
30	3	310	CHL	C3C-C4C-NC	-3.24	106.94	110.57
30	4	609	CHL	C3C-C4C-NC	-3.24	106.94	110.57
30	Y	307	CHL	C4D-CHA-C1A	3.24	125.19	121.25
30	1	601	CHL	C4B-CHC-C1C	3.24	134.02	126.34
30	0	609	CHL	C3C-C4C-NC	-3.24	106.94	110.57
35	9	317	RRX	C33-C5-C4	3.24	119.84	113.62
30	Y	301	CHL	CMA-C3A-C4A	3.24	120.47	111.77
31	R	303	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
31	C	610	CLA	C1-C2-C3	-3.24	120.45	126.04
43	z	101	BCR	C38-C26-C25	-3.24	120.89	124.53
35	4	615	RRX	C33-C5-C4	3.24	119.83	113.62
31	q	313	CLA	C2D-C1D-ND	3.23	112.49	110.10
30	y	607	CHL	C3C-C4C-NC	-3.23	106.94	110.57
31	G	610	CLA	C2C-C1C-NC	3.23	113.00	109.97
31	s	314	CLA	C2C-C1C-NC	3.23	113.00	109.97
31	p	612	CLA	C2D-C1D-ND	3.23	112.49	110.10
31	r	304	CLA	C2D-C1D-ND	3.23	112.49	110.10
30	0	605	CHL	C1-C2-C3	-3.23	120.45	126.04
36	n	319	NEX	C31-C30-C29	3.23	131.92	127.31
31	g	304	CLA	CHD-C1D-ND	-3.23	121.48	124.45
36	S	319	NEX	C17-C1-C6	-3.23	107.58	110.47
43	D	405	BCR	C35-C13-C14	-3.23	118.40	122.92
30	s	308	CHL	C3C-C4C-NC	-3.23	106.95	110.57
30	y	601	CHL	C1-C2-C3	-3.23	120.47	126.04
31	y	603	CLA	C1-C2-C3	-3.23	120.47	126.04
30	0	608	CHL	C4D-CHA-C1A	3.23	125.17	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	607	CLA	C1-C2-C3	-3.22	120.47	126.04
31	s	303	CLA	C1-C2-C3	-3.22	120.47	126.04
31	r	305	CLA	CHD-C1D-ND	-3.22	121.49	124.45
31	2	610	CLA	C1-C2-C3	-3.22	120.47	126.04
31	6	315	CLA	C1-C2-C3	-3.22	120.47	126.04
43	A	410	BCR	C4-C5-C6	-3.22	118.05	122.73
31	r	304	CLA	CHD-C1D-ND	-3.22	121.49	124.45
31	p	603	CLA	C2C-C1C-NC	3.22	112.99	109.97
31	7	304	CLA	CHD-C1D-ND	-3.22	121.50	124.45
43	H	101	BCR	C20-C21-C22	-3.22	122.72	127.31
32	0	616	LUT	C35-C15-C14	-3.22	116.88	123.47
31	B	602	CLA	CHD-C1D-ND	-3.22	121.50	124.45
35	2	614	RRX	C29-C28-C27	3.22	114.71	110.30
31	p	603	CLA	C1-C2-C3	-3.22	120.48	126.04
31	a	407	CLA	CHD-C1D-ND	-3.22	121.50	124.45
31	b	603	CLA	CHD-C1D-ND	-3.22	121.50	124.45
31	R	304	CLA	C1-C2-C3	-3.22	120.48	126.04
31	n	304	CLA	CHD-C1D-ND	-3.22	121.50	124.45
30	y	601	CHL	C1-O2A-CGA	3.22	124.88	116.44
31	8	602	CLA	C1-C2-C3	-3.21	120.48	126.04
31	4	610	CLA	C2D-C1D-ND	3.21	112.47	110.10
31	8	613	CLA	C2D-C1D-ND	3.21	112.47	110.10
31	0	602	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	s	310	CLA	CHD-C1D-ND	-3.21	121.50	124.45
35	G	614	RRX	C33-C5-C4	3.21	119.79	113.62
31	4	602	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	C	608	CLA	CHD-C1D-ND	-3.21	121.50	124.45
30	G	623	CHL	C2C-C3C-C4C	3.21	108.78	106.49
31	S	304	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	3	311	CLA	CHD-C1D-ND	-3.21	121.50	124.45
32	1	616	LUT	C21-C26-C27	-3.21	108.64	112.70
31	8	603	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	8	614	CLA	CHD-C1D-ND	-3.21	121.50	124.45
43	C	615	BCR	C36-C18-C17	-3.21	118.43	122.92
30	6	308	CHL	C4D-CHA-C1A	3.21	125.15	121.25
31	4	604	CLA	C2C-C1C-NC	3.21	112.98	109.97
30	3	308	CHL	CMA-C3A-C4A	3.21	120.39	111.77
30	1	619	CHL	C3B-C4B-NB	-3.21	107.54	110.52
32	p	616	LUT	C21-C26-C27	-3.21	108.65	112.70
31	2	613	CLA	CHD-C1D-ND	-3.21	121.51	124.45
31	n	314	CLA	C2C-C1C-NC	3.21	112.98	109.97
30	5	608	CHL	C4D-CHA-C1A	3.21	125.15	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	316	CLA	CHD-C1D-ND	-3.21	121.51	124.45
43	B	617	BCR	C38-C26-C27	3.21	119.77	113.62
30	2	605	CHL	C4D-CHA-C1A	3.20	125.15	121.25
32	0	617	LUT	C31-C30-C29	-3.20	122.74	127.31
31	y	603	CLA	CHD-C1D-ND	-3.20	121.51	124.45
31	G	611	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	a	407	CLA	C2C-C1C-NC	3.20	112.97	109.97
30	Y	302	CHL	C1-O2A-CGA	3.20	124.84	116.44
30	5	608	CHL	C3C-C4C-NC	-3.20	106.98	110.57
35	g	315	RRX	C20-C19-C18	-3.20	117.42	126.42
31	C	607	CLA	C2C-C1C-NC	3.20	112.97	109.97
30	g	306	CHL	CMA-C3A-C4A	3.20	120.38	111.77
30	6	302	CHL	C3C-C4C-NC	-3.20	106.98	110.57
31	6	315	CLA	C2D-C1D-ND	3.20	112.46	110.10
30	9	308	CHL	C1-C2-C3	-3.20	120.51	126.04
31	G	604	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	7	314	CLA	C2C-C1C-NC	3.20	112.97	109.97
32	N	316	LUT	C1-C6-C5	-3.20	118.11	122.61
31	A	407	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	6	311	CLA	C2D-C1D-ND	3.20	112.46	110.10
31	8	612	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	g	313	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	N	303	CLA	C1-C2-C3	-3.20	120.51	126.04
30	s	309	CHL	C3B-C4B-NB	-3.20	107.55	110.52
30	y	605	CHL	C2C-C3C-C4C	3.20	108.77	106.49
31	7	315	CLA	CHD-C1D-ND	-3.20	121.52	124.45
43	b	620	BCR	C30-C25-C26	-3.19	118.11	122.61
31	s	312	CLA	C2C-C1C-NC	3.19	112.96	109.97
36	R	319	NEX	C38-C25-C26	-3.19	116.91	122.26
43	d	406	BCR	C30-C25-C26	-3.19	118.11	122.61
43	t	101	BCR	C23-C24-C25	-3.19	118.23	127.20
30	N	307	CHL	C2C-C3C-C4C	3.19	108.77	106.49
30	Y	302	CHL	C2C-C3C-C4C	3.19	108.77	106.49
31	3	312	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	Y	314	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	n	305	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	3	304	CLA	CHD-C1D-ND	-3.19	121.52	124.45
31	G	613	CLA	CHD-C1D-ND	-3.19	121.52	124.45
31	y	604	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	1	612	CLA	CHD-C1D-ND	-3.19	121.52	124.45
30	9	311	CHL	C3C-C4C-NC	-3.19	106.99	110.57
32	R	317	LUT	C8-C7-C6	-3.19	118.24	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	c	614	BCR	C1-C6-C5	-3.19	118.12	122.61
31	0	613	CLA	C2C-C1C-NC	3.19	112.96	109.97
30	5	609	CHL	C3C-C4C-NC	-3.19	106.99	110.57
31	3	301	CLA	C2D-C1D-ND	3.19	112.45	110.10
31	N	313	CLA	C1-C2-C3	-3.19	120.53	126.04
31	5	614	CLA	C1-C2-C3	-3.19	120.53	126.04
31	s	316	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	N	311	CLA	C2D-C1D-ND	3.19	112.45	110.10
36	R	301	NEX	C40-C33-C34	-3.19	118.46	122.92
30	5	606	CHL	CMA-C3A-C4A	3.18	120.33	111.77
31	6	305	CLA	CHD-C1D-ND	-3.18	121.53	124.45
30	p	606	CHL	C1-C2-C3	-3.18	121.60	126.75
31	n	303	CLA	C2D-C1D-ND	3.18	112.45	110.10
31	2	603	CLA	CHD-C1D-ND	-3.18	121.53	124.45
32	6	317	LUT	C8-C7-C6	-3.18	118.27	127.20
30	4	607	CHL	C2C-C3C-C4C	3.18	108.76	106.49
30	q	308	CHL	C1-O2A-CGA	3.18	124.79	116.44
31	Y	311	CLA	C2C-C1C-NC	3.18	112.95	109.97
43	C	615	BCR	C38-C26-C25	-3.18	120.96	124.53
30	7	307	CHL	C1-O2A-CGA	3.18	124.79	116.44
30	n	309	CHL	C3C-C4C-NC	-3.18	107.00	110.57
31	R	311	CLA	C2C-C1C-NC	3.18	112.95	109.97
31	n	316	CLA	CHD-C1D-ND	-3.18	121.53	124.45
30	p	605	CHL	C4D-CHA-C1A	3.18	125.11	121.25
31	5	612	CLA	C2D-C1D-ND	3.18	112.44	110.10
30	Y	301	CHL	C2C-C3C-C4C	3.17	108.75	106.49
31	6	312	CLA	CMA-C3A-C4A	3.17	120.31	111.77
31	G	604	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	y	615	CLA	C2D-C1D-ND	3.17	112.44	110.10
30	3	307	CHL	C3C-C4C-NC	-3.17	107.01	110.57
32	y	616	LUT	C10-C11-C12	-3.17	113.31	123.22
32	S	317	LUT	C11-C10-C9	-3.17	122.78	127.31
30	4	605	CHL	C4D-CHA-C1A	3.17	125.11	121.25
43	a	410	BCR	C8-C7-C6	-3.17	118.29	127.20
31	b	610	CLA	C2C-C1C-NC	3.17	112.94	109.97
32	S	318	LUT	C7-C8-C9	-3.17	121.44	126.23
30	2	606	CHL	C4D-CHA-C1A	3.17	125.11	121.25
30	s	309	CHL	C3C-C4C-NC	-3.17	107.02	110.57
30	q	310	CHL	C4D-CHA-C1A	3.17	125.11	121.25
31	N	304	CLA	C2C-C1C-NC	3.17	112.94	109.97
31	N	312	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	d	404	CLA	CHD-C1D-ND	-3.17	121.54	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	p	614	CLA	C1D-ND-C4D	-3.17	104.08	106.33
30	g	309	CHL	C4D-CHA-C1A	3.17	125.11	121.25
31	g	311	CLA	C2C-C1C-NC	3.17	112.94	109.97
31	r	303	CLA	C3B-C4B-NB	-3.17	107.58	110.52
32	n	317	LUT	C7-C8-C9	-3.17	121.45	126.23
30	q	310	CHL	C1-O2A-CGA	3.17	124.75	116.44
30	N	307	CHL	CMA-C3A-C4A	3.17	120.29	111.77
43	T	101	BCR	C15-C14-C13	-3.17	122.79	127.31
31	N	304	CLA	CHD-C1D-ND	-3.17	121.54	124.45
30	2	601	CHL	C1-O2A-CGA	3.17	124.75	116.44
30	r	308	CHL	C4D-CHA-C1A	3.17	125.10	121.25
30	6	308	CHL	C3C-C4C-NC	-3.17	107.02	110.57
31	B	606	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	Y	303	CLA	C2C-C1C-NC	3.16	112.94	109.97
31	2	611	CLA	C1-C2-C3	-3.16	120.57	126.04
30	1	619	CHL	CAA-C2A-C3A	-3.16	104.12	112.78
31	0	611	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	y	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	p	612	CLA	C2C-C1C-NC	3.16	112.93	109.97
31	2	609	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	y	602	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	Y	313	CLA	CMA-C3A-C4A	3.16	120.27	111.77
32	3	318	LUT	C15-C35-C34	-3.16	117.00	123.47
31	7	313	CLA	CHD-C1D-ND	-3.16	121.55	124.45
34	W	201	LMG	O8-C28-C29	3.16	121.82	111.91
31	C	602	CLA	C2C-C1C-NC	3.16	112.93	109.97
43	v	101	BCR	C4-C5-C6	-3.16	118.15	122.73
31	1	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	g	310	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	2	609	CLA	C2D-C1D-ND	3.16	112.43	110.10
30	1	606	CHL	C3C-C4C-NC	-3.16	107.03	110.57
32	S	318	LUT	C18-C5-C6	-3.16	120.98	124.53
31	0	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45
30	p	606	CHL	C4D-CHA-C1A	3.16	125.09	121.25
43	d	406	BCR	C1-C6-C5	-3.16	118.17	122.61
31	3	314	CLA	C2C-C1C-NC	3.16	112.93	109.97
35	2	614	RRX	C33-C5-C4	3.16	119.68	113.62
30	q	310	CHL	C4B-CHC-C1C	3.15	133.82	126.34
42	A	408	PHO	CMB-C2B-C3B	3.15	130.58	124.68
31	B	612	CLA	C2D-C1D-ND	3.15	112.43	110.10
31	8	604	CLA	C2C-C1C-NC	3.15	112.93	109.97
32	8	615	LUT	C7-C8-C9	-3.15	121.47	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	609	CHL	C4D-CHA-C1A	3.15	125.08	121.25
30	q	310	CHL	C2B-C1B-NB	-3.15	108.12	110.23
30	7	307	CHL	C3B-C4B-NB	-3.15	107.59	110.52
31	b	613	CLA	C1D-ND-C4D	-3.15	104.10	106.33
30	G	601	CHL	C3C-C4C-NC	-3.15	107.04	110.57
31	2	612	CLA	CMA-C3A-C4A	3.15	120.24	111.77
31	c	605	CLA	C2C-C1C-NC	3.15	112.92	109.97
30	2	608	CHL	C3C-C4C-NC	-3.15	107.04	110.57
31	B	609	CLA	C2C-C1C-NC	3.15	112.92	109.97
34	g	322	LMG	O8-C28-C29	3.15	121.79	111.91
31	S	312	CLA	C1-C2-C3	-3.15	120.60	126.04
43	B	617	BCR	C8-C7-C6	-3.15	118.36	127.20
31	n	303	CLA	CHD-C1D-ND	-3.15	121.56	124.45
30	g	302	CHL	C1-C2-C3	-3.15	120.60	126.04
31	p	615	CLA	C3B-C4B-NB	-3.15	107.60	110.52
32	3	318	LUT	C18-C5-C4	3.15	120.18	114.36
30	Y	309	CHL	C4B-CHC-C1C	3.15	133.80	126.34
43	v	101	BCR	C30-C25-C26	-3.14	118.18	122.61
31	6	314	CLA	C2C-C1C-NC	3.14	112.92	109.97
30	q	310	CHL	CMA-C3A-C4A	3.14	120.22	111.77
31	3	301	CLA	C3B-C4B-NB	-3.14	107.60	110.52
31	5	602	CLA	C2D-C1D-ND	3.14	112.42	110.10
30	4	606	CHL	C1-C2-C3	-3.14	121.67	126.75
31	G	604	CLA	C1-C2-C3	-3.14	120.61	126.04
30	4	609	CHL	C4D-CHA-C1A	3.14	125.07	121.25
31	N	321	CLA	CHD-C1D-ND	-3.14	121.57	124.45
37	9	322	XAT	C7-C8-C9	-3.14	120.65	125.53
30	0	608	CHL	C2C-C3C-C4C	3.14	108.73	106.49
32	R	317	LUT	C1-C6-C5	-3.14	118.19	122.61
31	7	316	CLA	C2C-C1C-NC	3.14	112.92	109.97
31	n	304	CLA	C2C-C1C-NC	3.14	112.92	109.97
42	A	408	PHO	O2D-CGD-O1D	-3.14	117.70	123.84
31	R	306	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
37	q	321	XAT	C7-C8-C9	-3.14	120.66	125.53
31	q	304	CLA	CHD-C1D-ND	-3.14	121.57	124.45
31	d	401	CLA	C2C-C1C-NC	3.14	112.91	109.97
30	5	606	CHL	C1-C2-C3	-3.14	121.67	126.75
30	y	609	CHL	C3C-C4C-NC	-3.14	107.05	110.57
31	A	409	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	8	611	CLA	CHD-C1D-ND	-3.14	121.57	124.45
43	v	101	BCR	C8-C7-C6	-3.14	118.39	127.20
31	R	303	CLA	C2C-C1C-NC	3.14	112.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	q	312	CLA	CHD-C1D-ND	-3.14	121.57	124.45
46	d	403	BCT	O3-C-O1	-3.14	111.41	119.55
31	b	608	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	n	313	CLA	CHD-C1D-ND	-3.14	121.57	124.45
30	n	309	CHL	CMA-C3A-C4A	3.14	120.20	111.77
31	b	617	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	Y	304	CLA	C1-C2-C3	-3.13	120.62	126.04
43	B	617	BCR	C21-C20-C19	-3.13	113.43	123.22
30	9	307	CHL	C4D-CHA-C1A	3.13	125.06	121.25
32	S	318	LUT	C8-C7-C6	-3.13	118.40	127.20
34	n	322	LMG	O1-C1-C2	3.13	113.20	108.30
31	5	604	CLA	C2C-C1C-NC	3.13	112.91	109.97
30	y	607	CHL	C2C-C3C-C4C	3.13	108.72	106.49
31	b	606	CLA	CHD-C1D-ND	-3.13	121.57	124.45
32	n	318	LUT	C31-C30-C29	-3.13	122.84	127.31
30	3	303	CHL	C3C-C4C-NC	-3.13	107.06	110.57
30	p	605	CHL	C3C-C4C-NC	-3.13	107.06	110.57
30	0	606	CHL	C4D-CHA-C1A	3.13	125.06	121.25
31	b	606	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	b	614	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	g	304	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	c	611	CLA	CHD-C1D-ND	-3.13	121.58	124.45
30	3	308	CHL	C3B-C4B-NB	-3.13	107.61	110.52
30	N	301	CHL	C4D-CHA-C1A	3.13	125.06	121.25
31	7	311	CLA	C1-C2-C3	-3.13	120.63	126.04
31	a	409	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	s	305	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	0	610	CLA	C2D-C1D-ND	3.13	112.41	110.10
38	0	621	SQD	O7-S-C6	-3.13	103.22	106.94
31	R	311	CLA	C1-C2-C3	-3.13	120.63	126.04
30	2	608	CHL	C4D-CHA-C1A	3.13	125.06	121.25
31	8	609	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	n	311	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	S	314	CLA	C2C-C1C-NC	3.13	112.90	109.97
31	0	610	CLA	CHD-C1D-ND	-3.13	121.58	124.45
30	R	309	CHL	C3C-C4C-NC	-3.13	107.06	110.57
30	g	307	CHL	CMA-C3A-C4A	3.13	120.18	111.77
31	b	614	CLA	CHD-C1D-ND	-3.13	121.58	124.45
31	r	303	CLA	O1D-CGD-CBD	-3.13	118.08	124.48
30	R	308	CHL	C3B-C4B-NB	-3.13	107.61	110.52
31	p	613	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	b	612	CLA	C2D-C1D-ND	3.13	112.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	316	CLA	C2C-C1C-NC	3.13	112.90	109.97
31	6	312	CLA	C2C-C1C-NC	3.13	112.90	109.97
31	Y	304	CLA	CHD-C1D-ND	-3.13	121.58	124.45
32	8	616	LUT	C31-C30-C29	-3.13	122.85	127.31
30	G	606	CHL	C3B-C4B-NB	-3.13	107.61	110.52
31	2	602	CLA	C1D-ND-C4D	-3.13	104.11	106.33
30	0	607	CHL	C3C-C4C-NC	-3.13	107.06	110.57
37	2	619	XAT	C7-C8-C9	-3.12	120.68	125.53
37	G	620	XAT	C7-C8-C9	-3.12	120.68	125.53
37	g	321	XAT	C7-C8-C9	-3.12	120.68	125.53
30	p	608	CHL	C3C-C4C-NC	-3.12	107.07	110.57
36	5	618	NEX	C17-C1-C6	-3.12	107.68	110.47
30	6	306	CHL	C3C-C4C-NC	-3.12	107.07	110.57
30	G	605	CHL	C3C-C4C-NC	-3.12	107.07	110.57
30	1	609	CHL	C4D-CHA-C1A	3.12	125.05	121.25
30	G	605	CHL	C4D-CHA-C1A	3.12	125.05	121.25
31	r	304	CLA	C2C-C1C-NC	3.12	112.90	109.97
37	4	619	XAT	C7-C8-C9	-3.12	120.69	125.53
31	g	311	CLA	C1-C2-C3	-3.12	120.65	126.04
31	Y	303	CLA	CHD-C1D-ND	-3.12	121.59	124.45
31	s	316	CLA	CHD-C1D-ND	-3.12	121.59	124.45
31	8	603	CLA	C2C-C1C-NC	3.12	112.89	109.97
32	y	617	LUT	C8-C7-C6	-3.12	118.44	127.20
31	4	603	CLA	C1-C2-C3	-3.12	120.65	126.04
30	6	302	CHL	C1-C2-C3	-3.12	120.65	126.04
43	a	410	BCR	C7-C8-C9	-3.12	121.53	126.23
31	9	305	CLA	C2C-C1C-NC	3.11	112.89	109.97
31	B	613	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	9	305	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	4	602	CLA	C2D-C1D-ND	3.11	112.40	110.10
32	r	317	LUT	C30-C31-C32	-3.11	113.50	123.22
30	y	609	CHL	C4B-CHC-C1C	3.11	133.72	126.34
31	6	313	CLA	C2D-C1D-ND	3.11	112.40	110.10
43	b	619	BCR	C24-C23-C22	-3.11	121.53	126.23
30	Y	309	CHL	C3C-C4C-NC	-3.11	107.08	110.57
30	q	308	CHL	C4B-CHC-C1C	3.11	133.72	126.34
47	e	102	HEM	C4C-NC-C1C	3.11	108.39	105.35
30	2	606	CHL	C3C-C4C-NC	-3.11	107.08	110.57
43	b	619	BCR	C8-C7-C6	-3.11	118.47	127.20
31	2	611	CLA	C2C-C1C-NC	3.11	112.89	109.97
30	S	307	CHL	C3B-C4B-NB	-3.11	107.63	110.52
33	t	102	LHG	C5-O7-C7	-3.11	110.14	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	309	CHL	C3B-C4B-NB	-3.11	107.63	110.52
31	B	610	CLA	C2C-C1C-NC	3.11	112.88	109.97
31	8	602	CLA	CHD-C1D-ND	-3.11	121.60	124.45
31	r	306	CLA	C2C-C1C-NC	3.11	112.88	109.97
31	r	311	CLA	C2C-C1C-NC	3.11	112.88	109.97
31	6	304	CLA	C2D-C1D-ND	3.11	112.39	110.10
30	0	609	CHL	C4D-CHA-C1A	3.11	125.03	121.25
30	p	609	CHL	C4D-CHA-C1A	3.11	125.03	121.25
30	3	307	CHL	C4D-CHA-C1A	3.11	125.03	121.25
30	7	309	CHL	C4D-CHA-C1A	3.11	125.03	121.25
31	b	608	CLA	CHD-C1D-ND	-3.10	121.60	124.45
30	s	307	CHL	C4B-CHC-C1C	3.10	133.70	126.34
30	4	608	CHL	C2C-C3C-C4C	3.10	108.70	106.49
33	b	628	LHG	O8-C23-C24	3.10	121.64	111.91
31	Y	314	CLA	CHD-C1D-ND	-3.10	121.60	124.45
31	0	615	CLA	C2D-C1D-ND	3.10	112.39	110.10
30	2	606	CHL	C1-C2-C3	-3.10	121.73	126.75
30	1	606	CHL	CMA-C3A-C4A	3.10	120.11	111.77
34	9	321	LMG	O8-C28-C29	3.10	121.64	111.91
30	n	307	CHL	C3C-C4C-NC	-3.10	107.09	110.57
31	S	305	CLA	C2C-C1C-NC	3.10	112.88	109.97
43	T	101	BCR	C30-C25-C26	-3.10	118.25	122.61
30	8	606	CHL	C3C-C4C-NC	-3.10	107.09	110.57
30	y	606	CHL	C3C-C4C-NC	-3.10	107.09	110.57
31	7	305	CLA	C2C-C1C-NC	3.10	112.88	109.97
31	s	315	CLA	C2C-C1C-NC	3.10	112.88	109.97
31	9	304	CLA	C1D-ND-C4D	-3.10	104.13	106.33
31	B	611	CLA	C2D-C1D-ND	3.10	112.39	110.10
30	y	606	CHL	C1-O2A-CGA	3.10	124.58	116.44
31	r	307	CLA	CHD-C1D-ND	-3.10	121.61	124.45
31	2	610	CLA	C2D-C1D-ND	3.10	112.39	110.10
31	p	611	CLA	C2D-C1D-ND	3.10	112.39	110.10
43	B	618	BCR	C24-C23-C22	-3.10	121.55	126.23
31	g	312	CLA	C2C-C1C-NC	3.10	112.87	109.97
30	4	607	CHL	C4B-CHC-C1C	3.10	133.69	126.34
30	q	307	CHL	C3C-C4C-NC	-3.10	107.10	110.57
31	Y	305	CLA	C2C-C1C-NC	3.10	112.87	109.97
31	S	310	CLA	C1-C2-C3	-3.10	120.69	126.04
32	N	316	LUT	C21-C26-C27	-3.10	108.79	112.70
30	1	609	CHL	C3C-C4C-NC	-3.10	107.10	110.57
31	g	305	CLA	CHD-C1D-ND	-3.10	121.61	124.45
31	N	313	CLA	C2C-C1C-NC	3.10	112.87	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	315	CLA	C2C-C1C-NC	3.10	112.87	109.97
32	g	316	LUT	C18-C5-C4	3.10	120.09	114.36
31	2	610	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	B	606	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	9	313	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	1	602	CLA	C1-C2-C3	-3.09	120.69	126.04
30	9	310	CHL	C3C-C4C-NC	-3.09	107.10	110.57
31	0	604	CLA	C2C-C1C-NC	3.09	112.87	109.97
32	p	617	LUT	C18-C5-C4	3.09	120.08	114.36
30	S	307	CHL	C4B-CHC-C1C	3.09	133.67	126.34
30	N	306	CHL	C3C-C4C-NC	-3.09	107.11	110.57
30	1	605	CHL	C4B-CHC-C1C	3.09	133.67	126.34
30	Y	307	CHL	C3B-C4B-NB	-3.09	107.65	110.52
31	n	313	CLA	C2D-C1D-ND	3.09	112.38	110.10
30	7	306	CHL	C3C-C4C-NC	-3.09	107.11	110.57
31	q	316	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	n	315	CLA	C2C-C1C-NC	3.09	112.87	109.97
30	1	608	CHL	C2C-C3C-C4C	3.09	108.69	106.49
30	0	606	CHL	CMA-C3A-C4A	3.09	120.07	111.77
31	3	313	CLA	C2D-C1D-ND	3.09	112.38	110.10
31	S	306	CLA	C1D-ND-C4D	-3.09	104.14	106.33
31	s	306	CLA	CHD-C1D-ND	-3.09	121.62	124.45
31	c	613	CLA	C2C-C1C-NC	3.09	112.86	109.97
30	S	308	CHL	C2C-C3C-C4C	3.09	108.69	106.49
30	N	302	CHL	C4B-CHC-C1C	3.09	133.66	126.34
32	s	318	LUT	C18-C5-C6	-3.09	121.06	124.53
32	q	318	LUT	C18-C5-C4	3.09	120.07	114.36
30	g	309	CHL	C2C-C3C-C4C	3.09	108.69	106.49
34	B	621	LMG	O8-C28-C29	3.09	121.59	111.91
30	y	605	CHL	C3B-C4B-NB	-3.09	107.65	110.52
31	4	604	CLA	CHD-C1D-ND	-3.09	121.62	124.45
31	A	409	CLA	CHD-C1D-ND	-3.09	121.62	124.45
31	S	303	CLA	C2D-C1D-ND	3.09	112.38	110.10
43	C	615	BCR	C23-C22-C21	3.09	123.68	118.94
30	p	609	CHL	C3C-C4C-NC	-3.09	107.11	110.57
36	g	317	NEX	C38-C25-C26	-3.09	117.09	122.26
31	7	313	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	r	303	CLA	C2C-C1C-NC	3.08	112.86	109.97
35	9	317	RRX	C29-C28-C27	3.08	114.53	110.30
31	R	315	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	g	310	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	N	315	CLA	CHD-C1D-ND	-3.08	121.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	312	CLA	CHD-C1D-ND	-3.08	121.62	124.45
30	4	601	CHL	C3C-C4C-NC	-3.08	107.11	110.57
31	b	609	CLA	C2C-C1C-NC	3.08	112.86	109.97
30	q	303	CHL	C3C-C4C-NC	-3.08	107.11	110.57
30	p	607	CHL	C3B-C4B-NB	-3.08	107.66	110.52
31	5	613	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	3	315	CLA	C2D-C1D-ND	3.08	112.37	110.10
30	Y	307	CHL	C3C-C4C-NC	-3.08	107.12	110.57
31	3	315	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	C	611	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	b	615	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	4	611	CLA	C2D-C1D-ND	3.08	112.37	110.10
33	g	319	LHG	O8-C23-C24	3.08	121.57	111.91
31	q	305	CLA	CMA-C3A-C4A	3.08	120.05	111.77
31	8	611	CLA	C2D-C1D-ND	3.08	112.37	110.10
31	c	607	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	7	316	CLA	CHD-C1D-ND	-3.08	121.63	124.45
30	s	302	CHL	C3C-C4C-NC	-3.08	107.12	110.57
35	4	615	RRX	C29-C28-C27	3.08	114.52	110.30
46	D	402	BCT	O2-C-O1	-3.08	111.56	119.55
47	E	101	HEM	C4C-NC-C1C	3.08	108.36	105.35
32	6	317	LUT	C15-C14-C13	-3.08	122.92	127.31
31	S	316	CLA	C2C-C1C-NC	3.08	112.85	109.97
31	s	304	CLA	C2C-C1C-NC	3.08	112.85	109.97
31	y	612	CLA	CHD-C1D-ND	-3.08	121.63	124.45
32	s	318	LUT	C11-C10-C9	-3.08	122.92	127.31
30	8	607	CHL	CMA-C3A-C4A	3.08	120.04	111.77
31	1	614	CLA	C2D-C1D-ND	3.07	112.37	110.10
31	S	304	CLA	C2D-C1D-ND	3.07	112.37	110.10
31	8	613	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	d	405	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	C	612	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
32	6	318	LUT	C21-C26-C27	-3.07	108.82	112.70
31	9	306	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	g	312	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	q	316	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	c	601	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
31	R	315	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	c	612	CLA	CHD-C1D-ND	-3.07	121.63	124.45
30	2	607	CHL	C1-O2A-CGA	3.07	124.50	116.44
31	c	606	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
34	k	101	LMG	O8-C28-C29	3.07	121.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	305	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	g	314	CLA	C2D-C1D-ND	3.07	112.37	110.10
31	Y	305	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	p	602	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	7	305	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	0	612	CLA	CHD-C1D-ND	-3.07	121.63	124.45
30	7	321	CHL	CMA-C3A-C4A	3.07	120.02	111.77
30	g	308	CHL	C3C-C4C-NC	-3.07	107.13	110.57
35	G	614	RRX	C29-C28-C27	3.07	114.50	110.30
31	p	614	CLA	C2D-C1D-ND	3.07	112.36	110.10
30	5	608	CHL	CMA-C3A-C4A	3.07	120.02	111.77
31	3	304	CLA	CMA-C3A-C4A	3.07	120.02	111.77
31	0	613	CLA	CHD-C1D-ND	-3.07	121.64	124.45
32	5	616	LUT	C31-C30-C29	-3.07	122.93	127.31
31	Y	314	CLA	C2D-C1D-ND	3.07	112.36	110.10
37	r	318	XAT	C6-C7-C8	-3.07	119.51	125.99
42	D	401	PHO	C2B-C1B-NB	-3.07	107.41	109.53
31	5	611	CLA	C1-C2-C3	-3.07	120.74	126.04
43	B	619	BCR	C1-C6-C5	-3.06	118.30	122.61
30	6	307	CHL	C3C-C4C-NC	-3.06	107.14	110.57
31	8	602	CLA	C2D-C1D-ND	3.06	112.36	110.10
30	y	607	CHL	C1-O2A-CGA	3.06	124.48	116.44
31	7	313	CLA	C1-C2-C3	-3.06	120.75	126.04
31	C	611	CLA	C2C-C1C-NC	3.06	112.84	109.97
31	b	615	CLA	C2D-C1D-ND	3.06	112.36	110.10
31	b	611	CLA	CHD-C1D-ND	-3.06	121.64	124.45
30	n	308	CHL	CMA-C3A-C4A	3.06	120.00	111.77
31	2	602	CLA	C2C-C1C-NC	3.06	112.84	109.97
30	1	601	CHL	C3B-C4B-NB	-3.06	107.68	110.52
30	7	302	CHL	C4B-CHC-C1C	3.06	133.60	126.34
30	N	309	CHL	C2C-C3C-C4C	3.06	108.67	106.49
30	8	601	CHL	C2C-C3C-C4C	3.06	108.67	106.49
36	2	616	NEX	C38-C25-C26	-3.06	117.13	122.26
31	s	304	CLA	C2D-C1D-ND	3.06	112.36	110.10
30	6	309	CHL	C2C-C3C-C4C	3.06	108.67	106.49
31	0	611	CLA	C2C-C1C-NC	3.06	112.84	109.97
30	y	609	CHL	C1-O2A-CGA	3.06	124.47	116.44
31	5	602	CLA	C2C-C1C-NC	3.06	112.84	109.97
30	N	301	CHL	C3B-C4B-NB	-3.06	107.68	110.52
30	g	307	CHL	C4D-CHA-C1A	3.06	124.97	121.25
43	B	619	BCR	C8-C7-C6	-3.06	118.62	127.20
30	R	308	CHL	C4B-CHC-C1C	3.06	133.59	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	611	CLA	C2C-C1C-NC	3.06	112.83	109.97
31	s	304	CLA	CHD-C1D-ND	-3.06	121.65	124.45
30	8	605	CHL	C2C-C3C-C4C	3.06	108.67	106.49
43	c	615	BCR	C30-C25-C26	-3.06	118.31	122.61
31	R	304	CLA	C2C-C1C-NC	3.06	112.83	109.97
30	y	607	CHL	C3B-C4B-NB	-3.05	107.68	110.52
31	9	314	CLA	C3B-C4B-NB	-3.05	107.68	110.52
31	2	603	CLA	C2D-C1D-ND	3.05	112.36	110.10
31	d	405	CLA	C2D-C1D-ND	3.05	112.36	110.10
31	9	313	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	3	306	CLA	C2C-C1C-NC	3.05	112.83	109.97
31	7	312	CLA	C2C-C1C-NC	3.05	112.83	109.97
30	p	601	CHL	C1-C2-C3	-3.05	121.81	126.75
30	0	608	CHL	C2B-C1B-NB	-3.05	108.19	110.23
31	C	601	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	G	612	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	7	303	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	9	306	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	2	607	CHL	C2C-C3C-C4C	3.05	108.67	106.49
36	q	319	NEX	O24-C25-C38	-3.05	111.40	115.06
30	0	605	CHL	C2B-C1B-NB	-3.05	108.19	110.23
31	5	611	CLA	C2C-C1C-NC	3.05	112.83	109.97
43	Z	101	BCR	C30-C25-C26	-3.05	118.31	122.61
32	p	616	LUT	C31-C30-C29	3.05	131.66	127.31
30	q	307	CHL	C4B-CHC-C1C	3.05	133.57	126.34
32	Y	315	LUT	C30-C31-C32	-3.05	113.70	123.22
31	0	613	CLA	CMA-C3A-C4A	3.05	119.97	111.77
30	R	310	CHL	C2C-C3C-C4C	3.05	108.66	106.49
31	c	608	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	n	302	CHL	C2C-C3C-C4C	3.05	108.66	106.49
30	n	306	CHL	C2C-C3C-C4C	3.05	108.66	106.49
31	y	611	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	B	610	CLA	C2D-C1D-ND	3.05	112.35	110.10
30	6	306	CHL	CMA-C3A-C4A	3.05	119.96	111.77
31	p	603	CLA	C1-O2A-CGA	3.05	124.44	116.44
31	S	305	CLA	CHD-C1D-ND	-3.05	121.66	124.45
31	n	304	CLA	CMA-C3A-C4A	3.05	119.96	111.77
30	q	311	CHL	C4D-CHA-C1A	3.05	124.95	121.25
30	7	302	CHL	C3C-C4C-NC	-3.05	107.16	110.57
31	6	303	CLA	C2C-C1C-NC	3.04	112.82	109.97
32	0	616	LUT	C1-C6-C5	-3.04	118.33	122.61
30	s	309	CHL	CMA-C3A-C4A	3.04	119.95	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	304	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	8	610	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	c	603	CLA	CMA-C3A-C4A	3.04	119.95	111.77
31	6	314	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	B	605	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	q	304	CLA	CMA-C3A-C4A	3.04	119.95	111.77
31	4	604	CLA	C2D-C1D-ND	3.04	112.34	110.10
31	Y	310	CLA	C2D-C1D-ND	3.04	112.34	110.10
31	9	315	CLA	CMA-C3A-C4A	3.04	119.95	111.77
30	p	601	CHL	CMA-C3A-C4A	3.04	119.94	111.77
32	6	317	LUT	C11-C10-C9	-3.04	122.97	127.31
31	2	613	CLA	C2C-C1C-NC	3.04	112.82	109.97
30	7	309	CHL	CMA-C3A-C4A	3.04	119.94	111.77
31	7	303	CLA	C2D-C1D-ND	3.04	112.34	110.10
30	3	302	CHL	C4B-CHC-C1C	3.04	133.54	126.34
31	6	313	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	N	314	CLA	C2C-C1C-NC	3.04	112.82	109.97
43	A	410	BCR	C23-C24-C25	-3.04	118.67	127.20
31	C	612	CLA	CHD-C1D-ND	-3.04	121.66	124.45
30	g	306	CHL	C3C-C4C-NC	-3.04	107.17	110.57
30	G	623	CHL	C4D-CHA-C1A	3.04	124.94	121.25
31	s	303	CLA	C2D-C1D-ND	3.04	112.34	110.10
30	r	309	CHL	C3C-C4C-NC	-3.04	107.17	110.57
31	G	609	CLA	C1-C2-C3	-3.04	120.79	126.04
31	a	409	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	4	603	CLA	C2C-C1C-NC	3.04	112.82	109.97
30	7	310	CHL	C4B-CHC-C1C	3.04	133.54	126.34
30	G	608	CHL	C4D-CHA-C1A	3.04	124.94	121.25
34	0	620	LMG	O1-C1-C2	3.04	113.04	108.30
31	4	603	CLA	CMA-C3A-C4A	3.04	119.93	111.77
32	1	615	LUT	C35-C15-C14	-3.03	117.26	123.47
30	5	606	CHL	C4B-CHC-C1C	3.03	133.54	126.34
30	n	308	CHL	C4B-CHC-C1C	3.03	133.54	126.34
31	B	602	CLA	C2C-C1C-NC	3.03	112.81	109.97
30	Y	301	CHL	C4D-CHA-C1A	3.03	124.94	121.25
31	2	611	CLA	C2D-C1D-ND	3.03	112.34	110.10
36	8	617	NEX	C38-C25-C26	-3.03	117.18	122.26
31	4	613	CLA	CHD-C1D-ND	-3.03	121.67	124.45
36	4	617	NEX	O24-C25-C38	-3.03	111.42	115.06
31	1	614	CLA	C2C-C1C-NC	3.03	112.81	109.97
30	8	607	CHL	C4D-CHA-C1A	3.03	124.94	121.25
31	B	605	CLA	C2C-C1C-NC	3.03	112.81	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	406	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
31	r	305	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	b	604	CLA	C1-C2-C3	-3.03	120.80	126.04
30	n	301	CHL	C4B-CHC-C1C	3.03	133.53	126.34
30	n	310	CHL	C4B-CHC-C1C	3.03	133.53	126.34
31	S	313	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
30	q	310	CHL	C2C-C3C-C4C	3.03	108.65	106.49
43	b	619	BCR	C38-C26-C27	3.03	119.44	113.62
32	1	615	LUT	C30-C31-C32	-3.03	113.76	123.22
31	5	614	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	q	313	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	c	611	CLA	CMA-C3A-C4A	3.03	119.91	111.77
36	0	618	NEX	C17-C1-C6	-3.03	107.76	110.47
31	p	611	CLA	C3B-C4B-NB	-3.03	107.71	110.52
30	7	306	CHL	C1-O2A-CGA	3.03	124.39	116.44
30	7	321	CHL	C4B-CHC-C1C	3.03	133.52	126.34
33	A	415	LHG	C5-O7-C7	-3.03	110.34	117.79
31	C	610	CLA	C2C-C1C-NC	3.03	112.81	109.97
30	7	307	CHL	C3C-C4C-NC	-3.03	107.18	110.57
32	r	317	LUT	C35-C15-C14	-3.03	117.27	123.47
30	g	308	CHL	C1-O2A-CGA	3.03	124.39	116.44
30	g	308	CHL	C4D-CHA-C1A	3.03	124.93	121.25
31	6	303	CLA	C2D-C1D-ND	3.03	112.33	110.10
31	N	321	CLA	C2D-C1D-ND	3.03	112.33	110.10
31	6	313	CLA	CMA-C3A-C4A	3.03	119.91	111.77
30	6	307	CHL	C1-C2-C3	-3.03	121.86	126.75
31	6	311	CLA	CMA-C3A-C4A	3.03	119.91	111.77
30	7	310	CHL	C3C-C4C-NC	-3.03	107.18	110.57
31	y	615	CLA	CHD-C1D-ND	-3.03	121.67	124.45
31	8	603	CLA	CMA-C3A-C4A	3.02	119.90	111.77
32	s	318	LUT	C31-C30-C29	-3.02	122.99	127.31
31	S	311	CLA	C2C-C1C-NC	3.02	112.81	109.97
31	q	314	CLA	C2C-C1C-NC	3.02	112.81	109.97
30	9	303	CHL	C4D-CHA-C1A	3.02	124.93	121.25
30	7	302	CHL	C1-O2A-CGA	3.02	124.38	116.44
34	C	619	LMG	O8-C28-C29	3.02	121.40	111.91
31	2	604	CLA	C2D-C1D-ND	3.02	112.33	110.10
32	s	318	LUT	C7-C8-C9	-3.02	121.67	126.23
31	y	612	CLA	C2C-C1C-NC	3.02	112.80	109.97
33	A	415	LHG	O8-C23-C24	3.02	121.39	111.91
30	n	301	CHL	C3C-C4C-NC	-3.02	107.18	110.57
31	B	610	CLA	CMA-C3A-C4A	3.02	119.90	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	404	CLA	C1-C2-C3	-3.02	120.82	126.04
31	5	604	CLA	C2D-C1D-ND	3.02	112.33	110.10
43	v	101	BCR	C23-C24-C25	-3.02	118.72	127.20
43	T	101	BCR	C2-C1-C6	3.02	115.13	110.48
31	3	301	CLA	CMA-C3A-C4A	3.02	119.89	111.77
31	s	314	CLA	CHD-C1D-ND	-3.02	121.68	124.45
32	r	317	LUT	C10-C11-C12	-3.02	113.79	123.22
31	5	612	CLA	CMA-C3A-C4A	3.02	119.89	111.77
33	K	102	LHG	O8-C23-C24	3.02	121.39	111.91
31	G	603	CLA	C2C-C1C-NC	3.02	112.80	109.97
31	q	305	CLA	CHD-C1D-ND	-3.02	121.68	124.45
36	Y	317	NEX	C17-C1-C6	-3.02	107.77	110.47
30	s	308	CHL	C2C-C3C-C4C	3.02	108.64	106.49
31	2	603	CLA	C2C-C1C-NC	3.02	112.80	109.97
31	3	315	CLA	CHD-C1D-ND	-3.02	121.68	124.45
30	7	310	CHL	C1-C2-C3	-3.02	120.82	126.04
30	6	302	CHL	C4D-CHA-C1A	3.02	124.92	121.25
30	n	309	CHL	C4D-CHA-C1A	3.02	124.92	121.25
37	g	321	XAT	C38-C25-C26	-3.02	117.20	122.26
31	C	605	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
31	b	611	CLA	C2C-C1C-NC	3.02	112.80	109.97
30	5	605	CHL	C3C-C4C-NC	-3.02	107.19	110.57
30	6	307	CHL	C4D-CHA-C1A	3.02	124.92	121.25
30	Y	308	CHL	CMA-C3A-C4A	3.02	119.88	111.77
31	3	304	CLA	C2D-C1D-ND	3.02	112.33	110.10
31	7	312	CLA	C2D-C1D-ND	3.02	112.33	110.10
31	8	610	CLA	C2D-C1D-ND	3.02	112.33	110.10
30	s	307	CHL	C3B-C4B-NB	-3.01	107.72	110.52
30	9	307	CHL	CMA-C3A-C4A	3.01	119.88	111.77
30	6	309	CHL	C4D-CHA-C1A	3.01	124.92	121.25
30	0	601	CHL	C3C-C4C-NC	-3.01	107.19	110.57
30	6	308	CHL	C2C-C3C-C4C	3.01	108.64	106.49
31	9	304	CLA	C2C-C1C-NC	3.01	112.80	109.97
43	B	619	BCR	C15-C16-C17	-3.01	117.30	123.47
30	0	608	CHL	C3B-C4B-NB	-3.01	107.72	110.52
37	r	318	XAT	C7-C8-C9	-3.01	120.85	125.53
31	4	602	CLA	C2C-C1C-NC	3.01	112.80	109.97
31	0	614	CLA	C2C-C1C-NC	3.01	112.80	109.97
31	8	614	CLA	C2C-C1C-NC	3.01	112.80	109.97
31	r	316	CLA	CMA-C3A-C4A	3.01	119.87	111.77
30	Y	309	CHL	C1-C2-C3	-3.01	120.83	126.04
30	6	310	CHL	CMA-C3A-C4A	3.01	119.87	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	307	CHL	CMA-C3A-C4A	3.01	119.87	111.77
31	3	312	CLA	CMA-C3A-C4A	3.01	119.87	111.77
35	g	315	RRX	C11-C12-C13	-3.01	117.95	126.42
31	6	315	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	9	312	CLA	C2D-C1D-ND	3.01	112.32	110.10
31	S	313	CLA	CHD-C1D-ND	-3.01	121.69	124.45
32	0	616	LUT	C15-C14-C13	-3.01	123.01	127.31
30	p	607	CHL	C4B-CHC-C1C	3.01	133.48	126.34
31	3	305	CLA	CMA-C3A-C4A	3.01	119.86	111.77
30	6	308	CHL	C3B-C4B-NB	-3.01	107.72	110.52
31	0	603	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	0	603	CLA	C1-C2-C3	-3.01	120.84	126.04
31	B	603	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	R	313	CLA	C2C-C1C-NC	3.01	112.79	109.97
34	0	620	LMG	C8-O7-C10	-3.01	110.39	117.79
31	6	305	CLA	C2C-C1C-NC	3.01	112.79	109.97
43	B	618	BCR	C16-C17-C18	-3.01	123.02	127.31
31	n	312	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	g	310	CLA	C1-C2-C3	-3.01	120.84	126.04
30	q	303	CHL	C4D-CHA-C1A	3.01	124.91	121.25
43	c	614	BCR	C27-C26-C25	-3.01	118.37	122.73
30	5	607	CHL	C3B-C4B-NB	-3.01	107.73	110.52
30	3	302	CHL	C2C-C3C-C4C	3.01	108.63	106.49
31	8	604	CLA	CHD-C1D-ND	-3.01	121.69	124.45
30	Y	308	CHL	C3C-C4C-NC	-3.00	107.20	110.57
30	1	607	CHL	C2C-C3C-C4C	3.00	108.63	106.49
31	g	313	CLA	CHD-C1D-ND	-3.00	121.69	124.45
31	D	404	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
31	5	610	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	5	614	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	8	612	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	c	605	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
31	S	306	CLA	CHD-C1D-ND	-3.00	121.69	124.45
31	b	612	CLA	CHD-C1D-ND	-3.00	121.69	124.45
31	2	603	CLA	CMA-C3A-C4A	3.00	119.84	111.77
31	6	314	CLA	C2D-C1D-ND	3.00	112.32	110.10
30	4	606	CHL	CMA-C3A-C4A	3.00	119.84	111.77
31	S	315	CLA	C2C-C1C-NC	3.00	112.78	109.97
30	9	308	CHL	C4B-CHC-C1C	3.00	133.46	126.34
31	5	613	CLA	CHD-C1D-ND	-3.00	121.69	124.45
31	C	603	CLA	CMA-C3A-C4A	3.00	119.84	111.77
31	b	611	CLA	C2D-C1D-ND	3.00	112.32	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	r	308	CHL	C3C-C4C-NC	-3.00	107.20	110.57
30	5	601	CHL	C3B-C4B-NB	-3.00	107.73	110.52
31	7	304	CLA	C3B-C4B-NB	-3.00	107.73	110.52
31	y	611	CLA	C3B-C4B-NB	-3.00	107.73	110.52
31	p	610	CLA	C1-C2-C3	-3.00	120.86	126.04
31	6	313	CLA	CHD-C1D-ND	-3.00	121.70	124.45
31	N	312	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	g	314	CLA	C3B-C4B-NB	-3.00	107.73	110.52
31	p	611	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	c	603	CLA	C2C-C1C-NC	3.00	112.78	109.97
37	q	321	XAT	C38-C25-C26	-3.00	117.24	122.26
31	5	604	CLA	CHD-C1D-ND	-3.00	121.70	124.45
31	B	609	CLA	CHD-C1D-ND	-3.00	121.70	124.45
31	y	610	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	y	614	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	2	609	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	4	614	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	B	612	CLA	C1-C2-C3	-3.00	120.86	126.04
31	9	306	CLA	C2D-C1D-ND	3.00	112.31	110.10
36	N	318	NEX	C39-C29-C30	-3.00	118.73	122.92
43	a	410	BCR	C16-C17-C18	-3.00	123.03	127.31
31	C	611	CLA	CMA-C3A-C4A	3.00	119.83	111.77
31	N	311	CLA	C2C-C1C-NC	3.00	112.78	109.97
34	0	622	LMG	O8-C28-C29	3.00	121.31	111.91
31	0	612	CLA	C2C-C1C-NC	2.99	112.78	109.97
31	7	311	CLA	C1D-ND-C4D	-2.99	104.21	106.33
31	6	314	CLA	CMA-C3A-C4A	2.99	119.82	111.77
31	8	610	CLA	C3B-C4B-NB	-2.99	107.74	110.52
31	r	304	CLA	C1-C2-C3	-2.99	120.87	126.04
43	T	101	BCR	C24-C23-C22	-2.99	121.71	126.23
37	2	619	XAT	C38-C25-C26	-2.99	117.24	122.26
31	6	311	CLA	C2C-C1C-NC	2.99	112.78	109.97
30	0	607	CHL	C1-C2-C3	-2.99	120.87	126.04
31	6	315	CLA	C1D-ND-C4D	-2.99	104.21	106.33
32	r	317	LUT	C15-C35-C34	-2.99	117.34	123.47
31	B	609	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	D	403	CLA	C2C-C1C-NC	2.99	112.78	109.97
43	h	101	BCR	C2-C1-C6	2.99	115.09	110.48
30	0	609	CHL	C1-O2A-CGA	2.99	124.29	116.44
30	9	307	CHL	C4B-CHC-C1C	2.99	133.43	126.34
31	C	609	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
31	1	610	CLA	C1D-ND-C4D	-2.99	104.21	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	610	CLA	C1D-ND-C4D	-2.99	104.21	106.33
31	N	310	CLA	CMA-C3A-C4A	2.99	119.81	111.77
31	N	303	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	c	611	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	5	611	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	N	310	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	n	314	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	B	610	CLA	CHD-C1D-ND	-2.99	121.71	124.45
31	9	315	CLA	CHD-C1D-ND	-2.99	121.71	124.45
30	3	303	CHL	C4B-CHC-C1C	2.99	133.43	126.34
31	1	611	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	2	612	CLA	CHD-C1D-ND	-2.99	121.71	124.45
31	N	315	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	s	303	CLA	C2C-C1C-NC	2.99	112.77	109.97
32	1	615	LUT	C10-C11-C12	-2.99	113.89	123.22
30	Y	301	CHL	C1-C2-C3	-2.99	120.88	126.04
31	n	305	CLA	CHD-C1D-ND	-2.99	121.71	124.45
30	G	623	CHL	C3B-C4B-NB	-2.99	107.74	110.52
31	3	305	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	6	304	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	4	614	CLA	CMA-C3A-C4A	2.99	119.80	111.77
30	9	303	CHL	C3C-C4C-NC	-2.99	107.22	110.57
45	C	618	DGD	O2G-C1B-C2B	2.99	117.94	111.50
30	8	608	CHL	C4B-CHC-C1C	2.99	133.42	126.34
30	g	306	CHL	C4B-CHC-C1C	2.99	133.42	126.34
31	N	305	CLA	C2D-C1D-ND	2.99	112.31	110.10
30	5	608	CHL	C4B-CHC-C1C	2.99	133.42	126.34
34	n	322	LMG	O8-C28-C29	2.99	121.28	111.91
31	4	610	CLA	C1-C2-C3	-2.99	120.88	126.04
31	r	313	CLA	C2C-C1C-NC	2.99	112.77	109.97
43	c	614	BCR	C38-C26-C27	2.98	119.35	113.62
31	n	312	CLA	C3B-C4B-NB	-2.98	107.75	110.52
30	0	608	CHL	C4B-CHC-C1C	2.98	133.42	126.34
30	7	308	CHL	C4D-CHA-C1A	2.98	124.88	121.25
30	r	308	CHL	CMA-C3A-C4A	2.98	119.79	111.77
31	N	304	CLA	C2D-C1D-ND	2.98	112.30	110.10
31	7	315	CLA	C2D-C1D-ND	2.98	112.30	110.10
31	n	316	CLA	C2D-C1D-ND	2.98	112.30	110.10
31	g	314	CLA	CHD-C1D-ND	-2.98	121.71	124.45
31	B	613	CLA	C2C-C1C-NC	2.98	112.77	109.97
30	1	619	CHL	C4D-CHA-C1A	2.98	124.88	121.25
31	c	607	CLA	CHD-C1D-ND	-2.98	121.71	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	606	CHL	C3C-C4C-NC	-2.98	107.23	110.57
31	N	303	CLA	C2D-C1D-ND	2.98	112.30	110.10
30	1	609	CHL	C4B-CHC-C1C	2.98	133.41	126.34
31	7	303	CLA	C2C-C1C-NC	2.98	112.77	109.97
37	4	619	XAT	C38-C25-C26	-2.98	117.26	122.26
31	Y	310	CLA	C1D-ND-C4D	-2.98	104.22	106.33
30	g	309	CHL	C4B-CHC-C1C	2.98	133.41	126.34
30	q	310	CHL	C3B-C4B-NB	-2.98	107.75	110.52
31	q	305	CLA	C2C-C1C-NC	2.98	112.76	109.97
34	b	622	LMG	O8-C28-C29	2.98	121.26	111.91
30	6	302	CHL	C1-O2A-CGA	2.98	124.26	116.44
31	y	604	CLA	CHD-C1D-ND	-2.98	121.72	124.45
31	g	314	CLA	C2C-C1C-NC	2.98	112.76	109.97
31	r	315	CLA	C1-O2A-CGA	2.98	124.26	116.44
36	6	319	NEX	C17-C1-C6	-2.98	107.81	110.47
30	r	310	CHL	C4B-CHC-C1C	2.98	133.40	126.34
31	8	604	CLA	C2D-C1D-ND	2.98	112.30	110.10
30	p	606	CHL	C3C-C4C-NC	-2.98	107.23	110.57
31	y	602	CLA	C2C-C1C-NC	2.98	112.76	109.97
30	r	309	CHL	C4D-CHA-C1A	2.98	124.87	121.25
31	7	315	CLA	C1-C2-C3	-2.98	120.89	126.04
31	S	304	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
31	a	407	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
31	g	312	CLA	C2D-C1D-ND	2.98	112.30	110.10
34	c	621	LMG	O8-C28-C29	2.98	121.25	111.91
33	5	619	LHG	C5-O7-C7	-2.98	110.46	117.79
31	4	602	CLA	CMA-C3A-C4A	2.98	119.77	111.77
36	n	319	NEX	C39-C29-C30	-2.98	118.75	122.92
33	e	101	LHG	C5-O7-C7	-2.98	110.46	117.79
42	D	401	PHO	O2D-CGD-O1D	-2.98	118.02	123.84
45	C	617	DGD	O2G-C1B-C2B	2.98	117.92	111.50
30	1	606	CHL	C3B-C4B-NB	-2.98	107.75	110.52
30	p	605	CHL	C2C-C3C-C4C	2.98	108.61	106.49
31	8	609	CLA	CMA-C3A-C4A	2.98	119.77	111.77
31	G	612	CLA	C2C-C1C-NC	2.97	112.76	109.97
35	2	614	RRX	C20-C19-C18	-2.97	118.06	126.42
31	n	303	CLA	CMA-C3A-C4A	2.97	119.77	111.77
30	N	302	CHL	C1-O2A-CGA	2.97	124.25	116.44
31	9	304	CLA	CMA-C3A-C4A	2.97	119.77	111.77
31	b	607	CLA	O2A-CGA-CBA	2.97	121.24	111.91
31	s	312	CLA	CHD-C1D-ND	-2.97	121.72	124.45
31	C	608	CLA	C2C-C1C-NC	2.97	112.76	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	N	301	CHL	C3C-C4C-NC	-2.97	107.24	110.57
32	7	317	LUT	C1-C6-C5	-2.97	118.42	122.61
37	9	322	XAT	C38-C25-C26	-2.97	117.28	122.26
43	V	101	BCR	C8-C7-C6	-2.97	118.85	127.20
30	G	623	CHL	C1-O2A-CGA	2.97	124.24	116.44
30	N	309	CHL	C4D-CHA-C1A	2.97	124.87	121.25
31	q	314	CLA	CHD-C1D-ND	-2.97	121.72	124.45
31	0	615	CLA	C2C-C1C-NC	2.97	112.76	109.97
31	r	311	CLA	O2A-CGA-CBA	2.97	121.24	111.91
31	C	602	CLA	C1-C2-C3	-2.97	120.90	126.04
31	5	603	CLA	C2D-C1D-ND	2.97	112.29	110.10
31	p	615	CLA	C2D-C1D-ND	2.97	112.29	110.10
31	r	304	CLA	CMA-C3A-C4A	2.97	119.76	111.77
32	8	615	LUT	C21-C26-C27	-2.97	108.94	112.70
31	1	611	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	3	313	CLA	CHD-C1D-ND	-2.97	121.72	124.45
30	0	608	CHL	CMA-C3A-C4A	2.97	119.75	111.77
31	R	307	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
30	G	601	CHL	C4D-CHA-C1A	2.97	124.86	121.25
31	1	604	CLA	C2C-C1C-NC	2.97	112.75	109.97
43	c	615	BCR	C33-C5-C4	2.97	119.32	113.62
31	2	613	CLA	C2D-C1D-ND	2.97	112.29	110.10
31	n	304	CLA	C2D-C1D-ND	2.97	112.29	110.10
31	8	602	CLA	CMA-C3A-C4A	2.97	119.75	111.77
30	y	606	CHL	C3B-C4B-NB	-2.97	107.76	110.52
31	0	610	CLA	C1D-ND-C4D	-2.97	104.23	106.33
30	4	605	CHL	C4B-CHC-C1C	2.97	133.37	126.34
30	Y	307	CHL	C4B-CHC-C1C	2.97	133.37	126.34
31	B	608	CLA	C2C-C1C-NC	2.97	112.75	109.97
31	2	609	CLA	C1-C2-C3	-2.97	120.91	126.04
43	v	101	BCR	C10-C11-C12	-2.97	113.96	123.22
30	2	607	CHL	CMA-C3A-C4A	2.97	119.74	111.77
30	8	608	CHL	C2C-C3C-C4C	2.97	108.60	106.49
30	n	310	CHL	C2C-C3C-C4C	2.97	108.60	106.49
43	B	618	BCR	C15-C16-C17	-2.97	117.40	123.47
31	b	602	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
30	y	608	CHL	CMA-C3A-C4A	2.96	119.74	111.77
31	r	305	CLA	CMA-C3A-C4A	2.96	119.74	111.77
31	5	612	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	y	610	CLA	C1D-ND-C4D	-2.96	104.23	106.33
36	6	319	NEX	C26-C27-C28	-2.96	119.73	125.99
30	9	309	CHL	C3C-C4C-NC	-2.96	107.25	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	602	CLA	C2D-C1D-ND	2.96	112.29	110.10
31	C	604	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	2	609	CLA	C1D-ND-C4D	-2.96	104.23	106.33
30	G	607	CHL	CMA-C3A-C4A	2.96	119.73	111.77
31	8	602	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	g	303	CLA	C1-O2A-CGA	2.96	124.21	116.44
36	N	318	NEX	C17-C1-C6	-2.96	107.82	110.47
31	B	616	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
37	G	620	XAT	C38-C25-C26	-2.96	117.30	122.26
31	p	602	CLA	CHD-C1D-ND	-2.96	121.73	124.45
30	R	309	CHL	C4D-CHA-C1A	2.96	124.85	121.25
31	r	313	CLA	CHD-C1D-ND	-2.96	121.73	124.45
33	A	417	LHG	O8-C23-C24	2.96	121.19	111.91
31	R	313	CLA	C2D-C1D-ND	2.96	112.28	110.10
30	6	309	CHL	C4B-CHC-C1C	2.96	133.35	126.34
31	N	321	CLA	C2C-C1C-NC	2.96	112.74	109.97
31	b	604	CLA	C2C-C1C-NC	2.96	112.74	109.97
30	2	605	CHL	C3C-C4C-NC	-2.96	107.25	110.57
30	4	606	CHL	C3C-C4C-NC	-2.96	107.25	110.57
32	0	616	LUT	C30-C31-C32	-2.96	113.99	123.22
31	B	607	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
30	0	601	CHL	C4B-CHC-C1C	2.96	133.35	126.34
31	D	403	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	G	604	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	N	315	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	p	610	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	N	312	CLA	C2C-C1C-NC	2.96	112.74	109.97
31	n	313	CLA	C2C-C1C-NC	2.96	112.74	109.97
30	8	601	CHL	C4B-CHC-C1C	2.96	133.35	126.34
31	B	615	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
36	0	618	NEX	C26-C27-C28	-2.96	119.74	125.99
31	1	614	CLA	C1-C2-C3	-2.96	120.93	126.04
30	9	307	CHL	C3B-C4B-NB	-2.96	107.77	110.52
35	9	317	RRX	C38-C26-C27	2.96	119.83	114.36
31	B	615	CLA	C1-C2-C3	-2.96	120.93	126.04
31	C	601	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
31	n	311	CLA	C1D-ND-C4D	-2.95	104.24	106.33
31	n	303	CLA	C2C-C1C-NC	2.95	112.74	109.97
32	n	317	LUT	C21-C26-C27	-2.95	108.97	112.70
31	c	601	CLA	C3B-C4B-NB	-2.95	107.77	110.52
31	b	613	CLA	C1-C2-C3	-2.95	120.93	126.04
30	7	321	CHL	C2C-C3C-C4C	2.95	108.59	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	603	CLA	C2C-C1C-NC	2.95	112.74	109.97
31	N	305	CLA	CHD-C1D-ND	-2.95	121.74	124.45
30	q	311	CHL	C3C-C4C-NC	-2.95	107.26	110.57
43	C	614	BCR	C1-C6-C5	-2.95	118.45	122.61
31	n	303	CLA	C1-C2-C3	-2.95	120.94	126.04
30	0	605	CHL	CHC-C1C-NC	2.95	128.68	124.20
31	R	306	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
30	2	605	CHL	C4B-CHC-C1C	2.95	133.34	126.34
31	s	305	CLA	C2D-C1D-ND	2.95	112.28	110.10
36	6	319	NEX	C38-C25-C26	-2.95	117.31	122.26
30	0	605	CHL	C4B-CHC-C1C	2.95	133.34	126.34
31	5	602	CLA	C1D-ND-C4D	-2.95	104.24	106.33
36	r	319	NEX	C38-C25-C26	-2.95	117.32	122.26
30	g	307	CHL	C2C-C3C-C4C	2.95	108.59	106.49
31	7	311	CLA	C2D-C1D-ND	2.95	112.28	110.10
36	6	319	NEX	C2-C1-C6	2.95	112.08	109.21
32	s	317	LUT	C21-C26-C27	-2.95	108.97	112.70
33	9	320	LHG	C5-O7-C7	-2.95	110.53	117.79
31	3	315	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	C	613	CLA	C2C-C1C-NC	2.95	112.73	109.97
30	p	607	CHL	C4D-CHA-C1A	2.95	124.84	121.25
30	s	308	CHL	CMA-C3A-C4A	2.95	119.70	111.77
31	9	312	CLA	CHD-C1D-ND	-2.95	121.74	124.45
31	9	305	CLA	C2D-C1D-ND	2.95	112.28	110.10
31	4	604	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	Y	303	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	G	602	CLA	C2C-C1C-NC	2.95	112.73	109.97
30	r	308	CHL	C1-C2-C3	-2.95	120.94	126.04
31	1	612	CLA	C1-C2-C3	-2.95	120.94	126.04
31	p	613	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
31	4	602	CLA	C1D-ND-C4D	-2.95	104.24	106.33
31	6	311	CLA	C1D-ND-C4D	-2.95	104.24	106.33
35	4	615	RRX	C38-C26-C27	2.95	119.82	114.36
43	B	619	BCR	C33-C5-C6	-2.95	121.22	124.53
31	y	602	CLA	CMA-C3A-C4A	2.95	119.69	111.77
33	s	322	LHG	O8-C23-C24	2.95	121.16	111.91
31	2	610	CLA	CHD-C1D-ND	-2.95	121.75	124.45
30	N	308	CHL	C4D-CHA-C1A	2.95	124.83	121.25
35	G	614	RRX	C38-C26-C27	2.95	119.81	114.36
30	3	307	CHL	C2C-C3C-C4C	2.95	108.59	106.49
30	n	308	CHL	C2C-C3C-C4C	2.95	108.59	106.49
31	y	611	CLA	C2D-C1D-ND	2.95	112.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	9	302	LMG	O8-C28-C29	2.95	121.15	111.91
31	B	615	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
31	b	607	CLA	C2C-C1C-NC	2.95	112.73	109.97
31	N	310	CLA	C1D-ND-C4D	-2.94	104.24	106.33
31	p	611	CLA	C1D-ND-C4D	-2.94	104.24	106.33
31	n	312	CLA	C2D-C1D-ND	2.94	112.27	110.10
31	6	303	CLA	CMA-C3A-C4A	2.94	119.69	111.77
30	0	601	CHL	C1-C2-C3	-2.94	120.95	126.04
30	n	302	CHL	C4B-CHC-C1C	2.94	133.32	126.34
36	0	618	NEX	C2-C1-C6	2.94	112.07	109.21
30	9	311	CHL	CMA-C3A-C4A	2.94	119.68	111.77
31	0	614	CLA	C2D-C1D-ND	2.94	112.27	110.10
43	a	410	BCR	C1-C6-C5	-2.94	118.47	122.61
31	N	310	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	S	312	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	c	612	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
31	1	611	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	p	612	CLA	CMA-C3A-C4A	2.94	119.68	111.77
31	8	611	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	1	611	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	A	409	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	q	306	CLA	CMA-C3A-C4A	2.94	119.68	111.77
31	s	305	CLA	CHD-C1D-ND	-2.94	121.75	124.45
30	s	308	CHL	C4D-CHA-C1A	2.94	124.83	121.25
30	5	609	CHL	C1-O2A-CGA	2.94	124.16	116.44
31	4	613	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	C	603	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	8	609	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	R	303	CLA	O1D-CGD-CBD	-2.94	118.47	124.48
31	2	604	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	p	614	CLA	C2C-C1C-NC	2.94	112.72	109.97
31	q	304	CLA	C2C-C1C-NC	2.94	112.72	109.97
30	S	309	CHL	CMA-C3A-C4A	2.94	119.67	111.77
31	N	313	CLA	CMA-C3A-C4A	2.94	119.67	111.77
31	1	611	CLA	C3B-C4B-NB	-2.94	107.79	110.52
32	0	616	LUT	C7-C8-C9	-2.94	121.80	126.23
34	C	619	LMG	C8-O7-C10	-2.94	110.56	117.79
31	R	314	CLA	C2C-C1C-NC	2.94	112.72	109.97
30	G	605	CHL	CMA-C3A-C4A	2.94	119.67	111.77
30	N	301	CHL	C4B-CHC-C1C	2.94	133.30	126.34
31	4	603	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	B	611	CLA	CHD-C1D-ND	-2.94	121.75	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	0	618	NEX	C38-C25-C26	-2.94	117.34	122.26
30	5	601	CHL	C4B-CHC-C1C	2.94	133.30	126.34
31	6	304	CLA	C3B-C4B-NB	-2.94	107.79	110.52
30	y	607	CHL	C4D-CHA-C1A	2.94	124.82	121.25
31	C	602	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
31	0	604	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
30	g	308	CHL	C1-C2-C3	-2.94	122.00	126.75
31	s	316	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
30	6	306	CHL	C4B-CHC-C1C	2.94	133.30	126.34
31	S	303	CLA	C1D-ND-C4D	-2.94	104.25	106.33
31	D	404	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	Y	312	CLA	C2C-C1C-NC	2.93	112.72	109.97
31	0	602	CLA	C2C-C1C-NC	2.93	112.72	109.97
31	S	305	CLA	C2D-C1D-ND	2.93	112.27	110.10
31	q	304	CLA	C2D-C1D-ND	2.93	112.27	110.10
31	s	304	CLA	CMA-C3A-C4A	2.93	119.66	111.77
30	9	310	CHL	C2C-C3C-C4C	2.93	108.58	106.49
31	n	311	CLA	C2C-C1C-NC	2.93	112.72	109.97
30	q	308	CHL	C3B-C4B-NB	-2.93	107.79	110.52
30	Y	308	CHL	C1-O2A-CGA	2.93	124.14	116.44
31	5	614	CLA	CMA-C3A-C4A	2.93	119.66	111.77
31	4	611	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	1	610	CLA	C2D-C1D-ND	2.93	112.27	110.10
31	b	614	CLA	C2D-C1D-ND	2.93	112.27	110.10
31	s	303	CLA	C1D-ND-C4D	-2.93	104.25	106.33
31	2	611	CLA	CHD-C1D-ND	-2.93	121.76	124.45
30	3	303	CHL	CMA-C3A-C4A	2.93	119.65	111.77
42	A	408	PHO	O1D-CGD-CBD	2.93	129.62	124.74
30	G	607	CHL	C4D-CHA-C1A	2.93	124.82	121.25
34	b	626	LMG	O8-C28-C29	2.93	121.11	111.91
43	b	619	BCR	C33-C5-C4	2.93	119.25	113.62
36	9	319	NEX	C38-C25-C26	-2.93	117.35	122.26
30	7	307	CHL	C4B-CHC-C1C	2.93	133.29	126.34
43	C	615	BCR	C27-C26-C25	-2.93	118.48	122.73
31	4	612	CLA	C3B-C4B-NB	-2.93	107.80	110.52
31	3	316	CLA	C2D-C1D-ND	2.93	112.26	110.10
32	1	616	LUT	C31-C30-C29	-2.93	123.13	127.31
31	5	602	CLA	CMA-C3A-C4A	2.93	119.64	111.77
36	G	616	NEX	C5-C6-C1	2.93	122.60	119.70
31	3	314	CLA	C2D-C1D-ND	2.93	112.26	110.10
31	n	305	CLA	C2D-C1D-ND	2.93	112.26	110.10
31	N	314	CLA	CMA-C3A-C4A	2.93	119.64	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	316	CLA	C2C-C1C-NC	2.93	112.72	109.97
30	4	609	CHL	C1-C2-C3	-2.93	120.98	126.04
31	7	303	CLA	CMA-C3A-C4A	2.93	119.64	111.77
37	9	322	XAT	C27-C28-C29	2.93	130.07	125.53
31	b	605	CLA	CMA-C3A-C4A	2.93	119.64	111.77
31	1	603	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
30	N	306	CHL	C3B-C4B-NB	-2.93	107.80	110.52
32	5	616	LUT	C21-C26-C27	-2.93	109.00	112.70
30	7	302	CHL	C1-C2-C3	-2.93	120.98	126.04
31	y	614	CLA	C2C-C1C-NC	2.92	112.71	109.97
30	S	309	CHL	C1-O2A-CGA	2.92	124.12	116.44
31	b	610	CLA	C2D-C1D-ND	2.92	112.26	110.10
31	3	301	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	y	603	CLA	C2C-C1C-NC	2.92	112.71	109.97
31	p	614	CLA	C1-C2-C3	-2.92	120.99	126.04
31	b	606	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
31	N	311	CLA	CMA-C3A-C4A	2.92	119.63	111.77
33	d	408	LHG	C5-O7-C7	-2.92	110.60	117.79
31	C	612	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
30	G	601	CHL	C1-C2-C3	-2.92	120.99	126.04
34	2	620	LMG	O8-C28-C29	2.92	121.08	111.91
31	7	314	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	6	312	CLA	C1-C2-C3	-2.92	120.99	126.04
31	9	316	CLA	C2D-C1D-ND	2.92	112.26	110.10
31	s	312	CLA	CMA-C3A-C4A	2.92	119.62	111.77
31	c	612	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
30	9	309	CHL	C3B-C4B-NB	-2.92	107.81	110.52
43	V	101	BCR	C23-C24-C25	-2.92	119.00	127.20
31	N	313	CLA	C2D-C1D-ND	2.92	112.26	110.10
31	2	610	CLA	C3B-C4B-NB	-2.92	107.81	110.52
37	q	321	XAT	C27-C28-C29	2.92	130.06	125.53
34	c	620	LMG	C8-O7-C10	-2.92	110.60	117.79
31	5	611	CLA	C3B-C4B-NB	-2.92	107.81	110.52
31	2	602	CLA	CMA-C3A-C4A	2.92	119.62	111.77
30	8	601	CHL	C4D-CHA-C1A	2.92	124.80	121.25
31	N	313	CLA	CHD-C1D-ND	-2.92	121.77	124.45
30	0	609	CHL	C4B-CHC-C1C	2.92	133.26	126.34
31	3	306	CLA	C1D-ND-C4D	-2.92	104.26	106.33
31	n	315	CLA	CMA-C3A-C4A	2.92	119.62	111.77
33	D	408	LHG	O8-C23-C24	2.92	121.06	111.91
31	C	610	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
31	a	409	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	605	CHL	C4B-CHC-C1C	2.92	133.26	126.34
31	4	612	CLA	C1D-ND-C4D	-2.92	104.26	106.33
44	A	416	PL9	C36-C34-C33	-2.92	115.22	121.12
30	G	606	CHL	CMA-C3A-C4A	2.92	119.61	111.77
31	c	602	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
31	4	610	CLA	C3B-C4B-NB	-2.92	107.81	110.52
31	B	605	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
31	1	602	CLA	CHD-C1D-ND	-2.92	121.78	124.45
31	r	314	CLA	C2D-C1D-ND	2.91	112.25	110.10
31	8	613	CLA	CMA-C3A-C4A	2.91	119.61	111.77
30	N	309	CHL	C4B-CHC-C1C	2.91	133.25	126.34
30	3	310	CHL	C4D-CHA-C1A	2.91	124.80	121.25
32	y	617	LUT	C30-C31-C32	-2.91	114.12	123.22
31	Y	303	CLA	C2D-C1D-ND	2.91	112.25	110.10
31	2	612	CLA	C2C-C1C-NC	2.91	112.70	109.97
31	7	304	CLA	CMA-C3A-C4A	2.91	119.60	111.77
30	0	607	CHL	C3B-C4B-NB	-2.91	107.81	110.52
31	y	615	CLA	C3B-C4B-NB	-2.91	107.81	110.52
31	C	613	CLA	C2D-C1D-ND	2.91	112.25	110.10
34	6	322	LMG	O8-C28-C29	2.91	121.05	111.91
30	y	606	CHL	C4D-CHA-C1A	2.91	124.79	121.25
31	r	304	CLA	C1D-ND-C4D	-2.91	104.27	106.33
36	2	616	NEX	C17-C1-C6	-2.91	107.87	110.47
31	g	304	CLA	CMA-C3A-C4A	2.91	119.60	111.77
31	N	312	CLA	C3B-C4B-NB	-2.91	107.81	110.52
31	s	315	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
32	6	317	LUT	C1-C6-C5	-2.91	118.52	122.61
31	R	315	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	7	312	CLA	CHD-C1D-ND	-2.91	121.78	124.45
30	p	606	CHL	C4B-CHC-C1C	2.91	133.24	126.34
31	Y	314	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	R	307	CLA	CHD-C1D-ND	-2.91	121.78	124.45
43	T	101	BCR	C11-C10-C9	-2.91	123.16	127.31
30	s	307	CHL	CMA-C3A-C4A	2.91	119.59	111.77
30	9	311	CHL	C4D-CHA-C1A	2.91	124.79	121.25
31	N	304	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	G	603	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	c	610	CLA	O2A-CGA-CBA	2.91	121.03	111.91
30	N	302	CHL	CMA-C3A-C4A	2.91	119.58	111.77
31	4	611	CLA	CMA-C3A-C4A	2.91	119.58	111.77
34	b	624	LMG	O8-C28-C29	2.91	121.03	111.91
34	d	411	LMG	O8-C28-C29	2.91	121.03	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	612	CLA	CHD-C1D-ND	-2.91	121.78	124.45
30	n	302	CHL	C4D-CHA-C1A	2.91	124.79	121.25
31	C	607	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
30	9	307	CHL	C3C-C4C-NC	-2.91	107.31	110.57
32	s	317	LUT	C11-C10-C9	-2.91	123.16	127.31
36	9	319	NEX	C2-C1-C6	2.90	112.03	109.21
31	5	603	CLA	C2C-C1C-NC	2.90	112.69	109.97
43	d	406	BCR	C20-C21-C22	-2.90	123.17	127.31
31	8	614	CLA	CMA-C3A-C4A	2.90	119.58	111.77
30	p	601	CHL	C3C-C4C-NC	-2.90	107.31	110.57
31	6	304	CLA	CHD-C1D-ND	-2.90	121.79	124.45
30	0	607	CHL	C4B-CHC-C1C	2.90	133.22	126.34
37	g	321	XAT	C27-C28-C29	2.90	130.03	125.53
31	B	614	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	G	602	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	8	612	CLA	CMA-C3A-C4A	2.90	119.57	111.77
30	y	608	CHL	C4B-CHC-C1C	2.90	133.22	126.34
31	c	602	CLA	C1-C2-C3	-2.90	121.02	126.04
43	B	618	BCR	C27-C26-C25	-2.90	118.52	122.73
32	3	318	LUT	C31-C30-C29	-2.90	123.17	127.31
34	7	320	LMG	C7-O1-C1	-2.90	108.07	113.74
31	N	311	CLA	C1D-ND-C4D	-2.90	104.27	106.33
31	9	314	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	N	303	CLA	CMA-C3A-C4A	2.90	119.57	111.77
31	B	607	CLA	CHD-C1D-ND	-2.90	121.79	124.45
31	2	609	CLA	CMA-C3A-C4A	2.90	119.57	111.77
31	n	311	CLA	CMA-C3A-C4A	2.90	119.57	111.77
34	Q1	101	LMG	O8-C28-C29	2.90	121.01	111.91
31	5	610	CLA	C2C-C1C-NC	2.90	112.69	109.97
31	n	314	CLA	CMA-C3A-C4A	2.90	119.56	111.77
31	B	614	CLA	CHD-C1D-ND	-2.90	121.79	124.45
30	p	609	CHL	C4B-CHC-C1C	2.90	133.21	126.34
31	C	606	CLA	C3B-C4B-NB	-2.90	107.83	110.52
31	G	603	CLA	C3B-C4B-NB	-2.90	107.83	110.52
33	2	617	LHG	C5-O7-C7	-2.90	110.66	117.79
31	d	404	CLA	C2D-C1D-ND	2.90	112.24	110.10
30	n	302	CHL	CMA-C3A-C4A	2.90	119.56	111.77
43	C	615	BCR	C23-C24-C25	-2.90	119.06	127.20
31	y	615	CLA	C2C-C1C-NC	2.90	112.69	109.97
30	3	307	CHL	C4B-CHC-C1C	2.90	133.21	126.34
43	T	101	BCR	C38-C26-C27	2.90	119.18	113.62
32	2	615	LUT	C11-C10-C9	-2.90	123.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	q	311	CHL	C4B-CHC-C1C	2.90	133.21	126.34
37	4	619	XAT	C27-C28-C29	2.90	130.03	125.53
34	b	629	LMG	O8-C28-C29	2.90	121.00	111.91
31	q	312	CLA	CMA-C3A-C4A	2.90	119.56	111.77
30	G	601	CHL	C3B-C4B-NB	-2.90	107.83	110.52
31	y	603	CLA	CMA-C3A-C4A	2.90	119.56	111.77
31	5	603	CLA	C1-C2-C3	-2.90	121.03	126.04
31	b	613	CLA	CHD-C1D-ND	-2.90	121.79	124.45
37	g	321	XAT	C18-C5-C6	-2.90	117.41	122.26
43	C	614	BCR	C11-C12-C13	-2.90	118.28	126.42
32	N	317	LUT	C18-C5-C6	-2.90	121.28	124.53
31	b	616	CLA	C1C-C2C-C3C	-2.89	103.91	106.96
31	p	612	CLA	CHD-C1D-ND	-2.89	121.79	124.45
31	n	316	CLA	C2C-C1C-NC	2.89	112.68	109.97
30	Y	308	CHL	C4D-CHA-C1A	2.89	124.77	121.25
30	0	601	CHL	CMA-C3A-C4A	2.89	119.55	111.77
31	a	406	CLA	C2D-C1D-ND	2.89	112.24	110.10
34	y	620	LMG	O8-C28-C29	2.89	120.99	111.91
31	5	611	CLA	C1D-ND-C4D	-2.89	104.28	106.33
31	8	609	CLA	C1D-ND-C4D	-2.89	104.28	106.33
37	G	620	XAT	C18-C5-C6	-2.89	117.41	122.26
35	G	614	RRX	C20-C19-C18	-2.89	118.29	126.42
30	9	308	CHL	C3C-C4C-NC	-2.89	107.33	110.57
32	Y	316	LUT	C30-C31-C32	-2.89	114.19	123.22
31	Y	312	CLA	C3B-C4B-NB	-2.89	107.83	110.52
30	n	307	CHL	C4D-CHA-C1A	2.89	124.77	121.25
31	C	606	CLA	C2C-C1C-NC	2.89	112.68	109.97
31	p	610	CLA	C2C-C1C-NC	2.89	112.68	109.97
31	g	313	CLA	C2D-C1D-ND	2.89	112.23	110.10
31	N	321	CLA	C3B-C4B-NB	-2.89	107.83	110.52
31	q	305	CLA	C3B-C4B-NB	-2.89	107.83	110.52
30	r	310	CHL	C4D-CHA-C1A	2.89	124.77	121.25
34	B	625	LMG	O8-C28-C29	2.89	120.98	111.91
31	G	609	CLA	C2C-C1C-NC	2.89	112.68	109.97
35	9	317	RRX	C20-C19-C18	-2.89	118.30	126.42
32	G	615	LUT	C1-C6-C5	-2.89	118.54	122.61
31	S	313	CLA	C2D-C1D-ND	2.89	112.23	110.10
30	4	609	CHL	C4B-CHC-C1C	2.89	133.19	126.34
30	8	601	CHL	CMA-C3A-C4A	2.89	119.53	111.77
30	S	309	CHL	C3B-C4B-NB	-2.89	107.84	110.52
31	y	614	CLA	C3B-C4B-NB	-2.89	107.84	110.52
34	5	620	LMG	O8-C28-C29	2.89	120.97	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	305	CLA	C2D-C1D-ND	2.89	112.23	110.10
35	4	615	RRX	C20-C19-C18	-2.89	118.31	126.42
37	2	619	XAT	C27-C28-C29	2.89	130.01	125.53
31	8	610	CLA	CMA-C3A-C4A	2.89	119.53	111.77
37	q	321	XAT	C18-C5-C6	-2.89	117.42	122.26
31	Y	312	CLA	CHD-C1D-ND	-2.89	121.80	124.45
31	p	613	CLA	CHD-C1D-ND	-2.89	121.80	124.45
31	B	601	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
30	n	301	CHL	C3B-C4B-NB	-2.89	107.84	110.52
31	q	314	CLA	C3B-C4B-NB	-2.89	107.84	110.52
45	c	618	DGD	O1G-C1A-C2A	2.89	120.97	111.91
30	5	606	CHL	C3C-C4C-NC	-2.89	107.33	110.57
32	5	616	LUT	C1-C6-C5	-2.89	118.55	122.61
43	D	405	BCR	C33-C5-C4	2.89	119.16	113.62
37	4	619	XAT	C18-C5-C6	-2.89	117.42	122.26
30	Y	308	CHL	C3B-C4B-NB	-2.89	107.84	110.52
30	4	605	CHL	C3C-C4C-NC	-2.89	107.33	110.57
31	R	316	CLA	C2D-C1D-ND	2.88	112.23	110.10
31	g	313	CLA	CMA-C3A-C4A	2.88	119.53	111.77
30	0	607	CHL	C2C-C3C-C4C	2.88	108.55	106.49
30	s	308	CHL	C4B-CHC-C1C	2.88	133.18	126.34
30	N	306	CHL	CMA-C3A-C4A	2.88	119.53	111.77
31	D	404	CLA	C2C-C1C-NC	2.88	112.67	109.97
32	S	317	LUT	C21-C26-C27	-2.88	109.06	112.70
31	6	313	CLA	C3B-C4B-NB	-2.88	107.84	110.52
31	b	610	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
30	q	309	CHL	C3C-C4C-NC	-2.88	107.34	110.57
31	Y	304	CLA	C3B-C4B-NB	-2.88	107.84	110.52
31	g	305	CLA	C2D-C1D-ND	2.88	112.23	110.10
30	8	606	CHL	C4D-CHA-C1A	2.88	124.76	121.25
45	c	617	DGD	O1G-C1A-C2A	2.88	120.95	111.91
30	8	607	CHL	C2C-C3C-C4C	2.88	108.54	106.49
31	N	311	CLA	C3B-C4B-NB	-2.88	107.84	110.52
35	2	614	RRX	C38-C26-C27	2.88	119.69	114.36
34	a	401	LMG	C8-O7-C10	-2.88	110.70	117.79
31	q	312	CLA	C2C-C1C-NC	2.88	112.67	109.97
33	j	102	LHG	C5-O7-C7	-2.88	110.70	117.79
31	9	315	CLA	C1-C2-C3	-2.88	121.06	126.04
30	g	308	CHL	C4B-CHC-C1C	2.88	133.17	126.34
31	1	612	CLA	O2A-CGA-CBA	2.88	120.95	111.91
31	3	305	CLA	CHD-C1D-ND	-2.88	121.81	124.45
42	D	401	PHO	O1D-CGD-CBD	2.88	129.54	124.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	312	CLA	C1D-ND-C4D	-2.88	104.29	106.33
30	1	607	CHL	C4D-CHA-C1A	2.88	124.75	121.25
31	Y	310	CLA	CMA-C3A-C4A	2.88	119.51	111.77
30	n	306	CHL	C3B-C4B-NB	-2.88	107.84	110.52
31	b	615	CLA	C2C-C1C-NC	2.88	112.67	109.97
30	8	605	CHL	C1-C2-C3	-2.88	121.06	126.04
30	G	608	CHL	C4B-CHC-C1C	2.88	133.17	126.34
31	9	316	CLA	CMA-C3A-C4A	2.88	119.51	111.77
34	I	101	LMG	O8-C28-C29	2.88	120.94	111.91
30	y	601	CHL	C4D-CHA-C1A	2.88	124.75	121.25
30	4	609	CHL	CMA-C3A-C4A	2.88	119.51	111.77
31	C	611	CLA	C1-C2-C3	-2.88	121.06	126.04
31	b	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	p	604	CLA	C2C-C1C-NC	2.88	112.67	109.97
31	b	609	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
31	s	314	CLA	CMA-C3A-C4A	2.88	119.51	111.77
31	7	312	CLA	C3B-C4B-NB	-2.88	107.85	110.52
31	S	314	CLA	C2D-C1D-ND	2.88	112.22	110.10
34	s	321	LMG	C7-O1-C1	-2.88	108.12	113.74
30	N	306	CHL	C4B-CHC-C1C	2.88	133.16	126.34
31	R	316	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
30	8	606	CHL	C1-C2-C3	-2.88	121.07	126.04
30	n	306	CHL	C1-C2-C3	-2.88	121.07	126.04
30	S	309	CHL	C4B-CHC-C1C	2.88	133.16	126.34
31	2	610	CLA	CMA-C3A-C4A	2.88	119.50	111.77
31	5	611	CLA	CMA-C3A-C4A	2.88	119.50	111.77
31	5	612	CLA	CHD-C1D-ND	-2.88	121.81	124.45
31	5	613	CLA	C1-C2-C3	-2.88	121.07	126.04
30	N	308	CHL	C2C-C3C-C4C	2.88	108.54	106.49
31	s	306	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
31	7	316	CLA	C2D-C1D-ND	2.88	112.22	110.10
31	R	311	CLA	O2A-CGA-CBA	2.88	120.93	111.91
31	b	610	CLA	CHD-C1D-ND	-2.87	121.81	124.45
31	n	314	CLA	CHD-C1D-ND	-2.87	121.81	124.45
31	4	612	CLA	C1C-C2C-C3C	-2.87	103.93	106.96
31	Y	304	CLA	C2C-C1C-NC	2.87	112.67	109.97
32	Y	315	LUT	C35-C15-C14	-2.87	117.59	123.47
31	B	614	CLA	CMA-C3A-C4A	2.87	119.50	111.77
31	p	610	CLA	CMA-C3A-C4A	2.87	119.50	111.77
31	Y	304	CLA	C2D-C1D-ND	2.87	112.22	110.10
31	p	612	CLA	C3B-C4B-NB	-2.87	107.85	110.52
43	Z	101	BCR	C11-C12-C13	-2.87	118.34	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	W	202	LMG	O8-C28-C29	2.87	120.92	111.91
43	B	619	BCR	C38-C26-C27	2.87	119.14	113.62
31	a	406	CLA	CHD-C1D-ND	-2.87	121.81	124.45
31	3	315	CLA	C3B-C4B-NB	-2.87	107.85	110.52
30	p	605	CHL	C4B-CHC-C1C	2.87	133.15	126.34
30	Y	301	CHL	C4B-CHC-C1C	2.87	133.15	126.34
30	6	309	CHL	C3B-C4B-NB	-2.87	107.85	110.52
31	Y	310	CLA	C2C-C1C-NC	2.87	112.66	109.97
30	r	308	CHL	C4B-CHC-C1C	2.87	133.15	126.34
37	G	620	XAT	C27-C28-C29	2.87	129.99	125.53
32	p	616	LUT	C7-C8-C9	-2.87	121.90	126.23
31	S	303	CLA	C2C-C1C-NC	2.87	112.66	109.97
30	8	607	CHL	C4B-CHC-C1C	2.87	133.15	126.34
30	2	605	CHL	C2C-C3C-C4C	2.87	108.53	106.49
31	N	315	CLA	CMA-C3A-C4A	2.87	119.49	111.77
31	6	305	CLA	C2D-C1D-ND	2.87	112.22	110.10
30	y	605	CHL	C2B-C1B-NB	-2.87	108.31	110.23
32	s	317	LUT	C8-C7-C6	-2.87	119.14	127.20
36	4	617	NEX	C17-C1-C6	-2.87	107.90	110.47
31	3	301	CLA	C2C-C1C-NC	2.87	112.66	109.97
37	9	322	XAT	C18-C5-C6	-2.87	117.45	122.26
36	g	317	NEX	C39-C29-C30	-2.87	118.90	122.92
31	S	306	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	4	608	CHL	C4D-CHA-C1A	2.87	124.74	121.25
31	1	614	CLA	CMA-C3A-C4A	2.87	119.48	111.77
30	G	608	CHL	C2C-C3C-C4C	2.87	108.53	106.49
30	y	607	CHL	C4B-CHC-C1C	2.87	133.14	126.34
30	9	308	CHL	C3B-C4B-NB	-2.87	107.86	110.52
31	b	607	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	N	307	CHL	C4D-CHA-C1A	2.87	124.74	121.25
30	R	308	CHL	CMA-C3A-C4A	2.87	119.48	111.77
31	n	312	CLA	CMA-C3A-C4A	2.87	119.48	111.77
30	5	601	CHL	C3C-C4C-NC	-2.87	107.36	110.57
30	R	308	CHL	C3C-C4C-NC	-2.87	107.36	110.57
30	7	309	CHL	C4B-CHC-C1C	2.87	133.13	126.34
31	B	602	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
31	3	314	CLA	CHD-C1D-ND	-2.87	121.82	124.45
31	Y	313	CLA	CHD-C1D-ND	-2.87	121.82	124.45
33	8	618	LHG	O8-C23-C24	2.87	120.90	111.91
31	4	612	CLA	C2C-C1C-NC	2.87	112.66	109.97
34	R	321	LMG	O8-C28-C29	2.86	120.90	111.91
32	y	616	LUT	C35-C15-C14	-2.86	117.61	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	610	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
30	9	310	CHL	C3B-C4B-NB	-2.86	107.86	110.52
31	p	614	CLA	C3B-C4B-NB	-2.86	107.86	110.52
30	n	309	CHL	C4B-CHC-C1C	2.86	133.13	126.34
31	p	603	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
31	R	307	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
31	q	305	CLA	C2D-C1D-ND	2.86	112.21	110.10
30	2	608	CHL	C4B-CHC-C1C	2.86	133.13	126.34
30	8	606	CHL	C1-O2A-CGA	2.86	123.96	116.44
31	5	615	CLA	CMA-C3A-C4A	2.86	119.47	111.77
32	y	616	LUT	C15-C14-C13	-2.86	123.22	127.31
30	1	607	CHL	C4B-CHC-C1C	2.86	133.13	126.34
30	G	623	CHL	C1-C2-C3	-2.86	121.09	126.04
37	2	619	XAT	C18-C5-C6	-2.86	117.46	122.26
31	7	313	CLA	C2D-C1D-ND	2.86	112.21	110.10
31	3	301	CLA	C1D-ND-C4D	-2.86	104.30	106.33
31	B	606	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
31	s	311	CLA	C1-C2-C3	-2.86	121.09	126.04
31	1	612	CLA	C2C-C1C-NC	2.86	112.65	109.97
30	N	308	CHL	C4B-CHC-C1C	2.86	133.12	126.34
31	3	314	CLA	CMA-C3A-C4A	2.86	119.46	111.77
33	n	320	LHG	O8-C23-C24	2.86	120.88	111.91
31	b	603	CLA	C3B-C4B-NB	-2.86	107.86	110.52
32	y	617	LUT	C15-C35-C34	-2.86	117.62	123.47
31	B	612	CLA	CHD-C1D-ND	-2.86	121.83	124.45
31	G	613	CLA	C2C-C1C-NC	2.86	112.65	109.97
31	7	311	CLA	C2C-C1C-NC	2.86	112.65	109.97
31	p	611	CLA	CMA-C3A-C4A	2.86	119.46	111.77
30	2	606	CHL	C4B-CHC-C1C	2.86	133.12	126.34
43	C	614	BCR	C24-C23-C22	-2.86	121.92	126.23
31	g	312	CLA	CMA-C3A-C4A	2.86	119.46	111.77
31	5	603	CLA	CMA-C3A-C4A	2.86	119.46	111.77
30	y	606	CHL	C4B-CHC-C1C	2.86	133.12	126.34
30	3	307	CHL	CMA-C3A-C4A	2.86	119.45	111.77
31	c	613	CLA	C2D-C1D-ND	2.86	112.21	110.10
31	y	613	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
31	c	608	CLA	C2C-C1C-NC	2.86	112.65	109.97
30	6	307	CHL	CMA-C3A-C4A	2.86	119.45	111.77
30	8	607	CHL	C1-O2A-CGA	2.86	123.94	116.44
31	S	306	CLA	CMA-C3A-C4A	2.86	119.45	111.77
31	N	304	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
31	r	315	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	601	CHL	C3B-C4B-NB	-2.86	107.86	110.52
30	7	309	CHL	C3B-C4B-NB	-2.86	107.86	110.52
31	R	306	CLA	CAA-C2A-C3A	-2.86	104.96	112.78
31	S	316	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
30	1	608	CHL	C3B-C4B-NB	-2.86	107.87	110.52
43	V	101	BCR	C10-C11-C12	-2.85	114.31	123.22
31	B	612	CLA	C1D-ND-C4D	-2.85	104.31	106.33
30	8	601	CHL	C3B-C4B-NB	-2.85	107.87	110.52
31	s	306	CLA	C3B-C4B-NB	-2.85	107.87	110.52
45	C	616	DGD	O1G-C1A-C2A	2.85	120.86	111.91
31	9	306	CLA	CMA-C3A-C4A	2.85	119.44	111.77
31	R	303	CLA	C2D-C1D-ND	2.85	112.21	110.10
31	S	306	CLA	C3B-C4B-NB	-2.85	107.87	110.52
31	G	611	CLA	CHD-C1D-ND	-2.85	121.83	124.45
31	y	615	CLA	C1D-ND-C4D	-2.85	104.31	106.33
30	p	605	CHL	CMA-C3A-C4A	2.85	119.44	111.77
32	5	616	LUT	C7-C8-C9	-2.85	121.93	126.23
31	y	604	CLA	C2D-C1D-ND	2.85	112.20	110.10
31	S	314	CLA	CHD-C1D-ND	-2.85	121.83	124.45
30	n	302	CHL	C1-O2A-CGA	2.85	123.92	116.44
31	7	312	CLA	CMA-C3A-C4A	2.85	119.43	111.77
30	S	308	CHL	C4D-CHA-C1A	2.85	124.72	121.25
30	y	606	CHL	CMA-C3A-C4A	2.85	119.43	111.77
45	c	616	DGD	O1G-C1A-C2A	2.85	120.85	111.91
30	Y	306	CHL	C2C-C3C-C4C	2.85	108.52	106.49
31	G	604	CLA	C1D-ND-C4D	-2.85	104.31	106.33
31	q	304	CLA	C1D-ND-C4D	-2.85	104.31	106.33
30	0	601	CHL	C3B-C4B-NB	-2.85	107.87	110.52
31	A	405	CLA	CHD-C1D-ND	-2.85	121.84	124.45
31	b	611	CLA	CMA-C3A-C4A	2.85	119.43	111.77
31	b	606	CLA	C2D-C1D-ND	2.85	112.20	110.10
30	p	608	CHL	C4D-CHA-C1A	2.85	124.72	121.25
30	g	308	CHL	C3B-C4B-NB	-2.85	107.87	110.52
31	b	611	CLA	C3B-C4B-NB	-2.85	107.87	110.52
43	c	614	BCR	C35-C13-C14	-2.85	118.93	122.92
31	a	407	CLA	CMA-C3A-C4A	2.85	119.43	111.77
43	c	614	BCR	C23-C22-C21	2.85	123.31	118.94
31	8	614	CLA	C2D-C1D-ND	2.85	112.20	110.10
31	r	305	CLA	C2D-C1D-ND	2.85	112.20	110.10
31	C	601	CLA	C3B-C4B-NB	-2.85	107.87	110.52
31	b	602	CLA	C3B-C4B-NB	-2.85	107.87	110.52
31	2	610	CLA	C1D-ND-C4D	-2.85	104.31	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	610	CLA	O2A-CGA-CBA	2.85	120.84	111.91
31	1	603	CLA	C1-C2-C3	-2.85	121.12	126.04
31	A	406	CLA	CAA-C2A-C3A	-2.85	104.99	112.78
30	n	307	CHL	C1-O2A-CGA	2.85	123.91	116.44
31	3	316	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
31	7	314	CLA	CMA-C3A-C4A	2.85	119.42	111.77
31	b	602	CLA	C2C-C1C-NC	2.84	112.64	109.97
31	3	312	CLA	C1-C2-C3	-2.84	121.12	126.04
31	B	613	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
30	8	601	CHL	C1-O2A-CGA	2.84	123.91	116.44
31	0	614	CLA	CMA-C3A-C4A	2.84	119.42	111.77
31	d	401	CLA	CMA-C3A-C4A	2.84	119.42	111.77
30	s	308	CHL	C3B-C4B-NB	-2.84	107.88	110.52
30	5	607	CHL	C4B-CHC-C1C	2.84	133.08	126.34
31	p	602	CLA	C2D-C1D-ND	2.84	112.20	110.10
31	c	602	CLA	CHD-C1D-ND	-2.84	121.84	124.45
31	C	606	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
31	p	610	CLA	C1D-ND-C4D	-2.84	104.32	106.33
31	r	305	CLA	C1-C2-C3	-2.84	121.13	126.04
31	p	611	CLA	CHD-C1D-ND	-2.84	121.84	124.45
30	G	601	CHL	CMA-C3A-C4A	2.84	119.41	111.77
31	6	315	CLA	CMA-C3A-C4A	2.84	119.41	111.77
31	1	610	CLA	C2C-C1C-NC	2.84	112.63	109.97
30	p	609	CHL	C3B-C4B-NB	-2.84	107.88	110.52
31	5	614	CLA	C3B-C4B-NB	-2.84	107.88	110.52
36	4	617	NEX	C26-C27-C28	-2.84	119.99	125.99
31	R	313	CLA	CHD-C1D-ND	-2.84	121.84	124.45
30	G	601	CHL	C4B-CHC-C1C	2.84	133.07	126.34
31	S	315	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
30	g	302	CHL	C2C-C3C-C4C	2.84	108.51	106.49
30	1	606	CHL	C4B-CHC-C1C	2.84	133.07	126.34
30	y	601	CHL	C4B-CHC-C1C	2.84	133.07	126.34
43	A	410	BCR	C33-C5-C4	2.84	119.07	113.62
30	n	307	CHL	C1-C2-C3	-2.84	121.13	126.04
31	6	303	CLA	C1D-ND-C4D	-2.84	104.32	106.33
31	n	304	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
43	T	101	BCR	C11-C12-C13	-2.84	118.44	126.42
30	Y	308	CHL	C4B-CHC-C1C	2.84	133.06	126.34
31	S	306	CLA	C2C-C1C-NC	2.84	112.63	109.97
31	3	306	CLA	C2D-C1D-ND	2.84	112.19	110.10
31	5	613	CLA	C2D-C1D-ND	2.84	112.19	110.10
30	6	306	CHL	C3B-C4B-NB	-2.84	107.88	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	612	CLA	C3B-C4B-NB	-2.84	107.88	110.52
31	G	602	CLA	CMA-C3A-C4A	2.84	119.39	111.77
30	6	308	CHL	C4B-CHC-C1C	2.84	133.06	126.34
31	C	613	CLA	CHD-C1D-ND	-2.84	121.85	124.45
31	p	614	CLA	CMA-C3A-C4A	2.84	119.39	111.77
31	g	314	CLA	CMA-C3A-C4A	2.84	119.39	111.77
30	5	609	CHL	C4B-CHC-C1C	2.83	133.06	126.34
31	r	306	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
31	c	612	CLA	C2D-C1D-ND	2.83	112.19	110.10
31	S	303	CLA	CMA-C3A-C4A	2.83	119.39	111.77
32	7	318	LUT	C11-C10-C9	-2.83	123.27	127.31
31	r	312	CLA	C2C-C1C-NC	2.83	112.63	109.97
30	G	606	CHL	C4D-CHA-C1A	2.83	124.70	121.25
30	4	608	CHL	C3B-C4B-NB	-2.83	107.89	110.52
30	6	306	CHL	C2C-C3C-C4C	2.83	108.51	106.49
31	n	303	CLA	C1D-ND-C4D	-2.83	104.32	106.33
30	8	605	CHL	C3B-C4B-NB	-2.83	107.89	110.52
30	q	303	CHL	C1-O2A-CGA	2.83	123.88	116.44
31	c	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	9	308	CHL	CMA-C3A-C4A	2.83	119.39	111.77
30	3	308	CHL	C2B-C1B-NB	-2.83	108.33	110.23
31	p	614	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
31	D	403	CLA	CHD-C1D-ND	-2.83	121.85	124.45
31	C	605	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
30	Y	302	CHL	C4D-CHA-C1A	2.83	124.69	121.25
30	Y	306	CHL	C4B-CHC-C1C	2.83	133.05	126.34
31	9	305	CLA	CMA-C3A-C4A	2.83	119.38	111.77
31	b	612	CLA	C1D-ND-C4D	-2.83	104.33	106.33
31	b	615	CLA	C1D-ND-C4D	-2.83	104.33	106.33
34	D	410	LMG	O8-C28-C29	2.83	120.79	111.91
30	1	605	CHL	C3C-C4C-NC	-2.83	107.40	110.57
31	C	609	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
31	c	610	CLA	C2C-C1C-NC	2.83	112.62	109.97
30	g	302	CHL	C3B-C4B-NB	-2.83	107.89	110.52
31	4	613	CLA	C3B-C4B-NB	-2.83	107.89	110.52
31	n	316	CLA	CMA-C3A-C4A	2.83	119.38	111.77
31	n	313	CLA	C1D-ND-C4D	-2.83	104.33	106.33
30	9	311	CHL	C4B-CHC-C1C	2.83	133.04	126.34
31	1	602	CLA	C2C-C1C-NC	2.83	112.62	109.97
30	n	302	CHL	C3B-C4B-NB	-2.83	107.89	110.52
37	r	318	XAT	C38-C25-C26	-2.83	117.52	122.26
31	1	613	CLA	CMA-C3A-C4A	2.83	119.37	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	613	CLA	O2A-CGA-CBA	2.83	120.78	111.91
31	r	304	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
31	r	305	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
31	6	316	CLA	CHD-C1D-ND	-2.83	121.86	124.45
31	B	601	CLA	C2C-C1C-NC	2.83	112.62	109.97
31	C	605	CLA	CHA-C4D-ND	2.83	138.41	132.50
31	8	610	CLA	CHD-C1D-ND	-2.83	121.86	124.45
31	5	614	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
31	S	304	CLA	C2C-C1C-NC	2.83	112.62	109.97
31	s	306	CLA	C2C-C1C-NC	2.83	112.62	109.97
31	2	613	CLA	CMA-C3A-C4A	2.83	119.37	111.77
30	g	309	CHL	C1-C2-C3	-2.83	121.16	126.04
31	Y	311	CLA	CHD-C1D-ND	-2.82	121.86	124.45
30	y	608	CHL	C3B-C4B-NB	-2.82	107.89	110.52
31	s	303	CLA	CMA-C3A-C4A	2.82	119.36	111.77
32	n	317	LUT	C8-C7-C6	-2.82	119.27	127.20
31	q	305	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
31	q	314	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
30	N	302	CHL	C3B-C4B-NB	-2.82	107.90	110.52
34	X	202	LMG	O8-C28-C29	2.82	120.76	111.91
31	b	609	CLA	C2D-C1D-ND	2.82	112.18	110.10
30	1	609	CHL	C3B-C4B-NB	-2.82	107.90	110.52
31	s	304	CLA	C3B-C4B-NB	-2.82	107.90	110.52
31	c	611	CLA	O2A-CGA-CBA	2.82	120.76	111.91
30	R	310	CHL	C1-C2-C3	-2.82	121.17	126.04
30	8	606	CHL	C2C-C3C-C4C	2.82	108.50	106.49
31	6	313	CLA	C1D-ND-C4D	-2.82	104.33	106.33
43	C	614	BCR	C21-C20-C19	-2.82	114.42	123.22
31	B	608	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
34	2	621	LMG	O8-C28-C29	2.82	120.75	111.91
32	R	317	LUT	C31-C32-C33	2.82	134.33	126.42
31	3	312	CLA	CHD-C1D-ND	-2.82	121.86	124.45
32	8	616	LUT	C21-C26-C27	-2.82	109.14	112.70
30	n	307	CHL	C2C-C3C-C4C	2.82	108.50	106.49
31	s	312	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
33	q	320	LHG	O8-C23-C24	2.82	120.75	111.91
31	c	607	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
31	d	405	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
31	B	614	CLA	C2C-C1C-NC	2.82	112.61	109.97
31	3	311	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
43	c	615	BCR	C36-C18-C17	-2.82	118.98	122.92
31	b	617	CLA	O2D-CGD-O1D	-2.82	118.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	308	CHL	C4B-CHC-C1C	2.82	133.01	126.34
30	Y	306	CHL	C3B-C4B-NB	-2.81	107.90	110.52
31	S	304	CLA	C3B-C4B-NB	-2.81	107.90	110.52
36	Y	317	NEX	C39-C29-C30	-2.81	118.98	122.92
31	N	321	CLA	C1D-ND-C4D	-2.81	104.34	106.33
30	4	608	CHL	C4B-CHC-C1C	2.81	133.01	126.34
43	B	617	BCR	C10-C11-C12	-2.81	114.44	123.22
30	2	607	CHL	C4B-CHC-C1C	2.81	133.01	126.34
30	6	302	CHL	C3B-C4B-NB	-2.81	107.91	110.52
43	T	101	BCR	C16-C17-C18	-2.81	123.30	127.31
31	8	611	CLA	C1D-ND-C4D	-2.81	104.34	106.33
30	5	606	CHL	C3B-C4B-NB	-2.81	107.91	110.52
31	0	610	CLA	C3B-C4B-NB	-2.81	107.91	110.52
32	n	318	LUT	C21-C26-C27	-2.81	109.15	112.70
31	C	604	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
30	g	302	CHL	C4D-CHA-C1A	2.81	124.67	121.25
43	c	615	BCR	C24-C23-C22	-2.81	121.99	126.23
31	r	312	CLA	C1-C2-C3	-2.81	121.18	126.04
31	g	305	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
30	6	302	CHL	C4B-CHC-C1C	2.81	133.00	126.34
30	9	303	CHL	C4B-CHC-C1C	2.81	133.00	126.34
31	7	304	CLA	C2C-C1C-NC	2.81	112.61	109.97
30	G	607	CHL	C3C-C4C-NC	-2.81	107.42	110.57
31	B	601	CLA	C3B-C4B-NB	-2.81	107.91	110.52
31	q	315	CLA	C1-C2-C3	-2.81	121.18	126.04
31	9	315	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
30	9	303	CHL	C3B-C4B-NB	-2.81	107.91	110.52
31	r	314	CLA	C2C-C1C-NC	2.81	112.60	109.97
30	g	307	CHL	C4B-CHC-C1C	2.81	133.00	126.34
31	5	613	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	B	611	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	s	305	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
30	5	605	CHL	C3B-C4B-NB	-2.81	107.91	110.52
31	y	614	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	c	601	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	C	607	CLA	C2D-C1D-ND	2.81	112.17	110.10
31	b	614	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
31	C	601	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	7	311	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	C	602	CLA	CHD-C1D-ND	-2.81	121.88	124.45
31	3	312	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
31	r	316	CLA	C1C-C2C-C3C	-2.81	104.01	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	612	CLA	C2D-C1D-ND	2.81	112.17	110.10
34	q	302	LMG	O8-C28-C29	2.81	120.71	111.91
31	7	316	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
31	n	305	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
31	3	306	CLA	CMA-C3A-C4A	2.80	119.31	111.77
30	q	308	CHL	C2B-C1B-NB	-2.80	108.35	110.23
31	B	606	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	2	603	CLA	C1D-ND-C4D	-2.80	104.34	106.33
31	N	314	CLA	C1D-ND-C4D	-2.80	104.34	106.33
31	3	314	CLA	C3B-C4B-NB	-2.80	107.91	110.52
32	8	615	LUT	C8-C7-C6	-2.80	119.33	127.20
31	9	315	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	R	303	CLA	CHD-C1D-ND	-2.80	121.88	124.45
30	6	307	CHL	C4B-CHC-C1C	2.80	132.99	126.34
31	C	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	p	606	CHL	CMA-C3A-C4A	2.80	119.31	111.77
36	G	616	NEX	C19-C9-C10	-2.80	119.00	122.92
30	N	302	CHL	C1-C2-C3	-2.80	121.20	126.04
31	d	401	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	g	313	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	C	601	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	q	314	CLA	CMA-C3A-C4A	2.80	119.30	111.77
31	9	314	CLA	CHD-C1D-ND	-2.80	121.88	124.45
31	2	603	CLA	C3B-C4B-NB	-2.80	107.92	110.52
31	8	612	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	1	612	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	g	310	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	s	316	CLA	C2D-C1D-ND	2.80	112.17	110.10
30	p	608	CHL	C3B-C4B-NB	-2.80	107.92	110.52
30	3	308	CHL	C4B-CHC-C1C	2.80	132.98	126.34
31	4	610	CLA	C2C-C1C-NC	2.80	112.59	109.97
31	1	614	CLA	C1D-ND-C4D	-2.80	104.35	106.33
30	G	605	CHL	C3B-C4B-NB	-2.80	107.92	110.52
30	2	607	CHL	C3B-C4B-NB	-2.80	107.92	110.52
30	4	601	CHL	CMA-C3A-C4A	2.80	119.29	111.77
31	4	613	CLA	CMA-C3A-C4A	2.80	119.29	111.77
43	c	615	BCR	C23-C24-C25	-2.80	119.35	127.20
31	C	601	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
31	c	611	CLA	C2D-C1D-ND	2.80	112.17	110.10
32	r	317	LUT	C7-C8-C9	-2.80	122.01	126.23
43	c	614	BCR	C20-C19-C18	2.80	134.27	126.42
31	7	313	CLA	C1C-C2C-C3C	-2.80	104.02	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	304	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
31	B	604	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	g	308	CHL	CMA-C3A-C4A	2.80	119.29	111.77
31	0	615	CLA	CMA-C3A-C4A	2.80	119.29	111.77
31	q	316	CLA	CMA-C3A-C4A	2.80	119.29	111.77
30	g	306	CHL	C3B-C4B-NB	-2.80	107.92	110.52
31	n	314	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
30	5	605	CHL	CMA-C3A-C4A	2.79	119.28	111.77
31	c	611	CLA	CAA-CBA-CGA	-2.79	105.09	113.25
31	N	314	CLA	O2A-CGA-CBA	2.79	120.67	111.91
31	G	613	CLA	C3B-C4B-NB	-2.79	107.92	110.52
31	8	610	CLA	C1D-ND-C4D	-2.79	104.35	106.33
31	c	601	CLA	C2D-C1D-ND	2.79	112.16	110.10
31	3	316	CLA	CMD-C2D-C3D	-2.79	121.19	127.61
31	s	310	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
34	b	622	LMG	O1-C1-C2	2.79	112.66	108.30
30	G	605	CHL	C2C-C3C-C4C	2.79	108.48	106.49
31	B	611	CLA	C2C-C1C-NC	2.79	112.59	109.97
30	G	623	CHL	C4B-CHC-C1C	2.79	132.96	126.34
31	3	313	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
31	S	311	CLA	C1-C2-C3	-2.79	121.22	126.04
43	C	615	BCR	C30-C25-C26	-2.79	118.68	122.61
31	3	316	CLA	CMA-C3A-C4A	2.79	119.27	111.77
31	6	316	CLA	CMA-C3A-C4A	2.79	119.27	111.77
31	G	602	CLA	C1D-ND-C4D	-2.79	104.35	106.33
30	q	307	CHL	C3B-C4B-NB	-2.79	107.93	110.52
31	3	316	CLA	C3B-C4B-NB	-2.79	107.93	110.52
30	3	310	CHL	C4B-CHC-C1C	2.79	132.95	126.34
31	7	303	CLA	C1-C2-C3	-2.79	121.22	126.04
31	g	303	CLA	CMA-C3A-C4A	2.79	119.26	111.77
31	B	609	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
31	s	306	CLA	CMA-C3A-C4A	2.79	119.26	111.77
31	C	611	CLA	O2A-CGA-CBA	2.79	120.65	111.91
30	8	605	CHL	C4B-CHC-C1C	2.79	132.94	126.34
36	n	319	NEX	C20-C13-C14	-2.79	119.02	122.92
32	3	317	LUT	C1-C6-C5	-2.79	118.69	122.61
43	b	620	BCR	C38-C26-C27	2.79	118.97	113.62
31	C	610	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	4	605	CHL	C3B-C4B-NB	-2.79	107.93	110.52
31	b	604	CLA	O2A-CGA-CBA	2.78	120.65	111.91
30	4	601	CHL	C4D-CHA-C1A	2.78	124.64	121.25
30	n	309	CHL	C2C-C3C-C4C	2.78	108.47	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	610	CLA	CHD-C1D-ND	-2.78	121.89	124.45
30	8	605	CHL	CMA-C3A-C4A	2.78	119.26	111.77
31	C	608	CLA	C2D-C1D-ND	2.78	112.16	110.10
31	G	603	CLA	C2D-C1D-ND	2.78	112.16	110.10
31	7	305	CLA	C2D-C1D-ND	2.78	112.16	110.10
31	2	611	CLA	C1D-ND-C4D	-2.78	104.36	106.33
32	r	317	LUT	C20-C13-C12	2.78	122.46	118.08
35	q	317	RRX	C35-C13-C14	-2.78	119.02	122.92
34	d	410	LMG	O8-C28-C29	2.78	120.64	111.91
31	n	312	CLA	CHD-C1D-ND	-2.78	121.90	124.45
31	p	602	CLA	CMA-C3A-C4A	2.78	119.25	111.77
30	p	608	CHL	C2C-C3C-C4C	2.78	108.47	106.49
31	r	314	CLA	C3B-C4B-NB	-2.78	107.93	110.52
31	y	612	CLA	C3B-C4B-NB	-2.78	107.93	110.52
30	G	606	CHL	C4B-CHC-C1C	2.78	132.94	126.34
31	D	404	CLA	C1D-ND-C4D	-2.78	104.36	106.33
30	S	307	CHL	CMA-C3A-C4A	2.78	119.25	111.77
31	6	304	CLA	C1-C2-C3	-2.78	121.23	126.04
31	9	305	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
34	D	411	LMG	O8-C28-C29	2.78	120.64	111.91
34	S	321	LMG	O8-C28-C29	2.78	120.64	111.91
36	8	617	NEX	C17-C1-C6	-2.78	107.98	110.47
31	2	602	CLA	C3B-C4B-NB	-2.78	107.94	110.52
31	1	604	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
31	1	613	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
31	R	305	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	b	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	2	602	CLA	CHD-C1D-ND	-2.78	121.90	124.45
30	p	608	CHL	C4B-CHC-C1C	2.78	132.93	126.34
34	q1	101	LMG	O8-C28-C29	2.78	120.63	111.91
31	c	604	CLA	C2D-C1D-ND	2.78	112.15	110.10
31	7	313	CLA	C4B-CHC-C1C	2.78	132.93	126.34
31	8	613	CLA	C1D-ND-C4D	-2.78	104.36	106.33
30	n	306	CHL	C4B-CHC-C1C	2.78	132.93	126.34
31	A	405	CLA	C2D-C1D-ND	2.78	112.15	110.10
31	N	312	CLA	CMA-C3A-C4A	2.78	119.24	111.77
36	5	618	NEX	C26-C27-C28	-2.78	120.12	125.99
35	g	315	RRX	C8-C7-C6	-2.78	119.41	127.20
31	N	303	CLA	C1D-ND-C4D	-2.78	104.36	106.33
31	a	409	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
30	G	608	CHL	C1-O2A-CGA	2.78	123.73	116.44
43	B	619	BCR	C23-C24-C25	-2.78	119.41	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	H	101	BCR	C38-C26-C27	2.78	118.95	113.62
31	7	304	CLA	C2D-C1D-ND	2.77	112.15	110.10
30	4	606	CHL	C2C-C3C-C4C	2.77	108.47	106.49
30	N	302	CHL	C2C-C3C-C4C	2.77	108.47	106.49
31	b	613	CLA	C2C-C1C-NC	2.77	112.57	109.97
30	4	606	CHL	C4D-CHA-C1A	2.77	124.62	121.25
31	4	604	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
30	n	306	CHL	CMA-C3A-C4A	2.77	119.23	111.77
31	N	311	CLA	CHD-C1D-ND	-2.77	121.91	124.45
31	R	306	CLA	O1D-CGD-CBD	-2.77	118.81	124.48
30	2	601	CHL	C3B-C4B-NB	-2.77	107.94	110.52
30	1	605	CHL	C3B-C4B-NB	-2.77	107.94	110.52
31	B	607	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	1	619	CHL	CHB-C4A-NA	2.77	128.34	124.51
30	N	301	CHL	CMA-C3A-C4A	2.77	119.22	111.77
31	G	612	CLA	CMA-C3A-C4A	2.77	119.22	111.77
31	4	613	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	C	611	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	0	602	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	s	311	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	3	315	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	0	615	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	n	315	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	C	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
31	B	608	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
31	R	304	CLA	O2A-CGA-CBA	2.77	120.60	111.91
34	s	321	LMG	O8-C28-C29	2.77	120.60	111.91
31	2	611	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
31	S	310	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
30	s	302	CHL	CHB-C4A-NA	2.77	128.34	124.51
31	y	602	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	b	616	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	2	607	CHL	C4D-CHA-C1A	2.77	124.62	121.25
30	6	310	CHL	C3B-C4B-NB	-2.77	107.95	110.52
31	R	313	CLA	C3B-C4B-NB	-2.77	107.95	110.52
31	C	605	CLA	C1-O2A-CGA	2.77	123.71	116.44
30	s	307	CHL	C3C-C4C-NC	-2.77	107.47	110.57
31	b	608	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
31	R	304	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
43	A	410	BCR	C1-C6-C5	-2.77	118.72	122.61
30	3	308	CHL	C3C-C4C-NC	-2.77	107.47	110.57
30	2	601	CHL	C4D-CHA-C1A	2.77	124.62	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	610	CLA	CMA-C3A-C4A	2.77	119.21	111.77
33	R	320	LHG	C5-O7-C7	-2.77	110.98	117.79
31	3	314	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	9	306	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	p	612	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	n	316	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	q	314	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
30	0	606	CHL	C3C-C4C-NC	-2.77	107.47	110.57
31	p	603	CLA	O2A-CGA-CBA	2.77	120.59	111.91
31	b	615	CLA	CMA-C3A-C4A	2.77	119.21	111.77
31	8	603	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
31	B	602	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
34	g	320	LMG	C8-O7-C10	-2.76	110.98	117.79
31	4	614	CLA	C2D-C1D-ND	2.76	112.14	110.10
30	7	310	CHL	CMA-C3A-C4A	2.76	119.20	111.77
31	A	407	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
31	r	315	CLA	C2D-C1D-ND	2.76	112.14	110.10
32	3	317	LUT	C8-C7-C6	-2.76	119.44	127.20
31	B	611	CLA	C1D-ND-C4D	-2.76	104.37	106.33
31	g	304	CLA	C3B-C4B-NB	-2.76	107.95	110.52
32	4	616	LUT	C21-C26-C27	-2.76	109.21	112.70
30	S	302	CHL	C4B-CHC-C1C	2.76	132.89	126.34
31	g	310	CLA	O2A-CGA-CBA	2.76	120.57	111.91
31	y	613	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
30	r	309	CHL	C4B-CHC-C1C	2.76	132.89	126.34
33	C	623	LHG	O8-C23-C24	2.76	120.57	111.91
32	3	318	LUT	C21-C26-C27	-2.76	109.21	112.70
30	q	303	CHL	C3B-C4B-NB	-2.76	107.95	110.52
31	5	613	CLA	C3B-C4B-NB	-2.76	107.95	110.52
31	6	314	CLA	C1D-ND-C4D	-2.76	104.37	106.33
31	C	607	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
31	S	316	CLA	CMA-C3A-C4A	2.76	119.19	111.77
35	g	315	RRX	C38-C26-C27	2.76	119.47	114.36
31	N	321	CLA	CMA-C3A-C4A	2.76	119.19	111.77
43	b	620	BCR	C33-C5-C4	2.76	118.92	113.62
31	N	314	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
30	q	307	CHL	C2C-C3C-C4C	2.76	108.46	106.49
34	a	413	LMG	O8-C28-C29	2.76	120.56	111.91
31	n	313	CLA	CMA-C3A-C4A	2.76	119.19	111.77
31	g	311	CLA	CHD-C1D-ND	-2.76	121.92	124.45
35	g	315	RRX	C34-C9-C10	-2.76	119.06	122.92
31	G	613	CLA	CMA-C3A-C4A	2.76	119.19	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	603	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
31	8	602	CLA	C1D-ND-C4D	-2.76	104.38	106.33
31	3	316	CLA	C1-C2-C3	-2.76	121.27	126.04
32	1	615	LUT	C31-C30-C29	-2.76	123.38	127.31
30	S	307	CHL	C3C-C4C-NC	-2.76	107.48	110.57
31	A	407	CLA	CMA-C3A-C4A	2.76	119.18	111.77
30	N	306	CHL	C4D-CHA-C1A	2.76	124.60	121.25
31	c	603	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
33	t	102	LHG	O8-C23-C24	2.76	120.56	111.91
31	D	403	CLA	C1-C2-C3	-2.76	121.28	126.04
31	6	305	CLA	C1D-ND-C4D	-2.76	104.38	106.33
31	5	604	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
30	Y	302	CHL	C4B-CHC-C1C	2.76	132.87	126.34
43	B	618	BCR	C20-C19-C18	-2.76	118.68	126.42
31	9	316	CLA	C1D-ND-C4D	-2.75	104.38	106.33
33	z	102	LHG	O8-C23-C24	2.75	120.55	111.91
31	4	612	CLA	CMA-C3A-C4A	2.75	119.17	111.77
31	b	612	CLA	C2C-C1C-NC	2.75	112.55	109.97
31	7	304	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
30	r	310	CHL	C2C-C3C-C4C	2.75	108.45	106.49
32	2	615	LUT	C18-C5-C4	2.75	119.46	114.36
31	r	312	CLA	C2D-C1D-ND	2.75	112.13	110.10
31	6	312	CLA	CHD-C1D-ND	-2.75	121.92	124.45
31	r	313	CLA	C3B-C4B-NB	-2.75	107.96	110.52
31	3	314	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	c	610	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	7	315	CLA	CMA-C3A-C4A	2.75	119.17	111.77
31	R	311	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	7	314	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	s	304	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
30	4	606	CHL	C3B-C4B-NB	-2.75	107.96	110.52
30	s	309	CHL	C1-O2A-CGA	2.75	123.66	116.44
31	c	602	CLA	C6-C5-C3	-2.75	106.24	113.45
32	0	617	LUT	C1-C6-C5	-2.75	118.74	122.61
31	5	603	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	5	613	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	c	611	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	5	605	CHL	C2B-C1B-NB	-2.75	108.39	110.23
31	y	603	CLA	C2D-C1D-ND	2.75	112.13	110.10
31	g	304	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
30	9	307	CHL	C2C-C3C-C4C	2.75	108.45	106.49
31	8	611	CLA	CMA-C3A-C4A	2.75	119.16	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	610	CLA	O2A-CGA-CBA	2.75	120.54	111.91
31	b	603	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	2	604	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	g	312	CLA	C1D-ND-C4D	-2.75	104.38	106.33
32	6	317	LUT	C30-C31-C32	-2.75	114.64	123.22
32	0	617	LUT	C18-C5-C4	2.75	119.44	114.36
30	n	307	CHL	C4B-CHC-C1C	2.75	132.85	126.34
31	r	306	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	4	601	CHL	C4B-CHC-C1C	2.75	132.85	126.34
31	r	312	CLA	O2A-CGA-CBA	2.75	120.53	111.91
30	Y	309	CHL	C3B-C4B-NB	-2.75	107.97	110.52
31	5	614	CLA	CHD-C1D-ND	-2.75	121.93	124.45
30	1	608	CHL	C4B-CHC-C1C	2.75	132.85	126.34
31	R	314	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	g	312	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	q	315	CLA	CMA-C3A-C4A	2.75	119.15	111.77
31	Y	304	CLA	CMA-C3A-C4A	2.75	119.15	111.77
30	y	608	CHL	C1-O2A-CGA	2.75	123.65	116.44
31	Y	314	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
43	h	101	BCR	C29-C30-C25	2.75	114.71	110.48
31	g	304	CLA	C2D-C1D-ND	2.75	112.13	110.10
31	y	610	CLA	CMA-C3A-C4A	2.75	119.15	111.77
31	p	613	CLA	C1D-ND-C4D	-2.74	104.39	106.33
31	1	610	CLA	CMA-C3A-C4A	2.74	119.15	111.77
36	3	319	NEX	C19-C9-C10	-2.74	119.08	122.92
32	6	317	LUT	C35-C15-C14	-2.74	117.85	123.47
31	6	314	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
31	b	607	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
31	y	615	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
30	N	309	CHL	C1-O2A-CGA	2.74	123.64	116.44
30	G	607	CHL	C3B-C4B-NB	-2.74	107.97	110.52
31	8	604	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
30	6	310	CHL	C4B-CHC-C1C	2.74	132.84	126.34
30	G	607	CHL	C4B-CHC-C1C	2.74	132.84	126.34
43	C	615	BCR	C35-C13-C12	-2.74	113.76	118.08
31	0	615	CLA	C3B-C4B-NB	-2.74	107.97	110.52
31	9	312	CLA	C2C-C1C-NC	2.74	112.54	109.97
31	y	610	CLA	C2C-C1C-NC	2.74	112.54	109.97
31	C	605	CLA	CHD-C1D-ND	-2.74	121.94	124.45
31	g	313	CLA	C1-C2-C3	-2.74	121.31	126.04
31	n	312	CLA	C1D-ND-C4D	-2.74	104.39	106.33
31	7	313	CLA	C3B-C4B-NB	-2.74	107.97	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	c	615	BCR	C19-C18-C17	2.74	123.14	118.94
31	B	603	CLA	O2A-CGA-CBA	2.74	120.50	111.91
30	8	606	CHL	C4B-CHC-C1C	2.74	132.83	126.34
34	W	203	LMG	O8-C28-C29	2.74	120.50	111.91
32	g	316	LUT	C11-C12-C13	-2.74	118.72	126.42
31	6	304	CLA	CMA-C3A-C4A	2.74	119.13	111.77
31	q	306	CLA	CHD-C1D-ND	-2.74	121.94	124.45
31	n	315	CLA	CHD-C1D-ND	-2.74	121.94	124.45
30	0	606	CHL	C1-O2A-CGA	2.74	123.62	116.44
31	q	306	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
31	b	604	CLA	CHD-C1D-ND	-2.74	121.94	124.45
30	4	609	CHL	C1-O2A-CGA	2.74	123.62	116.44
32	n	318	LUT	C18-C5-C4	2.74	119.42	114.36
31	G	603	CLA	C1D-ND-C4D	-2.74	104.39	106.33
31	p	613	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
31	b	616	CLA	C1-C2-C3	-2.74	121.31	126.04
31	1	614	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
31	3	304	CLA	C1D-ND-C4D	-2.74	104.39	106.33
31	A	409	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	B	605	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	Y	311	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	g	310	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	b	602	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
32	5	616	LUT	C8-C7-C6	-2.73	119.52	127.20
34	7	320	LMG	O8-C28-C29	2.73	120.49	111.91
32	5	617	LUT	C15-C35-C34	-2.73	117.88	123.47
31	A	409	CLA	C2D-C1D-ND	2.73	112.12	110.10
31	s	316	CLA	C4B-CHC-C1C	2.73	132.82	126.34
30	7	302	CHL	C3B-C4B-NB	-2.73	107.98	110.52
30	n	307	CHL	CMA-C3A-C4A	2.73	119.12	111.77
31	C	602	CLA	C6-C5-C3	-2.73	106.29	113.45
34	A	418	LMG	C8-O7-C10	-2.73	111.06	117.79
31	N	314	CLA	CHD-C1D-ND	-2.73	121.94	124.45
31	c	613	CLA	CHD-C1D-ND	-2.73	121.94	124.45
31	5	603	CLA	C1D-ND-C4D	-2.73	104.39	106.33
31	N	315	CLA	C1D-ND-C4D	-2.73	104.39	106.33
30	g	309	CHL	C3B-C4B-NB	-2.73	107.98	110.52
31	n	304	CLA	C1D-ND-C4D	-2.73	104.39	106.33
43	A	410	BCR	C11-C12-C13	-2.73	118.75	126.42
36	3	319	NEX	C38-C25-C26	-2.73	117.69	122.26
31	c	609	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
34	6	321	LMG	O8-C28-C29	2.73	120.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	604	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
31	g	311	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	7	302	CHL	CMA-C3A-C4A	2.73	119.11	111.77
37	R	318	XAT	C6-C7-C8	-2.73	120.22	125.99
30	s	302	CHL	C4B-CHC-C1C	2.73	132.81	126.34
30	8	606	CHL	CMA-C3A-C4A	2.73	119.11	111.77
32	1	615	LUT	C15-C14-C13	-2.73	123.42	127.31
31	G	603	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
31	n	315	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
32	0	616	LUT	C11-C10-C9	-2.73	123.42	127.31
31	B	613	CLA	C2D-C1D-ND	2.73	112.11	110.10
30	n	301	CHL	C1-O2A-CGA	2.73	123.60	116.44
31	Y	303	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
31	0	604	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
31	9	305	CLA	C3B-C4B-NB	-2.73	107.98	110.52
30	1	619	CHL	C4B-CHC-C1C	2.73	132.81	126.34
31	A	407	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
31	2	613	CLA	C1D-ND-C4D	-2.73	104.40	106.33
31	3	313	CLA	C1D-ND-C4D	-2.73	104.40	106.33
31	r	315	CLA	C2C-C1C-NC	2.73	112.53	109.97
31	c	610	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	d	405	CLA	CHD-C1D-ND	-2.72	121.95	124.45
32	7	317	LUT	C30-C31-C32	-2.72	114.71	123.22
30	0	605	CHL	CHD-C4C-C3C	2.72	128.84	124.84
30	2	605	CHL	C3B-C4B-NB	-2.72	107.99	110.52
30	5	609	CHL	C3B-C4B-NB	-2.72	107.99	110.52
33	B	624	LHG	O8-C23-C24	2.72	120.45	111.91
31	r	307	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
31	q	315	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	c	607	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	3	313	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	R	303	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	2	610	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
31	G	604	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
32	8	616	LUT	C18-C5-C4	2.72	119.40	114.36
31	p	615	CLA	C2C-C1C-NC	2.72	112.52	109.97
30	q	303	CHL	C4B-CHC-C1C	2.72	132.79	126.34
31	B	610	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	r	313	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
34	W	202	LMG	O1-C1-C2	2.72	112.55	108.30
48	R	302	LMU	C1B-O1B-C4'	-2.72	111.23	117.96
31	6	313	CLA	C1C-C2C-C3C	-2.72	104.10	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	310	CHL	C1-O2A-CGA	2.72	123.58	116.44
31	c	606	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	p	615	CLA	C1D-ND-C4D	-2.72	104.40	106.33
31	y	613	CLA	CMA-C3A-C4A	2.72	119.08	111.77
31	6	316	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
31	c	611	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
30	3	303	CHL	C3B-C4B-NB	-2.72	107.99	110.52
31	7	303	CLA	C1D-ND-C4D	-2.72	104.40	106.33
30	q	311	CHL	C3B-C4B-NB	-2.72	107.99	110.52
30	G	608	CHL	C3B-C4B-NB	-2.72	108.00	110.52
31	s	313	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
31	A	405	CLA	C2C-C1C-NC	2.72	112.52	109.97
32	y	616	LUT	C7-C8-C9	-2.72	122.13	126.23
31	9	306	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
32	g	316	LUT	C39-C29-C30	-2.71	119.12	122.92
31	1	612	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	8	612	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	g	305	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	6	315	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
31	7	315	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
31	c	613	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
31	R	306	CLA	C2D-C1D-ND	2.71	112.10	110.10
31	s	311	CLA	C2C-C1C-NC	2.71	112.51	109.97
30	7	306	CHL	C4B-CHC-C1C	2.71	132.77	126.34
31	4	614	CLA	O2A-CGA-CBA	2.71	120.42	111.91
32	q	318	LUT	C11-C12-C13	-2.71	118.80	126.42
31	7	312	CLA	C1D-ND-C4D	-2.71	104.41	106.33
30	2	601	CHL	C4B-CHC-C1C	2.71	132.77	126.34
43	C	615	BCR	C24-C23-C22	-2.71	122.14	126.23
32	9	318	LUT	C21-C26-C27	-2.71	109.28	112.70
31	7	311	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	6	304	CLA	C1D-ND-C4D	-2.71	104.41	106.33
30	0	606	CHL	C4B-CHC-C1C	2.71	132.76	126.34
31	B	603	CLA	CHD-C1D-ND	-2.71	121.96	124.45
31	1	602	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
30	2	601	CHL	CMA-C3A-C4A	2.71	119.05	111.77
31	4	604	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	g	304	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	R	303	CLA	CMA-C3A-C4A	2.71	119.05	111.77
36	r	301	NEX	C5-C6-C1	2.71	122.38	119.70
30	R	309	CHL	C4B-CHC-C1C	2.71	132.76	126.34
31	p	603	CLA	CMA-C3A-C4A	2.71	119.05	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	y	601	CHL	C2C-C3C-C4C	2.71	108.42	106.49
34	r	321	LMG	O1-C1-C2	2.71	112.53	108.30
31	p	612	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	r	311	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	1	613	CLA	C2D-C1D-ND	2.71	112.10	110.10
32	8	615	LUT	C11-C10-C9	-2.71	123.45	127.31
31	N	314	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	S	312	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	y	610	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	c	607	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
30	N	307	CHL	C4B-CHC-C1C	2.71	132.76	126.34
31	Y	311	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
33	S	322	LHG	O8-C23-C24	2.71	120.40	111.91
30	g	306	CHL	C2C-C3C-C4C	2.71	108.42	106.49
34	6	321	LMG	C8-O7-C10	-2.71	111.13	117.79
31	c	604	CLA	C2C-C1C-NC	2.71	112.51	109.97
43	t	101	BCR	C16-C15-C14	2.71	129.02	123.47
30	2	607	CHL	C2B-C1B-NB	-2.71	108.42	110.23
31	d	404	CLA	O2A-CGA-CBA	2.71	120.40	111.91
31	1	611	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	5	610	CLA	CMA-C3A-C4A	2.71	119.04	111.77
31	B	612	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	8	614	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
32	0	617	LUT	C10-C11-C12	-2.70	114.78	123.22
30	4	607	CHL	C4D-CHA-C1A	2.70	124.54	121.25
30	Y	307	CHL	C1-C2-C3	-2.70	121.37	126.04
31	1	613	CLA	CHD-C1D-ND	-2.70	121.97	124.45
31	3	305	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
30	r	310	CHL	C1-C2-C3	-2.70	121.37	126.04
31	3	315	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	s	314	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
30	Y	306	CHL	CMA-C3A-C4A	2.70	119.03	111.77
30	3	302	CHL	C2B-C1B-NB	-2.70	108.42	110.23
31	R	311	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
31	6	313	CLA	C1-C2-C3	-2.70	121.37	126.04
30	q	307	CHL	CMA-C3A-C4A	2.70	119.03	111.77
31	p	615	CLA	O1D-CGD-CBD	-2.70	118.96	124.48
31	g	314	CLA	C1D-ND-C4D	-2.70	104.42	106.33
30	2	601	CHL	C1-C2-C3	-2.70	121.37	126.04
31	C	601	CLA	C2C-C1C-NC	2.70	112.50	109.97
30	7	310	CHL	C3B-C4B-NB	-2.70	108.01	110.52
31	B	611	CLA	C3B-C4B-NB	-2.70	108.01	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	314	CLA	O2A-CGA-CBA	2.70	120.38	111.91
34	w	204	LMG	O8-C28-C29	2.70	120.38	111.91
33	N	319	LHG	O8-C23-C24	2.70	120.38	111.91
31	C	603	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	8	613	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	g	311	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
31	b	611	CLA	C1D-ND-C4D	-2.70	104.42	106.33
31	d	404	CLA	C2C-C1C-NC	2.70	112.50	109.97
43	b	620	BCR	C11-C12-C13	-2.70	118.84	126.42
30	7	306	CHL	C3B-C4B-NB	-2.70	108.01	110.52
31	4	603	CLA	C3B-C4B-NB	-2.70	108.01	110.52
31	n	311	CLA	C3B-C4B-NB	-2.70	108.01	110.52
32	0	616	LUT	C18-C5-C4	2.70	119.35	114.36
34	w	203	LMG	C9-C8-C7	-2.70	105.41	111.79
31	S	304	CLA	CHA-C4D-ND	2.70	138.14	132.50
31	b	613	CLA	C3B-C4B-NB	-2.70	108.01	110.52
31	N	305	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	r	313	CLA	C2D-C1D-ND	2.70	112.09	110.10
31	N	310	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
30	y	609	CHL	CHC-C1C-NC	2.70	128.29	124.20
31	q	312	CLA	O1D-CGD-CBD	-2.70	118.97	124.48
37	R	318	XAT	C18-C5-C6	-2.70	117.74	122.26
31	c	608	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
34	k	101	LMG	C8-O7-C10	-2.70	111.16	117.79
31	N	321	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	B	601	CLA	C2D-C1D-ND	2.69	112.09	110.10
32	n	317	LUT	C11-C10-C9	-2.69	123.46	127.31
31	3	312	CLA	C3B-C4B-NB	-2.69	108.02	110.52
34	d	409	LMG	O8-C28-C29	2.69	120.36	111.91
30	S	302	CHL	CMA-C3A-C4A	2.69	119.01	111.77
31	y	614	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	4	610	CLA	CMA-C3A-C4A	2.69	119.01	111.77
31	2	612	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	S	305	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	b	604	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
30	y	609	CHL	C3B-C4B-NB	-2.69	108.02	110.52
30	4	605	CHL	CMA-C3A-C4A	2.69	119.01	111.77
31	S	314	CLA	CMA-C3A-C4A	2.69	119.01	111.77
30	1	601	CHL	CMA-C3A-C2A	2.69	124.69	113.83
31	q	313	CLA	CHD-C1D-ND	-2.69	121.98	124.45
31	Y	310	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
30	9	310	CHL	C4D-CHA-C1A	2.69	124.53	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	316	CLA	CMA-C3A-C4A	2.69	119.01	111.77
34	q	301	LMG	O8-C28-C29	2.69	120.36	111.91
37	r	318	XAT	C26-C27-C28	-2.69	120.30	125.99
31	N	310	CLA	C3B-C4B-NB	-2.69	108.02	110.52
31	4	610	CLA	C1D-ND-C4D	-2.69	104.42	106.33
43	b	619	BCR	C23-C24-C25	-2.69	119.64	127.20
31	b	612	CLA	CMA-C3A-C4A	2.69	119.01	111.77
31	y	604	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	Y	311	CLA	C1-C2-C3	-2.69	121.39	126.04
31	5	615	CLA	CHA-C1A-NA	-2.69	120.24	126.40
34	k	102	LMG	O8-C28-C29	2.69	120.35	111.91
31	6	303	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	S	311	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	S	305	CLA	C1D-ND-C4D	-2.69	104.42	106.33
31	7	304	CLA	C1D-ND-C4D	-2.69	104.42	106.33
31	8	603	CLA	C1D-ND-C4D	-2.69	104.42	106.33
31	r	305	CLA	C1D-ND-C4D	-2.69	104.42	106.33
32	7	317	LUT	C18-C5-C4	2.69	119.34	114.36
43	b	619	BCR	C7-C8-C9	-2.69	122.17	126.23
30	g	302	CHL	C4B-CHC-C1C	2.69	132.72	126.34
31	0	611	CLA	C3B-C4B-NB	-2.69	108.02	110.52
31	1	610	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	R	312	CLA	C2C-C1C-NC	2.69	112.49	109.97
30	6	310	CHL	C1-C2-C3	-2.69	121.39	126.04
31	b	604	CLA	CHA-C4D-ND	2.69	138.12	132.50
31	4	614	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	5	614	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	8	613	CLA	CHD-C1D-ND	-2.69	121.98	124.45
31	5	610	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
30	R	309	CHL	C3B-C4B-NB	-2.69	108.02	110.52
30	s	309	CHL	C4D-CHA-C1A	2.69	124.52	121.25
31	6	304	CLA	C4B-CHC-C1C	2.69	132.71	126.34
31	6	316	CLA	C2D-C1D-ND	2.69	112.08	110.10
31	B	602	CLA	C2D-C1D-ND	2.69	112.08	110.10
31	G	609	CLA	C2D-C1D-ND	2.69	112.08	110.10
31	C	611	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	p	610	CLA	C3B-C4B-NB	-2.69	108.02	110.52
30	5	605	CHL	C4B-CHC-C1C	2.69	132.71	126.34
31	c	604	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
30	2	608	CHL	C3B-C4B-NB	-2.69	108.02	110.52
31	N	303	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
31	a	409	CLA	C2D-C1D-ND	2.68	112.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	301	CHL	CMA-C3A-C4A	2.68	118.99	111.77
30	p	601	CHL	C4B-CHC-C1C	2.68	132.70	126.34
31	s	305	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	7	311	CLA	C3B-C4B-NB	-2.68	108.03	110.52
31	q	314	CLA	C2D-C1D-ND	2.68	112.08	110.10
31	r	307	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
31	d	404	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	B	612	CLA	C2C-C1C-NC	2.68	112.48	109.97
34	s	321	LMG	O1-C1-C2	2.68	112.49	108.30
31	6	311	CLA	C1-C2-C3	-2.68	121.41	126.04
34	C	624	LMG	O8-C28-C29	2.68	120.32	111.91
31	5	604	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	q	305	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	d	404	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
30	g	309	CHL	C1-O2A-CGA	2.68	123.47	116.44
31	5	613	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	4	604	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
31	s	314	CLA	O2A-CGA-CBA	2.68	120.31	111.91
31	5	615	CLA	CHA-C4D-ND	2.68	138.10	132.50
31	2	613	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	p	615	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	y	614	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	C	612	CLA	C2D-C1D-ND	2.68	112.08	110.10
31	q	306	CLA	C2D-C1D-ND	2.68	112.08	110.10
30	p	601	CHL	C4D-CHA-C1A	2.68	124.51	121.25
31	3	306	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
30	q	309	CHL	C2B-C1B-NB	-2.68	108.44	110.23
31	N	312	CLA	C4B-CHC-C1C	2.68	132.69	126.34
31	s	313	CLA	C2D-C1D-ND	2.68	112.08	110.10
31	n	315	CLA	C3B-C4B-NB	-2.68	108.03	110.52
30	Y	302	CHL	C1-C2-C3	-2.67	121.42	126.04
31	C	605	CLA	C2D-C1D-ND	2.67	112.08	110.10
31	R	314	CLA	C3B-C4B-NB	-2.67	108.03	110.52
34	G	621	LMG	O8-C28-C29	2.67	120.30	111.91
31	Y	303	CLA	C1D-ND-C4D	-2.67	104.44	106.33
31	S	312	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
30	4	609	CHL	C2C-C3C-C4C	2.67	108.39	106.49
30	s	309	CHL	C4B-CHC-C1C	2.67	132.68	126.34
31	8	609	CLA	C3B-C4B-NB	-2.67	108.04	110.52
31	3	301	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	5	602	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
34	N	320	LMG	O8-C28-C29	2.67	120.29	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n	314	CLA	C1D-ND-C4D	-2.67	104.44	106.33
31	4	613	CLA	O2A-CGA-CBA	2.67	120.29	111.91
31	G	609	CLA	O2A-CGA-CBA	2.67	120.29	111.91
31	2	603	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
30	4	608	CHL	CMA-C3A-C4A	2.67	118.95	111.77
31	S	311	CLA	C2D-C1D-ND	2.67	112.07	110.10
31	s	304	CLA	C1D-ND-C4D	-2.67	104.44	106.33
36	N	318	NEX	C2-C1-C6	2.67	111.81	109.21
36	9	319	NEX	C39-C29-C30	-2.67	119.18	122.92
30	1	606	CHL	C4D-CHA-C1A	2.67	124.50	121.25
30	n	306	CHL	C4D-CHA-C1A	2.67	124.50	121.25
31	5	615	CLA	CMD-C2D-C3D	-2.67	121.47	127.61
31	R	314	CLA	C2D-C1D-ND	2.67	112.07	110.10
31	8	604	CLA	C1D-ND-C4D	-2.67	104.44	106.33
31	3	315	CLA	C1-C2-C3	-2.67	121.43	126.04
31	4	613	CLA	C4B-CHC-C1C	2.67	132.67	126.34
31	8	612	CLA	O2A-CGA-CBA	2.67	120.28	111.91
31	0	614	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	1	602	CLA	CMA-C3A-C4A	2.67	118.94	111.77
30	8	605	CHL	C4D-CHA-C1A	2.67	124.50	121.25
31	9	312	CLA	C3B-C4B-NB	-2.67	108.04	110.52
34	x	202	LMG	O8-C28-C29	2.67	120.28	111.91
32	N	317	LUT	C21-C26-C27	-2.67	109.33	112.70
31	Y	313	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	0	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
33	1	617	LHG	C5-O7-C7	-2.67	111.23	117.79
31	B	615	CLA	C2D-C1D-ND	2.67	112.07	110.10
31	2	602	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	C	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	s	303	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	4	612	CLA	C4B-CHC-C1C	2.67	132.66	126.34
33	3	320	LHG	C6-C5-C4	-2.67	105.48	111.79
31	0	611	CLA	C1-C2-C3	-2.67	121.43	126.04
31	4	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	c	613	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
31	B	610	CLA	C1D-ND-C4D	-2.66	104.44	106.33
31	N	313	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	7	305	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	n	314	CLA	O2A-CGA-CBA	2.66	120.27	111.91
31	q	305	CLA	C4B-CHC-C1C	2.66	132.65	126.34
33	j	102	LHG	O8-C23-C24	2.66	120.26	111.91
31	b	602	CLA	C2D-C1D-ND	2.66	112.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	614	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
33	b	625	LHG	O8-C23-C24	2.66	120.26	111.91
31	4	603	CLA	C4B-CHC-C1C	2.66	132.65	126.34
31	7	312	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	4	612	CLA	CHD-C1D-ND	-2.66	122.01	124.45
34	b	622	LMG	C8-O7-C10	-2.66	111.24	117.79
31	r	316	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
31	0	611	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	s	312	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
34	n	322	LMG	O7-C10-O9	-2.66	117.27	123.70
30	s	302	CHL	CMA-C3A-C4A	2.66	118.92	111.77
31	b	606	CLA	O2A-CGA-CBA	2.66	120.26	111.91
34	b	601	LMG	O8-C28-C29	2.66	120.26	111.91
30	3	307	CHL	C3B-C4B-NB	-2.66	108.05	110.52
30	2	605	CHL	CMA-C3A-C4A	2.66	118.92	111.77
30	1	608	CHL	C4D-CHA-C1A	2.66	124.49	121.25
31	C	606	CLA	C2D-C1D-ND	2.66	112.06	110.10
31	Y	311	CLA	C1-O2A-CGA	2.66	123.42	116.44
31	y	615	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	4	611	CLA	C1D-ND-C4D	-2.66	104.45	106.33
30	6	310	CHL	C4D-CHA-C1A	2.66	124.48	121.25
34	D	412	LMG	O8-C28-C29	2.66	120.25	111.91
31	0	610	CLA	C2C-C1C-NC	2.66	112.46	109.97
31	G	611	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	b	615	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
30	S	302	CHL	CHB-C4A-NA	2.66	128.19	124.51
30	y	601	CHL	C3B-C4B-NB	-2.66	108.05	110.52
31	q	316	CLA	C2D-C1D-ND	2.66	112.06	110.10
31	n	303	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	9	314	CLA	C2C-C1C-NC	2.66	112.46	109.97
31	y	611	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
32	2	615	LUT	C8-C7-C6	-2.66	119.74	127.20
31	S	304	CLA	CHA-C1A-NA	-2.66	120.32	126.40
30	9	310	CHL	C4B-CHC-C1C	2.66	132.64	126.34
34	w	204	LMG	C8-O7-C10	-2.66	111.25	117.79
30	5	607	CHL	C2B-C1B-NB	-2.66	108.45	110.23
31	B	614	CLA	C3B-C4B-NB	-2.65	108.05	110.52
30	n	302	CHL	C1-C2-C3	-2.65	121.45	126.04
30	0	607	CHL	C1-O2A-CGA	2.65	123.41	116.44
30	2	606	CHL	CMA-C3A-C4A	2.65	118.91	111.77
34	A	414	LMG	O8-C28-C29	2.65	120.23	111.91
34	w	202	LMG	O8-C28-C29	2.65	120.23	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	608	CHL	C2C-C3C-C4C	2.65	108.38	106.49
31	9	314	CLA	C4B-CHC-C1C	2.65	132.63	126.34
31	B	610	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
30	8	601	CHL	C1-C2-C3	-2.65	121.46	126.04
36	y	618	NEX	C38-C25-C26	-2.65	117.82	122.26
31	N	315	CLA	C3B-C4B-NB	-2.65	108.06	110.52
30	n	309	CHL	C1-O2A-CGA	2.65	123.40	116.44
31	Y	305	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	r	314	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	G	602	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
30	p	607	CHL	C2B-C1B-NB	-2.65	108.46	110.23
30	r	310	CHL	CMA-C3A-C4A	2.65	118.89	111.77
48	K	101	LMU	O5'-C1'-C2'	2.65	115.96	110.35
31	Y	305	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
31	p	610	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
34	D	409	LMG	O8-C28-C29	2.65	120.22	111.91
31	Y	314	CLA	C1D-ND-C4D	-2.65	104.45	106.33
33	M	101	LHG	C5-O7-C7	-2.65	111.27	117.79
31	0	612	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	Y	312	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
32	9	318	LUT	C31-C32-C33	-2.65	118.98	126.42
30	2	608	CHL	C1-O2A-CGA	2.65	123.39	116.44
31	9	313	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
30	9	307	CHL	C2B-C1B-NB	-2.65	108.46	110.23
36	g	317	NEX	C17-C1-C6	-2.65	108.10	110.47
30	G	601	CHL	C2C-C3C-C4C	2.65	108.38	106.49
30	Y	301	CHL	C3B-C4B-NB	-2.65	108.06	110.52
31	2	609	CLA	C3B-C4B-NB	-2.65	108.06	110.52
31	7	315	CLA	C1D-ND-C4D	-2.65	104.46	106.33
31	c	608	CLA	C2D-C1D-ND	2.64	112.05	110.10
31	4	603	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	B	604	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	8	609	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	R	312	CLA	CMD-C2D-C3D	-2.64	121.53	127.61
47	E	101	HEM	CHD-C1D-C2D	-2.64	120.85	124.98
30	G	623	CHL	CMA-C3A-C4A	2.64	118.88	111.77
32	6	317	LUT	C18-C5-C4	2.64	119.25	114.36
43	Z	101	BCR	C2-C1-C6	2.64	114.55	110.48
31	0	615	CLA	CHD-C1D-ND	-2.64	122.03	124.45
31	c	605	CLA	CHD-C1D-ND	-2.64	122.03	124.45
31	q	304	CLA	C3B-C4B-NB	-2.64	108.06	110.52
31	n	311	CLA	C1C-C2C-C3C	-2.64	104.18	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	603	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
34	n	321	LMG	O1-C1-C2	2.64	112.43	108.30
33	9	320	LHG	O8-C23-C24	2.64	120.20	111.91
32	Y	316	LUT	C18-C5-C4	2.64	119.25	114.36
31	r	303	CLA	C1D-ND-C4D	-2.64	104.46	106.33
31	2	609	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	c	610	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
31	2	603	CLA	C4B-CHC-C1C	2.64	132.60	126.34
31	B	603	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	0	603	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	q	304	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
45	C	617	DGD	O1G-C1A-C2A	2.64	120.19	111.91
30	6	302	CHL	CMA-C3A-C4A	2.64	118.87	111.77
31	7	316	CLA	C1D-ND-C4D	-2.64	104.46	106.33
31	G	613	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
30	9	310	CHL	C2B-C1B-NB	-2.64	108.46	110.23
31	C	606	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	9	316	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
30	Y	306	CHL	C4D-CHA-C1A	2.64	124.46	121.25
30	0	609	CHL	C3B-C4B-NB	-2.64	108.07	110.52
31	g	311	CLA	C3B-C4B-NB	-2.64	108.07	110.52
30	9	303	CHL	C1-O2A-CGA	2.64	123.36	116.44
30	N	306	CHL	C2C-C3C-C4C	2.64	108.37	106.49
31	s	316	CLA	CMA-C3A-C4A	2.64	118.86	111.77
30	1	601	CHL	CHC-C1C-NC	2.64	128.20	124.20
33	c	622	LHG	O8-C23-C24	2.64	120.18	111.91
31	4	602	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
31	8	613	CLA	C3B-C4B-NB	-2.63	108.07	110.52
31	5	612	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	G	611	CLA	CHA-C4D-ND	2.63	138.01	132.50
32	1	616	LUT	C11-C10-C9	-2.63	123.55	127.31
43	B	618	BCR	C23-C24-C25	-2.63	119.81	127.20
33	6	320	LHG	O8-C23-C24	2.63	120.17	111.91
31	N	305	CLA	C1D-ND-C4D	-2.63	104.47	106.33
31	A	409	CLA	CMA-C3A-C4A	2.63	118.85	111.77
31	Y	310	CLA	C3B-C4B-NB	-2.63	108.07	110.52
31	N	315	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	p	614	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	c	602	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	2	613	CLA	C3B-C4B-NB	-2.63	108.07	110.52
31	n	313	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	7	314	CLA	C2D-C1D-ND	2.63	112.04	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	608	CHL	C1-C2-C3	-2.63	121.49	126.04
30	9	310	CHL	CMA-C3A-C4A	2.63	118.84	111.77
33	M	101	LHG	O8-C23-C24	2.63	120.16	111.91
31	a	406	CLA	C2C-C1C-NC	2.63	112.44	109.97
31	0	602	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	a	409	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	8	613	CLA	O2A-CGA-CBA	2.63	120.16	111.91
45	C	618	DGD	O1G-C1A-C2A	2.63	120.16	111.91
35	g	315	RRX	C35-C13-C14	-2.63	119.24	122.92
31	3	304	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	p	615	CLA	CMA-C3A-C4A	2.63	118.84	111.77
34	w	203	LMG	C7-O1-C1	-2.63	108.61	113.74
31	5	611	CLA	CHD-C1D-ND	-2.63	122.04	124.45
34	G	619	LMG	C8-O7-C10	-2.63	111.32	117.79
31	g	311	CLA	CMA-C3A-C4A	2.63	118.83	111.77
31	3	312	CLA	C2D-C1D-ND	2.63	112.04	110.10
31	C	607	CLA	C3B-C4B-NB	-2.63	108.08	110.52
32	9	318	LUT	C11-C12-C13	-2.63	119.04	126.42
31	D	403	CLA	O2A-CGA-CBA	2.63	120.15	111.91
43	h	101	BCR	C8-C7-C6	-2.63	119.83	127.20
36	R	319	NEX	C17-C1-C6	-2.63	108.12	110.47
31	B	613	CLA	C3B-C4B-NB	-2.63	108.08	110.52
34	2	618	LMG	O8-C28-C29	2.63	120.15	111.91
30	1	607	CHL	CMA-C3A-C4A	2.63	118.83	111.77
31	y	602	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
30	5	601	CHL	C2B-C1B-NB	-2.63	108.47	110.23
33	G	618	LHG	O8-C23-C24	2.63	120.15	111.91
31	2	609	CLA	O1D-CGD-CBD	-2.62	119.11	124.48
32	g	316	LUT	C31-C32-C33	-2.62	119.04	126.42
31	b	611	CLA	C4B-CHC-C1C	2.62	132.56	126.34
31	D	404	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	R	313	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	c	609	CLA	C1-C2-C3	-2.62	121.50	126.04
32	1	616	LUT	C30-C31-C32	-2.62	115.03	123.22
31	S	315	CLA	CMD-C2D-C3D	-2.62	121.58	127.61
31	b	608	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	y	612	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
30	Y	309	CHL	CHC-C1C-NC	2.62	128.18	124.20
33	L	101	LHG	O8-C23-C24	2.62	120.14	111.91
31	1	604	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
31	7	303	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	p	611	CLA	C1C-C2C-C3C	-2.62	104.20	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	613	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	C	609	CLA	C2D-C1D-ND	2.62	112.04	110.10
31	0	612	CLA	C2D-C1D-ND	2.62	112.04	110.10
30	0	606	CHL	C3B-C4B-NB	-2.62	108.08	110.52
43	c	615	BCR	C37-C22-C21	-2.62	119.25	122.92
34	f	101	LMG	O8-C28-C29	2.62	120.13	111.91
31	Y	312	CLA	C2D-C1D-ND	2.62	112.03	110.10
31	6	311	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	9	312	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	g	303	CLA	C4B-CHC-C1C	2.62	132.55	126.34
31	3	311	CLA	CMA-C3A-C4A	2.62	118.81	111.77
31	1	612	CLA	C4B-CHC-C1C	2.62	132.55	126.34
31	Y	312	CLA	C4B-CHC-C1C	2.62	132.55	126.34
31	0	613	CLA	C2D-C1D-ND	2.62	112.03	110.10
31	b	607	CLA	C2D-C1D-ND	2.62	112.03	110.10
31	c	607	CLA	O2A-CGA-CBA	2.62	120.12	111.91
30	G	607	CHL	C2B-C1B-NB	-2.62	108.48	110.23
31	0	612	CLA	CHA-C4D-ND	2.62	137.97	132.50
31	R	311	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
30	3	308	CHL	C4D-CHA-C1A	2.62	124.43	121.25
36	R	301	NEX	C39-C29-C30	-2.62	119.26	122.92
36	Y	317	NEX	C40-C33-C34	-2.62	119.26	122.92
31	5	610	CLA	C3B-C4B-NB	-2.62	108.09	110.52
32	y	617	LUT	C10-C11-C12	-2.62	115.05	123.22
31	8	610	CLA	C1C-C2C-C3C	-2.62	104.21	106.96
43	D	405	BCR	C4-C5-C6	-2.62	118.93	122.73
31	S	310	CLA	CMA-C3A-C4A	2.62	118.80	111.77
33	7	319	LHG	O8-C23-C24	2.61	120.11	111.91
31	S	312	CLA	C2D-C1D-ND	2.61	112.03	110.10
33	s	320	LHG	C6-C5-C4	-2.61	105.60	111.79
33	6	320	LHG	C5-O7-C7	-2.61	111.35	117.79
31	9	305	CLA	C4B-CHC-C1C	2.61	132.54	126.34
31	g	303	CLA	C2C-C1C-NC	2.61	112.42	109.97
43	H	101	BCR	C16-C15-C14	-2.61	118.12	123.47
31	0	602	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	q	316	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	9	316	CLA	C3B-C4B-NB	-2.61	108.09	110.52
31	y	613	CLA	C3B-C4B-NB	-2.61	108.09	110.52
31	B	604	CLA	CHA-C4D-ND	2.61	137.97	132.50
31	p	615	CLA	C4B-CHC-C1C	2.61	132.54	126.34
31	p	604	CLA	C2D-C1D-ND	2.61	112.03	110.10
31	1	611	CLA	C1C-C2C-C3C	-2.61	104.21	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	304	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	n	316	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
43	A	410	BCR	C8-C7-C6	-2.61	119.86	127.20
30	p	605	CHL	C3B-C4B-NB	-2.61	108.09	110.52
30	y	607	CHL	CMA-C3A-C4A	2.61	118.80	111.77
31	B	603	CLA	CMA-C3A-C4A	2.61	118.80	111.77
31	6	312	CLA	O2A-CGA-CBA	2.61	120.11	111.91
31	p	614	CLA	C4B-CHC-C1C	2.61	132.53	126.34
30	2	608	CHL	C1-C2-C3	-2.61	121.53	126.04
31	r	306	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
31	q	313	CLA	C1D-ND-C4D	-2.61	104.48	106.33
36	G	616	NEX	C38-C25-C26	-2.61	117.89	122.26
30	5	605	CHL	C2C-C3C-C4C	2.61	108.35	106.49
31	G	610	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	8	611	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	2	611	CLA	O2A-CGA-CBA	2.61	120.10	111.91
31	4	611	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
34	C	622	LMG	O8-C28-C29	2.61	120.09	111.91
32	6	318	LUT	C1-C6-C5	-2.61	118.94	122.61
30	p	606	CHL	C3B-C4B-NB	-2.61	108.09	110.52
31	B	606	CLA	C1-C2-C3	-2.61	121.53	126.04
31	s	304	CLA	C4B-CHC-C1C	2.61	132.52	126.34
31	R	312	CLA	C2D-C1D-ND	2.61	112.03	110.10
33	1	617	LHG	O8-C23-C24	2.61	120.09	111.91
31	p	602	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
33	D	407	LHG	O8-C23-C24	2.61	120.09	111.91
34	6	323	LMG	O8-C28-C29	2.61	120.09	111.91
31	N	313	CLA	C1D-ND-C4D	-2.61	104.48	106.33
31	s	315	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
31	8	614	CLA	C3B-C4B-NB	-2.61	108.10	110.52
31	4	610	CLA	CHA-C4D-ND	2.61	137.95	132.50
31	5	612	CLA	C1D-ND-C4D	-2.61	104.48	106.33
31	5	614	CLA	C1D-ND-C4D	-2.61	104.48	106.33
31	8	602	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
31	n	315	CLA	O2A-CGA-CBA	2.61	120.08	111.91
31	B	604	CLA	CHD-C1D-ND	-2.61	122.06	124.45
32	S	317	LUT	C8-C7-C6	-2.60	119.89	127.20
31	S	314	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
30	4	607	CHL	C1-C2-C3	-2.60	121.54	126.04
31	B	606	CLA	O2A-CGA-CBA	2.60	120.08	111.91
31	b	617	CLA	O2A-CGA-CBA	2.60	120.08	111.91
33	C	623	LHG	C5-O7-C7	-2.60	111.38	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	314	CLA	C4B-CHC-C1C	2.60	132.51	126.34
45	C	620	DGD	C2G-O2G-C1B	-2.60	111.38	117.79
31	G	612	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	N	312	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	S	310	CLA	C2D-C1D-ND	2.60	112.02	110.10
32	3	317	LUT	C18-C5-C4	2.60	119.18	114.36
47	e	102	HEM	CHD-C1D-C2D	-2.60	120.91	124.98
31	R	316	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	6	312	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	s	310	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	G	604	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	d	405	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
34	J	101	LMG	O8-C28-C29	2.60	120.07	111.91
31	D	403	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	R	312	CLA	C3B-C4B-NB	-2.60	108.10	110.52
31	3	305	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	9	314	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
32	1	616	LUT	C15-C35-C34	-2.60	118.15	123.47
43	z	101	BCR	C4-C5-C6	-2.60	118.96	122.73
31	R	313	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	n	316	CLA	C3B-C4B-NB	-2.60	108.10	110.52
31	3	313	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	r	303	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
34	B	622	LMG	C8-O7-C10	-2.60	111.39	117.79
31	s	312	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	9	312	CLA	C1D-ND-C4D	-2.60	104.49	106.33
31	b	609	CLA	CMA-C3A-C4A	2.60	118.76	111.77
30	6	306	CHL	C4A-NA-C1A	2.60	107.87	106.71
31	c	602	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
34	j	101	LMG	O8-C28-C29	2.60	120.06	111.91
31	1	602	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	n	305	CLA	C1D-ND-C4D	-2.60	104.49	106.33
32	1	616	LUT	C8-C7-C6	-2.60	119.91	127.20
31	B	607	CLA	C3B-C4B-NB	-2.60	108.11	110.52
30	5	609	CHL	C2C-C3C-C4C	2.60	108.34	106.49
30	S	309	CHL	C4D-CHA-C1A	2.60	124.41	121.25
30	4	607	CHL	C1-O2A-CGA	2.60	123.26	116.44
31	b	611	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
31	g	314	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
32	G	615	LUT	C39-C29-C30	-2.60	119.29	122.92
34	b	624	LMG	O1-C1-C2	2.59	112.35	108.30
30	r	309	CHL	C3B-C4B-NB	-2.59	108.11	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	607	CLA	C3B-C4B-NB	-2.59	108.11	110.52
31	R	304	CLA	C2D-C1D-ND	2.59	112.02	110.10
31	8	603	CLA	C2D-C1D-ND	2.59	112.02	110.10
31	8	610	CLA	C4B-CHC-C1C	2.59	132.49	126.34
30	7	302	CHL	CHC-C1C-NC	2.59	128.14	124.20
31	8	602	CLA	C3B-C4B-NB	-2.59	108.11	110.52
31	y	613	CLA	C2D-C1D-ND	2.59	112.02	110.10
31	5	611	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	n	312	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	B	609	CLA	O2A-CGA-CBA	2.59	120.05	111.91
31	5	611	CLA	C4B-CHC-C1C	2.59	132.49	126.34
31	S	303	CLA	C4B-CHC-C1C	2.59	132.49	126.34
36	0	618	NEX	C19-C9-C10	-2.59	119.29	122.92
31	B	610	CLA	C4B-CHC-C1C	2.59	132.49	126.34
31	7	304	CLA	C4B-CHC-C1C	2.59	132.49	126.34
31	0	612	CLA	C3B-C4B-NB	-2.59	108.11	110.52
31	C	604	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	3	301	CLA	C4B-CHC-C1C	2.59	132.49	126.34
31	1	610	CLA	C3B-C4B-NB	-2.59	108.11	110.52
31	G	613	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
31	b	605	CLA	CHA-C4D-ND	2.59	137.92	132.50
31	3	315	CLA	C4B-CHC-C1C	2.59	132.48	126.34
30	y	601	CHL	CMA-C3A-C4A	2.59	118.74	111.77
31	1	611	CLA	C4B-CHC-C1C	2.59	132.48	126.34
31	p	612	CLA	C4B-CHC-C1C	2.59	132.48	126.34
30	3	309	CHL	C2B-C1B-NB	-2.59	108.50	110.23
31	0	611	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	3	316	CLA	CHA-C4D-ND	2.59	137.91	132.50
31	2	604	CLA	C1D-ND-C4D	-2.59	104.50	106.33
43	B	617	BCR	C2-C1-C6	2.59	114.47	110.48
31	p	604	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
31	b	615	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
31	2	604	CLA	CMA-C3A-C4A	2.59	118.73	111.77
31	c	602	CLA	C1-O2A-CGA	2.59	123.23	116.44
43	H	101	BCR	C33-C5-C4	2.59	118.59	113.62
31	0	602	CLA	O2A-CGA-CBA	2.59	120.03	111.91
31	y	612	CLA	C2D-C1D-ND	2.59	112.01	110.10
32	1	615	LUT	C1-C6-C5	-2.59	118.97	122.61
30	1	607	CHL	C3B-C4B-NB	-2.59	108.11	110.52
31	7	316	CLA	C3B-C4B-NB	-2.59	108.11	110.52
31	G	610	CLA	CMA-C3A-C4A	2.59	118.73	111.77
31	3	312	CLA	O2D-CGD-O1D	-2.59	118.78	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	313	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
31	9	313	CLA	CMA-C3A-C4A	2.59	118.72	111.77
30	4	609	CHL	CHB-C4A-NA	2.59	128.09	124.51
34	1	618	LMG	O8-C28-C29	2.59	120.02	111.91
31	C	605	CLA	C3B-C4B-NB	-2.59	108.12	110.52
30	4	606	CHL	C4B-CHC-C1C	2.59	132.47	126.34
30	Y	302	CHL	CMA-C3A-C4A	2.59	118.72	111.77
30	0	601	CHL	C1-O2A-CGA	2.59	123.23	116.44
31	A	407	CLA	C2D-C1D-ND	2.59	112.01	110.10
31	B	608	CLA	C2D-C1D-ND	2.59	112.01	110.10
30	2	606	CHL	C3B-C4B-NB	-2.58	108.12	110.52
31	4	603	CLA	C2D-C1D-ND	2.58	112.01	110.10
31	y	610	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	B	614	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
31	B	604	CLA	CMD-C2D-C3D	-2.58	121.67	127.61
31	6	312	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
36	q	319	NEX	C40-C33-C34	-2.58	119.31	122.92
32	6	318	LUT	C18-C5-C4	2.58	119.14	114.36
31	D	403	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	r	312	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	y	615	CLA	C4B-CHC-C1C	2.58	132.46	126.34
32	y	616	LUT	C39-C29-C28	2.58	122.14	118.08
37	R	318	XAT	C26-C27-C28	-2.58	120.53	125.99
31	q	313	CLA	CMA-C3A-C4A	2.58	118.71	111.77
31	r	313	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	r	315	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
30	1	601	CHL	CHB-C4A-NA	2.58	128.08	124.51
30	S	308	CHL	CMA-C3A-C4A	2.58	118.71	111.77
30	2	606	CHL	C2C-C3C-C4C	2.58	108.33	106.49
31	7	305	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
31	6	305	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	B	614	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	b	605	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	9	305	CLA	C1D-ND-C4D	-2.58	104.50	106.33
31	3	311	CLA	O2A-CGA-CBA	2.58	120.00	111.91
34	0	620	LMG	O8-C28-C29	2.58	120.00	111.91
31	a	407	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
30	R	310	CHL	CHB-C4A-NA	2.58	128.08	124.51
30	y	605	CHL	C4B-CHC-C1C	2.58	132.45	126.34
31	7	313	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
43	c	615	BCR	C23-C22-C21	2.58	122.90	118.94
31	R	312	CLA	C1C-C2C-C3C	-2.58	104.25	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	303	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	G	611	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
30	p	608	CHL	CMA-C3A-C4A	2.58	118.70	111.77
34	C	621	LMG	O8-C28-C29	2.58	120.00	111.91
31	G	610	CLA	C2D-C1D-ND	2.58	112.00	110.10
31	b	612	CLA	C4B-CHC-C1C	2.58	132.45	126.34
31	N	303	CLA	C3B-C4B-NB	-2.58	108.12	110.52
31	g	303	CLA	C3B-C4B-NB	-2.58	108.12	110.52
30	G	608	CHL	CMA-C3A-C2A	2.58	124.22	113.83
31	9	314	CLA	CHA-C4D-ND	2.58	137.89	132.50
31	9	304	CLA	O2A-CGA-CBA	2.58	119.99	111.91
31	9	313	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	c	601	CLA	CHA-C4D-ND	2.58	137.89	132.50
31	S	316	CLA	C2D-C1D-ND	2.58	112.00	110.10
31	C	609	CLA	C1-C2-C3	-2.58	121.59	126.04
36	p	618	NEX	C26-C27-C28	-2.58	120.55	125.99
31	4	610	CLA	CHD-C1D-ND	-2.57	122.09	124.45
36	p	618	NEX	C17-C1-C6	-2.57	108.17	110.47
31	a	407	CLA	C2D-C1D-ND	2.57	112.00	110.10
30	7	308	CHL	C3B-C4B-NB	-2.57	108.13	110.52
31	B	610	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
31	3	304	CLA	C4B-CHC-C1C	2.57	132.44	126.34
30	2	601	CHL	C2C-C3C-C4C	2.57	108.32	106.49
31	B	608	CLA	CMA-C3A-C4A	2.57	118.69	111.77
30	9	311	CHL	CHC-C1C-NC	2.57	128.11	124.20
31	d	405	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
31	3	313	CLA	C4B-CHC-C1C	2.57	132.44	126.34
31	y	611	CLA	C1-O2A-CGA	2.57	123.19	116.44
43	h	101	BCR	C15-C16-C17	-2.57	118.21	123.47
30	g	308	CHL	C2B-C1B-NB	-2.57	108.51	110.23
30	4	608	CHL	C1-O2A-CGA	2.57	123.19	116.44
31	6	305	CLA	CMA-C3A-C4A	2.57	118.68	111.77
31	c	603	CLA	O2A-CGA-CBA	2.57	119.97	111.91
31	6	311	CLA	C3B-C4B-NB	-2.57	108.13	110.52
31	5	610	CLA	C4B-CHC-C1C	2.57	132.43	126.34
32	y	617	LUT	C11-C10-C9	-2.57	123.64	127.31
34	c	620	LMG	O8-C28-C29	2.57	119.97	111.91
30	p	601	CHL	C3B-C4B-NB	-2.57	108.13	110.52
31	5	602	CLA	C4B-CHC-C1C	2.57	132.43	126.34
31	6	304	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
31	a	409	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
31	C	602	CLA	CMA-C3A-C4A	2.57	118.67	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Y	319	LMG	O8-C28-C29	2.57	119.97	111.91
31	B	608	CLA	CHD-C1D-ND	-2.57	122.09	124.45
31	y	611	CLA	C4B-CHC-C1C	2.57	132.43	126.34
31	7	305	CLA	CHA-C4D-ND	2.57	137.87	132.50
31	3	306	CLA	C3B-C4B-NB	-2.57	108.13	110.52
43	d	406	BCR	C11-C12-C13	2.57	133.63	126.42
30	R	310	CHL	C4B-CHC-C1C	2.57	132.43	126.34
31	6	312	CLA	C1-O2A-CGA	2.56	123.17	116.44
31	B	605	CLA	C2D-C1D-ND	2.56	111.99	110.10
31	B	601	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
37	2	619	XAT	C26-C27-C28	-2.56	120.57	125.99
31	6	304	CLA	OBD-CAD-C3D	-2.56	122.35	128.52
31	g	311	CLA	CHA-C4D-ND	2.56	137.86	132.50
31	B	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
31	R	315	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
31	N	313	CLA	C3B-C4B-NB	-2.56	108.14	110.52
31	R	313	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
31	y	611	CLA	C2C-C1C-NC	2.56	112.37	109.97
31	g	311	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
31	n	311	CLA	C4B-CHC-C1C	2.56	132.41	126.34
30	R	310	CHL	CMA-C3A-C4A	2.56	118.66	111.77
31	b	616	CLA	C2D-C1D-ND	2.56	111.99	110.10
31	c	605	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
32	p	617	LUT	C15-C14-C13	-2.56	123.65	127.31
31	n	312	CLA	C4B-CHC-C1C	2.56	132.41	126.34
31	N	311	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
43	B	618	BCR	C33-C5-C4	2.56	118.53	113.62
33	5	619	LHG	O8-C23-C24	2.56	119.94	111.91
31	6	312	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
44	A	416	PL9	C7-C8-C9	-2.56	122.53	126.79
36	R	301	NEX	C20-C13-C14	-2.56	119.34	122.92
31	s	314	CLA	C2D-C1D-ND	2.56	111.99	110.10
31	y	612	CLA	C4B-CHC-C1C	2.56	132.41	126.34
31	5	604	CLA	CMA-C3A-C4A	2.56	118.65	111.77
31	6	312	CLA	C3B-C4B-NB	-2.56	108.14	110.52
31	S	306	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
31	C	613	CLA	CBA-CAA-C2A	2.56	121.42	113.86
31	a	407	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
31	q	312	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
30	s	308	CHL	C4A-NA-C1A	2.56	107.86	106.71
31	0	612	CLA	C4B-CHC-C1C	2.56	132.41	126.34
31	7	312	CLA	C4B-CHC-C1C	2.56	132.41	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	613	CLA	C2D-C1D-ND	2.56	111.99	110.10
36	6	319	NEX	C19-C9-C10	-2.56	119.34	122.92
32	0	616	LUT	C39-C29-C28	2.56	122.11	118.08
31	N	304	CLA	C1D-ND-C4D	-2.56	104.52	106.33
32	7	318	LUT	C1-C6-C5	-2.56	119.01	122.61
31	6	313	CLA	C4B-CHC-C1C	2.56	132.40	126.34
31	c	610	CLA	C1-O2A-CGA	2.56	123.15	116.44
31	Y	312	CLA	CHA-C4D-ND	2.56	137.85	132.50
37	G	620	XAT	C26-C27-C28	-2.56	120.59	125.99
34	X	203	LMG	O8-C28-C29	2.56	119.93	111.91
31	A	409	CLA	CAA-C2A-C3A	-2.55	105.78	112.78
31	4	602	CLA	C4B-CHC-C1C	2.55	132.40	126.34
43	v	101	BCR	C38-C26-C27	2.55	118.52	113.62
31	s	303	CLA	C4B-CHC-C1C	2.55	132.40	126.34
31	3	304	CLA	C3B-C4B-NB	-2.55	108.15	110.52
31	G	602	CLA	C3B-C4B-NB	-2.55	108.15	110.52
31	Y	305	CLA	C1D-ND-C4D	-2.55	104.52	106.33
31	9	314	CLA	C1D-ND-C4D	-2.55	104.52	106.33
30	y	607	CHL	C1-C2-C3	-2.55	121.63	126.04
31	1	604	CLA	O2A-CGA-CBA	2.55	119.92	111.91
31	r	316	CLA	O2A-CGA-CBA	2.55	119.92	111.91
30	6	309	CHL	CHD-C4C-C3C	2.55	128.59	124.84
31	r	312	CLA	C3B-C4B-NB	-2.55	108.15	110.52
31	y	614	CLA	C4B-CHC-C1C	2.55	132.39	126.34
31	s	306	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
31	R	306	CLA	CHA-C4D-ND	2.55	137.84	132.50
36	q	319	NEX	C17-C1-C6	-2.55	108.19	110.47
30	S	309	CHL	C2C-C3C-C4C	2.55	108.31	106.49
31	d	401	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
31	2	609	CLA	C4B-CHC-C1C	2.55	132.39	126.34
30	G	605	CHL	C2B-C1B-NB	-2.55	108.52	110.23
31	9	304	CLA	C4B-CHC-C1C	2.55	132.39	126.34
43	t	101	BCR	C29-C30-C25	2.55	114.41	110.48
32	p	616	LUT	C19-C9-C10	-2.55	119.35	122.92
31	7	304	CLA	CHA-C4D-ND	2.55	137.83	132.50
31	3	316	CLA	CBA-CAA-C2A	-2.55	106.34	113.86
30	y	608	CHL	C2C-C3C-C4C	2.55	108.31	106.49
31	Y	313	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
32	4	616	LUT	C1-C6-C5	-2.55	119.02	122.61
43	b	620	BCR	C23-C24-C25	-2.55	120.05	127.20
43	h	101	BCR	C23-C24-C25	-2.55	120.05	127.20
31	9	315	CLA	C1D-ND-C4D	-2.55	104.53	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	1	610	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
31	b	609	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
30	3	309	CHL	CMA-C3A-C4A	2.55	118.62	111.77
30	2	605	CHL	C4A-NA-C1A	2.55	107.85	106.71
34	G	622	LMG	O8-C28-C29	2.55	119.90	111.91
31	0	614	CLA	C1D-ND-C4D	-2.55	104.53	106.33
31	R	307	CLA	C3B-C4B-NB	-2.55	108.15	110.52
31	b	615	CLA	C3B-C4B-NB	-2.55	108.15	110.52
30	9	311	CHL	C1-O2A-CGA	2.55	123.12	116.44
30	7	306	CHL	C4D-CHA-C1A	2.55	124.35	121.25
31	q	316	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
31	b	613	CLA	CMA-C3A-C4A	2.55	118.61	111.77
31	Y	304	CLA	C4B-CHC-C1C	2.55	132.38	126.34
35	2	614	RRX	C8-C7-C6	-2.55	120.05	127.20
31	7	313	CLA	CHA-C4D-ND	2.55	137.82	132.50
33	d	408	LHG	O8-C23-C24	2.54	119.89	111.91
31	N	321	CLA	C4B-CHC-C1C	2.54	132.37	126.34
31	y	613	CLA	CHA-C4D-ND	2.54	137.82	132.50
30	0	608	CHL	C1-O2A-CGA	2.54	123.12	116.44
31	B	606	CLA	CHA-C4D-ND	2.54	137.82	132.50
30	5	605	CHL	C4D-CHA-C1A	2.54	124.34	121.25
31	9	304	CLA	C3B-C4B-NB	-2.54	108.16	110.52
31	b	612	CLA	C3B-C4B-NB	-2.54	108.16	110.52
31	7	305	CLA	CMD-C2D-C3D	-2.54	121.76	127.61
33	0	619	LHG	C6-C5-C4	-2.54	105.77	111.79
43	b	619	BCR	C30-C25-C26	-2.54	119.03	122.61
31	B	607	CLA	CHA-C4D-ND	2.54	137.82	132.50
33	4	618	LHG	O8-C23-C24	2.54	119.89	111.91
37	q	321	XAT	C26-C27-C28	-2.54	120.62	125.99
31	a	409	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	s	305	CLA	CMA-C3A-C4A	2.54	118.61	111.77
31	y	604	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
31	3	314	CLA	C4B-CHC-C1C	2.54	132.37	126.34
31	p	614	CLA	CHA-C4D-ND	2.54	137.81	132.50
37	4	619	XAT	C26-C27-C28	-2.54	120.62	125.99
31	5	602	CLA	C3B-C4B-NB	-2.54	108.16	110.52
31	5	603	CLA	C3B-C4B-NB	-2.54	108.16	110.52
31	q	306	CLA	C3B-C4B-NB	-2.54	108.16	110.52
31	G	603	CLA	C4B-CHC-C1C	2.54	132.36	126.34
31	8	611	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
31	A	409	CLA	O2A-CGA-CBA	2.54	119.88	111.91
30	6	306	CHL	C2B-C1B-NB	-2.54	108.53	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	316	CLA	C2D-C1D-ND	2.54	111.98	110.10
30	n	310	CHL	CMA-C3A-C2A	2.54	124.08	113.83
32	q	318	LUT	C21-C26-C27	-2.54	109.49	112.70
31	N	305	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
31	1	612	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
31	y	612	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
31	Y	303	CLA	C4B-CHC-C1C	2.54	132.36	126.34
34	w	201	LMG	O8-C28-C29	2.54	119.88	111.91
31	b	608	CLA	CMA-C3A-C4A	2.54	118.60	111.77
31	4	602	CLA	C3B-C4B-NB	-2.54	108.16	110.52
43	B	618	BCR	C38-C26-C25	-2.54	121.68	124.53
31	b	606	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
31	Y	313	CLA	C2D-C1D-ND	2.54	111.97	110.10
30	y	605	CHL	C4D-CHA-C1A	2.54	124.34	121.25
31	R	314	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
31	p	611	CLA	C4B-CHC-C1C	2.54	132.36	126.34
31	B	614	CLA	C1D-ND-C4D	-2.54	104.53	106.33
31	1	604	CLA	C2D-C1D-ND	2.54	111.97	110.10
31	0	611	CLA	C2D-C1D-ND	2.54	111.97	110.10
31	S	313	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
31	3	311	CLA	C4B-CHC-C1C	2.54	132.35	126.34
31	Y	310	CLA	C4B-CHC-C1C	2.54	132.35	126.34
31	q	306	CLA	CHA-C4D-ND	2.54	137.80	132.50
30	g	302	CHL	CMA-C3A-C4A	2.54	118.59	111.77
30	N	308	CHL	C3B-C4B-NB	-2.54	108.16	110.52
31	1	602	CLA	C4B-CHC-C1C	2.54	132.35	126.34
43	C	614	BCR	C15-C16-C17	-2.54	118.28	123.47
31	r	307	CLA	CAA-C2A-C3A	-2.54	105.84	112.78
34	w	205	LMG	O8-C28-C29	2.54	119.86	111.91
31	C	612	CLA	O2A-CGA-CBA	2.53	119.86	111.91
31	A	406	CLA	CMA-C3A-C4A	2.53	118.58	111.77
31	7	314	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
30	6	307	CHL	C3B-C4B-NB	-2.53	108.16	110.52
31	Y	311	CLA	C3B-C4B-NB	-2.53	108.16	110.52
31	Y	312	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
31	p	604	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
35	q	317	RRX	C29-C28-C27	2.53	113.77	110.30
31	C	607	CLA	O2A-CGA-CBA	2.53	119.86	111.91
32	1	616	LUT	C10-C11-C12	-2.53	115.31	123.22
31	2	604	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	G	612	CLA	C2D-C1D-ND	2.53	111.97	110.10
34	n	321	LMG	O8-C28-C29	2.53	119.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	305	CLA	C3B-C4B-NB	-2.53	108.17	110.52
31	S	303	CLA	C3B-C4B-NB	-2.53	108.17	110.52
31	B	607	CLA	CMA-C3A-C4A	2.53	118.58	111.77
31	R	312	CLA	O2A-CGA-CBA	2.53	119.86	111.91
31	C	601	CLA	C4B-CHC-C1C	2.53	132.34	126.34
31	S	313	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	c	605	CLA	CHA-C4D-ND	2.53	137.79	132.50
33	3	320	LHG	O8-C23-C24	2.53	119.85	111.91
30	S	302	CHL	CHC-C1C-NC	2.53	128.04	124.20
31	B	609	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	6	302	CHL	C2C-C3C-C4C	2.53	108.29	106.49
31	b	612	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
31	4	610	CLA	O2A-CGA-CBA	2.53	119.85	111.91
31	n	313	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
34	q	301	LMG	C8-O7-C10	-2.53	111.56	117.79
36	n	319	NEX	C38-C25-C26	-2.53	118.02	122.26
37	9	322	XAT	C26-C27-C28	-2.53	120.64	125.99
33	L	101	LHG	C5-O7-C7	-2.53	111.56	117.79
32	y	616	LUT	C15-C35-C34	-2.53	118.29	123.47
30	0	607	CHL	CMA-C3A-C4A	2.53	118.57	111.77
31	6	311	CLA	C4B-CHC-C1C	2.53	132.34	126.34
31	C	608	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
31	G	610	CLA	C3B-C4B-NB	-2.53	108.17	110.52
30	q	310	CHL	CHD-C4C-C3C	2.53	128.56	124.84
43	b	618	BCR	C1-C6-C5	-2.53	119.05	122.61
31	q	313	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
31	N	303	CLA	C4B-CHC-C1C	2.53	132.34	126.34
31	8	614	CLA	C1D-ND-C4D	-2.53	104.54	106.33
31	S	305	CLA	CMA-C3A-C4A	2.53	118.57	111.77
33	r	320	LHG	C5-O7-C7	-2.53	111.57	117.79
37	g	321	XAT	C26-C27-C28	-2.53	120.65	125.99
31	B	611	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
34	p	620	LMG	O8-C28-C29	2.53	119.84	111.91
31	2	610	CLA	C4B-CHC-C1C	2.53	132.33	126.34
35	q	317	RRX	C23-C24-C25	-2.53	120.11	127.20
31	b	607	CLA	CHA-C4D-ND	2.53	137.78	132.50
31	n	303	CLA	C4B-CHC-C1C	2.53	132.33	126.34
30	8	607	CHL	C3B-C4B-NB	-2.53	108.17	110.52
31	b	611	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
30	N	309	CHL	C3B-C4B-NB	-2.53	108.17	110.52
31	1	614	CLA	C3B-C4B-NB	-2.53	108.17	110.52
31	d	404	CLA	C1D-ND-C4D	-2.53	104.54	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	416	LMG	C8-O7-C10	-2.53	111.57	117.79
31	3	313	CLA	O2A-CGA-CBA	2.53	119.83	111.91
31	S	312	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
31	B	612	CLA	CMA-C3A-C4A	2.52	118.56	111.77
31	d	405	CLA	CMA-C3A-C4A	2.52	118.56	111.77
31	p	613	CLA	C3B-C4B-NB	-2.52	108.17	110.52
34	r	321	LMG	O8-C28-C29	2.52	119.83	111.91
43	b	618	BCR	C38-C26-C27	2.52	118.46	113.62
31	b	613	CLA	C6-C5-C3	-2.52	106.84	113.45
31	y	613	CLA	C4B-CHC-C1C	2.52	132.32	126.34
31	G	602	CLA	C4B-CHC-C1C	2.52	132.32	126.34
32	y	616	LUT	C31-C30-C29	-2.52	123.71	127.31
31	0	610	CLA	C1-C2-C3	-2.52	121.68	126.04
31	B	616	CLA	O2A-CGA-CBA	2.52	119.82	111.91
31	n	303	CLA	C3B-C4B-NB	-2.52	108.18	110.52
31	s	306	CLA	C4B-CHC-C1C	2.52	132.32	126.34
31	3	305	CLA	C1D-ND-C4D	-2.52	104.54	106.33
30	4	609	CHL	CHC-C1C-NC	2.52	128.03	124.20
33	D	408	LHG	C5-O7-C7	-2.52	111.59	117.79
31	y	602	CLA	C3B-C4B-NB	-2.52	108.18	110.52
31	s	311	CLA	C6-C5-C3	-2.52	106.85	113.45
31	3	316	CLA	C4B-CHC-C1C	2.52	132.31	126.34
31	n	316	CLA	C4B-CHC-C1C	2.52	132.31	126.34
31	y	610	CLA	C4B-CHC-C1C	2.52	132.31	126.34
30	5	607	CHL	CHC-C1C-NC	2.52	128.03	124.20
31	4	603	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	B	614	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	1	602	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
31	N	310	CLA	C4B-CHC-C1C	2.52	132.31	126.34
36	y	618	NEX	C39-C29-C30	-2.52	119.40	122.92
31	y	612	CLA	CHA-C4D-ND	2.52	137.77	132.50
43	T	101	BCR	C29-C30-C25	2.52	114.36	110.48
31	p	603	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
31	Y	313	CLA	O2A-CGA-CBA	2.52	119.81	111.91
36	G	616	NEX	C20-C13-C14	-2.52	119.40	122.92
31	p	604	CLA	O2A-CGA-CBA	2.52	119.81	111.91
32	Y	316	LUT	C18-C5-C6	-2.52	121.70	124.53
31	q	305	CLA	CHA-C4D-ND	2.52	137.76	132.50
32	p	617	LUT	C8-C7-C6	-2.52	120.14	127.20
31	8	609	CLA	C4B-CHC-C1C	2.52	132.30	126.34
36	4	617	NEX	C39-C29-C30	-2.51	119.40	122.92
30	6	309	CHL	C2B-C1B-NB	-2.51	108.55	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	313	CLA	CHA-C4D-ND	2.51	137.76	132.50
31	5	612	CLA	C3B-C4B-NB	-2.51	108.18	110.52
31	0	612	CLA	CMA-C3A-C4A	2.51	118.53	111.77
31	y	604	CLA	C1D-ND-C4D	-2.51	104.55	106.33
30	2	608	CHL	CHC-C1C-NC	2.51	128.02	124.20
33	0	619	LHG	O8-C23-C24	2.51	119.80	111.91
31	G	612	CLA	O2A-CGA-CBA	2.51	119.80	111.91
31	0	615	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
33	D	407	LHG	C5-O7-C7	-2.51	111.60	117.79
34	B	622	LMG	O8-C28-C29	2.51	119.79	111.91
31	B	603	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	G	610	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	q	314	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	1	610	CLA	C4B-CHC-C1C	2.51	132.30	126.34
31	C	601	CLA	O2A-CGA-CBA	2.51	119.79	111.91
31	q	314	CLA	C1D-ND-C4D	-2.51	104.55	106.33
31	B	605	CLA	CHA-C4D-ND	2.51	137.75	132.50
36	R	301	NEX	C31-C30-C29	2.51	130.89	127.31
30	7	321	CHL	C3B-C4B-NB	-2.51	108.19	110.52
31	n	313	CLA	C3B-C4B-NB	-2.51	108.19	110.52
31	y	603	CLA	C3B-C4B-NB	-2.51	108.19	110.52
30	1	608	CHL	C2B-C1B-NB	-2.51	108.55	110.23
31	R	303	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
30	3	303	CHL	C1-O2A-CGA	2.51	123.03	116.44
30	7	310	CHL	CHC-C1C-NC	2.51	128.01	124.20
31	G	613	CLA	C4B-CHC-C1C	2.51	132.29	126.34
31	1	612	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	2	604	CLA	C3B-C4B-NB	-2.51	108.19	110.52
31	s	303	CLA	C3B-C4B-NB	-2.51	108.19	110.52
30	7	306	CHL	CHB-C4A-NA	2.51	127.98	124.51
32	9	318	LUT	C40-C33-C34	-2.51	119.41	122.92
31	8	602	CLA	C4B-CHC-C1C	2.51	132.29	126.34
31	R	315	CLA	CHA-C4D-ND	2.51	137.75	132.50
30	9	311	CHL	CHD-C4C-C3C	2.51	128.53	124.84
31	q	316	CLA	CHA-C4D-ND	2.51	137.74	132.50
34	3	321	LMG	O8-C28-C29	2.51	119.78	111.91
31	B	602	CLA	C3B-C4B-NB	-2.51	108.19	110.52
43	a	410	BCR	C19-C18-C17	-2.51	115.09	118.94
31	N	313	CLA	O2A-CGA-CBA	2.51	119.77	111.91
31	r	315	CLA	O2A-CGA-CBA	2.51	119.77	111.91
31	c	606	CLA	C2D-C1D-ND	2.51	111.95	110.10
31	8	611	CLA	C3B-C4B-NB	-2.51	108.19	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	619	CHL	CMA-C3A-C2A	2.51	123.94	113.83
34	2	618	LMG	C8-O7-C10	-2.51	111.62	117.79
37	r	318	XAT	C18-C5-C6	-2.51	118.06	122.26
31	2	613	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
43	C	615	BCR	C37-C22-C21	-2.50	119.41	122.92
31	c	609	CLA	C2D-C1D-ND	2.50	111.95	110.10
31	6	316	CLA	CHA-C4D-ND	2.50	137.74	132.50
31	5	614	CLA	C4B-CHC-C1C	2.50	132.28	126.34
30	8	608	CHL	CMA-C3A-C2A	2.50	123.93	113.83
31	Y	304	CLA	C1D-ND-C4D	-2.50	104.56	106.33
31	G	603	CLA	O2A-CGA-CBA	2.50	119.77	111.91
30	g	309	CHL	CMA-C3A-C2A	2.50	123.93	113.83
30	n	308	CHL	C3B-C4B-NB	-2.50	108.19	110.52
32	p	617	LUT	C21-C26-C25	2.50	115.90	111.42
31	G	611	CLA	C2D-C1D-ND	2.50	111.95	110.10
34	G	619	LMG	O8-C28-C29	2.50	119.76	111.91
30	n	309	CHL	C3B-C4B-NB	-2.50	108.19	110.52
31	b	614	CLA	C1D-ND-C4D	-2.50	104.56	106.33
31	b	613	CLA	C4B-CHC-C1C	2.50	132.27	126.34
31	A	406	CLA	C2D-C1D-ND	2.50	111.95	110.10
36	R	319	NEX	C26-C27-C28	-2.50	120.70	125.99
32	y	616	LUT	C19-C9-C8	2.50	122.02	118.08
30	S	308	CHL	C4B-CHC-C1C	2.50	132.27	126.34
42	A	408	PHO	C1C-C2C-C3C	-2.50	106.53	108.61
30	4	605	CHL	C2B-C1B-NB	-2.50	108.56	110.23
31	y	602	CLA	C4B-CHC-C1C	2.50	132.27	126.34
30	G	608	CHL	CHB-C4A-NA	2.50	127.97	124.51
35	G	614	RRX	C8-C7-C6	-2.50	120.18	127.20
31	s	311	CLA	C4B-CHC-C1C	2.50	132.27	126.34
30	8	608	CHL	CHD-C4C-C3C	2.50	128.52	124.84
31	N	315	CLA	C4B-CHC-C1C	2.50	132.27	126.34
31	3	315	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
31	s	310	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
33	r	320	LHG	O8-C23-C24	2.50	119.75	111.91
31	6	305	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
32	s	318	LUT	C30-C31-C32	-2.50	115.42	123.22
30	1	609	CHL	CHC-C1C-NC	2.50	128.00	124.20
31	B	604	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
31	2	602	CLA	CHA-C4D-ND	2.50	137.73	132.50
31	b	609	CLA	CHD-C1D-ND	-2.50	122.16	124.45
35	4	615	RRX	C8-C7-C6	-2.50	120.19	127.20
45	c	617	DGD	O6E-C1E-O5D	2.50	115.89	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	603	CLA	CHA-C4D-ND	2.50	137.72	132.50
31	7	311	CLA	C4B-CHC-C1C	2.50	132.26	126.34
31	S	311	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
34	J	102	LMG	O8-C28-C29	2.50	119.75	111.91
30	p	607	CHL	C1-O2A-CGA	2.50	123.00	116.44
33	p	619	LHG	O8-C23-C24	2.50	119.74	111.91
30	1	605	CHL	CHC-C1C-NC	2.50	127.99	124.20
43	a	410	BCR	C33-C5-C4	2.50	118.41	113.62
34	m	102	LMG	C4-C3-C2	-2.50	106.47	110.82
31	g	312	CLA	CHA-C4D-ND	2.50	137.72	132.50
32	Y	315	LUT	C39-C29-C28	2.50	122.01	118.08
31	r	303	CLA	CHA-C4D-ND	2.50	137.72	132.50
30	q	303	CHL	CMA-C3A-C4A	2.50	118.48	111.77
30	n	306	CHL	C2B-C1B-NB	-2.50	108.56	110.23
30	3	303	CHL	CHC-C1C-NC	2.50	127.99	124.20
31	3	311	CLA	C2D-C1D-ND	2.50	111.94	110.10
30	5	608	CHL	C3B-C4B-NB	-2.50	108.20	110.52
30	Y	309	CHL	C1-O2A-CGA	2.50	122.99	116.44
31	5	614	CLA	CHA-C4D-ND	2.50	137.72	132.50
31	2	611	CLA	CMA-C3A-C4A	2.49	118.48	111.77
31	g	313	CLA	C1D-ND-C4D	-2.49	104.56	106.33
30	4	608	CHL	C2B-C1B-NB	-2.49	108.56	110.23
36	s	319	NEX	C4-C3-C2	2.49	115.59	110.77
34	g	320	LMG	O8-C28-C29	2.49	119.73	111.91
31	c	607	CLA	CHA-C4D-ND	2.49	137.71	132.50
30	S	302	CHL	C4D-CHA-C1A	2.49	124.28	121.25
30	4	609	CHL	C3B-C4B-NB	-2.49	108.20	110.52
31	7	304	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
36	s	319	NEX	C38-C25-C26	-2.49	118.08	122.26
31	y	615	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
43	D	405	BCR	C20-C21-C22	-2.49	123.75	127.31
43	V	101	BCR	C15-C14-C13	-2.49	123.75	127.31
31	G	603	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	G	602	CLA	C1-C2-C3	-2.49	121.73	126.04
35	9	317	RRX	C8-C7-C6	-2.49	120.20	127.20
31	a	407	CLA	C4B-CHC-C1C	2.49	132.25	126.34
31	8	603	CLA	C3B-C4B-NB	-2.49	108.20	110.52
31	C	611	CLA	CHA-C4D-ND	2.49	137.71	132.50
36	N	318	NEX	C31-C30-C29	2.49	130.86	127.31
31	5	613	CLA	C4B-CHC-C1C	2.49	132.24	126.34
31	R	304	CLA	C4B-CHC-C1C	2.49	132.24	126.34
31	c	612	CLA	O2A-CGA-CBA	2.49	119.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	311	CHL	CMA-C3A-C2A	2.49	123.87	113.83
32	r	317	LUT	C19-C9-C8	2.49	122.00	118.08
43	D	405	BCR	C1-C6-C7	2.49	122.82	115.78
31	9	305	CLA	CHA-C4D-ND	2.49	137.71	132.50
30	6	307	CHL	C2C-C3C-C4C	2.49	108.26	106.49
31	3	305	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	N	311	CLA	C4B-CHC-C1C	2.49	132.24	126.34
31	c	613	CLA	CHA-C4D-ND	2.49	137.70	132.50
43	b	618	BCR	C21-C20-C19	-2.49	115.45	123.22
36	p	618	NEX	C20-C13-C14	-2.49	119.44	122.92
31	R	307	CLA	C2D-C1D-ND	2.49	111.94	110.10
30	6	310	CHL	C2C-C3C-C4C	2.49	108.26	106.49
31	y	615	CLA	CHA-C4D-ND	2.49	137.70	132.50
43	d	406	BCR	C33-C5-C4	2.49	118.39	113.62
30	2	605	CHL	C2B-C1B-NB	-2.49	108.56	110.23
31	2	609	CLA	O2A-CGA-CBA	2.49	119.71	111.91
32	G	615	LUT	C8-C7-C6	-2.49	120.22	127.20
30	q	309	CHL	C2C-C3C-C4C	2.49	108.26	106.49
31	6	304	CLA	CHA-C4D-ND	2.49	137.70	132.50
31	c	611	CLA	CHA-C4D-ND	2.49	137.70	132.50
30	y	605	CHL	CMA-C3A-C4A	2.49	118.45	111.77
31	S	315	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
30	5	605	CHL	CHB-C4A-NA	2.48	127.95	124.51
31	d	401	CLA	C2D-C1D-ND	2.48	111.94	110.10
31	b	602	CLA	CHA-C4D-ND	2.48	137.70	132.50
31	s	315	CLA	CHA-C4D-ND	2.48	137.70	132.50
31	s	315	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
31	5	604	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	0	610	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
31	g	304	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	6	303	CLA	C4B-CHC-C1C	2.48	132.23	126.34
31	B	605	CLA	O2A-CGA-CBA	2.48	119.70	111.91
31	B	613	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	C	610	CLA	CHA-C4D-ND	2.48	137.69	132.50
36	n	319	NEX	C19-C9-C10	-2.48	119.44	122.92
31	2	611	CLA	C4B-CHC-C1C	2.48	132.23	126.34
31	6	313	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	b	612	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
36	r	319	NEX	C39-C29-C30	-2.48	119.45	122.92
30	q	303	CHL	C2B-C1B-NB	-2.48	108.57	110.23
31	C	608	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
31	7	305	CLA	C1D-ND-C4D	-2.48	104.57	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	316	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
33	S	320	LHG	C5-O7-C7	-2.48	111.68	117.79
31	C	612	CLA	CMA-C3A-C4A	2.48	118.44	111.77
31	p	614	CLA	O2A-CGA-CBA	2.48	119.69	111.91
30	3	302	CHL	CHD-C4C-C3C	2.48	128.49	124.84
42	A	408	PHO	C1-C2-C3	-2.48	121.75	126.04
45	c	617	DGD	C2G-O2G-C1B	-2.48	111.68	117.79
31	1	602	CLA	O2A-CGA-CBA	2.48	119.69	111.91
30	3	309	CHL	CHB-C4A-NA	2.48	127.94	124.51
43	b	618	BCR	C37-C22-C23	2.48	121.98	118.08
31	D	403	CLA	C1D-ND-C4D	-2.48	104.57	106.33
30	y	608	CHL	CHC-C1C-NC	2.48	127.97	124.20
31	p	604	CLA	C3B-C4B-NB	-2.48	108.21	110.52
30	q	308	CHL	C3C-C4C-NC	-2.48	107.79	110.57
32	1	615	LUT	C20-C13-C12	2.48	121.98	118.08
31	C	601	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	r	311	CLA	C2D-C1D-ND	2.48	111.93	110.10
30	R	308	CHL	C2B-C1B-NB	-2.48	108.57	110.23
31	R	316	CLA	O2A-CGA-CBA	2.48	119.69	111.91
31	S	315	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	p	612	CLA	CHA-C4D-ND	2.48	137.68	132.50
36	q	319	NEX	C20-C13-C14	-2.48	119.45	122.92
30	p	607	CHL	CHC-C1C-NC	2.48	127.96	124.20
31	r	303	CLA	C4B-CHC-C1C	2.48	132.22	126.34
31	N	305	CLA	C3B-C4B-NB	-2.48	108.22	110.52
31	9	306	CLA	C3B-C4B-NB	-2.48	108.22	110.52
31	4	612	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	s	304	CLA	CHA-C4D-ND	2.48	137.68	132.50
30	5	601	CHL	C4A-NA-C1A	2.48	107.82	106.71
31	7	316	CLA	C4B-CHC-C1C	2.48	132.22	126.34
36	r	301	NEX	C38-C25-C26	-2.48	118.11	122.26
31	1	610	CLA	O2A-CGA-CBA	2.48	119.68	111.91
31	N	305	CLA	CHA-C4D-ND	2.48	137.68	132.50
32	G	615	LUT	C10-C11-C12	-2.48	115.48	123.22
30	2	601	CHL	CHB-C4A-NA	2.48	127.94	124.51
30	9	311	CHL	CHB-C4A-NA	2.48	127.94	124.51
43	a	410	BCR	C38-C26-C27	2.48	118.38	113.62
31	9	315	CLA	C3B-C4B-NB	-2.48	108.22	110.52
31	s	315	CLA	C3B-C4B-NB	-2.48	108.22	110.52
31	B	611	CLA	C4B-CHC-C1C	2.48	132.21	126.34
31	b	608	CLA	CHA-C4D-ND	2.48	137.68	132.50
30	n	306	CHL	C1-O2A-CGA	2.48	122.94	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	602	CLA	C4B-CHC-C1C	2.48	132.21	126.34
31	r	312	CLA	C4B-CHC-C1C	2.48	132.21	126.34
31	0	604	CLA	C2D-C1D-ND	2.48	111.93	110.10
32	N	316	LUT	C31-C30-C29	-2.48	123.78	127.31
31	5	612	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	Y	304	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	C	603	CLA	CMD-C2D-C3D	-2.48	121.92	127.61
31	7	315	CLA	O2A-CGA-CBA	2.48	119.68	111.91
31	G	609	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
31	Y	311	CLA	C2D-C1D-ND	2.48	111.93	110.10
31	9	313	CLA	C3B-C4B-NB	-2.47	108.22	110.52
34	A	412	LMG	O8-C28-C29	2.47	119.67	111.91
31	2	613	CLA	CHA-C4D-ND	2.47	137.68	132.50
31	p	613	CLA	CHA-C4D-ND	2.47	137.68	132.50
30	8	605	CHL	C2B-C1B-NB	-2.47	108.57	110.23
33	a	415	LHG	C5-O7-C7	-2.47	111.70	117.79
31	Y	314	CLA	C4B-CHC-C1C	2.47	132.21	126.34
31	0	602	CLA	C4B-CHC-C1C	2.47	132.21	126.34
30	N	309	CHL	CMA-C3A-C2A	2.47	123.81	113.83
31	G	610	CLA	CHA-C1A-NA	-2.47	120.73	126.40
30	p	609	CHL	C1-O2A-CGA	2.47	122.93	116.44
32	S	318	LUT	C35-C15-C14	-2.47	118.41	123.47
31	B	607	CLA	O2A-CGA-CBA	2.47	119.67	111.91
31	Y	305	CLA	CHA-C4D-ND	2.47	137.67	132.50
30	2	601	CHL	C2B-C1B-NB	-2.47	108.57	110.23
31	r	307	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	b	614	CLA	CMA-C3A-C4A	2.47	118.42	111.77
32	0	617	LUT	C30-C31-C32	-2.47	115.50	123.22
30	2	608	CHL	CMA-C3A-C2A	2.47	123.80	113.83
30	Y	302	CHL	CHB-C4A-NA	2.47	127.93	124.51
30	Y	302	CHL	C3B-C4B-NB	-2.47	108.22	110.52
43	c	614	BCR	C1-C6-C7	2.47	122.77	115.78
31	B	606	CLA	C2D-C1D-ND	2.47	111.92	110.10
31	c	603	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
31	0	614	CLA	C3B-C4B-NB	-2.47	108.22	110.52
31	y	603	CLA	C1D-ND-C4D	-2.47	104.58	106.33
30	s	309	CHL	C2C-C3C-C4C	2.47	108.25	106.49
36	S	319	NEX	C26-C27-C28	-2.47	120.77	125.99
33	S	320	LHG	O8-C23-C24	2.47	119.66	111.91
34	B	621	LMG	C8-O7-C10	-2.47	111.71	117.79
31	N	304	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	A	407	CLA	C4B-CHC-C1C	2.47	132.19	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	610	CLA	O2A-CGA-CBA	2.47	119.66	111.91
30	g	302	CHL	CHB-C4A-NA	2.47	127.93	124.51
32	Y	315	LUT	C15-C35-C34	-2.47	118.42	123.47
31	q	315	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	b	615	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	1	604	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
31	C	602	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
31	N	311	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
43	b	619	BCR	C15-C16-C17	-2.47	118.42	123.47
31	R	303	CLA	CHA-C4D-ND	2.47	137.66	132.50
30	G	606	CHL	C1-O2A-CGA	2.47	122.92	116.44
31	r	307	CLA	CMA-C3A-C4A	2.47	118.41	111.77
31	G	609	CLA	C4B-CHC-C1C	2.47	132.19	126.34
32	1	615	LUT	C15-C35-C34	-2.47	118.42	123.47
31	1	604	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	4	604	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	C	602	CLA	C2D-C1D-ND	2.47	111.92	110.10
31	3	305	CLA	C4B-CHC-C1C	2.47	132.19	126.34
33	S	322	LHG	C5-O7-C7	-2.47	111.72	117.79
31	6	303	CLA	C3B-C4B-NB	-2.47	108.23	110.52
31	6	315	CLA	C3B-C4B-NB	-2.47	108.23	110.52
31	S	315	CLA	C3B-C4B-NB	-2.47	108.23	110.52
31	g	312	CLA	C3B-C4B-NB	-2.47	108.23	110.52
32	7	318	LUT	C18-C5-C4	2.47	118.92	114.36
31	B	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
30	6	310	CHL	CHB-C4A-NA	2.47	127.92	124.51
31	S	306	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	9	305	CLA	O2A-CGA-CBA	2.47	119.64	111.91
31	b	613	CLA	O2A-CGA-CBA	2.47	119.64	111.91
31	7	315	CLA	C3B-C4B-NB	-2.47	108.23	110.52
31	q	316	CLA	C3B-C4B-NB	-2.47	108.23	110.52
43	V	101	BCR	C30-C25-C24	2.47	122.75	115.78
31	2	610	CLA	CHA-C4D-ND	2.46	137.66	132.50
33	s	320	LHG	O8-C23-C24	2.46	119.64	111.91
34	c	624	LMG	O8-C28-C29	2.46	119.64	111.91
31	s	310	CLA	CMA-C3A-C4A	2.46	118.40	111.77
30	3	310	CHL	CHC-C1C-NC	2.46	127.94	124.20
30	4	601	CHL	CHB-C4A-NA	2.46	127.92	124.51
43	H	101	BCR	C23-C24-C25	-2.46	120.28	127.20
44	a	414	PL9	C40-C39-C41	2.46	119.41	115.27
30	n	310	CHL	CHD-C4C-C3C	2.46	128.46	124.84
43	C	615	BCR	C34-C9-C8	-2.46	114.20	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	N	318	NEX	C38-C25-C26	-2.46	118.13	122.26
31	8	604	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
32	Y	316	LUT	C8-C7-C6	-2.46	120.29	127.20
31	2	613	CLA	C4B-CHC-C1C	2.46	132.18	126.34
31	7	316	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
42	D	401	PHO	C1C-C2C-C3C	-2.46	106.56	108.61
36	2	616	NEX	C16-C1-C6	-2.46	108.27	110.47
31	p	604	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
31	B	612	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
33	0	619	LHG	C5-O7-C7	-2.46	111.73	117.79
31	r	313	CLA	CMA-C3A-C4A	2.46	118.38	111.77
34	x	202	LMG	O1-C7-C8	-2.46	104.96	110.90
30	p	608	CHL	C1-O2A-CGA	2.46	122.90	116.44
31	G	613	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	6	312	CLA	C4B-CHC-C1C	2.46	132.17	126.34
30	8	605	CHL	C1-O2A-CGA	2.46	122.90	116.44
31	1	611	CLA	C1-C2-C3	-2.46	121.79	126.04
31	0	610	CLA	C4B-CHC-C1C	2.46	132.17	126.34
31	g	304	CLA	C4B-CHC-C1C	2.46	132.17	126.34
31	g	311	CLA	C2D-C1D-ND	2.46	111.92	110.10
31	s	312	CLA	C3B-C4B-NB	-2.46	108.23	110.52
36	Y	317	NEX	C38-C25-C26	-2.46	118.14	122.26
31	c	602	CLA	C4B-CHC-C1C	2.46	132.17	126.34
31	r	304	CLA	C4B-CHC-C1C	2.46	132.17	126.34
31	R	307	CLA	C4B-CHC-C1C	2.46	132.17	126.34
31	G	609	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
30	s	302	CHL	C4A-NA-C1A	2.46	107.81	106.71
31	b	609	CLA	C1D-ND-C4D	-2.46	104.59	106.33
30	p	606	CHL	C2C-C3C-C4C	2.46	108.24	106.49
31	r	307	CLA	C3B-C4B-NB	-2.46	108.23	110.52
31	b	603	CLA	CMA-C3A-C4A	2.46	118.38	111.77
31	B	607	CLA	C2D-C1D-ND	2.46	111.92	110.10
30	3	310	CHL	CMA-C3A-C2A	2.46	123.74	113.83
30	0	609	CHL	CMA-C3A-C2A	2.46	123.74	113.83
30	1	605	CHL	C2B-C1B-NB	-2.46	108.58	110.23
31	1	614	CLA	O2A-CGA-CBA	2.46	119.62	111.91
31	g	304	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
36	3	319	NEX	C17-C1-C6	-2.46	108.27	110.47
31	g	310	CLA	C4B-CHC-C1C	2.46	132.16	126.34
31	g	311	CLA	C4B-CHC-C1C	2.46	132.16	126.34
32	N	317	LUT	C11-C12-C13	-2.45	119.52	126.42
31	B	612	CLA	O2A-CGA-CBA	2.45	119.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	604	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	g	305	CLA	CHA-C4D-ND	2.45	137.63	132.50
30	g	302	CHL	C1-O2A-CGA	2.45	122.88	116.44
31	G	612	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	7	303	CLA	C4B-CHC-C1C	2.45	132.16	126.34
33	G	618	LHG	C5-O7-C7	-2.45	111.75	117.79
31	1	613	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
30	9	308	CHL	C2B-C1B-NB	-2.45	108.59	110.23
30	r	310	CHL	C2B-C1B-NB	-2.45	108.59	110.23
31	n	313	CLA	C4B-CHC-C1C	2.45	132.16	126.34
30	q	309	CHL	C4D-CHA-C1A	2.45	124.23	121.25
31	s	311	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
31	3	315	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	B	601	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	9	306	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	y	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	8	604	CLA	CMA-C3A-C4A	2.45	118.37	111.77
32	g	316	LUT	C19-C9-C10	-2.45	119.49	122.92
30	Y	301	CHL	CHD-C4C-C3C	2.45	128.44	124.84
31	2	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
43	C	615	BCR	C38-C26-C27	2.45	118.33	113.62
43	b	618	BCR	C33-C5-C4	2.45	118.33	113.62
30	g	306	CHL	C2B-C1B-NB	-2.45	108.59	110.23
31	B	606	CLA	C3B-C4B-NB	-2.45	108.24	110.52
31	S	306	CLA	C4B-CHC-C1C	2.45	132.15	126.34
45	c	619	DGD	O1G-C1A-C2A	2.45	119.60	111.91
31	N	313	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	g	314	CLA	CHA-C4D-ND	2.45	137.63	132.50
30	0	609	CHL	C2C-C3C-C4C	2.45	108.24	106.49
30	q	303	CHL	C2C-C3C-C4C	2.45	108.24	106.49
31	5	604	CLA	C3B-C4B-NB	-2.45	108.24	110.52
31	B	611	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
31	p	613	CLA	O2A-C1-C2	2.45	115.07	108.64
32	Y	316	LUT	C31-C30-C29	-2.45	123.81	127.31
31	5	611	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	0	615	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	7	303	CLA	CHA-C4D-ND	2.45	137.62	132.50
33	y	619	LHG	O8-C23-C24	2.45	119.59	111.91
31	B	605	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
32	p	616	LUT	C8-C7-C6	-2.45	120.32	127.20
34	w	201	LMG	C8-O7-C10	-2.45	111.76	117.79
31	r	314	CLA	CMA-C3A-C4A	2.45	118.35	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	p	618	NEX	C16-C1-C6	-2.45	108.28	110.47
31	C	603	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	R	304	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
30	q	311	CHL	CMA-C3A-C4A	2.45	118.35	111.77
31	G	603	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
31	3	314	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	n	312	CLA	CHA-C4D-ND	2.45	137.62	132.50
43	H	101	BCR	C30-C25-C26	-2.45	119.17	122.61
31	r	306	CLA	C2D-C1D-ND	2.45	111.91	110.10
34	7	301	LMG	O8-C28-C29	2.45	119.58	111.91
31	g	313	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	n	305	CLA	CHA-C4D-ND	2.45	137.62	132.50
30	5	609	CHL	CHC-C1C-NC	2.45	127.91	124.20
31	r	314	CLA	C4B-CHC-C1C	2.45	132.14	126.34
31	q	312	CLA	CHA-C4D-ND	2.45	137.61	132.50
31	6	316	CLA	C4B-CHC-C1C	2.44	132.14	126.34
30	Y	308	CHL	C2B-C1B-NB	-2.44	108.59	110.23
31	n	312	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
31	r	316	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
31	c	601	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
31	n	304	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	r	305	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	p	610	CLA	C4B-CHC-C1C	2.44	132.14	126.34
42	D	401	PHO	C4A-C3A-C2A	-2.44	100.51	102.84
31	7	312	CLA	CHA-C4D-ND	2.44	137.61	132.50
32	3	318	LUT	C8-C7-C6	-2.44	120.34	127.20
31	q	315	CLA	C1D-ND-C4D	-2.44	104.60	106.33
31	c	610	CLA	CAA-CBA-CGA	-2.44	106.11	113.25
30	q	309	CHL	C4B-CHC-C1C	2.44	132.13	126.34
31	b	612	CLA	O2A-CGA-CBA	2.44	119.58	111.91
31	g	303	CLA	O2A-CGA-CBA	2.44	119.58	111.91
31	R	316	CLA	CMA-C3A-C4A	2.44	118.34	111.77
30	0	609	CHL	CHB-C4A-NA	2.44	127.89	124.51
31	9	312	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	S	305	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	n	314	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	d	404	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	B	613	CLA	CMA-C3A-C4A	2.44	118.34	111.77
36	8	617	NEX	C39-C29-C30	-2.44	119.50	122.92
31	q	315	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
31	g	303	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
43	z	101	BCR	C34-C9-C10	-2.44	119.50	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	604	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	0	603	CLA	C3B-C4B-NB	-2.44	108.25	110.52
30	5	609	CHL	C2B-C1B-NB	-2.44	108.60	110.23
31	r	315	CLA	CMA-C3A-C4A	2.44	118.33	111.77
31	3	313	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	Y	313	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	8	610	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	8	604	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	Y	314	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	8	612	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	9	316	CLA	C4B-CHC-C1C	2.44	132.12	126.34
31	a	409	CLA	C4B-CHC-C1C	2.44	132.12	126.34
31	7	314	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	G	613	CLA	O2A-CGA-CBA	2.44	119.56	111.91
31	N	313	CLA	C4B-CHC-C1C	2.44	132.12	126.34
31	c	606	CLA	CHD-C1D-ND	-2.44	122.21	124.45
45	c	617	DGD	C3G-O3G-C1D	-2.44	108.97	113.74
43	z	101	BCR	C29-C30-C25	2.44	114.23	110.48
31	8	613	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	p	611	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	g	311	CLA	CHA-C1A-NA	-2.44	120.81	126.40
31	S	305	CLA	C4B-CHC-C1C	2.44	132.12	126.34
30	q	311	CHL	CHC-C1C-NC	2.44	127.90	124.20
31	5	603	CLA	C4B-CHC-C1C	2.44	132.12	126.34
31	N	314	CLA	C4B-CHC-C1C	2.44	132.12	126.34
31	8	614	CLA	C4B-CHC-C1C	2.44	132.12	126.34
31	r	311	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
31	G	602	CLA	CHA-C4D-ND	2.44	137.60	132.50
30	8	601	CHL	C2B-C1B-NB	-2.44	108.60	110.23
31	d	401	CLA	CMD-C2D-C3D	-2.44	122.01	127.61
31	7	303	CLA	C3B-C4B-NB	-2.44	108.25	110.52
36	p	618	NEX	C40-C33-C34	-2.44	119.51	122.92
31	b	603	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	8	611	CLA	C4B-CHC-C1C	2.44	132.12	126.34
31	3	304	CLA	O2A-CGA-CBA	2.44	119.56	111.91
31	4	611	CLA	CHA-C4D-ND	2.44	137.60	132.50
43	A	410	BCR	C35-C13-C14	-2.44	119.51	122.92
33	2	617	LHG	O8-C23-C24	2.44	119.55	111.91
31	B	612	CLA	C4B-CHC-C1C	2.44	132.12	126.34
32	r	317	LUT	C22-C23-C24	2.44	114.51	111.74
30	1	609	CHL	CMA-C3A-C2A	2.44	123.65	113.83
31	3	312	CLA	C4B-CHC-C1C	2.44	132.11	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	608	CHL	C3B-C4B-NB	-2.44	108.26	110.52
45	c	619	DGD	C3G-O3G-C1D	-2.43	108.98	113.74
34	w	203	LMG	O8-C28-O10	-2.43	117.45	123.59
31	C	604	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	8	602	CLA	CHA-C4D-ND	2.43	137.59	132.50
34	6	321	LMG	O1-C1-C2	2.43	112.10	108.30
30	3	309	CHL	C1-O2A-CGA	2.43	122.83	116.44
31	g	304	CLA	O2A-CGA-CBA	2.43	119.55	111.91
31	s	305	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	A	409	CLA	C4B-CHC-C1C	2.43	132.11	126.34
31	b	602	CLA	C4B-CHC-C1C	2.43	132.11	126.34
31	N	315	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	n	315	CLA	CHA-C4D-ND	2.43	137.59	132.50
30	Y	308	CHL	CHB-C4A-NA	2.43	127.88	124.51
30	y	601	CHL	CHB-C4A-NA	2.43	127.88	124.51
30	R	309	CHL	CMA-C3A-C4A	2.43	118.31	111.77
31	R	315	CLA	C4B-CHC-C1C	2.43	132.11	126.34
31	7	316	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	s	311	CLA	O2A-CGA-CBA	2.43	119.54	111.91
31	S	312	CLA	C4B-CHC-C1C	2.43	132.10	126.34
31	b	615	CLA	C4B-CHC-C1C	2.43	132.10	126.34
36	s	319	NEX	O24-C25-C38	-2.43	112.14	115.06
43	b	618	BCR	C8-C7-C6	-2.43	120.38	127.20
31	2	613	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
31	b	607	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
30	p	608	CHL	C2B-C1B-NB	-2.43	108.60	110.23
30	G	605	CHL	C1-O2A-CGA	2.43	123.79	116.73
31	c	608	CLA	C1-C2-C3	-2.43	121.84	126.04
31	s	312	CLA	CHA-C4D-ND	2.43	137.58	132.50
34	b	623	LMG	O8-C28-C29	2.43	119.53	111.91
30	6	310	CHL	CHC-C1C-NC	2.43	127.89	124.20
36	5	618	NEX	C38-C25-C26	-2.43	118.19	122.26
30	n	302	CHL	C2B-C1B-NB	-2.43	108.60	110.23
31	C	613	CLA	CHA-C4D-ND	2.43	137.58	132.50
31	R	312	CLA	CHA-C4D-ND	2.43	137.58	132.50
30	1	607	CHL	C1-C2-C3	-2.43	121.84	126.04
31	d	401	CLA	C4B-CHC-C1C	2.43	132.10	126.34
31	p	610	CLA	CHA-C4D-ND	2.43	137.58	132.50
31	0	611	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
31	7	315	CLA	C4B-CHC-C1C	2.43	132.10	126.34
31	1	614	CLA	C4B-CHC-C1C	2.43	132.09	126.34
36	q	319	NEX	C19-C9-C10	-2.43	119.52	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	p	603	CLA	CHA-C4D-ND	2.43	137.58	132.50
30	1	601	CHL	C2B-C1B-NB	-2.43	108.61	110.23
43	Z	101	BCR	C21-C20-C19	-2.43	115.64	123.22
31	8	610	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
31	s	311	CLA	C3B-C4B-NB	-2.43	108.26	110.52
32	N	317	LUT	C15-C35-C34	-2.43	118.50	123.47
43	V	101	BCR	C7-C8-C9	-2.43	122.57	126.23
30	5	607	CHL	CHD-C4C-C3C	2.43	128.41	124.84
30	N	309	CHL	CHD-C4C-C3C	2.43	128.41	124.84
34	a	401	LMG	O8-C28-C29	2.43	119.52	111.91
31	y	610	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
31	N	303	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	s	313	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	S	312	CLA	CMA-C3A-C4A	2.43	118.29	111.77
31	8	604	CLA	C3B-C4B-NB	-2.43	108.27	110.52
31	4	614	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	B	602	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	b	613	CLA	C16-C15-C13	-2.42	108.08	115.92
31	6	312	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	n	303	CLA	CHA-C4D-ND	2.42	137.57	132.50
43	z	101	BCR	C11-C12-C13	-2.42	119.61	126.42
30	9	311	CHL	C1-C2-C3	-2.42	121.85	126.04
31	d	401	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
31	R	312	CLA	CMA-C3A-C4A	2.42	118.29	111.77
31	8	613	CLA	C4B-CHC-C1C	2.42	132.09	126.34
43	h	101	BCR	C33-C5-C4	2.42	118.27	113.62
31	3	304	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	p	604	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	B	609	CLA	C1D-ND-C4D	-2.42	104.61	106.33
31	Y	305	CLA	C4B-CHC-C1C	2.42	132.09	126.34
31	s	316	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
32	1	615	LUT	C39-C29-C28	2.42	121.90	118.08
31	2	611	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	3	312	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	b	614	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	2	609	CLA	CHA-C4D-ND	2.42	137.57	132.50
30	9	303	CHL	CMA-C3A-C4A	2.42	118.28	111.77
31	C	609	CLA	O2A-CGA-CBA	2.42	119.51	111.91
31	N	321	CLA	CHA-C4D-ND	2.42	137.57	132.50
30	p	607	CHL	CHD-C4C-C3C	2.42	128.40	124.84
34	4	621	LMG	O8-C28-C29	2.42	119.51	111.91
32	5	617	LUT	C22-C23-C24	2.42	114.50	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	610	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	r	303	CLA	CHD-C1D-ND	-2.42	122.23	124.45
30	5	608	CHL	CHC-C1C-NC	2.42	127.88	124.20
31	y	611	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
32	S	317	LUT	C35-C15-C14	-2.42	118.52	123.47
31	9	315	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	c	603	CLA	CHA-C4D-ND	2.42	137.56	132.50
30	Y	306	CHL	CHD-C4C-C3C	2.42	128.40	124.84
31	S	304	CLA	C4B-CHC-C1C	2.42	132.08	126.34
31	q	314	CLA	C4B-CHC-C1C	2.42	132.08	126.34
33	p	619	LHG	C5-O7-C7	-2.42	111.83	117.79
36	Y	317	NEX	C16-C1-C6	-2.42	108.31	110.47
31	R	312	CLA	C4B-CHC-C1C	2.42	132.08	126.34
31	G	613	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
30	G	606	CHL	C2C-C3C-C4C	2.42	108.21	106.49
31	p	611	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
30	0	601	CHL	CHC-C1C-NC	2.42	127.87	124.20
30	4	606	CHL	C1-O2A-CGA	2.42	122.79	116.44
31	b	604	CLA	CMA-C3A-C4A	2.42	118.28	111.77
44	A	416	PL9	C32-C33-C34	-2.42	121.83	127.66
31	q	312	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
31	r	304	CLA	C3B-C4B-NB	-2.42	108.27	110.52
31	b	614	CLA	C4B-CHC-C1C	2.42	132.07	126.34
36	r	301	NEX	C20-C13-C14	-2.42	119.53	122.92
31	0	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	b	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	g	313	CLA	C4B-CHC-C1C	2.42	132.07	126.34
30	S	302	CHL	C4A-NA-C1A	2.42	107.79	106.71
31	6	304	CLA	O2A-CGA-CBA	2.42	119.50	111.91
34	4	620	LMG	O8-C28-C29	2.42	119.50	111.91
31	C	613	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
34	c	621	LMG	C8-O7-C10	-2.42	111.84	117.79
31	G	604	CLA	C4B-CHC-C1C	2.42	132.07	126.34
31	b	612	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	8	603	CLA	O2A-CGA-CBA	2.42	119.49	111.91
32	7	317	LUT	C15-C35-C34	-2.42	118.52	123.47
31	1	603	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
31	y	610	CLA	O2A-CGA-CBA	2.42	119.49	111.91
31	G	612	CLA	C4B-CHC-C1C	2.42	132.07	126.34
31	D	404	CLA	CMA-C3A-C4A	2.42	118.27	111.77
31	4	613	CLA	C1-O2A-CGA	2.42	122.78	116.44
31	B	601	CLA	C4B-CHC-C1C	2.42	132.07	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	305	CLA	C4B-CHC-C1C	2.42	132.07	126.34
31	n	305	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
31	A	409	CLA	C1D-ND-C4D	-2.42	104.62	106.33
31	s	314	CLA	CHA-C4D-ND	2.42	137.55	132.50
36	r	301	NEX	C40-C33-C34	-2.42	119.54	122.92
30	Y	306	CHL	C2B-C1B-NB	-2.42	108.61	110.23
36	9	319	NEX	C17-C1-C6	-2.41	108.31	110.47
43	c	615	BCR	C29-C30-C25	2.41	114.20	110.48
32	9	318	LUT	C38-C25-C24	-2.41	118.39	123.56
31	5	610	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
31	r	313	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
31	N	311	CLA	CHA-C4D-ND	2.41	137.55	132.50
48	K	101	LMU	C1'-C2'-C3'	2.41	115.02	110.00
31	S	311	CLA	C4B-CHC-C1C	2.41	132.06	126.34
36	G	616	NEX	C39-C29-C30	-2.41	119.54	122.92
30	p	605	CHL	C2B-C1B-NB	-2.41	108.61	110.23
31	s	305	CLA	C3B-C4B-NB	-2.41	108.28	110.52
30	p	601	CHL	CHB-C4A-NA	2.41	127.85	124.51
31	B	610	CLA	CHA-C4D-ND	2.41	137.55	132.50
34	Y	319	LMG	C8-O7-C10	-2.41	111.85	117.79
32	Y	315	LUT	C20-C13-C12	2.41	121.88	118.08
31	7	313	CLA	C1D-ND-C4D	-2.41	104.62	106.33
32	n	317	LUT	C31-C30-C29	-2.41	123.87	127.31
31	q	315	CLA	CHD-C1D-ND	-2.41	122.24	124.45
30	3	310	CHL	CHB-C4A-NA	2.41	127.85	124.51
30	S	309	CHL	CHB-C4A-NA	2.41	127.85	124.51
30	5	601	CHL	CHC-C1C-NC	2.41	127.86	124.20
33	a	415	LHG	O8-C23-C24	2.41	119.48	111.91
34	a	413	LMG	C3-C4-C5	2.41	114.54	110.24
30	N	309	CHL	C1-C2-C3	-2.41	121.87	126.04
31	6	315	CLA	C4B-CHC-C1C	2.41	132.06	126.34
33	3	320	LHG	C5-O7-C7	-2.41	111.85	117.79
31	B	616	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
31	b	608	CLA	C2D-C1D-ND	2.41	111.88	110.10
31	s	316	CLA	C3B-C4B-NB	-2.41	108.28	110.52
30	5	609	CHL	CMA-C3A-C2A	2.41	123.56	113.83
31	R	314	CLA	C4B-CHC-C1C	2.41	132.06	126.34
31	7	305	CLA	C4B-CHC-C1C	2.41	132.06	126.34
31	c	609	CLA	CHA-C4D-ND	2.41	137.54	132.50
30	N	301	CHL	C1-O2A-CGA	2.41	122.77	116.44
31	q	315	CLA	C3B-C4B-NB	-2.41	108.28	110.52
31	0	614	CLA	O2D-CGD-O1D	-2.41	119.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	604	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
31	C	611	CLA	C4B-CHC-C1C	2.41	132.05	126.34
31	n	304	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	c	613	CLA	C1-O2A-CGA	2.41	122.77	116.44
31	y	603	CLA	C4B-CHC-C1C	2.41	132.05	126.34
31	n	314	CLA	CHA-C4D-ND	2.41	137.54	132.50
30	7	321	CHL	CHD-C4C-C3C	2.41	128.38	124.84
31	g	314	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
31	6	311	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	C	602	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	R	304	CLA	C1D-ND-C4D	-2.41	104.62	106.33
31	1	611	CLA	CHA-C4D-ND	2.41	137.54	132.50
32	8	615	LUT	C31-C30-C29	-2.41	123.87	127.31
31	3	306	CLA	C4B-CHC-C1C	2.41	132.05	126.34
31	y	602	CLA	O2A-CGA-CBA	2.41	119.47	111.91
34	A	418	LMG	O8-C28-C29	2.41	119.47	111.91
31	R	307	CLA	CHA-C4D-ND	2.41	137.53	132.50
30	0	609	CHL	CHC-C1C-NC	2.41	127.86	124.20
30	g	308	CHL	CHC-C1C-NC	2.41	127.86	124.20
31	q	304	CLA	CHA-C4D-ND	2.41	137.53	132.50
30	6	307	CHL	C4A-NA-C1A	2.41	107.79	106.71
30	S	308	CHL	C4A-NA-C1A	2.41	107.79	106.71
31	b	605	CLA	C4B-CHC-C1C	2.41	132.05	126.34
31	0	614	CLA	CHA-C4D-ND	2.41	137.53	132.50
32	7	318	LUT	C21-C26-C27	-2.41	109.66	112.70
30	3	310	CHL	CHD-C4C-C3C	2.41	128.38	124.84
31	5	603	CLA	O2A-CGA-CBA	2.41	119.46	111.91
31	5	603	CLA	CHA-C4D-ND	2.41	137.53	132.50
31	5	610	CLA	CHA-C4D-ND	2.41	137.53	132.50
31	S	303	CLA	O2A-CGA-CBA	2.41	119.46	111.91
30	g	309	CHL	CHD-C4C-C3C	2.41	128.38	124.84
43	b	619	BCR	C29-C30-C25	2.41	114.18	110.48
31	C	602	CLA	C1-O2A-CGA	2.41	122.75	116.44
31	p	610	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
43	t	101	BCR	C1-C6-C5	-2.41	119.23	122.61
32	s	317	LUT	C30-C31-C32	-2.40	115.71	123.22
31	8	604	CLA	C4B-CHC-C1C	2.40	132.04	126.34
31	5	615	CLA	C3B-C4B-NB	-2.40	108.28	110.52
36	Y	317	NEX	C31-C30-C29	2.40	130.74	127.31
34	r	321	LMG	O6-C1-C2	-2.40	105.26	110.35
30	9	309	CHL	CHC-C1C-NC	2.40	127.85	124.20
30	p	601	CHL	CHC-C1C-NC	2.40	127.85	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	311	CLA	O2A-CGA-CBA	2.40	119.45	111.91
30	n	302	CHL	CHD-C4C-C3C	2.40	128.37	124.84
31	0	613	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	9	316	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	6	314	CLA	O2A-CGA-CBA	2.40	119.45	111.91
31	Y	310	CLA	O2A-CGA-CBA	2.40	119.45	111.91
36	r	301	NEX	C39-C29-C30	-2.40	119.56	122.92
31	q	313	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	B	605	CLA	C4B-CHC-C1C	2.40	132.04	126.34
31	C	602	CLA	C4B-CHC-C1C	2.40	132.04	126.34
31	c	601	CLA	C4B-CHC-C1C	2.40	132.04	126.34
30	N	302	CHL	CHC-C1C-NC	2.40	127.85	124.20
31	A	407	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
32	7	317	LUT	C11-C12-C13	-2.40	119.67	126.42
48	R	302	LMU	O5'-C5'-C4'	-2.40	104.69	109.75
31	c	604	CLA	C4B-CHC-C1C	2.40	132.04	126.34
31	Y	303	CLA	CHA-C4D-ND	2.40	137.53	132.50
33	b	625	LHG	C5-O7-C7	-2.40	111.88	117.79
31	8	611	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	0	614	CLA	C4B-CHC-C1C	2.40	132.03	126.34
35	g	315	RRX	C33-C5-C4	2.40	118.23	113.62
30	4	605	CHL	C2C-C3C-C4C	2.40	108.20	106.49
30	7	309	CHL	C2B-C1B-NB	-2.40	108.62	110.23
32	8	616	LUT	C30-C31-C32	-2.40	115.72	123.22
44	A	416	PL9	C27-C28-C29	-2.40	121.88	127.66
31	s	303	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
43	c	614	BCR	C19-C18-C17	2.40	122.62	118.94
31	3	306	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	b	606	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	g	313	CLA	C3B-C4B-NB	-2.40	108.29	110.52
31	N	304	CLA	C4B-CHC-C1C	2.40	132.03	126.34
31	y	614	CLA	CHA-C4D-ND	2.40	137.52	132.50
36	R	301	NEX	C38-C25-C26	-2.40	118.24	122.26
30	S	308	CHL	CHB-C4A-NA	2.40	127.83	124.51
31	5	612	CLA	C4B-CHC-C1C	2.40	132.03	126.34
31	S	314	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	6	314	CLA	C3B-C4B-NB	-2.40	108.29	110.52
31	Y	303	CLA	C3B-C4B-NB	-2.40	108.29	110.52
32	n	318	LUT	C30-C31-C32	-2.40	115.73	123.22
30	S	309	CHL	CHC-C1C-NC	2.40	127.84	124.20
31	8	612	CLA	C4B-CHC-C1C	2.40	132.03	126.34
30	n	308	CHL	CHD-C4C-C3C	2.40	128.37	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	603	CLA	C1D-ND-C4D	-2.40	104.63	106.33
34	m	102	LMG	O8-C28-C29	2.40	119.44	111.91
32	r	317	LUT	C40-C33-C32	2.40	121.86	118.08
31	r	303	CLA	CMA-C3A-C4A	2.40	118.22	111.77
31	8	614	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	Y	303	CLA	O2A-CGA-CBA	2.40	119.43	111.91
30	8	601	CHL	CHD-C4C-C3C	2.40	128.37	124.84
31	R	313	CLA	C4B-CHC-C1C	2.40	132.03	126.34
33	l	101	LHG	O8-C23-C24	2.40	119.43	111.91
30	2	608	CHL	C2C-C3C-C4C	2.40	108.20	106.49
31	r	312	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	B	614	CLA	C4B-CHC-C1C	2.40	132.02	126.34
31	S	305	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
31	N	310	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
32	0	616	LUT	C20-C13-C12	2.40	121.85	118.08
31	7	315	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	r	316	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	c	604	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
30	3	303	CHL	C2C-C3C-C4C	2.40	108.20	106.49
31	a	406	CLA	C4B-CHC-C1C	2.40	132.02	126.34
47	E	101	HEM	CBA-CAA-C2A	-2.40	105.97	112.63
30	6	302	CHL	CHC-C1C-NC	2.40	127.84	124.20
31	s	316	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	n	304	CLA	O2A-CGA-CBA	2.40	119.43	111.91
31	q	305	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
31	4	614	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
31	n	314	CLA	C4B-CHC-C1C	2.40	132.02	126.34
30	n	310	CHL	C3B-C4B-NB	-2.40	108.29	110.52
31	N	304	CLA	C3B-C4B-NB	-2.40	108.29	110.52
31	n	303	CLA	O2A-CGA-CBA	2.39	119.42	111.91
31	r	311	CLA	C4B-CHC-C1C	2.39	132.02	126.34
31	5	615	CLA	O1D-CGD-CBD	-2.39	119.58	124.48
30	7	306	CHL	C2C-C3C-C4C	2.39	108.20	106.49
30	G	608	CHL	CHC-C1C-NC	2.39	127.83	124.20
31	b	603	CLA	C2D-C1D-ND	2.39	111.87	110.10
31	G	602	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
31	9	306	CLA	C4B-CHC-C1C	2.39	132.01	126.34
31	6	314	CLA	CHA-C4D-ND	2.39	137.50	132.50
32	7	318	LUT	C15-C35-C34	-2.39	118.57	123.47
36	y	618	NEX	C40-C33-C34	-2.39	119.57	122.92
31	G	611	CLA	CMA-C3A-C4A	2.39	118.20	111.77
31	R	307	CLA	CMA-C3A-C4A	2.39	118.20	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	615	CLA	C2D-C1D-ND	2.39	111.87	110.10
31	6	303	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	c	606	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	q	312	CLA	O2A-CGA-CBA	2.39	119.41	111.91
31	6	303	CLA	O2A-CGA-CBA	2.39	119.41	111.91
31	R	304	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
31	n	313	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	c	601	CLA	C2C-C1C-NC	2.39	112.21	109.97
31	N	305	CLA	C4B-CHC-C1C	2.39	132.01	126.34
31	b	605	CLA	CHA-C1A-NA	-2.39	120.92	126.40
31	b	608	CLA	O2A-CGA-CBA	2.39	119.41	111.91
31	y	604	CLA	C4B-CHC-C1C	2.39	132.01	126.34
31	5	613	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	b	613	CLA	CHA-C4D-ND	2.39	137.50	132.50
33	S	320	LHG	C6-C5-C4	-2.39	106.14	111.79
32	g	316	LUT	C40-C33-C34	-2.39	119.58	122.92
30	3	307	CHL	CHD-C4C-C3C	2.39	128.35	124.84
31	5	604	CLA	C4B-CHC-C1C	2.39	132.00	126.34
31	9	312	CLA	C4B-CHC-C1C	2.39	132.00	126.34
31	n	315	CLA	C4B-CHC-C1C	2.39	132.00	126.34
31	8	612	CLA	CHA-C4D-ND	2.39	137.50	132.50
43	t	101	BCR	C28-C27-C26	-2.39	109.81	114.08
31	1	610	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	s	303	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	S	305	CLA	CHA-C4D-ND	2.39	137.50	132.50
32	0	617	LUT	C8-C7-C6	-2.39	120.50	127.20
31	G	610	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
30	R	310	CHL	C4D-CHA-C1A	2.39	124.16	121.25
31	4	602	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	C	606	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	r	306	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	Y	305	CLA	C3B-C4B-NB	-2.39	108.30	110.52
31	3	314	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
31	n	305	CLA	CMA-C3A-C4A	2.39	118.19	111.77
30	Y	307	CHL	CMA-C3A-C2A	2.39	123.46	113.83
31	6	305	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	R	316	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	S	310	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	d	401	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	r	304	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	r	313	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	s	306	CLA	CHA-C4D-ND	2.39	137.49	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	a	412	SQD	O5-C1-O6	-2.39	104.32	109.97
30	6	310	CHL	CMA-C3A-C2A	2.39	123.46	113.83
31	B	611	CLA	O2A-CGA-CBA	2.39	119.40	111.91
30	9	308	CHL	CHC-C1C-NC	2.39	127.82	124.20
31	8	603	CLA	C4B-CHC-C1C	2.39	132.00	126.34
30	0	608	CHL	CHD-C4C-C3C	2.39	128.35	124.84
32	n	317	LUT	C35-C15-C14	-2.39	118.59	123.47
31	n	305	CLA	C4B-CHC-C1C	2.39	132.00	126.34
31	r	305	CLA	C4B-CHC-C1C	2.39	132.00	126.34
31	c	602	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	r	311	CLA	CAA-C2A-C3A	-2.39	106.25	112.78
31	7	313	CLA	CMD-C2D-C3D	-2.39	122.13	127.61
31	g	305	CLA	C4B-CHC-C1C	2.39	132.00	126.34
31	r	305	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
31	D	403	CLA	CHA-C4D-ND	2.38	137.49	132.50
30	g	309	CHL	CHC-C1C-NC	2.38	127.82	124.20
31	g	312	CLA	C4B-CHC-C1C	2.38	131.99	126.34
34	D	409	LMG	O1-C7-C8	-2.38	105.15	110.90
35	G	614	RRX	C37-C22-C21	-2.38	119.58	122.92
43	B	618	BCR	C10-C11-C12	-2.38	115.78	123.22
30	n	301	CHL	CHC-C1C-NC	2.38	127.82	124.20
31	c	606	CLA	C4B-CHC-C1C	2.38	131.99	126.34
32	5	617	LUT	C8-C7-C6	-2.38	120.51	127.20
31	1	604	CLA	C4B-CHC-C1C	2.38	131.99	126.34
30	N	307	CHL	C1-O2A-CGA	2.38	122.69	116.44
30	r	309	CHL	C2B-C1B-NB	-2.38	108.64	110.23
31	y	602	CLA	CHA-C4D-ND	2.38	137.48	132.50
36	r	319	NEX	C26-C27-C28	-2.38	120.96	125.99
31	0	611	CLA	O2A-CGA-CBA	2.38	119.38	111.91
31	R	313	CLA	CHA-C4D-ND	2.38	137.48	132.50
30	q	303	CHL	CHC-C1C-NC	2.38	127.82	124.20
31	4	604	CLA	C3B-C4B-NB	-2.38	108.31	110.52
43	c	614	BCR	C33-C5-C4	2.38	118.19	113.62
30	N	306	CHL	C2B-C1B-NB	-2.38	108.64	110.23
30	G	605	CHL	CHB-C4A-NA	2.38	127.80	124.51
30	y	608	CHL	CHD-C4C-C3C	2.38	128.34	124.84
31	0	612	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
31	c	613	CLA	CHA-C1A-NA	-2.38	120.95	126.40
31	B	603	CLA	C4B-CHC-C1C	2.38	131.98	126.34
31	p	602	CLA	O2A-CGA-CBA	2.38	119.38	111.91
30	8	606	CHL	C2B-C1B-NB	-2.38	108.64	110.23
31	0	603	CLA	O2A-CGA-CBA	2.38	119.37	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	616	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	n	316	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	r	315	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	A	405	CLA	CAA-C2A-C1A	-2.38	104.18	111.97
31	S	314	CLA	C1-O2A-CGA	2.38	122.68	116.44
31	6	314	CLA	C4B-CHC-C1C	2.38	131.98	126.34
31	r	305	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	y	610	CLA	CHA-C4D-ND	2.38	137.47	132.50
30	R	309	CHL	C2B-C1B-NB	-2.38	108.64	110.23
30	0	607	CHL	C2B-C1B-NB	-2.38	108.64	110.23
30	q	307	CHL	C2B-C1B-NB	-2.38	108.64	110.23
31	R	303	CLA	C4B-CHC-C1C	2.38	131.98	126.34
31	9	313	CLA	C2D-C1D-ND	2.38	111.86	110.10
43	D	405	BCR	C23-C24-C25	-2.38	120.53	127.20
31	5	611	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
31	R	314	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	0	602	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	g	311	CLA	O2A-CGA-CBA	2.38	119.37	111.91
35	9	317	RRX	C37-C22-C21	-2.38	119.59	122.92
31	0	611	CLA	C4B-CHC-C1C	2.38	131.98	126.34
44	A	416	PL9	C40-C39-C41	2.38	119.27	115.27
36	S	319	NEX	O24-C25-C38	-2.38	112.21	115.06
31	1	613	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	A	405	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	N	310	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	9	315	CLA	C4B-CHC-C1C	2.38	131.97	126.34
36	3	319	NEX	C40-C33-C34	-2.38	119.59	122.92
31	7	311	CLA	CMD-C2D-C3D	-2.38	122.15	127.61
31	c	605	CLA	C1-O2A-CGA	2.38	122.68	116.44
31	4	602	CLA	O2A-CGA-CBA	2.38	119.36	111.91
31	4	614	CLA	C4B-CHC-C1C	2.37	131.97	126.34
31	c	604	CLA	CHA-C4D-ND	2.37	137.47	132.50
47	E	101	HEM	C4D-ND-C1D	2.37	107.53	105.07
31	q	315	CLA	O1D-CGD-CBD	-2.37	119.62	124.48
31	2	611	CLA	C3B-C4B-NB	-2.37	108.31	110.52
31	d	401	CLA	C3B-C4B-NB	-2.37	108.31	110.52
43	B	619	BCR	C35-C13-C14	-2.37	119.60	122.92
31	5	612	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
31	N	312	CLA	CHA-C4D-ND	2.37	137.47	132.50
44	a	414	PL9	C22-C23-C24	-2.37	121.94	127.66
33	Y	318	LHG	O8-C23-C24	2.37	119.36	111.91
30	1	605	CHL	C1-O2A-CGA	2.37	122.67	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	308	CHL	CHD-C4C-C3C	2.37	128.33	124.84
31	R	306	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
43	B	617	BCR	C3-C4-C5	-2.37	109.84	114.08
31	q	314	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
31	B	607	CLA	C4B-CHC-C1C	2.37	131.96	126.34
31	s	310	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	p	610	CLA	O2A-CGA-CBA	2.37	119.35	111.91
31	7	303	CLA	O2A-CGA-CBA	2.37	119.35	111.91
30	p	605	CHL	C4A-NA-C1A	2.37	107.77	106.71
31	0	604	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	G	610	CLA	C4B-CHC-C1C	2.37	131.96	126.34
31	3	316	CLA	O2A-CGA-CBA	2.37	119.35	111.91
34	7	322	LMG	C8-O7-C10	-2.37	111.95	117.79
31	c	605	CLA	C3B-C4B-NB	-2.37	108.32	110.52
31	c	607	CLA	C4B-CHC-C1C	2.37	131.96	126.34
31	1	611	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
31	1	602	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	b	617	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	C	608	CLA	C4B-CHC-C1C	2.37	131.96	126.34
30	s	302	CHL	CHC-C1C-NC	2.37	127.80	124.20
31	n	304	CLA	C4B-CHC-C1C	2.37	131.96	126.34
35	G	614	RRX	C36-C18-C17	-2.37	119.60	122.92
32	p	616	LUT	C31-C32-C33	2.37	133.07	126.42
31	1	614	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	R	311	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	4	613	CLA	CHA-C4D-ND	2.37	137.45	132.50
31	c	608	CLA	CHA-C4D-ND	2.37	137.45	132.50
34	6	323	LMG	O6-C5-C6	2.37	112.33	106.44
31	3	316	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
31	B	612	CLA	C6-C5-C3	-2.37	107.24	113.45
31	p	603	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
30	p	609	CHL	CHC-C1C-NC	2.37	127.80	124.20
30	1	606	CHL	C2C-C3C-C4C	2.37	108.18	106.49
43	c	615	BCR	C7-C8-C9	-2.37	122.66	126.23
31	0	603	CLA	C4B-CHC-C1C	2.37	131.95	126.34
31	p	602	CLA	C4B-CHC-C1C	2.37	131.95	126.34
31	R	303	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
31	0	610	CLA	C1-O2A-CGA	2.37	122.66	116.44
32	8	615	LUT	C35-C15-C14	-2.37	118.62	123.47
31	2	612	CLA	C3B-C4B-NB	-2.37	108.32	110.52
32	y	616	LUT	C18-C5-C4	2.37	118.74	114.36
31	2	612	CLA	CHA-C4D-ND	2.37	137.45	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	8	615	LUT	C30-C31-C32	-2.37	115.83	123.22
32	n	317	LUT	C30-C31-C32	-2.37	115.83	123.22
35	q	317	RRX	C11-C10-C9	-2.37	123.93	127.31
31	B	613	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
32	n	318	LUT	C8-C7-C6	-2.37	120.56	127.20
31	r	313	CLA	O2A-CGA-CBA	2.37	119.33	111.91
31	c	601	CLA	O2A-CGA-CBA	2.37	119.33	111.91
31	y	613	CLA	C6-C5-C3	-2.36	107.25	113.45
31	s	305	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	s	314	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	9	314	CLA	CMA-C3A-C4A	2.36	118.13	111.77
34	w	202	LMG	C8-O7-C10	-2.36	111.97	117.79
31	B	606	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
34	7	322	LMG	O8-C28-C29	2.36	119.33	111.91
31	N	315	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
30	R	309	CHL	C2C-C3C-C4C	2.36	108.17	106.49
31	S	303	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	S	316	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	Y	311	CLA	C4B-CHC-C1C	2.36	131.94	126.34
31	A	406	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
30	N	306	CHL	CHB-C4A-NA	2.36	127.78	124.51
31	c	602	CLA	C2D-C1D-ND	2.36	111.84	110.10
31	7	311	CLA	CHA-C4D-ND	2.36	137.44	132.50
34	c	624	LMG	C8-O7-C10	-2.36	111.98	117.79
31	3	316	CLA	C1D-ND-C4D	-2.36	104.66	106.33
31	c	604	CLA	C3B-C4B-NB	-2.36	108.33	110.52
43	C	614	BCR	C2-C1-C6	2.36	114.11	110.48
31	0	610	CLA	CHA-C4D-ND	2.36	137.44	132.50
32	7	317	LUT	C8-C7-C6	-2.36	120.57	127.20
31	c	608	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
31	N	314	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	Y	314	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	3	311	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
36	3	319	NEX	C26-C27-C28	-2.36	121.00	125.99
31	5	610	CLA	O2A-CGA-CBA	2.36	119.31	111.91
30	n	302	CHL	CHC-C1C-NC	2.36	127.78	124.20
31	8	609	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	q	304	CLA	C4B-CHC-C1C	2.36	131.93	126.34
31	r	312	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
31	a	406	CLA	CHA-C4D-ND	2.36	137.43	132.50
44	A	416	PL9	C22-C23-C24	-2.36	121.98	127.66
31	4	604	CLA	C4B-CHC-C1C	2.36	131.93	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	305	CLA	C4B-CHC-C1C	2.36	131.93	126.34
31	s	313	CLA	C3B-C4B-NB	-2.36	108.33	110.52
31	B	609	CLA	C4B-CHC-C1C	2.36	131.93	126.34
30	y	609	CHL	CHD-C4C-C3C	2.36	128.31	124.84
32	6	317	LUT	C39-C29-C28	2.36	121.79	118.08
31	3	306	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
36	2	616	NEX	C26-C27-C28	-2.36	121.01	125.99
31	Y	312	CLA	O2A-CGA-CBA	2.36	119.31	111.91
36	y	618	NEX	C2-C1-C6	2.36	111.50	109.21
30	8	601	CHL	CHC-C1C-NC	2.36	127.78	124.20
31	Y	305	CLA	O2A-CGA-CBA	2.36	119.30	111.91
31	N	321	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
31	g	305	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
30	s	307	CHL	C2B-C1B-NB	-2.36	108.65	110.23
30	3	310	CHL	C2C-C3C-C4C	2.36	108.17	106.49
43	H	101	BCR	C8-C7-C6	-2.36	120.58	127.20
30	G	608	CHL	CHD-C4C-C3C	2.36	128.30	124.84
31	2	604	CLA	C4B-CHC-C1C	2.36	131.93	126.34
31	R	304	CLA	CHA-C4D-ND	2.36	137.43	132.50
31	0	603	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
43	v	101	BCR	C33-C5-C4	2.36	118.14	113.62
30	1	619	CHL	C2B-C1B-NB	-2.36	108.65	110.23
31	c	605	CLA	CMD-C2D-C3D	-2.36	122.20	127.61
31	Y	311	CLA	CHA-C4D-ND	2.35	137.43	132.50
31	q	313	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
31	3	316	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
31	5	612	CLA	O2A-CGA-CBA	2.35	119.30	111.91
31	s	306	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
30	g	308	CHL	C2C-C3C-C4C	2.35	108.17	106.49
31	B	611	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	S	315	CLA	C4B-CHC-C1C	2.35	131.92	126.34
32	3	318	LUT	C20-C13-C14	-2.35	119.63	122.92
31	5	602	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	Y	310	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	d	404	CLA	C4B-CHC-C1C	2.35	131.92	126.34
31	N	310	CLA	O2A-CGA-CBA	2.35	119.29	111.91
30	r	308	CHL	C2B-C1B-NB	-2.35	108.66	110.23
31	6	316	CLA	C1D-ND-C4D	-2.35	104.66	106.33
31	c	612	CLA	CHA-C4D-ND	2.35	137.42	132.50
30	1	601	CHL	CHD-C4C-C3C	2.35	128.30	124.84
32	9	318	LUT	C18-C5-C4	2.35	118.71	114.36
35	4	615	RRX	C37-C22-C21	-2.35	119.63	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	607	CHL	C1-O2A-CGA	2.35	122.61	116.44
30	4	609	CHL	CHD-C4C-C3C	2.35	128.30	124.84
30	9	303	CHL	C2C-C3C-C4C	2.35	108.17	106.49
31	9	313	CLA	O2A-CGA-CBA	2.35	119.29	111.91
31	R	311	CLA	C4B-CHC-C1C	2.35	131.91	126.34
31	9	313	CLA	C4B-CHC-C1C	2.35	131.91	126.34
36	s	319	NEX	C39-C29-C30	-2.35	119.63	122.92
32	8	616	LUT	C8-C7-C6	-2.35	120.60	127.20
31	Y	313	CLA	C4B-CHC-C1C	2.35	131.91	126.34
31	q	306	CLA	C4B-CHC-C1C	2.35	131.91	126.34
31	y	604	CLA	C3B-C4B-NB	-2.35	108.33	110.52
31	5	610	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
31	a	409	CLA	C1D-ND-C4D	-2.35	104.67	106.33
31	r	307	CLA	C4B-CHC-C1C	2.35	131.91	126.34
31	y	611	CLA	CHA-C4D-ND	2.35	137.41	132.50
30	3	310	CHL	C3B-C4B-NB	-2.35	108.34	110.52
32	0	617	LUT	C15-C35-C34	-2.35	118.66	123.47
31	1	603	CLA	C4B-CHC-C1C	2.35	131.91	126.34
30	Y	306	CHL	CHB-C4A-NA	2.35	127.76	124.51
31	N	303	CLA	O2A-CGA-CBA	2.35	119.28	111.91
30	9	309	CHL	C2B-C1B-NB	-2.35	108.66	110.23
31	S	312	CLA	CHA-C4D-ND	2.35	137.41	132.50
34	d	409	LMG	C8-O7-C10	-2.35	112.01	117.79
30	1	607	CHL	CHD-C4C-C3C	2.35	128.29	124.84
30	p	609	CHL	CMA-C3A-C2A	2.35	123.30	113.83
31	C	607	CLA	CHA-C4D-ND	2.35	137.41	132.50
31	4	611	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
31	c	609	CLA	C6-C5-C3	-2.35	107.30	113.45
43	b	620	BCR	C8-C7-C6	-2.35	120.61	127.20
31	q	316	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
31	R	315	CLA	C2D-C1D-ND	2.34	111.83	110.10
30	q	307	CHL	CHC-C1C-NC	2.34	127.76	124.20
34	a	416	LMG	O8-C28-C29	2.34	119.27	111.91
31	1	603	CLA	CMA-C3A-C4A	2.34	118.07	111.77
31	2	610	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
31	9	304	CLA	CHA-C4D-ND	2.34	137.40	132.50
31	6	305	CLA	C3B-C4B-NB	-2.34	108.34	110.52
31	q	306	CLA	C6-C5-C3	-2.34	107.31	113.45
35	2	614	RRX	C27-C26-C25	-2.34	115.63	120.85
31	p	613	CLA	C4B-CHC-C1C	2.34	131.90	126.34
31	g	310	CLA	CHA-C4D-ND	2.34	137.40	132.50
30	3	309	CHL	C4B-CHC-C1C	2.34	131.89	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	601	CLA	O2A-CGA-CBA	2.34	119.26	111.91
43	c	615	BCR	C35-C13-C14	-2.34	119.64	122.92
31	B	613	CLA	C4B-CHC-C1C	2.34	131.89	126.34
31	S	314	CLA	C4B-CHC-C1C	2.34	131.89	126.34
31	S	304	CLA	CMA-C3A-C4A	2.34	118.06	111.77
44	a	414	PL9	C27-C28-C29	-2.34	122.02	127.66
31	q	305	CLA	O2A-CGA-CBA	2.34	119.25	111.91
31	q	304	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
32	S	318	LUT	C31-C32-C33	-2.34	119.84	126.42
30	1	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
32	p	616	LUT	C18-C5-C4	2.34	118.69	114.36
34	x	202	LMG	C8-O7-C10	-2.34	112.03	117.79
31	y	611	CLA	C1D-ND-C4D	-2.34	104.67	106.33
35	9	317	RRX	C35-C13-C14	-2.34	119.65	122.92
43	d	406	BCR	C38-C26-C27	2.34	118.11	113.62
43	C	614	BCR	C8-C7-C6	-2.34	120.63	127.20
30	Y	302	CHL	CHD-C4C-C3C	2.34	128.28	124.84
31	8	602	CLA	O2A-CGA-CBA	2.34	119.25	111.91
31	A	406	CLA	CHA-C4D-ND	2.34	137.39	132.50
31	7	313	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
31	7	313	CLA	O2A-CGA-CBA	2.34	119.24	111.91
31	C	613	CLA	CMA-C3A-C4A	2.34	118.06	111.77
31	B	609	CLA	CHA-C4D-ND	2.34	137.39	132.50
43	V	101	BCR	C11-C10-C9	-2.34	123.97	127.31
31	0	613	CLA	C4B-CHC-C1C	2.34	131.88	126.34
31	G	604	CLA	C3B-C4B-NB	-2.34	108.35	110.52
31	6	304	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
31	g	305	CLA	CMA-C3A-C4A	2.34	118.05	111.77
35	2	614	RRX	C36-C18-C17	-2.34	119.65	122.92
30	n	307	CHL	C2B-C1B-NB	-2.34	108.67	110.23
31	C	603	CLA	O2A-CGA-CBA	2.34	119.24	111.91
32	N	317	LUT	C19-C9-C10	-2.34	119.65	122.92
31	p	602	CLA	CHA-C4D-ND	2.34	137.38	132.50
36	r	301	NEX	C26-C27-C28	-2.34	121.06	125.99
31	C	610	CLA	C2D-C1D-ND	2.34	111.83	110.10
31	y	611	CLA	C1-C2-C3	-2.34	122.00	126.04
35	4	615	RRX	C36-C18-C17	-2.34	119.65	122.92
31	4	603	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
31	9	316	CLA	CMD-C2D-C3D	-2.33	122.24	127.61
31	D	404	CLA	C3B-C4B-NB	-2.33	108.35	110.52
30	6	309	CHL	CHC-C1C-NC	2.33	127.75	124.20
31	2	604	CLA	O2D-CGD-O1D	-2.33	119.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	303	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
30	N	309	CHL	CHB-C4A-NA	2.33	127.74	124.51
31	d	405	CLA	C1D-ND-C4D	-2.33	104.68	106.33
31	G	609	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	9	306	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	b	610	CLA	CHA-C4D-ND	2.33	137.38	132.50
31	A	406	CLA	C4B-CHC-C1C	2.33	131.87	126.34
31	S	313	CLA	C4B-CHC-C1C	2.33	131.87	126.34
30	8	605	CHL	CHD-C4C-C3C	2.33	128.27	124.84
34	p	620	LMG	C8-O7-C10	-2.33	112.05	117.79
31	b	602	CLA	O2A-CGA-CBA	2.33	119.23	111.91
30	q	311	CHL	CHB-C4A-NA	2.33	127.74	124.51
36	G	616	NEX	C26-C27-C28	-2.33	121.06	125.99
31	y	613	CLA	C16-C15-C13	-2.33	108.38	115.92
38	B	620	SQD	O3-C3-C2	-2.33	104.96	110.35
31	8	612	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	b	613	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	s	306	CLA	O2A-CGA-CBA	2.33	119.22	111.91
30	0	609	CHL	C2B-C1B-NB	-2.33	108.67	110.23
30	n	310	CHL	CHC-C1C-NC	2.33	127.74	124.20
31	7	312	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
45	C	620	DGD	O1G-C1A-C2A	2.33	119.22	111.91
31	R	315	CLA	CMA-C3A-C4A	2.33	118.04	111.77
30	N	307	CHL	C1-C2-C3	-2.33	122.01	126.04
43	b	620	BCR	C21-C20-C19	-2.33	115.94	123.22
30	5	601	CHL	CMA-C3A-C4A	2.33	118.04	111.77
32	s	317	LUT	C35-C15-C14	-2.33	118.70	123.47
30	3	307	CHL	C2B-C1B-NB	-2.33	108.67	110.23
31	6	305	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
31	C	604	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
31	3	301	CLA	CHA-C4D-ND	2.33	137.37	132.50
31	C	612	CLA	CHA-C4D-ND	2.33	137.37	132.50
30	0	601	CHL	CMA-C3A-C2A	2.33	123.22	113.83
31	Y	304	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	r	313	CLA	C4B-CHC-C1C	2.33	131.86	126.34
31	r	315	CLA	C4B-CHC-C1C	2.33	131.86	126.34
31	p	604	CLA	CMA-C3A-C4A	2.33	118.03	111.77
31	n	314	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	y	603	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
30	2	608	CHL	CHB-C4A-NA	2.33	127.73	124.51
31	S	310	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
36	0	618	NEX	C40-C33-C34	-2.33	119.66	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	1	603	CLA	O2A-CGA-CBA	2.33	119.21	111.91
31	0	615	CLA	C4B-CHC-C1C	2.33	131.86	126.34
34	a	413	LMG	O1-C1-C2	2.33	111.94	108.30
31	G	609	CLA	CHA-C4D-ND	2.33	137.37	132.50
47	e	102	HEM	C4D-ND-C1D	2.33	107.48	105.07
30	Y	308	CHL	CHC-C1C-NC	2.33	127.73	124.20
31	R	312	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
38	Y	320	SQD	O3-C3-C2	-2.33	104.97	110.35
31	7	305	CLA	C3B-C4B-NB	-2.33	108.36	110.52
31	B	604	CLA	C4B-CHC-C1C	2.33	131.85	126.34
31	B	615	CLA	CHA-C4D-ND	2.33	137.36	132.50
31	n	304	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
31	g	314	CLA	O2A-CGA-CBA	2.33	119.20	111.91
31	A	406	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
31	D	403	CLA	C4B-CHC-C1C	2.32	131.85	126.34
31	S	311	CLA	O2A-CGA-CBA	2.32	119.20	111.91
30	S	309	CHL	CHD-C4C-C3C	2.32	128.26	124.84
35	2	614	RRX	C37-C22-C21	-2.32	119.67	122.92
31	c	609	CLA	C4B-CHC-C1C	2.32	131.85	126.34
30	n	306	CHL	CHD-C4C-C3C	2.32	128.26	124.84
31	S	311	CLA	CHA-C4D-ND	2.32	137.36	132.50
31	g	313	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	R	315	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
31	R	315	CLA	O2A-CGA-CBA	2.32	119.20	111.91
30	4	607	CHL	CHD-C4C-C3C	2.32	128.25	124.84
31	C	608	CLA	CHA-C4D-ND	2.32	137.36	132.50
31	a	407	CLA	CHA-C4D-ND	2.32	137.36	132.50
44	a	414	PL9	C36-C34-C33	-2.32	116.42	121.12
31	n	311	CLA	CHA-C4D-ND	2.32	137.36	132.50
32	S	318	LUT	C40-C33-C34	-2.32	119.67	122.92
31	p	604	CLA	C1D-ND-C4D	-2.32	104.69	106.33
31	r	304	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	b	602	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
31	G	602	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	9	306	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	c	613	CLA	C2A-C1A-CHA	2.32	127.92	123.86
31	N	312	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	y	614	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	2	612	CLA	C4B-CHC-C1C	2.32	131.84	126.34
31	s	312	CLA	C4B-CHC-C1C	2.32	131.84	126.34
31	0	612	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
30	Y	307	CHL	CHC-C1C-NC	2.32	127.72	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	9	302	LMG	C8-O7-C10	-2.32	112.08	117.79
33	R	320	LHG	O8-C23-C24	2.32	119.19	111.91
38	s	301	SQD	O3-C3-C2	-2.32	104.99	110.35
31	0	603	CLA	CHA-C4D-ND	2.32	137.35	132.50
32	G	615	LUT	C20-C13-C12	2.32	121.73	118.08
30	6	306	CHL	CHC-C1C-NC	2.32	127.72	124.20
31	N	313	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
31	S	304	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
31	6	303	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
31	B	609	CLA	C3B-C4B-NB	-2.32	108.36	110.52
31	n	305	CLA	C3B-C4B-NB	-2.32	108.36	110.52
31	c	605	CLA	C4B-CHC-C1C	2.32	131.83	126.34
31	y	613	CLA	CHD-C1D-ND	-2.32	122.33	124.45
35	9	317	RRX	C27-C26-C25	-2.32	115.69	120.85
31	3	301	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
31	c	605	CLA	C1-C2-C3	-2.32	122.04	126.04
31	R	314	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
43	c	614	BCR	C37-C22-C21	-2.32	119.68	122.92
31	G	612	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
31	c	608	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
30	7	307	CHL	CHC-C1C-NC	2.31	127.72	124.20
31	6	315	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
31	p	615	CLA	CHA-C4D-ND	2.31	137.34	132.50
31	C	606	CLA	C4B-CHC-C1C	2.31	131.83	126.34
30	5	608	CHL	CHD-C4C-C3C	2.31	128.24	124.84
31	b	610	CLA	CAA-CBA-CGA	-2.31	106.49	113.25
35	G	614	RRX	C35-C13-C14	-2.31	119.68	122.92
38	B	623	SQD	O3-C3-C2	-2.31	105.00	110.35
31	1	603	CLA	C2D-C1D-ND	2.31	111.81	110.10
35	9	317	RRX	C36-C18-C17	-2.31	119.68	122.92
31	r	312	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
30	9	303	CHL	C2B-C1B-NB	-2.31	108.68	110.23
44	A	416	PL9	C37-C38-C39	-2.31	122.09	127.66
31	R	304	CLA	C3B-C4B-NB	-2.31	108.37	110.52
31	b	604	CLA	C3B-C4B-NB	-2.31	108.37	110.52
31	c	603	CLA	C2D-C1D-ND	2.31	111.81	110.10
31	s	311	CLA	CHA-C4D-ND	2.31	137.33	132.50
36	S	319	NEX	C38-C25-C26	-2.31	118.39	122.26
30	g	306	CHL	CHB-C4A-NA	2.31	127.71	124.51
30	7	309	CHL	CHD-C4C-C3C	2.31	128.24	124.84
31	R	307	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
31	C	608	CLA	O2D-CGD-O1D	-2.31	119.32	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	314	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
30	5	607	CHL	C4D-CHA-C1A	2.31	124.06	121.25
30	1	606	CHL	CHC-C1C-NC	2.31	127.71	124.20
30	R	308	CHL	CHC-C1C-NC	2.31	127.71	124.20
32	S	317	LUT	C1-C6-C5	-2.31	119.36	122.61
30	9	309	CHL	C2C-C3C-C4C	2.31	108.14	106.49
30	p	605	CHL	CHD-C4C-C3C	2.31	128.23	124.84
38	b	621	SQD	O3-C3-C2	-2.31	105.01	110.35
36	n	319	NEX	C12-C13-C14	2.31	122.48	118.94
31	7	315	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
31	2	603	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
31	R	316	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
31	y	602	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
31	B	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
30	N	307	CHL	CMA-C3A-C2A	2.31	123.14	113.83
31	0	604	CLA	O2A-CGA-CBA	2.31	119.15	111.91
30	5	606	CHL	C2C-C3C-C4C	2.31	108.13	106.49
30	9	311	CHL	C2C-C3C-C4C	2.31	108.13	106.49
30	R	310	CHL	C2B-C1B-NB	-2.31	108.69	110.23
30	1	609	CHL	C1-O2A-CGA	2.31	122.50	116.44
34	9	301	LMG	O8-C9-C8	2.31	115.15	108.43
31	3	315	CLA	O2A-CGA-CBA	2.31	119.15	111.91
31	3	311	CLA	CHA-C4D-ND	2.31	137.32	132.50
31	S	315	CLA	O2A-CGA-CBA	2.31	119.15	111.91
31	g	305	CLA	C3B-C4B-NB	-2.31	108.38	110.52
31	Y	313	CLA	C1-O2A-CGA	2.31	122.50	116.44
30	7	308	CHL	C1-C2-C3	-2.31	122.05	126.04
30	2	606	CHL	CHD-C4C-C3C	2.31	128.23	124.84
31	9	316	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
37	r	318	XAT	O4-C5-C18	-2.31	112.29	115.06
31	r	312	CLA	C1D-ND-C4D	-2.31	104.70	106.33
31	7	303	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
30	R	309	CHL	CHC-C1C-NC	2.30	127.70	124.20
35	4	615	RRX	C27-C26-C25	-2.30	115.71	120.85
30	4	601	CHL	C2B-C1B-NB	-2.30	108.69	110.23
31	4	610	CLA	C4B-CHC-C1C	2.30	131.80	126.34
31	b	603	CLA	C4B-CHC-C1C	2.30	131.80	126.34
36	6	319	NEX	C40-C33-C34	-2.30	119.69	122.92
30	p	609	CHL	CHB-C4A-NA	2.30	127.70	124.51
35	G	614	RRX	C27-C26-C25	-2.30	115.71	120.85
31	B	602	CLA	C4B-CHC-C1C	2.30	131.80	126.34
31	0	610	CLA	O2A-CGA-CBA	2.30	119.14	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	614	CLA	O2A-CGA-CBA	2.30	119.14	111.91
32	4	616	LUT	C19-C9-C10	-2.30	119.70	122.92
31	9	314	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
31	B	607	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
30	7	310	CHL	CHD-C4C-C3C	2.30	128.23	124.84
31	9	312	CLA	CMA-C3A-C4A	2.30	117.96	111.77
31	s	311	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
31	G	604	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
32	7	318	LUT	C30-C31-C32	-2.30	116.03	123.22
31	r	316	CLA	C3B-C4B-NB	-2.30	108.38	110.52
30	0	605	CHL	C4D-CHA-C1A	2.30	124.05	121.25
31	5	615	CLA	C4B-CHC-C1C	2.30	131.80	126.34
31	8	612	CLA	C1-C2-C3	-2.30	122.06	126.04
31	N	321	CLA	O2A-CGA-CBA	2.30	119.13	111.91
30	N	302	CHL	C2B-C1B-NB	-2.30	108.69	110.23
31	n	311	CLA	O2A-CGA-CBA	2.30	119.13	111.91
31	s	303	CLA	C6-C7-C8	-2.30	108.48	115.92
31	p	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
31	S	311	CLA	CMA-C3A-C4A	2.30	117.96	111.77
38	R	322	SQD	O3-C3-C2	-2.30	105.03	110.35
38	S	301	SQD	O3-C3-C2	-2.30	105.03	110.35
31	5	613	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
31	N	304	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
30	4	605	CHL	CHC-C1C-NC	2.30	127.69	124.20
31	1	602	CLA	C3B-C4B-NB	-2.30	108.38	110.52
31	9	305	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
31	1	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
31	A	405	CLA	C4B-CHC-C1C	2.30	131.79	126.34
35	g	315	RRX	C36-C18-C17	-2.30	119.70	122.92
36	4	617	NEX	C40-C33-C34	-2.30	119.70	122.92
31	C	606	CLA	O2A-CGA-CBA	2.30	119.12	111.91
31	y	603	CLA	O2A-CGA-CBA	2.30	119.12	111.91
30	n	306	CHL	CHB-C4A-NA	2.30	127.69	124.51
31	A	407	CLA	CHA-C4D-ND	2.30	137.31	132.50
33	F1	301	LHG	O8-C23-C24	2.30	119.12	111.91
32	Y	316	LUT	C11-C12-C13	-2.30	119.96	126.42
31	1	613	CLA	C4B-CHC-C1C	2.30	131.79	126.34
34	b	626	LMG	C8-O7-C10	-2.30	112.13	117.79
38	6	301	SQD	O3-C3-C2	-2.30	105.04	110.35
38	m	101	SQD	O3-C3-C2	-2.30	105.04	110.35
31	d	405	CLA	CHA-C4D-ND	2.30	137.31	132.50
31	A	405	CLA	O2A-CGA-CBA	2.30	119.12	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	311	CLA	CMA-C3A-C4A	2.30	117.95	111.77
30	5	609	CHL	CHB-C4A-NA	2.30	127.69	124.51
30	4	608	CHL	CHD-C4C-C3C	2.30	128.22	124.84
30	5	606	CHL	CMA-C3A-C2A	2.30	123.09	113.83
43	b	620	BCR	C15-C16-C17	-2.30	118.77	123.47
43	B	618	BCR	C37-C22-C23	2.30	121.69	118.08
36	r	301	NEX	C16-C1-C6	-2.30	108.42	110.47
31	C	612	CLA	C6-C5-C3	-2.30	107.43	113.45
31	N	303	CLA	C6-C5-C3	-2.30	107.43	113.45
31	0	613	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
31	B	603	CLA	C2D-C1D-ND	2.30	111.80	110.10
31	S	314	CLA	O2A-CGA-CBA	2.30	119.11	111.91
43	h	101	BCR	C30-C25-C26	-2.30	119.38	122.61
31	g	312	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
31	b	616	CLA	CHA-C4D-ND	2.30	137.30	132.50
31	Y	304	CLA	O2A-CGA-CBA	2.29	119.11	111.91
31	5	614	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
31	C	607	CLA	C1-C2-C3	-2.29	122.08	126.04
30	8	605	CHL	CHB-C4A-NA	2.29	127.68	124.51
30	6	302	CHL	CHD-C4C-C3C	2.29	128.21	124.84
31	r	307	CLA	CHA-C1A-NA	-2.29	121.15	126.40
31	S	315	CLA	C2D-C1D-ND	2.29	111.79	110.10
31	B	613	CLA	C1D-ND-C4D	-2.29	104.71	106.33
31	B	604	CLA	CHA-C1A-NA	-2.29	121.15	126.40
31	1	611	CLA	O2A-CGA-CBA	2.29	119.10	111.91
31	c	611	CLA	C4B-CHC-C1C	2.29	131.78	126.34
30	7	307	CHL	C2C-C3C-C4C	2.29	108.12	106.49
35	4	615	RRX	C35-C13-C14	-2.29	119.71	122.92
31	s	311	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
30	Y	309	CHL	CHD-C4C-C3C	2.29	128.21	124.84
30	q	311	CHL	CHD-C4C-C3C	2.29	128.21	124.84
38	X	201	SQD	O3-C3-C2	-2.29	105.05	110.35
31	s	314	CLA	C4B-CHC-C1C	2.29	131.77	126.34
31	y	615	CLA	C6-C5-C3	-2.29	107.45	113.45
31	1	603	CLA	CHA-C4D-ND	2.29	137.29	132.50
36	0	618	NEX	C31-C30-C29	2.29	130.58	127.31
31	B	608	CLA	CHA-C4D-ND	2.29	137.29	132.50
31	r	311	CLA	CHA-C4D-ND	2.29	137.29	132.50
30	q	303	CHL	CHB-C4A-NA	2.29	127.68	124.51
37	R	318	XAT	C39-C29-C30	-2.29	119.72	122.92
36	8	617	NEX	C26-C27-C28	-2.29	121.15	125.99
31	5	604	CLA	O2D-CGD-O1D	-2.29	119.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	604	CLA	C4B-CHC-C1C	2.29	131.77	126.34
31	8	614	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
30	N	301	CHL	CHC-C1C-NC	2.29	127.68	124.20
31	R	312	CLA	C1D-ND-C4D	-2.29	104.71	106.33
30	4	606	CHL	CMA-C3A-C2A	2.29	123.06	113.83
31	3	306	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
30	1	609	CHL	CHB-C4A-NA	2.29	127.68	124.51
43	b	619	BCR	C37-C22-C21	-2.29	119.72	122.92
34	W	202	LMG	O6-C1-O1	-2.29	104.55	109.97
32	s	318	LUT	C35-C15-C14	-2.29	118.79	123.47
31	p	615	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
30	6	310	CHL	C2B-C1B-NB	-2.29	108.70	110.23
30	s	309	CHL	C2B-C1B-NB	-2.29	108.70	110.23
31	0	614	CLA	C6-C5-C3	-2.29	107.45	113.45
32	1	616	LUT	C18-C5-C4	2.29	118.59	114.36
30	3	302	CHL	CHC-C1C-NC	2.29	127.67	124.20
36	6	319	NEX	C31-C30-C29	2.29	130.57	127.31
31	5	613	CLA	O2A-CGA-CBA	2.29	119.09	111.91
31	g	304	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
31	4	603	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
30	2	601	CHL	CHC-C1C-NC	2.29	127.67	124.20
30	4	608	CHL	CHC-C1C-NC	2.29	127.67	124.20
30	Y	302	CHL	CHC-C1C-NC	2.29	127.67	124.20
31	q	316	CLA	C4B-CHC-C1C	2.29	131.76	126.34
30	G	601	CHL	CHC-C1C-NC	2.29	127.67	124.20
30	N	309	CHL	CHC-C1C-NC	2.29	127.67	124.20
36	2	616	NEX	C39-C29-C30	-2.29	119.72	122.92
31	3	311	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
31	4	610	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	n	316	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
43	B	619	BCR	C34-C9-C10	-2.29	119.72	122.92
43	A	410	BCR	C38-C26-C27	2.28	118.00	113.62
36	n	319	NEX	C40-C33-C34	-2.28	119.72	122.92
30	p	609	CHL	C2B-C1B-NB	-2.28	108.70	110.23
31	q	305	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
31	s	315	CLA	C4B-CHC-C1C	2.28	131.75	126.34
30	4	609	CHL	CMA-C3A-C2A	2.28	123.04	113.83
33	z	102	LHG	O7-C7-O9	-2.28	118.18	123.70
31	3	314	CLA	O2A-CGA-CBA	2.28	119.07	111.91
31	b	611	CLA	O2A-CGA-CBA	2.28	119.07	111.91
31	b	610	CLA	C4B-CHC-C1C	2.28	131.75	126.34
43	C	615	BCR	C7-C6-C5	-2.28	115.93	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	r	301	NEX	C19-C9-C10	-2.28	119.73	122.92
30	7	307	CHL	C2B-C1B-NB	-2.28	108.70	110.23
31	2	609	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
32	y	617	LUT	C40-C33-C32	2.28	121.67	118.08
30	7	306	CHL	CHC-C1C-NC	2.28	127.66	124.20
30	r	309	CHL	CHC-C1C-NC	2.28	127.66	124.20
43	b	618	BCR	C10-C11-C12	-2.28	116.10	123.22
31	b	614	CLA	C3B-C4B-NB	-2.28	108.40	110.52
31	G	610	CLA	O2A-CGA-CBA	2.28	119.06	111.91
31	R	314	CLA	CMA-C3A-C4A	2.28	117.90	111.77
31	y	603	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
30	S	309	CHL	C2B-C1B-NB	-2.28	108.70	110.23
31	3	304	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
31	8	614	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
43	C	614	BCR	C29-C30-C25	2.28	113.99	110.48
43	H	101	BCR	C29-C30-C25	2.28	113.99	110.48
31	c	608	CLA	C4B-CHC-C1C	2.28	131.74	126.34
30	y	606	CHL	CHC-C1C-NC	2.28	127.66	124.20
32	2	615	LUT	C2-C3-C4	2.28	113.42	110.30
31	b	606	CLA	C1D-ND-C4D	-2.28	104.72	106.33
31	4	614	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
31	8	609	CLA	O2A-CGA-CBA	2.28	119.06	111.91
31	2	602	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
38	A	413	SQD	O3-C3-C2	-2.28	105.08	110.35
34	4	620	LMG	C8-O7-C10	-2.28	112.19	117.79
31	y	615	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
31	r	315	CLA	C1-C2-C3	-2.28	122.11	126.04
31	1	604	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
30	N	307	CHL	C2B-C1B-NB	-2.28	108.71	110.23
31	b	603	CLA	CHA-C1A-NA	-2.28	121.19	126.40
31	G	602	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
32	r	317	LUT	C39-C29-C28	2.28	121.66	118.08
31	n	314	CLA	C1-C2-C3	-2.28	122.11	126.04
30	p	606	CHL	CHD-C4C-C3C	2.28	128.19	124.84
31	Y	312	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
31	S	310	CLA	C1-O2A-CGA	2.28	122.41	116.44
30	G	607	CHL	CHC-C1C-NC	2.28	127.66	124.20
31	Y	310	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
30	y	607	CHL	CHB-C4A-NA	2.28	127.66	124.51
32	r	317	LUT	C8-C9-C10	-2.27	115.45	118.94
31	9	312	CLA	CHA-C1A-NA	-2.27	121.19	126.40
30	g	306	CHL	CMA-C3A-C2A	2.27	123.00	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	305	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
32	y	616	LUT	C11-C10-C9	-2.27	124.06	127.31
30	N	308	CHL	CMA-C3A-C2A	2.27	123.00	113.83
31	q	315	CLA	CHA-C1A-NA	-2.27	121.19	126.40
31	s	315	CLA	O2A-CGA-CBA	2.27	119.04	111.91
31	d	405	CLA	C4B-CHC-C1C	2.27	131.73	126.34
31	6	315	CLA	CHA-C4D-ND	2.27	137.25	132.50
31	S	303	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
31	0	603	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
30	8	607	CHL	CHC-C1C-NC	2.27	127.65	124.20
31	B	610	CLA	O2A-CGA-CBA	2.27	119.04	111.91
30	N	308	CHL	CHB-C4A-NA	2.27	127.66	124.51
36	n	319	NEX	C11-C10-C9	2.27	130.55	127.31
36	S	319	NEX	C40-C33-C34	-2.27	119.74	122.92
31	S	311	CLA	C3B-C4B-NB	-2.27	108.41	110.52
31	d	405	CLA	C3B-C4B-NB	-2.27	108.41	110.52
43	C	614	BCR	C38-C26-C27	2.27	117.98	113.62
31	R	316	CLA	C1D-ND-C4D	-2.27	104.72	106.33
32	8	616	LUT	C15-C35-C34	-2.27	118.82	123.47
30	G	601	CHL	C2B-C1B-NB	-2.27	108.71	110.23
31	D	404	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
30	g	307	CHL	CMA-C3A-C2A	2.27	122.99	113.83
31	n	316	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
33	e	101	LHG	O8-C23-O10	-2.27	117.86	123.59
30	G	607	CHL	CHB-C4A-NA	2.27	127.65	124.51
31	a	406	CLA	C1D-ND-C4D	-2.27	104.72	106.33
32	N	316	LUT	C11-C12-C13	-2.27	120.04	126.42
31	Y	314	CLA	O2A-CGA-CBA	2.27	119.03	111.91
31	S	316	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
30	0	608	CHL	CHC-C1C-NC	2.27	127.65	124.20
34	b	624	LMG	C8-O7-C10	-2.27	112.20	117.79
30	3	302	CHL	CHB-C4A-NA	2.27	127.65	124.51
43	A	410	BCR	C29-C30-C25	2.27	113.97	110.48
31	b	605	CLA	O2A-CGA-CBA	2.27	119.02	111.91
31	Y	304	CLA	C6-C5-C3	-2.27	107.51	113.45
30	r	308	CHL	CHC-C1C-NC	2.27	127.64	124.20
30	5	607	CHL	C2C-C3C-C4C	2.27	108.11	106.49
30	5	605	CHL	C4A-NA-C1A	2.27	107.72	106.71
31	Y	304	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
31	4	614	CLA	C1D-ND-C4D	-2.27	104.72	106.33
30	9	303	CHL	CHC-C1C-NC	2.27	127.64	124.20
30	N	301	CHL	C2B-C1B-NB	-2.27	108.71	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	g	309	CHL	C2B-C1B-NB	-2.27	108.71	110.23
31	C	604	CLA	CMA-C3A-C4A	2.27	117.86	111.77
31	R	306	CLA	CHA-C1A-NA	-2.27	121.21	126.40
31	p	613	CLA	CMA-C3A-C4A	2.27	117.86	111.77
31	g	310	CLA	C3B-C4B-NB	-2.26	108.41	110.52
31	b	609	CLA	CHA-C4D-ND	2.26	137.24	132.50
31	c	601	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
30	r	308	CHL	CMA-C3A-C2A	2.26	122.96	113.83
31	r	315	CLA	C1D-ND-C4D	-2.26	104.73	106.33
31	N	303	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
31	Y	305	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
31	9	306	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
30	1	606	CHL	CHB-C4A-NA	2.26	127.64	124.51
37	g	321	XAT	C25-C24-C23	-2.26	108.27	112.75
31	0	604	CLA	C4B-CHC-C1C	2.26	131.71	126.34
31	r	316	CLA	C4B-CHC-C1C	2.26	131.71	126.34
31	7	304	CLA	O2A-CGA-CBA	2.26	119.01	111.91
31	N	303	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
36	2	616	NEX	C19-C9-C10	-2.26	119.75	122.92
30	r	308	CHL	C2C-C3C-C4C	2.26	108.10	106.49
31	r	314	CLA	CHA-C4D-ND	2.26	137.23	132.50
30	6	302	CHL	CHB-C4A-NA	2.26	127.64	124.51
30	r	308	CHL	CHB-C4A-NA	2.26	127.64	124.51
31	N	304	CLA	O2A-CGA-CBA	2.26	119.00	111.91
31	S	314	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
31	9	315	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
31	5	603	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	6	311	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
30	7	306	CHL	C2B-C1B-NB	-2.26	108.72	110.23
31	4	612	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
38	A	411	SQD	O3-C3-C2	-2.26	105.13	110.35
30	7	310	CHL	CMA-C3A-C2A	2.26	122.94	113.83
31	N	321	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
30	S	307	CHL	C2B-C1B-NB	-2.26	108.72	110.23
31	b	616	CLA	C3B-C4B-NB	-2.26	108.42	110.52
30	4	601	CHL	CHC-C1C-NC	2.26	127.63	124.20
31	b	604	CLA	C4B-CHC-C1C	2.26	131.69	126.34
30	q	307	CHL	CHD-C4C-C3C	2.26	128.16	124.84
31	7	316	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	b	615	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
43	z	101	BCR	C21-C20-C19	-2.26	116.17	123.22
36	n	319	NEX	C28-C29-C30	2.26	122.41	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	311	CLA	C3B-C4B-NB	-2.26	108.42	110.52
31	6	314	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	9	312	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	g	314	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	a	406	CLA	C3B-C4B-NB	-2.26	108.42	110.52
31	p	604	CLA	C4B-CHC-C1C	2.26	131.69	126.34
43	a	410	BCR	C29-C30-C25	2.26	113.95	110.48
30	N	302	CHL	CMA-C3A-C2A	2.26	122.93	113.83
31	6	316	CLA	CHA-C1A-NA	-2.26	121.23	126.40
31	b	610	CLA	CHA-C1A-NA	-2.25	121.23	126.40
31	4	602	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
32	5	617	LUT	C18-C5-C4	2.25	118.53	114.36
31	4	610	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
35	4	615	RRX	C34-C9-C10	-2.25	119.77	122.92
30	p	609	CHL	C2C-C3C-C4C	2.25	108.10	106.49
31	r	306	CLA	C4B-CHC-C1C	2.25	131.69	126.34
37	4	619	XAT	C25-C24-C23	-2.25	108.29	112.75
31	q	312	CLA	C4B-CHC-C1C	2.25	132.56	125.70
43	z	101	BCR	C23-C24-C25	-2.25	120.87	127.20
36	q	319	NEX	C26-C27-C28	-2.25	121.23	125.99
30	s	308	CHL	C2B-C1B-NB	-2.25	108.72	110.23
37	q	321	XAT	C25-C24-C23	-2.25	108.29	112.75
31	q	304	CLA	O2A-CGA-CBA	2.25	118.98	111.91
31	S	310	CLA	C4B-CHC-C1C	2.25	131.68	126.34
31	s	310	CLA	C4B-CHC-C1C	2.25	131.68	126.34
30	s	309	CHL	CHB-C4A-NA	2.25	127.63	124.51
30	6	307	CHL	CHD-C4C-C3C	2.25	128.15	124.84
31	6	311	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
31	R	313	CLA	O2A-CGA-CBA	2.25	118.98	111.91
31	b	615	CLA	O2A-CGA-CBA	2.25	118.98	111.91
30	2	606	CHL	CHC-C1C-NC	2.25	127.62	124.20
31	r	304	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
30	g	306	CHL	CHD-C4C-C3C	2.25	128.15	124.84
31	C	609	CLA	CHA-C4D-ND	2.25	137.21	132.50
38	a	412	SQD	O3-C3-C2	-2.25	105.14	110.35
36	p	618	NEX	C5-C4-C3	2.25	114.41	111.75
38	g	301	SQD	O3-C3-C2	-2.25	105.14	110.35
43	z	101	BCR	C1-C6-C5	-2.25	119.44	122.61
30	p	607	CHL	C2C-C3C-C4C	2.25	108.09	106.49
30	q	311	CHL	C2C-C3C-C4C	2.25	108.09	106.49
31	B	606	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
43	b	620	BCR	C1-C6-C5	-2.25	119.44	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	p	601	CHL	C4A-NA-C1A	2.25	107.72	106.71
43	B	619	BCR	C21-C20-C19	-2.25	116.19	123.22
30	7	309	CHL	C1-O2A-CGA	2.25	122.35	116.44
31	7	314	CLA	C4B-CHC-C1C	2.25	131.68	126.34
31	q	304	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
36	N	318	NEX	C11-C10-C9	2.25	130.52	127.31
30	7	308	CHL	CHB-C4A-NA	2.25	127.62	124.51
31	1	603	CLA	C3B-C4B-NB	-2.25	108.43	110.52
43	v	101	BCR	C16-C15-C14	-2.25	118.87	123.47
31	6	303	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
31	B	607	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
30	7	308	CHL	CMA-C3A-C4A	2.25	117.82	111.77
31	C	608	CLA	CMA-C3A-C4A	2.25	117.82	111.77
36	s	319	NEX	C26-C27-C28	-2.25	121.24	125.99
31	s	306	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
47	e	102	HEM	CHA-C4D-C3D	-2.25	121.11	125.33
30	6	309	CHL	CMA-C3A-C2A	2.25	122.90	113.83
30	5	601	CHL	C1-O2A-CGA	2.25	122.34	116.44
31	p	615	CLA	CHA-C1A-NA	-2.25	121.25	126.40
37	2	619	XAT	C25-C24-C23	-2.25	108.30	112.75
32	S	317	LUT	C30-C31-C32	-2.25	116.20	123.22
31	0	615	CLA	CHA-C1A-NA	-2.25	121.25	126.40
31	1	614	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
30	r	309	CHL	C2C-C3C-C4C	2.25	108.09	106.49
35	2	614	RRX	C35-C13-C14	-2.25	119.78	122.92
30	8	608	CHL	CHC-C1C-NC	2.25	127.61	124.20
31	5	611	CLA	O2A-CGA-CBA	2.25	118.96	111.91
31	a	406	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
31	s	303	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
44	A	416	PL9	C31-C32-C33	-2.25	104.50	111.88
31	G	613	CLA	C1D-ND-C4D	-2.25	104.74	106.33
31	b	608	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
30	G	607	CHL	C1-O2A-CGA	2.25	122.34	116.44
30	1	606	CHL	C2B-C1B-NB	-2.25	108.73	110.23
37	G	620	XAT	C25-C24-C23	-2.25	108.31	112.75
38	G	617	SQD	O3-C3-C2	-2.25	105.16	110.35
32	n	318	LUT	C15-C35-C34	-2.25	118.87	123.47
43	V	101	BCR	C16-C15-C14	-2.25	118.87	123.47
31	4	612	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
30	S	302	CHL	CHD-C4C-C3C	2.25	128.14	124.84
31	R	305	CLA	CHA-C4D-ND	2.25	137.20	132.50
31	c	603	CLA	C4B-CHC-C1C	2.25	131.66	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	303	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
43	z	101	BCR	C15-C16-C17	-2.24	118.88	123.47
30	7	309	CHL	CMA-C3A-C2A	2.24	122.88	113.83
36	y	618	NEX	C19-C9-C10	-2.24	119.78	122.92
31	y	612	CLA	O2A-CGA-CBA	2.24	118.95	111.91
31	c	607	CLA	CHA-C1A-NA	-2.24	121.26	126.40
31	c	603	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
31	6	305	CLA	C6-C5-C3	-2.24	107.57	113.45
31	G	604	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
30	1	606	CHL	CHD-C4C-C3C	2.24	128.14	124.84
30	2	601	CHL	CHD-C4C-C3C	2.24	128.14	124.84
30	7	321	CHL	CHC-C1C-NC	2.24	127.61	124.20
35	9	317	RRX	C34-C9-C10	-2.24	119.78	122.92
43	Z	101	BCR	C23-C24-C25	-2.24	120.90	127.20
31	A	405	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
31	g	305	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
30	G	605	CHL	CMA-C3A-C2A	2.24	122.87	113.83
34	A	414	LMG	C8-O7-C10	-2.24	112.27	117.79
30	1	608	CHL	CMA-C3A-C2A	2.24	122.87	113.83
30	2	607	CHL	CHB-C4A-NA	2.24	127.61	124.51
31	S	316	CLA	C3B-C4B-NB	-2.24	108.44	110.52
43	c	614	BCR	C36-C18-C17	-2.24	119.78	122.92
31	D	404	CLA	CHA-C4D-ND	2.24	137.19	132.50
31	R	303	CLA	O2A-CGA-CBA	2.24	118.94	111.91
43	C	615	BCR	C29-C30-C25	2.24	113.93	110.48
30	5	608	CHL	C1-O2A-CGA	2.24	122.32	116.44
30	N	301	CHL	CHB-C4A-NA	2.24	127.61	124.51
31	s	304	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
31	r	305	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
31	3	305	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
31	c	610	CLA	C4B-CHC-C1C	2.24	131.65	126.34
38	G	624	SQD	O3-C3-C2	-2.24	105.17	110.35
31	C	613	CLA	C4B-CHC-C1C	2.24	131.65	126.34
37	9	322	XAT	C25-C24-C23	-2.24	108.32	112.75
30	3	302	CHL	C4D-CHA-C1A	2.24	123.97	121.25
30	G	606	CHL	CHC-C1C-NC	2.24	127.60	124.20
38	a	411	SQD	O3-C3-C2	-2.24	105.17	110.35
31	g	312	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
34	W	201	LMG	O8-C28-O10	-2.24	117.94	123.59
36	Y	317	NEX	O24-C25-C38	-2.24	112.37	115.06
32	9	318	LUT	C20-C13-C14	-2.24	119.79	122.92
37	r	318	XAT	C40-C33-C34	-2.24	119.79	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	315	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
31	S	305	CLA	O2A-CGA-CBA	2.24	118.93	111.91
43	c	615	BCR	C11-C12-C13	-2.24	120.13	126.42
30	y	605	CHL	CHB-C4A-NA	2.24	127.61	124.51
30	r	309	CHL	CMA-C3A-C4A	2.24	117.79	111.77
30	r	310	CHL	CHD-C4C-C3C	2.24	128.13	124.84
36	S	319	NEX	C2-C1-C6	2.24	111.39	109.21
31	c	604	CLA	CMA-C3A-C4A	2.24	117.78	111.77
35	G	614	RRX	C34-C9-C10	-2.24	119.79	122.92
30	S	307	CHL	CMA-C3A-C2A	2.24	122.85	113.83
31	0	603	CLA	CMA-C3A-C4A	2.24	117.78	111.77
31	b	605	CLA	CHD-C1D-ND	-2.24	122.40	124.45
31	4	613	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
31	A	406	CLA	O2A-CGA-CBA	2.24	118.92	111.91
31	g	303	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
31	C	613	CLA	CHA-C1A-NA	-2.24	121.28	126.40
31	r	304	CLA	C6-C5-C3	-2.24	107.59	113.45
31	r	312	CLA	C1-O2A-CGA	2.24	122.31	116.44
31	D	404	CLA	C4B-CHC-C1C	2.24	131.64	126.34
31	A	409	CLA	CHA-C4D-ND	2.24	137.18	132.50
31	c	609	CLA	O2A-CGA-CBA	2.24	118.92	111.91
31	B	608	CLA	C4B-CHC-C1C	2.23	131.64	126.34
30	G	623	CHL	CMA-C3A-C2A	2.23	122.84	113.83
30	n	301	CHL	C2B-C1B-NB	-2.23	108.73	110.23
36	s	319	NEX	C40-C33-C34	-2.23	119.79	122.92
31	r	315	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
34	b	622	LMG	C7-O1-C1	2.23	118.10	113.74
31	s	314	CLA	C1-O2A-CGA	2.23	122.31	116.44
31	y	614	CLA	O2A-CGA-CBA	2.23	118.92	111.91
30	9	309	CHL	CHD-C4C-C3C	2.23	128.12	124.84
31	5	614	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
31	B	608	CLA	O2A-CGA-CBA	2.23	118.92	111.91
31	N	313	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	a	409	CLA	CHA-C4D-ND	2.23	137.17	132.50
31	q	313	CLA	C4B-CHC-C1C	2.23	132.50	125.70
36	p	618	NEX	C2-C1-C6	2.23	111.38	109.21
31	c	608	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	c	612	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	c	608	CLA	C3B-C4B-NB	-2.23	108.44	110.52
31	4	603	CLA	OBD-CAD-C3D	-2.23	123.15	128.52
31	G	611	CLA	C4B-CHC-C1C	2.23	131.63	126.34
36	q	319	NEX	C38-C25-C26	-2.23	118.52	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	R	318	XAT	C40-C33-C34	-2.23	119.80	122.92
30	8	607	CHL	CHD-C4C-C3C	2.23	128.12	124.84
31	1	612	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	B	601	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	b	606	CLA	C4B-CHC-C1C	2.23	131.63	126.34
31	S	304	CLA	C1D-ND-C4D	-2.23	104.75	106.33
33	4	618	LHG	C6-C5-C4	-2.23	106.51	111.79
31	C	604	CLA	C2D-C1D-ND	2.23	111.75	110.10
30	s	302	CHL	CHD-C4C-C3C	2.23	128.12	124.84
30	Y	308	CHL	CMA-C3A-C2A	2.23	122.83	113.83
30	6	307	CHL	CHC-C1C-NC	2.23	127.59	124.20
32	y	616	LUT	C20-C13-C12	2.23	121.59	118.08
30	4	606	CHL	CHB-C4A-NA	2.23	127.60	124.51
30	N	308	CHL	CHD-C4C-C3C	2.23	128.12	124.84
31	n	304	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	s	316	CLA	C1D-ND-C4D	-2.23	104.75	106.33
30	q	309	CHL	CHB-C4A-NA	2.23	127.59	124.51
31	4	602	CLA	C6-C5-C3	-2.23	107.61	113.45
30	q	308	CHL	CHC-C1C-NC	2.23	127.58	124.20
33	A	417	LHG	O8-C23-O10	-2.23	117.97	123.59
31	9	315	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
36	g	317	NEX	C26-C27-C28	-2.23	121.28	125.99
30	s	308	CHL	CHD-C4C-C3C	2.23	128.12	124.84
31	7	304	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
31	8	603	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
36	q	319	NEX	C39-C29-C30	-2.23	119.80	122.92
44	a	414	PL9	O2-C1-C6	2.23	124.45	120.59
31	B	613	CLA	O2A-CGA-CBA	2.23	118.90	111.91
32	4	616	LUT	C8-C7-C6	-2.23	120.95	127.20
31	p	603	CLA	C3B-C4B-NB	-2.23	108.45	110.52
32	1	616	LUT	C1-C6-C5	-2.23	119.48	122.61
38	0	621	SQD	O3-C3-C2	-2.23	105.20	110.35
30	N	302	CHL	CHD-C4C-C3C	2.23	128.11	124.84
31	R	306	CLA	C2A-C1A-CHA	2.23	127.75	123.86
30	N	301	CHL	C2C-C3C-C4C	2.23	108.08	106.49
31	6	304	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
31	n	313	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
32	1	616	LUT	C38-C25-C24	-2.23	118.80	123.56
36	p	618	NEX	C39-C29-C30	-2.23	119.81	122.92
36	8	617	NEX	C16-C1-C6	-2.23	108.48	110.47
34	2	620	LMG	O8-C28-O10	-2.23	117.97	123.59
31	D	404	CLA	C1-O2A-CGA	2.23	122.28	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	B	619	BCR	C30-C25-C26	-2.23	119.48	122.61
31	r	303	CLA	O2A-CGA-CBA	2.23	118.89	111.91
30	q	310	CHL	CHC-C1C-NC	2.23	127.58	124.20
31	y	615	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
31	b	617	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
31	4	604	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
30	7	310	CHL	CHB-C4A-NA	2.22	127.59	124.51
31	1	614	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
32	0	616	LUT	C10-C11-C12	-2.22	116.28	123.22
32	Y	316	LUT	C35-C15-C14	-2.22	118.92	123.47
31	G	612	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
31	S	303	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
31	D	403	CLA	C3B-C4B-NB	-2.22	108.45	110.52
30	9	303	CHL	CHB-C4A-NA	2.22	127.58	124.51
43	z	101	BCR	C8-C7-C6	-2.22	120.96	127.20
31	B	614	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
36	R	319	NEX	C39-C29-C30	-2.22	119.81	122.92
31	2	612	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
31	9	305	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
31	C	607	CLA	C4B-CHC-C1C	2.22	131.60	126.34
31	N	315	CLA	O2A-CGA-CBA	2.22	118.88	111.91
31	r	305	CLA	O2A-CGA-CBA	2.22	118.88	111.91
30	6	309	CHL	CHB-C4A-NA	2.22	127.58	124.51
31	q	306	CLA	C1D-ND-C4D	-2.22	104.76	106.33
34	b	622	LMG	O6-C1-O1	-2.22	104.72	109.97
30	5	606	CHL	CHC-C1C-NC	2.22	127.57	124.20
31	y	613	CLA	CHA-C1A-NA	-2.22	121.32	126.40
31	q	312	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
30	r	310	CHL	CHB-C4A-NA	2.22	127.58	124.51
32	9	318	LUT	C8-C7-C6	-2.22	120.97	127.20
38	r	322	SQD	O3-C3-C2	-2.22	105.22	110.35
31	s	311	CLA	C1D-ND-C4D	-2.22	104.76	106.33
31	s	310	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
35	2	614	RRX	C34-C9-C10	-2.22	119.82	122.92
30	n	308	CHL	CHC-C1C-NC	2.22	127.57	124.20
31	7	303	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
32	0	616	LUT	C19-C9-C8	2.22	121.57	118.08
32	y	617	LUT	C39-C29-C28	2.22	121.57	118.08
31	8	609	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
31	R	311	CLA	C2D-C1D-ND	2.22	111.74	110.10
30	5	608	CHL	CMA-C3A-C2A	2.22	122.77	113.83
32	0	616	LUT	C38-C25-C24	-2.22	118.82	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	309	CHL	CMA-C3A-C2A	2.22	122.77	113.83
30	4	601	CHL	C1-O2A-CGA	2.22	122.26	116.44
34	b	624	LMG	O7-C10-O9	-2.22	118.35	123.70
42	D	401	PHO	C1-C2-C3	-2.22	122.21	126.04
30	r	310	CHL	CHC-C1C-NC	2.22	127.56	124.20
35	q	317	RRX	C32-C1-C6	2.22	113.89	110.30
31	6	316	CLA	O2A-CGA-CBA	2.22	118.86	111.91
30	G	606	CHL	CMA-C3A-C2A	2.22	122.77	113.83
31	g	303	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
31	n	315	CLA	CHA-C1A-NA	-2.22	121.32	126.40
31	q	315	CLA	O2A-CGA-CBA	2.22	118.86	111.91
30	3	308	CHL	C4A-NA-C1A	2.22	107.70	106.71
30	y	601	CHL	CHC-C1C-NC	2.22	127.56	124.20
31	8	613	CLA	CHA-C1A-NA	-2.22	121.33	126.40
43	B	618	BCR	C29-C30-C25	2.22	113.89	110.48
31	B	607	CLA	C16-C15-C13	-2.21	108.76	115.92
30	s	307	CHL	CMA-C3A-C2A	2.21	122.76	113.83
31	s	304	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
30	G	623	CHL	CHB-C4A-NA	2.21	127.57	124.51
31	8	602	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
32	s	317	LUT	C1-C6-C5	-2.21	119.50	122.61
31	3	314	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
31	6	316	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
32	7	318	LUT	C8-C7-C6	-2.21	120.99	127.20
30	p	606	CHL	CMA-C3A-C2A	2.21	122.76	113.83
31	b	617	CLA	C2D-C1D-ND	2.21	111.73	110.10
31	3	313	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
32	g	316	LUT	C20-C13-C14	-2.21	119.82	122.92
31	R	316	CLA	C3B-C4B-NB	-2.21	108.46	110.52
30	5	607	CHL	C1-O2A-CGA	2.21	122.25	116.44
30	g	309	CHL	CHB-C4A-NA	2.21	127.57	124.51
30	s	302	CHL	C4D-CHA-C1A	2.21	123.94	121.25
31	B	609	CLA	CHA-C1A-NA	-2.21	121.33	126.40
30	1	609	CHL	CHD-C4C-C3C	2.21	128.09	124.84
32	Y	316	LUT	C38-C25-C24	-2.21	118.83	123.56
31	g	303	CLA	CHA-C4D-ND	2.21	137.13	132.50
31	b	607	CLA	C3B-C4B-NB	-2.21	108.46	110.52
31	c	611	CLA	C3B-C4B-NB	-2.21	108.46	110.52
30	2	606	CHL	C1-O2A-CGA	2.21	122.25	116.44
31	S	305	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
34	9	301	LMG	C4-C3-C2	2.21	114.68	110.82
31	1	612	CLA	C1D-ND-C4D	-2.21	104.76	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	6	317	LUT	C10-C11-C12	-2.21	116.32	123.22
31	7	316	CLA	O2A-CGA-CBA	2.21	118.85	111.91
31	6	316	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	0	614	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	4	613	CLA	C1D-ND-C4D	-2.21	104.77	106.33
31	b	610	CLA	C1D-ND-C4D	-2.21	104.77	106.33
31	s	313	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	R	312	CLA	C1-C2-C3	-2.21	122.22	126.04
30	2	605	CHL	CHD-C4C-C3C	2.21	128.09	124.84
30	5	609	CHL	CHD-C4C-C3C	2.21	128.09	124.84
30	G	605	CHL	CHD-C4C-C3C	2.21	128.09	124.84
31	S	313	CLA	C6-C5-C3	-2.21	107.66	113.45
30	y	608	CHL	CMA-C3A-C2A	2.21	122.74	113.83
30	N	306	CHL	CMA-C3A-C2A	2.21	122.74	113.83
34	b	622	LMG	O7-C10-O9	-2.21	118.36	123.70
30	G	623	CHL	C2B-C1B-NB	-2.21	108.75	110.23
31	C	610	CLA	CHA-C1A-NA	-2.21	121.34	126.40
30	7	306	CHL	CMA-C3A-C2A	2.21	122.74	113.83
48	K	101	LMU	C1-O1'-C1'	-2.21	110.18	113.84
30	S	307	CHL	CHC-C1C-NC	2.21	127.55	124.20
31	7	305	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
31	8	611	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	y	614	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
30	n	301	CHL	C2C-C3C-C4C	2.21	108.06	106.49
31	0	602	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
31	b	616	CLA	C1-O2A-CGA	2.21	122.24	116.44
36	R	301	NEX	C17-C1-C6	-2.21	108.50	110.47
30	7	306	CHL	CHD-C4C-C3C	2.21	128.09	124.84
31	C	609	CLA	C4B-CHC-C1C	2.21	131.57	126.34
31	p	603	CLA	C4B-CHC-C1C	2.21	131.57	126.34
30	4	608	CHL	CHB-C4A-NA	2.21	127.56	124.51
31	6	314	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
31	c	604	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
43	V	101	BCR	C33-C5-C4	2.21	117.86	113.62
36	8	617	NEX	C40-C33-C34	-2.21	119.83	122.92
32	5	616	LUT	C18-C5-C4	2.21	118.44	114.36
31	2	604	CLA	O2A-CGA-CBA	2.21	118.83	111.91
31	C	607	CLA	C6-C5-C3	-2.21	107.67	113.45
31	0	604	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
31	8	602	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
30	9	311	CHL	C3B-C4B-NB	-2.21	108.47	110.52
31	c	607	CLA	OBD-CAD-C3D	-2.21	123.21	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	z	101	BCR	C16-C15-C14	-2.21	118.96	123.47
37	r	318	XAT	C39-C29-C30	-2.20	119.83	122.92
31	N	312	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
31	S	306	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
30	y	608	CHL	CHB-C4A-NA	2.20	127.56	124.51
31	b	607	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
32	s	317	LUT	C15-C35-C34	-2.20	118.96	123.47
31	6	315	CLA	O2A-CGA-CBA	2.20	118.82	111.91
31	4	613	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
31	R	307	CLA	CHA-C1A-NA	-2.20	121.35	126.40
30	Y	301	CHL	CMA-C3A-C2A	2.20	122.72	113.83
30	p	605	CHL	CHC-C1C-NC	2.20	127.55	124.20
31	N	314	CLA	CHA-C1A-NA	-2.20	121.35	126.40
32	g	316	LUT	C8-C7-C6	-2.20	121.01	127.20
30	Y	309	CHL	C3A-C2A-C1A	2.20	104.64	101.34
30	G	608	CHL	C2B-C1B-NB	-2.20	108.75	110.23
30	y	607	CHL	C2B-C1B-NB	-2.20	108.75	110.23
31	n	311	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
31	R	313	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
31	2	609	CLA	CHA-C1A-NA	-2.20	121.35	126.40
31	N	315	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
34	w	203	LMG	C8-O7-C10	-2.20	112.37	117.79
30	5	601	CHL	CHB-C4A-NA	2.20	127.56	124.51
30	G	601	CHL	CHB-C4A-NA	2.20	127.56	124.51
43	B	618	BCR	C38-C26-C27	2.20	117.85	113.62
30	2	608	CHL	CHD-C4C-C3C	2.20	128.08	124.84
30	1	619	CHL	CHA-C1A-NA	-2.20	121.36	126.40
31	7	315	CLA	CHA-C1A-NA	-2.20	121.36	126.40
31	5	604	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
43	a	410	BCR	C36-C18-C17	-2.20	119.84	122.92
31	6	313	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
46	D	402	BCT	O3-C-O1	-2.20	113.84	119.55
31	N	311	CLA	O2A-CGA-CBA	2.20	118.81	111.91
30	y	606	CHL	CMA-C3A-C2A	2.20	122.70	113.83
31	3	314	CLA	C6-C5-C3	-2.20	107.69	113.45
31	b	606	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
31	G	610	CLA	C2A-C1A-CHA	2.20	127.70	123.86
31	8	609	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
31	2	612	CLA	O2A-CGA-CBA	2.20	118.81	111.91
32	7	317	LUT	C39-C29-C28	2.20	121.54	118.08
30	s	307	CHL	CHC-C1C-NC	2.20	127.54	124.20
34	6	321	LMG	O7-C10-O9	-2.20	118.39	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	609	CLA	C4B-CHC-C1C	2.20	131.55	126.34
31	5	602	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
31	R	304	CLA	CMA-C3A-C4A	2.20	117.68	111.77
31	B	613	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
31	b	605	CLA	C2D-C1D-ND	2.20	111.72	110.10
32	s	317	LUT	C18-C5-C4	2.20	118.42	114.36
34	W	201	LMG	C8-O7-C10	-2.20	112.38	117.79
43	b	620	BCR	C16-C15-C14	-2.20	118.97	123.47
31	5	602	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
31	N	305	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
30	p	601	CHL	C1-O2A-CGA	2.20	122.20	116.44
31	2	603	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
31	5	614	CLA	O2A-CGA-CBA	2.20	118.80	111.91
30	2	607	CHL	CHC-C1C-NC	2.20	127.53	124.20
43	d	406	BCR	C23-C24-C25	-2.20	121.04	127.20
31	4	610	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
31	G	604	CLA	O2A-CGA-CBA	2.20	118.80	111.91
31	n	305	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
30	p	606	CHL	CHC-C1C-NC	2.19	127.53	124.20
31	d	404	CLA	CMD-C2D-C3D	-2.19	122.56	127.61
30	0	601	CHL	CHB-C4A-NA	2.19	127.55	124.51
30	0	609	CHL	C1-C2-C3	-2.19	122.25	126.04
30	s	308	CHL	CHC-C1C-NC	2.19	127.53	124.20
30	y	608	CHL	C2B-C1B-NB	-2.19	108.76	110.23
31	n	303	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
31	r	315	CLA	C3B-C4B-NB	-2.19	108.48	110.52
31	7	314	CLA	O2A-CGA-CBA	2.19	118.79	111.91
31	c	604	CLA	C1D-ND-C4D	-2.19	104.78	106.33
30	1	606	CHL	CMA-C3A-C2A	2.19	122.67	113.83
31	7	315	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
34	k	102	LMG	C8-O7-C10	-2.19	112.39	117.79
31	p	602	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
32	7	317	LUT	C35-C15-C14	-2.19	118.98	123.47
30	y	606	CHL	CHB-C4A-NA	2.19	127.54	124.51
31	s	313	CLA	C1D-ND-C4D	-2.19	104.78	106.33
31	5	615	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	d	404	CLA	C3B-C4B-NB	-2.19	108.48	110.52
38	M	102	SQD	O3-C3-C2	-2.19	105.28	110.35
30	y	606	CHL	C2C-C3C-C4C	2.19	108.05	106.49
31	n	303	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
31	b	608	CLA	C4B-CHC-C1C	2.19	131.53	126.34
31	r	306	CLA	CHA-C1A-NA	-2.19	121.38	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	p	612	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
33	l	101	LHG	C5-O7-C7	-2.19	112.40	117.79
30	G	623	CHL	CHD-C4C-C3C	2.19	128.06	124.84
31	5	603	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	y	602	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	4	612	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	s	304	CLA	CHA-C1A-NA	-2.19	121.38	126.40
31	C	608	CLA	C6-C5-C3	-2.19	107.71	113.45
31	s	311	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	0	615	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
30	3	303	CHL	CHB-C4A-NA	2.19	127.54	124.51
30	n	302	CHL	CMA-C3A-C2A	2.19	122.66	113.83
36	5	618	NEX	C39-C29-C30	-2.19	119.86	122.92
31	4	610	CLA	CMC-C2C-C1C	2.19	128.37	125.04
31	4	610	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	9	304	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	y	612	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
32	p	617	LUT	C15-C35-C34	2.19	127.96	123.47
31	4	604	CLA	O2A-CGA-CBA	2.19	118.78	111.91
30	g	302	CHL	CHC-C1C-NC	2.19	127.52	124.20
31	b	612	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	N	310	CLA	C11-C10-C8	-2.19	108.85	115.92
30	8	601	CHL	CMA-C3A-C2A	2.19	122.66	113.83
31	0	602	CLA	C3B-C4B-NB	-2.19	108.48	110.52
30	7	308	CHL	C1-O2A-CGA	2.19	122.19	116.44
31	R	315	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
30	q	303	CHL	C1-C2-C3	-2.19	122.26	126.04
31	8	604	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	q	304	CLA	C6-C5-C3	-2.19	107.72	113.45
31	y	604	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	a	406	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
31	b	609	CLA	O2A-CGA-CBA	2.19	118.77	111.91
31	r	311	CLA	C1-O2A-CGA	2.19	122.18	116.44
31	2	604	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
32	r	317	LUT	C12-C13-C14	-2.19	115.59	118.94
30	1	606	CHL	C1-C2-C3	-2.19	122.26	126.04
31	c	606	CLA	O2A-CGA-CBA	2.19	118.77	111.91
31	C	612	CLA	C4B-CHC-C1C	2.19	131.52	126.34
31	r	311	CLA	C3B-C4B-NB	-2.19	108.49	110.52
30	2	605	CHL	CHC-C1C-NC	2.19	127.52	124.20
31	R	316	CLA	C4B-CHC-C1C	2.18	131.52	126.34
43	D	405	BCR	C11-C10-C9	2.18	130.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	609	CHL	C2B-C1B-NB	-2.18	108.77	110.23
31	c	613	CLA	C4B-CHC-C1C	2.18	131.52	126.34
30	3	307	CHL	CHC-C1C-NC	2.18	127.52	124.20
31	q	306	CLA	O2A-CGA-CBA	2.18	118.76	111.91
34	C	621	LMG	O7-C10-O9	-2.18	118.43	123.70
31	R	311	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
35	g	315	RRX	C8-C9-C10	2.18	122.29	118.94
32	s	318	LUT	C22-C23-C24	2.18	114.22	111.74
31	Y	304	CLA	CHA-C1A-NA	-2.18	121.40	126.40
30	7	308	CHL	C4A-NA-C1A	2.18	107.69	106.71
30	N	308	CHL	CHC-C1C-NC	2.18	127.51	124.20
31	B	607	CLA	CBA-CAA-C2A	-2.18	107.42	113.86
31	r	304	CLA	O2A-CGA-CBA	2.18	118.75	111.91
32	S	317	LUT	C15-C35-C34	-2.18	119.00	123.47
32	q	318	LUT	C38-C25-C24	-2.18	118.89	123.56
30	0	601	CHL	C2B-C1B-NB	-2.18	108.77	110.23
32	1	615	LUT	C19-C9-C8	2.18	121.51	118.08
30	6	308	CHL	CMA-C3A-C4A	2.18	117.63	111.77
31	B	608	CLA	C3B-C4B-NB	-2.18	108.49	110.52
32	p	617	LUT	C2-C3-C4	2.18	113.29	110.30
31	9	313	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
34	9	321	LMG	C8-O7-C10	-2.18	112.42	117.79
36	6	319	NEX	C20-C13-C14	-2.18	119.87	122.92
31	s	312	CLA	O2A-CGA-CBA	2.18	118.75	111.91
32	1	615	LUT	C12-C13-C14	-2.18	115.60	118.94
34	q	301	LMG	O7-C10-O9	-2.18	118.43	123.70
31	N	305	CLA	CMA-C3A-C4A	2.18	117.63	111.77
35	2	614	RRX	C1-C6-C7	2.18	121.94	115.78
31	S	315	CLA	C1D-ND-C4D	-2.18	104.79	106.33
30	p	606	CHL	C1-O2A-CGA	2.18	122.16	116.44
43	H	101	BCR	C11-C12-C13	-2.18	120.30	126.42
30	4	601	CHL	C2C-C3C-C4C	2.18	108.04	106.49
31	6	316	CLA	C3B-C4B-NB	-2.18	108.49	110.52
30	7	302	CHL	CHD-C4C-C3C	2.18	128.04	124.84
31	B	606	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
31	C	607	CLA	CMA-C3A-C4A	2.18	117.63	111.77
31	c	612	CLA	C4B-CHC-C1C	2.18	131.50	126.34
32	S	318	LUT	C39-C29-C30	-2.18	119.87	122.92
31	C	606	CLA	CMA-C3A-C4A	2.18	117.62	111.77
31	c	613	CLA	CBA-CAA-C2A	2.18	120.29	113.86
32	G	615	LUT	C38-C25-C24	-2.18	118.90	123.56
36	R	319	NEX	C19-C9-C10	-2.18	119.87	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	304	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
31	g	313	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
31	R	311	CLA	C1-O2A-CGA	2.18	122.15	116.44
34	s	321	LMG	C8-O7-C10	-2.18	112.43	117.79
30	7	307	CHL	CMA-C3A-C2A	2.18	122.60	113.83
34	B	625	LMG	C9-C8-C7	-2.18	106.64	111.79
31	0	613	CLA	O2A-CGA-CBA	2.18	118.73	111.91
31	0	603	CLA	C2D-C1D-ND	2.18	111.71	110.10
30	3	303	CHL	CHD-C4C-C3C	2.17	128.04	124.84
31	B	614	CLA	O2A-CGA-CBA	2.17	118.73	111.91
31	g	313	CLA	O2A-CGA-CBA	2.17	118.73	111.91
43	c	615	BCR	C34-C9-C10	-2.17	119.88	122.92
31	B	609	CLA	C6-C5-C3	-2.17	107.75	113.45
30	G	606	CHL	CHB-C4A-NA	2.17	127.52	124.51
43	z	101	BCR	C2-C1-C6	2.17	113.83	110.48
31	S	310	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
31	S	313	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
31	S	306	CLA	O2A-CGA-CBA	2.17	118.73	111.91
30	y	607	CHL	CMA-C3A-C2A	2.17	122.59	113.83
36	4	617	NEX	C38-C25-C26	-2.17	118.62	122.26
32	Y	315	LUT	C11-C10-C9	-2.17	124.21	127.31
30	2	606	CHL	CMA-C3A-C2A	2.17	122.59	113.83
31	A	407	CLA	O2A-CGA-CBA	2.17	118.73	111.91
31	1	610	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
30	4	605	CHL	CHB-C4A-NA	2.17	127.52	124.51
31	6	304	CLA	CHA-C1A-NA	-2.17	121.42	126.40
43	D	405	BCR	C20-C19-C18	-2.17	120.31	126.42
30	Y	302	CHL	CMA-C3A-C2A	2.17	122.59	113.83
31	0	602	CLA	C1D-ND-C4D	-2.17	104.79	106.33
31	B	605	CLA	C3B-C4B-NB	-2.17	108.50	110.52
31	R	311	CLA	C3B-C4B-NB	-2.17	108.50	110.52
30	7	302	CHL	CHB-C4A-NA	2.17	127.52	124.51
31	C	605	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
31	s	316	CLA	CHA-C1A-NA	-2.17	121.43	126.40
31	B	603	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
31	R	306	CLA	C4B-CHC-C1C	2.17	131.49	126.34
31	6	313	CLA	O2A-CGA-CBA	2.17	118.72	111.91
34	w	203	LMG	C30-C29-C28	-2.17	105.73	113.62
30	7	310	CHL	C2B-C1B-NB	-2.17	108.78	110.23
31	n	303	CLA	C6-C5-C3	-2.17	107.76	113.45
30	0	607	CHL	CHC-C1C-NC	2.17	127.50	124.20
30	g	308	CHL	CHD-C4C-C3C	2.17	128.03	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	q	306	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
31	0	612	CLA	CHA-C1A-NA	-2.17	121.43	126.40
32	q	318	LUT	C15-C35-C34	-2.17	119.03	123.47
31	c	608	CLA	CHA-C1A-NA	-2.17	121.43	126.40
32	9	318	LUT	C39-C29-C30	-2.17	119.89	122.92
31	y	614	CLA	CHA-C1A-NA	-2.17	121.43	126.40
31	5	613	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
31	0	613	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
35	9	317	RRX	C1-C6-C7	2.17	121.91	115.78
31	b	617	CLA	CHA-C1A-NA	-2.17	121.43	126.40
32	N	316	LUT	C30-C31-C32	-2.17	116.45	123.22
34	B	621	LMG	O7-C10-O9	-2.17	118.47	123.70
31	B	616	CLA	C4B-CHC-C1C	2.17	131.48	126.34
35	4	615	RRX	C1-C6-C7	2.17	121.91	115.78
31	5	602	CLA	O2A-CGA-CBA	2.17	118.70	111.91
31	b	611	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
31	6	304	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
31	2	612	CLA	C1D-ND-C4D	-2.17	104.80	106.33
31	4	611	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	A	405	CLA	CMD-C2D-C3D	-2.16	122.63	127.61
31	c	609	CLA	CMA-C3A-C4A	2.16	117.59	111.77
31	5	615	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
36	5	618	NEX	C40-C33-C34	-2.16	119.89	122.92
36	8	617	NEX	C19-C9-C10	-2.16	119.89	122.92
43	b	618	BCR	C2-C1-C6	2.16	113.81	110.48
31	B	615	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
30	q	311	CHL	CMA-C3A-C2A	2.16	122.56	113.83
36	0	618	NEX	C20-C13-C14	-2.16	119.89	122.92
31	3	315	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	c	610	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	S	311	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
31	a	407	CLA	O2A-CGA-CBA	2.16	118.70	111.91
30	s	309	CHL	CHC-C1C-NC	2.16	127.48	124.20
31	g	310	CLA	CMA-C3A-C4A	2.16	117.59	111.77
31	3	312	CLA	C1-O2A-CGA	2.16	122.12	116.44
31	p	603	CLA	C2D-C1D-ND	2.16	111.70	110.10
30	3	303	CHL	CMA-C3A-C2A	2.16	122.55	113.83
34	6	323	LMG	C1-O6-C5	2.16	117.93	113.69
31	5	612	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
32	n	317	LUT	C38-C25-C24	-2.16	118.93	123.56
38	b	627	SQD	O3-C3-C2	-2.16	105.35	110.35
30	0	607	CHL	CHD-C4C-C3C	2.16	128.02	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	6	318	LUT	C15-C35-C34	-2.16	119.05	123.47
31	d	405	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	Y	314	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
36	N	318	NEX	O24-C25-C38	-2.16	112.47	115.06
31	B	602	CLA	CMA-C3A-C4A	2.16	117.58	111.77
31	a	409	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	b	614	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	s	315	CLA	C2D-C1D-ND	2.16	111.70	110.10
30	N	306	CHL	CHD-C4C-C3C	2.16	128.01	124.84
36	n	319	NEX	C16-C1-C6	-2.16	108.54	110.47
31	N	305	CLA	CHA-C1A-NA	-2.16	121.45	126.40
43	V	101	BCR	C15-C16-C17	-2.16	119.05	123.47
31	S	304	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
31	3	304	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
30	p	601	CHL	CHD-C4C-C3C	2.16	128.01	124.84
31	C	605	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	9	305	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	C	611	CLA	CHA-C1A-NA	-2.16	121.45	126.40
30	G	606	CHL	C2B-C1B-NB	-2.16	108.78	110.23
30	q	311	CHL	C2B-C1B-NB	-2.16	108.78	110.23
31	S	303	CLA	C11-C10-C8	-2.16	108.94	115.92
36	S	319	NEX	C39-C29-C30	-2.16	119.90	122.92
34	y	620	LMG	C9-C8-C7	-2.16	106.68	111.79
31	b	602	CLA	C1D-ND-C4D	-2.16	104.80	106.33
31	C	610	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
31	s	305	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
35	q	317	RRX	C19-C18-C17	2.16	122.25	118.94
31	b	617	CLA	C1-O2A-CGA	2.16	122.11	116.44
31	B	613	CLA	CHA-C1A-NA	-2.16	121.46	126.40
32	N	316	LUT	C18-C5-C4	2.16	118.35	114.36
31	G	602	CLA	CHA-C1A-NA	-2.16	121.46	126.40
31	r	303	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
32	p	616	LUT	C15-C35-C34	2.16	127.89	123.47
31	g	305	CLA	O2A-CGA-CBA	2.16	118.67	111.91
30	6	309	CHL	C1-O2A-CGA	2.16	122.10	116.44
32	1	616	LUT	C39-C29-C28	2.16	121.47	118.08
35	g	315	RRX	C23-C24-C25	-2.16	121.15	127.20
31	D	404	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
31	s	314	CLA	CHA-C1A-NA	-2.16	121.46	126.40
30	n	309	CHL	CHB-C4A-NA	2.16	127.49	124.51
31	S	316	CLA	C4B-CHC-C1C	2.16	131.45	126.34
34	Q1	101	LMG	C8-O7-C10	-2.16	112.48	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	316	CLA	CHA-C1A-NA	-2.16	121.46	126.40
31	c	602	CLA	CHA-C1A-NA	-2.16	121.46	126.40
32	n	317	LUT	C18-C5-C4	2.16	118.35	114.36
31	0	614	CLA	O2A-CGA-CBA	2.16	118.67	111.91
31	p	602	CLA	C1D-ND-C4D	-2.16	104.80	106.33
32	8	615	LUT	C38-C25-C24	-2.15	118.95	123.56
31	S	313	CLA	CMA-C3A-C4A	2.15	117.56	111.77
32	3	318	LUT	C11-C10-C9	-2.15	124.23	127.31
31	A	409	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
43	b	618	BCR	C36-C18-C19	2.15	121.47	118.08
31	3	315	CLA	CHA-C1A-NA	-2.15	121.47	126.40
30	0	607	CHL	CMA-C3A-C2A	2.15	122.52	113.83
30	y	606	CHL	C2B-C1B-NB	-2.15	108.79	110.23
42	D	401	PHO	O2A-CGA-O1A	-2.15	118.16	123.59
31	s	310	CLA	C3B-C4B-NB	-2.15	108.52	110.52
31	2	604	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	r	307	CLA	C2D-C1D-ND	2.15	111.69	110.10
30	6	308	CHL	CHC-C1C-NC	2.15	127.47	124.20
43	t	101	BCR	C3-C4-C5	-2.15	110.23	114.08
31	9	312	CLA	C1-O2A-CGA	2.15	122.09	116.44
31	2	603	CLA	O2A-CGA-CBA	2.15	118.66	111.91
31	R	314	CLA	O2A-CGA-CBA	2.15	118.66	111.91
30	n	309	CHL	CHC-C1C-NC	2.15	127.47	124.20
30	n	306	CHL	CMA-C3A-C2A	2.15	122.51	113.83
31	B	608	CLA	C1D-ND-C4D	-2.15	104.81	106.33
31	8	612	CLA	C6-C5-C3	-2.15	107.81	113.45
31	n	314	CLA	C6-C5-C3	-2.15	107.81	113.45
31	9	312	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
32	1	615	LUT	C18-C5-C4	2.15	118.34	114.36
31	y	612	CLA	CHA-C1A-NA	-2.15	121.47	126.40
32	n	317	LUT	C39-C29-C28	2.15	121.47	118.08
43	b	618	BCR	C35-C13-C12	2.15	121.47	118.08
31	R	305	CLA	C1-O2A-CGA	2.15	122.09	116.44
30	n	301	CHL	CHB-C4A-NA	2.15	127.49	124.51
30	y	607	CHL	CHD-C4C-C3C	2.15	128.00	124.84
36	N	318	NEX	C4-C3-C2	2.15	114.93	110.77
38	g	318	SQD	O3-C3-C2	-2.15	105.38	110.35
31	p	611	CLA	O2A-CGA-CBA	2.15	118.66	111.91
30	g	306	CHL	CHC-C1C-NC	2.15	127.47	124.20
31	q	316	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	C	607	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
30	4	609	CHL	C2B-C1B-NB	-2.15	108.79	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	G	614	RRX	C1-C6-C7	2.15	121.86	115.78
31	0	602	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
31	c	609	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
36	r	319	NEX	C20-C13-C14	-2.15	119.91	122.92
31	4	602	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
31	c	612	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
34	Q1	101	LMG	O1-C1-C2	2.15	111.66	108.30
30	1	607	CHL	CHC-C1C-NC	2.15	127.46	124.20
31	B	616	CLA	C2D-C1D-ND	2.15	111.69	110.10
30	2	606	CHL	CHB-C4A-NA	2.15	127.48	124.51
32	Y	315	LUT	C31-C30-C29	-2.15	124.25	127.31
32	N	316	LUT	C15-C35-C34	-2.15	119.08	123.47
31	c	603	CLA	C3B-C4B-NB	-2.15	108.52	110.52
30	G	601	CHL	C1-O2A-CGA	2.15	122.08	116.44
30	5	605	CHL	CMA-C3A-C2A	2.15	122.49	113.83
30	5	605	CHL	CHC-C1C-NC	2.15	127.46	124.20
32	8	615	LUT	C18-C5-C4	2.15	118.33	114.36
36	r	319	NEX	O24-C25-C38	-2.15	112.48	115.06
30	6	308	CHL	C2B-C1B-NB	-2.15	108.79	110.23
30	4	605	CHL	C4A-NA-C1A	2.15	107.67	106.71
31	R	306	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	r	314	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
30	2	601	CHL	CMA-C3A-C2A	2.15	122.48	113.83
31	8	612	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
31	q	316	CLA	O2A-CGA-CBA	2.15	118.64	111.91
31	9	312	CLA	O2A-CGA-CBA	2.15	118.64	111.91
31	S	310	CLA	C3B-C4B-NB	-2.15	108.53	110.52
34	w	203	LMG	O7-C10-O9	-2.15	118.52	123.70
30	7	302	CHL	C2B-C1B-NB	-2.15	108.79	110.23
31	s	310	CLA	O2A-CGA-CBA	2.15	118.64	111.91
31	1	614	CLA	CHA-C1A-NA	-2.14	121.49	126.40
30	n	301	CHL	CHD-C4C-C3C	2.14	127.99	124.84
30	R	309	CHL	CHB-C4A-NA	2.14	127.48	124.51
32	0	616	LUT	C31-C30-C29	-2.14	124.25	127.31
30	7	302	CHL	CMA-C3A-C2A	2.14	122.48	113.83
30	g	302	CHL	CMA-C3A-C2A	2.14	122.48	113.83
31	c	613	CLA	CMA-C3A-C4A	2.14	117.53	111.77
35	g	315	RRX	C37-C22-C21	-2.14	119.92	122.92
31	C	608	CLA	C3B-C4B-NB	-2.14	108.53	110.52
44	A	416	PL9	C41-C39-C38	-2.14	116.78	121.12
32	s	317	LUT	C20-C13-C12	2.14	121.45	118.08
31	1	612	CLA	CHA-C1A-NA	-2.14	121.49	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	609	CLA	C6-C7-C8	-2.14	108.99	115.92
30	3	302	CHL	CMA-C3A-C2A	2.14	122.47	113.83
31	b	616	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
31	B	612	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
31	3	313	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
31	Y	314	CLA	CHA-C1A-NA	-2.14	121.49	126.40
30	6	308	CHL	CHD-C4C-C3C	2.14	127.99	124.84
30	1	619	CHL	CHC-C4B-NB	-2.14	121.99	124.26
31	S	316	CLA	CHA-C1A-NA	-2.14	121.49	126.40
32	G	615	LUT	C15-C35-C34	2.14	127.86	123.47
31	s	303	CLA	C6-C5-C3	-2.14	107.84	113.45
31	p	612	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
31	d	405	CLA	C1-O2A-CGA	2.14	122.06	116.44
30	1	605	CHL	CMA-C3A-C2A	2.14	122.46	113.83
30	g	307	CHL	C2B-C1B-NB	-2.14	108.80	110.23
31	Y	305	CLA	CMA-C3A-C4A	2.14	117.53	111.77
36	Y	317	NEX	C20-C13-C14	-2.14	119.92	122.92
31	5	612	CLA	CHA-C1A-NA	-2.14	121.50	126.40
31	8	614	CLA	O2A-CGA-CBA	2.14	118.62	111.91
31	3	301	CLA	C6-C5-C3	-2.14	107.84	113.45
31	q	313	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	C	608	CLA	C1D-ND-C4D	-2.14	104.81	106.33
31	q	306	CLA	CHA-C1A-NA	-2.14	121.50	126.40
43	h	101	BCR	C31-C1-C6	-2.14	106.83	110.30
31	0	610	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
43	Z	101	BCR	C16-C15-C14	-2.14	119.09	123.47
30	4	601	CHL	CMA-C3A-C2A	2.14	122.46	113.83
30	8	605	CHL	CMA-C3A-C2A	2.14	122.46	113.83
30	2	608	CHL	C2B-C1B-NB	-2.14	108.80	110.23
30	g	302	CHL	C2B-C1B-NB	-2.14	108.80	110.23
31	G	603	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
30	9	307	CHL	CHD-C4C-C3C	2.14	127.98	124.84
30	G	605	CHL	CHC-C1C-NC	2.14	127.45	124.20
32	s	318	LUT	C15-C35-C34	-2.14	119.09	123.47
31	C	606	CLA	C1D-ND-C4D	-2.14	104.82	106.33
36	3	319	NEX	C39-C29-C30	-2.14	119.93	122.92
31	7	304	CLA	CHA-C1A-NA	-2.14	121.50	126.40
30	Y	301	CHL	CHB-C4A-NA	2.14	127.47	124.51
32	p	617	LUT	C38-C25-C24	-2.14	118.98	123.56
31	s	311	CLA	CMA-C3A-C4A	2.14	117.52	111.77
31	9	304	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	s	316	CLA	CMD-C2D-C3D	-2.14	122.70	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	611	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
31	9	313	CLA	CHA-C1A-NA	-2.14	121.50	126.40
31	3	305	CLA	CHA-C1A-NA	-2.14	121.50	126.40
31	c	612	CLA	CHA-C1A-NA	-2.14	121.50	126.40
30	0	609	CHL	CHD-C4C-C3C	2.14	127.98	124.84
31	3	311	CLA	C1D-ND-C4D	-2.14	104.82	106.33
31	n	305	CLA	CHA-C1A-NA	-2.14	121.50	126.40
30	R	309	CHL	CHD-C4C-C3C	2.14	127.98	124.84
43	C	614	BCR	C34-C9-C10	-2.14	119.93	122.92
31	c	605	CLA	C2D-C1D-ND	2.14	111.68	110.10
31	A	405	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
36	9	319	NEX	C26-C27-C28	-2.13	121.48	125.99
31	B	615	CLA	C6-C5-C3	-2.13	107.86	113.45
34	c	620	LMG	O7-C10-O9	-2.13	118.54	123.70
31	C	611	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
43	h	101	BCR	C20-C19-C18	-2.13	120.42	126.42
34	m	102	LMG	O7-C10-O9	-2.13	118.54	123.70
31	s	314	CLA	C3B-C4B-NB	-2.13	108.53	110.52
31	5	602	CLA	CHA-C1A-NA	-2.13	121.51	126.40
30	5	601	CHL	C2C-C3C-C4C	2.13	108.01	106.49
30	0	601	CHL	C2C-C3C-C4C	2.13	108.01	106.49
31	1	611	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	a	409	CLA	C3B-C4B-NB	-2.13	108.54	110.52
34	A	414	LMG	C1-O6-C5	-2.13	109.50	113.69
30	3	303	CHL	C2B-C1B-NB	-2.13	108.80	110.23
30	Y	309	CHL	C2B-C1B-NB	-2.13	108.80	110.23
36	3	319	NEX	C20-C13-C14	-2.13	119.94	122.92
31	8	614	CLA	CHA-C1A-NA	-2.13	121.51	126.40
31	0	610	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	9	304	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
33	y	619	LHG	C6-C5-C4	-2.13	106.75	111.79
31	N	313	CLA	CHA-C1A-NA	-2.13	121.52	126.40
30	5	606	CHL	CHD-C4C-C3C	2.13	127.97	124.84
31	B	601	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	N	304	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	0	615	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
43	D	405	BCR	C1-C6-C5	-2.13	119.61	122.61
31	d	405	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	N	310	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
31	p	614	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
30	7	309	CHL	CHC-C1C-NC	2.13	127.44	124.20
30	7	310	CHL	C1-O2A-CGA	2.13	122.03	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	316	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	2	610	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	n	314	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	s	313	CLA	C4B-CHC-C1C	2.13	131.39	126.34
47	E	101	HEM	C1A-CHA-C4D	-2.13	121.29	126.34
31	2	602	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
34	S	321	LMG	C8-O7-C10	-2.13	112.55	117.79
30	1	619	CHL	CHC-C1C-NC	2.13	127.43	124.20
30	2	605	CHL	CHB-C4A-NA	2.13	127.46	124.51
31	s	311	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
33	g	319	LHG	C5-O7-C7	-2.13	112.55	117.79
31	Y	314	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
31	3	316	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	8	602	CLA	CHA-C1A-NA	-2.13	121.52	126.40
33	Y	318	LHG	C6-C5-C4	-2.13	106.75	111.79
31	q	313	CLA	CHA-C1A-NA	-2.13	121.53	126.40
31	B	606	CLA	C4B-CHC-C1C	2.13	131.38	126.34
31	B	611	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
31	A	405	CLA	C1D-ND-C4D	-2.13	104.82	106.33
32	y	617	LUT	C35-C15-C14	-2.13	119.12	123.47
31	r	305	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
31	2	613	CLA	O2A-CGA-CBA	2.13	118.58	111.91
30	0	601	CHL	CHD-C4C-C3C	2.13	127.97	124.84
31	S	314	CLA	CHA-C1A-NA	-2.13	121.53	126.40
31	B	610	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
30	6	308	CHL	CHB-C4A-NA	2.13	127.45	124.51
30	0	605	CHL	CHB-C4A-NA	2.13	127.45	124.51
31	Y	303	CLA	C6-C5-C3	-2.13	107.88	113.45
33	t	102	LHG	O7-C7-O9	-2.13	118.56	123.70
31	p	612	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
30	N	306	CHL	CHC-C1C-NC	2.13	127.43	124.20
31	C	601	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
31	n	314	CLA	CHA-C1A-NA	-2.13	121.53	126.40
31	B	602	CLA	C6-C7-C8	-2.13	109.05	115.92
44	a	414	PL9	C12-C13-C14	-2.12	122.54	127.66
31	7	316	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
31	a	406	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
31	G	611	CLA	CHA-C1A-NA	-2.12	121.53	126.40
30	6	310	CHL	C4A-NA-C1A	2.12	107.66	106.71
31	r	303	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
31	n	316	CLA	O2A-CGA-CBA	2.12	118.57	111.91
31	s	305	CLA	O2A-CGA-CBA	2.12	118.57	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	G	615	LUT	C18-C5-C4	2.12	118.29	114.36
37	G	620	XAT	C40-C33-C34	-2.12	119.95	122.92
30	7	307	CHL	CHD-C4C-C3C	2.12	127.96	124.84
32	n	317	LUT	C10-C11-C12	-2.12	116.59	123.22
34	C	619	LMG	O8-C28-O10	-2.12	118.23	123.59
31	r	311	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
31	b	616	CLA	C6-C5-C3	-2.12	107.89	113.45
30	G	601	CHL	CMA-C3A-C2A	2.12	122.39	113.83
30	y	605	CHL	C4A-NA-C1A	2.12	107.66	106.71
31	9	312	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
31	6	314	CLA	C6-C5-C3	-2.12	107.89	113.45
30	3	308	CHL	CHC-C1C-NC	2.12	127.42	124.20
30	n	310	CHL	CHB-C4A-NA	2.12	127.45	124.51
31	3	311	CLA	CHA-C1A-NA	-2.12	121.54	126.40
33	4	618	LHG	C5-O7-C7	-2.12	112.57	117.79
31	r	306	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
31	B	606	CLA	C6-C5-C3	-2.12	107.89	113.45
31	D	404	CLA	O2A-CGA-CBA	2.12	118.56	111.91
31	n	315	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
32	G	615	LUT	C31-C32-C33	-2.12	120.46	126.42
31	C	607	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
32	8	615	LUT	C39-C29-C28	2.12	121.42	118.08
31	G	613	CLA	CHA-C1A-NA	-2.12	121.54	126.40
30	q	309	CHL	CMA-C3A-C2A	2.12	122.38	113.83
31	D	403	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
31	8	604	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	C	605	CLA	C7-C6-C5	-2.12	107.60	113.36
31	4	603	CLA	O2A-CGA-CBA	2.12	118.56	111.91
31	A	407	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
31	S	310	CLA	O2A-CGA-CBA	2.12	118.56	111.91
31	4	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	g	310	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
36	5	618	NEX	C19-C9-C10	-2.12	119.96	122.92
31	9	304	CLA	C1-O2A-CGA	2.12	122.00	116.44
30	Y	301	CHL	CHC-C1C-NC	2.12	127.42	124.20
30	9	310	CHL	CMA-C3A-C2A	2.12	122.37	113.83
36	y	618	NEX	C26-C27-C28	-2.12	121.52	125.99
45	C	618	DGD	C1D-O6D-C5D	-2.12	109.53	113.69
34	0	622	LMG	C8-O7-C10	-2.12	112.58	117.79
32	r	317	LUT	C38-C25-C24	-2.12	119.03	123.56
30	r	310	CHL	C1-O2A-CGA	2.12	122.00	116.44
38	y	621	SQD	O3-C3-C2	-2.12	105.46	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	604	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	p	602	CLA	C3B-C4B-NB	-2.12	108.55	110.52
31	C	601	CLA	C1D-ND-C4D	-2.12	104.83	106.33
31	3	312	CLA	O2A-CGA-CBA	2.12	118.55	111.91
32	y	617	LUT	C38-C25-C24	-2.12	119.03	123.56
43	C	614	BCR	C29-C28-C27	2.12	116.10	111.38
30	4	607	CHL	C2B-C1B-NB	-2.12	108.81	110.23
31	n	311	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	c	610	CLA	C3B-C4B-NB	-2.11	108.55	110.52
31	2	611	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
43	V	101	BCR	C21-C20-C19	-2.11	116.62	123.22
30	8	605	CHL	CHC-C1C-NC	2.11	127.41	124.20
31	b	603	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
31	c	607	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
30	y	601	CHL	CHD-C4C-C3C	2.11	127.95	124.84
30	R	308	CHL	CMA-C3A-C2A	2.11	122.35	113.83
31	3	311	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
31	s	306	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
32	7	317	LUT	C31-C30-C29	-2.11	124.29	127.31
31	S	304	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
31	6	311	CLA	O2A-CGA-CBA	2.11	118.54	111.91
31	R	313	CLA	CHA-C1A-NA	-2.11	121.56	126.40
31	q	305	CLA	CHA-C1A-NA	-2.11	121.56	126.40
31	A	407	CLA	C1D-ND-C4D	-2.11	104.83	106.33
30	8	607	CHL	CMA-C3A-C2A	2.11	122.35	113.83
31	r	312	CLA	C6-C5-C3	-2.11	107.92	113.45
31	C	610	CLA	C4B-CHC-C1C	2.11	131.35	126.34
31	p	603	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
31	0	604	CLA	C3B-C4B-NB	-2.11	108.56	110.52
30	3	307	CHL	CHB-C4A-NA	2.11	127.43	124.51
30	1	609	CHL	C2C-C3C-C4C	2.11	107.99	106.49
30	R	308	CHL	C2C-C3C-C4C	2.11	107.99	106.49
31	8	612	CLA	CHA-C1A-NA	-2.11	121.56	126.40
31	q	315	CLA	C4B-CHC-C1C	2.11	131.34	126.34
32	8	615	LUT	C10-C11-C12	-2.11	116.63	123.22
30	R	308	CHL	CHD-C4C-C3C	2.11	127.94	124.84
32	S	317	LUT	C20-C13-C12	2.11	121.40	118.08
31	G	609	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
31	2	603	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	R	314	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	A	405	CLA	CMA-C3A-C4A	2.11	117.44	111.77
31	S	313	CLA	C3B-C4B-NB	-2.11	108.56	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	611	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	b	617	CLA	CMA-C3A-C4A	2.11	117.44	111.77
30	y	609	CHL	C2B-C1B-NB	-2.11	108.82	110.23
30	0	608	CHL	CMA-C3A-C2A	2.11	122.34	113.83
32	4	616	LUT	C11-C12-C13	-2.11	120.49	126.42
31	r	314	CLA	O2A-CGA-CBA	2.11	118.53	111.91
31	p	610	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
31	9	315	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	7	313	CLA	C6-C5-C3	-2.11	107.93	113.45
36	R	319	NEX	C16-C1-C6	-2.11	108.58	110.47
31	S	311	CLA	CHA-C1A-NA	-2.11	121.57	126.40
36	2	616	NEX	C40-C33-C34	-2.11	119.97	122.92
30	8	601	CHL	CHB-C4A-NA	2.11	127.43	124.51
31	B	606	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
31	S	316	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
32	y	617	LUT	C19-C9-C8	2.11	121.40	118.08
31	g	310	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
31	6	313	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
43	B	617	BCR	C33-C5-C4	2.11	117.66	113.62
31	r	304	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
34	m	102	LMG	C8-O7-C10	-2.11	112.61	117.79
30	Y	306	CHL	C4A-NA-C1A	2.11	107.65	106.71
30	q	310	CHL	CMA-C3A-C2A	2.11	122.33	113.83
31	1	611	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	3	304	CLA	CHA-C1A-NA	-2.11	121.57	126.40
30	S	308	CHL	CHD-C4C-C3C	2.11	127.94	124.84
32	4	616	LUT	C15-C35-C34	-2.11	119.16	123.47
31	p	603	CLA	CHA-C1A-NA	-2.11	121.58	126.40
37	g	321	XAT	C40-C33-C34	-2.11	119.97	122.92
30	n	309	CHL	CHD-C4C-C3C	2.11	127.94	124.84
31	3	313	CLA	CHA-C1A-NA	-2.11	121.58	126.40
31	1	604	CLA	C1-O2A-CGA	2.11	121.97	116.44
31	B	602	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
31	G	609	CLA	C3B-C4B-NB	-2.11	108.56	110.52
43	T	101	BCR	C8-C7-C6	-2.10	121.29	127.20
31	Y	312	CLA	C1D-ND-C4D	-2.10	104.84	106.33
30	Y	308	CHL	C2C-C3C-C4C	2.10	107.99	106.49
31	6	312	CLA	CHA-C1A-NA	-2.10	121.58	126.40
36	8	617	NEX	C20-C13-C14	-2.10	119.98	122.92
31	5	612	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
36	y	618	NEX	C31-C30-C29	2.10	130.31	127.31
30	3	302	CHL	C3A-C2A-C1A	2.10	104.49	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	307	CHL	CHB-C4A-NA	2.10	127.42	124.51
43	a	410	BCR	C10-C11-C12	-2.10	116.66	123.22
31	S	311	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
37	9	322	XAT	C40-C33-C34	-2.10	119.98	122.92
43	Z	101	BCR	C15-C16-C17	-2.10	119.17	123.47
31	C	606	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	0	614	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	7	314	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	S	311	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
31	b	617	CLA	C4B-CHC-C1C	2.10	131.32	126.34
31	7	312	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	r	307	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	5	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	p	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	g	313	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	d	401	CLA	C1D-ND-C4D	-2.10	104.84	106.33
31	0	613	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
34	W	202	LMG	C8-O7-C10	-2.10	112.62	117.79
31	g	314	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	4	611	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	q	306	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
31	7	305	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	9	312	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
30	3	308	CHL	CHB-C4A-NA	2.10	127.42	124.51
31	2	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	4	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	s	311	CLA	CHA-C1A-NA	-2.10	121.59	126.40
30	n	306	CHL	CHC-C1C-NC	2.10	127.39	124.20
32	G	615	LUT	C11-C10-C9	-2.10	124.31	127.31
31	0	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	y	610	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	1	602	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
31	p	604	CLA	C1-O2A-CGA	2.10	121.95	116.44
30	5	605	CHL	CHD-C4C-C3C	2.10	127.92	124.84
31	5	613	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	y	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
37	q	321	XAT	C40-C33-C34	-2.10	119.98	122.92
31	c	606	CLA	C6-C7-C8	-2.10	109.14	115.92
31	7	314	CLA	C1-O2A-CGA	2.10	121.95	116.44
31	S	316	CLA	C1D-ND-C4D	-2.10	104.84	106.33
30	4	607	CHL	CHD-C1D-C2D	2.10	129.88	125.48
30	p	601	CHL	C2C-C3C-C4C	2.10	107.98	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	613	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
32	q	318	LUT	C19-C9-C10	-2.10	119.99	122.92
31	s	303	CLA	C11-C10-C8	-2.10	109.14	115.92
32	5	617	LUT	C21-C26-C27	-2.10	110.05	112.70
31	7	304	CLA	OBD-CAD-C3D	-2.10	123.48	128.52
30	Y	307	CHL	C2C-C3C-C4C	2.10	107.98	106.49
30	p	601	CHL	C2B-C1B-NB	-2.10	108.83	110.23
30	7	308	CHL	CHC-C1C-NC	2.10	127.38	124.20
32	r	317	LUT	C11-C10-C9	-2.10	124.32	127.31
31	n	303	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
30	N	307	CHL	CHB-C4A-NA	2.09	127.41	124.51
30	n	302	CHL	CHB-C4A-NA	2.09	127.41	124.51
31	a	407	CLA	C6-C5-C3	-2.09	107.96	113.45
34	G	621	LMG	C8-O7-C10	-2.09	112.63	117.79
36	g	317	NEX	C40-C33-C34	-2.09	119.99	122.92
31	g	310	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
36	3	319	NEX	O24-C25-C38	-2.09	112.55	115.06
37	4	619	XAT	C40-C33-C34	-2.09	119.99	122.92
31	C	602	CLA	CHA-C1A-NA	-2.09	121.60	126.40
30	y	609	CHL	C3A-C2A-C1A	2.09	104.47	101.34
30	y	606	CHL	C1-C2-C3	-2.09	122.42	126.04
31	s	313	CLA	CMA-C3A-C4A	2.09	117.40	111.77
32	6	317	LUT	C38-C25-C24	-2.09	119.08	123.56
30	1	607	CHL	CHB-C4A-NA	2.09	127.41	124.51
35	g	315	RRX	C19-C18-C17	2.09	122.15	118.94
31	3	314	CLA	CHA-C1A-NA	-2.09	121.61	126.40
31	1	604	CLA	C3B-C4B-NB	-2.09	108.57	110.52
31	n	311	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
31	9	314	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
30	7	321	CHL	C1-O2A-CGA	2.09	121.93	116.44
31	C	607	CLA	CHA-C1A-NA	-2.09	121.61	126.40
36	5	618	NEX	O24-C25-C38	-2.09	112.55	115.06
30	Y	307	CHL	CHB-C4A-NA	2.09	127.40	124.51
31	0	615	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	c	607	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
33	A	415	LHG	O8-C23-O10	-2.09	118.31	123.59
32	p	617	LUT	C19-C9-C10	-2.09	119.99	122.92
30	Y	302	CHL	C4A-NA-C1A	2.09	107.65	106.71
31	7	303	CLA	CHA-C1A-NA	-2.09	121.61	126.40
36	N	318	NEX	C15-C14-C13	-2.09	124.33	127.31
30	4	607	CHL	CHC-C1C-NC	2.09	127.37	124.20
30	S	302	CHL	C3B-C4B-NB	-2.09	108.58	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	604	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	c	609	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
36	r	319	NEX	C19-C9-C10	-2.09	120.00	122.92
31	c	607	CLA	CMA-C3A-C4A	2.09	117.39	111.77
30	9	310	CHL	CHC-C1C-NC	2.09	127.37	124.20
30	G	607	CHL	CMA-C3A-C2A	2.09	122.26	113.83
31	3	301	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
34	p	620	LMG	C7-O1-C1	-2.09	109.66	113.74
30	g	308	CHL	CMA-C3A-C2A	2.09	122.25	113.83
36	8	617	NEX	C2-C1-C6	2.09	111.24	109.21
43	c	614	BCR	C8-C7-C6	-2.09	121.34	127.20
30	r	308	CHL	CHD-C4C-C3C	2.09	127.91	124.84
47	E	101	HEM	CHA-C4D-C3D	-2.09	121.41	125.33
31	6	304	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
31	q	313	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
43	v	101	BCR	C35-C13-C12	2.09	121.37	118.08
32	6	318	LUT	C30-C31-C32	-2.09	116.70	123.22
30	p	609	CHL	CHD-C4C-C3C	2.09	127.91	124.84
31	b	605	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
34	q	301	LMG	O6-C5-C6	2.09	111.63	106.44
31	p	614	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
31	Y	310	CLA	CHA-C1A-NA	-2.09	121.62	126.40
31	r	314	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
34	D	410	LMG	C8-O7-C10	-2.09	112.65	117.79
31	S	306	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	0	603	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
31	A	405	CLA	C3B-C4B-NB	-2.09	108.58	110.52
31	0	613	CLA	CHA-C1A-NA	-2.09	121.62	126.40
45	C	620	DGD	O2G-C1B-O1B	-2.09	118.66	123.70
31	C	602	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
30	n	308	CHL	CMA-C3A-C2A	2.09	122.24	113.83
31	g	314	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
31	C	611	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
31	A	405	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
30	0	607	CHL	CHB-C4A-NA	2.08	127.39	124.51
36	s	319	NEX	C2-C1-C6	2.08	111.24	109.21
31	0	602	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
30	4	609	CHL	C4A-NA-C1A	2.08	107.64	106.71
31	1	611	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
31	C	607	CLA	C6-C7-C8	-2.08	109.18	115.92
31	N	305	CLA	O2A-CGA-CBA	2.08	118.45	111.91
31	8	602	CLA	C6-C5-C3	-2.08	107.99	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	315	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	y	604	CLA	O2A-CGA-CBA	2.08	118.44	111.91
30	6	306	CHL	CHD-C4C-C3C	2.08	127.90	124.84
43	V	101	BCR	C35-C13-C12	2.08	121.36	118.08
31	n	305	CLA	O2A-CGA-CBA	2.08	118.44	111.91
31	1	604	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	7	307	CHL	CHB-C4A-NA	2.08	127.39	124.51
31	2	612	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
31	A	409	CLA	C3B-C4B-NB	-2.08	108.58	110.52
31	C	608	CLA	O2A-CGA-CBA	2.08	118.44	111.91
30	7	321	CHL	CMA-C3A-C2A	2.08	122.23	113.83
32	6	318	LUT	C8-C7-C6	-2.08	121.36	127.20
30	6	310	CHL	C1-O2A-CGA	2.08	121.91	116.44
30	4	605	CHL	CHD-C4C-C3C	2.08	127.90	124.84
30	G	601	CHL	CHD-C4C-C3C	2.08	127.90	124.84
30	N	301	CHL	CHD-C4C-C3C	2.08	127.90	124.84
31	C	603	CLA	C4B-CHC-C1C	2.08	131.27	126.34
30	6	306	CHL	C3A-C2A-C1A	2.08	104.46	101.34
36	S	319	NEX	C19-C9-C10	-2.08	120.01	122.92
30	Y	307	CHL	C2B-C1B-NB	-2.08	108.84	110.23
45	c	617	DGD	C6D-O5D-C1E	2.08	117.80	113.74
31	0	602	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	0	612	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
31	G	611	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
31	B	615	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	C	609	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	S	314	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	7	311	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	d	401	CLA	C1-O2A-CGA	2.08	121.90	116.44
31	8	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40
34	j	101	LMG	C8-O7-C10	-2.08	112.67	117.79
36	R	301	NEX	O24-C25-C38	-2.08	112.57	115.06
31	B	603	CLA	C1-C2-C3	-2.08	122.45	126.04
30	4	606	CHL	C2B-C1B-NB	-2.08	108.84	110.23
30	y	601	CHL	CMA-C3A-C2A	2.08	122.21	113.83
31	p	610	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
31	r	313	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	3	306	CLA	OBD-CAD-C3D	-2.08	123.52	128.52
31	p	610	CLA	C6-C5-C3	-2.08	108.01	113.45
30	n	308	CHL	C1-O2A-CGA	2.08	121.89	116.44
31	6	305	CLA	O2A-CGA-CBA	2.08	118.43	111.91
31	9	316	CLA	CHA-C1A-NA	-2.08	121.64	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	401	CLA	O2A-CGA-CBA	2.08	118.42	111.91
31	b	613	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
31	p	610	CLA	CHA-C1A-NA	-2.08	121.64	126.40
32	N	317	LUT	C2-C3-C4	2.08	113.15	110.30
31	3	313	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
31	y	615	CLA	O2A-CGA-CBA	2.08	118.42	111.91
31	9	304	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	C	607	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
32	Y	315	LUT	C19-C9-C8	2.08	121.35	118.08
31	N	315	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	S	310	CLA	CHA-C1A-NA	-2.08	121.64	126.40
30	p	608	CHL	CHC-C1C-NC	2.07	127.35	124.20
31	S	313	CLA	O2A-CGA-CBA	2.07	118.42	111.91
44	A	416	PL9	O2-C1-C6	2.07	124.18	120.59
30	8	607	CHL	CHB-C4A-NA	2.07	127.38	124.51
31	N	304	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	b	607	CLA	C1D-ND-C4D	-2.07	104.86	106.33
31	8	613	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
42	d	402	PHO	C1C-C2C-C3C	-2.07	106.89	108.61
34	g	320	LMG	O7-C10-O9	-2.07	118.69	123.70
38	A	411	SQD	O8-S-C6	-2.07	102.44	105.74
31	g	311	CLA	C2A-C1A-CHA	2.07	127.48	123.86
30	6	308	CHL	C4A-NA-C1A	2.07	107.64	106.71
31	5	614	CLA	CHA-C1A-NA	-2.07	121.65	126.40
31	b	609	CLA	C3B-C4B-NB	-2.07	108.59	110.52
31	B	602	CLA	O2A-CGA-CBA	2.07	118.41	111.91
37	R	318	XAT	C19-C9-C10	-2.07	120.02	122.92
30	g	302	CHL	CHD-C4C-C3C	2.07	127.88	124.84
31	6	311	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	6	313	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	S	313	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
31	p	602	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
33	b	628	LHG	C5-O7-C7	-2.07	112.69	117.79
30	9	308	CHL	C2C-C3C-C4C	2.07	107.97	106.49
31	b	611	CLA	CHA-C1A-NA	-2.07	121.66	126.40
30	S	308	CHL	CMA-C3A-C2A	2.07	122.18	113.83
30	9	309	CHL	C1-C2-C3	-2.07	122.46	126.04
31	S	315	CLA	CHA-C1A-NA	-2.07	121.66	126.40
31	9	305	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
31	G	609	CLA	C1D-ND-C4D	-2.07	104.86	106.33
31	3	306	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
31	4	611	CLA	C4B-CHC-C1C	2.07	132.00	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	609	CHL	C1-C2-C3	-2.07	122.47	126.04
31	5	611	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
31	q	306	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
31	R	303	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
30	q	307	CHL	CHB-C4A-NA	2.07	127.37	124.51
30	3	307	CHL	CMA-C3A-C2A	2.07	122.17	113.83
43	z	101	BCR	C38-C26-C27	2.07	117.59	113.62
34	c	621	LMG	O8-C28-O10	-2.07	118.37	123.59
31	S	311	CLA	C1D-ND-C4D	-2.07	104.87	106.33
31	y	613	CLA	C1D-ND-C4D	-2.07	104.87	106.33
31	c	607	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
31	n	303	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
31	A	407	CLA	C1-O2A-CGA	2.07	121.87	116.44
31	r	313	CLA	C1-O2A-CGA	2.07	121.87	116.44
30	Y	308	CHL	CHD-C4C-C3C	2.07	127.88	124.84
30	g	307	CHL	CHB-C4A-NA	2.07	127.37	124.51
34	d	411	LMG	O7-C10-O9	-2.07	118.71	123.70
31	y	604	CLA	CMA-C3A-C4A	2.07	117.33	111.77
31	g	304	CLA	CHA-C1A-NA	-2.07	121.67	126.40
36	0	618	NEX	C4-C3-C2	2.07	114.76	110.77
32	3	318	LUT	C30-C31-C32	-2.07	116.77	123.22
32	y	616	LUT	C40-C33-C32	2.07	121.33	118.08
31	B	609	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	Y	314	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	B	609	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
30	q	307	CHL	CMA-C3A-C2A	2.07	122.16	113.83
38	B	623	SQD	O8-S-C6	-2.07	102.45	105.74
31	5	604	CLA	O2A-CGA-CBA	2.07	118.39	111.91
31	7	312	CLA	O2A-CGA-CBA	2.07	118.39	111.91
31	s	314	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
37	2	619	XAT	C40-C33-C34	-2.07	120.03	122.92
43	H	101	BCR	C34-C9-C10	-2.07	120.03	122.92
43	Z	101	BCR	C8-C7-C6	-2.07	121.40	127.20
30	S	307	CHL	CHB-C4A-NA	2.06	127.37	124.51
31	C	604	CLA	C3B-C4B-NB	-2.06	108.60	110.52
34	6	322	LMG	C8-O7-C10	-2.06	112.71	117.79
37	2	619	XAT	C19-C9-C10	-2.06	120.03	122.92
30	9	309	CHL	CMA-C3A-C2A	2.06	122.15	113.83
31	1	602	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	g	310	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	c	611	CLA	CHA-C1A-NA	-2.06	121.67	126.40
31	1	602	CLA	CMD-C2D-C3D	-2.06	122.87	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	0	610	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
31	b	606	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
44	a	414	PL9	C20-C19-C21	2.06	118.74	115.27
31	0	610	CLA	CHA-C1A-NA	-2.06	121.67	126.40
36	6	319	NEX	C4-C3-C2	2.06	114.76	110.77
30	p	606	CHL	CHB-C4A-NA	2.06	127.36	124.51
31	A	406	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	B	603	CLA	C3B-C4B-NB	-2.06	108.60	110.52
30	G	607	CHL	C4A-NA-C1A	2.06	107.63	106.71
31	A	406	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	C	608	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	r	315	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
31	y	612	CLA	C1-O2A-CGA	2.06	121.85	116.44
31	s	303	CLA	O2A-CGA-CBA	2.06	118.38	111.91
30	G	623	CHL	CHC-C1C-NC	2.06	127.33	124.20
44	a	414	PL9	O2-C1-C2	-2.06	117.06	121.78
31	6	314	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	c	601	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	q	315	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
31	N	315	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
30	p	605	CHL	CHB-C4A-NA	2.06	127.36	124.51
31	7	313	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	g	312	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	1	602	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
31	q	316	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
30	p	608	CHL	CHB-C4A-NA	2.06	127.36	124.51
31	b	604	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	4	614	CLA	C1-O2A-CGA	2.06	121.85	116.44
36	R	319	NEX	C2-C1-C6	2.06	111.21	109.21
36	9	319	NEX	C4-C3-C2	2.06	114.75	110.77
31	s	315	CLA	CHA-C1A-NA	-2.06	121.68	126.40
32	Y	316	LUT	C2-C3-C4	2.06	113.12	110.30
32	3	317	LUT	C30-C31-C32	-2.06	116.79	123.22
31	r	303	CLA	CHA-C1A-NA	-2.06	121.69	126.40
31	8	613	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
31	c	611	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
32	q	318	LUT	C2-C3-C4	2.06	113.12	110.30
31	Y	303	CLA	CHA-C1A-NA	-2.06	121.69	126.40
31	C	604	CLA	C6-C7-C8	-2.06	109.27	115.92
31	C	613	CLA	C3B-C4B-NB	-2.06	108.61	110.52
31	R	315	CLA	C3B-C4B-NB	-2.06	108.61	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	D	409	LMG	C8-O7-C10	-2.06	112.73	117.79
31	g	310	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
31	1	610	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
31	Y	303	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
32	5	617	LUT	C20-C13-C14	-2.06	120.04	122.92
32	Y	316	LUT	C19-C9-C10	-2.06	120.04	122.92
30	n	307	CHL	CHB-C4A-NA	2.06	127.36	124.51
38	b	621	SQD	O8-S-C6	-2.06	102.46	105.74
33	C	623	LHG	O7-C7-O9	-2.06	118.73	123.70
30	9	303	CHL	CMA-C3A-C2A	2.06	122.12	113.83
32	y	616	LUT	C8-C9-C10	-2.06	115.79	118.94
31	3	301	CLA	CHA-C1A-NA	-2.06	121.69	126.40
31	c	611	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	6	311	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
31	B	615	CLA	CMA-C3A-C4A	2.05	117.29	111.77
31	g	310	CLA	CHA-C1A-NA	-2.05	121.69	126.40
30	y	607	CHL	CHC-C1C-NC	2.05	127.32	124.20
31	s	316	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
31	s	303	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
31	B	614	CLA	CHA-C1A-NA	-2.05	121.69	126.40
31	3	301	CLA	O2A-CGA-CBA	2.05	118.35	111.91
31	7	312	CLA	CHA-C1A-NA	-2.05	121.70	126.40
30	r	308	CHL	C1-O2A-CGA	2.05	121.83	116.44
31	n	303	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	n	312	CLA	O2A-CGA-CBA	2.05	118.35	111.91
30	9	308	CHL	CHD-C4C-C3C	2.05	127.86	124.84
44	a	414	PL9	C32-C33-C34	-2.05	122.72	127.66
38	x	201	SQD	O3-C3-C2	-2.05	105.60	110.35
31	c	609	CLA	C16-C15-C13	-2.05	109.28	115.92
32	n	317	LUT	C15-C35-C34	-2.05	119.27	123.47
31	N	303	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	8	603	CLA	CHA-C1A-NA	-2.05	121.70	126.40
43	B	617	BCR	C30-C25-C26	-2.05	119.72	122.61
42	a	408	PHO	C1C-C2C-C3C	-2.05	106.90	108.61
31	R	305	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
31	2	611	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	b	617	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	8	610	CLA	O2A-CGA-CBA	2.05	118.35	111.91
31	s	305	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	1	612	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
31	3	315	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	0	613	CLA	C1D-ND-C4D	-2.05	104.88	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	p	612	CLA	CHA-C1A-NA	-2.05	121.70	126.40
32	Y	315	LUT	C28-C29-C30	-2.05	115.79	118.94
47	e	102	HEM	C4A-NA-C1A	2.05	107.36	105.35
30	6	310	CHL	CHD-C4C-C3C	2.05	127.85	124.84
30	Y	306	CHL	C3A-C2A-C1A	2.05	104.41	101.34
31	b	612	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
30	9	308	CHL	CHB-C4A-NA	2.05	127.35	124.51
32	1	616	LUT	C20-C13-C12	2.05	121.31	118.08
35	q	317	RRX	C38-C26-C27	2.05	118.15	114.36
30	Y	306	CHL	CHC-C1C-NC	2.05	127.31	124.20
31	n	315	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
31	r	314	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	3	312	CLA	C1D-ND-C4D	-2.05	104.88	106.33
30	G	607	CHL	C2C-C3C-C4C	2.05	107.95	106.49
31	B	615	CLA	C4B-CHC-C1C	2.05	131.20	126.34
31	N	311	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
31	5	610	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	Y	312	CLA	C6-C5-C3	-2.05	108.08	113.45
30	8	605	CHL	C4A-NA-C1A	2.05	107.63	106.71
43	c	614	BCR	C24-C25-C26	-2.05	116.50	121.46
31	5	602	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	b	615	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	y	602	CLA	CHA-C1A-NA	-2.05	121.71	126.40
32	6	317	LUT	C20-C13-C12	2.05	121.30	118.08
31	S	305	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	N	314	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
32	3	317	LUT	C35-C15-C14	-2.05	119.28	123.47
31	R	311	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	G	611	CLA	C3B-C4B-NB	-2.05	108.62	110.52
47	e	102	HEM	C1A-CHA-C4D	-2.05	121.48	126.34
30	7	310	CHL	C2C-C3C-C4C	2.05	107.95	106.49
30	6	302	CHL	CMA-C3A-C2A	2.05	122.08	113.83
31	9	306	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
31	G	603	CLA	CHA-C1A-NA	-2.05	121.71	126.40
30	0	606	CHL	CHC-C1C-NC	2.05	127.31	124.20
31	1	614	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	c	610	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
30	R	308	CHL	CHB-C4A-NA	2.05	127.34	124.51
31	c	603	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
44	A	416	PL9	O2-C1-C2	-2.05	117.09	121.78
31	B	611	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	N	321	CLA	CHA-C1A-NA	-2.04	121.72	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	407	CLA	CHA-C1A-NA	-2.04	121.72	126.40
44	a	414	PL9	C7-C8-C9	-2.04	123.39	126.79
34	G	622	LMG	C8-O7-C10	-2.04	112.76	117.79
31	S	313	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
31	c	613	CLA	C1-C2-C3	-2.04	122.51	126.04
31	0	610	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
30	2	605	CHL	CMA-C3A-C2A	2.04	122.07	113.83
34	2	621	LMG	C9-C8-C7	-2.04	106.95	111.79
31	3	314	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
30	1	619	CHL	C3A-C2A-C1A	2.04	104.40	101.34
31	Y	312	CLA	CMA-C3A-C4A	2.04	117.26	111.77
31	B	605	CLA	C1D-ND-C4D	-2.04	104.88	106.33
31	r	311	CLA	C1D-ND-C4D	-2.04	104.88	106.33
32	s	318	LUT	C39-C29-C28	2.04	121.30	118.08
31	s	314	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
31	1	610	CLA	CHA-C1A-NA	-2.04	121.72	126.40
31	C	612	CLA	CHA-C1A-NA	-2.04	121.72	126.40
30	n	307	CHL	CMA-C3A-C2A	2.04	122.06	113.83
31	1	613	CLA	C3B-C4B-NB	-2.04	108.62	110.52
31	g	310	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	Y	313	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
31	7	314	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
32	8	615	LUT	C15-C35-C34	-2.04	119.29	123.47
32	9	318	LUT	C19-C9-C10	-2.04	120.06	122.92
36	r	319	NEX	C40-C33-C34	-2.04	120.06	122.92
30	Y	307	CHL	CHD-C4C-C3C	2.04	127.84	124.84
31	S	313	CLA	CHA-C1A-NA	-2.04	121.72	126.40
31	R	313	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	c	601	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
30	8	608	CHL	CHB-C4A-NA	2.04	127.33	124.51
31	7	314	CLA	C3B-C4B-NB	-2.04	108.62	110.52
32	s	318	LUT	C20-C13-C12	2.04	121.29	118.08
31	n	316	CLA	CHA-C1A-NA	-2.04	121.72	126.40
32	y	617	LUT	C1-C6-C5	-2.04	119.74	122.61
31	y	615	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	1	613	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	Y	312	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	r	307	CLA	O2A-CGA-CBA	2.04	118.31	111.91
32	8	616	LUT	C38-C25-C24	-2.04	119.19	123.56
36	4	617	NEX	C19-C9-C10	-2.04	120.07	122.92
31	A	407	CLA	C3B-C4B-NB	-2.04	108.62	110.52
31	4	613	CLA	CAA-C2A-C3A	-2.04	107.19	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	616	LUT	C35-C15-C14	-2.04	119.30	123.47
32	n	318	LUT	C38-C25-C24	-2.04	119.20	123.56
43	B	617	BCR	C37-C22-C23	2.04	121.29	118.08
31	9	315	CLA	O2A-CGA-CBA	2.04	118.31	111.91
31	y	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	G	612	CLA	C3B-C4B-NB	-2.04	108.62	110.52
31	B	616	CLA	CHA-C1A-NA	-2.04	121.73	126.40
37	R	318	XAT	C20-C13-C14	-2.04	120.07	122.92
31	r	315	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
31	b	610	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	G	609	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	b	612	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	4	602	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	0	612	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	0	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B	601	CLA	C1D-ND-C4D	-2.04	104.89	106.33
47	E	101	HEM	CHA-C1A-NA	2.04	127.59	123.85
37	G	620	XAT	C19-C9-C10	-2.04	120.07	122.92
31	6	303	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	R	314	CLA	C1-O2A-CGA	2.04	121.79	116.44
30	5	606	CHL	CHB-C4A-NA	2.04	127.33	124.51
31	4	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	A	407	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
30	6	302	CHL	C2B-C1B-NB	-2.04	108.87	110.23
31	N	310	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	6	303	CLA	C6-C5-C3	-2.04	108.12	113.45
31	3	305	CLA	O2A-CGA-CBA	2.04	118.30	111.91
31	2	609	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B	601	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	7	313	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B	601	CLA	CHA-C1A-NA	-2.04	121.74	126.40
30	8	606	CHL	CMA-C3A-C2A	2.04	122.04	113.83
31	p	614	CLA	CHA-C1A-NA	-2.04	121.74	126.40
31	8	604	CLA	O2A-CGA-CBA	2.04	118.29	111.91
31	7	311	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
36	y	618	NEX	C4-C3-C2	2.04	114.70	110.77
31	4	610	CLA	C6-C5-C3	-2.03	108.12	113.45
44	a	414	PL9	C37-C38-C39	-2.03	122.76	127.66
36	g	317	NEX	C19-C9-C10	-2.03	120.07	122.92
31	8	609	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
32	s	317	LUT	C19-C9-C8	2.03	121.28	118.08
31	C	606	CLA	CHA-C1A-NA	-2.03	121.74	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
34	9	321	LMG	O8-C28-O10	-2.03	118.46	123.59
30	n	301	CHL	CMA-C3A-C2A	2.03	122.03	113.83
31	b	605	CLA	C2A-C1A-CHA	2.03	127.41	123.86
31	c	603	CLA	CHA-C1A-NA	-2.03	121.74	126.40
31	r	312	CLA	CMA-C3A-C4A	2.03	117.24	111.77
30	8	606	CHL	CHB-C4A-NA	2.03	127.32	124.51
31	0	612	CLA	C1D-ND-C4D	-2.03	104.89	106.33
31	c	608	CLA	C1D-ND-C4D	-2.03	104.89	106.33
31	p	611	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
45	C	617	DGD	O1G-C1A-O1A	-2.03	118.46	123.59
37	R	318	XAT	C24-C23-C22	-2.03	106.85	110.77
31	C	613	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	R	306	CLA	O2A-CGA-CBA	2.03	118.28	111.91
32	Y	316	LUT	C15-C35-C34	-2.03	119.31	123.47
31	N	311	CLA	CHA-C1A-NA	-2.03	121.75	126.40
33	g	319	LHG	O8-C23-O10	-2.03	118.47	123.59
37	4	619	XAT	C19-C9-C10	-2.03	120.08	122.92
32	Y	316	LUT	C39-C29-C28	2.03	121.28	118.08
31	b	614	CLA	CHA-C1A-NA	-2.03	121.75	126.40
31	n	304	CLA	CHA-C1A-NA	-2.03	121.75	126.40
31	C	610	CLA	C3B-C4B-NB	-2.03	108.63	110.52
31	Y	310	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
30	g	307	CHL	CHC-C1C-NC	2.03	127.28	124.20
38	a	412	SQD	O8-S-C6	-2.03	102.50	105.74
31	s	304	CLA	CAA-C2A-C3A	-2.03	109.19	114.26
31	c	605	CLA	C6-C5-C3	-2.03	108.13	113.45
30	q	310	CHL	CHB-C4A-NA	2.03	127.32	124.51
31	c	612	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	n	315	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
36	N	318	NEX	C19-C9-C10	-2.03	120.08	122.92
43	b	619	BCR	C10-C11-C12	-2.03	116.88	123.22
32	y	616	LUT	C12-C13-C14	-2.03	115.83	118.94
34	k	101	LMG	O8-C28-O10	-2.03	118.47	123.59
31	N	314	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	R	307	CLA	O2A-CGA-CBA	2.03	118.28	111.91
36	8	617	NEX	O24-C25-C38	-2.03	112.62	115.06
37	g	321	XAT	C19-C9-C10	-2.03	120.08	122.92
31	y	613	CLA	C6-C7-C8	-2.03	109.36	115.92
30	y	606	CHL	CHD-C4C-C3C	2.03	127.82	124.84
31	N	312	CLA	CHA-C1A-NA	-2.03	121.75	126.40
48	c	623	LMU	O5B-C1B-C2B	2.03	114.64	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	315	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
36	9	319	NEX	C19-C9-C10	-2.03	120.08	122.92
31	c	608	CLA	C1-O2A-CGA	2.03	121.76	116.44
31	b	604	CLA	C2D-C1D-ND	2.03	111.60	110.10
31	G	611	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
31	r	304	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	R	316	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
32	0	617	LUT	C38-C25-C24	-2.03	119.22	123.56
32	n	317	LUT	C20-C13-C12	2.03	121.27	118.08
34	c	620	LMG	O8-C28-O10	-2.03	118.48	123.59
30	1	607	CHL	CMA-C3A-C2A	2.03	122.00	113.83
31	B	607	CLA	C1D-ND-C4D	-2.03	104.90	106.33
31	B	610	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	b	607	CLA	C4B-CHC-C1C	2.03	131.14	126.34
31	a	406	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
32	N	317	LUT	C30-C31-C32	-2.03	116.90	123.22
34	d	410	LMG	O8-C28-O10	-2.03	118.48	123.59
31	C	613	CLA	C2A-C1A-CHA	2.03	127.40	123.86
34	2	621	LMG	O7-C10-O9	-2.03	118.81	123.70
34	w	204	LMG	O7-C10-O9	-2.03	118.81	123.70
31	b	616	CLA	C4B-CHC-C1C	2.03	131.14	126.34
36	r	301	NEX	C31-C30-C29	2.02	130.20	127.31
31	q	312	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
31	B	610	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
31	A	405	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	5	610	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
30	7	302	CHL	C2C-C3C-C4C	2.02	107.93	106.49
31	b	613	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	5	611	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	y	604	CLA	CHA-C1A-NA	-2.02	121.76	126.40
37	9	322	XAT	C19-C9-C10	-2.02	120.09	122.92
36	g	317	NEX	C31-C30-C29	2.02	130.20	127.31
31	4	614	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	S	312	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	G	602	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
31	c	604	CLA	O2A-CGA-CBA	2.02	118.26	111.91
34	J	101	LMG	C8-O7-C10	-2.02	112.81	117.79
31	c	604	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	c	609	CLA	C11-C10-C8	-2.02	109.38	115.92
31	s	313	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	S	311	CLA	C6-C5-C3	-2.02	108.15	113.45
34	b	624	LMG	O6-C5-C4	2.02	113.37	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	311	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
36	S	319	NEX	C20-C13-C14	-2.02	120.09	122.92
34	B	625	LMG	O8-C28-O10	-2.02	118.49	123.59
31	2	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	4	614	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
31	y	614	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
31	7	303	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
43	B	619	BCR	C29-C30-C25	2.02	113.59	110.48
44	a	414	PL9	O1-C4-C3	-2.02	118.49	120.72
30	2	607	CHL	CHD-C4C-C3C	2.02	127.81	124.84
31	S	304	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	1	603	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
31	R	305	CLA	C2D-C1D-ND	2.02	111.59	110.10
31	0	613	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
32	8	615	LUT	C20-C13-C12	2.02	121.26	118.08
30	s	307	CHL	C2C-C3C-C4C	2.02	107.93	106.49
31	Y	305	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	R	312	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
31	c	604	CLA	C1-O2A-CGA	2.02	121.74	116.44
38	x	201	SQD	O5-C1-O6	-2.02	105.19	109.97
31	2	612	CLA	C1-O2A-CGA	2.02	121.74	116.44
30	4	601	CHL	CHD-C4C-C3C	2.02	127.81	124.84
30	R	310	CHL	C3A-C2A-C1A	2.02	104.36	101.34
30	R	310	CHL	CHC-C1C-NC	2.02	127.27	124.20
32	4	616	LUT	C20-C13-C14	-2.02	120.09	122.92
31	c	613	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	N	310	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
31	q	315	CLA	C11-C10-C8	-2.02	109.39	115.92
30	6	308	CHL	CMA-C3A-C2A	2.02	121.97	113.83
36	n	319	NEX	C11-C12-C13	2.02	132.09	126.42
30	N	302	CHL	CHB-C4A-NA	2.02	127.30	124.51
43	C	614	BCR	C33-C5-C4	2.02	117.49	113.62
31	9	305	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	1	603	CLA	CHA-C1A-NA	-2.02	121.78	126.40
30	G	605	CHL	C4A-NA-C1A	2.02	107.61	106.71
31	R	315	CLA	C6-C5-C3	-2.02	108.17	113.45
31	3	304	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	r	316	CLA	C1D-ND-C4D	-2.02	104.90	106.33
31	y	604	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
31	4	604	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	304	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
43	d	406	BCR	C21-C20-C19	-2.02	116.92	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	612	CLA	CHA-C1A-NA	-2.02	121.78	126.40
45	c	617	DGD	O5D-C6D-C5D	2.02	112.78	109.05
31	b	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	311	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	316	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	q	304	CLA	C6-C7-C8	-2.02	109.40	115.92
31	y	603	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
34	b	601	LMG	C9-C8-C7	-2.02	107.02	111.79
30	9	310	CHL	CHB-C4A-NA	2.02	127.30	124.51
31	5	612	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
31	r	304	CLA	C6-C7-C8	-2.01	109.41	115.92
32	Y	315	LUT	C18-C5-C4	2.01	118.09	114.36
32	y	616	LUT	C38-C25-C24	-2.01	119.25	123.56
31	Y	304	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
31	n	316	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
30	g	308	CHL	CHB-C4A-NA	2.01	127.30	124.51
34	7	322	LMG	O7-C10-O9	-2.01	118.83	123.70
31	C	603	CLA	CHA-C1A-NA	-2.01	121.79	126.40
31	R	314	CLA	CHA-C1A-NA	-2.01	121.79	126.40
30	G	606	CHL	CHD-C4C-C3C	2.01	127.80	124.84
31	R	316	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
30	3	309	CHL	CMA-C3A-C2A	2.01	121.95	113.83
31	1	613	CLA	O2A-CGA-CBA	2.01	118.23	111.91
30	5	608	CHL	CHB-C4A-NA	2.01	127.30	124.51
32	Y	315	LUT	C38-C25-C24	-2.01	119.25	123.56
43	v	101	BCR	C30-C25-C24	2.01	121.47	115.78
31	7	314	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
44	a	414	PL9	C31-C32-C33	-2.01	105.27	111.88
31	4	610	CLA	C6-C7-C8	-2.01	109.41	115.92
31	B	604	CLA	O2A-CGA-CBA	2.01	118.22	111.91
45	c	617	DGD	O2G-C1B-O1B	-2.01	118.84	123.70
31	2	609	CLA	C11-C10-C8	-2.01	109.41	115.92
43	d	406	BCR	C29-C30-C25	2.01	113.58	110.48
31	b	614	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
30	9	308	CHL	CMA-C3A-C2A	2.01	121.94	113.83
32	8	615	LUT	C19-C9-C8	2.01	121.25	118.08
31	G	609	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
32	8	616	LUT	C35-C15-C14	-2.01	119.35	123.47
37	q	321	XAT	C19-C9-C10	-2.01	120.11	122.92
31	8	613	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	s	313	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	y	612	CLA	CMD-C2D-C3D	-2.01	122.99	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	612	CLA	C3B-C4B-NB	-2.01	108.65	110.52
31	Y	311	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	N	303	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
31	S	303	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	8	610	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	q	314	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
31	0	604	CLA	C1D-ND-C4D	-2.01	104.91	106.33
31	7	304	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
30	S	309	CHL	C4A-NA-C1A	2.01	107.61	106.71
31	c	603	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
33	A	415	LHG	O7-C7-O9	-2.01	118.85	123.70
34	G	622	LMG	O7-C10-O9	-2.01	118.85	123.70
31	d	405	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
31	c	608	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	g	314	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
34	D	411	LMG	O8-C28-O10	-2.01	118.53	123.59
31	2	613	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	B	610	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	C	602	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	N	303	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
47	E	101	HEM	C4A-NA-C1A	2.01	107.31	105.35
32	n	317	LUT	C19-C9-C8	2.01	121.24	118.08
31	8	610	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
31	r	306	CLA	C3B-C4B-NB	-2.01	108.65	110.52
31	s	310	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	S	314	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
31	n	311	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
32	6	317	LUT	C19-C9-C8	2.01	121.24	118.08
38	x	201	SQD	O8-S-C6	-2.01	102.54	105.74
34	b	624	LMG	O6-C1-C2	-2.01	106.10	110.35
31	4	613	CLA	CHA-C1A-NA	-2.00	121.81	126.40
31	r	314	CLA	C1D-ND-C4D	-2.00	104.91	106.33
30	q	303	CHL	CMA-C3A-C2A	2.00	121.91	113.83
31	G	602	CLA	C1-O2A-CGA	2.00	121.70	116.44
31	n	312	CLA	CMD-C2D-C3D	-2.00	123.00	127.61
34	B	622	LMG	O7-C10-O9	-2.00	118.86	123.70
31	2	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	N	312	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
33	s	322	LHG	O7-C7-O9	-2.00	118.86	123.70
43	b	619	BCR	C35-C13-C14	-2.00	120.12	122.92
31	N	312	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
36	2	616	NEX	C20-C13-C14	-2.00	120.12	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	313	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
31	y	602	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
38	s	301	SQD	O8-S-C6	-2.00	102.55	105.74
31	S	303	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
31	c	606	CLA	CHA-C1A-NA	-2.00	121.81	126.40
31	y	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
31	C	613	CLA	C1D-ND-C4D	-2.00	104.91	106.33
33	D	408	LHG	O8-C23-O10	-2.00	118.54	123.59
31	1	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	2	603	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	9	316	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	C	601	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
31	C	609	CLA	CMA-C3A-C4A	2.00	117.15	111.77
31	Y	313	CLA	CHA-C1A-NA	-2.00	121.82	126.40
31	C	611	CLA	C3B-C4B-NB	-2.00	108.66	110.52
31	b	610	CLA	C3B-C4B-NB	-2.00	108.66	110.52
34	b	626	LMG	O8-C28-O10	-2.00	118.54	123.59
38	0	621	SQD	O8-S-C6	-2.00	102.55	105.74
32	s	317	LUT	C39-C29-C28	2.00	121.23	118.08
31	g	313	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	G	610	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
34	D	410	LMG	O8-C28-O10	-2.00	118.54	123.59

There are no chirality outliers.

All (7923) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	1	601	CHL	CHA-CBD-CGD-O1D
30	1	601	CHL	CHA-CBD-CGD-O2D
30	1	606	CHL	CAD-CBD-CGD-O1D
30	1	606	CHL	CAD-CBD-CGD-O2D
30	1	607	CHL	C1A-C2A-CAA-CBA
30	1	607	CHL	C3A-C2A-CAA-CBA
30	1	609	CHL	C11-C12-C13-C14
30	2	601	CHL	C1A-C2A-CAA-CBA
30	2	601	CHL	C3A-C2A-CAA-CBA
30	2	605	CHL	CHA-CBD-CGD-O1D
30	2	605	CHL	CHA-CBD-CGD-O2D
30	3	302	CHL	C2-C1-O2A-CGA
30	3	302	CHL	CHA-CBD-CGD-O1D
30	3	302	CHL	CAD-CBD-CGD-O1D
30	3	302	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	3	307	CHL	CAD-CBD-CGD-O1D
30	3	307	CHL	CAD-CBD-CGD-O2D
30	3	308	CHL	CHA-CBD-CGD-O1D
30	3	308	CHL	CHA-CBD-CGD-O2D
30	3	309	CHL	CHA-CBD-CGD-O1D
30	3	309	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	C1A-C2A-CAA-CBA
30	4	601	CHL	C3A-C2A-CAA-CBA
30	4	605	CHL	CHA-CBD-CGD-O1D
30	4	605	CHL	CHA-CBD-CGD-O2D
30	4	607	CHL	C1A-C2A-CAA-CBA
30	4	607	CHL	C2-C1-O2A-CGA
30	5	607	CHL	CAD-CBD-CGD-O2D
30	5	609	CHL	CHA-CBD-CGD-O1D
30	5	609	CHL	CHA-CBD-CGD-O2D
30	6	302	CHL	C1A-C2A-CAA-CBA
30	6	302	CHL	C3A-C2A-CAA-CBA
30	6	306	CHL	CHA-CBD-CGD-O1D
30	6	306	CHL	CHA-CBD-CGD-O2D
30	6	307	CHL	C1A-C2A-CAA-CBA
30	G	601	CHL	C1A-C2A-CAA-CBA
30	G	601	CHL	CHA-CBD-CGD-O1D
30	G	601	CHL	CHA-CBD-CGD-O2D
30	G	601	CHL	C11-C12-C13-C14
30	G	605	CHL	C1A-C2A-CAA-CBA
30	G	606	CHL	CHA-CBD-CGD-O1D
30	G	606	CHL	CHA-CBD-CGD-O2D
30	G	608	CHL	C11-C12-C13-C14
30	N	306	CHL	CHA-CBD-CGD-O1D
30	N	306	CHL	CHA-CBD-CGD-O2D
30	R	310	CHL	C2A-CAA-CBA-CGA
30	Y	302	CHL	C3A-C2A-CAA-CBA
30	0	605	CHL	C2-C1-O2A-CGA
30	0	605	CHL	CAD-CBD-CGD-O2D
30	0	605	CHL	C4-C3-C5-C6
30	0	606	CHL	C1A-C2A-CAA-CBA
30	7	302	CHL	C3A-C2A-CAA-CBA
30	7	306	CHL	CAD-CBD-CGD-O1D
30	7	306	CHL	CAD-CBD-CGD-O2D
30	7	307	CHL	CBD-CGD-O2D-CED
30	7	308	CHL	C1A-C2A-CAA-CBA
30	8	608	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	8	608	CHL	C3A-C2A-CAA-CBA
30	9	307	CHL	CHA-CBD-CGD-O1D
30	9	307	CHL	CHA-CBD-CGD-O2D
30	9	308	CHL	C2-C3-C5-C6
30	9	308	CHL	C4-C3-C5-C6
30	9	309	CHL	CBD-CGD-O2D-CED
30	9	310	CHL	C1A-C2A-CAA-CBA
30	9	310	CHL	C3A-C2A-CAA-CBA
30	9	311	CHL	CHA-CBD-CGD-O1D
30	9	311	CHL	CHA-CBD-CGD-O2D
30	p	601	CHL	C1A-C2A-CAA-CBA
30	p	601	CHL	C3A-C2A-CAA-CBA
30	p	605	CHL	CHA-CBD-CGD-O1D
30	p	605	CHL	CHA-CBD-CGD-O2D
30	p	607	CHL	CAD-CBD-CGD-O1D
30	p	607	CHL	CAD-CBD-CGD-O2D
30	q	303	CHL	C1A-C2A-CAA-CBA
30	q	303	CHL	C3A-C2A-CAA-CBA
30	q	307	CHL	CHA-CBD-CGD-O1D
30	q	307	CHL	CHA-CBD-CGD-O2D
30	q	309	CHL	C1A-C2A-CAA-CBA
30	q	309	CHL	C2-C1-O2A-CGA
30	q	309	CHL	CAD-CBD-CGD-O1D
30	q	309	CHL	CAD-CBD-CGD-O2D
30	q	311	CHL	C1A-C2A-CAA-CBA
30	g	302	CHL	C1A-C2A-CAA-CBA
30	g	302	CHL	CHA-CBD-CGD-O1D
30	g	302	CHL	CHA-CBD-CGD-O2D
30	g	302	CHL	C11-C12-C13-C14
30	g	306	CHL	C1A-C2A-CAA-CBA
30	g	307	CHL	CHA-CBD-CGD-O1D
30	g	307	CHL	CHA-CBD-CGD-O2D
30	g	309	CHL	C11-C12-C13-C14
30	n	310	CHL	C1A-C2A-CAA-CBA
30	y	601	CHL	C3A-C2A-CAA-CBA
31	1	603	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	CHA-CBD-CGD-O1D
31	1	604	CLA	CHA-CBD-CGD-O2D
31	1	610	CLA	CBD-CGD-O2D-CED
31	1	610	CLA	C11-C10-C8-C9
31	1	611	CLA	C2-C1-O2A-CGA
31	1	612	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	1	613	CLA	CBD-CGD-O2D-CED
31	1	614	CLA	C1A-C2A-CAA-CBA
31	1	614	CLA	C2-C1-O2A-CGA
31	1	614	CLA	CBD-CGD-O2D-CED
31	2	602	CLA	CBD-CGD-O2D-CED
31	2	609	CLA	C2-C1-O2A-CGA
31	2	609	CLA	CHA-CBD-CGD-O1D
31	2	609	CLA	CHA-CBD-CGD-O2D
31	2	609	CLA	CBD-CGD-O2D-CED
31	2	610	CLA	C1A-C2A-CAA-CBA
31	2	611	CLA	C2-C1-O2A-CGA
31	2	612	CLA	CHA-CBD-CGD-O1D
31	2	612	CLA	CHA-CBD-CGD-O2D
31	2	613	CLA	C1A-C2A-CAA-CBA
31	2	613	CLA	C3A-C2A-CAA-CBA
31	2	613	CLA	C2-C1-O2A-CGA
31	2	613	CLA	CBD-CGD-O2D-CED
31	3	305	CLA	C1A-C2A-CAA-CBA
31	3	305	CLA	CBD-CGD-O2D-CED
31	3	306	CLA	C3A-C2A-CAA-CBA
31	3	312	CLA	C1A-C2A-CAA-CBA
31	3	312	CLA	C3A-C2A-CAA-CBA
31	3	312	CLA	C2-C1-O2A-CGA
31	3	312	CLA	CHA-CBD-CGD-O1D
31	3	312	CLA	CHA-CBD-CGD-O2D
31	3	312	CLA	CBD-CGD-O2D-CED
31	3	313	CLA	C2-C1-O2A-CGA
31	3	316	CLA	C2-C1-O2A-CGA
31	3	316	CLA	CBD-CGD-O2D-CED
31	4	604	CLA	C3A-C2A-CAA-CBA
31	4	604	CLA	CAD-CBD-CGD-O1D
31	4	604	CLA	CAD-CBD-CGD-O2D
31	4	604	CLA	C2-C3-C5-C6
31	4	610	CLA	C2-C1-O2A-CGA
31	4	610	CLA	CHA-CBD-CGD-O1D
31	4	610	CLA	CHA-CBD-CGD-O2D
31	4	610	CLA	C2-C3-C5-C6
31	4	610	CLA	C4-C3-C5-C6
31	4	612	CLA	CHA-CBD-CGD-O2D
31	4	614	CLA	CBA-CGA-O2A-C1
31	4	614	CLA	O1A-CGA-O2A-C1
31	5	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	5	603	CLA	CBA-CGA-O2A-C1
31	5	603	CLA	O1A-CGA-O2A-C1
31	5	611	CLA	C3A-C2A-CAA-CBA
31	5	611	CLA	CHA-CBD-CGD-O1D
31	5	611	CLA	CHA-CBD-CGD-O2D
31	5	612	CLA	CBA-CGA-O2A-C1
31	5	612	CLA	O1A-CGA-O2A-C1
31	5	612	CLA	CHA-CBD-CGD-O1D
31	5	612	CLA	CHA-CBD-CGD-O2D
31	5	613	CLA	C2-C1-O2A-CGA
31	5	614	CLA	C1A-C2A-CAA-CBA
31	5	614	CLA	CBD-CGD-O2D-CED
31	5	615	CLA	C1A-C2A-CAA-CBA
31	5	615	CLA	C2B-C3B-CAB-CBB
31	5	615	CLA	C4B-C3B-CAB-CBB
31	5	615	CLA	CBD-CGD-O2D-CED
31	6	304	CLA	C1A-C2A-CAA-CBA
31	6	304	CLA	C2-C1-O2A-CGA
31	6	305	CLA	C1A-C2A-CAA-CBA
31	6	305	CLA	C3A-C2A-CAA-CBA
31	6	305	CLA	CHA-CBD-CGD-O1D
31	6	311	CLA	C1A-C2A-CAA-CBA
31	6	311	CLA	C3A-C2A-CAA-CBA
31	6	312	CLA	C2-C1-O2A-CGA
31	6	312	CLA	CHA-CBD-CGD-O1D
31	6	312	CLA	CHA-CBD-CGD-O2D
31	6	316	CLA	C1A-C2A-CAA-CBA
31	6	316	CLA	C3A-C2A-CAA-CBA
31	6	316	CLA	C2-C1-O2A-CGA
31	6	316	CLA	CBD-CGD-O2D-CED
31	A	406	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C3A-C2A-CAA-CBA
31	A	406	CLA	CHA-CBD-CGD-O1D
31	A	406	CLA	CHA-CBD-CGD-O2D
31	A	407	CLA	CHA-CBD-CGD-O1D
31	A	407	CLA	CHA-CBD-CGD-O2D
31	A	409	CLA	C2-C3-C5-C6
31	A	409	CLA	C4-C3-C5-C6
31	B	601	CLA	CHA-CBD-CGD-O1D
31	B	601	CLA	CHA-CBD-CGD-O2D
31	B	602	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	B	602	CLA	CHA-CBD-CGD-O1D
31	B	602	CLA	CHA-CBD-CGD-O2D
31	B	602	CLA	C2-C3-C5-C6
31	B	602	CLA	C4-C3-C5-C6
31	B	603	CLA	CBD-CGD-O2D-CED
31	B	603	CLA	C2-C3-C5-C6
31	B	603	CLA	C4-C3-C5-C6
31	B	604	CLA	C1A-C2A-CAA-CBA
31	B	604	CLA	C2-C3-C5-C6
31	B	604	CLA	C4-C3-C5-C6
31	B	605	CLA	CBD-CGD-O2D-CED
31	B	606	CLA	C2B-C3B-CAB-CBB
31	B	606	CLA	C4B-C3B-CAB-CBB
31	B	606	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	C1A-C2A-CAA-CBA
31	B	607	CLA	C3A-C2A-CAA-CBA
31	B	607	CLA	CHA-CBD-CGD-O1D
31	B	607	CLA	CHA-CBD-CGD-O2D
31	B	607	CLA	CAD-CBD-CGD-O1D
31	B	607	CLA	CAD-CBD-CGD-O2D
31	B	609	CLA	C1A-C2A-CAA-CBA
31	B	609	CLA	C3A-C2A-CAA-CBA
31	B	609	CLA	CBD-CGD-O2D-CED
31	B	609	CLA	C11-C10-C8-C9
31	B	610	CLA	C2-C1-O2A-CGA
31	B	610	CLA	C11-C12-C13-C14
31	B	612	CLA	C1A-C2A-CAA-CBA
31	B	612	CLA	C3A-C2A-CAA-CBA
31	B	612	CLA	C2-C1-O2A-CGA
31	B	613	CLA	CBD-CGD-O2D-CED
31	B	613	CLA	C4-C3-C5-C6
31	B	614	CLA	C2A-CAA-CBA-CGA
31	B	614	CLA	CBD-CGD-O2D-CED
31	B	614	CLA	C6-C7-C8-C9
31	C	601	CLA	CHA-CBD-CGD-O1D
31	C	601	CLA	CHA-CBD-CGD-O2D
31	C	601	CLA	CAD-CBD-CGD-O1D
31	C	601	CLA	CAD-CBD-CGD-O2D
31	C	602	CLA	CHA-CBD-CGD-O1D
31	C	602	CLA	CHA-CBD-CGD-O2D
31	C	602	CLA	CAD-CBD-CGD-O1D
31	C	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	C	604	CLA	CHA-CBD-CGD-O2D
31	C	605	CLA	CHA-CBD-CGD-O1D
31	C	605	CLA	CHA-CBD-CGD-O2D
31	C	606	CLA	C1A-C2A-CAA-CBA
31	C	606	CLA	C3A-C2A-CAA-CBA
31	C	606	CLA	CHA-CBD-CGD-O1D
31	C	606	CLA	CHA-CBD-CGD-O2D
31	C	606	CLA	CAD-CBD-CGD-O1D
31	C	607	CLA	C2B-C3B-CAB-CBB
31	C	607	CLA	C4B-C3B-CAB-CBB
31	C	607	CLA	CHA-CBD-CGD-O1D
31	C	607	CLA	CHA-CBD-CGD-O2D
31	C	608	CLA	CHA-CBD-CGD-O1D
31	C	608	CLA	CHA-CBD-CGD-O2D
31	C	609	CLA	C2-C1-O2A-CGA
31	C	610	CLA	C1A-C2A-CAA-CBA
31	C	612	CLA	CBA-CGA-O2A-C1
31	C	612	CLA	O1A-CGA-O2A-C1
31	C	613	CLA	C1A-C2A-CAA-CBA
31	D	403	CLA	C6-C7-C8-C9
31	D	404	CLA	C1A-C2A-CAA-CBA
31	D	404	CLA	C4-C3-C5-C6
31	G	603	CLA	C1A-C2A-CAA-CBA
31	G	603	CLA	CBA-CGA-O2A-C1
31	G	604	CLA	C1A-C2A-CAA-CBA
31	G	604	CLA	C3A-C2A-CAA-CBA
31	G	610	CLA	C1A-C2A-CAA-CBA
31	G	610	CLA	C3A-C2A-CAA-CBA
31	G	610	CLA	C2-C3-C5-C6
31	G	610	CLA	C4-C3-C5-C6
31	G	612	CLA	CBD-CGD-O2D-CED
31	G	613	CLA	C2-C1-O2A-CGA
31	N	305	CLA	C1A-C2A-CAA-CBA
31	N	305	CLA	CHA-CBD-CGD-O1D
31	N	305	CLA	CAD-CBD-CGD-O1D
31	N	305	CLA	C11-C10-C8-C9
31	N	310	CLA	C1A-C2A-CAA-CBA
31	N	310	CLA	C3A-C2A-CAA-CBA
31	N	311	CLA	C1A-C2A-CAA-CBA
31	N	311	CLA	C3A-C2A-CAA-CBA
31	N	313	CLA	C6-C7-C8-C9
31	N	314	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	N	314	CLA	C3A-C2A-CAA-CBA
31	N	321	CLA	C2-C1-O2A-CGA
31	N	321	CLA	CBD-CGD-O2D-CED
31	R	303	CLA	C3A-C2A-CAA-CBA
31	R	304	CLA	CHA-CBD-CGD-O1D
31	R	304	CLA	CHA-CBD-CGD-O2D
31	R	306	CLA	C1A-C2A-CAA-CBA
31	R	306	CLA	C3A-C2A-CAA-CBA
31	R	306	CLA	CHA-CBD-CGD-O2D
31	R	312	CLA	C1A-C2A-CAA-CBA
31	R	312	CLA	C3A-C2A-CAA-CBA
31	R	313	CLA	CBD-CGD-O2D-CED
31	R	314	CLA	C2-C1-O2A-CGA
31	R	314	CLA	CBD-CGD-O2D-CED
31	R	315	CLA	C2-C1-O2A-CGA
31	R	316	CLA	C1A-C2A-CAA-CBA
31	R	316	CLA	C3A-C2A-CAA-CBA
31	R	316	CLA	CHA-CBD-CGD-O1D
31	S	303	CLA	C1A-C2A-CAA-CBA
31	S	303	CLA	C3A-C2A-CAA-CBA
31	S	304	CLA	C1A-C2A-CAA-CBA
31	S	304	CLA	C3A-C2A-CAA-CBA
31	S	306	CLA	C2-C1-O2A-CGA
31	S	310	CLA	C1A-C2A-CAA-CBA
31	S	310	CLA	C3A-C2A-CAA-CBA
31	S	310	CLA	CBD-CGD-O2D-CED
31	S	310	CLA	C2-C3-C5-C6
31	S	310	CLA	C4-C3-C5-C6
31	S	312	CLA	C1A-C2A-CAA-CBA
31	S	312	CLA	C3A-C2A-CAA-CBA
31	S	312	CLA	C2A-CAA-CBA-CGA
31	S	312	CLA	C2-C1-O2A-CGA
31	S	312	CLA	CHA-CBD-CGD-O1D
31	S	312	CLA	CHA-CBD-CGD-O2D
31	S	313	CLA	CHA-CBD-CGD-O1D
31	S	314	CLA	CHA-CBD-CGD-O1D
31	S	314	CLA	CHA-CBD-CGD-O2D
31	S	314	CLA	CBD-CGD-O2D-CED
31	S	314	CLA	C11-C10-C8-C9
31	S	315	CLA	C3A-C2A-CAA-CBA
31	S	316	CLA	CBA-CGA-O2A-C1
31	S	316	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	Y	305	CLA	CHA-CBD-CGD-O1D
31	Y	305	CLA	CHA-CBD-CGD-O2D
31	Y	305	CLA	CAD-CBD-CGD-O1D
31	Y	305	CLA	CAD-CBD-CGD-O2D
31	Y	311	CLA	C1A-C2A-CAA-CBA
31	Y	311	CLA	C3A-C2A-CAA-CBA
31	Y	313	CLA	CBD-CGD-O2D-CED
31	0	602	CLA	C2-C3-C5-C6
31	0	602	CLA	C4-C3-C5-C6
31	0	603	CLA	C1A-C2A-CAA-CBA
31	0	603	CLA	C3A-C2A-CAA-CBA
31	0	603	CLA	C2-C1-O2A-CGA
31	0	603	CLA	CHA-CBD-CGD-O2D
31	0	604	CLA	C1A-C2A-CAA-CBA
31	0	604	CLA	C3A-C2A-CAA-CBA
31	0	604	CLA	CHA-CBD-CGD-O1D
31	0	604	CLA	CHA-CBD-CGD-O2D
31	0	604	CLA	CAD-CBD-CGD-O1D
31	0	610	CLA	C1A-C2A-CAA-CBA
31	0	610	CLA	C3A-C2A-CAA-CBA
31	0	610	CLA	C2-C3-C5-C6
31	0	610	CLA	C4-C3-C5-C6
31	0	610	CLA	C11-C10-C8-C9
31	0	611	CLA	C2-C1-O2A-CGA
31	0	611	CLA	CHA-CBD-CGD-O1D
31	0	611	CLA	CHA-CBD-CGD-O2D
31	0	612	CLA	CBA-CGA-O2A-C1
31	0	612	CLA	O1A-CGA-O2A-C1
31	0	613	CLA	CBD-CGD-O2D-CED
31	0	614	CLA	C1A-C2A-CAA-CBA
31	0	614	CLA	C3A-C2A-CAA-CBA
31	0	614	CLA	CBD-CGD-O2D-CED
31	0	614	CLA	O1D-CGD-O2D-CED
31	0	615	CLA	C1A-C2A-CAA-CBA
31	0	615	CLA	C3A-C2A-CAA-CBA
31	7	305	CLA	CHA-CBD-CGD-O1D
31	7	305	CLA	CHA-CBD-CGD-O2D
31	7	312	CLA	C1A-C2A-CAA-CBA
31	7	312	CLA	C3A-C2A-CAA-CBA
31	7	314	CLA	CBD-CGD-O2D-CED
31	7	315	CLA	C1A-C2A-CAA-CBA
31	7	315	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	7	315	CLA	CHA-CBD-CGD-O1D
31	7	315	CLA	CHA-CBD-CGD-O2D
31	7	315	CLA	CBD-CGD-O2D-CED
31	7	316	CLA	C1A-C2A-CAA-CBA
31	7	316	CLA	C2-C1-O2A-CGA
31	8	603	CLA	CBA-CGA-O2A-C1
31	8	603	CLA	O1A-CGA-O2A-C1
31	8	604	CLA	C1A-C2A-CAA-CBA
31	8	609	CLA	C1A-C2A-CAA-CBA
31	8	609	CLA	C3A-C2A-CAA-CBA
31	8	609	CLA	C6-C7-C8-C9
31	8	610	CLA	C1A-C2A-CAA-CBA
31	8	610	CLA	C3A-C2A-CAA-CBA
31	8	612	CLA	C2-C1-O2A-CGA
31	8	612	CLA	CBD-CGD-O2D-CED
31	8	612	CLA	C6-C7-C8-C9
31	8	613	CLA	C1A-C2A-CAA-CBA
31	8	613	CLA	C3A-C2A-CAA-CBA
31	8	613	CLA	C2-C1-O2A-CGA
31	8	614	CLA	CBD-CGD-O2D-CED
31	9	304	CLA	C1A-C2A-CAA-CBA
31	9	304	CLA	C2-C1-O2A-CGA
31	9	306	CLA	C1A-C2A-CAA-CBA
31	9	306	CLA	C3A-C2A-CAA-CBA
31	9	306	CLA	CHA-CBD-CGD-O1D
31	9	306	CLA	CHA-CBD-CGD-O2D
31	9	312	CLA	C1A-C2A-CAA-CBA
31	9	312	CLA	CHA-CBD-CGD-O1D
31	9	312	CLA	CHA-CBD-CGD-O2D
31	9	313	CLA	CHA-CBD-CGD-O1D
31	9	313	CLA	CHA-CBD-CGD-O2D
31	9	314	CLA	C2-C1-O2A-CGA
31	9	314	CLA	CBD-CGD-O2D-CED
31	9	315	CLA	CBD-CGD-O2D-CED
31	p	610	CLA	C2A-CAA-CBA-CGA
31	p	610	CLA	CHA-CBD-CGD-O1D
31	p	610	CLA	CHA-CBD-CGD-O2D
31	p	610	CLA	CBD-CGD-O2D-CED
31	p	611	CLA	C1A-C2A-CAA-CBA
31	p	611	CLA	C3A-C2A-CAA-CBA
31	p	611	CLA	CHA-CBD-CGD-O1D
31	p	611	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	p	611	CLA	C11-C10-C8-C7
31	p	612	CLA	CHA-CBD-CGD-O2D
31	p	613	CLA	CBD-CGD-O2D-CED
31	p	614	CLA	CBD-CGD-O2D-CED
31	p	614	CLA	O1D-CGD-O2D-CED
31	q	305	CLA	CHA-CBD-CGD-O1D
31	q	305	CLA	CHA-CBD-CGD-O2D
31	q	312	CLA	C2A-CAA-CBA-CGA
31	q	312	CLA	O1A-CGA-O2A-C1
31	q	312	CLA	CBD-CGD-O2D-CED
31	q	313	CLA	CHA-CBD-CGD-O1D
31	q	313	CLA	CHA-CBD-CGD-O2D
31	q	314	CLA	CAD-CBD-CGD-O1D
31	q	314	CLA	CAD-CBD-CGD-O2D
31	q	316	CLA	C1A-C2A-CAA-CBA
31	q	316	CLA	C3A-C2A-CAA-CBA
31	q	316	CLA	CBD-CGD-O2D-CED
31	a	407	CLA	C1A-C2A-CAA-CBA
31	a	407	CLA	CHA-CBD-CGD-O1D
31	a	407	CLA	CHA-CBD-CGD-O2D
31	a	409	CLA	C2-C3-C5-C6
31	a	409	CLA	C4-C3-C5-C6
31	b	602	CLA	C1A-C2A-CAA-CBA
31	b	602	CLA	C3A-C2A-CAA-CBA
31	b	603	CLA	C1A-C2A-CAA-CBA
31	b	603	CLA	CBA-CGA-O2A-C1
31	b	603	CLA	O1A-CGA-O2A-C1
31	b	603	CLA	C4-C3-C5-C6
31	b	604	CLA	CBD-CGD-O2D-CED
31	b	605	CLA	C1A-C2A-CAA-CBA
31	b	605	CLA	CHA-CBD-CGD-O1D
31	b	605	CLA	CHA-CBD-CGD-O2D
31	b	605	CLA	CAD-CBD-CGD-O1D
31	b	605	CLA	CAD-CBD-CGD-O2D
31	b	606	CLA	CBD-CGD-O2D-CED
31	b	606	CLA	C4-C3-C5-C6
31	b	607	CLA	CHA-CBD-CGD-O1D
31	b	607	CLA	CHA-CBD-CGD-O2D
31	b	607	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	C1A-C2A-CAA-CBA
31	b	608	CLA	C3A-C2A-CAA-CBA
31	b	608	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	b	608	CLA	CHA-CBD-CGD-O2D
31	b	608	CLA	CAD-CBD-CGD-O1D
31	b	608	CLA	CAD-CBD-CGD-O2D
31	b	609	CLA	C1A-C2A-CAA-CBA
31	b	609	CLA	C2-C3-C5-C6
31	b	609	CLA	C4-C3-C5-C6
31	b	610	CLA	C1A-C2A-CAA-CBA
31	b	610	CLA	C3A-C2A-CAA-CBA
31	b	610	CLA	CHA-CBD-CGD-O1D
31	b	610	CLA	CHA-CBD-CGD-O2D
31	b	610	CLA	CAD-CBD-CGD-O1D
31	b	610	CLA	CBD-CGD-O2D-CED
31	b	610	CLA	C11-C10-C8-C9
31	b	613	CLA	C1A-C2A-CAA-CBA
31	b	613	CLA	C3A-C2A-CAA-CBA
31	b	614	CLA	CBD-CGD-O2D-CED
31	b	614	CLA	C2-C3-C5-C6
31	b	614	CLA	C4-C3-C5-C6
31	b	615	CLA	C6-C7-C8-C9
31	b	616	CLA	CHA-CBD-CGD-O1D
31	b	616	CLA	CHA-CBD-CGD-O2D
31	b	617	CLA	CBA-CGA-O2A-C1
31	b	617	CLA	O1A-CGA-O2A-C1
31	c	601	CLA	CAD-CBD-CGD-O1D
31	c	601	CLA	CAD-CBD-CGD-O2D
31	c	602	CLA	CHA-CBD-CGD-O1D
31	c	602	CLA	CHA-CBD-CGD-O2D
31	c	602	CLA	CAD-CBD-CGD-O1D
31	c	602	CLA	CAD-CBD-CGD-O2D
31	c	603	CLA	CBD-CGD-O2D-CED
31	c	604	CLA	CHA-CBD-CGD-O1D
31	c	604	CLA	CHA-CBD-CGD-O2D
31	c	605	CLA	CHA-CBD-CGD-O1D
31	c	605	CLA	CHA-CBD-CGD-O2D
31	c	605	CLA	CAD-CBD-CGD-O1D
31	c	605	CLA	CAD-CBD-CGD-O2D
31	c	606	CLA	C1A-C2A-CAA-CBA
31	c	606	CLA	C3A-C2A-CAA-CBA
31	c	606	CLA	CHA-CBD-CGD-O1D
31	c	606	CLA	CHA-CBD-CGD-O2D
31	c	606	CLA	CAD-CBD-CGD-O1D
31	c	608	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	c	608	CLA	CHA-CBD-CGD-O2D
31	c	609	CLA	C2-C1-O2A-CGA
31	c	609	CLA	C6-C7-C8-C9
31	c	610	CLA	CBA-CGA-O2A-C1
31	c	610	CLA	O1A-CGA-O2A-C1
31	c	612	CLA	CBA-CGA-O2A-C1
31	c	612	CLA	O1A-CGA-O2A-C1
31	c	613	CLA	C1A-C2A-CAA-CBA
31	d	401	CLA	CHA-CBD-CGD-O1D
31	d	401	CLA	CHA-CBD-CGD-O2D
31	d	404	CLA	C2-C3-C5-C6
31	d	404	CLA	C4-C3-C5-C6
31	d	405	CLA	C1A-C2A-CAA-CBA
31	d	405	CLA	C3A-C2A-CAA-CBA
31	d	405	CLA	CBD-CGD-O2D-CED
31	g	303	CLA	C2-C1-O2A-CGA
31	g	304	CLA	C1A-C2A-CAA-CBA
31	g	304	CLA	C3A-C2A-CAA-CBA
31	g	305	CLA	C1A-C2A-CAA-CBA
31	g	305	CLA	C3A-C2A-CAA-CBA
31	g	311	CLA	C1A-C2A-CAA-CBA
31	g	311	CLA	C3A-C2A-CAA-CBA
31	g	311	CLA	C6-C7-C8-C10
31	g	313	CLA	CHA-CBD-CGD-O1D
31	g	313	CLA	CHA-CBD-CGD-O2D
31	g	314	CLA	CBD-CGD-O2D-CED
31	n	304	CLA	CBA-CGA-O2A-C1
31	n	304	CLA	O1A-CGA-O2A-C1
31	n	305	CLA	C1A-C2A-CAA-CBA
31	n	311	CLA	C1A-C2A-CAA-CBA
31	n	311	CLA	C3A-C2A-CAA-CBA
31	n	312	CLA	C1A-C2A-CAA-CBA
31	n	312	CLA	C3A-C2A-CAA-CBA
31	n	314	CLA	C2-C1-O2A-CGA
31	n	314	CLA	CBD-CGD-O2D-CED
31	n	314	CLA	C6-C7-C8-C9
31	n	315	CLA	C1A-C2A-CAA-CBA
31	n	315	CLA	C3A-C2A-CAA-CBA
31	n	315	CLA	C2-C1-O2A-CGA
31	r	303	CLA	C1A-C2A-CAA-CBA
31	r	303	CLA	C3A-C2A-CAA-CBA
31	r	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	r	303	CLA	CHA-CBD-CGD-O2D
31	r	306	CLA	C1A-C2A-CAA-CBA
31	r	306	CLA	C3A-C2A-CAA-CBA
31	r	311	CLA	CBD-CGD-O2D-CED
31	r	312	CLA	C1A-C2A-CAA-CBA
31	r	312	CLA	C3A-C2A-CAA-CBA
31	r	313	CLA	CBD-CGD-O2D-CED
31	r	314	CLA	C2-C1-O2A-CGA
31	r	314	CLA	CHA-CBD-CGD-O1D
31	r	315	CLA	C1A-C2A-CAA-CBA
31	r	315	CLA	C3A-C2A-CAA-CBA
31	r	315	CLA	C2-C1-O2A-CGA
31	r	316	CLA	C1A-C2A-CAA-CBA
31	r	316	CLA	C3A-C2A-CAA-CBA
31	r	316	CLA	CHA-CBD-CGD-O1D
31	r	316	CLA	CHA-CBD-CGD-O2D
31	s	303	CLA	C3A-C2A-CAA-CBA
31	s	303	CLA	CBA-CGA-O2A-C1
31	s	303	CLA	O1A-CGA-O2A-C1
31	s	304	CLA	C1A-C2A-CAA-CBA
31	s	306	CLA	CHA-CBD-CGD-O2D
31	s	310	CLA	C1A-C2A-CAA-CBA
31	s	310	CLA	C3A-C2A-CAA-CBA
31	s	312	CLA	C1A-C2A-CAA-CBA
31	s	312	CLA	C3A-C2A-CAA-CBA
31	s	312	CLA	CHA-CBD-CGD-O1D
31	s	312	CLA	CHA-CBD-CGD-O2D
31	s	313	CLA	CHA-CBD-CGD-O1D
31	s	313	CLA	CHA-CBD-CGD-O2D
31	s	314	CLA	CBD-CGD-O2D-CED
31	s	315	CLA	C3A-C2A-CAA-CBA
31	s	316	CLA	C1A-C2A-CAA-CBA
31	s	316	CLA	CBA-CGA-O2A-C1
31	s	316	CLA	CBD-CGD-O2D-CED
31	y	604	CLA	CHA-CBD-CGD-O1D
31	y	604	CLA	CHA-CBD-CGD-O2D
31	y	604	CLA	CAD-CBD-CGD-O1D
31	y	612	CLA	C6-C7-C8-C9
31	y	614	CLA	CBA-CGA-O2A-C1
31	y	614	CLA	O1A-CGA-O2A-C1
31	y	615	CLA	C1A-C2A-CAA-CBA
31	y	615	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	y	615	CLA	CHA-CBD-CGD-O1D
31	y	615	CLA	CHA-CBD-CGD-O2D
32	1	616	LUT	C7-C8-C9-C10
32	1	616	LUT	C7-C8-C9-C19
32	3	317	LUT	C11-C12-C13-C14
32	3	317	LUT	C11-C12-C13-C20
32	3	318	LUT	C11-C12-C13-C14
32	3	318	LUT	C11-C12-C13-C20
32	4	616	LUT	C7-C8-C9-C10
32	4	616	LUT	C7-C8-C9-C19
32	4	616	LUT	C31-C32-C33-C34
32	4	616	LUT	C31-C32-C33-C40
32	5	616	LUT	C11-C12-C13-C14
32	5	616	LUT	C11-C12-C13-C20
32	5	616	LUT	C31-C32-C33-C34
32	5	616	LUT	C31-C32-C33-C40
32	5	617	LUT	C7-C8-C9-C10
32	5	617	LUT	C7-C8-C9-C19
32	5	617	LUT	C31-C32-C33-C34
32	5	617	LUT	C31-C32-C33-C40
32	6	317	LUT	C11-C12-C13-C14
32	6	317	LUT	C11-C12-C13-C20
32	6	317	LUT	C31-C32-C33-C34
32	6	317	LUT	C31-C32-C33-C40
32	6	318	LUT	C7-C8-C9-C10
32	6	318	LUT	C7-C8-C9-C19
32	6	318	LUT	C31-C32-C33-C34
32	6	318	LUT	C31-C32-C33-C40
32	G	615	LUT	C21-C26-C27-C28
32	G	615	LUT	C25-C26-C27-C28
32	G	615	LUT	C31-C32-C33-C40
32	G	615	LUT	C33-C34-C35-C15
32	N	316	LUT	C11-C12-C13-C14
32	N	316	LUT	C11-C12-C13-C20
32	N	317	LUT	C31-C32-C33-C34
32	N	317	LUT	C31-C32-C33-C40
32	R	317	LUT	C11-C12-C13-C14
32	R	317	LUT	C11-C12-C13-C20
32	S	317	LUT	C7-C8-C9-C10
32	S	317	LUT	C7-C8-C9-C19
32	S	317	LUT	C11-C12-C13-C14
32	S	317	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
32	S	317	LUT	C31-C32-C33-C34
32	S	317	LUT	C31-C32-C33-C40
32	S	318	LUT	C11-C12-C13-C14
32	S	318	LUT	C11-C12-C13-C20
32	S	318	LUT	C21-C26-C27-C28
32	S	318	LUT	C27-C28-C29-C30
32	S	318	LUT	C27-C28-C29-C39
32	S	318	LUT	C31-C32-C33-C34
32	S	318	LUT	C31-C32-C33-C40
32	0	616	LUT	C11-C12-C13-C14
32	0	616	LUT	C11-C12-C13-C20
32	7	317	LUT	C11-C12-C13-C14
32	7	317	LUT	C11-C12-C13-C20
32	7	318	LUT	C7-C8-C9-C10
32	7	318	LUT	C7-C8-C9-C19
32	8	615	LUT	C7-C8-C9-C10
32	8	615	LUT	C7-C8-C9-C19
32	8	615	LUT	C11-C12-C13-C14
32	8	615	LUT	C11-C12-C13-C20
32	8	615	LUT	C31-C32-C33-C34
32	8	615	LUT	C31-C32-C33-C40
32	8	616	LUT	C31-C32-C33-C34
32	8	616	LUT	C31-C32-C33-C40
32	p	617	LUT	C7-C8-C9-C10
32	q	318	LUT	C11-C12-C13-C14
32	q	318	LUT	C11-C12-C13-C20
32	q	318	LUT	C31-C32-C33-C34
32	q	318	LUT	C31-C32-C33-C40
32	g	316	LUT	C11-C12-C13-C20
32	g	316	LUT	C21-C26-C27-C28
32	g	316	LUT	C25-C26-C27-C28
32	g	316	LUT	C31-C32-C33-C34
32	g	316	LUT	C31-C32-C33-C40
32	n	317	LUT	C7-C8-C9-C10
32	n	317	LUT	C7-C8-C9-C19
32	n	317	LUT	C11-C12-C13-C14
32	n	317	LUT	C11-C12-C13-C20
32	n	317	LUT	C31-C32-C33-C34
32	n	317	LUT	C31-C32-C33-C40
32	n	318	LUT	C31-C32-C33-C34
32	n	318	LUT	C31-C32-C33-C40
32	r	317	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	r	317	LUT	C11-C12-C13-C20
32	s	317	LUT	C7-C8-C9-C10
32	s	317	LUT	C7-C8-C9-C19
32	s	317	LUT	C11-C12-C13-C14
32	s	317	LUT	C11-C12-C13-C20
32	s	317	LUT	C31-C32-C33-C34
32	s	317	LUT	C31-C32-C33-C40
32	s	318	LUT	C11-C12-C13-C14
32	s	318	LUT	C11-C12-C13-C20
32	y	617	LUT	C7-C8-C9-C10
32	y	617	LUT	C7-C8-C9-C19
33	1	617	LHG	O1-C1-C2-C3
33	1	617	LHG	C1-C2-C3-O3
33	1	617	LHG	C3-O3-P-O4
33	1	617	LHG	C4-O6-P-O4
33	2	617	LHG	C3-O3-P-O4
33	2	617	LHG	C4-O6-P-O3
33	2	617	LHG	C4-O6-P-O4
33	2	617	LHG	C4-O6-P-O5
33	3	320	LHG	C4-O6-P-O3
33	3	320	LHG	C4-O6-P-O4
33	3	320	LHG	C4-O6-P-O5
33	3	320	LHG	O7-C5-C6-O8
33	4	618	LHG	C1-C2-C3-O3
33	4	618	LHG	C4-O6-P-O3
33	4	618	LHG	C4-O6-P-O4
33	4	618	LHG	C4-O6-P-O5
33	4	618	LHG	O9-C7-O7-C5
33	4	618	LHG	C8-C7-O7-C5
33	5	619	LHG	O1-C1-C2-O2
33	5	619	LHG	C3-O3-P-O5
33	5	619	LHG	C3-O3-P-O6
33	5	619	LHG	C4-O6-P-O5
33	5	619	LHG	O9-C7-O7-C5
33	6	320	LHG	C4-O6-P-O3
33	6	320	LHG	C4-O6-P-O4
33	6	320	LHG	C4-O6-P-O5
33	A	415	LHG	O1-C1-C2-C3
33	A	415	LHG	C4-O6-P-O4
33	A	415	LHG	O7-C5-C6-O8
33	A	417	LHG	C3-O3-P-O5
33	A	417	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
33	A	417	LHG	O6-C4-C5-O7
33	C	623	LHG	O1-C1-C2-C3
33	C	623	LHG	C1-C2-C3-O3
33	C	623	LHG	C4-O6-P-O5
33	C	623	LHG	C8-C7-O7-C5
33	D	407	LHG	O1-C1-C2-C3
33	D	407	LHG	C1-C2-C3-O3
33	D	407	LHG	C3-O3-P-O5
33	D	407	LHG	C3-O3-P-O6
33	D	407	LHG	C4-O6-P-O5
33	D	408	LHG	O1-C1-C2-C3
33	D	408	LHG	C1-C2-C3-O3
33	D	408	LHG	C4-O6-P-O3
33	D	408	LHG	C4-O6-P-O5
33	G	618	LHG	C4-O6-P-O4
33	G	618	LHG	C4-O6-P-O5
33	K	102	LHG	O1-C1-C2-O2
33	K	102	LHG	O1-C1-C2-C3
33	K	102	LHG	C1-C2-C3-O3
33	K	102	LHG	C3-O3-P-O4
33	K	102	LHG	C3-O3-P-O5
33	K	102	LHG	C3-O3-P-O6
33	K	102	LHG	C4-O6-P-O5
33	K	102	LHG	O9-C7-O7-C5
33	K	102	LHG	C8-C7-O7-C5
33	L	101	LHG	C4-O6-P-O5
33	M	101	LHG	C3-O3-P-O5
33	M	101	LHG	O7-C5-C6-O8
33	M	101	LHG	C8-C7-O7-C5
33	N	319	LHG	O1-C1-C2-O2
33	N	319	LHG	O1-C1-C2-C3
33	N	319	LHG	C3-O3-P-O5
33	N	319	LHG	C4-O6-P-O4
33	R	320	LHG	O1-C1-C2-C3
33	R	320	LHG	C4-O6-P-O4
33	S	320	LHG	O1-C1-C2-O2
33	S	320	LHG	O1-C1-C2-C3
33	S	320	LHG	C1-C2-C3-O3
33	S	320	LHG	C3-O3-P-O5
33	S	320	LHG	C4-O6-P-O3
33	S	320	LHG	C4-O6-P-O4
33	S	320	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
33	S	322	LHG	C1-C2-C3-O3
33	S	322	LHG	O2-C2-C3-O3
33	Y	318	LHG	C1-C2-C3-O3
33	Y	318	LHG	C3-O3-P-O4
33	0	619	LHG	O1-C1-C2-C3
33	0	619	LHG	C4-O6-P-O5
33	0	619	LHG	O7-C5-C6-O8
33	0	619	LHG	C8-C7-O7-C5
33	7	319	LHG	C1-C2-C3-O3
33	7	319	LHG	C4-O6-P-O4
33	8	618	LHG	O1-C1-C2-O2
33	8	618	LHG	C1-C2-C3-O3
33	8	618	LHG	O2-C2-C3-O3
33	8	618	LHG	C4-O6-P-O4
33	8	618	LHG	C4-C5-O7-C7
33	9	320	LHG	O1-C1-C2-C3
33	9	320	LHG	C1-C2-C3-O3
33	9	320	LHG	C4-O6-P-O5
33	p	619	LHG	O1-C1-C2-O2
33	p	619	LHG	C1-C2-C3-O3
33	p	619	LHG	C4-O6-P-O4
33	p	619	LHG	C8-C7-O7-C5
33	q	320	LHG	O1-C1-C2-C3
33	q	320	LHG	C1-C2-C3-O3
33	q	320	LHG	C3-O3-P-O4
33	q	320	LHG	C4-O6-P-O4
33	a	415	LHG	C1-C2-C3-O3
33	a	415	LHG	C3-O3-P-O6
33	a	415	LHG	C4-O6-P-O3
33	a	415	LHG	O6-C4-C5-O7
33	b	625	LHG	C4-O6-P-O5
33	b	628	LHG	C3-O3-P-O5
33	b	628	LHG	C4-O6-P-O4
33	c	622	LHG	O1-C1-C2-C3
33	c	622	LHG	C3-O3-P-O5
33	c	622	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C1-C2-C3-O3
33	d	408	LHG	C4-O6-P-O5
33	e	101	LHG	C4-O6-P-O4
33	g	319	LHG	O1-C1-C2-C3
33	g	319	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
33	j	102	LHG	C3-O3-P-O4
33	j	102	LHG	C3-O3-P-O5
33	j	102	LHG	C3-O3-P-O6
33	j	102	LHG	O7-C5-C6-O8
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
33	n	320	LHG	O1-C1-C2-O2
33	n	320	LHG	C1-C2-C3-O3
33	n	320	LHG	O2-C2-C3-O3
33	n	320	LHG	C4-O6-P-O4
33	r	320	LHG	O1-C1-C2-C3
33	r	320	LHG	C4-O6-P-O4
33	s	320	LHG	C1-C2-C3-O3
33	s	320	LHG	C4-O6-P-O3
33	s	320	LHG	C4-O6-P-O4
33	s	320	LHG	C4-O6-P-O5
33	s	320	LHG	O7-C5-C6-O8
33	s	322	LHG	C4-O6-P-O3
33	s	322	LHG	C8-C7-O7-C5
33	t	102	LHG	O1-C1-C2-C3
33	t	102	LHG	C1-C2-C3-O3
33	t	102	LHG	C4-O6-P-O3
33	y	619	LHG	C1-C2-C3-O3
33	y	619	LHG	C3-O3-P-O4
33	y	619	LHG	C3-O3-P-O5
33	y	619	LHG	C3-O3-P-O6
33	z	102	LHG	O1-C1-C2-C3
33	z	102	LHG	C1-C2-C3-O3
33	z	102	LHG	C4-O6-P-O3
33	z	102	LHG	C4-O6-P-O5
33	z	102	LHG	O6-C4-C5-O7
33	z	102	LHG	O9-C7-O7-C5
33	z	102	LHG	C8-C7-O7-C5
33	F1	301	LHG	O2-C2-C3-O3
33	F1	301	LHG	C3-O3-P-O5
33	F1	301	LHG	O7-C5-C6-O8
34	4	620	LMG	O6-C1-O1-C7
34	4	620	LMG	C11-C10-O7-C8
34	4	621	LMG	O6-C1-O1-C7
34	4	621	LMG	C11-C10-O7-C8
34	5	620	LMG	C11-C10-O7-C8
34	6	321	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	6	322	LMG	C2-C1-O1-C7
34	6	322	LMG	O6-C1-O1-C7
34	6	322	LMG	O9-C10-O7-C8
34	6	322	LMG	C11-C10-O7-C8
34	6	323	LMG	O10-C28-O8-C9
34	A	412	LMG	O6-C1-O1-C7
34	A	412	LMG	C9-C8-O7-C10
34	A	414	LMG	O9-C10-O7-C8
34	A	414	LMG	C11-C10-O7-C8
34	A	418	LMG	C11-C10-O7-C8
34	B	622	LMG	C11-C10-O7-C8
34	B	625	LMG	O10-C28-O8-C9
34	C	621	LMG	O9-C10-O7-C8
34	C	621	LMG	C11-C10-O7-C8
34	C	622	LMG	C11-C10-O7-C8
34	G	622	LMG	C2-C1-O1-C7
34	G	622	LMG	O6-C1-O1-C7
34	G	622	LMG	C11-C10-O7-C8
34	I	101	LMG	C11-C10-O7-C8
34	J	102	LMG	C11-C10-O7-C8
34	N	320	LMG	C8-C7-O1-C1
34	N	320	LMG	C11-C10-O7-C8
34	W	202	LMG	O6-C1-O1-C7
34	W	203	LMG	O1-C7-C8-O7
34	W	203	LMG	C11-C10-O7-C8
34	X	202	LMG	C11-C10-O7-C8
34	X	203	LMG	O7-C8-C9-O8
34	Y	319	LMG	O6-C1-O1-C7
34	0	620	LMG	C2-C1-O1-C7
34	0	620	LMG	O6-C1-O1-C7
34	0	620	LMG	C11-C10-O7-C8
34	0	622	LMG	C2-C1-O1-C7
34	0	622	LMG	O6-C1-O1-C7
34	7	301	LMG	C2-C1-O1-C7
34	7	301	LMG	O6-C1-O1-C7
34	7	301	LMG	C8-C7-O1-C1
34	7	301	LMG	C11-C10-O7-C8
34	7	322	LMG	C8-C7-O1-C1
34	7	322	LMG	C11-C10-O7-C8
34	9	301	LMG	O9-C10-O7-C8
34	9	301	LMG	C11-C10-O7-C8
34	9	302	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	9	321	LMG	O6-C1-O1-C7
34	9	321	LMG	C11-C10-O7-C8
34	p	620	LMG	C11-C10-O7-C8
34	q	301	LMG	C2-C1-O1-C7
34	q	301	LMG	C8-C7-O1-C1
34	q	302	LMG	O9-C10-O7-C8
34	a	401	LMG	O9-C10-O7-C8
34	a	401	LMG	C11-C10-O7-C8
34	a	413	LMG	C11-C10-O7-C8
34	b	601	LMG	O6-C1-O1-C7
34	b	601	LMG	C11-C10-O7-C8
34	b	622	LMG	O6-C1-O1-C7
34	b	623	LMG	C11-C10-O7-C8
34	b	624	LMG	O6-C1-O1-C7
34	b	624	LMG	C8-C9-O8-C28
34	b	624	LMG	C11-C10-O7-C8
34	b	624	LMG	O10-C28-O8-C9
34	b	629	LMG	C11-C10-O7-C8
34	c	620	LMG	O6-C1-O1-C7
34	c	621	LMG	C11-C10-O7-C8
34	c	624	LMG	C11-C10-O7-C8
34	f	101	LMG	C11-C10-O7-C8
34	g	322	LMG	O6-C1-O1-C7
34	j	101	LMG	O10-C28-O8-C9
34	k	101	LMG	C11-C10-O7-C8
34	k	102	LMG	C2-C1-O1-C7
34	k	102	LMG	O6-C1-O1-C7
34	k	102	LMG	C11-C10-O7-C8
34	m	102	LMG	O6-C1-O1-C7
34	m	102	LMG	C11-C10-O7-C8
34	n	321	LMG	O6-C1-O1-C7
34	n	322	LMG	O6-C1-O1-C7
34	w	201	LMG	O6-C1-O1-C7
34	w	201	LMG	O1-C7-C8-O7
34	w	203	LMG	C11-C10-O7-C8
34	w	204	LMG	C2-C1-O1-C7
34	w	204	LMG	O6-C1-O1-C7
34	w	204	LMG	O9-C10-O7-C8
34	w	204	LMG	C11-C10-O7-C8
34	w	205	LMG	C2-C1-O1-C7
34	w	205	LMG	O6-C1-O1-C7
34	w	205	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	x	202	LMG	O9-C10-O7-C8
34	x	202	LMG	C11-C10-O7-C8
34	y	620	LMG	C11-C10-O7-C8
34	Q1	101	LMG	O6-C1-O1-C7
34	Q1	101	LMG	O9-C10-O7-C8
34	Q1	101	LMG	C11-C10-O7-C8
34	q1	101	LMG	C8-C7-O1-C1
34	q1	101	LMG	C11-C10-O7-C8
35	2	614	RRX	C23-C24-C25-C30
35	2	614	RRX	C23-C24-C25-C26
35	2	614	RRX	C37-C22-C23-C24
35	2	614	RRX	C21-C22-C23-C24
35	2	614	RRX	C36-C18-C19-C20
35	2	614	RRX	C17-C18-C19-C20
35	2	614	RRX	C11-C12-C13-C14
35	2	614	RRX	C11-C12-C13-C35
35	2	614	RRX	C7-C8-C9-C10
35	2	614	RRX	C7-C8-C9-C34
35	4	615	RRX	C23-C24-C25-C30
35	4	615	RRX	C23-C24-C25-C26
35	4	615	RRX	C37-C22-C23-C24
35	4	615	RRX	C21-C22-C23-C24
35	4	615	RRX	C36-C18-C19-C20
35	4	615	RRX	C17-C18-C19-C20
35	4	615	RRX	C11-C12-C13-C14
35	4	615	RRX	C11-C12-C13-C35
35	4	615	RRX	C9-C10-C11-C12
35	4	615	RRX	C7-C8-C9-C10
35	4	615	RRX	C7-C8-C9-C34
35	4	615	RRX	C1-C6-C7-C8
35	G	614	RRX	C23-C24-C25-C30
35	G	614	RRX	C23-C24-C25-C26
35	G	614	RRX	C37-C22-C23-C24
35	G	614	RRX	C21-C22-C23-C24
35	G	614	RRX	C36-C18-C19-C20
35	G	614	RRX	C17-C18-C19-C20
35	G	614	RRX	C11-C12-C13-C14
35	G	614	RRX	C11-C12-C13-C35
35	G	614	RRX	C9-C10-C11-C12
35	G	614	RRX	C7-C8-C9-C10
35	G	614	RRX	C7-C8-C9-C34
35	G	614	RRX	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
35	9	317	RRX	C23-C24-C25-C30
35	9	317	RRX	C23-C24-C25-C26
35	9	317	RRX	C37-C22-C23-C24
35	9	317	RRX	C21-C22-C23-C24
35	9	317	RRX	C36-C18-C19-C20
35	9	317	RRX	C17-C18-C19-C20
35	9	317	RRX	C11-C12-C13-C14
35	9	317	RRX	C11-C12-C13-C35
35	9	317	RRX	C9-C10-C11-C12
35	9	317	RRX	C7-C8-C9-C10
35	9	317	RRX	C7-C8-C9-C34
35	9	317	RRX	C1-C6-C7-C8
35	q	317	RRX	C23-C24-C25-C30
35	q	317	RRX	C37-C22-C23-C24
35	q	317	RRX	C21-C22-C23-C24
35	q	317	RRX	C7-C8-C9-C10
35	q	317	RRX	C7-C8-C9-C34
35	g	315	RRX	C37-C22-C23-C24
35	g	315	RRX	C7-C8-C9-C10
36	2	616	NEX	C10-C11-C12-C13
36	2	616	NEX	C12-C13-C14-C15
36	2	616	NEX	C20-C13-C14-C15
36	2	616	NEX	C28-C29-C30-C31
36	2	616	NEX	C39-C29-C30-C31
36	2	616	NEX	C31-C32-C33-C34
36	2	616	NEX	C31-C32-C33-C40
36	3	319	NEX	C32-C33-C34-C35
36	3	319	NEX	C40-C33-C34-C35
36	4	617	NEX	C10-C11-C12-C13
36	4	617	NEX	C26-C27-C28-C29
36	4	617	NEX	C39-C29-C30-C31
36	5	618	NEX	C10-C11-C12-C13
36	5	618	NEX	C11-C12-C13-C14
36	5	618	NEX	C11-C12-C13-C20
36	5	618	NEX	C14-C15-C35-C34
36	5	618	NEX	C30-C31-C32-C33
36	6	319	NEX	C28-C29-C30-C31
36	6	319	NEX	C39-C29-C30-C31
36	6	319	NEX	C29-C30-C31-C32
36	6	319	NEX	C30-C31-C32-C33
36	N	318	NEX	C10-C11-C12-C13
36	N	318	NEX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	N	318	NEX	C11-C12-C13-C20
36	N	318	NEX	C32-C33-C34-C35
36	N	318	NEX	C40-C33-C34-C35
36	0	618	NEX	C28-C29-C30-C31
36	0	618	NEX	C39-C29-C30-C31
36	0	618	NEX	C29-C30-C31-C32
36	0	618	NEX	C30-C31-C32-C33
36	8	617	NEX	C11-C12-C13-C14
36	8	617	NEX	C11-C12-C13-C20
36	9	319	NEX	C9-C10-C11-C12
36	9	319	NEX	C10-C11-C12-C13
36	9	319	NEX	C14-C15-C35-C34
36	p	618	NEX	C11-C10-C9-C8
36	p	618	NEX	C11-C10-C9-C19
36	q	319	NEX	C10-C11-C12-C13
36	q	319	NEX	C11-C12-C13-C14
36	q	319	NEX	C11-C12-C13-C20
36	q	319	NEX	C14-C15-C35-C34
36	q	319	NEX	C32-C33-C34-C35
36	q	319	NEX	C40-C33-C34-C35
36	g	317	NEX	C10-C11-C12-C13
36	g	317	NEX	C11-C12-C13-C14
36	g	317	NEX	C11-C12-C13-C20
36	g	317	NEX	C12-C13-C14-C15
36	g	317	NEX	C20-C13-C14-C15
36	g	317	NEX	C28-C29-C30-C31
36	g	317	NEX	C39-C29-C30-C31
36	n	319	NEX	C11-C10-C9-C8
36	n	319	NEX	C11-C10-C9-C19
36	n	319	NEX	C10-C11-C12-C13
36	n	319	NEX	C11-C12-C13-C14
36	n	319	NEX	C11-C12-C13-C20
36	r	319	NEX	C7-C8-C9-C10
36	r	319	NEX	C28-C29-C30-C31
37	2	619	XAT	C21-C26-C27-C28
37	2	619	XAT	C25-C26-C27-C28
37	2	619	XAT	O24-C26-C27-C28
37	2	619	XAT	C26-C27-C28-C29
37	4	619	XAT	C21-C26-C27-C28
37	4	619	XAT	C25-C26-C27-C28
37	4	619	XAT	O24-C26-C27-C28
37	4	619	XAT	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
37	G	620	XAT	C21-C26-C27-C28
37	G	620	XAT	C25-C26-C27-C28
37	G	620	XAT	O24-C26-C27-C28
37	G	620	XAT	C26-C27-C28-C29
37	9	322	XAT	C21-C26-C27-C28
37	9	322	XAT	C25-C26-C27-C28
37	9	322	XAT	O24-C26-C27-C28
37	9	322	XAT	C26-C27-C28-C29
37	q	321	XAT	C21-C26-C27-C28
37	q	321	XAT	C25-C26-C27-C28
37	q	321	XAT	O24-C26-C27-C28
37	q	321	XAT	C26-C27-C28-C29
37	g	321	XAT	C21-C26-C27-C28
37	g	321	XAT	C25-C26-C27-C28
37	g	321	XAT	O24-C26-C27-C28
37	g	321	XAT	C26-C27-C28-C29
38	6	301	SQD	O5-C5-C6-S
38	A	411	SQD	O47-C45-C46-O48
38	A	413	SQD	C2-C1-O6-C44
38	A	413	SQD	O5-C1-O6-C44
38	A	413	SQD	O5-C5-C6-S
38	B	620	SQD	O5-C1-O6-C44
38	B	620	SQD	O49-C7-O47-C45
38	B	620	SQD	C8-C7-O47-C45
38	B	623	SQD	C2-C1-O6-C44
38	B	623	SQD	O5-C1-O6-C44
38	B	623	SQD	O5-C5-C6-S
38	G	617	SQD	C2-C1-O6-C44
38	G	617	SQD	C8-C7-O47-C45
38	G	617	SQD	O5-C5-C6-S
38	R	322	SQD	O5-C5-C6-S
38	S	301	SQD	O6-C44-C45-O47
38	Y	320	SQD	O5-C1-O6-C44
38	Y	320	SQD	C8-C7-O47-C45
38	0	621	SQD	C2-C1-O6-C44
38	0	621	SQD	O5-C1-O6-C44
38	0	621	SQD	C8-C7-O47-C45
38	0	621	SQD	O5-C5-C6-S
38	a	412	SQD	C2-C1-O6-C44
38	a	412	SQD	O5-C1-O6-C44
38	a	412	SQD	O5-C5-C6-S
38	b	621	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
38	b	621	SQD	O5-C5-C6-S
38	b	627	SQD	O5-C5-C6-S
38	g	301	SQD	O5-C1-O6-C44
38	g	301	SQD	O5-C5-C6-S
38	g	318	SQD	C2-C1-O6-C44
38	g	318	SQD	O5-C1-O6-C44
38	r	322	SQD	C2-C1-O6-C44
38	r	322	SQD	O5-C1-O6-C44
38	r	322	SQD	O49-C7-O47-C45
38	r	322	SQD	C8-C7-O47-C45
38	r	322	SQD	O5-C5-C6-S
38	s	301	SQD	C2-C1-O6-C44
38	s	301	SQD	O5-C1-O6-C44
38	s	301	SQD	O5-C5-C6-S
38	x	201	SQD	O5-C5-C6-S
38	y	621	SQD	O6-C44-C45-O47
38	y	621	SQD	C8-C7-O47-C45
42	A	408	PHO	C11-C10-C8-C9
43	B	617	BCR	C7-C8-C9-C10
43	B	617	BCR	C7-C8-C9-C34
43	B	617	BCR	C11-C12-C13-C14
43	B	617	BCR	C11-C12-C13-C35
43	B	617	BCR	C37-C22-C23-C24
43	B	618	BCR	C7-C8-C9-C10
43	B	618	BCR	C7-C8-C9-C34
43	B	618	BCR	C11-C12-C13-C14
43	B	618	BCR	C11-C12-C13-C35
43	B	618	BCR	C17-C18-C19-C20
43	B	618	BCR	C36-C18-C19-C20
43	B	619	BCR	C1-C6-C7-C8
43	B	619	BCR	C7-C8-C9-C34
43	B	619	BCR	C11-C12-C13-C14
43	B	619	BCR	C11-C12-C13-C35
43	C	614	BCR	C11-C12-C13-C14
43	C	614	BCR	C11-C12-C13-C35
43	C	614	BCR	C17-C18-C19-C20
43	C	614	BCR	C36-C18-C19-C20
43	C	614	BCR	C21-C22-C23-C24
43	C	614	BCR	C37-C22-C23-C24
43	C	615	BCR	C11-C12-C13-C14
43	C	615	BCR	C11-C12-C13-C35
43	D	405	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
43	D	405	BCR	C11-C12-C13-C35
43	D	405	BCR	C17-C18-C19-C20
43	D	405	BCR	C36-C18-C19-C20
43	D	405	BCR	C19-C20-C21-C22
43	D	405	BCR	C23-C24-C25-C30
43	H	101	BCR	C7-C8-C9-C10
43	H	101	BCR	C7-C8-C9-C34
43	T	101	BCR	C9-C10-C11-C12
43	T	101	BCR	C21-C22-C23-C24
43	T	101	BCR	C37-C22-C23-C24
43	V	101	BCR	C11-C12-C13-C14
43	V	101	BCR	C11-C12-C13-C35
43	V	101	BCR	C37-C22-C23-C24
43	Z	101	BCR	C11-C12-C13-C14
43	Z	101	BCR	C11-C12-C13-C35
43	a	410	BCR	C1-C6-C7-C8
43	b	618	BCR	C5-C6-C7-C8
43	b	618	BCR	C11-C12-C13-C14
43	b	618	BCR	C11-C12-C13-C35
43	b	618	BCR	C13-C14-C15-C16
43	b	618	BCR	C37-C22-C23-C24
43	b	619	BCR	C7-C8-C9-C10
43	b	619	BCR	C7-C8-C9-C34
43	b	619	BCR	C9-C10-C11-C12
43	b	619	BCR	C17-C18-C19-C20
43	b	619	BCR	C36-C18-C19-C20
43	b	620	BCR	C11-C12-C13-C14
43	b	620	BCR	C11-C12-C13-C35
43	b	620	BCR	C17-C18-C19-C20
43	b	620	BCR	C36-C18-C19-C20
43	c	614	BCR	C5-C6-C7-C8
43	c	614	BCR	C17-C18-C19-C20
43	c	614	BCR	C36-C18-C19-C20
43	c	614	BCR	C21-C22-C23-C24
43	c	614	BCR	C37-C22-C23-C24
43	c	614	BCR	C23-C24-C25-C26
43	c	615	BCR	C7-C8-C9-C10
43	c	615	BCR	C7-C8-C9-C34
43	c	615	BCR	C11-C12-C13-C14
43	c	615	BCR	C11-C12-C13-C35
43	d	406	BCR	C17-C18-C19-C20
43	d	406	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
43	d	406	BCR	C23-C24-C25-C26
43	h	101	BCR	C7-C8-C9-C10
43	h	101	BCR	C7-C8-C9-C34
43	t	101	BCR	C5-C6-C7-C8
43	t	101	BCR	C11-C12-C13-C14
43	t	101	BCR	C11-C12-C13-C35
43	v	101	BCR	C7-C8-C9-C34
43	v	101	BCR	C11-C12-C13-C14
43	v	101	BCR	C11-C12-C13-C35
43	z	101	BCR	C7-C8-C9-C10
43	z	101	BCR	C7-C8-C9-C34
44	A	416	PL9	C7-C8-C9-C11
44	A	416	PL9	C12-C13-C14-C16
44	A	416	PL9	C17-C18-C19-C21
44	A	416	PL9	C32-C33-C34-C36
44	A	416	PL9	C45-C44-C46-C47
44	a	414	PL9	C7-C8-C9-C10
44	a	414	PL9	C7-C8-C9-C11
44	a	414	PL9	C9-C11-C12-C13
44	a	414	PL9	C27-C28-C29-C31
44	a	414	PL9	C32-C33-C34-C35
44	a	414	PL9	C32-C33-C34-C36
44	a	414	PL9	C37-C38-C39-C40
44	a	414	PL9	C37-C38-C39-C41
45	C	616	DGD	C2A-C1A-O1G-C1G
45	C	616	DGD	O1A-C1A-O1G-C1G
45	C	618	DGD	C2D-C1D-O3G-C3G
45	C	618	DGD	O6D-C1D-O3G-C3G
45	C	620	DGD	C2A-C1A-O1G-C1G
45	C	620	DGD	O1A-C1A-O1G-C1G
45	C	620	DGD	C2B-C1B-O2G-C2G
45	c	616	DGD	O1B-C1B-O2G-C2G
45	c	617	DGD	O1B-C1B-O2G-C2G
45	c	617	DGD	O6E-C1E-O5D-C6D
45	c	618	DGD	C2B-C1B-O2G-C2G
45	c	619	DGD	C2B-C1B-O2G-C2G
48	R	302	LMU	O5'-C1'-O1'-C1
31	1	614	CLA	O1D-CGD-O2D-CED
31	3	316	CLA	O1D-CGD-O2D-CED
31	5	615	CLA	O1D-CGD-O2D-CED
31	6	316	CLA	O1D-CGD-O2D-CED
31	N	315	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	8	614	CLA	O1D-CGD-O2D-CED
31	9	315	CLA	O1D-CGD-O2D-CED
31	p	613	CLA	O1D-CGD-O2D-CED
31	p	615	CLA	O1D-CGD-O2D-CED
31	g	305	CLA	O1D-CGD-O2D-CED
31	n	316	CLA	O1D-CGD-O2D-CED
31	r	314	CLA	O1D-CGD-O2D-CED
31	s	314	CLA	O1D-CGD-O2D-CED
31	9	306	CLA	C5-C6-C7-C8
31	2	609	CLA	O1D-CGD-O2D-CED
31	6	314	CLA	O1D-CGD-O2D-CED
31	A	405	CLA	O1D-CGD-O2D-CED
31	N	321	CLA	O1D-CGD-O2D-CED
31	7	315	CLA	O1D-CGD-O2D-CED
31	8	611	CLA	O1D-CGD-O2D-CED
31	n	313	CLA	O1D-CGD-O2D-CED
30	2	607	CHL	CBD-CGD-O2D-CED
30	4	606	CHL	CBD-CGD-O2D-CED
30	0	605	CHL	CBD-CGD-O2D-CED
30	p	608	CHL	CBD-CGD-O2D-CED
31	1	611	CLA	CBD-CGD-O2D-CED
31	2	603	CLA	CBD-CGD-O2D-CED
31	2	604	CLA	CBD-CGD-O2D-CED
31	2	610	CLA	CBD-CGD-O2D-CED
31	2	611	CLA	CBD-CGD-O2D-CED
31	2	612	CLA	CBD-CGD-O2D-CED
31	3	304	CLA	CBD-CGD-O2D-CED
31	3	314	CLA	CBD-CGD-O2D-CED
31	3	315	CLA	CBD-CGD-O2D-CED
31	4	602	CLA	CBD-CGD-O2D-CED
31	4	603	CLA	CBD-CGD-O2D-CED
31	4	610	CLA	CBD-CGD-O2D-CED
31	4	611	CLA	CBD-CGD-O2D-CED
31	4	613	CLA	CBD-CGD-O2D-CED
31	4	614	CLA	CBD-CGD-O2D-CED
31	5	603	CLA	CBD-CGD-O2D-CED
31	5	610	CLA	CBD-CGD-O2D-CED
31	5	613	CLA	CBD-CGD-O2D-CED
31	6	303	CLA	CBD-CGD-O2D-CED
31	6	304	CLA	CBD-CGD-O2D-CED
31	6	311	CLA	CBD-CGD-O2D-CED
31	6	312	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	6	314	CLA	CBD-CGD-O2D-CED
31	A	405	CLA	CBD-CGD-O2D-CED
31	A	409	CLA	CBD-CGD-O2D-CED
31	B	601	CLA	CBD-CGD-O2D-CED
31	B	602	CLA	CBD-CGD-O2D-CED
31	B	608	CLA	CBD-CGD-O2D-CED
31	B	616	CLA	CBD-CGD-O2D-CED
31	C	602	CLA	CBD-CGD-O2D-CED
31	C	603	CLA	CBD-CGD-O2D-CED
31	C	604	CLA	CBD-CGD-O2D-CED
31	C	606	CLA	CBD-CGD-O2D-CED
31	C	611	CLA	CBD-CGD-O2D-CED
31	C	612	CLA	CBD-CGD-O2D-CED
31	D	404	CLA	CBD-CGD-O2D-CED
31	G	609	CLA	CBD-CGD-O2D-CED
31	G	611	CLA	CBD-CGD-O2D-CED
31	G	613	CLA	CBD-CGD-O2D-CED
31	N	312	CLA	CBD-CGD-O2D-CED
31	N	313	CLA	CBD-CGD-O2D-CED
31	N	315	CLA	CBD-CGD-O2D-CED
31	R	303	CLA	CBD-CGD-O2D-CED
31	R	305	CLA	CBD-CGD-O2D-CED
31	R	311	CLA	CBD-CGD-O2D-CED
31	R	312	CLA	CBD-CGD-O2D-CED
31	S	304	CLA	CBD-CGD-O2D-CED
31	S	305	CLA	CBD-CGD-O2D-CED
31	S	315	CLA	CBD-CGD-O2D-CED
31	Y	305	CLA	CBD-CGD-O2D-CED
31	Y	310	CLA	CBD-CGD-O2D-CED
31	0	603	CLA	CBD-CGD-O2D-CED
31	0	604	CLA	CBD-CGD-O2D-CED
31	0	611	CLA	CBD-CGD-O2D-CED
31	7	304	CLA	CBD-CGD-O2D-CED
31	7	305	CLA	CBD-CGD-O2D-CED
31	7	311	CLA	CBD-CGD-O2D-CED
31	8	609	CLA	CBD-CGD-O2D-CED
31	8	611	CLA	CBD-CGD-O2D-CED
31	8	613	CLA	CBD-CGD-O2D-CED
31	9	306	CLA	CBD-CGD-O2D-CED
31	9	313	CLA	CBD-CGD-O2D-CED
31	p	602	CLA	CBD-CGD-O2D-CED
31	p	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	p	604	CLA	CBD-CGD-O2D-CED
31	p	615	CLA	CBD-CGD-O2D-CED
31	q	304	CLA	CBD-CGD-O2D-CED
31	q	305	CLA	CBD-CGD-O2D-CED
31	q	306	CLA	CBD-CGD-O2D-CED
31	q	314	CLA	CBD-CGD-O2D-CED
31	q	315	CLA	CBD-CGD-O2D-CED
31	a	406	CLA	CBD-CGD-O2D-CED
31	a	409	CLA	CBD-CGD-O2D-CED
31	b	602	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	CBD-CGD-O2D-CED
31	b	609	CLA	CBD-CGD-O2D-CED
31	b	615	CLA	CBD-CGD-O2D-CED
31	b	617	CLA	CBD-CGD-O2D-CED
31	c	602	CLA	CBD-CGD-O2D-CED
31	c	606	CLA	CBD-CGD-O2D-CED
31	c	610	CLA	CBD-CGD-O2D-CED
31	c	611	CLA	CBD-CGD-O2D-CED
31	c	613	CLA	CBD-CGD-O2D-CED
31	g	305	CLA	CBD-CGD-O2D-CED
31	g	311	CLA	CBD-CGD-O2D-CED
31	g	312	CLA	CBD-CGD-O2D-CED
31	g	313	CLA	CBD-CGD-O2D-CED
31	n	313	CLA	CBD-CGD-O2D-CED
31	n	315	CLA	CBD-CGD-O2D-CED
31	n	316	CLA	CBD-CGD-O2D-CED
31	r	305	CLA	CBD-CGD-O2D-CED
31	r	306	CLA	CBD-CGD-O2D-CED
31	r	312	CLA	CBD-CGD-O2D-CED
31	r	314	CLA	CBD-CGD-O2D-CED
31	r	315	CLA	CBD-CGD-O2D-CED
31	r	316	CLA	CBD-CGD-O2D-CED
31	s	304	CLA	CBD-CGD-O2D-CED
31	s	311	CLA	CBD-CGD-O2D-CED
31	y	603	CLA	CBD-CGD-O2D-CED
31	y	604	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	O1A-CGA-O2A-C1
31	1	611	CLA	O1A-CGA-O2A-C1
31	2	610	CLA	O1A-CGA-O2A-C1
31	5	604	CLA	O1A-CGA-O2A-C1
31	5	610	CLA	O1A-CGA-O2A-C1
31	5	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	6	313	CLA	O1A-CGA-O2A-C1
31	6	315	CLA	O1A-CGA-O2A-C1
31	B	601	CLA	O1A-CGA-O2A-C1
31	B	602	CLA	O1A-CGA-O2A-C1
31	B	614	CLA	O1A-CGA-O2A-C1
31	B	616	CLA	O1A-CGA-O2A-C1
31	G	603	CLA	O1A-CGA-O2A-C1
31	N	304	CLA	O1A-CGA-O2A-C1
31	R	316	CLA	O1A-CGA-O2A-C1
31	S	306	CLA	O1A-CGA-O2A-C1
31	p	610	CLA	O1A-CGA-O2A-C1
31	b	615	CLA	O1A-CGA-O2A-C1
31	g	304	CLA	O1A-CGA-O2A-C1
31	r	312	CLA	O1A-CGA-O2A-C1
31	r	313	CLA	O1A-CGA-O2A-C1
33	K	102	LHG	O10-C23-O8-C6
34	4	620	LMG	O10-C28-O8-C9
34	A	418	LMG	O10-C28-O8-C9
34	B	621	LMG	O10-C28-O8-C9
34	C	624	LMG	O10-C28-O8-C9
34	D	410	LMG	O10-C28-O8-C9
34	G	621	LMG	O10-C28-O8-C9
34	0	620	LMG	O10-C28-O8-C9
34	a	416	LMG	O10-C28-O8-C9
34	b	629	LMG	O10-C28-O8-C9
34	f	101	LMG	O10-C28-O8-C9
34	w	203	LMG	O10-C28-O8-C9
38	0	621	SQD	O10-C23-O48-C46
38	g	301	SQD	O10-C23-O48-C46
31	4	612	CLA	O1A-CGA-O2A-C1
31	5	615	CLA	O1A-CGA-O2A-C1
31	S	316	CLA	O1A-CGA-O2A-C1
31	q	314	CLA	O1A-CGA-O2A-C1
48	c	623	LMU	C4B-C5B-C6B-O6B
30	7	307	CHL	O1D-CGD-O2D-CED
30	9	309	CHL	O1D-CGD-O2D-CED
31	2	602	CLA	O1D-CGD-O2D-CED
31	2	612	CLA	O1D-CGD-O2D-CED
31	4	613	CLA	O1D-CGD-O2D-CED
31	5	614	CLA	O1D-CGD-O2D-CED
31	6	311	CLA	O1D-CGD-O2D-CED
31	S	314	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	0	613	CLA	O1D-CGD-O2D-CED
31	q	314	CLA	O1D-CGD-O2D-CED
31	q	315	CLA	O1D-CGD-O2D-CED
31	a	406	CLA	O1D-CGD-O2D-CED
31	g	313	CLA	O1D-CGD-O2D-CED
31	n	314	CLA	O1D-CGD-O2D-CED
31	4	612	CLA	CBA-CGA-O2A-C1
31	5	615	CLA	CBA-CGA-O2A-C1
31	9	316	CLA	CBA-CGA-O2A-C1
31	q	314	CLA	CBA-CGA-O2A-C1
48	r	302	LMU	O5B-C1B-O1B-C4'
30	4	606	CHL	O1D-CGD-O2D-CED
31	2	613	CLA	O1D-CGD-O2D-CED
31	3	305	CLA	O1D-CGD-O2D-CED
31	3	312	CLA	O1D-CGD-O2D-CED
31	B	605	CLA	O1D-CGD-O2D-CED
31	C	603	CLA	O1D-CGD-O2D-CED
31	R	314	CLA	O1D-CGD-O2D-CED
31	S	310	CLA	O1D-CGD-O2D-CED
31	S	316	CLA	O1D-CGD-O2D-CED
31	Y	313	CLA	O1D-CGD-O2D-CED
31	7	314	CLA	O1D-CGD-O2D-CED
31	8	612	CLA	O1D-CGD-O2D-CED
31	9	314	CLA	O1D-CGD-O2D-CED
31	p	610	CLA	O1D-CGD-O2D-CED
31	q	312	CLA	O1D-CGD-O2D-CED
31	b	607	CLA	O1D-CGD-O2D-CED
31	c	603	CLA	O1D-CGD-O2D-CED
31	r	313	CLA	O1D-CGD-O2D-CED
31	s	316	CLA	O1D-CGD-O2D-CED
31	1	604	CLA	CBA-CGA-O2A-C1
31	1	611	CLA	CBA-CGA-O2A-C1
31	2	610	CLA	CBA-CGA-O2A-C1
31	5	604	CLA	CBA-CGA-O2A-C1
31	5	610	CLA	CBA-CGA-O2A-C1
31	5	614	CLA	CBA-CGA-O2A-C1
31	6	313	CLA	CBA-CGA-O2A-C1
31	6	315	CLA	CBA-CGA-O2A-C1
31	B	616	CLA	CBA-CGA-O2A-C1
31	S	306	CLA	CBA-CGA-O2A-C1
31	0	611	CLA	CBA-CGA-O2A-C1
31	p	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	q	312	CLA	CBA-CGA-O2A-C1
31	b	615	CLA	CBA-CGA-O2A-C1
31	g	304	CLA	CBA-CGA-O2A-C1
31	r	312	CLA	CBA-CGA-O2A-C1
31	r	313	CLA	CBA-CGA-O2A-C1
33	K	102	LHG	C24-C23-O8-C6
34	A	418	LMG	C29-C28-O8-C9
34	B	621	LMG	C29-C28-O8-C9
34	D	410	LMG	C29-C28-O8-C9
34	G	621	LMG	C29-C28-O8-C9
34	a	416	LMG	C29-C28-O8-C9
34	f	101	LMG	C29-C28-O8-C9
34	w	203	LMG	C29-C28-O8-C9
34	x	202	LMG	C29-C28-O8-C9
38	B	620	SQD	C24-C23-O48-C46
38	g	301	SQD	C24-C23-O48-C46
30	1	607	CHL	CBD-CGD-O2D-CED
30	q	307	CHL	CBD-CGD-O2D-CED
30	q	309	CHL	CBD-CGD-O2D-CED
30	q	310	CHL	CBD-CGD-O2D-CED
30	g	308	CHL	CBD-CGD-O2D-CED
30	n	301	CHL	CBD-CGD-O2D-CED
31	1	602	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	CBD-CGD-O2D-CED
31	3	311	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	CBD-CGD-O2D-CED
31	C	610	CLA	CBD-CGD-O2D-CED
31	C	613	CLA	CBD-CGD-O2D-CED
31	G	603	CLA	CBD-CGD-O2D-CED
31	G	604	CLA	CBD-CGD-O2D-CED
31	G	610	CLA	CBD-CGD-O2D-CED
31	N	303	CLA	CBD-CGD-O2D-CED
31	N	310	CLA	CBD-CGD-O2D-CED
31	R	307	CLA	CBD-CGD-O2D-CED
31	R	315	CLA	CBD-CGD-O2D-CED
31	R	316	CLA	CBD-CGD-O2D-CED
31	S	312	CLA	CBD-CGD-O2D-CED
31	Y	304	CLA	CBD-CGD-O2D-CED
31	Y	311	CLA	CBD-CGD-O2D-CED
31	Y	312	CLA	CBD-CGD-O2D-CED
31	0	602	CLA	CBD-CGD-O2D-CED
31	0	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	0	612	CLA	CBD-CGD-O2D-CED
31	7	303	CLA	CBD-CGD-O2D-CED
31	8	602	CLA	CBD-CGD-O2D-CED
31	8	603	CLA	CBD-CGD-O2D-CED
31	8	604	CLA	CBD-CGD-O2D-CED
31	9	304	CLA	CBD-CGD-O2D-CED
31	9	312	CLA	CBD-CGD-O2D-CED
31	9	316	CLA	CBD-CGD-O2D-CED
31	b	603	CLA	CBD-CGD-O2D-CED
31	b	612	CLA	CBD-CGD-O2D-CED
31	b	616	CLA	CBD-CGD-O2D-CED
31	c	604	CLA	CBD-CGD-O2D-CED
31	c	612	CLA	CBD-CGD-O2D-CED
31	d	404	CLA	CBD-CGD-O2D-CED
31	g	303	CLA	CBD-CGD-O2D-CED
31	g	304	CLA	CBD-CGD-O2D-CED
31	g	310	CLA	CBD-CGD-O2D-CED
31	n	303	CLA	CBD-CGD-O2D-CED
31	n	304	CLA	CBD-CGD-O2D-CED
31	n	305	CLA	CBD-CGD-O2D-CED
31	n	311	CLA	CBD-CGD-O2D-CED
31	r	303	CLA	CBD-CGD-O2D-CED
31	r	307	CLA	CBD-CGD-O2D-CED
31	s	310	CLA	CBD-CGD-O2D-CED
31	s	312	CLA	CBD-CGD-O2D-CED
31	s	315	CLA	CBD-CGD-O2D-CED
31	y	615	CLA	CBD-CGD-O2D-CED
31	3	315	CLA	O1A-CGA-O2A-C1
31	5	611	CLA	O1A-CGA-O2A-C1
31	5	613	CLA	O1A-CGA-O2A-C1
31	6	312	CLA	O1A-CGA-O2A-C1
31	6	314	CLA	O1A-CGA-O2A-C1
31	B	610	CLA	O1A-CGA-O2A-C1
31	R	303	CLA	O1A-CGA-O2A-C1
31	R	311	CLA	O1A-CGA-O2A-C1
31	R	312	CLA	O1A-CGA-O2A-C1
31	R	313	CLA	O1A-CGA-O2A-C1
31	R	315	CLA	O1A-CGA-O2A-C1
31	S	303	CLA	O1A-CGA-O2A-C1
31	Y	304	CLA	O1A-CGA-O2A-C1
31	Y	305	CLA	O1A-CGA-O2A-C1
31	0	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	0	615	CLA	O1A-CGA-O2A-C1
31	7	304	CLA	O1A-CGA-O2A-C1
31	7	305	CLA	O1A-CGA-O2A-C1
31	7	316	CLA	O1A-CGA-O2A-C1
31	9	305	CLA	O1A-CGA-O2A-C1
31	9	313	CLA	O1A-CGA-O2A-C1
31	9	314	CLA	O1A-CGA-O2A-C1
31	p	603	CLA	O1A-CGA-O2A-C1
31	p	604	CLA	O1A-CGA-O2A-C1
31	p	614	CLA	O1A-CGA-O2A-C1
31	q	306	CLA	O1A-CGA-O2A-C1
31	g	314	CLA	O1A-CGA-O2A-C1
31	r	303	CLA	O1A-CGA-O2A-C1
31	r	311	CLA	O1A-CGA-O2A-C1
31	y	603	CLA	O1A-CGA-O2A-C1
33	p	619	LHG	O10-C23-O8-C6
33	q	320	LHG	O10-C23-O8-C6
33	z	102	LHG	O10-C23-O8-C6
34	1	618	LMG	O10-C28-O8-C9
34	2	618	LMG	O10-C28-O8-C9
34	6	321	LMG	O10-C28-O8-C9
34	6	322	LMG	O10-C28-O8-C9
34	D	409	LMG	O10-C28-O8-C9
34	G	619	LMG	O10-C28-O8-C9
34	G	622	LMG	O10-C28-O8-C9
34	I	101	LMG	O10-C28-O8-C9
34	J	101	LMG	O10-C28-O8-C9
34	N	320	LMG	O10-C28-O8-C9
34	R	321	LMG	O10-C28-O8-C9
34	W	201	LMG	O10-C28-O8-C9
34	W	202	LMG	O10-C28-O8-C9
34	X	202	LMG	O10-C28-O8-C9
34	7	320	LMG	O10-C28-O8-C9
34	7	322	LMG	O10-C28-O8-C9
34	9	302	LMG	O10-C28-O8-C9
34	9	321	LMG	O10-C28-O8-C9
34	p	620	LMG	O10-C28-O8-C9
34	q	301	LMG	O10-C28-O8-C9
34	q	302	LMG	O10-C28-O8-C9
34	a	401	LMG	O10-C28-O8-C9
34	b	601	LMG	O10-C28-O8-C9
34	b	626	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	c	620	LMG	O10-C28-O8-C9
34	c	624	LMG	O10-C28-O8-C9
34	g	320	LMG	O10-C28-O8-C9
34	g	322	LMG	O10-C28-O8-C9
34	m	102	LMG	O10-C28-O8-C9
34	n	322	LMG	O10-C28-O8-C9
34	x	202	LMG	O10-C28-O8-C9
34	Q1	101	LMG	O10-C28-O8-C9
34	q1	101	LMG	O10-C28-O8-C9
38	B	620	SQD	O10-C23-O48-C46
38	G	624	SQD	O10-C23-O48-C46
38	R	322	SQD	O10-C23-O48-C46
38	X	201	SQD	O10-C23-O48-C46
31	9	316	CLA	O1A-CGA-O2A-C1
31	s	316	CLA	O1A-CGA-O2A-C1
31	1	610	CLA	O1D-CGD-O2D-CED
31	1	613	CLA	O1D-CGD-O2D-CED
31	q	316	CLA	O1D-CGD-O2D-CED
31	b	606	CLA	O1D-CGD-O2D-CED
31	b	614	CLA	O1D-CGD-O2D-CED
31	1	603	CLA	O1D-CGD-O2D-CED
31	5	602	CLA	O1D-CGD-O2D-CED
31	B	613	CLA	O1D-CGD-O2D-CED
31	B	614	CLA	O1D-CGD-O2D-CED
31	G	612	CLA	O1D-CGD-O2D-CED
31	R	313	CLA	O1D-CGD-O2D-CED
31	b	610	CLA	O1D-CGD-O2D-CED
31	d	405	CLA	O1D-CGD-O2D-CED
31	g	314	CLA	O1D-CGD-O2D-CED
31	r	311	CLA	O1D-CGD-O2D-CED
30	4	609	CHL	CBD-CGD-O2D-CED
30	N	301	CHL	CBD-CGD-O2D-CED
30	Y	308	CHL	CBD-CGD-O2D-CED
31	5	612	CLA	CBD-CGD-O2D-CED
31	6	305	CLA	CBD-CGD-O2D-CED
31	C	601	CLA	CBD-CGD-O2D-CED
31	N	305	CLA	CBD-CGD-O2D-CED
31	7	313	CLA	CBD-CGD-O2D-CED
31	c	601	CLA	CBD-CGD-O2D-CED
31	c	607	CLA	CBD-CGD-O2D-CED
31	B	603	CLA	O1D-CGD-O2D-CED
31	B	606	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	B	609	CLA	O1D-CGD-O2D-CED
31	N	313	CLA	O1D-CGD-O2D-CED
31	R	311	CLA	O1D-CGD-O2D-CED
31	S	315	CLA	O1D-CGD-O2D-CED
31	b	604	CLA	O1D-CGD-O2D-CED
31	s	311	CLA	O1D-CGD-O2D-CED
33	1	617	LHG	O9-C7-O7-C5
33	C	623	LHG	O9-C7-O7-C5
33	0	619	LHG	O9-C7-O7-C5
33	7	319	LHG	O9-C7-O7-C5
33	p	619	LHG	O9-C7-O7-C5
33	s	322	LHG	O9-C7-O7-C5
34	2	621	LMG	O9-C10-O7-C8
34	4	620	LMG	O9-C10-O7-C8
34	4	621	LMG	O9-C10-O7-C8
34	A	412	LMG	O9-C10-O7-C8
34	B	622	LMG	O9-C10-O7-C8
34	C	622	LMG	O9-C10-O7-C8
34	G	622	LMG	O9-C10-O7-C8
34	I	101	LMG	O9-C10-O7-C8
34	J	102	LMG	O9-C10-O7-C8
34	N	320	LMG	O9-C10-O7-C8
34	W	203	LMG	O9-C10-O7-C8
34	0	620	LMG	O9-C10-O7-C8
34	7	301	LMG	O9-C10-O7-C8
34	9	321	LMG	O9-C10-O7-C8
34	p	620	LMG	O9-C10-O7-C8
34	a	413	LMG	O9-C10-O7-C8
34	a	416	LMG	O9-C10-O7-C8
34	b	601	LMG	O9-C10-O7-C8
34	b	623	LMG	O9-C10-O7-C8
34	b	624	LMG	O9-C10-O7-C8
34	b	629	LMG	O9-C10-O7-C8
34	c	620	LMG	O9-C10-O7-C8
34	c	621	LMG	O9-C10-O7-C8
34	c	624	LMG	O9-C10-O7-C8
34	f	101	LMG	O9-C10-O7-C8
34	g	320	LMG	O9-C10-O7-C8
34	k	101	LMG	O9-C10-O7-C8
34	k	102	LMG	O9-C10-O7-C8
34	m	102	LMG	O9-C10-O7-C8
34	w	203	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	y	620	LMG	O9-C10-O7-C8
34	q1	101	LMG	O9-C10-O7-C8
38	G	617	SQD	O49-C7-O47-C45
38	0	621	SQD	O49-C7-O47-C45
38	b	621	SQD	O49-C7-O47-C45
38	y	621	SQD	O49-C7-O47-C45
45	C	620	DGD	O1B-C1B-O2G-C2G
45	c	619	DGD	O1B-C1B-O2G-C2G
48	K	101	LMU	C4B-C5B-C6B-O6B
31	p	612	CLA	O1A-CGA-O2A-C1
31	p	615	CLA	O1A-CGA-O2A-C1
31	1	613	CLA	C3-C5-C6-C7
31	2	603	CLA	C3-C5-C6-C7
31	2	611	CLA	C3-C5-C6-C7
31	2	612	CLA	C3-C5-C6-C7
31	2	613	CLA	C3-C5-C6-C7
31	3	301	CLA	C3-C5-C6-C7
31	4	602	CLA	C3-C5-C6-C7
31	6	304	CLA	C3-C5-C6-C7
31	6	305	CLA	C3-C5-C6-C7
31	6	311	CLA	C3-C5-C6-C7
31	6	313	CLA	C3-C5-C6-C7
31	6	314	CLA	C3-C5-C6-C7
31	A	409	CLA	C3-C5-C6-C7
31	B	602	CLA	C3-C5-C6-C7
31	B	604	CLA	C3-C5-C6-C7
31	C	604	CLA	C3-C5-C6-C7
31	C	609	CLA	C3-C5-C6-C7
31	D	403	CLA	C3-C5-C6-C7
31	G	603	CLA	C3-C5-C6-C7
31	G	612	CLA	C3-C5-C6-C7
31	N	304	CLA	C3-C5-C6-C7
31	R	312	CLA	C3-C5-C6-C7
31	S	311	CLA	C3-C5-C6-C7
31	S	313	CLA	C3-C5-C6-C7
31	Y	305	CLA	C3-C5-C6-C7
31	0	604	CLA	C3-C5-C6-C7
31	0	610	CLA	C3-C5-C6-C7
31	0	613	CLA	C3-C5-C6-C7
31	8	612	CLA	C3-C5-C6-C7
31	p	603	CLA	C3-C5-C6-C7
31	q	315	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	a	409	CLA	C3-C5-C6-C7
31	b	605	CLA	C3-C5-C6-C7
31	b	608	CLA	C3-C5-C6-C7
31	b	615	CLA	C3-C5-C6-C7
31	b	617	CLA	C3-C5-C6-C7
31	c	606	CLA	C3-C5-C6-C7
31	c	608	CLA	C3-C5-C6-C7
31	c	613	CLA	C3-C5-C6-C7
31	d	405	CLA	C3-C5-C6-C7
31	n	314	CLA	C3-C5-C6-C7
31	r	315	CLA	C3-C5-C6-C7
31	s	311	CLA	C3-C5-C6-C7
31	s	313	CLA	C3-C5-C6-C7
31	y	612	CLA	C3-C5-C6-C7
31	y	614	CLA	C3-C5-C6-C7
42	D	401	PHO	C3-C5-C6-C7
42	d	402	PHO	C3-C5-C6-C7
30	5	607	CHL	CBA-CGA-O2A-C1
31	3	315	CLA	CBA-CGA-O2A-C1
31	4	613	CLA	CBA-CGA-O2A-C1
31	5	613	CLA	CBA-CGA-O2A-C1
31	6	304	CLA	CBA-CGA-O2A-C1
31	6	312	CLA	CBA-CGA-O2A-C1
31	6	314	CLA	CBA-CGA-O2A-C1
31	A	409	CLA	CBA-CGA-O2A-C1
31	B	601	CLA	CBA-CGA-O2A-C1
31	B	610	CLA	CBA-CGA-O2A-C1
31	B	614	CLA	CBA-CGA-O2A-C1
31	N	304	CLA	CBA-CGA-O2A-C1
31	R	303	CLA	CBA-CGA-O2A-C1
31	R	311	CLA	CBA-CGA-O2A-C1
31	R	313	CLA	CBA-CGA-O2A-C1
31	R	316	CLA	CBA-CGA-O2A-C1
31	S	303	CLA	CBA-CGA-O2A-C1
31	Y	304	CLA	CBA-CGA-O2A-C1
31	0	615	CLA	CBA-CGA-O2A-C1
31	7	305	CLA	CBA-CGA-O2A-C1
31	9	305	CLA	CBA-CGA-O2A-C1
31	9	313	CLA	CBA-CGA-O2A-C1
31	p	614	CLA	CBA-CGA-O2A-C1
31	q	306	CLA	CBA-CGA-O2A-C1
31	a	409	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	c	609	CLA	CBA-CGA-O2A-C1
31	y	603	CLA	CBA-CGA-O2A-C1
33	q	320	LHG	C24-C23-O8-C6
33	z	102	LHG	C24-C23-O8-C6
34	1	618	LMG	C29-C28-O8-C9
34	2	618	LMG	C29-C28-O8-C9
34	4	620	LMG	C29-C28-O8-C9
34	6	323	LMG	C29-C28-O8-C9
34	B	625	LMG	C29-C28-O8-C9
34	C	624	LMG	C29-C28-O8-C9
34	D	409	LMG	C29-C28-O8-C9
34	G	619	LMG	C29-C28-O8-C9
34	I	101	LMG	C29-C28-O8-C9
34	J	101	LMG	C29-C28-O8-C9
34	N	320	LMG	C29-C28-O8-C9
34	R	321	LMG	C29-C28-O8-C9
34	0	620	LMG	C29-C28-O8-C9
34	7	320	LMG	C29-C28-O8-C9
34	7	322	LMG	C29-C28-O8-C9
34	9	321	LMG	C29-C28-O8-C9
34	q	301	LMG	C29-C28-O8-C9
34	b	601	LMG	C29-C28-O8-C9
34	b	624	LMG	C29-C28-O8-C9
34	b	626	LMG	C29-C28-O8-C9
34	b	629	LMG	C29-C28-O8-C9
34	c	620	LMG	C29-C28-O8-C9
34	j	101	LMG	C29-C28-O8-C9
34	m	102	LMG	C29-C28-O8-C9
34	n	322	LMG	C29-C28-O8-C9
34	Q1	101	LMG	C29-C28-O8-C9
34	q1	101	LMG	C29-C28-O8-C9
38	G	624	SQD	C24-C23-O48-C46
38	X	201	SQD	C24-C23-O48-C46
38	0	621	SQD	C24-C23-O48-C46
31	9	313	CLA	C2-C1-O2A-CGA
31	1	610	CLA	C5-C6-C7-C8
33	1	617	LHG	C8-C7-O7-C5
33	5	619	LHG	C8-C7-O7-C5
33	7	319	LHG	C8-C7-O7-C5
34	2	621	LMG	C11-C10-O7-C8
34	6	321	LMG	C11-C10-O7-C8
34	q	302	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	a	416	LMG	C11-C10-O7-C8
34	c	620	LMG	C11-C10-O7-C8
34	g	320	LMG	C11-C10-O7-C8
34	w	205	LMG	C11-C10-O7-C8
45	c	616	DGD	C2B-C1B-O2G-C2G
45	c	617	DGD	C2B-C1B-O2G-C2G
31	3	314	CLA	O1D-CGD-O2D-CED
31	3	315	CLA	O1D-CGD-O2D-CED
31	4	602	CLA	O1D-CGD-O2D-CED
31	C	606	CLA	O1D-CGD-O2D-CED
31	S	304	CLA	O1D-CGD-O2D-CED
31	9	313	CLA	O1D-CGD-O2D-CED
31	n	315	CLA	O1D-CGD-O2D-CED
30	7	310	CHL	CBD-CGD-O2D-CED
31	3	313	CLA	CBD-CGD-O2D-CED
31	C	609	CLA	CBD-CGD-O2D-CED
31	y	602	CLA	CBD-CGD-O2D-CED
31	y	610	CLA	CBD-CGD-O2D-CED
31	N	310	CLA	O1A-CGA-O2A-C1
48	c	623	LMU	O5B-C5B-C6B-O6B
31	p	612	CLA	CBA-CGA-O2A-C1
31	p	615	CLA	CBA-CGA-O2A-C1
31	D	403	CLA	C4-C3-C5-C6
31	p	602	CLA	C4-C3-C5-C6
31	b	605	CLA	C4-C3-C5-C6
31	s	310	CLA	C4-C3-C5-C6
31	D	404	CLA	C2-C3-C5-C6
30	R	309	CHL	CBD-CGD-O2D-CED
30	0	607	CHL	CBD-CGD-O2D-CED
31	1	612	CLA	CBD-CGD-O2D-CED
31	B	611	CLA	CBD-CGD-O2D-CED
31	p	611	CLA	CBD-CGD-O2D-CED
31	p	612	CLA	CBD-CGD-O2D-CED
31	b	611	CLA	CBD-CGD-O2D-CED
31	c	609	CLA	CBD-CGD-O2D-CED
30	y	605	CHL	C2A-CAA-CBA-CGA
31	2	609	CLA	C2A-CAA-CBA-CGA
31	3	312	CLA	C2A-CAA-CBA-CGA
31	6	314	CLA	C2A-CAA-CBA-CGA
31	B	606	CLA	C2A-CAA-CBA-CGA
31	D	404	CLA	C2A-CAA-CBA-CGA
31	R	316	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	S	303	CLA	C2A-CAA-CBA-CGA
31	7	312	CLA	C2A-CAA-CBA-CGA
31	9	316	CLA	C2A-CAA-CBA-CGA
31	a	406	CLA	C2A-CAA-CBA-CGA
31	r	312	CLA	C2A-CAA-CBA-CGA
31	s	312	CLA	C2A-CAA-CBA-CGA
31	s	314	CLA	C2A-CAA-CBA-CGA
31	A	409	CLA	O1A-CGA-O2A-C1
31	a	409	CLA	O1A-CGA-O2A-C1
30	0	605	CHL	O1D-CGD-O2D-CED
31	2	611	CLA	O1D-CGD-O2D-CED
31	5	603	CLA	O1D-CGD-O2D-CED
31	b	615	CLA	O1D-CGD-O2D-CED
33	G	618	LHG	C13-C14-C15-C16
34	2	620	LMG	C17-C18-C19-C20
34	2	620	LMG	C35-C36-C37-C38
34	2	620	LMG	C38-C39-C40-C41
34	4	620	LMG	C17-C18-C19-C20
34	4	620	LMG	C35-C36-C37-C38
34	4	620	LMG	C38-C39-C40-C41
34	B	621	LMG	C17-C18-C19-C20
34	B	621	LMG	C20-C21-C22-C23
34	C	619	LMG	C20-C21-C22-C23
34	C	619	LMG	C35-C36-C37-C38
34	C	624	LMG	C17-C18-C19-C20
34	D	410	LMG	C17-C18-C19-C20
34	D	410	LMG	C20-C21-C22-C23
34	D	411	LMG	C17-C18-C19-C20
34	D	411	LMG	C20-C21-C22-C23
34	D	411	LMG	C35-C36-C37-C38
34	D	412	LMG	C35-C36-C37-C38
34	D	412	LMG	C38-C39-C40-C41
34	G	621	LMG	C20-C21-C22-C23
34	G	621	LMG	C35-C36-C37-C38
34	G	621	LMG	C38-C39-C40-C41
34	J	101	LMG	C20-C21-C22-C23
34	J	101	LMG	C35-C36-C37-C38
34	S	321	LMG	C17-C18-C19-C20
34	W	201	LMG	C38-C39-C40-C41
34	9	301	LMG	C20-C21-C22-C23
34	9	301	LMG	C35-C36-C37-C38
34	9	301	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
34	q	301	LMG	C17-C18-C19-C20
34	q	301	LMG	C35-C36-C37-C38
34	q	301	LMG	C38-C39-C40-C41
34	b	622	LMG	C17-C18-C19-C20
34	b	622	LMG	C20-C21-C22-C23
34	b	626	LMG	C17-C18-C19-C20
34	b	626	LMG	C20-C21-C22-C23
34	c	624	LMG	C35-C36-C37-C38
34	c	624	LMG	C38-C39-C40-C41
34	d	410	LMG	C17-C18-C19-C20
34	d	410	LMG	C20-C21-C22-C23
34	d	410	LMG	C35-C36-C37-C38
34	d	411	LMG	C35-C36-C37-C38
34	d	411	LMG	C38-C39-C40-C41
34	g	322	LMG	C35-C36-C37-C38
34	g	322	LMG	C38-C39-C40-C41
34	k	101	LMG	C17-C18-C19-C20
34	k	101	LMG	C35-C36-C37-C38
34	s	321	LMG	C17-C18-C19-C20
34	w	201	LMG	C35-C36-C37-C38
45	C	617	DGD	CBB-CCB-CDB-CEB
45	C	618	DGD	CEA-CFA-CGA-CHA
45	C	618	DGD	C8B-C9B-CAB-CBB
45	C	618	DGD	CBB-CCB-CDB-CEB
45	C	620	DGD	CBA-CCA-CDA-CEA
45	C	620	DGD	CBB-CCB-CDB-CEB
45	C	620	DGD	CEB-CFB-CGB-CHB
45	c	616	DGD	C8A-C9A-CAA-CBA
45	c	616	DGD	CBB-CCB-CDB-CEB
45	c	616	DGD	CEB-CFB-CGB-CHB
45	c	617	DGD	C8B-C9B-CAB-CBB
45	c	617	DGD	CBB-CCB-CDB-CEB
45	c	618	DGD	C8A-C9A-CAA-CBA
45	c	618	DGD	CBB-CCB-CDB-CEB
45	c	619	DGD	CEA-CFA-CGA-CHA
45	c	619	DGD	CBB-CCB-CDB-CEB
45	c	619	DGD	CEB-CFB-CGB-CHB
30	4	607	CHL	C3-C5-C6-C7
30	7	302	CHL	C3-C5-C6-C7
31	1	602	CLA	C3-C5-C6-C7
31	1	604	CLA	C3-C5-C6-C7
31	1	610	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	3	304	CLA	C3-C5-C6-C7
31	3	316	CLA	C3-C5-C6-C7
31	B	614	CLA	C3-C5-C6-C7
31	C	612	CLA	C3-C5-C6-C7
31	R	315	CLA	C3-C5-C6-C7
31	R	316	CLA	C3-C5-C6-C7
31	Y	303	CLA	C3-C5-C6-C7
31	0	614	CLA	C3-C5-C6-C7
31	9	312	CLA	C3-C5-C6-C7
31	q	306	CLA	C3-C5-C6-C7
31	a	406	CLA	C3-C5-C6-C7
31	b	603	CLA	C3-C5-C6-C7
31	c	603	CLA	C3-C5-C6-C7
31	c	604	CLA	C3-C5-C6-C7
31	g	304	CLA	C3-C5-C6-C7
31	s	312	CLA	C3-C5-C6-C7
31	y	602	CLA	C3-C5-C6-C7
31	y	613	CLA	C3-C5-C6-C7
31	1	612	CLA	CBA-CGA-O2A-C1
31	2	603	CLA	CBA-CGA-O2A-C1
31	2	609	CLA	CBA-CGA-O2A-C1
31	2	611	CLA	CBA-CGA-O2A-C1
31	2	613	CLA	CBA-CGA-O2A-C1
31	5	611	CLA	CBA-CGA-O2A-C1
31	C	609	CLA	CBA-CGA-O2A-C1
31	N	314	CLA	CBA-CGA-O2A-C1
31	R	312	CLA	CBA-CGA-O2A-C1
31	R	315	CLA	CBA-CGA-O2A-C1
31	Y	305	CLA	CBA-CGA-O2A-C1
31	0	610	CLA	CBA-CGA-O2A-C1
31	7	304	CLA	CBA-CGA-O2A-C1
31	7	316	CLA	CBA-CGA-O2A-C1
31	8	613	CLA	CBA-CGA-O2A-C1
31	9	314	CLA	CBA-CGA-O2A-C1
31	p	603	CLA	CBA-CGA-O2A-C1
31	p	604	CLA	CBA-CGA-O2A-C1
31	b	613	CLA	CBA-CGA-O2A-C1
31	c	611	CLA	CBA-CGA-O2A-C1
31	g	314	CLA	CBA-CGA-O2A-C1
31	n	311	CLA	CBA-CGA-O2A-C1
31	n	315	CLA	CBA-CGA-O2A-C1
31	r	303	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	r	311	CLA	CBA-CGA-O2A-C1
31	r	316	CLA	CBA-CGA-O2A-C1
33	p	619	LHG	C24-C23-O8-C6
34	4	621	LMG	C29-C28-O8-C9
34	6	321	LMG	C29-C28-O8-C9
34	6	322	LMG	C29-C28-O8-C9
34	D	411	LMG	C29-C28-O8-C9
34	G	622	LMG	C29-C28-O8-C9
34	W	201	LMG	C29-C28-O8-C9
34	W	202	LMG	C29-C28-O8-C9
34	X	202	LMG	C29-C28-O8-C9
34	9	302	LMG	C29-C28-O8-C9
34	p	620	LMG	C29-C28-O8-C9
34	q	302	LMG	C29-C28-O8-C9
34	a	401	LMG	C29-C28-O8-C9
34	c	624	LMG	C29-C28-O8-C9
34	d	410	LMG	C29-C28-O8-C9
34	g	320	LMG	C29-C28-O8-C9
34	g	322	LMG	C29-C28-O8-C9
38	R	322	SQD	C24-C23-O48-C46
42	A	408	PHO	CBA-CGA-O2A-C1
34	W	201	LMG	C41-C42-C43-C44
34	w	202	LMG	C38-C39-C40-C41
34	w	202	LMG	C41-C42-C43-C44
31	D	404	CLA	O1D-CGD-O2D-CED
31	R	305	CLA	O1D-CGD-O2D-CED
31	S	305	CLA	O1D-CGD-O2D-CED
31	Y	305	CLA	O1D-CGD-O2D-CED
31	0	611	CLA	O1D-CGD-O2D-CED
31	7	304	CLA	O1D-CGD-O2D-CED
31	p	604	CLA	O1D-CGD-O2D-CED
31	g	311	CLA	O1D-CGD-O2D-CED
44	A	416	PL9	C32-C33-C34-C35
30	N	306	CHL	CBD-CGD-O2D-CED
31	A	407	CLA	CBD-CGD-O2D-CED
31	B	610	CLA	CBD-CGD-O2D-CED
31	G	602	CLA	CBD-CGD-O2D-CED
31	d	401	CLA	CBD-CGD-O2D-CED
31	s	306	CLA	CBD-CGD-O2D-CED
31	y	612	CLA	CBD-CGD-O2D-CED
30	2	607	CHL	O1D-CGD-O2D-CED
31	2	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	4	610	CLA	O1D-CGD-O2D-CED
31	4	614	CLA	O1D-CGD-O2D-CED
31	5	613	CLA	O1D-CGD-O2D-CED
31	6	304	CLA	O1D-CGD-O2D-CED
31	B	602	CLA	O1D-CGD-O2D-CED
31	G	613	CLA	O1D-CGD-O2D-CED
31	R	312	CLA	O1D-CGD-O2D-CED
31	Y	310	CLA	O1D-CGD-O2D-CED
31	9	306	CLA	O1D-CGD-O2D-CED
31	p	603	CLA	O1D-CGD-O2D-CED
31	q	305	CLA	O1D-CGD-O2D-CED
31	b	608	CLA	O1D-CGD-O2D-CED
31	c	610	CLA	O1D-CGD-O2D-CED
31	c	611	CLA	O1D-CGD-O2D-CED
31	g	312	CLA	O1D-CGD-O2D-CED
31	r	306	CLA	O1D-CGD-O2D-CED
31	r	312	CLA	O1D-CGD-O2D-CED
31	s	304	CLA	O1D-CGD-O2D-CED
31	y	603	CLA	O1D-CGD-O2D-CED
33	M	101	LHG	O9-C7-O7-C5
34	5	620	LMG	O9-C10-O7-C8
34	6	321	LMG	O9-C10-O7-C8
34	6	323	LMG	O9-C10-O7-C8
34	A	418	LMG	O9-C10-O7-C8
34	X	202	LMG	O9-C10-O7-C8
34	7	322	LMG	O9-C10-O7-C8
38	Y	320	SQD	O49-C7-O47-C45
45	c	618	DGD	O1B-C1B-O2G-C2G
30	5	607	CHL	O1A-CGA-O2A-C1
31	1	603	CLA	O1A-CGA-O2A-C1
31	2	603	CLA	O1A-CGA-O2A-C1
31	2	604	CLA	O1A-CGA-O2A-C1
31	2	609	CLA	O1A-CGA-O2A-C1
31	4	613	CLA	O1A-CGA-O2A-C1
31	6	304	CLA	O1A-CGA-O2A-C1
31	6	316	CLA	O1A-CGA-O2A-C1
31	C	609	CLA	O1A-CGA-O2A-C1
31	N	314	CLA	O1A-CGA-O2A-C1
31	8	609	CLA	O1A-CGA-O2A-C1
31	n	311	CLA	O1A-CGA-O2A-C1
31	r	316	CLA	O1A-CGA-O2A-C1
34	2	621	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	4	621	LMG	O10-C28-O8-C9
38	a	411	SQD	O10-C23-O48-C46
33	l	101	LHG	C11-C12-C13-C14
31	C	602	CLA	O1D-CGD-O2D-CED
31	C	611	CLA	O1D-CGD-O2D-CED
31	8	609	CLA	O1D-CGD-O2D-CED
31	b	617	CLA	O1D-CGD-O2D-CED
35	2	614	RRX	C19-C20-C21-C22
35	4	615	RRX	C19-C20-C21-C22
35	G	614	RRX	C19-C20-C21-C22
35	9	317	RRX	C19-C20-C21-C22
43	C	614	BCR	C19-C20-C21-C22
43	D	405	BCR	C13-C14-C15-C16
43	T	101	BCR	C15-C16-C17-C18
43	V	101	BCR	C13-C14-C15-C16
31	7	311	CLA	C5-C6-C7-C8
48	R	302	LMU	C3'-C4'-O1B-C1B
30	1	606	CHL	CBD-CGD-O2D-CED
30	5	601	CHL	CBD-CGD-O2D-CED
30	G	607	CHL	CBD-CGD-O2D-CED
30	Y	307	CHL	CBD-CGD-O2D-CED
30	8	607	CHL	CBD-CGD-O2D-CED
30	q	308	CHL	CBD-CGD-O2D-CED
30	n	309	CHL	CBD-CGD-O2D-CED
31	4	612	CLA	CBD-CGD-O2D-CED
31	B	615	CLA	CBD-CGD-O2D-CED
31	C	607	CLA	CBD-CGD-O2D-CED
31	D	403	CLA	CBD-CGD-O2D-CED
31	N	311	CLA	CBD-CGD-O2D-CED
31	S	311	CLA	CBD-CGD-O2D-CED
31	Y	303	CLA	CBD-CGD-O2D-CED
31	3	304	CLA	O1D-CGD-O2D-CED
31	6	303	CLA	O1D-CGD-O2D-CED
31	B	616	CLA	O1D-CGD-O2D-CED
31	C	604	CLA	O1D-CGD-O2D-CED
31	b	602	CLA	O1D-CGD-O2D-CED
31	b	609	CLA	O1D-CGD-O2D-CED
31	c	602	CLA	O1D-CGD-O2D-CED
31	c	606	CLA	O1D-CGD-O2D-CED
33	1	617	LHG	O2-C2-C3-O3
33	3	320	LHG	O2-C2-C3-O3
33	5	619	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	A	417	LHG	O2-C2-C3-O3
33	B	624	LHG	O2-C2-C3-O3
33	C	623	LHG	O2-C2-C3-O3
33	K	102	LHG	O2-C2-C3-O3
33	N	319	LHG	O2-C2-C3-O3
33	R	320	LHG	O2-C2-C3-O3
33	Y	318	LHG	O2-C2-C3-O3
33	9	320	LHG	O2-C2-C3-O3
33	p	619	LHG	O2-C2-C3-O3
33	b	628	LHG	O2-C2-C3-O3
33	j	102	LHG	O2-C2-C3-O3
33	s	322	LHG	O2-C2-C3-O3
33	z	102	LHG	O2-C2-C3-O3
31	2	604	CLA	C3-C5-C6-C7
31	B	609	CLA	C3-C5-C6-C7
31	Y	312	CLA	C3-C5-C6-C7
31	Y	314	CLA	C3-C5-C6-C7
31	0	602	CLA	C3-C5-C6-C7
31	0	615	CLA	C3-C5-C6-C7
31	7	312	CLA	C3-C5-C6-C7
31	7	314	CLA	C3-C5-C6-C7
31	8	602	CLA	C3-C5-C6-C7
31	8	604	CLA	C3-C5-C6-C7
31	b	610	CLA	C3-C5-C6-C7
31	b	612	CLA	C3-C5-C6-C7
31	n	303	CLA	C3-C5-C6-C7
31	n	305	CLA	C3-C5-C6-C7
31	r	304	CLA	C3-C5-C6-C7
31	1	614	CLA	CBA-CGA-O2A-C1
31	2	604	CLA	CBA-CGA-O2A-C1
31	3	313	CLA	CBA-CGA-O2A-C1
31	4	610	CLA	CBA-CGA-O2A-C1
31	6	311	CLA	CBA-CGA-O2A-C1
31	G	613	CLA	CBA-CGA-O2A-C1
31	N	310	CLA	CBA-CGA-O2A-C1
31	N	315	CLA	CBA-CGA-O2A-C1
31	S	310	CLA	CBA-CGA-O2A-C1
31	7	315	CLA	CBA-CGA-O2A-C1
31	8	609	CLA	CBA-CGA-O2A-C1
31	g	305	CLA	CBA-CGA-O2A-C1
31	r	307	CLA	CBA-CGA-O2A-C1
31	s	314	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	5	619	LHG	C24-C23-O8-C6
38	a	411	SQD	C24-C23-O48-C46
31	0	610	CLA	O1A-CGA-O2A-C1
31	b	613	CLA	O1A-CGA-O2A-C1
31	c	609	CLA	O1A-CGA-O2A-C1
31	s	314	CLA	O1A-CGA-O2A-C1
42	A	408	PHO	O1A-CGA-O2A-C1
30	p	608	CHL	O1D-CGD-O2D-CED
31	1	611	CLA	O1D-CGD-O2D-CED
31	2	603	CLA	O1D-CGD-O2D-CED
31	B	608	CLA	O1D-CGD-O2D-CED
31	C	612	CLA	O1D-CGD-O2D-CED
31	G	609	CLA	O1D-CGD-O2D-CED
31	G	611	CLA	O1D-CGD-O2D-CED
31	0	604	CLA	O1D-CGD-O2D-CED
31	7	305	CLA	O1D-CGD-O2D-CED
31	7	311	CLA	O1D-CGD-O2D-CED
31	8	613	CLA	O1D-CGD-O2D-CED
31	p	602	CLA	O1D-CGD-O2D-CED
31	q	304	CLA	O1D-CGD-O2D-CED
31	r	305	CLA	O1D-CGD-O2D-CED
31	r	315	CLA	O1D-CGD-O2D-CED
31	r	316	CLA	O1D-CGD-O2D-CED
33	N	319	LHG	C8-C7-O7-C5
33	8	618	LHG	C8-C7-O7-C5
33	n	320	LHG	C8-C7-O7-C5
34	1	618	LMG	C11-C10-O7-C8
34	2	618	LMG	C11-C10-O7-C8
34	6	323	LMG	C11-C10-O7-C8
34	A	412	LMG	C11-C10-O7-C8
34	B	621	LMG	C11-C10-O7-C8
34	J	101	LMG	C11-C10-O7-C8
34	7	320	LMG	C11-C10-O7-C8
34	s	321	LMG	C11-C10-O7-C8
33	2	617	LHG	C13-C14-C15-C16
30	3	303	CHL	CBD-CGD-O2D-CED
30	4	607	CHL	CBD-CGD-O2D-CED
30	9	311	CHL	CBD-CGD-O2D-CED
31	q	313	CLA	CBD-CGD-O2D-CED
31	s	305	CLA	CBD-CGD-O2D-CED
48	K	101	LMU	O5B-C5B-C6B-O6B
33	2	617	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	2	617	LHG	C28-C29-C30-C31
33	S	320	LHG	C28-C29-C30-C31
33	l	101	LHG	C9-C10-C11-C12
33	r	320	LHG	C11-C12-C13-C14
33	s	320	LHG	C28-C29-C30-C31
31	0	610	CLA	C5-C6-C7-C8
34	x	202	LMG	C8-C9-O8-C28
38	M	102	SQD	C45-C46-O48-C23
45	c	616	DGD	C2G-C1G-O1G-C1A
31	0	603	CLA	O1D-CGD-O2D-CED
31	1	614	CLA	O1A-CGA-O2A-C1
31	2	611	CLA	O1A-CGA-O2A-C1
31	G	613	CLA	O1A-CGA-O2A-C1
34	D	411	LMG	O10-C28-O8-C9
34	d	410	LMG	O10-C28-O8-C9
33	q	320	LHG	C26-C27-C28-C29
33	b	625	LHG	C31-C32-C33-C34
33	s	322	LHG	C28-C29-C30-C31
36	N	318	NEX	C14-C15-C35-C34
31	4	611	CLA	O1D-CGD-O2D-CED
31	5	610	CLA	O1D-CGD-O2D-CED
31	6	312	CLA	O1D-CGD-O2D-CED
33	5	619	LHG	C7-C8-C9-C10
33	G	618	LHG	C11-C10-C9-C8
33	b	625	LHG	C25-C26-C27-C28
33	g	319	LHG	C26-C27-C28-C29
30	6	308	CHL	CBD-CGD-O2D-CED
31	N	304	CLA	C5-C6-C7-C8
31	1	614	CLA	C3-C5-C6-C7
31	3	314	CLA	C3-C5-C6-C7
31	5	611	CLA	C3-C5-C6-C7
31	N	305	CLA	C3-C5-C6-C7
31	7	311	CLA	C3-C5-C6-C7
31	1	603	CLA	CBA-CGA-O2A-C1
31	6	316	CLA	CBA-CGA-O2A-C1
33	t	102	LHG	C24-C23-O8-C6
34	2	621	LMG	C29-C28-O8-C9
31	A	409	CLA	O1D-CGD-O2D-CED
31	a	409	CLA	O1D-CGD-O2D-CED
48	R	302	LMU	O5B-C5B-C6B-O6B
33	8	618	LHG	O9-C7-O7-C5
33	n	320	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
48	r	302	LMU	C4B-C5B-C6B-O6B
33	c	622	LHG	C33-C34-C35-C36
33	K	102	LHG	C2-C3-O3-P
31	4	610	CLA	O1A-CGA-O2A-C1
31	7	315	CLA	O1A-CGA-O2A-C1
31	8	613	CLA	O1A-CGA-O2A-C1
31	c	611	CLA	O1A-CGA-O2A-C1
31	g	305	CLA	O1A-CGA-O2A-C1
30	9	309	CHL	C3-C5-C6-C7
31	4	602	CLA	C8-C10-C11-C12
31	6	311	CLA	C5-C6-C7-C8
31	G	603	CLA	C5-C6-C7-C8
30	1	619	CHL	C4-C3-C5-C6
30	2	608	CHL	C4-C3-C5-C6
30	5	609	CHL	C4-C3-C5-C6
30	6	308	CHL	C4-C3-C5-C6
30	Y	302	CHL	C4-C3-C5-C6
30	0	609	CHL	C4-C3-C5-C6
30	y	606	CHL	C4-C3-C5-C6
31	B	605	CLA	C4-C3-C5-C6
30	1	619	CHL	C2-C3-C5-C6
30	2	608	CHL	C2-C3-C5-C6
30	5	609	CHL	C2-C3-C5-C6
30	6	308	CHL	C2-C3-C5-C6
30	Y	302	CHL	C2-C3-C5-C6
30	0	609	CHL	C2-C3-C5-C6
30	y	606	CHL	C2-C3-C5-C6
31	B	605	CLA	C2-C3-C5-C6
31	B	613	CLA	C2-C3-C5-C6
31	b	603	CLA	C2-C3-C5-C6
31	b	606	CLA	C2-C3-C5-C6
30	1	608	CHL	CBD-CGD-O2D-CED
31	9	305	CLA	CBD-CGD-O2D-CED
33	e	101	LHG	C7-C8-C9-C10
31	2	613	CLA	C2A-CAA-CBA-CGA
31	B	610	CLA	C2A-CAA-CBA-CGA
31	9	312	CLA	C2A-CAA-CBA-CGA
31	p	614	CLA	C2A-CAA-CBA-CGA
31	N	312	CLA	O1D-CGD-O2D-CED
31	R	303	CLA	O1D-CGD-O2D-CED
31	8	603	CLA	O1D-CGD-O2D-CED
31	g	304	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	1	612	CLA	O1A-CGA-O2A-C1
31	2	613	CLA	O1A-CGA-O2A-C1
31	3	312	CLA	O1A-CGA-O2A-C1
31	3	313	CLA	O1A-CGA-O2A-C1
31	6	311	CLA	O1A-CGA-O2A-C1
31	N	315	CLA	O1A-CGA-O2A-C1
31	S	310	CLA	O1A-CGA-O2A-C1
31	n	315	CLA	O1A-CGA-O2A-C1
31	r	307	CLA	O1A-CGA-O2A-C1
31	s	310	CLA	O1A-CGA-O2A-C1
34	q	301	LMG	O6-C1-O1-C7
38	G	617	SQD	O5-C1-O6-C44
38	M	102	SQD	O5-C1-O6-C44
38	S	301	SQD	O5-C1-O6-C44
38	b	621	SQD	O5-C1-O6-C44
38	b	627	SQD	O5-C1-O6-C44
31	2	610	CLA	O1D-CGD-O2D-CED
31	q	306	CLA	O1D-CGD-O2D-CED
44	A	416	PL9	C19-C21-C22-C23
31	3	312	CLA	CBA-CGA-O2A-C1
31	B	605	CLA	CBA-CGA-O2A-C1
31	B	612	CLA	CBA-CGA-O2A-C1
31	C	611	CLA	CBA-CGA-O2A-C1
31	R	307	CLA	CBA-CGA-O2A-C1
31	Y	313	CLA	CBA-CGA-O2A-C1
31	c	607	CLA	CBA-CGA-O2A-C1
31	s	310	CLA	CBA-CGA-O2A-C1
31	y	604	CLA	CBA-CGA-O2A-C1
45	C	618	DGD	C2A-C1A-O1G-C1G
45	c	619	DGD	C2A-C1A-O1G-C1G
31	N	315	CLA	C5-C6-C7-C8
33	q	320	LHG	C34-C35-C36-C37
33	g	319	LHG	C11-C10-C9-C8
30	9	307	CHL	CBD-CGD-O2D-CED
31	4	603	CLA	O1D-CGD-O2D-CED
48	r	302	LMU	O5B-C5B-C6B-O6B
33	d	408	LHG	C31-C32-C33-C34
48	r	302	LMU	C5-C6-C7-C8
31	B	601	CLA	O1D-CGD-O2D-CED
31	B	607	CLA	O1D-CGD-O2D-CED
31	C	613	CLA	O1D-CGD-O2D-CED
31	N	303	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	Y	304	CLA	O1D-CGD-O2D-CED
31	9	304	CLA	O1D-CGD-O2D-CED
31	9	312	CLA	O1D-CGD-O2D-CED
31	c	612	CLA	O1D-CGD-O2D-CED
31	c	613	CLA	O1D-CGD-O2D-CED
31	d	404	CLA	O1D-CGD-O2D-CED
31	n	311	CLA	O1D-CGD-O2D-CED
31	s	310	CLA	O1D-CGD-O2D-CED
31	y	604	CLA	O1D-CGD-O2D-CED
33	t	102	LHG	O10-C23-O8-C6
33	R	320	LHG	C8-C7-O7-C5
34	2	620	LMG	C11-C10-O7-C8
34	0	622	LMG	C11-C10-O7-C8
34	w	202	LMG	C11-C10-O7-C8
31	5	613	CLA	C5-C6-C7-C8
33	j	102	LHG	C24-C25-C26-C27
44	A	416	PL9	C12-C13-C14-C15
30	n	301	CHL	O1D-CGD-O2D-CED
31	1	604	CLA	O1D-CGD-O2D-CED
31	3	311	CLA	O1D-CGD-O2D-CED
31	C	610	CLA	O1D-CGD-O2D-CED
31	G	610	CLA	O1D-CGD-O2D-CED
31	R	316	CLA	O1D-CGD-O2D-CED
31	7	303	CLA	O1D-CGD-O2D-CED
31	b	616	CLA	O1D-CGD-O2D-CED
31	c	604	CLA	O1D-CGD-O2D-CED
31	g	303	CLA	O1D-CGD-O2D-CED
31	s	312	CLA	O1D-CGD-O2D-CED
31	7	312	CLA	CBD-CGD-O2D-CED
31	y	611	CLA	CBD-CGD-O2D-CED
31	g	304	CLA	C5-C6-C7-C8
31	s	303	CLA	C8-C10-C11-C12
31	9	304	CLA	C2C-C3C-CAC-CBC
31	s	315	CLA	O1D-CGD-O2D-CED
33	2	617	LHG	C1-C2-C3-O3
33	5	619	LHG	C1-C2-C3-O3
33	6	320	LHG	C1-C2-C3-O3
33	A	417	LHG	C1-C2-C3-O3
33	G	618	LHG	C1-C2-C3-O3
33	L	101	LHG	C1-C2-C3-O3
33	N	319	LHG	C1-C2-C3-O3
33	b	625	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	c	622	LHG	C1-C2-C3-O3
33	g	319	LHG	C1-C2-C3-O3
33	j	102	LHG	C1-C2-C3-O3
33	l	101	LHG	C1-C2-C3-O3
33	F1	301	LHG	C1-C2-C3-O3
33	N	319	LHG	O9-C7-O7-C5
34	1	618	LMG	O9-C10-O7-C8
34	2	618	LMG	O9-C10-O7-C8
34	J	101	LMG	O9-C10-O7-C8
34	s	321	LMG	O9-C10-O7-C8
31	3	311	CLA	O1A-CGA-O2A-C1
31	A	406	CLA	O1A-CGA-O2A-C1
31	B	612	CLA	O1A-CGA-O2A-C1
31	C	611	CLA	O1A-CGA-O2A-C1
31	R	307	CLA	O1A-CGA-O2A-C1
31	p	611	CLA	O1A-CGA-O2A-C1
33	5	619	LHG	O10-C23-O8-C6
45	C	618	DGD	O1A-C1A-O1G-C1G
31	B	607	CLA	C3-C5-C6-C7
31	c	611	CLA	C3-C5-C6-C7
31	N	310	CLA	O1D-CGD-O2D-CED
31	Y	312	CLA	O1D-CGD-O2D-CED
31	0	602	CLA	O1D-CGD-O2D-CED
31	8	602	CLA	O1D-CGD-O2D-CED
31	b	612	CLA	O1D-CGD-O2D-CED
31	n	304	CLA	O1D-CGD-O2D-CED
31	r	303	CLA	O1D-CGD-O2D-CED
31	1	602	CLA	CBA-CGA-O2A-C1
31	3	311	CLA	CBA-CGA-O2A-C1
31	3	316	CLA	CBA-CGA-O2A-C1
31	A	406	CLA	CBA-CGA-O2A-C1
31	C	607	CLA	CBA-CGA-O2A-C1
31	C	610	CLA	CBA-CGA-O2A-C1
31	G	604	CLA	CBA-CGA-O2A-C1
31	G	610	CLA	CBA-CGA-O2A-C1
31	N	305	CLA	CBA-CGA-O2A-C1
31	N	321	CLA	CBA-CGA-O2A-C1
31	R	314	CLA	CBA-CGA-O2A-C1
31	0	603	CLA	CBA-CGA-O2A-C1
31	8	604	CLA	CBA-CGA-O2A-C1
31	8	614	CLA	CBA-CGA-O2A-C1
31	9	304	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	9	312	CLA	CBA-CGA-O2A-C1
31	p	611	CLA	CBA-CGA-O2A-C1
31	q	316	CLA	CBA-CGA-O2A-C1
31	a	407	CLA	CBA-CGA-O2A-C1
31	b	606	CLA	CBA-CGA-O2A-C1
31	b	612	CLA	CBA-CGA-O2A-C1
31	d	405	CLA	CBA-CGA-O2A-C1
31	g	311	CLA	CBA-CGA-O2A-C1
31	n	305	CLA	CBA-CGA-O2A-C1
31	n	316	CLA	CBA-CGA-O2A-C1
33	G	618	LHG	C24-C23-O8-C6
38	M	102	SQD	C24-C23-O48-C46
38	m	101	SQD	C24-C23-O48-C46
42	a	408	PHO	CBA-CGA-O2A-C1
45	c	618	DGD	C2A-C1A-O1G-C1G
30	N	309	CHL	CBD-CGD-O2D-CED
31	4	604	CLA	CBD-CGD-O2D-CED
33	M	101	LHG	C34-C35-C36-C37
35	2	614	RRX	C9-C10-C11-C12
36	5	618	NEX	C29-C30-C31-C32
36	N	318	NEX	C13-C14-C15-C35
43	B	618	BCR	C19-C20-C21-C22
43	B	619	BCR	C9-C10-C11-C12
43	T	101	BCR	C19-C20-C21-C22
43	c	615	BCR	C9-C10-C11-C12
33	d	408	LHG	C23-C24-C25-C26
33	p	619	LHG	C24-C25-C26-C27
31	c	612	CLA	C5-C6-C7-C8
33	6	320	LHG	C11-C10-C9-C8
31	r	307	CLA	O1D-CGD-O2D-CED
31	2	613	CLA	C5-C6-C7-C8
33	M	101	LHG	C26-C27-C28-C29
33	b	628	LHG	C29-C30-C31-C32
33	y	619	LHG	C29-C30-C31-C32
48	R	302	LMU	C4B-C5B-C6B-O6B
31	A	409	CLA	C8-C10-C11-C12
31	B	606	CLA	C13-C15-C16-C17
31	a	409	CLA	C8-C10-C11-C12
33	4	618	LHG	O2-C2-C3-O3
33	6	320	LHG	O2-C2-C3-O3
33	A	415	LHG	O2-C2-C3-O3
33	D	407	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	O2-C2-C3-O3
33	S	320	LHG	O2-C2-C3-O3
33	7	319	LHG	O2-C2-C3-O3
33	a	415	LHG	O2-C2-C3-O3
33	d	408	LHG	O2-C2-C3-O3
33	l	101	LHG	O2-C2-C3-O3
33	t	102	LHG	O2-C2-C3-O3
33	y	619	LHG	O2-C2-C3-O3
33	3	320	LHG	C7-C8-C9-C10
33	S	322	LHG	C23-C24-C25-C26
33	p	619	LHG	C7-C8-C9-C10
33	b	625	LHG	C23-C24-C25-C26
33	F1	301	LHG	C23-C24-C25-C26
31	5	603	CLA	C3-C5-C6-C7
34	4	621	LMG	C2-C1-O1-C7
34	W	202	LMG	C2-C1-O1-C7
34	9	301	LMG	C2-C1-O1-C7
34	a	413	LMG	C2-C1-O1-C7
34	b	624	LMG	C2-C1-O1-C7
34	m	102	LMG	C2-C1-O1-C7
34	n	321	LMG	C2-C1-O1-C7
34	n	322	LMG	C2-C1-O1-C7
34	r	321	LMG	C2-C1-O1-C7
34	Q1	101	LMG	C2-C1-O1-C7
38	B	620	SQD	C2-C1-O6-C44
38	M	102	SQD	C2-C1-O6-C44
38	b	627	SQD	C2-C1-O6-C44
33	4	618	LHG	O7-C5-C6-O8
33	R	320	LHG	O7-C5-C6-O8
33	8	618	LHG	O7-C5-C6-O8
33	9	320	LHG	O7-C5-C6-O8
33	e	101	LHG	O7-C5-C6-O8
33	n	320	LHG	O7-C5-C6-O8
45	c	617	DGD	C2A-C1A-O1G-C1G
33	C	623	LHG	C26-C27-C28-C29
34	q	302	LMG	C31-C32-C33-C34
31	1	602	CLA	O1A-CGA-O2A-C1
31	G	610	CLA	O1A-CGA-O2A-C1
31	N	305	CLA	O1A-CGA-O2A-C1
31	8	604	CLA	O1A-CGA-O2A-C1
31	8	614	CLA	O1A-CGA-O2A-C1
31	a	407	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	d	405	CLA	O1A-CGA-O2A-C1
31	n	305	CLA	O1A-CGA-O2A-C1
31	3	301	CLA	C4-C3-C5-C6
30	G	601	CHL	C2-C3-C5-C6
30	7	310	CHL	C2-C3-C5-C6
31	D	403	CLA	C2-C3-C5-C6
31	p	602	CLA	C2-C3-C5-C6
31	b	605	CLA	C2-C3-C5-C6
31	s	310	CLA	C2-C3-C5-C6
44	A	416	PL9	C43-C44-C46-C47
30	1	605	CHL	C6-C7-C8-C9
30	1	605	CHL	C11-C10-C8-C9
30	1	607	CHL	C14-C13-C15-C16
30	3	310	CHL	C11-C10-C8-C9
30	6	308	CHL	C11-C10-C8-C9
30	6	308	CHL	C14-C13-C15-C16
30	6	310	CHL	C11-C10-C8-C9
30	G	623	CHL	C11-C10-C8-C9
30	G	623	CHL	C14-C13-C15-C16
30	N	306	CHL	C11-C10-C8-C9
30	N	309	CHL	C11-C10-C8-C9
30	Y	309	CHL	C11-C10-C8-C9
30	0	607	CHL	C11-C10-C8-C9
30	0	607	CHL	C14-C13-C15-C16
30	7	306	CHL	C11-C10-C8-C9
30	7	307	CHL	C11-C10-C8-C9
30	7	308	CHL	C14-C13-C15-C16
30	8	605	CHL	C11-C10-C8-C9
30	9	303	CHL	C14-C13-C15-C16
30	9	311	CHL	C6-C7-C8-C9
30	9	311	CHL	C11-C10-C8-C9
30	g	302	CHL	C11-C10-C8-C9
30	n	306	CHL	C11-C10-C8-C9
30	y	601	CHL	C11-C10-C8-C9
30	y	607	CHL	C14-C13-C15-C16
31	1	604	CLA	C6-C7-C8-C9
31	2	602	CLA	C11-C10-C8-C9
31	2	610	CLA	C6-C7-C8-C9
31	3	316	CLA	C6-C7-C8-C9
31	5	602	CLA	C6-C7-C8-C9
31	5	610	CLA	C6-C7-C8-C9
31	5	611	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	6	303	CLA	C6-C7-C8-C9
31	6	303	CLA	C11-C10-C8-C9
31	6	312	CLA	C11-C10-C8-C9
31	A	406	CLA	C14-C13-C15-C16
31	A	409	CLA	C6-C7-C8-C9
31	B	605	CLA	C11-C10-C8-C9
31	B	607	CLA	C11-C12-C13-C14
31	C	601	CLA	C11-C12-C13-C14
31	C	607	CLA	C14-C13-C15-C16
31	C	608	CLA	C11-C10-C8-C9
31	C	613	CLA	C11-C12-C13-C14
31	D	404	CLA	C6-C7-C8-C9
31	N	303	CLA	C11-C10-C8-C9
31	N	303	CLA	C11-C12-C13-C14
31	N	310	CLA	C6-C7-C8-C9
31	R	304	CLA	C6-C7-C8-C9
31	R	311	CLA	C11-C10-C8-C9
31	R	316	CLA	C14-C13-C15-C16
31	S	305	CLA	C6-C7-C8-C9
31	Y	311	CLA	C11-C12-C13-C14
31	Y	312	CLA	C11-C12-C13-C14
31	7	311	CLA	C11-C10-C8-C9
31	7	313	CLA	C11-C10-C8-C9
31	9	304	CLA	C11-C10-C8-C9
31	p	602	CLA	C6-C7-C8-C9
31	p	610	CLA	C6-C7-C8-C9
31	a	409	CLA	C6-C7-C8-C9
31	b	605	CLA	C6-C7-C8-C9
31	b	606	CLA	C14-C13-C15-C16
31	b	609	CLA	C14-C13-C15-C16
31	b	611	CLA	C6-C7-C8-C9
31	b	611	CLA	C11-C12-C13-C14
31	b	612	CLA	C6-C7-C8-C9
31	b	612	CLA	C11-C12-C13-C14
31	b	614	CLA	C6-C7-C8-C9
31	b	616	CLA	C11-C10-C8-C9
31	c	608	CLA	C6-C7-C8-C9
31	c	613	CLA	C14-C13-C15-C16
31	d	404	CLA	C6-C7-C8-C9
31	g	313	CLA	C6-C7-C8-C9
31	n	311	CLA	C6-C7-C8-C9
31	r	304	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	r	311	CLA	C11-C10-C8-C9
31	s	310	CLA	C6-C7-C8-C9
31	s	312	CLA	C6-C7-C8-C9
31	y	613	CLA	C11-C10-C8-C9
30	q	310	CHL	O1D-CGD-O2D-CED
31	1	602	CLA	O1D-CGD-O2D-CED
31	S	312	CLA	O1D-CGD-O2D-CED
31	Y	311	CLA	O1D-CGD-O2D-CED
31	g	310	CLA	O1D-CGD-O2D-CED
31	y	615	CLA	O1D-CGD-O2D-CED
31	2	602	CLA	C2C-C3C-CAC-CBC
31	C	603	CLA	C8-C10-C11-C12
31	C	610	CLA	C13-C15-C16-C17
31	c	610	CLA	C15-C16-C17-C18
42	A	408	PHO	C8-C10-C11-C12
30	4	608	CHL	C2A-CAA-CBA-CGA
30	N	306	CHL	C2A-CAA-CBA-CGA
30	Y	307	CHL	C2A-CAA-CBA-CGA
30	q	310	CHL	C2A-CAA-CBA-CGA
31	1	614	CLA	C2A-CAA-CBA-CGA
31	3	306	CLA	C2A-CAA-CBA-CGA
31	4	610	CLA	C2A-CAA-CBA-CGA
31	4	613	CLA	C2A-CAA-CBA-CGA
31	B	604	CLA	C2A-CAA-CBA-CGA
31	7	315	CLA	C2A-CAA-CBA-CGA
32	3	318	LUT	C7-C8-C9-C19
32	5	617	LUT	C11-C12-C13-C20
32	6	318	LUT	C11-C12-C13-C20
32	G	615	LUT	C7-C8-C9-C19
32	G	615	LUT	C27-C28-C29-C39
32	N	316	LUT	C7-C8-C9-C19
32	N	316	LUT	C31-C32-C33-C40
32	N	317	LUT	C11-C12-C13-C20
32	R	317	LUT	C7-C8-C9-C19
32	R	317	LUT	C31-C32-C33-C40
32	8	616	LUT	C7-C8-C9-C19
32	p	616	LUT	C7-C8-C9-C19
32	p	616	LUT	C11-C12-C13-C20
32	g	316	LUT	C27-C28-C29-C39
32	n	318	LUT	C7-C8-C9-C19
36	6	319	NEX	C31-C32-C33-C40
36	R	319	NEX	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
36	0	618	NEX	C31-C32-C33-C40
36	p	618	NEX	C11-C12-C13-C20
37	2	619	XAT	C27-C28-C29-C39
37	4	619	XAT	C27-C28-C29-C39
37	G	620	XAT	C27-C28-C29-C39
37	9	322	XAT	C27-C28-C29-C39
37	q	321	XAT	C27-C28-C29-C39
37	g	321	XAT	C27-C28-C29-C39
43	B	617	BCR	C36-C18-C19-C20
43	C	614	BCR	C7-C8-C9-C34
43	V	101	BCR	C36-C18-C19-C20
43	Z	101	BCR	C7-C8-C9-C34
43	a	410	BCR	C36-C18-C19-C20
43	b	618	BCR	C36-C18-C19-C20
43	b	619	BCR	C11-C12-C13-C35
43	b	619	BCR	C37-C22-C23-C24
43	c	614	BCR	C7-C8-C9-C34
43	c	614	BCR	C11-C12-C13-C35
43	d	406	BCR	C11-C12-C13-C35
43	d	406	BCR	C37-C22-C23-C24
43	h	101	BCR	C11-C12-C13-C35
43	v	101	BCR	C36-C18-C19-C20
43	v	101	BCR	C37-C22-C23-C24
32	3	318	LUT	C7-C8-C9-C10
32	5	617	LUT	C11-C12-C13-C14
32	G	615	LUT	C7-C8-C9-C10
32	G	615	LUT	C27-C28-C29-C30
32	N	316	LUT	C7-C8-C9-C10
32	R	317	LUT	C7-C8-C9-C10
32	R	317	LUT	C31-C32-C33-C34
32	Y	316	LUT	C7-C8-C9-C10
32	7	317	LUT	C7-C8-C9-C10
32	8	616	LUT	C7-C8-C9-C10
32	p	616	LUT	C7-C8-C9-C10
32	p	616	LUT	C31-C32-C33-C34
32	g	316	LUT	C27-C28-C29-C30
32	n	318	LUT	C7-C8-C9-C10
35	g	315	RRX	C21-C22-C23-C24
36	6	319	NEX	C31-C32-C33-C34
36	0	618	NEX	C31-C32-C33-C34
37	2	619	XAT	C27-C28-C29-C30
37	4	619	XAT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
37	G	620	XAT	C27-C28-C29-C30
37	9	322	XAT	C27-C28-C29-C30
37	q	321	XAT	C27-C28-C29-C30
37	g	321	XAT	C27-C28-C29-C30
43	B	617	BCR	C17-C18-C19-C20
43	C	614	BCR	C7-C8-C9-C10
43	V	101	BCR	C17-C18-C19-C20
43	b	618	BCR	C21-C22-C23-C24
43	b	619	BCR	C11-C12-C13-C14
43	c	614	BCR	C7-C8-C9-C10
43	c	614	BCR	C11-C12-C13-C14
43	d	406	BCR	C11-C12-C13-C14
43	d	406	BCR	C21-C22-C23-C24
43	h	101	BCR	C11-C12-C13-C14
43	v	101	BCR	C17-C18-C19-C20
34	3	321	LMG	C11-C10-O7-C8
34	B	625	LMG	C11-C10-O7-C8
34	W	201	LMG	C11-C10-O7-C8
34	X	203	LMG	C11-C10-O7-C8
34	n	321	LMG	C11-C10-O7-C8
33	A	417	LHG	C31-C32-C33-C34
34	r	321	LMG	C11-C12-C13-C14
33	M	101	LHG	C23-C24-C25-C26
33	F1	301	LHG	C7-C8-C9-C10
31	3	316	CLA	O1A-CGA-O2A-C1
31	N	321	CLA	O1A-CGA-O2A-C1
31	9	304	CLA	O1A-CGA-O2A-C1
31	q	316	CLA	O1A-CGA-O2A-C1
31	b	606	CLA	O1A-CGA-O2A-C1
31	n	316	CLA	O1A-CGA-O2A-C1
42	a	408	PHO	O1A-CGA-O2A-C1
31	6	312	CLA	C5-C6-C7-C8
31	B	603	CLA	C15-C16-C17-C18
31	B	616	CLA	C5-C6-C7-C8
31	b	612	CLA	C8-C10-C11-C12
31	c	601	CLA	C8-C10-C11-C12
30	1	607	CHL	O1D-CGD-O2D-CED
30	g	308	CHL	O1D-CGD-O2D-CED
31	n	303	CLA	O1D-CGD-O2D-CED
33	C	623	LHG	C33-C34-C35-C36
30	7	306	CHL	CBD-CGD-O2D-CED
31	G	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	G	604	CLA	O1D-CGD-O2D-CED
31	G	610	CLA	C3-C5-C6-C7
31	g	303	CLA	C3-C5-C6-C7
31	c	608	CLA	CBA-CGA-O2A-C1
33	g	319	LHG	C24-C23-O8-C6
34	A	412	LMG	C29-C28-O8-C9
31	1	613	CLA	C15-C16-C17-C18
31	R	311	CLA	C5-C6-C7-C8
31	S	303	CLA	C5-C6-C7-C8
31	S	312	CLA	C10-C11-C12-C13
31	0	602	CLA	C5-C6-C7-C8
31	q	306	CLA	C5-C6-C7-C8
31	a	407	CLA	C13-C15-C16-C17
31	b	607	CLA	C13-C15-C16-C17
31	c	606	CLA	C8-C10-C11-C12
31	s	310	CLA	C5-C6-C7-C8
31	y	613	CLA	C8-C10-C11-C12
34	w	202	LMG	C29-C30-C31-C32
33	2	617	LHG	C7-C8-C9-C10
33	4	618	LHG	C23-C24-C25-C26
33	A	415	LHG	C7-C8-C9-C10
33	D	407	LHG	C23-C24-C25-C26
33	0	619	LHG	C7-C8-C9-C10
33	9	320	LHG	C7-C8-C9-C10
34	n	322	LMG	C28-C29-C30-C31
38	b	627	SQD	C7-C8-C9-C10
31	R	315	CLA	O1D-CGD-O2D-CED
31	N	304	CLA	CBD-CGD-O2D-CED
36	g	317	NEX	C14-C15-C35-C34
30	y	607	CHL	C8-C10-C11-C12
31	1	612	CLA	C8-C10-C11-C12
31	A	409	CLA	C5-C6-C7-C8
31	B	606	CLA	C8-C10-C11-C12
31	B	609	CLA	C8-C10-C11-C12
31	C	613	CLA	C5-C6-C7-C8
31	G	604	CLA	C5-C6-C7-C8
31	S	303	CLA	C8-C10-C11-C12
31	S	314	CLA	C13-C15-C16-C17
31	8	612	CLA	C5-C6-C7-C8
31	p	602	CLA	C5-C6-C7-C8
31	a	409	CLA	C5-C6-C7-C8
31	b	606	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	n	314	CLA	C5-C6-C7-C8
31	s	311	CLA	C8-C10-C11-C12
31	s	311	CLA	C10-C11-C12-C13
31	s	312	CLA	C13-C15-C16-C17
31	y	611	CLA	C13-C15-C16-C17
44	D	406	PL9	C47-C48-C49-C51
31	R	307	CLA	O1D-CGD-O2D-CED
31	9	316	CLA	O1D-CGD-O2D-CED
31	n	305	CLA	O1D-CGD-O2D-CED
33	C	623	LHG	O1-C1-C2-O2
33	D	407	LHG	O1-C1-C2-O2
33	S	322	LHG	O1-C1-C2-O2
33	7	319	LHG	O1-C1-C2-O2
33	9	320	LHG	O1-C1-C2-O2
33	b	628	LHG	O1-C1-C2-O2
33	l	101	LHG	O1-C1-C2-O2
33	z	102	LHG	O1-C1-C2-O2
33	3	320	LHG	C23-C24-C25-C26
33	6	320	LHG	C23-C24-C25-C26
33	B	624	LHG	C7-C8-C9-C10
33	B	624	LHG	C23-C24-C25-C26
33	C	623	LHG	C7-C8-C9-C10
33	C	623	LHG	C23-C24-C25-C26
33	G	618	LHG	C23-C24-C25-C26
33	K	102	LHG	C7-C8-C9-C10
33	M	101	LHG	C7-C8-C9-C10
33	N	319	LHG	C23-C24-C25-C26
33	7	319	LHG	C7-C8-C9-C10
33	b	628	LHG	C7-C8-C9-C10
33	b	628	LHG	C23-C24-C25-C26
33	g	319	LHG	C23-C24-C25-C26
33	s	320	LHG	C7-C8-C9-C10
33	s	320	LHG	C23-C24-C25-C26
33	t	102	LHG	C7-C8-C9-C10
33	z	102	LHG	C23-C24-C25-C26
34	J	101	LMG	C10-C11-C12-C13
34	n	321	LMG	C28-C29-C30-C31
45	C	616	DGD	O6E-C5E-C6E-O5E
38	s	301	SQD	C30-C31-C32-C33
31	6	315	CLA	CBD-CGD-O2D-CED
42	d	402	PHO	CBD-CGD-O2D-CED
30	1	601	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	y	607	CHL	C5-C6-C7-C8
31	R	305	CLA	C8-C10-C11-C12
31	7	313	CLA	C13-C15-C16-C17
31	a	406	CLA	C15-C16-C17-C18
31	y	610	CLA	C8-C10-C11-C12
31	N	313	CLA	C3-C5-C6-C7
31	3	306	CLA	CBA-CGA-O2A-C1
31	B	603	CLA	CBA-CGA-O2A-C1
31	R	304	CLA	CBA-CGA-O2A-C1
31	S	305	CLA	CBA-CGA-O2A-C1
31	b	614	CLA	CBA-CGA-O2A-C1
31	0	610	CLA	O1D-CGD-O2D-CED
31	0	612	CLA	O1D-CGD-O2D-CED
31	8	604	CLA	O1D-CGD-O2D-CED
31	b	603	CLA	O1D-CGD-O2D-CED
34	x	202	LMG	O6-C5-C6-O5
34	2	620	LMG	O9-C10-O7-C8
34	B	621	LMG	O9-C10-O7-C8
34	W	201	LMG	O9-C10-O7-C8
34	0	622	LMG	O9-C10-O7-C8
34	7	320	LMG	O9-C10-O7-C8
31	1	603	CLA	C2-C1-O2A-CGA
31	1	604	CLA	C2-C1-O2A-CGA
31	3	315	CLA	C2-C1-O2A-CGA
31	6	315	CLA	C2-C1-O2A-CGA
31	A	407	CLA	C2-C1-O2A-CGA
31	B	601	CLA	C2-C1-O2A-CGA
31	C	602	CLA	C2-C1-O2A-CGA
31	0	614	CLA	C2-C1-O2A-CGA
31	7	305	CLA	C2-C1-O2A-CGA
31	9	312	CLA	C2-C1-O2A-CGA
31	p	604	CLA	C2-C1-O2A-CGA
31	p	614	CLA	C2-C1-O2A-CGA
31	q	306	CLA	C2-C1-O2A-CGA
31	a	407	CLA	C2-C1-O2A-CGA
31	b	605	CLA	C2-C1-O2A-CGA
31	b	613	CLA	C2-C1-O2A-CGA
31	b	614	CLA	C2-C1-O2A-CGA
31	b	616	CLA	C2-C1-O2A-CGA
31	c	602	CLA	C2-C1-O2A-CGA
31	d	401	CLA	C2-C1-O2A-CGA
31	d	405	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
33	9	320	LHG	C24-C25-C26-C27
31	2	602	CLA	C13-C15-C16-C17
31	6	312	CLA	C10-C11-C12-C13
31	B	602	CLA	C15-C16-C17-C18
31	B	614	CLA	C8-C10-C11-C12
31	G	610	CLA	C5-C6-C7-C8
33	4	618	LHG	C7-C8-C9-C10
33	S	320	LHG	C23-C24-C25-C26
33	0	619	LHG	C23-C24-C25-C26
33	7	319	LHG	C23-C24-C25-C26
33	q	320	LHG	C7-C8-C9-C10
45	c	618	DGD	C1B-C2B-C3B-C4B
30	G	606	CHL	CBD-CGD-O2D-CED
30	r	309	CHL	CBD-CGD-O2D-CED
31	7	316	CLA	CBD-CGD-O2D-CED
34	5	620	LMG	C12-C13-C14-C15
34	G	619	LMG	C11-C10-O7-C8
34	Y	319	LMG	C11-C10-O7-C8
31	B	608	CLA	C15-C16-C17-C18
31	S	312	CLA	C5-C6-C7-C8
31	b	607	CLA	C10-C11-C12-C13
30	G	601	CHL	C4-C3-C5-C6
30	Y	309	CHL	C11-C12-C13-C15
30	q	309	CHL	C6-C7-C8-C10
31	1	611	CLA	C11-C10-C8-C7
31	1	612	CLA	C6-C7-C8-C10
31	3	316	CLA	C11-C10-C8-C7
31	4	613	CLA	C11-C10-C8-C7
31	6	314	CLA	C11-C10-C8-C7
31	B	605	CLA	C11-C12-C13-C15
31	C	603	CLA	C6-C7-C8-C10
31	0	610	CLA	C6-C7-C8-C10
31	7	312	CLA	C11-C10-C8-C7
31	a	406	CLA	C11-C10-C8-C7
31	b	608	CLA	C11-C10-C8-C7
31	b	613	CLA	C6-C7-C8-C10
31	b	614	CLA	C11-C12-C13-C15
31	c	603	CLA	C6-C7-C8-C10
48	r	302	LMU	C1-C2-C3-C4
31	Y	304	CLA	C3-C5-C6-C7
31	C	607	CLA	O1A-CGA-O2A-C1
31	C	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	G	604	CLA	O1A-CGA-O2A-C1
31	Y	313	CLA	O1A-CGA-O2A-C1
31	0	603	CLA	O1A-CGA-O2A-C1
31	b	612	CLA	O1A-CGA-O2A-C1
38	m	101	SQD	O10-C23-O48-C46
32	3	318	LUT	C9-C10-C11-C12
32	4	616	LUT	C9-C10-C11-C12
36	g	317	NEX	C13-C14-C15-C35
36	n	319	NEX	C9-C10-C11-C12
43	B	618	BCR	C9-C10-C11-C12
43	D	405	BCR	C15-C16-C17-C18
43	V	101	BCR	C15-C16-C17-C18
43	b	620	BCR	C9-C10-C11-C12
43	c	614	BCR	C15-C16-C17-C18
31	C	608	CLA	CBA-CGA-O2A-C1
33	b	625	LHG	C24-C23-O8-C6
30	5	608	CHL	C2A-CAA-CBA-CGA
30	G	623	CHL	C2A-CAA-CBA-CGA
30	Y	301	CHL	C2A-CAA-CBA-CGA
30	Y	302	CHL	C2A-CAA-CBA-CGA
30	0	601	CHL	C2A-CAA-CBA-CGA
30	0	607	CHL	C2A-CAA-CBA-CGA
30	8	601	CHL	C2A-CAA-CBA-CGA
30	9	308	CHL	C2A-CAA-CBA-CGA
30	n	302	CHL	C2A-CAA-CBA-CGA
30	y	607	CHL	C2A-CAA-CBA-CGA
31	2	604	CLA	C2A-CAA-CBA-CGA
31	5	603	CLA	C2A-CAA-CBA-CGA
31	5	610	CLA	C2A-CAA-CBA-CGA
31	R	312	CLA	C2A-CAA-CBA-CGA
31	p	603	CLA	C2A-CAA-CBA-CGA
30	4	609	CHL	O1D-CGD-O2D-CED
30	N	301	CHL	O1D-CGD-O2D-CED
30	q	307	CHL	O1D-CGD-O2D-CED
30	q	309	CHL	O1D-CGD-O2D-CED
31	5	612	CLA	O1D-CGD-O2D-CED
31	6	305	CLA	O1D-CGD-O2D-CED
31	C	601	CLA	O1D-CGD-O2D-CED
31	7	313	CLA	O1D-CGD-O2D-CED
31	c	601	CLA	O1D-CGD-O2D-CED
31	c	607	CLA	O1D-CGD-O2D-CED
31	y	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	4	613	CLA	C8-C10-C11-C12
31	D	403	CLA	C15-C16-C17-C18
31	7	313	CLA	C8-C10-C11-C12
31	8	612	CLA	C8-C10-C11-C12
31	b	607	CLA	C8-C10-C11-C12
31	b	613	CLA	C8-C10-C11-C12
31	b	617	CLA	C5-C6-C7-C8
31	c	611	CLA	C5-C6-C7-C8
31	n	314	CLA	C8-C10-C11-C12
31	s	310	CLA	C8-C10-C11-C12
31	y	611	CLA	C15-C16-C17-C18
31	y	612	CLA	C15-C16-C17-C18
31	B	605	CLA	O1A-CGA-O2A-C1
31	R	314	CLA	O1A-CGA-O2A-C1
31	c	607	CLA	O1A-CGA-O2A-C1
33	G	618	LHG	O10-C23-O8-C6
38	M	102	SQD	O10-C23-O48-C46
30	N	308	CHL	CBD-CGD-O2D-CED
30	y	607	CHL	CBD-CGD-O2D-CED
34	B	621	LMG	O6-C1-O1-C7
34	j	101	LMG	O6-C1-O1-C7
38	X	201	SQD	O5-C1-O6-C44
31	2	602	CLA	C15-C16-C17-C18
31	C	603	CLA	C10-C11-C12-C13
31	S	313	CLA	C5-C6-C7-C8
31	g	310	CLA	C8-C10-C11-C12
31	y	602	CLA	O1D-CGD-O2D-CED
44	A	416	PL9	C44-C46-C47-C48
44	D	406	PL9	C44-C46-C47-C48
33	7	319	LHG	C10-C11-C12-C13
33	8	618	LHG	C23-C24-C25-C26
33	c	622	LHG	C7-C8-C9-C10
33	n	320	LHG	C23-C24-C25-C26
36	8	617	NEX	C10-C11-C12-C13
36	p	618	NEX	C30-C31-C32-C33
36	q	319	NEX	C30-C31-C32-C33
37	R	318	XAT	C10-C11-C12-C13
37	r	318	XAT	C10-C11-C12-C13
33	4	618	LHG	C16-C17-C18-C19
34	2	618	LMG	C35-C36-C37-C38
34	6	321	LMG	C35-C36-C37-C38
34	A	418	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
34	C	621	LMG	C35-C36-C37-C38
34	G	619	LMG	C35-C36-C37-C38
34	W	203	LMG	C35-C36-C37-C38
34	X	203	LMG	C35-C36-C37-C38
34	Y	319	LMG	C35-C36-C37-C38
34	0	620	LMG	C35-C36-C37-C38
34	0	622	LMG	C35-C36-C37-C38
34	7	301	LMG	C17-C18-C19-C20
34	a	416	LMG	C35-C36-C37-C38
34	f	101	LMG	C35-C36-C37-C38
34	g	320	LMG	C35-C36-C37-C38
34	w	204	LMG	C35-C36-C37-C38
45	C	616	DGD	C8B-C9B-CAB-CBB
48	R	302	LMU	O1'-C1-C2-C3
31	C	609	CLA	O1D-CGD-O2D-CED
34	W	203	LMG	O6-C5-C6-O5
33	2	617	LHG	O2-C2-C3-O3
33	D	408	LHG	O2-C2-C3-O3
33	G	618	LHG	O2-C2-C3-O3
33	0	619	LHG	O2-C2-C3-O3
33	q	320	LHG	O2-C2-C3-O3
33	b	625	LHG	O2-C2-C3-O3
33	c	622	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
33	g	319	LHG	O2-C2-C3-O3
33	s	320	LHG	O2-C2-C3-O3
33	R	320	LHG	O9-C7-O7-C5
34	3	321	LMG	O9-C10-O7-C8
34	B	625	LMG	O9-C10-O7-C8
34	X	203	LMG	O9-C10-O7-C8
31	2	602	CLA	C3-C5-C6-C7
31	3	311	CLA	C3-C5-C6-C7
31	N	321	CLA	C3-C5-C6-C7
31	7	315	CLA	C3-C5-C6-C7
31	1	604	CLA	C8-C10-C11-C12
31	1	610	CLA	C8-C10-C11-C12
31	C	605	CLA	C5-C6-C7-C8
31	C	611	CLA	C13-C15-C16-C17
31	D	403	CLA	C13-C15-C16-C17
31	G	612	CLA	C5-C6-C7-C8
31	Y	312	CLA	C10-C11-C12-C13
31	Y	313	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	Y	313	CLA	C13-C15-C16-C17
31	0	602	CLA	C13-C15-C16-C17
31	b	604	CLA	C5-C6-C7-C8
31	r	305	CLA	C8-C10-C11-C12
31	s	305	CLA	C8-C10-C11-C12
31	4	604	CLA	CBA-CGA-O2A-C1
31	G	612	CLA	CBA-CGA-O2A-C1
34	6	323	LMG	C35-C36-C37-C38
34	w	203	LMG	C35-C36-C37-C38
34	Q1	101	LMG	C35-C36-C37-C38
38	B	623	SQD	C14-C15-C16-C17
30	Y	308	CHL	O1D-CGD-O2D-CED
31	9	312	CLA	O1A-CGA-O2A-C1
31	g	311	CLA	O1A-CGA-O2A-C1
31	y	604	CLA	O1A-CGA-O2A-C1
45	c	617	DGD	O1A-C1A-O1G-C1G
45	c	618	DGD	O1A-C1A-O1G-C1G
45	c	619	DGD	O1A-C1A-O1G-C1G
33	D	407	LHG	C7-C8-C9-C10
33	L	101	LHG	C23-C24-C25-C26
33	b	625	LHG	C7-C8-C9-C10
33	l	101	LHG	C7-C8-C9-C10
38	a	412	SQD	C7-C8-C9-C10
33	G	618	LHG	C24-C25-C26-C27
33	K	102	LHG	C25-C26-C27-C28
34	6	322	LMG	C17-C18-C19-C20
34	W	202	LMG	C35-C36-C37-C38
34	c	620	LMG	C35-C36-C37-C38
34	x	202	LMG	C35-C36-C37-C38
34	y	620	LMG	C35-C36-C37-C38
31	3	313	CLA	O1D-CGD-O2D-CED
30	1	607	CHL	C5-C6-C7-C8
30	G	623	CHL	C8-C10-C11-C12
31	5	602	CLA	C5-C6-C7-C8
31	A	406	CLA	C13-C15-C16-C17
31	B	604	CLA	C8-C10-C11-C12
31	Y	310	CLA	C5-C6-C7-C8
31	9	304	CLA	C5-C6-C7-C8
31	b	611	CLA	C5-C6-C7-C8
31	b	612	CLA	C13-C15-C16-C17
31	b	614	CLA	C5-C6-C7-C8
31	b	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	c	608	CLA	C10-C11-C12-C13
31	r	305	CLA	C5-C6-C7-C8
31	r	316	CLA	C5-C6-C7-C8
31	s	311	CLA	C15-C16-C17-C18
31	y	610	CLA	C5-C6-C7-C8
33	L	101	LHG	C30-C31-C32-C33
33	0	619	LHG	C9-C10-C11-C12
30	8	601	CHL	CBD-CGD-O2D-CED
30	n	302	CHL	CBD-CGD-O2D-CED
31	B	603	CLA	O1A-CGA-O2A-C1
31	b	614	CLA	O1A-CGA-O2A-C1
33	r	320	LHG	C8-C7-O7-C5
34	9	302	LMG	C11-C10-O7-C8
34	g	322	LMG	C20-C21-C22-C23
30	4	607	CHL	C5-C6-C7-C8
30	y	609	CHL	C5-C6-C7-C8
31	2	610	CLA	C8-C10-C11-C12
31	B	611	CLA	C8-C10-C11-C12
31	B	613	CLA	C5-C6-C7-C8
31	C	605	CLA	C13-C15-C16-C17
31	C	610	CLA	C8-C10-C11-C12
31	C	610	CLA	C15-C16-C17-C18
31	S	311	CLA	C8-C10-C11-C12
31	p	610	CLA	C5-C6-C7-C8
31	b	615	CLA	C8-C10-C11-C12
31	b	617	CLA	C10-C11-C12-C13
31	s	314	CLA	C13-C15-C16-C17
33	1	617	LHG	C3-O3-P-O6
33	1	617	LHG	C4-O6-P-O3
33	2	617	LHG	C3-O3-P-O6
33	5	619	LHG	C4-O6-P-O3
33	A	415	LHG	C3-O3-P-O6
33	A	415	LHG	C4-O6-P-O3
33	D	407	LHG	C4-O6-P-O3
33	D	408	LHG	C3-O3-P-O6
33	G	618	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O3
33	M	101	LHG	C3-O3-P-O6
33	N	319	LHG	C3-O3-P-O6
33	N	319	LHG	C4-O6-P-O3
33	R	320	LHG	C4-O6-P-O3
33	S	322	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
33	S	322	LHG	C4-O6-P-O3
33	Y	318	LHG	C4-O6-P-O3
33	7	319	LHG	C4-O6-P-O3
33	8	618	LHG	C4-O6-P-O3
33	p	619	LHG	C4-O6-P-O3
33	q	320	LHG	C3-O3-P-O6
33	q	320	LHG	C4-O6-P-O3
33	b	628	LHG	C4-O6-P-O3
33	c	622	LHG	C3-O3-P-O6
33	c	622	LHG	C4-O6-P-O3
33	d	408	LHG	C4-O6-P-O3
33	e	101	LHG	C3-O3-P-O6
33	g	319	LHG	C4-O6-P-O3
33	j	102	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O3
33	n	320	LHG	C4-O6-P-O3
33	r	320	LHG	C4-O6-P-O3
33	t	102	LHG	C3-O3-P-O6
33	y	619	LHG	C4-O6-P-O3
33	F1	301	LHG	C3-O3-P-O6
33	a	415	LHG	C7-C8-C9-C10
34	A	414	LMG	C28-C29-C30-C31
44	d	407	PL9	C47-C48-C49-C51
31	C	601	CLA	C3-C5-C6-C7
31	8	614	CLA	C3-C5-C6-C7
31	n	316	CLA	C3-C5-C6-C7
31	Y	314	CLA	CBA-CGA-O2A-C1
31	0	602	CLA	CBA-CGA-O2A-C1
31	a	406	CLA	CBA-CGA-O2A-C1
31	c	605	CLA	CBA-CGA-O2A-C1
31	c	613	CLA	CBA-CGA-O2A-C1
31	r	314	CLA	CBA-CGA-O2A-C1
34	0	622	LMG	C29-C28-O8-C9
31	B	611	CLA	O1D-CGD-O2D-CED
31	N	305	CLA	O1D-CGD-O2D-CED
31	C	602	CLA	C13-C15-C16-C17
31	G	602	CLA	O1D-CGD-O2D-CED
31	p	611	CLA	O1D-CGD-O2D-CED
33	B	624	LHG	C29-C30-C31-C32
31	r	312	CLA	C8-C10-C11-C12
33	K	102	LHG	C23-C24-C25-C26
33	N	319	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	r	320	LHG	C23-C24-C25-C26
34	7	301	LMG	C28-C29-C30-C31
34	b	623	LMG	C28-C29-C30-C31
38	6	301	SQD	C23-C24-C25-C26
38	B	620	SQD	C7-C8-C9-C10
31	p	612	CLA	O1D-CGD-O2D-CED
31	y	612	CLA	O1D-CGD-O2D-CED
33	3	320	LHG	C1-C2-C3-O3
33	A	415	LHG	C1-C2-C3-O3
33	B	624	LHG	C1-C2-C3-O3
33	R	320	LHG	C1-C2-C3-O3
33	0	619	LHG	C1-C2-C3-O3
33	b	628	LHG	C1-C2-C3-O3
33	e	101	LHG	C1-C2-C3-O3
33	s	322	LHG	C1-C2-C3-O3
33	r	320	LHG	O9-C7-O7-C5
34	G	619	LMG	O9-C10-O7-C8
34	Y	319	LMG	O9-C10-O7-C8
34	9	302	LMG	O9-C10-O7-C8
34	n	321	LMG	O9-C10-O7-C8
34	n	322	LMG	O9-C10-O7-C8
34	w	202	LMG	O9-C10-O7-C8
30	3	310	CHL	C4-C3-C5-C6
30	7	310	CHL	C4-C3-C5-C6
30	y	601	CHL	C4-C3-C5-C6
31	7	311	CLA	C4-C3-C5-C6
33	8	618	LHG	C24-C25-C26-C27
33	n	320	LHG	C24-C25-C26-C27
31	Y	310	CLA	C8-C10-C11-C12
31	g	310	CLA	C5-C6-C7-C8
33	A	417	LHG	C29-C30-C31-C32
30	1	619	CHL	C2A-CAA-CBA-CGA
30	3	307	CHL	C2A-CAA-CBA-CGA
30	3	309	CHL	C2A-CAA-CBA-CGA
30	4	605	CHL	C2A-CAA-CBA-CGA
30	5	601	CHL	C2A-CAA-CBA-CGA
30	5	605	CHL	C2A-CAA-CBA-CGA
30	6	308	CHL	C2A-CAA-CBA-CGA
30	G	606	CHL	C2A-CAA-CBA-CGA
30	N	302	CHL	C2A-CAA-CBA-CGA
30	R	308	CHL	C2A-CAA-CBA-CGA
30	7	302	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	7	309	CHL	C2A-CAA-CBA-CGA
30	8	605	CHL	C2A-CAA-CBA-CGA
30	9	307	CHL	C2A-CAA-CBA-CGA
30	9	310	CHL	C2A-CAA-CBA-CGA
30	p	605	CHL	C2A-CAA-CBA-CGA
30	p	606	CHL	C2A-CAA-CBA-CGA
30	p	607	CHL	C2A-CAA-CBA-CGA
30	p	608	CHL	C2A-CAA-CBA-CGA
30	n	306	CHL	C2A-CAA-CBA-CGA
30	r	308	CHL	C2A-CAA-CBA-CGA
30	y	601	CHL	C2A-CAA-CBA-CGA
31	3	311	CLA	C2A-CAA-CBA-CGA
31	G	612	CLA	C2A-CAA-CBA-CGA
31	b	615	CLA	C2A-CAA-CBA-CGA
31	r	316	CLA	C2A-CAA-CBA-CGA
31	3	314	CLA	C6-C7-C8-C9
31	4	603	CLA	C6-C7-C8-C9
31	p	603	CLA	C6-C7-C8-C10
30	7	321	CHL	C3-C5-C6-C7
30	n	308	CHL	C3-C5-C6-C7
31	p	613	CLA	C3-C5-C6-C7
31	s	310	CLA	C3-C5-C6-C7
30	7	310	CHL	O1D-CGD-O2D-CED
31	N	303	CLA	CBA-CGA-O2A-C1
31	S	314	CLA	CBA-CGA-O2A-C1
31	7	303	CLA	CBA-CGA-O2A-C1
31	D	404	CLA	C8-C10-C11-C12
33	L	101	LHG	C7-C8-C9-C10
31	b	605	CLA	C8-C10-C11-C12
43	h	101	BCR	C9-C10-C11-C12
43	v	101	BCR	C13-C14-C15-C16
33	A	417	LHG	C7-C8-C9-C10
33	7	319	LHG	C11-C12-C13-C14
33	g	319	LHG	C11-C12-C13-C14
33	g	319	LHG	C28-C29-C30-C31
34	D	409	LMG	C32-C33-C34-C35
34	q	301	LMG	C16-C17-C18-C19
30	0	607	CHL	O1D-CGD-O2D-CED
31	1	612	CLA	O1D-CGD-O2D-CED
31	c	609	CLA	O1D-CGD-O2D-CED
33	6	320	LHG	C8-C7-O7-C5
33	D	407	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
33	9	320	LHG	C8-C7-O7-C5
33	j	102	LHG	C8-C7-O7-C5
34	C	619	LMG	C11-C10-O7-C8
34	W	202	LMG	C11-C10-O7-C8
34	n	322	LMG	C11-C10-O7-C8
34	w	201	LMG	C11-C10-O7-C8
31	C	609	CLA	C13-C15-C16-C17
31	p	611	CLA	C8-C10-C11-C12
36	2	616	NEX	C40-C33-C34-C35
36	3	319	NEX	C11-C10-C9-C19
36	4	617	NEX	C20-C13-C14-C15
36	N	318	NEX	C20-C13-C14-C15
36	N	318	NEX	C39-C29-C30-C31
36	R	319	NEX	C39-C29-C30-C31
36	R	319	NEX	C40-C33-C34-C35
36	8	617	NEX	C11-C10-C9-C19
36	8	617	NEX	C40-C33-C34-C35
36	p	618	NEX	C39-C29-C30-C31
36	n	319	NEX	C40-C33-C34-C35
36	r	301	NEX	C39-C29-C30-C31
36	r	319	NEX	C39-C29-C30-C31
37	R	318	XAT	C20-C13-C14-C15
31	6	315	CLA	C3-C5-C6-C7
31	c	601	CLA	C3-C5-C6-C7
33	1	617	LHG	C11-C12-C13-C14
33	5	619	LHG	C11-C10-C9-C8
33	S	320	LHG	C29-C30-C31-C32
33	S	322	LHG	C13-C14-C15-C16
33	c	622	LHG	C11-C12-C13-C14
33	c	622	LHG	C13-C14-C15-C16
33	l	101	LHG	C13-C14-C15-C16
33	s	322	LHG	C13-C14-C15-C16
34	W	203	LMG	C30-C31-C32-C33
38	y	621	SQD	C25-C26-C27-C28
31	3	306	CLA	O1A-CGA-O2A-C1
31	A	407	CLA	O1D-CGD-O2D-CED
31	B	610	CLA	O1D-CGD-O2D-CED
31	S	311	CLA	O1D-CGD-O2D-CED
31	b	611	CLA	O1D-CGD-O2D-CED
31	d	401	CLA	O1D-CGD-O2D-CED
31	2	611	CLA	C6-C7-C8-C9
31	6	305	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	0	604	CLA	C6-C7-C8-C9
31	c	612	CLA	C6-C7-C8-C9
31	g	305	CLA	C6-C7-C8-C9
31	r	315	CLA	C6-C7-C8-C9
31	r	316	CLA	C16-C17-C18-C20
31	b	610	CLA	CBA-CGA-O2A-C1
31	c	604	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C11-C12-C13-C14
33	L	101	LHG	C11-C10-C9-C8
33	R	320	LHG	C13-C14-C15-C16
33	S	320	LHG	C9-C10-C11-C12
33	b	625	LHG	C13-C14-C15-C16
33	b	628	LHG	C11-C12-C13-C14
33	s	320	LHG	C29-C30-C31-C32
33	z	102	LHG	C9-C10-C11-C12
33	n	320	LHG	C4-C5-O7-C7
34	q1	101	LMG	C7-C8-O7-C10
33	6	320	LHG	O9-C7-O7-C5
33	D	407	LHG	O9-C7-O7-C5
33	9	320	LHG	O9-C7-O7-C5
33	j	102	LHG	O9-C7-O7-C5
34	C	619	LMG	O9-C10-O7-C8
34	G	621	LMG	O9-C10-O7-C8
34	W	202	LMG	O9-C10-O7-C8
34	w	201	LMG	O9-C10-O7-C8
31	b	616	CLA	C13-C15-C16-C17
31	g	313	CLA	C8-C10-C11-C12
31	r	312	CLA	C5-C6-C7-C8
33	q	320	LHG	C23-C24-C25-C26
34	D	410	LMG	C10-C11-C12-C13
31	a	407	CLA	CBD-CGD-O2D-CED
33	Y	318	LHG	C28-C29-C30-C31
33	g	319	LHG	C34-C35-C36-C37
33	r	320	LHG	C26-C27-C28-C29
33	z	102	LHG	C11-C12-C13-C14
38	B	620	SQD	C31-C32-C33-C34
38	a	411	SQD	C10-C11-C12-C13
31	G	612	CLA	O1A-CGA-O2A-C1
31	c	613	CLA	O1A-CGA-O2A-C1
33	4	618	LHG	C11-C10-C9-C8
33	4	618	LHG	C28-C29-C30-C31
33	D	408	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	M	101	LHG	C30-C31-C32-C33
33	S	322	LHG	C11-C12-C13-C14
33	8	618	LHG	C31-C32-C33-C34
33	n	320	LHG	C31-C32-C33-C34
33	y	619	LHG	C28-C29-C30-C31
38	r	322	SQD	C27-C28-C29-C30
38	s	301	SQD	C11-C10-C9-C8
31	B	615	CLA	O1D-CGD-O2D-CED
31	C	611	CLA	C15-C16-C17-C18
33	D	407	LHG	C13-C14-C15-C16
33	K	102	LHG	C13-C14-C15-C16
33	N	319	LHG	C13-C14-C15-C16
33	8	618	LHG	C15-C16-C17-C18
33	c	622	LHG	C29-C30-C31-C32
33	n	320	LHG	C15-C16-C17-C18
34	4	620	LMG	C16-C17-C18-C19
48	c	623	LMU	O1'-C1-C2-C3
31	y	603	CLA	C3-C5-C6-C7
33	d	408	LHG	C7-C8-C9-C10
30	N	306	CHL	O1D-CGD-O2D-CED
30	R	309	CHL	O1D-CGD-O2D-CED
34	R	321	LMG	C2-C1-O1-C7
34	q	302	LMG	C2-C1-O1-C7
34	j	101	LMG	C2-C1-O1-C7
36	2	616	NEX	C32-C33-C34-C35
36	3	319	NEX	C11-C10-C9-C8
36	4	617	NEX	C12-C13-C14-C15
36	4	617	NEX	C28-C29-C30-C31
36	N	318	NEX	C12-C13-C14-C15
36	N	318	NEX	C28-C29-C30-C31
36	R	319	NEX	C28-C29-C30-C31
36	R	319	NEX	C32-C33-C34-C35
36	8	617	NEX	C11-C10-C9-C8
36	8	617	NEX	C32-C33-C34-C35
36	p	618	NEX	C28-C29-C30-C31
36	q	319	NEX	C28-C29-C30-C31
36	n	319	NEX	C32-C33-C34-C35
36	r	301	NEX	C28-C29-C30-C31
37	R	318	XAT	C12-C13-C14-C15
38	6	301	SQD	C2-C1-O6-C44
38	R	322	SQD	C2-C1-O6-C44
38	X	201	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
45	C	617	DGD	C2E-C1E-O5D-C6D
45	c	617	DGD	C2E-C1E-O5D-C6D
31	r	315	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C15-C16-C17-C18
33	C	623	LHG	C11-C10-C9-C8
33	Y	318	LHG	C11-C10-C9-C8
33	8	618	LHG	C28-C29-C30-C31
33	9	320	LHG	C25-C26-C27-C28
33	p	619	LHG	C11-C12-C13-C14
33	p	619	LHG	C26-C27-C28-C29
33	b	625	LHG	C26-C27-C28-C29
33	c	622	LHG	C9-C10-C11-C12
33	n	320	LHG	C26-C27-C28-C29
33	n	320	LHG	C28-C29-C30-C31
34	D	411	LMG	C32-C33-C34-C35
34	b	601	LMG	C30-C31-C32-C33
38	A	411	SQD	C12-C13-C14-C15
30	9	303	CHL	C8-C10-C11-C12
31	2	602	CLA	C5-C6-C7-C8
31	c	603	CLA	C8-C10-C11-C12
31	N	303	CLA	O1A-CGA-O2A-C1
31	S	305	CLA	O1A-CGA-O2A-C1
34	0	622	LMG	O10-C28-O8-C9
31	1	602	CLA	C11-C12-C13-C15
31	2	603	CLA	C6-C7-C8-C10
31	0	615	CLA	C6-C7-C8-C10
31	q	306	CLA	C6-C7-C8-C10
31	s	311	CLA	C16-C17-C18-C19
30	G	607	CHL	O1D-CGD-O2D-CED
30	Y	307	CHL	O1D-CGD-O2D-CED
30	8	607	CHL	O1D-CGD-O2D-CED
31	Y	303	CLA	O1D-CGD-O2D-CED
31	s	306	CLA	O1D-CGD-O2D-CED
34	d	409	LMG	O6-C5-C6-O5
30	1	607	CHL	C4-C3-C5-C6
31	2	612	CLA	C4-C3-C5-C6
31	A	405	CLA	C4-C3-C5-C6
31	B	609	CLA	C4-C3-C5-C6
31	S	303	CLA	C4-C3-C5-C6
31	a	406	CLA	C4-C3-C5-C6
31	b	610	CLA	C4-C3-C5-C6
31	s	314	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	N	319	LHG	C31-C32-C33-C34
33	R	320	LHG	C11-C12-C13-C14
33	Y	318	LHG	C11-C12-C13-C14
33	8	618	LHG	C26-C27-C28-C29
33	e	101	LHG	C26-C27-C28-C29
33	e	101	LHG	C28-C29-C30-C31
34	d	410	LMG	C32-C33-C34-C35
30	3	310	CHL	C2-C3-C5-C6
30	q	309	CHL	C2-C3-C5-C6
30	1	607	CHL	C11-C12-C13-C14
30	0	607	CHL	C6-C7-C8-C9
31	1	610	CLA	C6-C7-C8-C9
31	1	613	CLA	C14-C13-C15-C16
31	4	610	CLA	C6-C7-C8-C9
31	C	605	CLA	C14-C13-C15-C16
31	S	312	CLA	C6-C7-C8-C9
31	Y	312	CLA	C11-C10-C8-C9
31	9	304	CLA	C6-C7-C8-C9
31	b	614	CLA	C11-C12-C13-C14
31	b	617	CLA	C6-C7-C8-C9
31	c	601	CLA	C11-C10-C8-C9
31	c	603	CLA	C6-C7-C8-C9
31	g	311	CLA	C6-C7-C8-C9
30	q	308	CHL	O1D-CGD-O2D-CED
33	1	617	LHG	C23-C24-C25-C26
33	p	619	LHG	C23-C24-C25-C26
33	s	322	LHG	C23-C24-C25-C26
33	5	619	LHG	C11-C12-C13-C14
33	6	320	LHG	C11-C12-C13-C14
33	D	407	LHG	C9-C10-C11-C12
33	D	407	LHG	C11-C12-C13-C14
33	G	618	LHG	C11-C12-C13-C14
33	q	320	LHG	C11-C12-C13-C14
33	q	320	LHG	C28-C29-C30-C31
33	b	625	LHG	C11-C12-C13-C14
33	e	101	LHG	C13-C14-C15-C16
33	g	319	LHG	C13-C14-C15-C16
38	0	621	SQD	C11-C12-C13-C14
31	6	313	CLA	C5-C6-C7-C8
31	C	602	CLA	C15-C16-C17-C18
31	q	315	CLA	C8-C10-C11-C12
30	5	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	6	307	CHL	C2A-CAA-CBA-CGA
30	7	321	CHL	C2A-CAA-CBA-CGA
30	n	308	CHL	C2A-CAA-CBA-CGA
31	9	304	CLA	C2A-CAA-CBA-CGA
31	c	610	CLA	C2A-CAA-CBA-CGA
31	r	315	CLA	C2A-CAA-CBA-CGA
31	y	615	CLA	C2A-CAA-CBA-CGA
31	C	608	CLA	O1A-CGA-O2A-C1
31	R	304	CLA	O1A-CGA-O2A-C1
31	S	314	CLA	O1A-CGA-O2A-C1
31	0	602	CLA	O1A-CGA-O2A-C1
31	c	608	CLA	O1A-CGA-O2A-C1
31	r	314	CLA	O1A-CGA-O2A-C1
33	b	625	LHG	O10-C23-O8-C6
33	g	319	LHG	O10-C23-O8-C6
34	A	412	LMG	O10-C28-O8-C9
32	Y	316	LUT	C7-C8-C9-C19
32	7	317	LUT	C7-C8-C9-C19
32	9	318	LUT	C7-C8-C9-C19
32	p	616	LUT	C31-C32-C33-C40
32	p	617	LUT	C7-C8-C9-C19
32	q	318	LUT	C7-C8-C9-C19
35	g	315	RRX	C7-C8-C9-C34
43	A	410	BCR	C7-C8-C9-C34
43	T	101	BCR	C11-C12-C13-C35
43	c	615	BCR	C37-C22-C23-C24
33	3	320	LHG	C26-C27-C28-C29
33	L	101	LHG	C11-C12-C13-C14
33	R	320	LHG	C26-C27-C28-C29
33	s	320	LHG	C26-C27-C28-C29
33	z	102	LHG	C13-C14-C15-C16
34	b	624	LMG	C13-C14-C15-C16
38	X	201	SQD	C25-C26-C27-C28
33	2	617	LHG	O1-C1-C2-C3
33	3	320	LHG	O1-C1-C2-C3
33	5	619	LHG	O1-C1-C2-C3
33	6	320	LHG	O1-C1-C2-C3
33	A	417	LHG	O1-C1-C2-C3
33	B	624	LHG	O1-C1-C2-C3
33	G	618	LHG	O1-C1-C2-C3
33	L	101	LHG	O1-C1-C2-C3
33	S	322	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	Y	318	LHG	O1-C1-C2-C3
33	7	319	LHG	O1-C1-C2-C3
33	8	618	LHG	O1-C1-C2-C3
33	p	619	LHG	O1-C1-C2-C3
33	b	625	LHG	O1-C1-C2-C3
33	b	628	LHG	O1-C1-C2-C3
33	e	101	LHG	O1-C1-C2-C3
33	j	102	LHG	O1-C1-C2-C3
33	l	101	LHG	O1-C1-C2-C3
33	n	320	LHG	O1-C1-C2-C3
33	s	320	LHG	O1-C1-C2-C3
33	s	322	LHG	O1-C1-C2-C3
33	y	619	LHG	O1-C1-C2-C3
33	F1	301	LHG	O1-C1-C2-C3
32	N	317	LUT	C7-C8-C9-C10
32	9	318	LUT	C7-C8-C9-C10
32	q	318	LUT	C7-C8-C9-C10
32	g	316	LUT	C11-C12-C13-C14
43	B	617	BCR	C21-C22-C23-C24
43	B	619	BCR	C7-C8-C9-C10
43	T	101	BCR	C11-C12-C13-C14
43	V	101	BCR	C21-C22-C23-C24
43	Z	101	BCR	C7-C8-C9-C10
43	b	618	BCR	C17-C18-C19-C20
43	b	619	BCR	C21-C22-C23-C24
43	c	615	BCR	C21-C22-C23-C24
43	v	101	BCR	C7-C8-C9-C10
43	v	101	BCR	C21-C22-C23-C24
31	3	315	CLA	C3-C5-C6-C7
31	5	602	CLA	C3-C5-C6-C7
31	R	304	CLA	C3-C5-C6-C7
31	S	305	CLA	C3-C5-C6-C7
31	7	304	CLA	C3-C5-C6-C7
34	b	626	LMG	O9-C10-O7-C8
30	Y	302	CHL	C10-C11-C12-C13
31	R	316	CLA	C13-C15-C16-C17
31	c	610	CLA	C13-C15-C16-C17
34	G	621	LMG	C11-C10-O7-C8
34	b	626	LMG	C11-C10-O7-C8
33	4	618	LHG	C11-C12-C13-C14
33	A	415	LHG	C29-C30-C31-C32
33	S	320	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
33	S	322	LHG	C33-C34-C35-C36
33	b	625	LHG	C28-C29-C30-C31
33	e	101	LHG	C25-C26-C27-C28
33	l	101	LHG	C34-C35-C36-C37
34	6	321	LMG	C29-C30-C31-C32
34	0	620	LMG	C13-C14-C15-C16
33	2	617	LHG	C23-C24-C25-C26
33	5	619	LHG	C23-C24-C25-C26
33	A	415	LHG	C23-C24-C25-C26
33	D	408	LHG	C7-C8-C9-C10
33	R	320	LHG	C23-C24-C25-C26
33	8	618	LHG	C7-C8-C9-C10
33	9	320	LHG	C23-C24-C25-C26
33	j	102	LHG	C23-C24-C25-C26
33	n	320	LHG	C7-C8-C9-C10
34	9	302	LMG	C10-C11-C12-C13
38	G	624	SQD	C23-C24-C25-C26
31	D	403	CLA	O1D-CGD-O2D-CED
33	D	408	LHG	C9-C10-C11-C12
33	D	408	LHG	C26-C27-C28-C29
33	L	101	LHG	C33-C34-C35-C36
33	N	319	LHG	C11-C10-C9-C8
33	S	320	LHG	C13-C14-C15-C16
33	q	320	LHG	C13-C14-C15-C16
33	a	415	LHG	C28-C29-C30-C31
33	b	625	LHG	C9-C10-C11-C12
33	b	625	LHG	C10-C11-C12-C13
33	b	628	LHG	C28-C29-C30-C31
33	d	408	LHG	C13-C14-C15-C16
33	z	102	LHG	C25-C26-C27-C28
33	F1	301	LHG	C11-C10-C9-C8
34	m	102	LMG	C30-C31-C32-C33
45	c	617	DGD	C3B-C4B-C5B-C6B
48	r	302	LMU	C6-C7-C8-C9
31	B	601	CLA	C4B-C3B-CAB-CBB
31	C	606	CLA	C4B-C3B-CAB-CBB
31	R	303	CLA	C4B-C3B-CAB-CBB
30	1	619	CHL	C11-C12-C13-C15
31	2	611	CLA	C6-C7-C8-C10
31	3	305	CLA	C6-C7-C8-C10
31	4	603	CLA	C6-C7-C8-C10
31	N	304	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	Y	304	CLA	C6-C7-C8-C9
31	g	305	CLA	C6-C7-C8-C10
31	r	315	CLA	C6-C7-C8-C10
31	r	316	CLA	C16-C17-C18-C19
31	y	603	CLA	C6-C7-C8-C9
34	b	626	LMG	C8-C9-O8-C28
34	q	302	LMG	O6-C1-O1-C7
38	6	301	SQD	O5-C1-O6-C44
38	R	322	SQD	O5-C1-O6-C44
45	C	617	DGD	O6E-C1E-O5D-C6D
31	S	311	CLA	C10-C11-C12-C13
31	d	404	CLA	C15-C16-C17-C18
42	a	408	PHO	C5-C6-C7-C8
30	1	606	CHL	O1D-CGD-O2D-CED
33	5	619	LHG	C9-C10-C11-C12
33	B	624	LHG	C13-C14-C15-C16
33	D	407	LHG	C34-C35-C36-C37
33	D	408	LHG	C11-C12-C13-C14
33	K	102	LHG	C11-C12-C13-C14
33	S	320	LHG	C11-C10-C9-C8
33	s	320	LHG	C13-C14-C15-C16
45	c	616	DGD	CAA-CBA-CCA-CDA
30	p	609	CHL	CBD-CGD-O2D-CED
31	C	608	CLA	CBD-CGD-O2D-CED
31	8	610	CLA	CBD-CGD-O2D-CED
31	n	312	CLA	CBD-CGD-O2D-CED
31	4	612	CLA	O1D-CGD-O2D-CED
33	4	618	LHG	C13-C14-C15-C16
33	M	101	LHG	C28-C29-C30-C31
33	M	101	LHG	C33-C34-C35-C36
33	8	618	LHG	C33-C34-C35-C36
33	n	320	LHG	C33-C34-C35-C36
33	s	320	LHG	C25-C26-C27-C28
33	y	619	LHG	C11-C10-C9-C8
34	a	416	LMG	C11-C12-C13-C14
34	a	416	LMG	C30-C31-C32-C33
33	l	101	LHG	C23-C24-C25-C26
45	C	616	DGD	C1A-C2A-C3A-C4A
30	G	601	CHL	C8-C10-C11-C12
31	0	603	CLA	C5-C6-C7-C8
31	c	605	CLA	O1A-CGA-O2A-C1
33	t	102	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
33	F1	301	LHG	C11-C12-C13-C14
34	6	321	LMG	C32-C33-C34-C35
38	B	620	SQD	C25-C26-C27-C28
31	G	602	CLA	C3-C5-C6-C7
31	8	603	CLA	C3-C5-C6-C7
31	s	305	CLA	C3-C5-C6-C7
31	C	606	CLA	CBA-CGA-O2A-C1
31	c	603	CLA	CBA-CGA-O2A-C1
45	C	617	DGD	C2A-C1A-O1G-C1G
33	d	408	LHG	C11-C12-C13-C14
33	y	619	LHG	C11-C12-C13-C14
34	D	412	LMG	C16-C17-C18-C19
34	n	321	LMG	C11-C12-C13-C14
48	R	302	LMU	C6-C7-C8-C9
30	4	607	CHL	O1D-CGD-O2D-CED
30	n	309	CHL	O1D-CGD-O2D-CED
30	3	303	CHL	C3A-C2A-CAA-CBA
30	4	608	CHL	C3A-C2A-CAA-CBA
30	6	307	CHL	C3A-C2A-CAA-CBA
30	G	601	CHL	C3A-C2A-CAA-CBA
30	0	606	CHL	C3A-C2A-CAA-CBA
30	7	306	CHL	C3A-C2A-CAA-CBA
30	7	308	CHL	C3A-C2A-CAA-CBA
30	g	302	CHL	C3A-C2A-CAA-CBA
30	n	310	CHL	C3A-C2A-CAA-CBA
31	1	603	CLA	C3A-C2A-CAA-CBA
31	1	614	CLA	C3A-C2A-CAA-CBA
31	2	603	CLA	C3A-C2A-CAA-CBA
31	3	305	CLA	C3A-C2A-CAA-CBA
31	4	603	CLA	C3A-C2A-CAA-CBA
31	5	603	CLA	C3A-C2A-CAA-CBA
31	5	615	CLA	C3A-C2A-CAA-CBA
31	6	304	CLA	C3A-C2A-CAA-CBA
31	6	313	CLA	C3A-C2A-CAA-CBA
31	B	604	CLA	C3A-C2A-CAA-CBA
31	B	610	CLA	C3A-C2A-CAA-CBA
31	C	612	CLA	C3A-C2A-CAA-CBA
31	C	613	CLA	C3A-C2A-CAA-CBA
31	G	603	CLA	C3A-C2A-CAA-CBA
31	N	304	CLA	C3A-C2A-CAA-CBA
31	R	307	CLA	C3A-C2A-CAA-CBA
31	Y	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	0	612	CLA	C3A-C2A-CAA-CBA
31	7	304	CLA	C3A-C2A-CAA-CBA
31	7	315	CLA	C3A-C2A-CAA-CBA
31	8	603	CLA	C3A-C2A-CAA-CBA
31	9	305	CLA	C3A-C2A-CAA-CBA
31	p	603	CLA	C3A-C2A-CAA-CBA
31	q	305	CLA	C3A-C2A-CAA-CBA
31	a	407	CLA	C3A-C2A-CAA-CBA
31	b	605	CLA	C3A-C2A-CAA-CBA
31	c	610	CLA	C3A-C2A-CAA-CBA
31	c	612	CLA	C3A-C2A-CAA-CBA
31	c	613	CLA	C3A-C2A-CAA-CBA
31	n	304	CLA	C3A-C2A-CAA-CBA
31	r	307	CLA	C3A-C2A-CAA-CBA
31	y	603	CLA	C3A-C2A-CAA-CBA
31	1	612	CLA	C15-C16-C17-C18
31	B	611	CLA	C13-C15-C16-C17
31	Y	312	CLA	C15-C16-C17-C18
31	q	305	CLA	C5-C6-C7-C8
31	c	610	CLA	C8-C10-C11-C12
34	X	202	LMG	C8-C9-O8-C28
31	9	304	CLA	C4C-C3C-CAC-CBC
33	M	101	LHG	C31-C32-C33-C34
33	8	618	LHG	C13-C14-C15-C16
33	n	320	LHG	C13-C14-C15-C16
34	B	625	LMG	C33-C34-C35-C36
34	D	409	LMG	C18-C19-C20-C21
31	C	607	CLA	O1D-CGD-O2D-CED
30	1	619	CHL	C11-C12-C13-C14
31	6	305	CLA	C6-C7-C8-C9
31	Y	305	CLA	C6-C7-C8-C9
31	0	604	CLA	C6-C7-C8-C10
33	2	617	LHG	C9-C10-C11-C12
33	4	618	LHG	C26-C27-C28-C29
33	B	624	LHG	C28-C29-C30-C31
33	D	408	LHG	C27-C28-C29-C30
33	M	101	LHG	C9-C10-C11-C12
33	q	320	LHG	C24-C25-C26-C27
33	a	415	LHG	C33-C34-C35-C36
33	b	628	LHG	C31-C32-C33-C34
33	t	102	LHG	C9-C10-C11-C12
34	b	624	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
34	x	202	LMG	C33-C34-C35-C36
34	y	620	LMG	C30-C31-C32-C33
33	S	320	LHG	C4-C5-C6-O8
34	D	409	LMG	O1-C7-C8-C9
38	B	620	SQD	O6-C44-C45-C46
38	M	102	SQD	C44-C45-C46-O48
31	N	321	CLA	C5-C6-C7-C8
31	7	315	CLA	C5-C6-C7-C8
33	1	617	LHG	C25-C26-C27-C28
33	5	619	LHG	C25-C26-C27-C28
33	A	415	LHG	C28-C29-C30-C31
33	D	408	LHG	C28-C29-C30-C31
33	L	101	LHG	C31-C32-C33-C34
33	j	102	LHG	C28-C29-C30-C31
33	t	102	LHG	C30-C31-C32-C33
34	C	619	LMG	C19-C20-C21-C22
34	c	621	LMG	C32-C33-C34-C35
36	2	616	NEX	C14-C15-C35-C34
37	R	318	XAT	C14-C15-C35-C34
31	B	616	CLA	C3-C5-C6-C7
31	a	407	CLA	C3-C5-C6-C7
38	s	301	SQD	C7-C8-C9-C10
33	S	320	LHG	C11-C12-C13-C14
33	d	408	LHG	C28-C29-C30-C31
31	4	604	CLA	O1A-CGA-O2A-C1
31	c	609	CLA	C10-C11-C12-C13
31	r	316	CLA	C8-C10-C11-C12
30	6	302	CHL	C4-C3-C5-C6
30	G	623	CHL	C4-C3-C5-C6
31	Y	311	CLA	C4-C3-C5-C6
31	0	603	CLA	C4-C3-C5-C6
31	7	314	CLA	C4-C3-C5-C6
31	y	611	CLA	C4-C3-C5-C6
31	9	306	CLA	CBA-CGA-O2A-C1
31	r	306	CLA	CBA-CGA-O2A-C1
31	A	405	CLA	C2-C3-C5-C6
31	Y	311	CLA	C2-C3-C5-C6
31	0	603	CLA	C2-C3-C5-C6
31	7	314	CLA	C2-C3-C5-C6
31	a	406	CLA	C2-C3-C5-C6
31	b	610	CLA	C2-C3-C5-C6
31	s	314	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	y	611	CLA	C2-C3-C5-C6
44	a	414	PL9	C12-C11-C9-C8
33	A	415	LHG	C8-C7-O7-C5
34	C	624	LMG	C11-C10-O7-C8
34	D	411	LMG	C11-C10-O7-C8
34	q	301	LMG	C11-C10-O7-C8
34	b	622	LMG	C11-C10-O7-C8
34	d	410	LMG	C11-C10-O7-C8
34	B	621	LMG	C8-C9-O8-C28
33	p	619	LHG	C10-C11-C12-C13
33	t	102	LHG	C26-C27-C28-C29
34	W	203	LMG	C4-C5-C6-O5
31	Y	311	CLA	C2A-CAA-CBA-CGA
31	Y	313	CLA	C2A-CAA-CBA-CGA
31	b	605	CLA	C2A-CAA-CBA-CGA
33	1	617	LHG	O1-C1-C2-O2
33	2	617	LHG	O1-C1-C2-O2
33	6	320	LHG	O1-C1-C2-O2
33	A	415	LHG	O1-C1-C2-O2
33	D	408	LHG	O1-C1-C2-O2
33	G	618	LHG	O1-C1-C2-O2
33	0	619	LHG	O1-C1-C2-O2
33	q	320	LHG	O1-C1-C2-O2
33	b	625	LHG	O1-C1-C2-O2
33	c	622	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
33	j	102	LHG	O1-C1-C2-O2
33	r	320	LHG	O1-C1-C2-O2
33	s	322	LHG	O1-C1-C2-O2
33	t	102	LHG	O1-C1-C2-O2
33	F1	301	LHG	O1-C1-C2-O2
33	4	618	LHG	C30-C31-C32-C33
33	D	407	LHG	C10-C11-C12-C13
33	M	101	LHG	C11-C10-C9-C8
33	0	619	LHG	C11-C12-C13-C14
33	j	102	LHG	C13-C14-C15-C16
34	B	622	LMG	C32-C33-C34-C35
34	B	622	LMG	C33-C34-C35-C36
45	C	617	DGD	C2A-C3A-C4A-C5A
31	3	316	CLA	C8-C10-C11-C12
31	q	313	CLA	O1D-CGD-O2D-CED
31	Y	314	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	b	610	CLA	O1A-CGA-O2A-C1
31	1	602	CLA	C11-C12-C13-C14
31	9	315	CLA	C6-C7-C8-C9
31	2	602	CLA	C2B-C3B-CAB-CBB
31	B	601	CLA	C2B-C3B-CAB-CBB
31	C	606	CLA	C2B-C3B-CAB-CBB
31	R	303	CLA	C2B-C3B-CAB-CBB
31	r	313	CLA	C2B-C3B-CAB-CBB
31	s	312	CLA	C2B-C3B-CAB-CBB
30	g	302	CHL	C5-C6-C7-C8
31	7	311	CLA	C8-C10-C11-C12
45	c	619	DGD	CCA-CDA-CEA-CFA
30	7	308	CHL	C3-C5-C6-C7
31	9	315	CLA	C3-C5-C6-C7
31	g	313	CLA	C3-C5-C6-C7
48	c	623	LMU	C1-C2-C3-C4
31	s	305	CLA	CBA-CGA-O2A-C1
33	p	619	LHG	C5-C6-O8-C23
33	A	417	LHG	C26-C27-C28-C29
31	7	303	CLA	O1A-CGA-O2A-C1
31	a	406	CLA	O1A-CGA-O2A-C1
33	j	102	LHG	C7-C8-C9-C10
31	Y	304	CLA	C5-C6-C7-C8
34	D	409	LMG	O6-C5-C6-O5
31	2	602	CLA	C4C-C3C-CAC-CBC
33	e	101	LHG	C33-C34-C35-C36
34	C	624	LMG	O9-C10-O7-C8
34	D	411	LMG	O9-C10-O7-C8
34	q	301	LMG	O9-C10-O7-C8
34	b	622	LMG	O9-C10-O7-C8
34	d	410	LMG	O9-C10-O7-C8
31	2	604	CLA	C2-C1-O2A-CGA
31	3	314	CLA	C2-C1-O2A-CGA
31	5	604	CLA	C2-C1-O2A-CGA
31	A	406	CLA	C2-C1-O2A-CGA
31	B	604	CLA	C2-C1-O2A-CGA
31	B	613	CLA	C2-C1-O2A-CGA
31	B	616	CLA	C2-C1-O2A-CGA
31	C	613	CLA	C2-C1-O2A-CGA
31	D	404	CLA	C2-C1-O2A-CGA
31	G	610	CLA	C2-C1-O2A-CGA
31	N	313	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	R	303	CLA	C2-C1-O2A-CGA
31	S	315	CLA	C2-C1-O2A-CGA
31	Y	304	CLA	C2-C1-O2A-CGA
31	Y	314	CLA	C2-C1-O2A-CGA
31	8	604	CLA	C2-C1-O2A-CGA
31	q	316	CLA	C2-C1-O2A-CGA
31	b	602	CLA	C2-C1-O2A-CGA
31	g	305	CLA	C2-C1-O2A-CGA
31	r	305	CLA	C2-C1-O2A-CGA
31	r	307	CLA	C2-C1-O2A-CGA
31	s	306	CLA	C2-C1-O2A-CGA
31	s	310	CLA	C2-C1-O2A-CGA
31	s	315	CLA	C2-C1-O2A-CGA
31	0	614	CLA	C5-C6-C7-C8
33	A	415	LHG	C31-C32-C33-C34
33	s	322	LHG	C26-C27-C28-C29
31	C	608	CLA	C5-C6-C7-C8
31	c	604	CLA	O1A-CGA-O2A-C1
31	r	315	CLA	O1A-CGA-O2A-C1
45	C	617	DGD	O1A-C1A-O1G-C1G
31	3	301	CLA	C6-C7-C8-C9
33	y	619	LHG	C27-C28-C29-C30
31	Y	304	CLA	C6-C7-C8-C10
31	8	603	CLA	C6-C7-C8-C9
31	c	612	CLA	C6-C7-C8-C10
33	s	322	LHG	C7-C8-C9-C10
34	b	622	LMG	C10-C11-C12-C13
31	1	612	CLA	C3-C5-C6-C7
31	p	602	CLA	C3-C5-C6-C7
32	5	616	LUT	C5-C6-C7-C8
32	p	617	LUT	C1-C6-C7-C8
35	2	614	RRX	C1-C6-C7-C8
35	q	317	RRX	C23-C24-C25-C26
43	A	410	BCR	C1-C6-C7-C8
43	A	410	BCR	C23-C24-C25-C26
43	B	617	BCR	C1-C6-C7-C8
43	B	618	BCR	C1-C6-C7-C8
43	C	614	BCR	C23-C24-C25-C26
43	D	405	BCR	C23-C24-C25-C26
43	T	101	BCR	C23-C24-C25-C26
43	V	101	BCR	C1-C6-C7-C8
43	V	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
43	V	101	BCR	C23-C24-C25-C26
43	V	101	BCR	C23-C24-C25-C30
43	a	410	BCR	C23-C24-C25-C26
43	b	618	BCR	C1-C6-C7-C8
43	b	618	BCR	C23-C24-C25-C26
43	b	619	BCR	C1-C6-C7-C8
43	b	619	BCR	C23-C24-C25-C26
43	c	614	BCR	C1-C6-C7-C8
43	c	615	BCR	C5-C6-C7-C8
43	d	406	BCR	C23-C24-C25-C30
43	t	101	BCR	C1-C6-C7-C8
43	v	101	BCR	C1-C6-C7-C8
43	v	101	BCR	C5-C6-C7-C8
43	v	101	BCR	C23-C24-C25-C30
33	A	417	LHG	C25-C26-C27-C28
33	D	407	LHG	C30-C31-C32-C33
33	D	407	LHG	C31-C32-C33-C34
33	N	319	LHG	C28-C29-C30-C31
33	Y	318	LHG	C33-C34-C35-C36
33	y	619	LHG	C13-C14-C15-C16
38	a	411	SQD	C9-C10-C11-C12
30	1	619	CHL	CBA-CGA-O2A-C1
30	G	605	CHL	CBA-CGA-O2A-C1
31	G	602	CLA	CBA-CGA-O2A-C1
31	R	306	CLA	CBA-CGA-O2A-C1
31	y	612	CLA	CBA-CGA-O2A-C1
31	y	613	CLA	CBA-CGA-O2A-C1
31	4	602	CLA	C5-C6-C7-C8
31	0	610	CLA	C8-C10-C11-C12
31	7	314	CLA	C13-C15-C16-C17
34	d	409	LMG	C11-C10-O7-C8
33	A	415	LHG	C11-C12-C13-C14
33	q	320	LHG	C11-C10-C9-C8
34	b	601	LMG	C15-C16-C17-C18
34	f	101	LMG	C32-C33-C34-C35
34	y	620	LMG	C29-C30-C31-C32
30	5	601	CHL	O1D-CGD-O2D-CED
31	N	311	CLA	O1D-CGD-O2D-CED
31	c	603	CLA	O1A-CGA-O2A-C1
30	9	310	CHL	CBD-CGD-O2D-CED
33	s	322	LHG	C11-C12-C13-C14
33	s	322	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
34	y	620	LMG	C12-C13-C14-C15
44	D	406	PL9	C47-C48-C49-C50
31	4	602	CLA	C13-C15-C16-C17
31	b	608	CLA	C15-C16-C17-C18
31	y	612	CLA	C8-C10-C11-C12
31	s	305	CLA	O1D-CGD-O2D-CED
33	t	102	LHG	C35-C36-C37-C38
30	1	605	CHL	C4-C3-C5-C6
30	1	609	CHL	C4-C3-C5-C6
30	4	601	CHL	C4-C3-C5-C6
30	N	302	CHL	C4-C3-C5-C6
30	Y	307	CHL	C4-C3-C5-C6
30	0	601	CHL	C4-C3-C5-C6
30	8	601	CHL	C4-C3-C5-C6
30	9	303	CHL	C4-C3-C5-C6
30	q	303	CHL	C4-C3-C5-C6
30	q	309	CHL	C4-C3-C5-C6
30	g	302	CHL	C4-C3-C5-C6
30	n	302	CHL	C4-C3-C5-C6
30	r	308	CHL	C4-C3-C5-C6
31	C	610	CLA	C4-C3-C5-C6
31	b	608	CLA	C4-C3-C5-C6
31	s	305	CLA	C4-C3-C5-C6
30	3	303	CHL	O1D-CGD-O2D-CED
30	1	601	CHL	C11-C12-C13-C15
30	1	605	CHL	C2-C3-C5-C6
30	1	605	CHL	C6-C7-C8-C10
30	1	607	CHL	C2-C3-C5-C6
30	1	609	CHL	C2-C3-C5-C6
30	G	623	CHL	C2-C3-C5-C6
30	N	302	CHL	C2-C3-C5-C6
30	Y	307	CHL	C2-C3-C5-C6
30	0	607	CHL	C2-C3-C5-C6
30	0	607	CHL	C6-C7-C8-C10
30	8	601	CHL	C2-C3-C5-C6
30	9	303	CHL	C2-C3-C5-C6
30	9	311	CHL	C6-C7-C8-C10
30	g	302	CHL	C2-C3-C5-C6
30	n	302	CHL	C2-C3-C5-C6
30	r	308	CHL	C2-C3-C5-C6
30	y	601	CHL	C2-C3-C5-C6
30	y	601	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
31	1	610	CLA	C6-C7-C8-C10
31	2	602	CLA	C12-C13-C15-C16
31	2	610	CLA	C11-C10-C8-C7
31	5	611	CLA	C11-C10-C8-C7
31	6	303	CLA	C11-C10-C8-C7
31	6	312	CLA	C11-C10-C8-C7
31	B	602	CLA	C11-C10-C8-C7
31	B	609	CLA	C2-C3-C5-C6
31	C	605	CLA	C12-C13-C15-C16
31	C	607	CLA	C11-C12-C13-C15
31	C	613	CLA	C11-C12-C13-C15
31	G	610	CLA	C6-C7-C8-C10
31	N	303	CLA	C6-C7-C8-C10
31	N	303	CLA	C11-C12-C13-C15
31	N	305	CLA	C6-C7-C8-C10
31	N	305	CLA	C11-C10-C8-C7
31	R	316	CLA	C12-C13-C15-C16
31	S	314	CLA	C6-C7-C8-C10
31	Y	312	CLA	C11-C10-C8-C7
31	Y	312	CLA	C11-C12-C13-C15
31	7	311	CLA	C6-C7-C8-C10
31	7	311	CLA	C11-C10-C8-C7
31	7	313	CLA	C6-C7-C8-C10
31	8	602	CLA	C6-C7-C8-C10
31	8	604	CLA	C6-C7-C8-C10
31	9	304	CLA	C6-C7-C8-C10
31	q	304	CLA	C6-C7-C8-C10
31	b	604	CLA	C6-C7-C8-C10
31	b	605	CLA	C6-C7-C8-C10
31	b	608	CLA	C2-C3-C5-C6
31	b	611	CLA	C11-C12-C13-C15
31	b	616	CLA	C11-C10-C8-C7
31	b	617	CLA	C6-C7-C8-C10
31	c	601	CLA	C11-C10-C8-C7
31	c	605	CLA	C2-C3-C5-C6
31	c	606	CLA	C6-C7-C8-C10
31	n	303	CLA	C6-C7-C8-C10
31	n	305	CLA	C6-C7-C8-C10
31	y	604	CLA	C2-C3-C5-C6
31	y	611	CLA	C11-C10-C8-C7
31	y	613	CLA	C11-C10-C8-C7
42	A	408	PHO	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
42	a	408	PHO	C11-C12-C13-C15
31	6	312	CLA	C3-C5-C6-C7
31	g	305	CLA	C3-C5-C6-C7
30	1	619	CHL	O1A-CGA-O2A-C1
31	G	602	CLA	O1A-CGA-O2A-C1
31	9	306	CLA	O1A-CGA-O2A-C1
31	y	612	CLA	O1A-CGA-O2A-C1
31	y	613	CLA	O1A-CGA-O2A-C1
33	b	628	LHG	C13-C14-C15-C16
33	j	102	LHG	C26-C27-C28-C29
30	7	307	CHL	C5-C6-C7-C8
31	3	312	CLA	C13-C15-C16-C17
31	C	605	CLA	C8-C10-C11-C12
31	D	404	CLA	C13-C15-C16-C17
35	g	315	RRX	C19-C20-C21-C22
36	8	617	NEX	C9-C10-C11-C12
43	b	618	BCR	C15-C16-C17-C18
31	n	304	CLA	C6-C7-C8-C9
33	S	320	LHG	O9-C7-O7-C5
34	D	410	LMG	O9-C10-O7-C8
34	g	322	LMG	O9-C10-O7-C8
38	a	412	SQD	O49-C7-O47-C45
38	a	412	SQD	C23-C24-C25-C26
30	2	606	CHL	CBA-CGA-O2A-C1
31	B	609	CLA	CBA-CGA-O2A-C1
31	B	613	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C16-C17-C18-C19
33	l	101	LHG	C25-C26-C27-C28
30	9	309	CHL	C2A-CAA-CBA-CGA
30	q	309	CHL	C2A-CAA-CBA-CGA
31	3	315	CLA	C2A-CAA-CBA-CGA
31	A	405	CLA	C2A-CAA-CBA-CGA
31	C	601	CLA	C2A-CAA-CBA-CGA
31	N	305	CLA	C2A-CAA-CBA-CGA
31	N	311	CLA	C2A-CAA-CBA-CGA
31	0	602	CLA	C2A-CAA-CBA-CGA
31	q	316	CLA	C2A-CAA-CBA-CGA
31	n	305	CLA	C2A-CAA-CBA-CGA
31	r	307	CLA	C2A-CAA-CBA-CGA
31	R	311	CLA	C8-C10-C11-C12
31	c	601	CLA	C15-C16-C17-C18
33	Y	318	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	9	305	CLA	O1D-CGD-O2D-CED
33	N	319	LHG	C33-C34-C35-C36
33	Y	318	LHG	C30-C31-C32-C33
34	m	102	LMG	C29-C30-C31-C32
38	a	412	SQD	C11-C10-C9-C8
45	c	616	DGD	C6A-C7A-C8A-C9A
33	1	617	LHG	C7-C8-C9-C10
34	m	102	LMG	C10-C11-C12-C13
38	x	201	SQD	C23-C24-C25-C26
31	y	611	CLA	O1D-CGD-O2D-CED
31	B	610	CLA	C5-C6-C7-C8
33	1	617	LHG	C26-C27-C28-C29
33	4	618	LHG	C14-C15-C16-C17
33	L	101	LHG	C13-C14-C15-C16
34	2	620	LMG	C18-C19-C20-C21
38	m	101	SQD	C26-C27-C28-C29
45	C	620	DGD	C4B-C5B-C6B-C7B
45	c	616	DGD	CCB-CDB-CEB-CFB
48	r	302	LMU	C2-C3-C4-C5
33	z	102	LHG	C5-C6-O8-C23
33	G	618	LHG	C33-C34-C35-C36
33	d	408	LHG	C26-C27-C28-C29
34	Q1	101	LMG	C31-C32-C33-C34
45	c	618	DGD	CCA-CDA-CEA-CFA
31	C	606	CLA	O1A-CGA-O2A-C1
31	r	306	CLA	O1A-CGA-O2A-C1
31	s	305	CLA	O1A-CGA-O2A-C1
30	n	310	CHL	CBD-CGD-O2D-CED
30	y	606	CHL	CBD-CGD-O2D-CED
31	7	304	CLA	C6-C7-C8-C9
31	q	312	CLA	C6-C7-C8-C9
34	R	321	LMG	O6-C1-O1-C7
31	B	605	CLA	C5-C6-C7-C8
31	B	608	CLA	C13-C15-C16-C17
30	6	308	CHL	O1D-CGD-O2D-CED
31	3	301	CLA	C5-C6-C7-C8
33	D	408	LHG	C16-C17-C18-C19
33	8	618	LHG	C11-C10-C9-C8
33	n	320	LHG	C11-C10-C9-C8
34	d	411	LMG	C13-C14-C15-C16
38	a	412	SQD	C9-C10-C11-C12
34	x	202	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
38	S	301	SQD	C7-C8-C9-C10
33	3	320	LHG	C8-C7-O7-C5
33	S	320	LHG	C8-C7-O7-C5
33	b	628	LHG	C8-C7-O7-C5
33	s	320	LHG	C8-C7-O7-C5
33	t	102	LHG	C8-C7-O7-C5
34	D	409	LMG	C11-C10-O7-C8
34	D	410	LMG	C11-C10-O7-C8
34	S	321	LMG	C11-C10-O7-C8
34	g	322	LMG	C11-C10-O7-C8
34	r	321	LMG	C11-C10-O7-C8
38	a	412	SQD	C8-C7-O47-C45
45	C	616	DGD	C2B-C1B-O2G-C2G
31	1	614	CLA	C5-C6-C7-C8
33	c	622	LHG	C34-C35-C36-C37
34	S	321	LMG	C14-C15-C16-C17
34	q	302	LMG	C11-C12-C13-C14
38	R	322	SQD	C11-C12-C13-C14
48	r	302	LMU	O1'-C1-C2-C3
31	G	612	CLA	C13-C15-C16-C17
31	c	605	CLA	C5-C6-C7-C8
33	4	618	LHG	C24-C25-C26-C27
33	j	102	LHG	C31-C32-C33-C34
33	A	415	LHG	O9-C7-O7-C5
33	b	628	LHG	O9-C7-O7-C5
34	D	409	LMG	O9-C10-O7-C8
34	S	321	LMG	O9-C10-O7-C8
34	d	409	LMG	O9-C10-O7-C8
34	r	321	LMG	O9-C10-O7-C8
45	C	616	DGD	O1B-C1B-O2G-C2G
31	S	310	CLA	C3-C5-C6-C7
31	n	304	CLA	C3-C5-C6-C7
34	g	322	LMG	C12-C13-C14-C15
34	n	321	LMG	C12-C13-C14-C15
34	4	620	LMG	C2-C1-O1-C7
34	B	625	LMG	C2-C1-O1-C7
34	C	621	LMG	C2-C1-O1-C7
34	C	624	LMG	C2-C1-O1-C7
34	9	302	LMG	C2-C1-O1-C7
34	9	321	LMG	C2-C1-O1-C7
34	b	601	LMG	C2-C1-O1-C7
34	b	626	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	b	629	LMG	C2-C1-O1-C7
45	C	617	DGD	C2D-C1D-O3G-C3G
45	c	619	DGD	C2D-C1D-O3G-C3G
31	b	608	CLA	C13-C15-C16-C17
33	1	617	LHG	O7-C5-C6-O8
33	S	320	LHG	O7-C5-C6-O8
33	7	319	LHG	O7-C5-C6-O8
33	b	625	LHG	O7-C5-C6-O8
33	r	320	LHG	O7-C5-C6-O8
33	s	322	LHG	O7-C5-C6-O8
34	A	418	LMG	O1-C7-C8-O7
34	D	412	LMG	O7-C8-C9-O8
34	R	321	LMG	O7-C8-C9-O8
34	a	416	LMG	O1-C7-C8-O7
34	n	321	LMG	O7-C8-C9-O8
38	6	301	SQD	O47-C45-C46-O48
38	G	624	SQD	O47-C45-C46-O48
34	7	322	LMG	O6-C5-C6-O5
38	s	301	SQD	C24-C23-O48-C46
33	2	617	LHG	C27-C28-C29-C30
33	r	320	LHG	C13-C14-C15-C16
31	3	314	CLA	C6-C7-C8-C10
31	9	305	CLA	C6-C7-C8-C9
33	2	617	LHG	C26-C27-C28-C29
33	e	101	LHG	C24-C25-C26-C27
33	n	320	LHG	C34-C35-C36-C37
33	s	322	LHG	C33-C34-C35-C36
45	c	616	DGD	C9B-CAB-CBB-CCB
34	g	320	LMG	O6-C5-C6-O5
34	w	202	LMG	O6-C5-C6-O5
34	Q1	101	LMG	O6-C5-C6-O5
31	C	601	CLA	C8-C10-C11-C12
31	s	312	CLA	C8-C10-C11-C12
30	R	309	CHL	C4-C3-C5-C6
30	0	607	CHL	C4-C3-C5-C6
30	7	302	CHL	C4-C3-C5-C6
30	9	311	CHL	C4-C3-C5-C6
30	r	309	CHL	C4-C3-C5-C6
31	7	315	CLA	C4-C3-C5-C6
31	y	604	CLA	C4-C3-C5-C6
34	0	620	LMG	C28-C29-C30-C31
30	3	302	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	N	306	CHL	C2-C3-C5-C6
30	q	303	CHL	C2-C3-C5-C6
31	2	612	CLA	C2-C3-C5-C6
31	3	301	CLA	C2-C3-C5-C6
31	C	610	CLA	C2-C3-C5-C6
31	S	303	CLA	C2-C3-C5-C6
31	s	305	CLA	C2-C3-C5-C6
44	D	406	PL9	C4-C3-C7-C8
44	a	414	PL9	C4-C3-C7-C8
44	d	407	PL9	C4-C3-C7-C8
33	B	624	LHG	C31-C32-C33-C34
33	8	618	LHG	C34-C35-C36-C37
30	1	606	CHL	C11-C10-C8-C9
30	2	608	CHL	C6-C7-C8-C9
30	Y	307	CHL	C11-C10-C8-C9
30	8	606	CHL	C11-C10-C8-C9
30	n	307	CHL	C11-C10-C8-C9
31	B	605	CLA	C11-C12-C13-C14
31	B	609	CLA	C6-C7-C8-C9
31	C	603	CLA	C6-C7-C8-C9
31	C	607	CLA	C11-C12-C13-C14
31	C	610	CLA	C14-C13-C15-C16
31	G	602	CLA	C6-C7-C8-C9
31	G	610	CLA	C6-C7-C8-C9
31	N	303	CLA	C6-C7-C8-C9
31	N	305	CLA	C6-C7-C8-C9
31	R	316	CLA	C6-C7-C8-C9
31	0	602	CLA	C11-C10-C8-C9
31	0	610	CLA	C6-C7-C8-C9
31	7	311	CLA	C6-C7-C8-C9
31	7	312	CLA	C11-C10-C8-C9
31	7	313	CLA	C6-C7-C8-C9
31	8	602	CLA	C6-C7-C8-C9
31	8	604	CLA	C6-C7-C8-C9
31	9	306	CLA	C6-C7-C8-C9
31	p	611	CLA	C6-C7-C8-C9
31	p	611	CLA	C11-C10-C8-C9
31	q	304	CLA	C6-C7-C8-C9
31	b	608	CLA	C11-C10-C8-C9
31	c	606	CLA	C6-C7-C8-C9
31	g	303	CLA	C14-C13-C15-C16
31	n	303	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	n	305	CLA	C6-C7-C8-C9
34	B	625	LMG	C8-C9-O8-C28
33	B	624	LHG	C10-C11-C12-C13
33	G	618	LHG	C30-C31-C32-C33
33	j	102	LHG	C34-C35-C36-C37
31	G	604	CLA	C3-C5-C6-C7
30	9	311	CHL	O1D-CGD-O2D-CED
30	q	308	CHL	C2A-CAA-CBA-CGA
31	R	306	CLA	C2A-CAA-CBA-CGA
31	8	604	CLA	C2A-CAA-CBA-CGA
31	b	613	CLA	C2A-CAA-CBA-CGA
31	d	405	CLA	C2A-CAA-CBA-CGA
33	C	623	LHG	C9-C10-C11-C12
33	S	322	LHG	C26-C27-C28-C29
33	7	319	LHG	C24-C25-C26-C27
34	B	622	LMG	O6-C5-C6-O5
34	R	321	LMG	O6-C5-C6-O5
34	w	201	LMG	O6-C5-C6-O5
45	C	620	DGD	O6E-C5E-C6E-O5E
32	2	615	LUT	C31-C32-C33-C40
32	3	318	LUT	C31-C32-C33-C40
32	N	317	LUT	C7-C8-C9-C19
32	s	318	LUT	C31-C32-C33-C40
43	T	101	BCR	C7-C8-C9-C34
43	V	101	BCR	C7-C8-C9-C34
43	a	410	BCR	C7-C8-C9-C34
43	z	101	BCR	C36-C18-C19-C20
31	7	312	CLA	O1D-CGD-O2D-CED
33	s	322	LHG	C31-C32-C33-C34
34	b	622	LMG	C19-C20-C21-C22
32	N	317	LUT	C11-C12-C13-C14
43	T	101	BCR	C7-C8-C9-C10
31	B	609	CLA	O1A-CGA-O2A-C1
31	R	306	CLA	O1A-CGA-O2A-C1
30	1	608	CHL	O1D-CGD-O2D-CED
30	3	303	CHL	C1A-C2A-CAA-CBA
30	4	608	CHL	C1A-C2A-CAA-CBA
30	4	609	CHL	C1A-C2A-CAA-CBA
30	Y	302	CHL	C1A-C2A-CAA-CBA
30	Y	308	CHL	C1A-C2A-CAA-CBA
30	7	302	CHL	C1A-C2A-CAA-CBA
30	7	306	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	s	309	CHL	C1A-C2A-CAA-CBA
30	y	601	CHL	C1A-C2A-CAA-CBA
30	y	608	CHL	C1A-C2A-CAA-CBA
31	1	602	CLA	C1A-C2A-CAA-CBA
31	1	603	CLA	C1A-C2A-CAA-CBA
31	1	610	CLA	C1A-C2A-CAA-CBA
31	2	602	CLA	C1A-C2A-CAA-CBA
31	2	603	CLA	C1A-C2A-CAA-CBA
31	2	604	CLA	C1A-C2A-CAA-CBA
31	2	609	CLA	C1A-C2A-CAA-CBA
31	3	304	CLA	C1A-C2A-CAA-CBA
31	3	306	CLA	C1A-C2A-CAA-CBA
31	3	315	CLA	C1A-C2A-CAA-CBA
31	3	316	CLA	C1A-C2A-CAA-CBA
31	4	602	CLA	C1A-C2A-CAA-CBA
31	4	603	CLA	C1A-C2A-CAA-CBA
31	4	604	CLA	C1A-C2A-CAA-CBA
31	4	610	CLA	C1A-C2A-CAA-CBA
31	4	611	CLA	C1A-C2A-CAA-CBA
31	5	602	CLA	C1A-C2A-CAA-CBA
31	5	603	CLA	C1A-C2A-CAA-CBA
31	5	604	CLA	C1A-C2A-CAA-CBA
31	5	611	CLA	C1A-C2A-CAA-CBA
31	6	303	CLA	C1A-C2A-CAA-CBA
31	6	313	CLA	C1A-C2A-CAA-CBA
31	6	314	CLA	C1A-C2A-CAA-CBA
31	6	315	CLA	C1A-C2A-CAA-CBA
31	A	407	CLA	C1A-C2A-CAA-CBA
31	B	610	CLA	C1A-C2A-CAA-CBA
31	C	601	CLA	C1A-C2A-CAA-CBA
31	C	603	CLA	C1A-C2A-CAA-CBA
31	C	608	CLA	C1A-C2A-CAA-CBA
31	C	611	CLA	C1A-C2A-CAA-CBA
31	C	612	CLA	C1A-C2A-CAA-CBA
31	G	602	CLA	C1A-C2A-CAA-CBA
31	G	609	CLA	C1A-C2A-CAA-CBA
31	N	304	CLA	C1A-C2A-CAA-CBA
31	R	303	CLA	C1A-C2A-CAA-CBA
31	R	307	CLA	C1A-C2A-CAA-CBA
31	S	311	CLA	C1A-C2A-CAA-CBA
31	S	315	CLA	C1A-C2A-CAA-CBA
31	S	316	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	Y	303	CLA	C1A-C2A-CAA-CBA
31	Y	304	CLA	C1A-C2A-CAA-CBA
31	Y	310	CLA	C1A-C2A-CAA-CBA
31	Y	314	CLA	C1A-C2A-CAA-CBA
31	0	612	CLA	C1A-C2A-CAA-CBA
31	7	303	CLA	C1A-C2A-CAA-CBA
31	7	304	CLA	C1A-C2A-CAA-CBA
31	7	305	CLA	C1A-C2A-CAA-CBA
31	7	311	CLA	C1A-C2A-CAA-CBA
31	8	602	CLA	C1A-C2A-CAA-CBA
31	8	603	CLA	C1A-C2A-CAA-CBA
31	9	305	CLA	C1A-C2A-CAA-CBA
31	9	313	CLA	C1A-C2A-CAA-CBA
31	p	602	CLA	C1A-C2A-CAA-CBA
31	p	603	CLA	C1A-C2A-CAA-CBA
31	p	604	CLA	C1A-C2A-CAA-CBA
31	p	610	CLA	C1A-C2A-CAA-CBA
31	p	613	CLA	C1A-C2A-CAA-CBA
31	p	614	CLA	C1A-C2A-CAA-CBA
31	q	304	CLA	C1A-C2A-CAA-CBA
31	q	305	CLA	C1A-C2A-CAA-CBA
31	q	312	CLA	C1A-C2A-CAA-CBA
31	b	604	CLA	C1A-C2A-CAA-CBA
31	b	607	CLA	C1A-C2A-CAA-CBA
31	b	615	CLA	C1A-C2A-CAA-CBA
31	c	601	CLA	C1A-C2A-CAA-CBA
31	c	603	CLA	C1A-C2A-CAA-CBA
31	c	608	CLA	C1A-C2A-CAA-CBA
31	c	610	CLA	C1A-C2A-CAA-CBA
31	c	611	CLA	C1A-C2A-CAA-CBA
31	d	401	CLA	C1A-C2A-CAA-CBA
31	g	303	CLA	C1A-C2A-CAA-CBA
31	g	310	CLA	C1A-C2A-CAA-CBA
31	n	303	CLA	C1A-C2A-CAA-CBA
31	n	304	CLA	C1A-C2A-CAA-CBA
31	r	304	CLA	C1A-C2A-CAA-CBA
31	r	307	CLA	C1A-C2A-CAA-CBA
31	r	313	CLA	C1A-C2A-CAA-CBA
31	s	303	CLA	C1A-C2A-CAA-CBA
31	s	311	CLA	C1A-C2A-CAA-CBA
31	s	315	CLA	C1A-C2A-CAA-CBA
31	y	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	y	603	CLA	C1A-C2A-CAA-CBA
31	y	604	CLA	C1A-C2A-CAA-CBA
31	y	610	CLA	C1A-C2A-CAA-CBA
31	y	614	CLA	C1A-C2A-CAA-CBA
31	C	603	CLA	C16-C17-C18-C20
31	C	612	CLA	C6-C7-C8-C9
31	N	304	CLA	C6-C7-C8-C10
31	7	304	CLA	C6-C7-C8-C10
31	8	603	CLA	C6-C7-C8-C10
31	9	315	CLA	C6-C7-C8-C10
31	p	611	CLA	C11-C12-C13-C15
31	q	312	CLA	C6-C7-C8-C10
31	n	304	CLA	C6-C7-C8-C10
31	y	603	CLA	C6-C7-C8-C10
33	3	320	LHG	O9-C7-O7-C5
33	b	625	LHG	C8-C7-O7-C5
33	9	320	LHG	C26-C27-C28-C29
33	g	319	LHG	C30-C31-C32-C33
34	k	101	LMG	C18-C19-C20-C21
38	x	201	SQD	C27-C28-C29-C30
43	C	614	BCR	C9-C10-C11-C12
43	c	614	BCR	C13-C14-C15-C16
43	v	101	BCR	C9-C10-C11-C12
31	N	304	CLA	O1D-CGD-O2D-CED
31	B	603	CLA	C10-C11-C12-C13
31	b	609	CLA	C5-C6-C7-C8
31	c	602	CLA	C8-C10-C11-C12
31	c	603	CLA	C15-C16-C17-C18
33	B	624	LHG	C3-O3-P-O6
33	Y	318	LHG	C3-O3-P-O6
33	b	625	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O3
33	L	101	LHG	C29-C30-C31-C32
34	6	323	LMG	C29-C30-C31-C32
38	B	623	SQD	C25-C26-C27-C28
34	b	623	LMG	C10-C11-C12-C13
34	C	621	LMG	O6-C5-C6-O5
44	d	407	PL9	C47-C48-C49-C50
31	q	305	CLA	C3-C5-C6-C7
31	y	604	CLA	C3-C5-C6-C7
31	4	604	CLA	O1D-CGD-O2D-CED
33	N	319	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
38	s	301	SQD	C9-C10-C11-C12
30	G	605	CHL	O1A-CGA-O2A-C1
31	4	610	CLA	C10-C11-C12-C13
31	C	605	CLA	CBA-CGA-O2A-C1
31	g	310	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C24-C23-O8-C6
34	G	619	LMG	O6-C5-C6-O5
33	1	617	LHG	O6-C4-C5-C6
33	2	617	LHG	O6-C4-C5-C6
33	6	320	LHG	O6-C4-C5-C6
33	A	417	LHG	O6-C4-C5-C6
33	G	618	LHG	O6-C4-C5-C6
33	N	319	LHG	O6-C4-C5-C6
33	R	320	LHG	O6-C4-C5-C6
33	8	618	LHG	O6-C4-C5-C6
33	9	320	LHG	O6-C4-C5-C6
33	a	415	LHG	O6-C4-C5-C6
33	n	320	LHG	O6-C4-C5-C6
33	z	102	LHG	O6-C4-C5-C6
33	F1	301	LHG	O6-C4-C5-C6
34	B	621	LMG	C29-C30-C31-C32
34	k	101	LMG	C30-C31-C32-C33
48	R	302	LMU	C5'-C4'-O1B-C1B
33	1	617	LHG	C11-C10-C9-C8
33	a	415	LHG	C31-C32-C33-C34
33	l	101	LHG	C31-C32-C33-C34
34	W	201	LMG	O6-C5-C6-O5
34	c	620	LMG	O6-C5-C6-O5
31	N	310	CLA	C5-C6-C7-C8
34	w	205	LMG	C8-C9-O8-C28
33	2	617	LHG	C10-C11-C12-C13
33	b	628	LHG	C11-C10-C9-C8
34	D	412	LMG	C36-C37-C38-C39
45	c	618	DGD	C3A-C4A-C5A-C6A
30	1	606	CHL	C3-C5-C6-C7
33	b	628	LHG	C30-C31-C32-C33
33	s	320	LHG	C11-C12-C13-C14
30	N	307	CHL	CBA-CGA-O2A-C1
45	c	616	DGD	C2A-C1A-O1G-C1G
34	k	102	LMG	O6-C5-C6-O5
30	3	302	CHL	C4-C3-C5-C6
31	c	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	s	313	CLA	C4-C3-C5-C6
31	y	613	CLA	C4-C3-C5-C6
31	c	610	CLA	C2-C3-C5-C6
31	s	304	CLA	C3A-C2A-CAA-CBA
33	B	624	LHG	C12-C13-C14-C15
38	b	621	SQD	C26-C27-C28-C29
31	B	611	CLA	C15-C16-C17-C18
31	c	611	CLA	C8-C10-C11-C12
33	6	320	LHG	C9-C10-C11-C12
33	A	417	LHG	C33-C34-C35-C36
33	D	408	LHG	C17-C18-C19-C20
33	b	628	LHG	C15-C16-C17-C18
34	D	409	LMG	C11-C12-C13-C14
33	r	320	LHG	C7-C8-C9-C10
30	2	606	CHL	O1A-CGA-O2A-C1
31	B	613	CLA	O1A-CGA-O2A-C1
31	C	605	CLA	O1A-CGA-O2A-C1
33	e	101	LHG	C11-C12-C13-C14
34	b	626	LMG	C31-C32-C33-C34
34	c	624	LMG	C29-C30-C31-C32
30	y	606	CHL	C2A-CAA-CBA-CGA
31	b	602	CLA	C2A-CAA-CBA-CGA
31	c	601	CLA	C2A-CAA-CBA-CGA
31	q	305	CLA	C6-C7-C8-C9
31	g	304	CLA	C6-C7-C8-C9
34	b	626	LMG	O6-C5-C6-O5
30	9	307	CHL	O1D-CGD-O2D-CED
33	1	617	LHG	C4-C5-C6-O8
33	5	619	LHG	C4-C5-C6-O8
33	D	408	LHG	C4-C5-C6-O8
33	L	101	LHG	C4-C5-C6-O8
33	R	320	LHG	C4-C5-C6-O8
33	S	322	LHG	C9-C10-C11-C12
33	0	619	LHG	C4-C5-C6-O8
33	e	101	LHG	C4-C5-C6-O8
33	j	102	LHG	C4-C5-C6-O8
33	r	320	LHG	C4-C5-C6-O8
34	2	618	LMG	O1-C7-C8-C9
34	A	414	LMG	O1-C7-C8-C9
34	A	418	LMG	O1-C7-C8-C9
34	B	621	LMG	C7-C8-C9-O8
34	B	625	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	C	621	LMG	C7-C8-C9-O8
34	G	619	LMG	O1-C7-C8-C9
34	N	320	LMG	O1-C7-C8-C9
34	W	203	LMG	O1-C7-C8-C9
34	X	203	LMG	C7-C8-C9-O8
34	7	322	LMG	O1-C7-C8-C9
34	9	301	LMG	O1-C7-C8-C9
34	b	629	LMG	C7-C8-C9-O8
34	g	320	LMG	O1-C7-C8-C9
34	n	322	LMG	C33-C34-C35-C36
34	r	321	LMG	O1-C7-C8-C9
34	s	321	LMG	C7-C8-C9-O8
38	6	301	SQD	O6-C44-C45-C46
38	A	411	SQD	C44-C45-C46-O48
38	A	413	SQD	C44-C45-C46-O48
38	B	623	SQD	O6-C44-C45-C46
38	G	617	SQD	C44-C45-C46-O48
38	R	322	SQD	O6-C44-C45-C46
38	S	301	SQD	C44-C45-C46-O48
38	b	627	SQD	C44-C45-C46-O48
38	r	322	SQD	O6-C44-C45-C46
38	y	621	SQD	C44-C45-C46-O48
33	j	102	LHG	C24-C23-O8-C6
34	C	624	LMG	O6-C5-C6-O5
31	1	604	CLA	C13-C15-C16-C17
31	0	604	CLA	C5-C6-C7-C8
31	r	316	CLA	C13-C15-C16-C17
33	b	628	LHG	C9-C10-C11-C12
33	t	102	LHG	C11-C12-C13-C14
45	c	616	DGD	CDB-CEB-CFB-CGB
34	2	618	LMG	C8-C7-O1-C1
34	2	620	LMG	C8-C7-O1-C1
34	2	621	LMG	C8-C7-O1-C1
34	6	323	LMG	C8-C7-O1-C1
34	G	619	LMG	C8-C7-O1-C1
34	G	621	LMG	C8-C7-O1-C1
34	I	101	LMG	C8-C7-O1-C1
34	J	102	LMG	C8-C7-O1-C1
34	R	321	LMG	C8-C7-O1-C1
34	W	202	LMG	C8-C7-O1-C1
34	Y	319	LMG	C8-C7-O1-C1
34	0	622	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
34	9	321	LMG	C8-C7-O1-C1
34	b	622	LMG	C8-C7-O1-C1
34	c	621	LMG	C8-C7-O1-C1
34	f	101	LMG	C8-C7-O1-C1
34	g	320	LMG	C8-C7-O1-C1
34	y	620	LMG	C8-C7-O1-C1
34	Q1	101	LMG	C8-C7-O1-C1
38	6	301	SQD	C45-C44-O6-C1
38	R	322	SQD	C45-C44-O6-C1
38	X	201	SQD	C45-C44-O6-C1
38	b	621	SQD	C45-C44-O6-C1
45	C	617	DGD	C5D-C6D-O5D-C1E
45	c	619	DGD	C5D-C6D-O5D-C1E
30	N	309	CHL	O1D-CGD-O2D-CED
33	C	623	LHG	C35-C36-C37-C38
33	9	320	LHG	C28-C29-C30-C31
34	D	409	LMG	C12-C13-C14-C15
31	B	607	CLA	C10-C11-C12-C13
31	9	305	CLA	C5-C6-C7-C8
31	b	610	CLA	C13-C15-C16-C17
33	A	417	LHG	C28-C29-C30-C31
33	p	619	LHG	C25-C26-C27-C28
33	F1	301	LHG	C9-C10-C11-C12
34	2	621	LMG	C31-C32-C33-C34
34	d	411	LMG	C12-C13-C14-C15
45	c	617	DGD	C7A-C8A-C9A-CAA
34	2	618	LMG	O7-C10-C11-C12
34	6	323	LMG	O7-C10-C11-C12
34	I	101	LMG	O6-C5-C6-O5
34	p	620	LMG	O6-C5-C6-O5
34	d	411	LMG	O6-C5-C6-O5
33	A	417	LHG	C23-C24-C25-C26
38	B	620	SQD	C23-C24-C25-C26
33	s	320	LHG	C10-C11-C12-C13
38	B	623	SQD	C12-C13-C14-C15
48	R	302	LMU	C1-C2-C3-C4
34	a	413	LMG	O6-C1-O1-C7
44	a	414	PL9	C39-C41-C42-C43
33	D	408	LHG	C33-C34-C35-C36
33	p	619	LHG	C28-C29-C30-C31
30	g	306	CHL	CBA-CGA-O2A-C1
34	2	618	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
34	s	321	LMG	O6-C5-C6-O5
45	C	618	DGD	O6E-C5E-C6E-O5E
33	3	320	LHG	O1-C1-C2-O2
33	L	101	LHG	O1-C1-C2-O2
33	R	320	LHG	O1-C1-C2-O2
33	Y	318	LHG	O1-C1-C2-O2
33	g	319	LHG	O1-C1-C2-O2
34	3	321	LMG	C8-C9-O8-C28
34	b	629	LMG	C8-C9-O8-C28
33	A	415	LHG	C33-C34-C35-C36
33	S	322	LHG	C35-C36-C37-C38
33	b	625	LHG	C29-C30-C31-C32
33	l	101	LHG	C16-C17-C18-C19
33	r	320	LHG	C25-C26-C27-C28
33	F1	301	LHG	C13-C14-C15-C16
38	r	322	SQD	C10-C11-C12-C13
38	s	301	SQD	C25-C26-C27-C28
33	s	322	LHG	C29-C30-C31-C32
30	g	302	CHL	CAA-CBA-CGA-O2A
48	K	101	LMU	C1-C2-C3-C4
33	B	624	LHG	C35-C36-C37-C38
33	S	320	LHG	C26-C27-C28-C29
33	b	628	LHG	C33-C34-C35-C36
33	l	101	LHG	C30-C31-C32-C33
34	w	205	LMG	C31-C32-C33-C34
38	s	301	SQD	C28-C29-C30-C31
31	5	610	CLA	C5-C6-C7-C8
31	7	313	CLA	C5-C6-C7-C8
31	8	609	CLA	C5-C6-C7-C8
42	A	408	PHO	C5-C6-C7-C8
34	S	321	LMG	O6-C5-C6-O5
36	2	616	NEX	C11-C10-C9-C19
36	3	319	NEX	C39-C29-C30-C31
36	N	318	NEX	C11-C10-C9-C19
36	R	301	NEX	C39-C29-C30-C31
36	q	319	NEX	C39-C29-C30-C31
36	g	317	NEX	C40-C33-C34-C35
37	2	619	XAT	C20-C13-C14-C15
37	4	619	XAT	C20-C13-C14-C15
37	G	620	XAT	C20-C13-C14-C15
37	9	322	XAT	C20-C13-C14-C15
37	q	321	XAT	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
37	g	321	XAT	C20-C13-C14-C15
45	c	618	DGD	O6E-C5E-C6E-O5E
30	N	306	CHL	C4-C3-C5-C6
31	c	603	CLA	C4-C3-C5-C6
31	c	610	CLA	C4-C3-C5-C6
31	n	316	CLA	C5-C6-C7-C8
48	K	101	LMU	C6-C7-C8-C9
31	c	603	CLA	C2-C3-C5-C6
31	r	316	CLA	C2-C3-C5-C6
34	6	322	LMG	C10-C11-C12-C13
31	0	615	CLA	C6-C7-C8-C9
31	b	603	CLA	C16-C17-C18-C20
31	7	313	CLA	CBA-CGA-O2A-C1
31	q	304	CLA	CBA-CGA-O2A-C1
33	M	101	LHG	C24-C23-O8-C6
33	F1	301	LHG	C24-C23-O8-C6
34	r	321	LMG	C29-C28-O8-C9
34	5	620	LMG	C8-C9-O8-C28
33	c	622	LHG	C30-C31-C32-C33
34	D	411	LMG	C37-C38-C39-C40
34	d	410	LMG	C37-C38-C39-C40
38	b	627	SQD	C16-C17-C18-C19
31	3	306	CLA	CBD-CGD-O2D-CED
31	R	315	CLA	C5-C6-C7-C8
31	S	312	CLA	C13-C15-C16-C17
31	b	603	CLA	C15-C16-C17-C18
31	c	609	CLA	C13-C15-C16-C17
31	7	315	CLA	C6-C7-C8-C9
33	6	320	LHG	C13-C14-C15-C16
33	0	619	LHG	C12-C13-C14-C15
38	b	621	SQD	C17-C18-C19-C20
33	N	319	LHG	C4-C5-O7-C7
34	3	321	LMG	C9-C8-O7-C10
34	7	320	LMG	C9-C8-O7-C10
45	c	619	DGD	C1G-C2G-O2G-C1B
31	a	407	CLA	O1D-CGD-O2D-CED
34	4	620	LMG	O6-C5-C6-O5
30	4	609	CHL	C2A-CAA-CBA-CGA
30	r	310	CHL	C2A-CAA-CBA-CGA
31	3	305	CLA	C2A-CAA-CBA-CGA
31	6	315	CLA	C2A-CAA-CBA-CGA
31	R	304	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	9	306	CLA	C8-C10-C11-C12
31	c	603	CLA	C10-C11-C12-C13
31	C	604	CLA	C2-C1-O2A-CGA
31	C	605	CLA	C2-C1-O2A-CGA
31	N	311	CLA	C2-C1-O2A-CGA
31	N	315	CLA	C2-C1-O2A-CGA
31	R	307	CLA	C2-C1-O2A-CGA
31	Y	311	CLA	C2-C1-O2A-CGA
31	Y	313	CLA	C2-C1-O2A-CGA
31	g	314	CLA	C2-C1-O2A-CGA
33	n	320	LHG	C11-C12-C13-C14
33	s	320	LHG	C31-C32-C33-C34
33	y	619	LHG	C9-C10-C11-C12
33	y	619	LHG	C35-C36-C37-C38
33	a	415	LHG	C23-C24-C25-C26
30	G	606	CHL	O1D-CGD-O2D-CED
30	7	306	CHL	O1D-CGD-O2D-CED
30	8	608	CHL	CBD-CGD-O2D-CED
48	K	101	LMU	O5'-C5'-C6'-O6'
31	b	604	CLA	C3-C5-C6-C7
33	8	618	LHG	C11-C12-C13-C14
33	q	320	LHG	C30-C31-C32-C33
33	q	320	LHG	C33-C34-C35-C36
33	s	322	LHG	C27-C28-C29-C30
31	B	608	CLA	C8-C10-C11-C12
31	C	601	CLA	C10-C11-C12-C13
31	b	604	CLA	C13-C15-C16-C17
42	A	408	PHO	C10-C11-C12-C13
33	j	102	LHG	C11-C12-C13-C14
30	4	607	CHL	CBA-CGA-O2A-C1
31	2	612	CLA	CBA-CGA-O2A-C1
31	B	611	CLA	CBA-CGA-O2A-C1
31	8	602	CLA	CBA-CGA-O2A-C1
31	y	611	CLA	CBA-CGA-O2A-C1
33	5	619	LHG	O6-C4-C5-O7
33	g	319	LHG	O6-C4-C5-O7
33	r	320	LHG	O6-C4-C5-O7
33	y	619	LHG	O6-C4-C5-O7
34	G	619	LMG	O7-C10-C11-C12
34	c	620	LMG	O7-C10-C11-C12
31	6	315	CLA	O1D-CGD-O2D-CED
31	C	612	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	c	603	CLA	C16-C17-C18-C20
31	g	304	CLA	C6-C7-C8-C10
31	r	304	CLA	C11-C12-C13-C15
33	e	101	LHG	C23-C24-C25-C26
34	C	622	LMG	C28-C29-C30-C31
33	R	320	LHG	C28-C29-C30-C31
34	x	202	LMG	C34-C35-C36-C37
48	R	302	LMU	O5B-C1B-O1B-C4'
31	7	316	CLA	O1D-CGD-O2D-CED
30	1	619	CHL	C5-C6-C7-C8
30	g	309	CHL	C5-C6-C7-C8
30	y	609	CHL	C8-C10-C11-C12
31	2	602	CLA	C10-C11-C12-C13
31	B	614	CLA	C10-C11-C12-C13
34	b	629	LMG	C33-C34-C35-C36
31	C	608	CLA	O1D-CGD-O2D-CED
31	7	313	CLA	O1A-CGA-O2A-C1
45	c	616	DGD	O1A-C1A-O1G-C1G
33	j	102	LHG	C11-C10-C9-C8
45	c	619	DGD	C4D-C5D-C6D-O5D
33	S	322	LHG	C7-C8-C9-C10
38	m	101	SQD	C23-C24-C25-C26
31	N	305	CLA	C5-C6-C7-C8
31	y	604	CLA	C5-C6-C7-C8
34	6	321	LMG	C2-C1-O1-C7
34	A	414	LMG	C2-C1-O1-C7
34	D	410	LMG	C2-C1-O1-C7
34	W	201	LMG	C2-C1-O1-C7
34	b	622	LMG	C2-C1-O1-C7
34	c	620	LMG	C2-C1-O1-C7
34	w	202	LMG	C2-C1-O1-C7
36	6	319	NEX	C32-C33-C34-C35
36	0	618	NEX	C32-C33-C34-C35
37	2	619	XAT	C12-C13-C14-C15
45	C	620	DGD	C2D-C1D-O3G-C3G
33	S	320	LHG	C30-C31-C32-C33
34	q1	101	LMG	C8-C9-O8-C28
30	5	601	CHL	CAA-CBA-CGA-O2A
34	g	320	LMG	O7-C10-C11-C12
33	6	320	LHG	O7-C5-C6-O8
34	2	620	LMG	O1-C7-C8-O7
34	2	620	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	5	620	LMG	O1-C7-C8-O7
34	D	409	LMG	O1-C7-C8-O7
34	G	621	LMG	O1-C7-C8-O7
34	I	101	LMG	O1-C7-C8-O7
34	0	620	LMG	O1-C7-C8-O7
34	7	322	LMG	O7-C8-C9-O8
34	w	205	LMG	O1-C7-C8-O7
34	x	202	LMG	O1-C7-C8-O7
45	C	617	DGD	O2G-C2G-C3G-O3G
45	C	620	DGD	O2G-C2G-C3G-O3G
31	2	604	CLA	C6-C7-C8-C9
33	2	617	LHG	C34-C35-C36-C37
33	9	320	LHG	C11-C10-C9-C8
34	q	301	LMG	C11-C12-C13-C14
33	t	102	LHG	O9-C7-O7-C5
30	1	606	CHL	C5-C6-C7-C8
31	6	316	CLA	C5-C6-C7-C8
31	d	405	CLA	C10-C11-C12-C13
31	n	311	CLA	C5-C6-C7-C8
31	g	310	CLA	O1A-CGA-O2A-C1
31	p	611	CLA	C11-C12-C13-C14
42	d	402	PHO	CHA-CBD-CGD-O1D
42	d	402	PHO	CHA-CBD-CGD-O2D
33	t	102	LHG	C11-C10-C9-C8
31	2	602	CLA	C4-C3-C5-C6
31	0	613	CLA	C4-C3-C5-C6
31	r	316	CLA	C4-C3-C5-C6
34	2	620	LMG	C34-C35-C36-C37
30	1	605	CHL	C11-C10-C8-C7
30	1	605	CHL	C12-C13-C15-C16
30	1	606	CHL	C11-C10-C8-C7
30	1	606	CHL	C11-C12-C13-C15
30	1	607	CHL	C12-C13-C15-C16
30	2	601	CHL	C11-C10-C8-C7
30	2	608	CHL	C6-C7-C8-C10
30	6	310	CHL	C11-C10-C8-C7
30	G	623	CHL	C12-C13-C15-C16
30	N	306	CHL	C11-C10-C8-C7
30	Y	301	CHL	C12-C13-C15-C16
30	Y	307	CHL	C11-C10-C8-C7
30	Y	309	CHL	C12-C13-C15-C16
30	7	302	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
30	7	302	CHL	C12-C13-C15-C16
30	7	306	CHL	C6-C7-C8-C10
30	7	306	CHL	C11-C12-C13-C15
30	7	306	CHL	C12-C13-C15-C16
30	7	307	CHL	C12-C13-C15-C16
30	7	308	CHL	C12-C13-C15-C16
30	8	605	CHL	C11-C10-C8-C7
30	8	605	CHL	C11-C12-C13-C15
30	8	605	CHL	C12-C13-C15-C16
30	8	606	CHL	C11-C10-C8-C7
30	9	311	CHL	C11-C10-C8-C7
30	g	302	CHL	C11-C10-C8-C7
30	n	306	CHL	C11-C10-C8-C7
30	n	306	CHL	C11-C12-C13-C15
30	n	306	CHL	C12-C13-C15-C16
30	n	307	CHL	C11-C10-C8-C7
30	y	607	CHL	C11-C12-C13-C15
31	1	613	CLA	C6-C7-C8-C10
31	2	602	CLA	C2-C3-C5-C6
31	4	602	CLA	C6-C7-C8-C10
31	6	311	CLA	C6-C7-C8-C10
31	6	314	CLA	C6-C7-C8-C10
31	B	607	CLA	C11-C10-C8-C7
31	B	607	CLA	C11-C12-C13-C15
31	B	609	CLA	C6-C7-C8-C10
31	B	615	CLA	C6-C7-C8-C10
31	C	601	CLA	C11-C12-C13-C15
31	C	602	CLA	C6-C7-C8-C10
31	C	603	CLA	C11-C12-C13-C15
31	C	605	CLA	C11-C10-C8-C7
31	C	608	CLA	C11-C10-C8-C7
31	C	610	CLA	C12-C13-C15-C16
31	D	403	CLA	C11-C12-C13-C15
31	D	404	CLA	C6-C7-C8-C10
31	G	602	CLA	C6-C7-C8-C10
31	N	303	CLA	C11-C10-C8-C7
31	N	313	CLA	C6-C7-C8-C10
31	N	313	CLA	C11-C12-C13-C15
31	R	304	CLA	C6-C7-C8-C10
31	R	304	CLA	C11-C10-C8-C7
31	R	311	CLA	C11-C10-C8-C7
31	R	316	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	Y	311	CLA	C11-C10-C8-C7
31	Y	311	CLA	C11-C12-C13-C15
31	0	602	CLA	C6-C7-C8-C10
31	0	603	CLA	C6-C7-C8-C10
31	0	610	CLA	C11-C10-C8-C7
31	7	312	CLA	C6-C7-C8-C10
31	8	612	CLA	C6-C7-C8-C10
31	9	304	CLA	C11-C10-C8-C7
31	9	306	CLA	C6-C7-C8-C10
31	9	306	CLA	C11-C10-C8-C7
31	p	611	CLA	C6-C7-C8-C10
31	b	606	CLA	C12-C13-C15-C16
31	b	608	CLA	C11-C12-C13-C15
31	b	612	CLA	C11-C12-C13-C15
31	c	603	CLA	C11-C12-C13-C15
31	c	608	CLA	C6-C7-C8-C10
31	c	611	CLA	C11-C10-C8-C7
31	c	613	CLA	C12-C13-C15-C16
31	d	405	CLA	C6-C7-C8-C10
31	g	310	CLA	C11-C12-C13-C15
31	n	314	CLA	C6-C7-C8-C10
31	r	305	CLA	C6-C7-C8-C10
31	r	311	CLA	C6-C7-C8-C10
31	s	314	CLA	C11-C10-C8-C7
31	s	314	CLA	C12-C13-C15-C16
31	y	602	CLA	C6-C7-C8-C10
31	y	610	CLA	C11-C12-C13-C15
42	D	401	PHO	C11-C10-C8-C7
31	3	313	CLA	CAA-CBA-CGA-O2A
31	4	603	CLA	C3-C5-C6-C7
31	S	303	CLA	C3-C5-C6-C7
30	N	307	CHL	O1A-CGA-O2A-C1
38	s	301	SQD	O10-C23-O48-C46
31	Y	314	CLA	C6-C7-C8-C9
33	c	622	LHG	C12-C13-C14-C15
34	B	622	LMG	C12-C13-C14-C15
30	Y	301	CHL	C14-C13-C15-C16
30	Y	309	CHL	C14-C13-C15-C16
30	7	307	CHL	C14-C13-C15-C16
30	7	310	CHL	C11-C12-C13-C14
30	8	605	CHL	C14-C13-C15-C16
30	n	306	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	1	612	CLA	C6-C7-C8-C9
31	1	613	CLA	C6-C7-C8-C9
31	2	602	CLA	C6-C7-C8-C9
31	2	609	CLA	C6-C7-C8-C9
31	3	304	CLA	C6-C7-C8-C9
31	4	602	CLA	C6-C7-C8-C9
31	6	304	CLA	C6-C7-C8-C9
31	6	311	CLA	C6-C7-C8-C9
31	6	314	CLA	C6-C7-C8-C9
31	B	602	CLA	C11-C12-C13-C14
31	B	603	CLA	C11-C12-C13-C14
31	B	604	CLA	C14-C13-C15-C16
31	B	605	CLA	C14-C13-C15-C16
31	B	615	CLA	C6-C7-C8-C9
31	B	616	CLA	C6-C7-C8-C9
31	C	601	CLA	C6-C7-C8-C9
31	C	603	CLA	C11-C12-C13-C14
31	C	605	CLA	C11-C10-C8-C9
31	C	608	CLA	C6-C7-C8-C9
31	D	403	CLA	C11-C12-C13-C14
31	R	311	CLA	C6-C7-C8-C9
31	Y	303	CLA	C6-C7-C8-C9
31	Y	303	CLA	C11-C10-C8-C9
31	0	602	CLA	C6-C7-C8-C9
31	0	603	CLA	C6-C7-C8-C9
31	0	613	CLA	C6-C7-C8-C9
31	7	312	CLA	C6-C7-C8-C9
31	7	314	CLA	C11-C12-C13-C14
31	8	604	CLA	C11-C10-C8-C9
31	8	612	CLA	C11-C12-C13-C14
31	b	604	CLA	C6-C7-C8-C9
31	b	605	CLA	C14-C13-C15-C16
31	b	616	CLA	C11-C12-C13-C14
31	c	607	CLA	C11-C12-C13-C14
31	d	405	CLA	C6-C7-C8-C9
31	g	303	CLA	C6-C7-C8-C9
31	n	305	CLA	C11-C10-C8-C9
31	n	314	CLA	C11-C12-C13-C14
31	y	602	CLA	C6-C7-C8-C9
42	D	401	PHO	C11-C12-C13-C14
31	c	605	CLA	CBD-CGD-O2D-CED
34	W	201	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
34	q	301	LMG	C18-C19-C20-C21
31	C	601	CLA	CBA-CGA-O2A-C1
31	Y	311	CLA	CBA-CGA-O2A-C1
30	1	609	CHL	C10-C11-C12-C13
31	B	603	CLA	C8-C10-C11-C12
31	C	613	CLA	C8-C10-C11-C12
31	C	613	CLA	C13-C15-C16-C17
31	b	610	CLA	C8-C10-C11-C12
30	1	608	CHL	C2A-CAA-CBA-CGA
31	B	603	CLA	C2A-CAA-CBA-CGA
31	p	615	CLA	C2A-CAA-CBA-CGA
33	2	617	LHG	C16-C17-C18-C19
38	R	322	SQD	C12-C13-C14-C15
32	6	317	LUT	C27-C28-C29-C39
43	C	615	BCR	C37-C22-C23-C24
43	D	405	BCR	C37-C22-C23-C24
43	T	101	BCR	C36-C18-C19-C20
31	6	316	CLA	C6-C7-C8-C9
31	r	305	CLA	C11-C12-C13-C15
33	1	617	LHG	C28-C29-C30-C31
33	M	101	LHG	C11-C12-C13-C14
32	2	615	LUT	C31-C32-C33-C34
32	G	615	LUT	C31-C32-C33-C34
36	R	319	NEX	C31-C32-C33-C34
33	B	624	LHG	C17-C18-C19-C20
33	K	102	LHG	C26-C27-C28-C29
34	X	203	LMG	C11-C12-C13-C14
30	N	307	CHL	C3-C5-C6-C7
31	C	611	CLA	C3-C5-C6-C7
31	9	305	CLA	C3-C5-C6-C7
30	N	308	CHL	O1D-CGD-O2D-CED
30	n	302	CHL	O1D-CGD-O2D-CED
31	s	313	CLA	C5-C6-C7-C8
33	D	407	LHG	C26-C27-C28-C29
33	L	101	LHG	C35-C36-C37-C38
44	A	416	PL9	C37-C38-C39-C41
30	9	309	CHL	CBA-CGA-O2A-C1
31	C	603	CLA	CBA-CGA-O2A-C1
31	7	314	CLA	CBA-CGA-O2A-C1
31	c	606	CLA	CBA-CGA-O2A-C1
33	3	320	LHG	C24-C23-O8-C6
33	C	623	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
34	3	321	LMG	C29-C28-O8-C9
31	9	312	CLA	C6-C7-C8-C9
34	d	409	LMG	C10-C11-C12-C13
31	A	405	CLA	C5-C6-C7-C8
31	7	305	CLA	C5-C6-C7-C8
31	r	315	CLA	C5-C6-C7-C8
30	8	601	CHL	O1D-CGD-O2D-CED
33	D	407	LHG	C35-C36-C37-C38
33	G	618	LHG	C28-C29-C30-C31
34	C	624	LMG	C15-C16-C17-C18
38	R	322	SQD	C26-C27-C28-C29
45	c	619	DGD	O6D-C5D-C6D-O5D
31	2	602	CLA	C4B-C3B-CAB-CBB
31	B	615	CLA	C4B-C3B-CAB-CBB
31	S	310	CLA	C4B-C3B-CAB-CBB
31	Y	311	CLA	C4B-C3B-CAB-CBB
31	0	615	CLA	C4B-C3B-CAB-CBB
31	b	602	CLA	C4B-C3B-CAB-CBB
31	b	603	CLA	C4B-C3B-CAB-CBB
31	b	616	CLA	C4B-C3B-CAB-CBB
31	r	313	CLA	C4B-C3B-CAB-CBB
31	r	316	CLA	C4B-C3B-CAB-CBB
31	s	312	CLA	C4B-C3B-CAB-CBB
30	2	601	CHL	C8-C10-C11-C12
33	A	415	LHG	O6-C4-C5-C6
33	D	408	LHG	O6-C4-C5-C6
33	K	102	LHG	O6-C4-C5-C6
33	S	320	LHG	O6-C4-C5-C6
33	j	102	LHG	O6-C4-C5-C6
33	r	320	LHG	O6-C4-C5-C6
33	s	320	LHG	O6-C4-C5-C6
33	y	619	LHG	O6-C4-C5-C6
33	q	320	LHG	C25-C26-C27-C28
33	b	628	LHG	C34-C35-C36-C37
33	R	320	LHG	C7-C8-C9-C10
45	c	616	DGD	C1B-C2B-C3B-C4B
33	0	619	LHG	C13-C14-C15-C16
34	w	204	LMG	C11-C12-C13-C14
31	1	612	CLA	C5-C6-C7-C8
31	B	606	CLA	C10-C11-C12-C13
31	R	304	CLA	C10-C11-C12-C13
31	0	611	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	8	612	CLA	C15-C16-C17-C18
31	n	314	CLA	C15-C16-C17-C18
31	2	613	CLA	CAA-CBA-CGA-O2A
30	y	607	CHL	O1D-CGD-O2D-CED
33	B	624	LHG	C25-C26-C27-C28
38	b	621	SQD	C35-C36-C37-C38
30	R	308	CHL	C4-C3-C5-C6
30	9	309	CHL	C4-C3-C5-C6
31	1	610	CLA	C4-C3-C5-C6
31	c	606	CLA	C4-C3-C5-C6
30	6	302	CHL	C2-C3-C5-C6
31	0	613	CLA	C2-C3-C5-C6
33	G	618	LHG	C7-C8-C9-C10
34	n	322	LMG	C10-C11-C12-C13
38	M	102	SQD	C23-C24-C25-C26
33	j	102	LHG	C30-C31-C32-C33
38	b	621	SQD	C30-C31-C32-C33
42	a	408	PHO	C8-C10-C11-C12
30	2	608	CHL	C11-C10-C8-C9
30	q	309	CHL	C11-C10-C8-C9
30	g	306	CHL	O1A-CGA-O2A-C1
34	r	321	LMG	O10-C28-O8-C9
33	y	619	LHG	C34-C35-C36-C37
34	9	301	LMG	C11-C12-C13-C14
38	a	411	SQD	C32-C33-C34-C35
31	n	312	CLA	O1D-CGD-O2D-CED
30	3	310	CHL	C11-C12-C13-C14
31	G	603	CLA	C6-C7-C8-C9
31	Y	312	CLA	C16-C17-C18-C19
31	c	601	CLA	C16-C17-C18-C20
34	w	204	LMG	O6-C5-C6-O5
33	b	628	LHG	C25-C26-C27-C28
30	0	607	CHL	C8-C10-C11-C12
30	8	605	CHL	C8-C10-C11-C12
30	n	306	CHL	C8-C10-C11-C12
30	3	302	CHL	CBA-CGA-O2A-C1
30	3	309	CHL	CBA-CGA-O2A-C1
31	6	303	CLA	CBA-CGA-O2A-C1
31	6	305	CLA	CBA-CGA-O2A-C1
31	7	312	CLA	CBA-CGA-O2A-C1
33	R	320	LHG	O8-C23-C24-C25
34	5	620	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	B	622	LMG	C28-C29-C30-C31
33	Y	318	LHG	C35-C36-C37-C38
34	4	620	LMG	C32-C33-C34-C35
34	0	620	LMG	C29-C30-C31-C32
33	N	319	LHG	C2-C3-O3-P
33	8	618	LHG	C5-C4-O6-P
33	n	320	LHG	C5-C4-O6-P
30	1	601	CHL	C3A-C2A-CAA-CBA
30	4	607	CHL	C3A-C2A-CAA-CBA
30	6	310	CHL	C3A-C2A-CAA-CBA
30	0	608	CHL	C3A-C2A-CAA-CBA
30	q	309	CHL	C3A-C2A-CAA-CBA
30	q	311	CHL	C3A-C2A-CAA-CBA
31	2	610	CLA	C3A-C2A-CAA-CBA
31	3	301	CLA	C3A-C2A-CAA-CBA
31	3	313	CLA	C3A-C2A-CAA-CBA
31	B	608	CLA	C3A-C2A-CAA-CBA
31	7	316	CLA	C3A-C2A-CAA-CBA
31	p	613	CLA	C3A-C2A-CAA-CBA
31	b	609	CLA	C3A-C2A-CAA-CBA
31	y	611	CLA	C3A-C2A-CAA-CBA
31	7	305	CLA	C8-C10-C11-C12
31	s	305	CLA	C5-C6-C7-C8
31	3	315	CLA	C6-C7-C8-C9
31	8	614	CLA	C5-C6-C7-C8
33	S	322	LHG	C24-C25-C26-C27
33	0	619	LHG	C26-C27-C28-C29
45	C	616	DGD	C5B-C6B-C7B-C8B
31	8	610	CLA	O1D-CGD-O2D-CED
36	R	319	NEX	C13-C14-C15-C35
36	q	319	NEX	C29-C30-C31-C32
43	b	618	BCR	C19-C20-C21-C22
43	d	406	BCR	C19-C20-C21-C22
43	h	101	BCR	C19-C20-C21-C22
33	G	618	LHG	C9-C10-C11-C12
33	L	101	LHG	C34-C35-C36-C37
34	C	624	LMG	C11-C12-C13-C14
34	C	624	LMG	C18-C19-C20-C21
38	A	413	SQD	C10-C11-C12-C13
31	5	613	CLA	C3-C5-C6-C7
31	8	614	CLA	C6-C7-C8-C9
31	n	316	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	D	408	LHG	C34-C35-C36-C37
31	q	305	CLA	C6-C7-C8-C10
31	r	304	CLA	C11-C12-C13-C14
30	7	321	CHL	CBA-CGA-O2A-C1
30	n	308	CHL	CBA-CGA-O2A-C1
31	C	604	CLA	CBA-CGA-O2A-C1
31	b	608	CLA	CBA-CGA-O2A-C1
31	n	303	CLA	CBA-CGA-O2A-C1
34	k	102	LMG	C29-C28-O8-C9
33	D	407	LHG	C25-C26-C27-C28
34	B	621	LMG	C37-C38-C39-C40
34	9	302	LMG	C31-C32-C33-C34
38	S	301	SQD	C27-C28-C29-C30
31	4	610	CLA	C8-C10-C11-C12
31	b	616	CLA	C10-C11-C12-C13
33	2	617	LHG	C4-C5-C6-O8
33	4	618	LHG	C4-C5-C6-O8
33	6	320	LHG	C4-C5-C6-O8
33	A	415	LHG	C4-C5-C6-O8
33	C	623	LHG	C4-C5-C6-O8
33	M	101	LHG	C4-C5-C6-O8
33	7	319	LHG	C4-C5-C6-O8
33	8	618	LHG	C4-C5-C6-O8
33	9	320	LHG	C4-C5-C6-O8
33	b	625	LHG	C4-C5-C6-O8
33	c	622	LHG	C4-C5-C6-O8
33	n	320	LHG	C4-C5-C6-O8
33	y	619	LHG	C4-C5-C6-O8
34	2	620	LMG	O1-C7-C8-C9
34	A	412	LMG	C7-C8-C9-O8
34	D	412	LMG	C7-C8-C9-O8
34	G	621	LMG	O1-C7-C8-C9
34	I	101	LMG	O1-C7-C8-C9
34	J	101	LMG	O1-C7-C8-C9
34	R	321	LMG	C7-C8-C9-O8
34	0	622	LMG	O1-C7-C8-C9
34	7	322	LMG	C7-C8-C9-O8
34	a	416	LMG	O1-C7-C8-C9
34	b	624	LMG	C7-C8-C9-O8
34	n	321	LMG	C7-C8-C9-O8
34	n	322	LMG	O1-C7-C8-C9
34	w	201	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	w	205	LMG	O1-C7-C8-C9
34	w	205	LMG	C7-C8-C9-O8
38	A	411	SQD	O6-C44-C45-C46
38	G	624	SQD	O6-C44-C45-C46
38	Y	320	SQD	O6-C44-C45-C46
38	Y	320	SQD	C44-C45-C46-O48
38	a	412	SQD	C44-C45-C46-O48
38	b	621	SQD	C44-C45-C46-O48
38	x	201	SQD	O6-C44-C45-C46
33	b	625	LHG	O9-C7-O7-C5
33	s	320	LHG	O9-C7-O7-C5
33	3	320	LHG	C9-C10-C11-C12
33	6	320	LHG	C28-C29-C30-C31
33	y	619	LHG	C26-C27-C28-C29
34	4	620	LMG	C34-C35-C36-C37
34	G	621	LMG	C34-C35-C36-C37
33	g	319	LHG	C7-C8-C9-C10
31	2	612	CLA	O1A-CGA-O2A-C1
34	x	202	LMG	C11-C12-C13-C14
45	C	616	DGD	C4A-C5A-C6A-C7A
30	7	302	CHL	C8-C10-C11-C12
31	B	606	CLA	C3-C5-C6-C7
31	5	615	CLA	C2C-C3C-CAC-CBC
33	Y	318	LHG	C31-C32-C33-C34
31	y	612	CLA	C5-C6-C7-C8
30	2	601	CHL	C4-C3-C5-C6
30	4	609	CHL	C4-C3-C5-C6
30	r	310	CHL	C4-C3-C5-C6
31	9	304	CLA	C4-C3-C5-C6
42	D	401	PHO	C4-C3-C5-C6
31	2	603	CLA	C6-C7-C8-C9
31	9	305	CLA	C6-C7-C8-C10
31	s	311	CLA	C16-C17-C18-C20
31	7	311	CLA	C2-C3-C5-C6
31	c	606	CLA	C2-C3-C5-C6
33	g	319	LHG	C33-C34-C35-C36
33	q	320	LHG	C29-C30-C31-C32
30	p	609	CHL	O1D-CGD-O2D-CED
31	N	313	CLA	C15-C16-C17-C18
33	A	417	LHG	C3-O3-P-O6
33	0	619	LHG	C4-O6-P-O3
33	B	624	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	j	102	LHG	O10-C23-O8-C6
33	e	101	LHG	C31-C32-C33-C34
30	5	609	CHL	C3-C5-C6-C7
30	4	607	CHL	C2A-CAA-CBA-CGA
30	8	607	CHL	C2A-CAA-CBA-CGA
30	n	309	CHL	C2A-CAA-CBA-CGA
31	b	608	CLA	C2A-CAA-CBA-CGA
31	s	303	CLA	C2A-CAA-CBA-CGA
33	e	101	LHG	O1-C1-C2-O2
31	1	611	CLA	C5-C6-C7-C8
31	s	303	CLA	C10-C11-C12-C13
33	K	102	LHG	C11-C10-C9-C8
33	7	319	LHG	C28-C29-C30-C31
33	e	101	LHG	C11-C10-C9-C8
33	s	322	LHG	C35-C36-C37-C38
34	A	418	LMG	C12-C13-C14-C15
45	C	620	DGD	C5A-C6A-C7A-C8A
33	1	617	LHG	O6-C4-C5-O7
33	C	623	LHG	O6-C4-C5-O7
33	D	408	LHG	O6-C4-C5-O7
33	M	101	LHG	O6-C4-C5-O7
33	R	320	LHG	O6-C4-C5-O7
33	8	618	LHG	O6-C4-C5-O7
33	q	320	LHG	O6-C4-C5-O7
33	n	320	LHG	O6-C4-C5-O7
33	s	320	LHG	O6-C4-C5-O7
31	b	602	CLA	CBA-CGA-O2A-C1
45	C	618	DGD	CAB-CBB-CCB-CDB
30	4	607	CHL	O1A-CGA-O2A-C1
31	C	601	CLA	O1A-CGA-O2A-C1
31	7	314	CLA	O1A-CGA-O2A-C1
31	8	602	CLA	O1A-CGA-O2A-C1
33	F1	301	LHG	O10-C23-O8-C6
34	3	321	LMG	O10-C28-O8-C9
38	B	623	SQD	C23-C24-C25-C26
31	C	603	CLA	C16-C17-C18-C19
31	Y	312	CLA	C16-C17-C18-C20
31	c	603	CLA	C16-C17-C18-C19
31	6	304	CLA	CAA-CBA-CGA-O2A
34	W	202	LMG	O7-C10-C11-C12
45	c	619	DGD	O1G-C1A-C2A-C3A
31	Y	311	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	b	602	CLA	C2B-C3B-CAB-CBB
31	b	616	CLA	C2B-C3B-CAB-CBB
33	N	319	LHG	C29-C30-C31-C32
33	R	320	LHG	C25-C26-C27-C28
33	l	101	LHG	C35-C36-C37-C38
34	4	620	LMG	C18-C19-C20-C21
31	2	609	CLA	C5-C6-C7-C8
31	B	611	CLA	O1A-CGA-O2A-C1
31	q	304	CLA	O1A-CGA-O2A-C1
31	y	611	CLA	O1A-CGA-O2A-C1
33	M	101	LHG	O10-C23-O8-C6
33	2	617	LHG	C35-C36-C37-C38
38	y	621	SQD	C13-C14-C15-C16
34	y	620	LMG	C10-C11-C12-C13
31	2	613	CLA	C6-C7-C8-C9
33	g	319	LHG	C35-C36-C37-C38
45	c	618	DGD	C6B-C7B-C8B-C9B
33	2	617	LHG	O7-C5-C6-O8
33	5	619	LHG	O7-C5-C6-O8
33	C	623	LHG	O7-C5-C6-O8
33	N	319	LHG	O7-C5-C6-O8
33	q	320	LHG	O7-C5-C6-O8
33	c	622	LHG	O7-C5-C6-O8
33	y	619	LHG	O7-C5-C6-O8
34	A	412	LMG	O7-C8-C9-O8
34	A	414	LMG	O1-C7-C8-O7
34	B	625	LMG	O7-C8-C9-O8
34	C	621	LMG	O7-C8-C9-O8
34	X	203	LMG	O1-C7-C8-O7
34	0	622	LMG	O1-C7-C8-O7
34	7	322	LMG	O1-C7-C8-O7
34	b	624	LMG	O7-C8-C9-O8
38	B	620	SQD	O6-C44-C45-O47
38	R	322	SQD	O6-C44-C45-O47
38	y	621	SQD	O47-C45-C46-O48
38	x	201	SQD	C24-C23-O48-C46
33	N	319	LHG	C34-C35-C36-C37
33	a	415	LHG	C9-C10-C11-C12
32	5	617	LUT	C9-C10-C11-C12
30	n	310	CHL	O1D-CGD-O2D-CED
30	6	310	CHL	C11-C12-C13-C14
31	G	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	G	604	CLA	C6-C7-C8-C9
31	Y	305	CLA	C6-C7-C8-C10
31	b	603	CLA	C16-C17-C18-C19
31	r	305	CLA	C11-C12-C13-C14
33	G	618	LHG	C34-C35-C36-C37
33	Y	318	LHG	C29-C30-C31-C32
45	c	617	DGD	CFB-CGB-CHB-CIB
45	c	618	DGD	O6D-C1D-O3G-C3G
31	3	312	CLA	C15-C16-C17-C18
31	b	605	CLA	CBD-CGD-O2D-CED
44	A	416	PL9	C9-C11-C12-C13
31	1	614	CLA	C6-C7-C8-C9
33	a	415	LHG	C24-C25-C26-C27
38	B	623	SQD	C26-C27-C28-C29
31	p	610	CLA	C3-C5-C6-C7
30	R	310	CHL	C2-C1-O2A-CGA
31	4	602	CLA	C2-C1-O2A-CGA
31	R	304	CLA	C2-C1-O2A-CGA
31	R	311	CLA	C2-C1-O2A-CGA
31	b	604	CLA	C2-C1-O2A-CGA
31	c	613	CLA	C2-C1-O2A-CGA
31	7	315	CLA	C2-C3-C5-C6
31	Y	311	CLA	O1A-CGA-O2A-C1
30	1	601	CHL	C11-C12-C13-C14
30	1	606	CHL	C11-C12-C13-C14
30	Y	301	CHL	C11-C12-C13-C14
30	7	302	CHL	C11-C12-C13-C14
30	7	308	CHL	C11-C12-C13-C14
30	y	601	CHL	C11-C12-C13-C14
31	6	313	CLA	C6-C7-C8-C9
31	B	603	CLA	C6-C7-C8-C9
31	B	614	CLA	C11-C10-C8-C9
31	N	310	CLA	C11-C12-C13-C14
31	R	304	CLA	C11-C10-C8-C9
31	R	312	CLA	C11-C10-C8-C9
31	S	303	CLA	C6-C7-C8-C9
31	7	305	CLA	C6-C7-C8-C9
31	q	315	CLA	C11-C10-C8-C9
31	b	604	CLA	C11-C12-C13-C14
31	b	605	CLA	C11-C12-C13-C14
31	b	606	CLA	C6-C7-C8-C9
31	b	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	c	601	CLA	C6-C7-C8-C9
31	c	601	CLA	C11-C12-C13-C14
31	c	603	CLA	C11-C12-C13-C14
31	c	603	CLA	C14-C13-C15-C16
31	n	305	CLA	C14-C13-C15-C16
31	r	311	CLA	C6-C7-C8-C9
31	s	305	CLA	C6-C7-C8-C9
31	s	313	CLA	C6-C7-C8-C9
31	y	610	CLA	C6-C7-C8-C9
31	y	612	CLA	C14-C13-C15-C16
42	D	401	PHO	C6-C7-C8-C9
42	a	408	PHO	C11-C10-C8-C9
38	R	322	SQD	C9-C10-C11-C12
33	B	624	LHG	C9-C10-C11-C12
33	b	625	LHG	C11-C10-C9-C8
30	7	307	CHL	C8-C10-C11-C12
31	c	601	CLA	C5-C6-C7-C8
31	4	604	CLA	C4-C3-C5-C6
33	3	320	LHG	C2-C3-O3-P
33	A	417	LHG	C2-C3-O3-P
33	7	319	LHG	C5-C4-O6-P
33	9	320	LHG	C5-C4-O6-P
33	p	619	LHG	C5-C4-O6-P
33	b	628	LHG	C2-C3-O3-P
33	y	619	LHG	C2-C3-O3-P
33	z	102	LHG	C2-C3-O3-P
33	F1	301	LHG	C2-C3-O3-P
33	G	618	LHG	C26-C27-C28-C29
33	G	618	LHG	C29-C30-C31-C32
33	8	618	LHG	C27-C28-C29-C30
33	n	320	LHG	C27-C28-C29-C30
34	J	102	LMG	C33-C34-C35-C36
30	2	606	CHL	C2A-CAA-CBA-CGA
31	1	602	CLA	C2A-CAA-CBA-CGA
31	G	602	CLA	C2A-CAA-CBA-CGA
30	9	311	CHL	C11-C12-C13-C15
31	6	316	CLA	C6-C7-C8-C10
31	p	603	CLA	C6-C7-C8-C9
31	B	615	CLA	C3-C5-C6-C7
31	r	311	CLA	C3-C5-C6-C7
32	2	615	LUT	C5-C6-C7-C8
32	5	616	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	S	318	LUT	C5-C6-C7-C8
32	p	617	LUT	C5-C6-C7-C8
32	s	318	LUT	C5-C6-C7-C8
35	q	317	RRX	C1-C6-C7-C8
43	B	617	BCR	C23-C24-C25-C26
43	B	619	BCR	C5-C6-C7-C8
43	B	619	BCR	C23-C24-C25-C30
43	C	614	BCR	C1-C6-C7-C8
43	b	618	BCR	C23-C24-C25-C30
43	b	619	BCR	C5-C6-C7-C8
43	b	620	BCR	C1-C6-C7-C8
43	v	101	BCR	C23-C24-C25-C26
42	A	408	PHO	C15-C16-C17-C18
33	3	320	LHG	C28-C29-C30-C31
33	C	623	LHG	C28-C29-C30-C31
33	z	102	LHG	C26-C27-C28-C29
34	a	416	LMG	C12-C13-C14-C15
33	b	628	LHG	C19-C20-C21-C22
38	B	623	SQD	C16-C17-C18-C19
32	6	318	LUT	C11-C12-C13-C14
32	N	316	LUT	C31-C32-C33-C34
32	p	616	LUT	C11-C12-C13-C14
36	p	618	NEX	C11-C12-C13-C14
43	A	410	BCR	C7-C8-C9-C10
43	C	615	BCR	C21-C22-C23-C24
43	D	405	BCR	C21-C22-C23-C24
43	z	101	BCR	C17-C18-C19-C20
31	7	304	CLA	C5-C6-C7-C8
31	b	605	CLA	C15-C16-C17-C18
31	r	304	CLA	C8-C10-C11-C12
30	r	309	CHL	O1D-CGD-O2D-CED
31	y	614	CLA	C6-C7-C8-C9
34	w	201	LMG	C33-C34-C35-C36
38	R	322	SQD	C31-C32-C33-C34
33	a	415	LHG	C26-C27-C28-C29
38	B	620	SQD	C18-C19-C20-C21
45	C	617	DGD	C6B-C7B-C8B-C9B
31	3	305	CLA	C6-C7-C8-C9
31	6	312	CLA	C11-C12-C13-C15
31	G	604	CLA	C6-C7-C8-C10
31	q	306	CLA	C6-C7-C8-C9
31	c	601	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	3	302	CHL	C11-C10-C8-C9
31	6	304	CLA	C11-C10-C8-C9
38	B	623	SQD	C19-C20-C21-C22
31	3	306	CLA	C5-C6-C7-C8
30	9	310	CHL	O1D-CGD-O2D-CED
34	a	413	LMG	C11-C12-C13-C14
30	y	606	CHL	O1D-CGD-O2D-CED
31	c	605	CLA	O1D-CGD-O2D-CED
33	l	101	LHG	C26-C27-C28-C29
34	c	624	LMG	C32-C33-C34-C35
33	S	322	LHG	O6-C4-C5-C6
33	q	320	LHG	O6-C4-C5-C6
33	c	622	LHG	O6-C4-C5-C6
33	D	407	LHG	C33-C34-C35-C36
33	y	619	LHG	C16-C17-C18-C19
30	1	607	CHL	C11-C10-C8-C7
30	G	601	CHL	C11-C12-C13-C15
30	G	608	CHL	C11-C12-C13-C15
30	G	623	CHL	C11-C12-C13-C15
30	Y	301	CHL	C11-C12-C13-C15
30	0	607	CHL	C12-C13-C15-C16
30	8	608	CHL	C12-C13-C15-C16
30	g	302	CHL	C11-C12-C13-C15
30	g	309	CHL	C11-C10-C8-C7
30	g	309	CHL	C11-C12-C13-C15
30	r	310	CHL	C2-C3-C5-C6
30	y	606	CHL	C11-C10-C8-C7
31	1	610	CLA	C11-C10-C8-C7
31	2	602	CLA	C6-C7-C8-C10
31	3	304	CLA	C6-C7-C8-C10
31	4	602	CLA	C11-C10-C8-C7
31	4	610	CLA	C11-C10-C8-C7
31	5	610	CLA	C6-C7-C8-C10
31	6	303	CLA	C6-C7-C8-C10
31	6	304	CLA	C6-C7-C8-C10
31	6	312	CLA	C6-C7-C8-C10
31	6	313	CLA	C6-C7-C8-C10
31	A	409	CLA	C6-C7-C8-C10
31	B	602	CLA	C11-C12-C13-C15
31	B	603	CLA	C6-C7-C8-C10
31	B	603	CLA	C11-C12-C13-C15
31	B	604	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	B	605	CLA	C11-C10-C8-C7
31	B	609	CLA	C11-C10-C8-C7
31	B	610	CLA	C11-C12-C13-C15
31	B	611	CLA	C6-C7-C8-C10
31	B	613	CLA	C11-C12-C13-C15
31	B	614	CLA	C6-C7-C8-C10
31	B	616	CLA	C6-C7-C8-C10
31	B	616	CLA	C11-C10-C8-C7
31	C	608	CLA	C6-C7-C8-C10
31	C	611	CLA	C11-C12-C13-C15
31	D	403	CLA	C6-C7-C8-C10
31	D	403	CLA	C11-C10-C8-C7
31	G	612	CLA	C11-C12-C13-C15
31	R	311	CLA	C6-C7-C8-C10
31	R	312	CLA	C11-C10-C8-C7
31	S	305	CLA	C6-C7-C8-C10
31	S	311	CLA	C11-C10-C8-C7
31	S	313	CLA	C6-C7-C8-C10
31	S	314	CLA	C11-C10-C8-C7
31	Y	303	CLA	C6-C7-C8-C10
31	0	613	CLA	C6-C7-C8-C10
31	7	305	CLA	C11-C10-C8-C7
31	8	602	CLA	C11-C10-C8-C7
31	8	604	CLA	C12-C13-C15-C16
31	8	612	CLA	C11-C12-C13-C15
31	q	315	CLA	C11-C10-C8-C7
31	a	409	CLA	C6-C7-C8-C10
31	b	604	CLA	C11-C12-C13-C15
31	b	605	CLA	C11-C12-C13-C15
31	b	605	CLA	C12-C13-C15-C16
31	b	610	CLA	C6-C7-C8-C10
31	b	610	CLA	C11-C10-C8-C7
31	b	612	CLA	C6-C7-C8-C10
31	b	613	CLA	C11-C12-C13-C15
31	b	615	CLA	C6-C7-C8-C10
31	b	616	CLA	C11-C12-C13-C15
31	c	607	CLA	C11-C12-C13-C15
31	c	609	CLA	C6-C7-C8-C10
31	g	303	CLA	C6-C7-C8-C10
31	g	313	CLA	C6-C7-C8-C10
31	n	303	CLA	C11-C10-C8-C7
31	n	305	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	n	314	CLA	C11-C12-C13-C15
31	r	304	CLA	C6-C7-C8-C10
31	s	305	CLA	C11-C12-C13-C15
31	s	311	CLA	C11-C10-C8-C7
31	s	312	CLA	C12-C13-C15-C16
31	y	612	CLA	C6-C7-C8-C10
31	y	612	CLA	C12-C13-C15-C16
30	1	609	CHL	C8-C10-C11-C12
31	6	304	CLA	C5-C6-C7-C8
31	s	312	CLA	C5-C6-C7-C8
43	H	101	BCR	C19-C20-C21-C22
43	T	101	BCR	C13-C14-C15-C16
43	a	410	BCR	C15-C16-C17-C18
43	b	619	BCR	C15-C16-C17-C18
43	b	619	BCR	C19-C20-C21-C22
43	b	620	BCR	C19-C20-C21-C22
43	c	614	BCR	C9-C10-C11-C12
43	c	614	BCR	C19-C20-C21-C22
43	h	101	BCR	C13-C14-C15-C16
30	3	310	CHL	C11-C12-C13-C15
30	9	311	CHL	C11-C12-C13-C14
31	3	306	CLA	C6-C7-C8-C9
33	5	619	LHG	C26-C27-C28-C29
34	j	101	LMG	O9-C10-O7-C8
33	6	320	LHG	C26-C27-C28-C29
34	B	625	LMG	C31-C32-C33-C34
30	Y	301	CHL	C5-C6-C7-C8
31	3	304	CLA	C8-C10-C11-C12
31	G	609	CLA	C5-C6-C7-C8
33	B	624	LHG	O7-C7-C8-C9
33	3	320	LHG	O10-C23-O8-C6
30	1	606	CHL	C2A-CAA-CBA-CGA
30	4	606	CHL	C2A-CAA-CBA-CGA
30	6	306	CHL	C2A-CAA-CBA-CGA
30	6	309	CHL	C2A-CAA-CBA-CGA
30	G	607	CHL	C2A-CAA-CBA-CGA
30	N	308	CHL	C2A-CAA-CBA-CGA
30	0	605	CHL	C2A-CAA-CBA-CGA
30	0	608	CHL	C2A-CAA-CBA-CGA
30	g	308	CHL	C2A-CAA-CBA-CGA
31	C	612	CLA	C2A-CAA-CBA-CGA
31	R	307	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	S	314	CLA	C2A-CAA-CBA-CGA
33	C	623	LHG	C31-C32-C33-C34
33	s	322	LHG	C9-C10-C11-C12
34	w	202	LMG	C39-C40-C41-C42
34	j	101	LMG	C11-C10-O7-C8
36	6	319	NEX	C40-C33-C34-C35
36	0	618	NEX	C40-C33-C34-C35
38	a	411	SQD	C31-C32-C33-C34
31	g	311	CLA	C3-C5-C6-C7
45	c	616	DGD	CAB-CBB-CCB-CDB
30	9	309	CHL	O1A-CGA-O2A-C1
31	S	310	CLA	C11-C12-C13-C15
30	4	601	CHL	CBA-CGA-O2A-C1
31	B	604	CLA	CBA-CGA-O2A-C1
31	Y	312	CLA	CBA-CGA-O2A-C1
31	b	605	CLA	CBA-CGA-O2A-C1
31	r	305	CLA	CBA-CGA-O2A-C1
33	A	415	LHG	C24-C23-O8-C6
38	B	623	SQD	C24-C23-O48-C46
33	0	619	LHG	C27-C28-C29-C30
30	2	608	CHL	C11-C10-C8-C7
30	3	302	CHL	C11-C10-C8-C7
30	q	309	CHL	C11-C10-C8-C7
33	2	617	LHG	C30-C31-C32-C33
33	g	319	LHG	C9-C10-C11-C12
30	0	609	CHL	C8-C10-C11-C12
31	C	612	CLA	C5-C6-C7-C8
31	s	303	CLA	C13-C15-C16-C17
33	b	625	LHG	C30-C31-C32-C33
33	d	408	LHG	C9-C10-C11-C12
30	0	606	CHL	CAD-CBD-CGD-O2D
31	2	602	CLA	CAD-CBD-CGD-O2D
31	2	611	CLA	CAD-CBD-CGD-O2D
31	B	612	CLA	CAD-CBD-CGD-O2D
31	G	603	CLA	CAD-CBD-CGD-O2D
31	G	604	CLA	CAD-CBD-CGD-O2D
31	S	304	CLA	CAD-CBD-CGD-O2D
31	Y	312	CLA	CAD-CBD-CGD-O2D
31	b	610	CLA	CAD-CBD-CGD-O2D
31	c	603	CLA	CAD-CBD-CGD-O2D
31	c	606	CLA	CAD-CBD-CGD-O2D
31	r	307	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	y	604	CLA	CAD-CBD-CGD-O2D
31	y	612	CLA	CAD-CBD-CGD-O2D
33	7	319	LHG	C4-C5-O7-C7
34	1	618	LMG	C9-C8-O7-C10
34	I	101	LMG	C7-C8-O7-C10
34	f	101	LMG	C9-C8-O7-C10
36	r	319	NEX	C7-C8-C9-C19
36	s	319	NEX	C7-C8-C9-C19
42	A	408	PHO	CAD-CBD-CGD-O2D
45	c	616	DGD	C1G-C2G-O2G-C1B
47	E	101	HEM	C2B-C3B-CAB-CBB
47	e	102	HEM	C2B-C3B-CAB-CBB
34	b	622	LMG	C34-C35-C36-C37
34	b	623	LMG	C31-C32-C33-C34
31	B	607	CLA	C8-C10-C11-C12
34	W	203	LMG	C10-C11-C12-C13
38	b	627	SQD	C12-C13-C14-C15
48	R	302	LMU	C5-C6-C7-C8
31	b	616	CLA	CBA-CGA-O2A-C1
34	r	321	LMG	O6-C1-O1-C7
30	8	605	CHL	C13-C15-C16-C17
30	n	306	CHL	C13-C15-C16-C17
30	7	302	CHL	C2-C3-C5-C6
31	3	306	CLA	C2C-C3C-CAC-CBC
45	C	618	DGD	C1B-C2B-C3B-C4B
33	3	320	LHG	C4-C5-C6-O8
33	C	623	LHG	C2-C3-O3-P
33	N	319	LHG	C5-C4-O6-P
33	S	322	LHG	C4-C5-C6-O8
33	Y	318	LHG	C2-C3-O3-P
33	s	320	LHG	C4-C5-C6-O8
33	s	322	LHG	C4-C5-C6-O8
33	F1	301	LHG	C5-C4-O6-P
33	F1	301	LHG	C4-C5-C6-O8
34	X	203	LMG	O1-C7-C8-C9
34	Y	319	LMG	O1-C7-C8-C9
34	0	620	LMG	O1-C7-C8-C9
34	c	621	LMG	O1-C7-C8-C9
34	f	101	LMG	C7-C8-C9-O8
38	6	301	SQD	C44-C45-C46-O48
38	S	301	SQD	O6-C44-C45-C46
38	a	412	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
38	r	322	SQD	C44-C45-C46-O48
38	y	621	SQD	O6-C44-C45-C46
45	C	618	DGD	O1G-C1G-C2G-C3G
45	c	619	DGD	O1G-C1G-C2G-C3G
31	C	603	CLA	O1A-CGA-O2A-C1
31	n	303	CLA	O1A-CGA-O2A-C1
31	r	305	CLA	O1A-CGA-O2A-C1
33	S	322	LHG	C30-C31-C32-C33
34	I	101	LMG	C31-C32-C33-C34
33	6	320	LHG	O6-C4-C5-O7
33	D	407	LHG	O6-C4-C5-O7
33	L	101	LHG	O6-C4-C5-O7
33	S	320	LHG	O6-C4-C5-O7
33	b	628	LHG	O6-C4-C5-O7
33	c	622	LHG	O6-C4-C5-O7
33	j	102	LHG	O6-C4-C5-O7
33	l	101	LHG	O6-C4-C5-O7
30	7	308	CHL	C5-C6-C7-C8
30	q	303	CHL	C5-C6-C7-C8
31	1	602	CLA	C5-C6-C7-C8
31	1	613	CLA	C13-C15-C16-C17
31	4	603	CLA	C5-C6-C7-C8
31	5	602	CLA	C8-C10-C11-C12
31	B	609	CLA	C15-C16-C17-C18
31	S	305	CLA	C5-C6-C7-C8
31	b	611	CLA	C8-C10-C11-C12
30	p	601	CHL	CAA-CBA-CGA-O2A
31	N	314	CLA	CAA-CBA-CGA-O2A
45	c	617	DGD	O1G-C1A-C2A-C3A
31	9	312	CLA	C5-C6-C7-C8
45	C	617	DGD	C2B-C3B-C4B-C5B
47	E	101	HEM	C4C-C3C-CAC-CBC
47	e	102	HEM	C4C-C3C-CAC-CBC
30	1	605	CHL	C2A-CAA-CBA-CGA
30	2	607	CHL	C2A-CAA-CBA-CGA
31	p	611	CLA	C2A-CAA-CBA-CGA
36	3	319	NEX	C14-C15-C35-C34
31	y	613	CLA	C5-C6-C7-C8
30	3	302	CHL	O1A-CGA-O2A-C1
31	B	611	CLA	C16-C17-C18-C19
30	3	302	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	5	601	CHL	CHA-CBD-CGD-O1D
30	0	601	CHL	CHA-CBD-CGD-O1D
30	8	601	CHL	CHA-CBD-CGD-O1D
30	9	303	CHL	CHA-CBD-CGD-O1D
30	p	601	CHL	CHA-CBD-CGD-O1D
30	p	601	CHL	CHA-CBD-CGD-O2D
30	q	303	CHL	CHA-CBD-CGD-O1D
30	n	302	CHL	CHA-CBD-CGD-O1D
30	s	308	CHL	CHA-CBD-CGD-O1D
30	s	308	CHL	CHA-CBD-CGD-O2D
30	y	601	CHL	CHA-CBD-CGD-O1D
31	1	602	CLA	CHA-CBD-CGD-O1D
31	1	602	CLA	CHA-CBD-CGD-O2D
31	2	604	CLA	CHA-CBD-CGD-O1D
31	2	604	CLA	CHA-CBD-CGD-O2D
31	3	313	CLA	CHA-CBD-CGD-O1D
31	3	313	CLA	CHA-CBD-CGD-O2D
31	4	603	CLA	CHA-CBD-CGD-O1D
31	4	603	CLA	CHA-CBD-CGD-O2D
31	4	612	CLA	CHA-CBD-CGD-O1D
31	5	603	CLA	CHA-CBD-CGD-O1D
31	5	603	CLA	CHA-CBD-CGD-O2D
31	5	604	CLA	CHA-CBD-CGD-O1D
31	5	604	CLA	CHA-CBD-CGD-O2D
31	5	614	CLA	CHA-CBD-CGD-O1D
31	5	614	CLA	CHA-CBD-CGD-O2D
31	6	304	CLA	CHA-CBD-CGD-O1D
31	6	304	CLA	CHA-CBD-CGD-O2D
31	6	305	CLA	CHA-CBD-CGD-O2D
31	6	313	CLA	CHA-CBD-CGD-O1D
31	6	313	CLA	CHA-CBD-CGD-O2D
31	B	605	CLA	CHA-CBD-CGD-O1D
31	B	605	CLA	CHA-CBD-CGD-O2D
31	B	606	CLA	CHA-CBD-CGD-O1D
31	B	606	CLA	CHA-CBD-CGD-O2D
31	B	609	CLA	CHA-CBD-CGD-O1D
31	B	609	CLA	CHA-CBD-CGD-O2D
31	C	609	CLA	CHA-CBD-CGD-O1D
31	C	612	CLA	CHA-CBD-CGD-O1D
31	C	612	CLA	CHA-CBD-CGD-O2D
31	G	602	CLA	CHA-CBD-CGD-O1D
31	G	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	N	303	CLA	CHA-CBD-CGD-O1D
31	N	303	CLA	CHA-CBD-CGD-O2D
31	N	304	CLA	CHA-CBD-CGD-O1D
31	N	305	CLA	CHA-CBD-CGD-O2D
31	R	303	CLA	CHA-CBD-CGD-O1D
31	R	303	CLA	CHA-CBD-CGD-O2D
31	R	306	CLA	CHA-CBD-CGD-O1D
31	R	316	CLA	CHA-CBD-CGD-O2D
31	S	313	CLA	CHA-CBD-CGD-O2D
31	Y	303	CLA	CHA-CBD-CGD-O1D
31	Y	303	CLA	CHA-CBD-CGD-O2D
31	Y	304	CLA	CHA-CBD-CGD-O1D
31	Y	304	CLA	CHA-CBD-CGD-O2D
31	0	603	CLA	CHA-CBD-CGD-O1D
31	7	303	CLA	CHA-CBD-CGD-O1D
31	7	303	CLA	CHA-CBD-CGD-O2D
31	7	304	CLA	CHA-CBD-CGD-O1D
31	7	304	CLA	CHA-CBD-CGD-O2D
31	7	313	CLA	CHA-CBD-CGD-O1D
31	7	313	CLA	CHA-CBD-CGD-O2D
31	8	602	CLA	CHA-CBD-CGD-O1D
31	8	602	CLA	CHA-CBD-CGD-O2D
31	8	604	CLA	CHA-CBD-CGD-O1D
31	8	604	CLA	CHA-CBD-CGD-O2D
31	9	304	CLA	CHA-CBD-CGD-O1D
31	9	304	CLA	CHA-CBD-CGD-O2D
31	9	305	CLA	CHA-CBD-CGD-O1D
31	9	305	CLA	CHA-CBD-CGD-O2D
31	p	612	CLA	CHA-CBD-CGD-O1D
31	p	613	CLA	CHA-CBD-CGD-O1D
31	p	613	CLA	CHA-CBD-CGD-O2D
31	q	304	CLA	CHA-CBD-CGD-O1D
31	q	304	CLA	CHA-CBD-CGD-O2D
31	q	312	CLA	CHA-CBD-CGD-O1D
31	q	312	CLA	CHA-CBD-CGD-O2D
31	b	602	CLA	CHA-CBD-CGD-O1D
31	b	602	CLA	CHA-CBD-CGD-O2D
31	b	611	CLA	CHA-CBD-CGD-O1D
31	b	611	CLA	CHA-CBD-CGD-O2D
31	c	607	CLA	CHA-CBD-CGD-O1D
31	c	607	CLA	CHA-CBD-CGD-O2D
31	c	609	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	g	303	CLA	CHA-CBD-CGD-O1D
31	n	303	CLA	CHA-CBD-CGD-O1D
31	n	303	CLA	CHA-CBD-CGD-O2D
31	n	305	CLA	CHA-CBD-CGD-O1D
31	n	305	CLA	CHA-CBD-CGD-O2D
31	r	305	CLA	CHA-CBD-CGD-O1D
31	r	305	CLA	CHA-CBD-CGD-O2D
31	r	314	CLA	CHA-CBD-CGD-O2D
31	s	304	CLA	CHA-CBD-CGD-O1D
31	s	304	CLA	CHA-CBD-CGD-O2D
31	s	305	CLA	CHA-CBD-CGD-O1D
31	s	305	CLA	CHA-CBD-CGD-O2D
31	s	306	CLA	CHA-CBD-CGD-O1D
31	y	603	CLA	CHA-CBD-CGD-O1D
31	y	603	CLA	CHA-CBD-CGD-O2D
31	3	305	CLA	C3-C5-C6-C7
30	3	309	CHL	O1A-CGA-O2A-C1
31	6	303	CLA	O1A-CGA-O2A-C1
31	C	604	CLA	O1A-CGA-O2A-C1
31	Y	312	CLA	O1A-CGA-O2A-C1
31	7	312	CLA	O1A-CGA-O2A-C1
31	b	608	CLA	O1A-CGA-O2A-C1
31	c	606	CLA	O1A-CGA-O2A-C1
33	C	623	LHG	O10-C23-O8-C6
34	k	102	LMG	O10-C28-O8-C9
33	q	320	LHG	C31-C32-C33-C34
36	2	616	NEX	C11-C10-C9-C8
36	3	319	NEX	C28-C29-C30-C31
36	N	318	NEX	C11-C10-C9-C8
36	g	317	NEX	C32-C33-C34-C35
37	4	619	XAT	C12-C13-C14-C15
37	G	620	XAT	C12-C13-C14-C15
37	9	322	XAT	C12-C13-C14-C15
37	q	321	XAT	C12-C13-C14-C15
37	g	321	XAT	C12-C13-C14-C15
34	j	101	LMG	C11-C12-C13-C14
33	D	408	LHG	O7-C5-C6-O8
33	Y	318	LHG	O7-C5-C6-O8
34	4	621	LMG	O1-C7-C8-O7
34	c	621	LMG	O1-C7-C8-O7
34	r	321	LMG	O1-C7-C8-O7
34	s	321	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	w	205	LMG	O7-C8-C9-O8
38	6	301	SQD	O6-C44-C45-O47
38	A	413	SQD	O6-C44-C45-O47
38	G	624	SQD	O6-C44-C45-O47
38	M	102	SQD	O47-C45-C46-O48
38	Y	320	SQD	O47-C45-C46-O48
38	g	318	SQD	O6-C44-C45-O47
38	s	301	SQD	O6-C44-C45-O47
38	x	201	SQD	O6-C44-C45-O47
45	C	620	DGD	O1G-C1G-C2G-O2G
45	c	618	DGD	O2G-C2G-C3G-O3G
30	N	309	CHL	CBA-CGA-O2A-C1
34	b	622	LMG	C16-C17-C18-C19
38	M	102	SQD	C25-C26-C27-C28
30	6	307	CHL	CBD-CGD-O2D-CED
31	0	611	CLA	C10-C11-C12-C13
31	c	606	CLA	C5-C6-C7-C8
31	6	305	CLA	O1A-CGA-O2A-C1
33	5	619	LHG	C28-C29-C30-C31
33	A	415	LHG	C27-C28-C29-C30
34	b	622	LMG	C18-C19-C20-C21
48	K	101	LMU	C2-C3-C4-C5
33	A	417	LHG	C11-C10-C9-C8
34	1	618	LMG	C11-C12-C13-C14
31	p	611	CLA	C5-C6-C7-C8
31	6	315	CLA	C4-C3-C5-C6
31	G	612	CLA	C4-C3-C5-C6
33	3	320	LHG	C11-C10-C9-C8
33	M	101	LHG	C29-C30-C31-C32
33	j	102	LHG	C9-C10-C11-C12
31	b	616	CLA	O1A-CGA-O2A-C1
34	b	629	LMG	C10-C11-C12-C13
31	y	613	CLA	C2-C3-C5-C6
31	3	306	CLA	O1D-CGD-O2D-CED
34	a	401	LMG	C11-C12-C13-C14
30	G	623	CHL	C11-C12-C13-C14
30	Y	309	CHL	C11-C12-C13-C14
30	0	607	CHL	C11-C12-C13-C14
30	7	306	CHL	C11-C12-C13-C14
30	8	605	CHL	C11-C12-C13-C14
30	n	306	CHL	C11-C12-C13-C14
30	y	607	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	3	316	CLA	C11-C10-C8-C9
31	4	610	CLA	C11-C10-C8-C9
31	4	613	CLA	C11-C10-C8-C9
31	b	613	CLA	C11-C12-C13-C14
31	c	605	CLA	C6-C7-C8-C9
31	g	313	CLA	C11-C10-C8-C9
42	d	402	PHO	O1D-CGD-O2D-CED
34	2	618	LMG	C8-C9-O8-C28
31	y	614	CLA	C5-C6-C7-C8
33	A	415	LHG	C34-C35-C36-C37
38	R	322	SQD	C32-C33-C34-C35
34	W	202	LMG	O6-C5-C6-O5
30	4	601	CHL	O1A-CGA-O2A-C1
38	x	201	SQD	O10-C23-O48-C46
33	S	322	LHG	C11-C10-C9-C8
33	7	319	LHG	C26-C27-C28-C29
31	N	310	CLA	C15-C16-C17-C18
31	b	610	CLA	C15-C16-C17-C18
38	6	301	SQD	C4-C5-C6-S
38	A	411	SQD	C5-C6-S-O8
38	A	413	SQD	C4-C5-C6-S
38	B	623	SQD	C4-C5-C6-S
38	G	617	SQD	C4-C5-C6-S
38	R	322	SQD	C4-C5-C6-S
38	0	621	SQD	C4-C5-C6-S
38	b	627	SQD	C4-C5-C6-S
38	r	322	SQD	C4-C5-C6-S
38	s	301	SQD	C5-C6-S-O8
33	c	622	LHG	C35-C36-C37-C38
33	t	102	LHG	C34-C35-C36-C37
30	y	608	CHL	C2A-CAA-CBA-CGA
31	c	606	CLA	C2A-CAA-CBA-CGA
31	y	611	CLA	C2A-CAA-CBA-CGA
33	r	320	LHG	O8-C23-C24-C25
34	X	203	LMG	O7-C10-C11-C12
34	g	322	LMG	O7-C10-C11-C12
34	2	620	LMG	C37-C38-C39-C40
31	b	602	CLA	O1A-CGA-O2A-C1
31	D	404	CLA	CBA-CGA-O2A-C1
32	7	318	LUT	C11-C12-C13-C20
32	p	617	LUT	C31-C32-C33-C40
32	g	316	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
43	b	620	BCR	C7-C8-C9-C34
33	6	320	LHG	C29-C30-C31-C32
34	W	201	LMG	C12-C13-C14-C15
48	c	623	LMU	C2-C3-C4-C5
31	C	605	CLA	C10-C11-C12-C13
33	b	628	LHG	C12-C13-C14-C15
33	s	322	LHG	C10-C11-C12-C13
38	B	620	SQD	C10-C11-C12-C13
38	x	201	SQD	C10-C11-C12-C13
32	7	318	LUT	C11-C12-C13-C14
32	p	617	LUT	C31-C32-C33-C34
32	g	316	LUT	C7-C8-C9-C10
32	s	318	LUT	C31-C32-C33-C34
43	T	101	BCR	C17-C18-C19-C20
43	a	410	BCR	C7-C8-C9-C10
43	b	620	BCR	C7-C8-C9-C10
38	a	412	SQD	C11-C12-C13-C14
30	1	601	CHL	C1A-C2A-CAA-CBA
30	6	310	CHL	C1A-C2A-CAA-CBA
30	0	608	CHL	C1A-C2A-CAA-CBA
31	1	611	CLA	C1A-C2A-CAA-CBA
31	3	313	CLA	C1A-C2A-CAA-CBA
31	5	610	CLA	C1A-C2A-CAA-CBA
31	B	608	CLA	C1A-C2A-CAA-CBA
31	N	303	CLA	C1A-C2A-CAA-CBA
31	Y	305	CLA	C1A-C2A-CAA-CBA
31	0	602	CLA	C1A-C2A-CAA-CBA
31	q	306	CLA	C1A-C2A-CAA-CBA
31	c	612	CLA	C1A-C2A-CAA-CBA
31	2	612	CLA	C16-C17-C18-C19
31	7	303	CLA	C11-C12-C13-C15
33	y	619	LHG	C14-C15-C16-C17
30	S	309	CHL	C2-C1-O2A-CGA
31	G	612	CLA	C2-C1-O2A-CGA
31	N	314	CLA	C2-C1-O2A-CGA
31	8	614	CLA	C2-C1-O2A-CGA
31	p	611	CLA	C2-C1-O2A-CGA
31	c	604	CLA	C2-C1-O2A-CGA
31	n	316	CLA	C2-C1-O2A-CGA
31	3	301	CLA	CBA-CGA-O2A-C1
31	y	615	CLA	CBA-CGA-O2A-C1
33	0	619	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
38	S	301	SQD	C24-C23-O48-C46
33	A	417	LHG	C24-C25-C26-C27
38	B	623	SQD	O10-C23-O48-C46
33	G	618	LHG	C3-O3-P-O6
33	M	101	LHG	C4-O6-P-O3
33	R	320	LHG	C3-O3-P-O6
33	b	628	LHG	C3-O3-P-O6
33	s	322	LHG	C3-O3-P-O6
30	8	608	CHL	O1D-CGD-O2D-CED
31	b	605	CLA	O1D-CGD-O2D-CED
33	D	407	LHG	C11-C10-C9-C8
31	B	614	CLA	C4-C3-C5-C6
34	D	412	LMG	O7-C10-C11-C12
31	s	314	CLA	C3-C5-C6-C7
33	S	322	LHG	C2-C3-O3-P
33	S	322	LHG	C5-C4-O6-P
33	9	320	LHG	C2-C3-O3-P
33	c	622	LHG	C2-C3-O3-P
33	j	102	LHG	C2-C3-O3-P
30	0	601	CHL	C2-C3-C5-C6
30	9	311	CHL	C2-C3-C5-C6
30	r	309	CHL	C2-C3-C5-C6
42	D	401	PHO	C2-C3-C5-C6
44	a	414	PL9	C13-C14-C16-C17
34	d	409	LMG	C32-C33-C34-C35
30	7	321	CHL	O1A-CGA-O2A-C1
30	n	308	CHL	O1A-CGA-O2A-C1
31	B	604	CLA	O1A-CGA-O2A-C1
31	1	603	CLA	C4B-C3B-CAB-CBB
31	6	312	CLA	C4B-C3B-CAB-CBB
31	G	613	CLA	C4B-C3B-CAB-CBB
31	R	307	CLA	C4B-C3B-CAB-CBB
31	R	313	CLA	C4B-C3B-CAB-CBB
31	0	611	CLA	C4B-C3B-CAB-CBB
31	9	313	CLA	C4B-C3B-CAB-CBB
31	c	601	CLA	C4B-C3B-CAB-CBB
31	g	311	CLA	C4B-C3B-CAB-CBB
31	r	307	CLA	C4B-C3B-CAB-CBB
33	5	619	LHG	C4-O6-P-O4
33	A	415	LHG	C3-O3-P-O5
33	A	415	LHG	C4-O6-P-O5
33	A	417	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	B	624	LHG	C3-O3-P-O4
33	D	407	LHG	C4-O6-P-O4
33	D	408	LHG	C3-O3-P-O5
33	L	101	LHG	C4-O6-P-O4
33	M	101	LHG	C3-O3-P-O4
33	N	319	LHG	C3-O3-P-O4
33	S	322	LHG	C3-O3-P-O5
33	S	322	LHG	C4-O6-P-O5
33	Y	318	LHG	C3-O3-P-O5
33	Y	318	LHG	C4-O6-P-O5
33	0	619	LHG	C4-O6-P-O4
33	p	619	LHG	C4-O6-P-O5
33	a	415	LHG	C3-O3-P-O5
33	a	415	LHG	C4-O6-P-O4
33	b	625	LHG	C4-O6-P-O4
33	c	622	LHG	C3-O3-P-O4
33	d	408	LHG	C4-O6-P-O4
33	e	101	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O5
33	g	319	LHG	C4-O6-P-O5
33	j	102	LHG	C4-O6-P-O5
33	r	320	LHG	C4-O6-P-O5
33	s	322	LHG	C4-O6-P-O4
33	t	102	LHG	C3-O3-P-O5
33	t	102	LHG	C4-O6-P-O4
33	y	619	LHG	C4-O6-P-O5
33	F1	301	LHG	C3-O3-P-O4
31	2	602	CLA	C16-C17-C18-C19
31	A	409	CLA	C11-C12-C13-C15
31	S	311	CLA	C16-C17-C18-C20
31	a	409	CLA	C11-C12-C13-C15
33	j	102	LHG	C18-C19-C20-C21
34	5	620	LMG	C31-C32-C33-C34
45	c	616	DGD	C4B-C5B-C6B-C7B
34	x	202	LMG	C4-C5-C6-O5
31	B	609	CLA	C13-C15-C16-C17
30	Y	309	CHL	CBA-CGA-O2A-C1
33	4	618	LHG	O6-C4-C5-C6
33	5	619	LHG	O6-C4-C5-C6
33	C	623	LHG	O6-C4-C5-C6
33	D	407	LHG	O6-C4-C5-C6
33	L	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	M	101	LHG	O6-C4-C5-C6
33	b	628	LHG	O6-C4-C5-C6
33	e	101	LHG	O6-C4-C5-C6
33	g	319	LHG	O6-C4-C5-C6
33	l	101	LHG	O6-C4-C5-C6
33	t	102	LHG	O6-C4-C5-C6
34	6	322	LMG	C11-C12-C13-C14
38	A	411	SQD	C9-C10-C11-C12
38	b	621	SQD	C9-C10-C11-C12
31	b	605	CLA	O1A-CGA-O2A-C1
31	y	615	CLA	O1A-CGA-O2A-C1
30	y	609	CHL	C10-C11-C12-C13
31	g	313	CLA	C15-C16-C17-C18
30	Y	308	CHL	C2A-CAA-CBA-CGA
30	s	309	CHL	C2A-CAA-CBA-CGA
31	b	617	CLA	C2A-CAA-CBA-CGA
31	r	306	CLA	C2A-CAA-CBA-CGA
31	A	406	CLA	C3-C5-C6-C7
30	2	608	CHL	C5-C6-C7-C8
33	s	322	LHG	C30-C31-C32-C33
33	2	617	LHG	C12-C13-C14-C15
33	3	320	LHG	C10-C11-C12-C13
34	C	619	LMG	C12-C13-C14-C15
34	D	410	LMG	C16-C17-C18-C19
38	A	411	SQD	C27-C28-C29-C30
38	m	101	SQD	C32-C33-C34-C35
45	C	618	DGD	C6A-C7A-C8A-C9A
30	4	601	CHL	CAD-CBD-CGD-O1D
30	4	607	CHL	CAD-CBD-CGD-O1D
30	5	601	CHL	CAD-CBD-CGD-O1D
30	0	601	CHL	CAD-CBD-CGD-O1D
30	0	605	CHL	C2-C3-C5-C6
30	8	601	CHL	CAD-CBD-CGD-O1D
30	9	303	CHL	CAD-CBD-CGD-O1D
30	p	601	CHL	CAD-CBD-CGD-O1D
30	q	303	CHL	CAD-CBD-CGD-O1D
30	n	302	CHL	CAD-CBD-CGD-O1D
30	s	308	CHL	CAD-CBD-CGD-O1D
30	y	601	CHL	CAD-CBD-CGD-O1D
31	6	305	CLA	CAD-CBD-CGD-O1D
31	B	605	CLA	CAD-CBD-CGD-O1D
31	B	609	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	C	603	CLA	CAD-CBD-CGD-O1D
31	C	604	CLA	CAD-CBD-CGD-O1D
31	C	605	CLA	CAD-CBD-CGD-O1D
31	C	612	CLA	CAD-CBD-CGD-O1D
31	S	306	CLA	CAD-CBD-CGD-O1D
31	0	615	CLA	CAD-CBD-CGD-O1D
31	8	604	CLA	CAD-CBD-CGD-O1D
31	b	606	CLA	CAD-CBD-CGD-O1D
31	c	604	CLA	CAD-CBD-CGD-O1D
31	n	305	CLA	CAD-CBD-CGD-O1D
38	A	411	SQD	C5-C6-S-O7
38	B	620	SQD	O5-C5-C6-S
38	a	411	SQD	O5-C5-C6-S
47	e	102	HEM	C4D-C3D-CAD-CBD
31	1	614	CLA	CAA-CBA-CGA-O2A
34	b	629	LMG	O7-C10-C11-C12
31	2	603	CLA	C5-C6-C7-C8
31	N	311	CLA	O1A-CGA-O2A-C1
33	p	619	LHG	C11-C10-C9-C8
31	N	311	CLA	CBA-CGA-O2A-C1
31	5	611	CLA	O1D-CGD-O2D-CED
31	y	604	CLA	C6-C7-C8-C10
42	a	408	PHO	C16-C17-C18-C19
30	6	306	CHL	CBD-CGD-O2D-CED
31	4	614	CLA	C4-C3-C5-C6
31	C	613	CLA	C4-C3-C5-C6
30	1	601	CHL	C6-C7-C8-C10
30	1	601	CHL	C12-C13-C15-C16
30	1	609	CHL	C11-C12-C13-C15
30	1	619	CHL	C11-C10-C8-C7
30	3	310	CHL	C11-C10-C8-C7
30	4	601	CHL	C6-C7-C8-C10
30	6	308	CHL	C11-C10-C8-C7
30	6	308	CHL	C12-C13-C15-C16
30	G	601	CHL	C12-C13-C15-C16
30	G	608	CHL	C12-C13-C15-C16
30	G	623	CHL	C11-C10-C8-C7
30	N	307	CHL	C11-C10-C8-C7
30	N	309	CHL	C11-C10-C8-C7
30	Y	309	CHL	C11-C10-C8-C7
30	0	607	CHL	C11-C10-C8-C7
30	7	307	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
30	7	310	CHL	C12-C13-C15-C16
30	7	321	CHL	C12-C13-C15-C16
30	9	303	CHL	C11-C10-C8-C7
30	9	303	CHL	C12-C13-C15-C16
30	g	302	CHL	C12-C13-C15-C16
30	g	309	CHL	C12-C13-C15-C16
30	n	308	CHL	C12-C13-C15-C16
30	n	310	CHL	C12-C13-C15-C16
30	y	601	CHL	C11-C10-C8-C7
30	y	607	CHL	C12-C13-C15-C16
31	1	604	CLA	C6-C7-C8-C10
31	2	609	CLA	C11-C10-C8-C7
31	2	610	CLA	C6-C7-C8-C10
31	5	602	CLA	C6-C7-C8-C10
31	5	602	CLA	C11-C10-C8-C7
31	5	610	CLA	C11-C10-C8-C7
31	6	311	CLA	C11-C12-C13-C15
31	6	313	CLA	C11-C10-C8-C7
31	A	409	CLA	C11-C10-C8-C7
31	B	602	CLA	C3A-C2A-CAA-CBA
31	B	606	CLA	C6-C7-C8-C10
31	B	614	CLA	C11-C10-C8-C7
31	B	614	CLA	C11-C12-C13-C15
31	B	615	CLA	C11-C12-C13-C15
31	C	602	CLA	C11-C12-C13-C15
31	C	606	CLA	C6-C7-C8-C10
31	G	602	CLA	C11-C12-C13-C15
31	G	609	CLA	C11-C12-C13-C15
31	N	313	CLA	C11-C10-C8-C7
31	S	303	CLA	C11-C10-C8-C7
31	S	312	CLA	C11-C10-C8-C7
31	Y	310	CLA	C11-C12-C13-C15
31	Y	312	CLA	C12-C13-C15-C16
31	7	313	CLA	C11-C10-C8-C7
31	p	610	CLA	C6-C7-C8-C10
31	p	615	CLA	C3A-C2A-CAA-CBA
31	q	304	CLA	C11-C10-C8-C7
31	a	409	CLA	C11-C10-C8-C7
31	b	615	CLA	C11-C12-C13-C15
31	b	616	CLA	C6-C7-C8-C10
31	c	605	CLA	C6-C7-C8-C10
31	c	607	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	c	611	CLA	C12-C13-C15-C16
31	d	404	CLA	C6-C7-C8-C10
31	d	404	CLA	C11-C10-C8-C7
31	g	313	CLA	C11-C10-C8-C7
31	r	311	CLA	C11-C10-C8-C7
31	s	303	CLA	C11-C10-C8-C7
31	s	312	CLA	C6-C7-C8-C10
31	s	313	CLA	C6-C7-C8-C10
31	y	613	CLA	C12-C13-C15-C16
32	S	318	LUT	C25-C26-C27-C28
33	2	617	LHG	O6-C4-C5-O7
33	4	618	LHG	O6-C4-C5-O7
33	A	415	LHG	O6-C4-C5-O7
33	B	624	LHG	O6-C4-C5-O7
33	G	618	LHG	O6-C4-C5-O7
33	K	102	LHG	O6-C4-C5-O7
33	N	319	LHG	O6-C4-C5-O7
33	S	322	LHG	O6-C4-C5-O7
33	7	319	LHG	O6-C4-C5-O7
33	9	320	LHG	O6-C4-C5-O7
33	e	101	LHG	O6-C4-C5-O7
33	t	102	LHG	O6-C4-C5-O7
34	n	321	LMG	C10-C11-C12-C13
42	A	408	PHO	C6-C7-C8-C10
33	4	618	LHG	C29-C30-C31-C32
33	A	415	LHG	O10-C23-O8-C6
33	4	618	LHG	C33-C34-C35-C36
33	S	322	LHG	C31-C32-C33-C34
31	6	311	CLA	C8-C10-C11-C12
31	n	304	CLA	C5-C6-C7-C8
33	a	415	LHG	C29-C30-C31-C32
38	b	621	SQD	C14-C15-C16-C17
30	N	309	CHL	O1A-CGA-O2A-C1
33	0	619	LHG	O10-C23-O8-C6
30	6	310	CHL	C2A-CAA-CBA-CGA
30	p	601	CHL	C2A-CAA-CBA-CGA
31	8	610	CLA	C2A-CAA-CBA-CGA
31	p	602	CLA	C2A-CAA-CBA-CGA
31	g	305	CLA	C2A-CAA-CBA-CGA
31	n	312	CLA	C2A-CAA-CBA-CGA
31	y	613	CLA	C2A-CAA-CBA-CGA
31	2	609	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C26-C27-C28-C29
33	F1	301	LHG	C26-C27-C28-C29
34	2	620	LMG	C16-C17-C18-C19
31	9	304	CLA	CAA-CBA-CGA-O2A
34	C	619	LMG	O7-C10-C11-C12
34	S	321	LMG	O7-C10-C11-C12
31	b	604	CLA	C8-C10-C11-C12
33	B	624	LHG	C14-C15-C16-C17
34	2	620	LMG	C7-C8-C9-O8
34	4	621	LMG	O1-C7-C8-C9
34	5	620	LMG	O1-C7-C8-C9
34	w	202	LMG	O1-C7-C8-C9
34	x	202	LMG	O1-C7-C8-C9
38	A	413	SQD	O6-C44-C45-C46
38	B	623	SQD	C44-C45-C46-O48
38	X	201	SQD	C44-C45-C46-O48
38	a	411	SQD	C44-C45-C46-O48
38	m	101	SQD	O6-C44-C45-C46
45	C	620	DGD	O1G-C1G-C2G-C3G
33	L	101	LHG	O7-C5-C6-O8
34	A	412	LMG	O1-C7-C8-O7
34	B	621	LMG	O7-C8-C9-O8
34	N	320	LMG	O1-C7-C8-O7
34	Y	319	LMG	O1-C7-C8-O7
34	9	301	LMG	O1-C7-C8-O7
34	b	629	LMG	O7-C8-C9-O8
34	f	101	LMG	O7-C8-C9-O8
34	g	320	LMG	O1-C7-C8-O7
34	w	202	LMG	O1-C7-C8-O7
34	w	204	LMG	O1-C7-C8-O7
38	A	411	SQD	O6-C44-C45-O47
38	A	413	SQD	O47-C45-C46-O48
38	B	623	SQD	O6-C44-C45-O47
38	B	623	SQD	O47-C45-C46-O48
38	G	617	SQD	O47-C45-C46-O48
38	a	411	SQD	O47-C45-C46-O48
38	a	412	SQD	O6-C44-C45-O47
38	a	412	SQD	O47-C45-C46-O48
38	b	627	SQD	O47-C45-C46-O48
38	m	101	SQD	O6-C44-C45-O47
38	r	322	SQD	O6-C44-C45-O47
38	r	322	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
33	1	617	LHG	C9-C10-C11-C12
34	5	620	LMG	C8-C7-O1-C1
34	C	624	LMG	C8-C7-O1-C1
34	D	411	LMG	C8-C7-O1-C1
34	G	622	LMG	C8-C7-O1-C1
34	W	203	LMG	C8-C7-O1-C1
34	X	203	LMG	C8-C7-O1-C1
34	q	302	LMG	C8-C7-O1-C1
34	d	410	LMG	C8-C7-O1-C1
34	g	322	LMG	C8-C7-O1-C1
34	j	101	LMG	C8-C7-O1-C1
34	w	205	LMG	C8-C7-O1-C1
38	A	411	SQD	C45-C44-O6-C1
38	G	617	SQD	C45-C44-O6-C1
38	x	201	SQD	C45-C44-O6-C1
45	C	617	DGD	C2G-C3G-O3G-C1D
45	c	617	DGD	C5D-C6D-O5D-C1E
31	3	306	CLA	C6-C7-C8-C10
31	6	312	CLA	C11-C12-C13-C14
31	G	609	CLA	C8-C10-C11-C12
31	N	313	CLA	C8-C10-C11-C12
31	c	606	CLA	C15-C16-C17-C18
34	r	321	LMG	C13-C14-C15-C16
38	A	413	SQD	C28-C29-C30-C31
48	r	302	LMU	C7-C8-C9-C10
33	1	617	LHG	C5-C4-O6-P
33	d	408	LHG	C11-C10-C9-C8
33	g	319	LHG	C25-C26-C27-C28
33	r	320	LHG	C28-C29-C30-C31
34	5	620	LMG	C29-C30-C31-C32
31	3	301	CLA	O1A-CGA-O2A-C1
38	S	301	SQD	O10-C23-O48-C46
31	2	609	CLA	C10-C11-C12-C13
44	D	406	PL9	C15-C14-C16-C17
30	4	609	CHL	C11-C10-C8-C9
38	A	411	SQD	C29-C30-C31-C32
33	L	101	LHG	C25-C26-C27-C28
30	7	321	CHL	C11-C12-C13-C14
30	q	303	CHL	C11-C12-C13-C14
30	n	308	CHL	C11-C12-C13-C14
31	3	304	CLA	C11-C10-C8-C9
31	3	312	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	4	602	CLA	C11-C10-C8-C9
31	6	312	CLA	C6-C7-C8-C9
31	B	607	CLA	C11-C10-C8-C9
31	B	611	CLA	C6-C7-C8-C9
31	B	616	CLA	C11-C10-C8-C9
31	C	602	CLA	C11-C12-C13-C14
31	C	611	CLA	C11-C12-C13-C14
31	D	403	CLA	C11-C10-C8-C9
31	D	404	CLA	C14-C13-C15-C16
31	G	612	CLA	C11-C10-C8-C9
31	G	612	CLA	C11-C12-C13-C14
31	N	313	CLA	C11-C12-C13-C14
31	S	313	CLA	C6-C7-C8-C9
31	7	305	CLA	C11-C10-C8-C9
31	8	602	CLA	C11-C10-C8-C9
31	8	604	CLA	C14-C13-C15-C16
31	b	610	CLA	C6-C7-C8-C9
31	b	616	CLA	C6-C7-C8-C9
31	c	607	CLA	C14-C13-C15-C16
31	n	303	CLA	C11-C10-C8-C9
31	r	316	CLA	C14-C13-C15-C16
31	s	305	CLA	C11-C12-C13-C14
31	s	311	CLA	C11-C10-C8-C9
31	s	312	CLA	C14-C13-C15-C16
31	s	314	CLA	C11-C10-C8-C9
31	B	603	CLA	C3-C5-C6-C7
31	S	310	CLA	C11-C12-C13-C14
31	S	311	CLA	C16-C17-C18-C19
33	S	320	LHG	C24-C25-C26-C27
33	d	408	LHG	C34-C35-C36-C37
38	G	624	SQD	O5-C1-O6-C44
30	Y	309	CHL	O1A-CGA-O2A-C1
31	D	404	CLA	O1A-CGA-O2A-C1
31	8	613	CLA	CAA-CBA-CGA-O2A
33	y	619	LHG	O1-C1-C2-O2
31	r	316	CLA	C15-C16-C17-C18
31	6	315	CLA	C6-C7-C8-C9
33	A	415	LHG	C13-C14-C15-C16
43	a	410	BCR	C18-C19-C20-C21
43	c	614	BCR	C18-C19-C20-C21
43	v	101	BCR	C15-C16-C17-C18
34	b	622	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	Y	302	CHL	O1A-CGA-O2A-C1
31	4	602	CLA	C16-C17-C18-C20
33	D	408	LHG	C31-C32-C33-C34
32	3	318	LUT	C31-C32-C33-C34
32	6	317	LUT	C27-C28-C29-C30
30	Y	301	CHL	CBA-CGA-O2A-C1
33	L	101	LHG	C10-C11-C12-C13
30	3	309	CHL	CBD-CGD-O2D-CED
31	1	603	CLA	C2B-C3B-CAB-CBB
31	6	312	CLA	C2B-C3B-CAB-CBB
31	B	615	CLA	C2B-C3B-CAB-CBB
31	S	310	CLA	C2B-C3B-CAB-CBB
31	0	615	CLA	C2B-C3B-CAB-CBB
31	q	316	CLA	C2B-C3B-CAB-CBB
31	b	603	CLA	C2B-C3B-CAB-CBB
31	b	607	CLA	C2B-C3B-CAB-CBB
31	r	307	CLA	C2B-C3B-CAB-CBB
31	r	316	CLA	C2B-C3B-CAB-CBB
33	c	622	LHG	C17-C18-C19-C20
34	W	201	LMG	C16-C17-C18-C19
31	1	604	CLA	C10-C11-C12-C13
31	N	303	CLA	C13-C15-C16-C17
33	7	319	LHG	C12-C13-C14-C15
31	1	613	CLA	C4-C3-C5-C6
31	7	315	CLA	CAA-CBA-CGA-O2A
34	d	411	LMG	O7-C10-C11-C12
31	B	605	CLA	C13-C15-C16-C17
31	C	613	CLA	C15-C16-C17-C18
31	q	315	CLA	C13-C15-C16-C17
38	m	101	SQD	C24-C25-C26-C27
31	B	612	CLA	C13-C15-C16-C17
30	1	608	CHL	C1-C2-C3-C4
30	2	607	CHL	C1-C2-C3-C4
30	3	303	CHL	C1-C2-C3-C4
30	3	309	CHL	C1-C2-C3-C4
30	5	608	CHL	C1-C2-C3-C4
30	6	309	CHL	C1-C2-C3-C4
30	G	606	CHL	C1-C2-C3-C4
30	N	301	CHL	C1-C2-C3-C4
30	N	308	CHL	C1-C2-C3-C4
30	Y	308	CHL	C1-C2-C3-C4
30	0	608	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
30	7	309	CHL	C1-C2-C3-C4
30	8	607	CHL	C1-C2-C3-C4
30	9	310	CHL	C1-C2-C3-C4
30	p	608	CHL	C1-C2-C3-C4
30	q	310	CHL	C1-C2-C3-C4
30	g	307	CHL	C1-C2-C3-C4
30	n	301	CHL	C1-C2-C3-C4
30	n	309	CHL	C1-C2-C3-C4
30	y	608	CHL	C1-C2-C3-C4
31	B	601	CLA	C1-C2-C3-C4
31	G	613	CLA	C1-C2-C3-C4
31	R	313	CLA	C1-C2-C3-C4
31	b	602	CLA	C1-C2-C3-C4
31	g	314	CLA	C1-C2-C3-C4
31	r	313	CLA	C1-C2-C3-C4
33	7	319	LHG	C9-C10-C11-C12
31	N	315	CLA	C3-C5-C6-C7
31	q	312	CLA	C3-C5-C6-C7
31	g	314	CLA	CAA-CBA-CGA-O2A
31	n	315	CLA	CAA-CBA-CGA-O2A
34	B	625	LMG	O7-C10-C11-C12
33	B	624	LHG	C30-C31-C32-C33
34	6	323	LMG	C9-C8-O7-C10
34	D	411	LMG	C9-C8-O7-C10
34	a	413	LMG	C7-C8-O7-C10
34	b	624	LMG	C7-C8-O7-C10
34	d	410	LMG	C9-C8-O7-C10
34	w	203	LMG	C9-C8-O7-C10
38	r	322	SQD	C46-C45-O47-C7
33	B	624	LHG	O6-C4-C5-C6
33	7	319	LHG	O6-C4-C5-C6
30	7	306	CHL	C2A-CAA-CBA-CGA
31	2	612	CLA	C2A-CAA-CBA-CGA
31	c	605	CLA	C2A-CAA-CBA-CGA
34	W	201	LMG	C11-C12-C13-C14
31	2	603	CLA	C2-C1-O2A-CGA
31	2	610	CLA	C2-C1-O2A-CGA
31	3	301	CLA	C2-C1-O2A-CGA
31	3	306	CLA	C2-C1-O2A-CGA
31	A	409	CLA	C2-C1-O2A-CGA
31	S	310	CLA	C2-C1-O2A-CGA
31	S	313	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	0	615	CLA	C2-C1-O2A-CGA
31	a	409	CLA	C2-C1-O2A-CGA
31	b	615	CLA	C2-C1-O2A-CGA
31	n	305	CLA	C2-C1-O2A-CGA
31	r	311	CLA	C2-C1-O2A-CGA
31	s	305	CLA	C2-C1-O2A-CGA
31	y	603	CLA	C2-C1-O2A-CGA
34	A	414	LMG	C29-C30-C31-C32
34	c	624	LMG	C31-C32-C33-C34
31	B	608	CLA	C16-C17-C18-C20
33	4	618	LHG	C9-C10-C11-C12
38	B	620	SQD	C14-C15-C16-C17
34	s	321	LMG	O7-C10-C11-C12
31	c	601	CLA	O1A-CGA-O2A-C1
30	6	307	CHL	O1D-CGD-O2D-CED
31	Y	310	CLA	C3-C5-C6-C7
31	b	613	CLA	C3-C5-C6-C7
33	a	415	LHG	C2-C3-O3-P
33	L	101	LHG	C14-C15-C16-C17
30	Y	302	CHL	CBA-CGA-O2A-C1
36	p	618	NEX	C13-C14-C15-C35
33	F1	301	LHG	O6-C4-C5-O7
31	B	605	CLA	C15-C16-C17-C18
31	8	603	CLA	C5-C6-C7-C8
31	R	311	CLA	C4-C3-C5-C6
31	b	604	CLA	C4-C3-C5-C6
34	9	301	LMG	C30-C31-C32-C33
34	b	623	LMG	C33-C34-C35-C36
31	d	404	CLA	C3-C5-C6-C7
32	1	615	LUT	C5-C6-C7-C8
43	T	101	BCR	C5-C6-C7-C8
31	G	612	CLA	C2-C3-C5-C6
33	D	408	LHG	C30-C31-C32-C33
34	b	626	LMG	C29-C30-C31-C32
33	7	319	LHG	C25-C26-C27-C28
45	C	617	DGD	C1A-C2A-C3A-C4A
31	B	607	CLA	CBA-CGA-O2A-C1
33	e	101	LHG	C10-C11-C12-C13
38	b	627	SQD	C13-C14-C15-C16
31	B	616	CLA	C13-C15-C16-C17
31	b	603	CLA	C13-C15-C16-C17
30	6	306	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	3	304	CLA	C11-C12-C13-C15
31	N	303	CLA	C16-C17-C18-C20
31	6	305	CLA	C2A-CAA-CBA-CGA
31	B	607	CLA	C2A-CAA-CBA-CGA
31	7	314	CLA	C2A-CAA-CBA-CGA
36	R	301	NEX	C28-C29-C30-C31
36	n	319	NEX	C28-C29-C30-C31
36	y	618	NEX	C28-C29-C30-C31
45	c	618	DGD	C2D-C1D-O3G-C3G
33	S	322	LHG	O7-C5-C6-O8
34	2	618	LMG	O1-C7-C8-O7
34	J	101	LMG	O1-C7-C8-O7
34	W	201	LMG	O1-C7-C8-O7
34	n	322	LMG	O1-C7-C8-O7
38	S	301	SQD	O47-C45-C46-O48
38	Y	320	SQD	O6-C44-C45-O47
31	s	311	CLA	C5-C6-C7-C8
33	b	628	LHG	C24-C25-C26-C27
33	d	408	LHG	C29-C30-C31-C32
34	6	322	LMG	C31-C32-C33-C34
34	f	101	LMG	C31-C32-C33-C34
33	4	618	LHG	C3-O3-P-O6
33	6	320	LHG	C3-O3-P-O6
33	B	624	LHG	C4-O6-P-O3
33	C	623	LHG	C4-O6-P-O3
33	K	102	LHG	C4-O6-P-O3
33	S	320	LHG	C3-O3-P-O6
33	0	619	LHG	C3-O3-P-O6
33	7	319	LHG	C3-O3-P-O6
33	8	618	LHG	C3-O3-P-O6
33	9	320	LHG	C4-O6-P-O3
33	d	408	LHG	C3-O3-P-O6
33	g	319	LHG	C3-O3-P-O6
33	n	320	LHG	C3-O3-P-O6
33	r	320	LHG	C3-O3-P-O6
33	s	320	LHG	C3-O3-P-O6
33	B	624	LHG	C26-C27-C28-C29
34	2	621	LMG	C30-C31-C32-C33
34	0	620	LMG	C32-C33-C34-C35
42	D	401	PHO	CHA-CBD-CGD-O1D
42	D	401	PHO	CHA-CBD-CGD-O2D
31	7	305	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	w	201	LMG	C29-C28-O8-C9
33	Y	318	LHG	C4-C5-C6-O8
33	q	320	LHG	C4-C5-C6-O8
34	W	201	LMG	O1-C7-C8-C9
34	7	301	LMG	C7-C8-C9-O8
34	y	620	LMG	O1-C7-C8-C9
38	G	624	SQD	C44-C45-C46-O48
45	C	620	DGD	C1G-C2G-C3G-O3G
31	7	313	CLA	C4-C3-C5-C6
44	a	414	PL9	C30-C29-C31-C32
33	t	102	LHG	C29-C30-C31-C32
34	6	321	LMG	C4-C5-C6-O5
30	3	302	CHL	C6-C7-C8-C10
30	4	601	CHL	C2-C3-C5-C6
30	7	306	CHL	C11-C10-C8-C7
30	7	321	CHL	C11-C12-C13-C15
30	n	308	CHL	C11-C12-C13-C15
31	6	303	CLA	C11-C12-C13-C15
31	A	406	CLA	C12-C13-C15-C16
31	R	311	CLA	C2-C3-C5-C6
31	S	311	CLA	C12-C13-C15-C16
31	0	602	CLA	C11-C10-C8-C7
31	7	314	CLA	C11-C12-C13-C15
31	b	611	CLA	C11-C10-C8-C7
31	s	313	CLA	C2-C3-C5-C6
31	y	612	CLA	C11-C10-C8-C7
42	a	408	PHO	C11-C10-C8-C7
31	4	610	CLA	CAA-CBA-CGA-O2A
38	r	322	SQD	C25-C26-C27-C28
30	1	601	CHL	C6-C7-C8-C9
30	4	601	CHL	C6-C7-C8-C9
30	q	309	CHL	C6-C7-C8-C9
31	1	611	CLA	C11-C10-C8-C9
31	2	609	CLA	C11-C10-C8-C9
31	6	311	CLA	C11-C12-C13-C14
31	B	614	CLA	C11-C12-C13-C14
31	B	615	CLA	C11-C12-C13-C14
31	G	609	CLA	C11-C12-C13-C14
31	N	313	CLA	C11-C10-C8-C9
31	S	303	CLA	C11-C10-C8-C9
31	S	312	CLA	C11-C10-C8-C9
31	Y	310	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	q	304	CLA	C11-C10-C8-C9
31	b	608	CLA	C11-C12-C13-C14
31	b	615	CLA	C11-C12-C13-C14
31	c	611	CLA	C11-C10-C8-C9
31	g	310	CLA	C11-C12-C13-C14
31	s	312	CLA	C11-C12-C13-C14
31	s	314	CLA	C14-C13-C15-C16
31	y	610	CLA	C11-C12-C13-C14
30	9	303	CHL	C10-C11-C12-C13
31	c	603	CLA	C5-C6-C7-C8
36	3	319	NEX	C13-C14-C15-C35
36	g	317	NEX	C9-C10-C11-C12
43	B	617	BCR	C9-C10-C11-C12
43	B	617	BCR	C13-C14-C15-C16
43	B	617	BCR	C19-C20-C21-C22
43	V	101	BCR	C9-C10-C11-C12
31	2	612	CLA	C16-C17-C18-C20
31	4	610	CLA	C11-C12-C13-C14
33	g	319	LHG	C31-C32-C33-C34
33	S	322	LHG	C25-C26-C27-C28
31	s	312	CLA	CBA-CGA-O2A-C1
33	D	408	LHG	C25-C26-C27-C28
31	5	611	CLA	CBD-CGD-O2D-CED
31	p	612	CLA	CAA-CBA-CGA-O2A
31	b	615	CLA	C15-C16-C17-C18
33	8	618	LHG	C17-C18-C19-C20
33	n	320	LHG	C17-C18-C19-C20
32	7	317	LUT	C27-C28-C29-C39
32	y	616	LUT	C7-C8-C9-C19
31	a	409	CLA	C11-C12-C13-C14
31	y	613	CLA	C16-C17-C18-C19
31	3	315	CLA	C5-C6-C7-C8
33	A	415	LHG	C11-C10-C9-C8
34	7	320	LMG	C33-C34-C35-C36
33	c	622	LHG	C24-C23-O8-C6
33	5	619	LHG	C2-C3-O3-P
33	5	619	LHG	C5-C4-O6-P
33	D	407	LHG	C2-C3-O3-P
33	s	322	LHG	C2-C3-O3-P
45	c	618	DGD	C1A-C2A-C3A-C4A
43	V	101	BCR	C7-C8-C9-C10
33	G	618	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
34	C	619	LMG	C32-C33-C34-C35
45	C	617	DGD	C3B-C4B-C5B-C6B
30	4	607	CHL	C11-C10-C8-C7
30	4	609	CHL	C11-C10-C8-C7
31	6	304	CLA	C11-C10-C8-C7
33	d	408	LHG	O9-C7-O7-C5
31	1	614	CLA	C4-C3-C5-C6
44	d	407	PL9	C16-C17-C18-C19
33	A	417	LHG	O1-C1-C2-O2
33	B	624	LHG	O1-C1-C2-O2
30	6	310	CHL	CBD-CGD-O2D-CED
31	6	315	CLA	C2-C3-C5-C6
31	Y	314	CLA	C5-C6-C7-C8
33	1	617	LHG	C27-C28-C29-C30
33	t	102	LHG	C24-C25-C26-C27
31	y	602	CLA	C11-C12-C13-C15
30	r	308	CHL	CBA-CGA-O2A-C1
31	c	601	CLA	CBA-CGA-O2A-C1
38	6	301	SQD	C24-C23-O48-C46
31	3	301	CLA	C2C-C3C-CAC-CBC
34	6	322	LMG	C8-C9-O8-C28
44	D	406	PL9	C2-C3-C7-C8
34	w	201	LMG	O10-C28-O8-C9
34	B	622	LMG	C29-C30-C31-C32
38	S	301	SQD	C30-C31-C32-C33
34	2	618	LMG	O9-C10-C11-C12
34	6	323	LMG	O9-C10-C11-C12
31	d	404	CLA	CAA-CBA-CGA-O2A
30	Y	301	CHL	O1A-CGA-O2A-C1
31	S	313	CLA	O1A-CGA-O2A-C1
38	6	301	SQD	O10-C23-O48-C46
33	d	408	LHG	C10-C11-C12-C13
31	3	312	CLA	C4B-C3B-CAB-CBB
31	C	601	CLA	C4B-C3B-CAB-CBB
31	0	603	CLA	C4B-C3B-CAB-CBB
31	q	316	CLA	C4B-C3B-CAB-CBB
31	b	607	CLA	C4B-C3B-CAB-CBB
31	c	604	CLA	C4B-C3B-CAB-CBB
31	c	605	CLA	C4B-C3B-CAB-CBB
31	s	315	CLA	C4B-C3B-CAB-CBB
31	6	304	CLA	C2A-CAA-CBA-CGA
31	B	616	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	g	310	CLA	C2A-CAA-CBA-CGA
31	A	409	CLA	C11-C12-C13-C14
30	g	302	CHL	CAA-CBA-CGA-O1A
34	A	418	LMG	O6-C1-O1-C7
32	Y	316	LUT	C29-C30-C31-C32
36	R	301	NEX	C13-C14-C15-C35
36	8	617	NEX	C13-C14-C15-C35
43	H	101	BCR	C9-C10-C11-C12
43	b	618	BCR	C9-C10-C11-C12
43	c	615	BCR	C19-C20-C21-C22
34	S	321	LMG	C18-C19-C20-C21
45	c	617	DGD	C7B-C8B-C9B-CAB
31	s	312	CLA	O1A-CGA-O2A-C1
31	R	316	CLA	C8-C10-C11-C12
31	7	312	CLA	C10-C11-C12-C13
31	c	610	CLA	C5-C6-C7-C8
34	d	409	LMG	C11-C12-C13-C14
34	d	410	LMG	C21-C22-C23-C24
33	C	623	LHG	C34-C35-C36-C37
33	e	101	LHG	C12-C13-C14-C15
30	5	607	CHL	CBD-CGD-O2D-CED
33	l	101	LHG	C29-C30-C31-C32
33	y	619	LHG	C25-C26-C27-C28
33	z	102	LHG	C11-C10-C9-C8
34	C	619	LMG	C39-C40-C41-C42
34	D	411	LMG	C21-C22-C23-C24
47	E	101	HEM	C4B-C3B-CAB-CBB
47	e	102	HEM	C4B-C3B-CAB-CBB
31	4	613	CLA	C3-C5-C6-C7
31	y	615	CLA	C3-C5-C6-C7
31	R	311	CLA	C2C-C3C-CAC-CBC
34	w	201	LMG	C12-C13-C14-C15
38	m	101	SQD	C25-C26-C27-C28
31	N	315	CLA	C4-C3-C5-C6
31	6	314	CLA	C8-C10-C11-C12
31	C	611	CLA	C8-C10-C11-C12
30	R	308	CHL	C2-C3-C5-C6
31	1	614	CLA	C2-C3-C5-C6
33	1	617	LHG	C24-C25-C26-C27
33	L	101	LHG	C16-C17-C18-C19
34	7	322	LMG	C30-C31-C32-C33
34	k	102	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
45	c	617	DGD	CAB-CBB-CCB-CDB
31	S	314	CLA	C2-C1-O2A-CGA
31	p	603	CLA	C2-C1-O2A-CGA
31	b	608	CLA	C2-C1-O2A-CGA
31	b	617	CLA	C2-C1-O2A-CGA
31	c	605	CLA	C2-C1-O2A-CGA
31	c	606	CLA	C2-C1-O2A-CGA
31	s	303	CLA	C2-C1-O2A-CGA
31	y	611	CLA	C2-C1-O2A-CGA
31	2	602	CLA	C16-C17-C18-C20
34	5	620	LMG	C33-C34-C35-C36
31	q	313	CLA	C2C-C3C-CAC-CBC
31	7	314	CLA	C8-C10-C11-C12
30	3	308	CHL	C2A-CAA-CBA-CGA
30	7	310	CHL	C2A-CAA-CBA-CGA
31	A	406	CLA	C2A-CAA-CBA-CGA
31	G	604	CLA	C2A-CAA-CBA-CGA
31	N	303	CLA	C2A-CAA-CBA-CGA
31	7	303	CLA	C2A-CAA-CBA-CGA
31	b	607	CLA	C2A-CAA-CBA-CGA
34	c	620	LMG	O1-C7-C8-O7
38	b	621	SQD	O47-C45-C46-O48
47	E	101	HEM	C4D-C3D-CAD-CBD
31	3	306	CLA	C4C-C3C-CAC-CBC
34	C	624	LMG	C16-C17-C18-C19
33	B	624	LHG	C2-C3-O3-P
30	3	309	CHL	C3A-C2A-CAA-CBA
30	5	607	CHL	C3A-C2A-CAA-CBA
30	7	309	CHL	C3A-C2A-CAA-CBA
30	9	309	CHL	C3A-C2A-CAA-CBA
30	p	608	CHL	C3A-C2A-CAA-CBA
31	1	612	CLA	C3A-C2A-CAA-CBA
31	C	610	CLA	C3A-C2A-CAA-CBA
31	b	603	CLA	C3A-C2A-CAA-CBA
31	s	312	CLA	C16-C17-C18-C19
33	8	618	LHG	C35-C36-C37-C38
33	n	320	LHG	C35-C36-C37-C38
31	2	609	CLA	CAA-CBA-CGA-O2A
31	D	403	CLA	CAA-CBA-CGA-O2A
31	0	614	CLA	CAA-CBA-CGA-O2A
34	R	321	LMG	O7-C10-C11-C12
31	5	615	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
33	A	415	LHG	C35-C36-C37-C38
33	M	101	LHG	C32-C33-C34-C35
34	s	321	LMG	C11-C12-C13-C14
43	a	410	BCR	C13-C14-C15-C16
34	W	201	LMG	C42-C43-C44-C45
31	q	315	CLA	C4-C3-C5-C6
44	A	416	PL9	C40-C39-C41-C42
33	D	407	LHG	C28-C29-C30-C31
33	G	618	LHG	C25-C26-C27-C28
33	e	101	LHG	C34-C35-C36-C37
34	C	621	LMG	C12-C13-C14-C15
34	7	320	LMG	C29-C30-C31-C32
30	1	605	CHL	C14-C13-C15-C16
30	6	308	CHL	C11-C12-C13-C14
30	7	302	CHL	C14-C13-C15-C16
31	1	613	CLA	C11-C12-C13-C14
31	6	314	CLA	C11-C10-C8-C9
31	6	314	CLA	C14-C13-C15-C16
31	B	606	CLA	C11-C12-C13-C14
31	B	611	CLA	C11-C12-C13-C14
31	C	603	CLA	C14-C13-C15-C16
31	R	305	CLA	C6-C7-C8-C9
31	8	609	CLA	C11-C12-C13-C14
31	b	608	CLA	C6-C7-C8-C9
31	r	312	CLA	C6-C7-C8-C9
34	k	102	LMG	C30-C31-C32-C33
30	2	605	CHL	CAA-CBA-CGA-O2A
30	3	307	CHL	CAA-CBA-CGA-O2A
30	5	605	CHL	CAA-CBA-CGA-O2A
30	9	307	CHL	CAA-CBA-CGA-O2A
33	2	617	LHG	C31-C32-C33-C34
38	A	411	SQD	C26-C27-C28-C29
32	2	615	LUT	C39-C29-C30-C31
32	G	615	LUT	C40-C33-C34-C35
32	R	317	LUT	C39-C29-C30-C31
32	9	318	LUT	C40-C33-C34-C35
32	p	616	LUT	C39-C29-C30-C31
32	p	617	LUT	C39-C29-C30-C31
33	N	319	LHG	C4-C5-C6-O8
34	A	412	LMG	O1-C7-C8-C9
34	W	203	LMG	C7-C8-C9-O8
34	b	623	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	r	321	LMG	C7-C8-C9-O8
35	2	614	RRX	C16-C17-C18-C36
35	4	615	RRX	C16-C17-C18-C36
35	G	614	RRX	C16-C17-C18-C36
35	9	317	RRX	C16-C17-C18-C36
35	q	317	RRX	C16-C17-C18-C36
35	g	315	RRX	C16-C17-C18-C36
36	5	618	NEX	C39-C29-C30-C31
36	n	319	NEX	C39-C29-C30-C31
36	s	319	NEX	C39-C29-C30-C31
36	y	618	NEX	C39-C29-C30-C31
37	4	619	XAT	C40-C33-C34-C35
37	g	321	XAT	C40-C33-C34-C35
43	A	410	BCR	C16-C17-C18-C36
43	C	615	BCR	C11-C10-C9-C34
43	C	615	BCR	C16-C17-C18-C36
43	D	405	BCR	C11-C10-C9-C34
43	a	410	BCR	C20-C21-C22-C37
43	c	615	BCR	C16-C17-C18-C36
43	d	406	BCR	C11-C10-C9-C34
43	t	101	BCR	C16-C17-C18-C36
45	C	617	DGD	C1G-C2G-C3G-O3G
45	c	617	DGD	O1G-C1G-C2G-C3G
38	6	301	SQD	O49-C7-O47-C45
33	d	408	LHG	C25-C26-C27-C28
31	0	604	CLA	C2A-CAA-CBA-CGA
33	Y	318	LHG	C26-C27-C28-C29
34	c	620	LMG	O9-C10-C11-C12
34	g	320	LMG	O9-C10-C11-C12
33	0	619	LHG	C28-C29-C30-C31
34	9	301	LMG	C15-C16-C17-C18
31	2	609	CLA	C11-C12-C13-C15
31	3	304	CLA	C11-C12-C13-C14
31	B	607	CLA	C16-C17-C18-C20
31	S	312	CLA	C16-C17-C18-C19
31	y	604	CLA	C6-C7-C8-C9
42	d	402	PHO	O2A-C1-C2-C3
31	r	304	CLA	CBA-CGA-O2A-C1
33	p	619	LHG	C9-C10-C11-C12
30	3	307	CHL	CAA-CBA-CGA-O1A
30	5	605	CHL	CAA-CBA-CGA-O1A
32	8	616	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
32	n	318	LUT	C11-C12-C13-C20
32	r	317	LUT	C7-C8-C9-C19
44	d	407	PL9	C2-C3-C7-C8
30	r	308	CHL	O1A-CGA-O2A-C1
34	d	411	LMG	C33-C34-C35-C36
38	B	620	SQD	C9-C10-C11-C12
45	c	616	DGD	C7A-C8A-C9A-CAA
47	e	102	HEM	C2D-C3D-CAD-CBD
30	3	310	CHL	C10-C11-C12-C13
31	y	614	CLA	CBD-CGD-O2D-CED
34	w	202	LMG	C14-C15-C16-C17
34	S	321	LMG	C10-C11-C12-C13
33	C	623	LHG	C29-C30-C31-C32
33	y	619	LHG	C31-C32-C33-C34
34	c	624	LMG	C15-C16-C17-C18
34	2	620	LMG	C7-C8-O7-C10
34	2	620	LMG	C9-C8-O7-C10
34	J	101	LMG	C9-C8-O7-C10
34	W	201	LMG	C9-C8-O7-C10
34	W	203	LMG	C7-C8-O7-C10
34	W	203	LMG	C9-C8-O7-C10
34	0	622	LMG	C7-C8-O7-C10
34	0	622	LMG	C9-C8-O7-C10
34	9	302	LMG	C9-C8-O7-C10
34	p	620	LMG	C7-C8-O7-C10
34	w	205	LMG	C7-C8-O7-C10
34	w	205	LMG	C9-C8-O7-C10
38	r	322	SQD	C44-C45-O47-C7
45	C	617	DGD	C3G-C2G-O2G-C1B
45	C	618	DGD	C1G-C2G-O2G-C1B
45	c	617	DGD	C1G-C2G-O2G-C1B
31	g	311	CLA	C5-C6-C7-C8
45	C	618	DGD	O6D-C5D-C6D-O5D
45	c	616	DGD	O6D-C5D-C6D-O5D
30	2	607	CHL	C1A-C2A-CAA-CBA
30	3	309	CHL	C1A-C2A-CAA-CBA
30	0	601	CHL	C1A-C2A-CAA-CBA
30	0	607	CHL	C1A-C2A-CAA-CBA
30	p	608	CHL	C1A-C2A-CAA-CBA
31	3	301	CLA	C1A-C2A-CAA-CBA
31	G	613	CLA	C1A-C2A-CAA-CBA
31	R	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	R	313	CLA	C1A-C2A-CAA-CBA
31	a	406	CLA	C1A-C2A-CAA-CBA
33	D	408	LHG	C35-C36-C37-C38
33	j	102	LHG	C10-C11-C12-C13
31	2	611	CLA	CAA-CBA-CGA-O2A
30	3	310	CHL	C6-C7-C8-C10
30	R	309	CHL	C2-C3-C5-C6
31	1	610	CLA	C12-C13-C15-C16
31	3	316	CLA	C6-C7-C8-C10
31	B	603	CLA	C11-C10-C8-C7
31	B	610	CLA	C11-C10-C8-C7
31	B	611	CLA	C11-C10-C8-C7
31	B	612	CLA	C11-C10-C8-C7
31	C	607	CLA	C11-C10-C8-C7
31	C	607	CLA	C12-C13-C15-C16
31	G	602	CLA	C11-C10-C8-C7
31	R	316	CLA	C11-C10-C8-C7
31	7	314	CLA	C11-C10-C8-C7
31	q	315	CLA	C11-C12-C13-C15
31	b	609	CLA	C12-C13-C15-C16
31	b	614	CLA	C6-C7-C8-C10
31	b	617	CLA	C11-C12-C13-C15
31	g	303	CLA	C12-C13-C15-C16
31	r	311	CLA	C2-C3-C5-C6
31	s	310	CLA	C6-C7-C8-C10
30	n	306	CHL	O1D-CGD-O2D-CED
31	N	305	CLA	C13-C15-C16-C17
31	D	404	CLA	C3-C5-C6-C7
31	7	303	CLA	C3-C5-C6-C7
30	q	309	CHL	O1A-CGA-O2A-C1
31	r	304	CLA	O1A-CGA-O2A-C1
30	9	307	CHL	CAA-CBA-CGA-O1A
33	0	619	LHG	C10-C11-C12-C13
33	d	408	LHG	C33-C34-C35-C36
38	6	301	SQD	O47-C7-C8-C9
38	a	411	SQD	C7-C8-C9-C10
31	R	305	CLA	O1A-CGA-O2A-C1
31	R	311	CLA	C4C-C3C-CAC-CBC
45	C	620	DGD	C9B-CAB-CBB-CCB
30	7	321	CHL	C10-C11-C12-C13
34	G	619	LMG	O9-C10-C11-C12
31	y	610	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	6	310	CHL	O1D-CGD-O2D-CED
30	9	311	CHL	C2A-CAA-CBA-CGA
31	1	613	CLA	C2A-CAA-CBA-CGA
31	4	602	CLA	C2A-CAA-CBA-CGA
31	C	606	CLA	C2A-CAA-CBA-CGA
31	8	602	CLA	C2A-CAA-CBA-CGA
30	4	609	CHL	C5-C6-C7-C8
30	n	308	CHL	C10-C11-C12-C13
31	S	312	CLA	C8-C10-C11-C12
38	m	101	SQD	C7-C8-C9-C10
38	x	201	SQD	O47-C7-C8-C9
44	a	414	PL9	C3-C7-C8-C9
30	2	605	CHL	CAA-CBA-CGA-O1A
33	c	622	LHG	C31-C32-C33-C34
30	4	608	CHL	O2A-C1-C2-C3
30	7	310	CHL	C8-C10-C11-C12
31	S	313	CLA	CBA-CGA-O2A-C1
33	a	415	LHG	C11-C10-C9-C8
30	5	607	CHL	O1D-CGD-O2D-CED
38	S	301	SQD	C31-C32-C33-C34
45	c	618	DGD	O6D-C5D-C6D-O5D
38	6	301	SQD	C8-C7-O47-C45
30	4	607	CHL	C11-C10-C8-C9
34	s	321	LMG	C13-C14-C15-C16
30	R	310	CHL	C4-C3-C5-C6
31	q	305	CLA	C4-C3-C5-C6
33	j	102	LHG	C29-C30-C31-C32
34	q	301	LMG	C37-C38-C39-C40
34	a	413	LMG	C29-C30-C31-C32
45	c	618	DGD	C6A-C7A-C8A-C9A
31	a	407	CLA	C8-C10-C11-C12
31	7	313	CLA	C2-C3-C5-C6
31	9	306	CLA	C2-C3-C5-C6
31	q	315	CLA	C2-C3-C5-C6
31	3	312	CLA	C2B-C3B-CAB-CBB
31	C	601	CLA	C2B-C3B-CAB-CBB
31	G	613	CLA	C2B-C3B-CAB-CBB
31	N	321	CLA	C2B-C3B-CAB-CBB
31	R	307	CLA	C2B-C3B-CAB-CBB
31	R	313	CLA	C2B-C3B-CAB-CBB
31	0	611	CLA	C2B-C3B-CAB-CBB
31	9	313	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	c	601	CLA	C2B-C3B-CAB-CBB
31	c	604	CLA	C2B-C3B-CAB-CBB
31	d	401	CLA	C2B-C3B-CAB-CBB
31	g	311	CLA	C2B-C3B-CAB-CBB
33	2	617	LHG	C25-C26-C27-C28
31	D	404	CLA	C10-C11-C12-C13
30	8	605	CHL	O1D-CGD-O2D-CED
33	l	101	LHG	C28-C29-C30-C31
34	5	620	LMG	C11-C12-C13-C14
38	Y	320	SQD	C13-C14-C15-C16
32	2	615	LUT	C28-C29-C30-C31
32	R	317	LUT	C28-C29-C30-C31
32	9	318	LUT	C32-C33-C34-C35
32	p	616	LUT	C28-C29-C30-C31
32	p	617	LUT	C28-C29-C30-C31
35	2	614	RRX	C16-C17-C18-C19
35	4	615	RRX	C16-C17-C18-C19
35	G	614	RRX	C16-C17-C18-C19
35	9	317	RRX	C16-C17-C18-C19
35	q	317	RRX	C16-C17-C18-C19
35	g	315	RRX	C16-C17-C18-C19
36	5	618	NEX	C28-C29-C30-C31
36	8	617	NEX	C28-C29-C30-C31
36	s	319	NEX	C28-C29-C30-C31
43	A	410	BCR	C16-C17-C18-C19
43	C	615	BCR	C11-C10-C9-C8
43	C	615	BCR	C16-C17-C18-C19
43	D	405	BCR	C11-C10-C9-C8
43	a	410	BCR	C20-C21-C22-C23
43	c	615	BCR	C16-C17-C18-C19
43	d	406	BCR	C11-C10-C9-C8
43	t	101	BCR	C16-C17-C18-C19
31	3	305	CLA	C5-C6-C7-C8
33	r	320	LHG	C24-C25-C26-C27
34	w	201	LMG	C16-C17-C18-C19
33	G	618	LHG	O7-C5-C6-O8
34	G	619	LMG	O1-C7-C8-O7
34	d	411	LMG	O7-C8-C9-O8
34	r	321	LMG	O7-C8-C9-O8
38	x	201	SQD	O47-C45-C46-O48
45	c	616	DGD	O2G-C2G-C3G-O3G
45	c	617	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
34	B	625	LMG	C10-C11-C12-C13
30	q	311	CHL	C2A-CAA-CBA-CGA
34	a	413	LMG	C34-C35-C36-C37
38	m	101	SQD	C13-C14-C15-C16
36	N	318	NEX	C33-C34-C35-C15
37	R	318	XAT	C13-C14-C15-C35
33	Y	318	LHG	C27-C28-C29-C30
33	q	320	LHG	C35-C36-C37-C38
38	A	413	SQD	C27-C28-C29-C30
31	B	608	CLA	C16-C17-C18-C19
31	0	614	CLA	C6-C7-C8-C9
33	K	102	LHG	C9-C10-C11-C12
33	b	625	LHG	C34-C35-C36-C37
33	d	408	LHG	C35-C36-C37-C38
34	5	620	LMG	C30-C31-C32-C33
34	b	629	LMG	C29-C30-C31-C32
31	p	602	CLA	C8-C10-C11-C12
34	J	101	LMG	C18-C19-C20-C21
31	6	303	CLA	C3-C5-C6-C7
30	G	608	CHL	C4-C3-C5-C6
30	8	605	CHL	C4-C3-C5-C6
31	Y	305	CLA	C2-C1-O2A-CGA
31	Y	312	CLA	C2-C1-O2A-CGA
31	p	610	CLA	C2-C1-O2A-CGA
31	B	607	CLA	O1A-CGA-O2A-C1
30	1	606	CHL	C8-C10-C11-C12
31	2	612	CLA	C8-C10-C11-C12
31	c	605	CLA	C10-C11-C12-C13
31	A	405	CLA	C14-C13-C15-C16
31	b	606	CLA	C11-C12-C13-C14
31	c	608	CLA	C11-C10-C8-C9
31	y	611	CLA	C11-C12-C13-C14
31	y	613	CLA	C6-C7-C8-C9
33	j	102	LHG	C35-C36-C37-C38
33	n	320	LHG	C16-C17-C18-C19
33	8	618	LHG	C16-C17-C18-C19
34	W	201	LMG	C40-C41-C42-C43
31	B	605	CLA	C8-C10-C11-C12
30	5	601	CHL	CAA-CBA-CGA-O1A
31	C	610	CLA	CAA-CBA-CGA-O2A
30	9	308	CHL	O1D-CGD-O2D-CED
33	C	623	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
33	G	618	LHG	C35-C36-C37-C38
31	b	605	CLA	C13-C15-C16-C17
31	c	602	CLA	C13-C15-C16-C17
47	E	101	HEM	C2D-C3D-CAD-CBD
31	C	605	CLA	C2A-CAA-CBA-CGA
31	0	613	CLA	C2A-CAA-CBA-CGA
31	q	304	CLA	C2A-CAA-CBA-CGA
31	b	604	CLA	C2A-CAA-CBA-CGA
31	5	602	CLA	C11-C12-C13-C15
31	N	303	CLA	C16-C17-C18-C19
31	y	612	CLA	C16-C17-C18-C20
32	p	616	LUT	C1-C6-C7-C8
43	B	618	BCR	C23-C24-C25-C30
43	B	619	BCR	C23-C24-C25-C26
43	h	101	BCR	C23-C24-C25-C30
34	d	410	LMG	C33-C34-C35-C36
31	1	612	CLA	CAA-CBA-CGA-O2A
33	F1	301	LHG	O7-C7-C8-C9
33	D	408	LHG	C14-C15-C16-C17
33	q	320	LHG	C9-C10-C11-C12
34	3	321	LMG	C7-C8-C9-O8
34	6	323	LMG	O1-C7-C8-C9
34	C	622	LMG	O1-C7-C8-C9
34	D	411	LMG	C33-C34-C35-C36
34	c	620	LMG	O1-C7-C8-C9
34	w	204	LMG	O1-C7-C8-C9
31	q	313	CLA	CAA-CBA-CGA-O2A
33	D	407	LHG	C27-C28-C29-C30
33	N	319	LHG	C35-C36-C37-C38
32	1	616	LUT	C29-C30-C31-C32
36	6	319	NEX	C13-C14-C15-C35
36	0	618	NEX	C13-C14-C15-C35
36	p	618	NEX	C29-C30-C31-C32
43	B	617	BCR	C15-C16-C17-C18
34	G	621	LMG	C11-C12-C13-C14
30	n	306	CHL	C4-C3-C5-C6
31	2	609	CLA	C4-C3-C5-C6
31	9	306	CLA	C4-C3-C5-C6
31	c	602	CLA	C4-C3-C5-C6
31	s	312	CLA	C4-C3-C5-C6
43	a	410	BCR	C17-C18-C19-C20
31	R	305	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	d	404	CLA	C13-C15-C16-C17
48	R	302	LMU	C2B-C1B-O1B-C4'
33	N	319	LHG	C10-C11-C12-C13
33	l	101	LHG	C33-C34-C35-C36
31	1	610	CLA	C2-C3-C5-C6
31	1	613	CLA	C2-C3-C5-C6
44	D	406	PL9	C13-C14-C16-C17
31	N	312	CLA	CAA-CBA-CGA-O2A
38	M	102	SQD	C45-C44-O6-C1
33	8	618	LHG	C14-C15-C16-C17
34	a	416	LMG	C8-C9-O8-C28
33	n	320	LHG	C14-C15-C16-C17
34	9	321	LMG	C13-C14-C15-C16
30	4	601	CHL	C10-C11-C12-C13
33	c	622	LHG	O10-C23-O8-C6
33	R	320	LHG	O10-C23-C24-C25
33	R	320	LHG	C10-C11-C12-C13
38	S	301	SQD	C12-C13-C14-C15
30	6	310	CHL	C11-C12-C13-C15
30	Y	302	CHL	C16-C17-C18-C20
45	c	618	DGD	C9A-CAA-CBA-CCA
31	4	613	CLA	C5-C6-C7-C8
31	B	603	CLA	C5-C6-C7-C8
31	B	610	CLA	C15-C16-C17-C18
31	p	610	CLA	C11-C10-C8-C9
34	D	409	LMG	C10-C11-C12-C13
33	s	322	LHG	C32-C33-C34-C35
34	0	622	LMG	C32-C33-C34-C35
31	c	612	CLA	C2A-CAA-CBA-CGA
34	1	618	LMG	C13-C14-C15-C16
30	9	308	CHL	CBD-CGD-O2D-CED
33	a	415	LHG	C24-C23-O8-C6
33	c	622	LHG	C16-C17-C18-C19
34	B	621	LMG	C10-C11-C12-C13
33	e	101	LHG	O9-C7-O7-C5
38	B	623	SQD	C13-C14-C15-C16
38	a	412	SQD	C24-C25-C26-C27
31	B	602	CLA	C4B-C3B-CAB-CBB
31	N	321	CLA	C4B-C3B-CAB-CBB
31	R	316	CLA	C4B-C3B-CAB-CBB
31	p	603	CLA	C4B-C3B-CAB-CBB
31	c	607	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	d	401	CLA	C4B-C3B-CAB-CBB
31	s	310	CLA	C4B-C3B-CAB-CBB
33	R	320	LHG	C12-C13-C14-C15
30	0	607	CHL	C13-C15-C16-C17
31	9	312	CLA	CAA-CBA-CGA-O2A
34	n	321	LMG	O7-C10-C11-C12
30	6	310	CHL	C4-C3-C5-C6
30	Y	309	CHL	C4-C3-C5-C6
30	p	609	CHL	C4-C3-C5-C6
34	c	620	LMG	C34-C35-C36-C37
34	k	102	LMG	C12-C13-C14-C15
34	s	321	LMG	C21-C22-C23-C24
30	1	606	CHL	C2-C3-C5-C6
30	2	601	CHL	C2-C3-C5-C6
31	2	612	CLA	C11-C12-C13-C15
31	A	405	CLA	C12-C13-C15-C16
31	Y	303	CLA	C11-C10-C8-C7
31	8	604	CLA	C11-C10-C8-C7
31	b	604	CLA	C2-C3-C5-C6
31	b	612	CLA	C11-C10-C8-C7
31	b	613	CLA	C11-C10-C8-C7
31	b	613	CLA	C12-C13-C15-C16
31	c	602	CLA	C6-C7-C8-C10
31	n	305	CLA	C11-C10-C8-C7
31	y	613	CLA	C6-C7-C8-C10
42	D	401	PHO	C6-C7-C8-C10
30	7	321	CHL	C5-C6-C7-C8
30	n	308	CHL	C5-C6-C7-C8
31	b	608	CLA	C5-C6-C7-C8
33	e	101	LHG	C30-C31-C32-C33
33	s	320	LHG	O1-C1-C2-O2
33	7	319	LHG	C11-C10-C9-C8
34	w	201	LMG	C36-C37-C38-C39
38	s	301	SQD	C14-C15-C16-C17
48	K	101	LMU	C9-C10-C11-C12
31	b	609	CLA	C8-C10-C11-C12
31	c	605	CLA	C13-C15-C16-C17
31	6	304	CLA	CAA-CBA-CGA-O1A
34	5	620	LMG	O9-C10-C11-C12
34	6	323	LMG	C2-C1-O1-C7
33	l	101	LHG	C5-C4-O6-P
38	X	201	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
38	g	301	SQD	O47-C45-C46-O48
31	2	613	CLA	CAA-CBA-CGA-O1A
31	3	313	CLA	CAA-CBA-CGA-O1A
30	7	308	CHL	CBD-CGD-O2D-CED
31	4	610	CLA	C5-C6-C7-C8
31	r	312	CLA	C3-C5-C6-C7
34	7	322	LMG	O7-C10-C11-C12
30	7	308	CHL	O1D-CGD-O2D-CED
31	1	612	CLA	C10-C11-C12-C13
31	a	407	CLA	C5-C6-C7-C8
31	g	310	CLA	C15-C16-C17-C18
33	b	625	LHG	C35-C36-C37-C38
31	R	305	CLA	CBA-CGA-O2A-C1
36	G	616	NEX	C39-C29-C30-C31
36	S	319	NEX	C39-C29-C30-C31
36	Y	317	NEX	C39-C29-C30-C31
36	8	617	NEX	C39-C29-C30-C31
36	9	319	NEX	C20-C13-C14-C15
36	9	319	NEX	C39-C29-C30-C31
37	2	619	XAT	C40-C33-C34-C35
37	G	620	XAT	C40-C33-C34-C35
37	9	322	XAT	C40-C33-C34-C35
37	q	321	XAT	C40-C33-C34-C35
45	c	616	DGD	C4A-C5A-C6A-C7A
34	D	410	LMG	C8-C9-O8-C28
30	1	606	CHL	C4-C3-C5-C6
30	y	607	CHL	C4-C3-C5-C6
30	y	609	CHL	C4-C3-C5-C6
31	S	312	CLA	C4-C3-C5-C6
31	c	612	CLA	C4-C3-C5-C6
31	y	612	CLA	C4-C3-C5-C6
30	Y	301	CHL	C8-C10-C11-C12
31	1	602	CLA	C10-C11-C12-C13
31	6	312	CLA	C8-C10-C11-C12
31	N	303	CLA	C8-C10-C11-C12
31	6	316	CLA	C2C-C3C-CAC-CBC
34	A	414	LMG	C11-C12-C13-C14
34	J	101	LMG	C30-C31-C32-C33
34	d	409	LMG	C16-C17-C18-C19
34	j	101	LMG	C29-C30-C31-C32
48	R	302	LMU	C4-C5-C6-C7
30	R	310	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	4	614	CLA	C2-C3-C5-C6
31	C	613	CLA	C2-C3-C5-C6
31	9	304	CLA	C2-C3-C5-C6
31	s	312	CLA	C2-C3-C5-C6
34	b	626	LMG	C30-C31-C32-C33
31	0	603	CLA	C11-C10-C8-C7
31	p	610	CLA	C11-C10-C8-C7
30	N	307	CHL	C11-C10-C8-C9
30	7	306	CHL	C14-C13-C15-C16
30	g	309	CHL	C11-C10-C8-C9
31	4	613	CLA	C6-C7-C8-C9
31	5	602	CLA	C11-C10-C8-C9
31	5	610	CLA	C11-C10-C8-C9
31	5	611	CLA	C11-C10-C8-C9
31	6	313	CLA	C11-C10-C8-C9
31	A	409	CLA	C11-C10-C8-C9
31	B	606	CLA	C6-C7-C8-C9
31	B	612	CLA	C11-C10-C8-C9
31	C	601	CLA	C11-C10-C8-C9
31	C	605	CLA	C6-C7-C8-C9
31	C	606	CLA	C6-C7-C8-C9
31	C	607	CLA	C11-C10-C8-C9
31	G	602	CLA	C11-C10-C8-C9
31	G	602	CLA	C11-C12-C13-C14
31	G	602	CLA	C14-C13-C15-C16
31	S	311	CLA	C11-C10-C8-C9
31	a	409	CLA	C11-C10-C8-C9
31	c	607	CLA	C11-C10-C8-C9
31	c	611	CLA	C14-C13-C15-C16
31	d	404	CLA	C11-C10-C8-C9
31	n	311	CLA	C11-C12-C13-C14
31	s	303	CLA	C11-C10-C8-C9
31	y	602	CLA	C11-C10-C8-C9
42	A	408	PHO	C6-C7-C8-C9
42	A	408	PHO	C14-C13-C15-C16
42	a	408	PHO	C14-C13-C15-C16
34	g	322	LMG	C34-C35-C36-C37
38	B	620	SQD	C27-C28-C29-C30
33	0	619	LHG	C25-C26-C27-C28
30	0	601	CHL	C3A-C2A-CAA-CBA
31	4	614	CLA	C3A-C2A-CAA-CBA
31	5	612	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	N	305	CLA	C3A-C2A-CAA-CBA
31	8	612	CLA	C3A-C2A-CAA-CBA
31	a	406	CLA	C3A-C2A-CAA-CBA
31	n	305	CLA	C3A-C2A-CAA-CBA
31	n	314	CLA	C3A-C2A-CAA-CBA
38	M	102	SQD	C17-C18-C19-C20
33	d	408	LHG	O7-C7-C8-C9
34	N	320	LMG	O7-C10-C11-C12
34	9	321	LMG	O8-C28-C29-C30
34	x	202	LMG	O8-C28-C29-C30
38	M	102	SQD	O47-C7-C8-C9
38	x	201	SQD	O48-C23-C24-C25
34	j	101	LMG	C18-C19-C20-C21
38	M	102	SQD	C16-C17-C18-C19
30	1	605	CHL	CAD-CBD-CGD-O2D
30	1	607	CHL	CAD-CBD-CGD-O2D
30	2	601	CHL	CAD-CBD-CGD-O2D
30	2	607	CHL	CAD-CBD-CGD-O2D
30	3	303	CHL	CAD-CBD-CGD-O2D
30	5	608	CHL	CAD-CBD-CGD-O2D
30	6	302	CHL	CAD-CBD-CGD-O2D
30	6	308	CHL	CAD-CBD-CGD-O2D
30	6	310	CHL	CAD-CBD-CGD-O2D
30	G	605	CHL	CAD-CBD-CGD-O2D
30	G	607	CHL	CAD-CBD-CGD-O2D
30	G	623	CHL	CAD-CBD-CGD-O2D
30	N	301	CHL	CAD-CBD-CGD-O2D
30	N	302	CHL	CAD-CBD-CGD-O2D
30	N	307	CHL	CAD-CBD-CGD-O2D
30	S	308	CHL	CAD-CBD-CGD-O2D
30	Y	302	CHL	CAD-CBD-CGD-O2D
30	Y	307	CHL	CAD-CBD-CGD-O2D
30	0	607	CHL	CAD-CBD-CGD-O2D
30	0	609	CHL	CAD-CBD-CGD-O2D
30	7	307	CHL	CAD-CBD-CGD-O2D
30	8	606	CHL	CAD-CBD-CGD-O2D
30	9	308	CHL	CAD-CBD-CGD-O2D
30	9	309	CHL	CAD-CBD-CGD-O2D
30	p	608	CHL	CAD-CBD-CGD-O2D
30	g	306	CHL	CAD-CBD-CGD-O2D
30	n	301	CHL	CAD-CBD-CGD-O2D
30	n	307	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	r	308	CHL	CAD-CBD-CGD-O2D
30	y	606	CHL	CAD-CBD-CGD-O2D
31	1	603	CLA	CAD-CBD-CGD-O2D
31	4	614	CLA	CAD-CBD-CGD-O2D
31	B	604	CLA	CAD-CBD-CGD-O2D
31	B	614	CLA	CAD-CBD-CGD-O2D
31	C	606	CLA	CAD-CBD-CGD-O2D
31	R	305	CLA	CAD-CBD-CGD-O2D
31	R	307	CLA	CAD-CBD-CGD-O2D
31	0	604	CLA	CAD-CBD-CGD-O2D
31	b	615	CLA	CAD-CBD-CGD-O2D
31	b	617	CLA	CAD-CBD-CGD-O2D
31	s	315	CLA	CAD-CBD-CGD-O2D
34	g	322	LMG	C9-C8-O7-C10
42	a	408	PHO	CAD-CBD-CGD-O2D
47	e	102	HEM	C1A-C2A-CAA-CBA
34	b	622	LMG	C39-C40-C41-C42
31	S	314	CLA	C15-C16-C17-C18
31	b	608	CLA	C8-C10-C11-C12
34	w	202	LMG	C21-C22-C23-C24
31	1	613	CLA	C2-C1-O2A-CGA
31	G	604	CLA	C2-C1-O2A-CGA
33	c	622	LHG	C25-C26-C27-C28
34	6	321	LMG	C10-C11-C12-C13
33	S	320	LHG	O7-C7-C8-C9
34	D	410	LMG	O8-C28-C29-C30
38	6	301	SQD	O48-C23-C24-C25
38	B	623	SQD	C31-C32-C33-C34
38	X	201	SQD	C10-C11-C12-C13
33	B	624	LHG	C11-C10-C9-C8
33	b	628	LHG	C14-C15-C16-C17
34	6	321	LMG	C14-C15-C16-C17
34	C	621	LMG	C32-C33-C34-C35
30	4	607	CHL	C4-C3-C5-C6
30	7	321	CHL	C4-C3-C5-C6
30	n	308	CHL	C4-C3-C5-C6
31	B	606	CLA	C4-C3-C5-C6
31	C	609	CLA	C4-C3-C5-C6
31	C	611	CLA	C4-C3-C5-C6
31	r	311	CLA	C4-C3-C5-C6
31	8	611	CLA	CAA-CBA-CGA-O2A
31	n	313	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	s	313	CLA	C4C-C3C-CAC-CBC
42	D	401	PHO	C8-C10-C11-C12
30	4	607	CHL	C2-C3-C5-C6
31	C	611	CLA	C2-C3-C5-C6
31	q	305	CLA	C2-C3-C5-C6
31	C	603	CLA	CAA-CBA-CGA-O2A
31	G	612	CLA	CAA-CBA-CGA-O2A
31	7	314	CLA	CAA-CBA-CGA-O2A
33	2	617	LHG	O8-C23-C24-C25
33	4	618	LHG	O8-C23-C24-C25
33	p	619	LHG	O8-C23-C24-C25
34	7	301	LMG	O7-C10-C11-C12
34	r	321	LMG	O7-C10-C11-C12
33	a	415	LHG	O10-C23-O8-C6
32	7	317	LUT	C27-C28-C29-C30
32	8	616	LUT	C11-C12-C13-C14
32	n	318	LUT	C11-C12-C13-C14
32	r	317	LUT	C7-C8-C9-C10
32	y	616	LUT	C7-C8-C9-C10
36	2	616	NEX	C11-C12-C13-C14
43	H	101	BCR	C17-C18-C19-C20
43	h	101	BCR	C17-C18-C19-C20
34	W	201	LMG	C7-C8-C9-O8
36	5	618	NEX	O24-C26-C27-C28
36	q	319	NEX	O24-C26-C27-C28
38	G	617	SQD	O6-C44-C45-C46
45	c	618	DGD	C1G-C2G-C3G-O3G
45	c	619	DGD	O1A-C1A-C2A-C3A
31	7	311	CLA	CBA-CGA-O2A-C1
33	Y	318	LHG	O9-C7-O7-C5
30	2	601	CHL	O1A-CGA-O2A-C1
30	2	601	CHL	C5-C6-C7-C8
31	C	605	CLA	CAA-CBA-CGA-O2A
31	S	314	CLA	CAA-CBA-CGA-O2A
31	Y	313	CLA	CAA-CBA-CGA-O2A
31	0	613	CLA	CAA-CBA-CGA-O2A
31	a	406	CLA	CAA-CBA-CGA-O2A
33	3	320	LHG	O8-C23-C24-C25
33	8	618	LHG	C19-C20-C21-C22
33	n	320	LHG	C19-C20-C21-C22
34	6	323	LMG	C34-C35-C36-C37
31	N	312	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	q	313	CLA	CAA-CBA-CGA-O1A
30	1	601	CHL	O2A-C1-C2-C3
30	2	606	CHL	O2A-C1-C2-C3
30	4	606	CHL	O2A-C1-C2-C3
30	5	606	CHL	O2A-C1-C2-C3
30	G	607	CHL	O2A-C1-C2-C3
30	G	623	CHL	O2A-C1-C2-C3
30	N	306	CHL	O2A-C1-C2-C3
30	8	605	CHL	O2A-C1-C2-C3
30	p	606	CHL	O2A-C1-C2-C3
30	q	308	CHL	O2A-C1-C2-C3
30	g	308	CHL	O2A-C1-C2-C3
30	n	306	CHL	O2A-C1-C2-C3
30	y	607	CHL	O2A-C1-C2-C3
31	2	610	CLA	O2A-C1-C2-C3
31	8	603	CLA	O2A-C1-C2-C3
31	n	304	CLA	O2A-C1-C2-C3
42	D	401	PHO	O2A-C1-C2-C3
33	b	625	LHG	C33-C34-C35-C36
34	4	621	LMG	C13-C14-C15-C16
31	n	303	CLA	C2A-CAA-CBA-CGA
31	s	305	CLA	C2A-CAA-CBA-CGA
30	1	605	CHL	C5-C6-C7-C8
31	b	603	CLA	C10-C11-C12-C13
45	C	618	DGD	C2B-C3B-C4B-C5B
31	6	316	CLA	CAA-CBA-CGA-O2A
31	7	312	CLA	CAA-CBA-CGA-O2A
33	S	320	LHG	O8-C23-C24-C25
33	0	619	LHG	O8-C23-C24-C25
33	l	101	LHG	O8-C23-C24-C25
34	C	622	LMG	O7-C10-C11-C12
34	W	202	LMG	O9-C10-C11-C12
33	S	322	LHG	O9-C7-O7-C5
38	A	411	SQD	C33-C34-C35-C36
31	7	311	CLA	O1A-CGA-O2A-C1
30	1	606	CHL	CHA-CBD-CGD-O1D
30	1	606	CHL	CHA-CBD-CGD-O2D
30	3	307	CHL	CHA-CBD-CGD-O1D
30	3	307	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	CHA-CBD-CGD-O2D
30	5	601	CHL	CHA-CBD-CGD-O2D
30	0	601	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	7	306	CHL	CHA-CBD-CGD-O1D
30	7	306	CHL	CHA-CBD-CGD-O2D
30	8	601	CHL	CHA-CBD-CGD-O2D
30	9	303	CHL	CHA-CBD-CGD-O2D
30	p	607	CHL	CHA-CBD-CGD-O1D
30	p	607	CHL	CHA-CBD-CGD-O2D
30	q	303	CHL	CHA-CBD-CGD-O2D
30	q	309	CHL	CHA-CBD-CGD-O1D
30	q	309	CHL	CHA-CBD-CGD-O2D
30	n	302	CHL	CHA-CBD-CGD-O2D
30	y	601	CHL	CHA-CBD-CGD-O2D
31	1	610	CLA	CHA-CBD-CGD-O2D
31	1	612	CLA	CHA-CBD-CGD-O1D
31	1	612	CLA	CHA-CBD-CGD-O2D
31	1	614	CLA	CHA-CBD-CGD-O1D
31	1	614	CLA	CHA-CBD-CGD-O2D
31	2	603	CLA	CHA-CBD-CGD-O1D
31	2	603	CLA	CHA-CBD-CGD-O2D
31	2	610	CLA	CHA-CBD-CGD-O1D
31	2	610	CLA	CHA-CBD-CGD-O2D
31	3	304	CLA	CHA-CBD-CGD-O1D
31	3	304	CLA	CHA-CBD-CGD-O2D
31	3	305	CLA	CHA-CBD-CGD-O1D
31	3	305	CLA	CHA-CBD-CGD-O2D
31	3	306	CLA	CHA-CBD-CGD-O1D
31	3	306	CLA	CHA-CBD-CGD-O2D
31	4	602	CLA	CHA-CBD-CGD-O1D
31	4	604	CLA	CHA-CBD-CGD-O1D
31	4	604	CLA	CHA-CBD-CGD-O2D
31	4	613	CLA	CHA-CBD-CGD-O1D
31	4	613	CLA	CHA-CBD-CGD-O2D
31	5	602	CLA	CHA-CBD-CGD-O1D
31	5	602	CLA	CHA-CBD-CGD-O2D
31	5	613	CLA	CHA-CBD-CGD-O1D
31	5	613	CLA	CHA-CBD-CGD-O2D
31	6	303	CLA	CHA-CBD-CGD-O1D
31	6	303	CLA	CHA-CBD-CGD-O2D
31	6	311	CLA	CHA-CBD-CGD-O1D
31	6	311	CLA	CHA-CBD-CGD-O2D
31	6	315	CLA	CHA-CBD-CGD-O1D
31	6	315	CLA	CHA-CBD-CGD-O2D
31	B	608	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	B	608	CLA	CHA-CBD-CGD-O2D
31	B	610	CLA	CHA-CBD-CGD-O1D
31	C	603	CLA	CHA-CBD-CGD-O1D
31	C	611	CLA	CHA-CBD-CGD-O1D
31	C	611	CLA	CHA-CBD-CGD-O2D
31	G	610	CLA	CHA-CBD-CGD-O2D
31	G	612	CLA	CHA-CBD-CGD-O1D
31	G	612	CLA	CHA-CBD-CGD-O2D
31	N	304	CLA	CHA-CBD-CGD-O2D
31	N	312	CLA	CHA-CBD-CGD-O1D
31	N	312	CLA	CHA-CBD-CGD-O2D
31	N	313	CLA	CHA-CBD-CGD-O2D
31	N	314	CLA	CHA-CBD-CGD-O1D
31	N	314	CLA	CHA-CBD-CGD-O2D
31	R	311	CLA	CHA-CBD-CGD-O1D
31	R	311	CLA	CHA-CBD-CGD-O2D
31	S	303	CLA	CHA-CBD-CGD-O1D
31	S	303	CLA	CHA-CBD-CGD-O2D
31	S	305	CLA	CHA-CBD-CGD-O2D
31	Y	310	CLA	CHA-CBD-CGD-O1D
31	Y	310	CLA	CHA-CBD-CGD-O2D
31	Y	313	CLA	CHA-CBD-CGD-O1D
31	Y	313	CLA	CHA-CBD-CGD-O2D
31	Y	314	CLA	CHA-CBD-CGD-O1D
31	Y	314	CLA	CHA-CBD-CGD-O2D
31	0	602	CLA	CHA-CBD-CGD-O1D
31	0	602	CLA	CHA-CBD-CGD-O2D
31	0	612	CLA	CHA-CBD-CGD-O1D
31	0	612	CLA	CHA-CBD-CGD-O2D
31	0	614	CLA	CHA-CBD-CGD-O1D
31	0	614	CLA	CHA-CBD-CGD-O2D
31	0	615	CLA	CHA-CBD-CGD-O1D
31	7	311	CLA	CHA-CBD-CGD-O1D
31	7	311	CLA	CHA-CBD-CGD-O2D
31	7	312	CLA	CHA-CBD-CGD-O1D
31	7	312	CLA	CHA-CBD-CGD-O2D
31	7	314	CLA	CHA-CBD-CGD-O1D
31	7	314	CLA	CHA-CBD-CGD-O2D
31	8	603	CLA	CHA-CBD-CGD-O1D
31	8	603	CLA	CHA-CBD-CGD-O2D
31	8	610	CLA	CHA-CBD-CGD-O2D
31	8	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	9	315	CLA	CHA-CBD-CGD-O1D
31	9	315	CLA	CHA-CBD-CGD-O2D
31	9	316	CLA	CHA-CBD-CGD-O1D
31	9	316	CLA	CHA-CBD-CGD-O2D
31	p	602	CLA	CHA-CBD-CGD-O1D
31	p	603	CLA	CHA-CBD-CGD-O1D
31	p	604	CLA	CHA-CBD-CGD-O1D
31	p	604	CLA	CHA-CBD-CGD-O2D
31	p	614	CLA	CHA-CBD-CGD-O1D
31	p	614	CLA	CHA-CBD-CGD-O2D
31	q	306	CLA	CHA-CBD-CGD-O1D
31	q	306	CLA	CHA-CBD-CGD-O2D
31	q	314	CLA	CHA-CBD-CGD-O1D
31	q	314	CLA	CHA-CBD-CGD-O2D
31	q	315	CLA	CHA-CBD-CGD-O1D
31	q	315	CLA	CHA-CBD-CGD-O2D
31	b	603	CLA	CHA-CBD-CGD-O1D
31	b	603	CLA	CHA-CBD-CGD-O2D
31	b	606	CLA	CHA-CBD-CGD-O1D
31	b	609	CLA	CHA-CBD-CGD-O1D
31	b	609	CLA	CHA-CBD-CGD-O2D
31	b	613	CLA	CHA-CBD-CGD-O1D
31	b	613	CLA	CHA-CBD-CGD-O2D
31	c	601	CLA	CHA-CBD-CGD-O1D
31	c	601	CLA	CHA-CBD-CGD-O2D
31	c	611	CLA	CHA-CBD-CGD-O1D
31	c	611	CLA	CHA-CBD-CGD-O2D
31	c	612	CLA	CHA-CBD-CGD-O1D
31	g	303	CLA	CHA-CBD-CGD-O2D
31	g	304	CLA	CHA-CBD-CGD-O1D
31	g	304	CLA	CHA-CBD-CGD-O2D
31	g	305	CLA	CHA-CBD-CGD-O1D
31	g	305	CLA	CHA-CBD-CGD-O2D
31	g	310	CLA	CHA-CBD-CGD-O1D
31	g	310	CLA	CHA-CBD-CGD-O2D
31	g	311	CLA	CHA-CBD-CGD-O1D
31	g	311	CLA	CHA-CBD-CGD-O2D
31	n	304	CLA	CHA-CBD-CGD-O1D
31	n	304	CLA	CHA-CBD-CGD-O2D
31	n	312	CLA	CHA-CBD-CGD-O2D
31	n	314	CLA	CHA-CBD-CGD-O2D
31	n	316	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	r	304	CLA	CHA-CBD-CGD-O1D
31	r	304	CLA	CHA-CBD-CGD-O2D
31	r	311	CLA	CHA-CBD-CGD-O1D
31	r	311	CLA	CHA-CBD-CGD-O2D
31	s	303	CLA	CHA-CBD-CGD-O2D
31	s	314	CLA	CHA-CBD-CGD-O1D
31	s	314	CLA	CHA-CBD-CGD-O2D
31	y	602	CLA	CHA-CBD-CGD-O1D
31	y	602	CLA	CHA-CBD-CGD-O2D
31	y	610	CLA	CHA-CBD-CGD-O2D
31	y	614	CLA	CHA-CBD-CGD-O1D
31	y	614	CLA	CHA-CBD-CGD-O2D
36	3	319	NEX	C9-C10-C11-C12
31	3	315	CLA	CAA-CBA-CGA-O2A
31	S	316	CLA	CAA-CBA-CGA-O2A
31	p	614	CLA	CAA-CBA-CGA-O2A
31	y	613	CLA	CAA-CBA-CGA-O2A
34	0	622	LMG	O7-C10-C11-C12
44	a	414	PL9	C17-C18-C19-C21
31	B	606	CLA	C2-C3-C5-C6
31	S	312	CLA	C2-C3-C5-C6
44	a	414	PL9	C38-C39-C41-C42
33	d	408	LHG	C8-C7-O7-C5
33	e	101	LHG	C8-C7-O7-C5
33	Y	318	LHG	O6-C4-C5-C6
36	G	616	NEX	C28-C29-C30-C31
36	S	319	NEX	C28-C29-C30-C31
36	Y	317	NEX	C28-C29-C30-C31
36	9	319	NEX	C28-C29-C30-C31
38	R	322	SQD	C29-C30-C31-C32
31	B	612	CLA	C10-C11-C12-C13
31	S	311	CLA	C5-C6-C7-C8
30	p	607	CHL	CAA-CBA-CGA-O2A
31	4	613	CLA	CAA-CBA-CGA-O2A
31	5	613	CLA	CAA-CBA-CGA-O2A
31	S	303	CLA	CAA-CBA-CGA-O2A
31	0	615	CLA	CAA-CBA-CGA-O2A
33	L	101	LHG	O7-C7-C8-C9
33	a	415	LHG	O8-C23-C24-C25
33	F1	301	LHG	O8-C23-C24-C25
34	b	601	LMG	O7-C10-C11-C12
34	k	101	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	S	301	SQD	O47-C7-C8-C9
34	g	322	LMG	C30-C31-C32-C33
34	2	618	LMG	O7-C8-C9-O8
34	2	621	LMG	O7-C8-C9-O8
34	3	321	LMG	O7-C8-C9-O8
45	C	618	DGD	O2G-C2G-C3G-O3G
30	2	601	CHL	CBA-CGA-O2A-C1
30	9	311	CHL	C8-C10-C11-C12
31	C	608	CLA	C13-C15-C16-C17
31	7	311	CLA	C13-C15-C16-C17
30	6	306	CHL	CAA-CBA-CGA-O1A
33	j	102	LHG	C33-C34-C35-C36
30	N	306	CHL	CAA-CBA-CGA-O2A
30	8	605	CHL	CAA-CBA-CGA-O2A
30	n	306	CHL	CAA-CBA-CGA-O2A
31	1	613	CLA	CAA-CBA-CGA-O2A
31	b	609	CLA	CAA-CBA-CGA-O2A
33	3	320	LHG	O7-C7-C8-C9
33	6	320	LHG	O7-C7-C8-C9
33	y	619	LHG	O8-C23-C24-C25
34	I	101	LMG	O7-C10-C11-C12
34	I	101	LMG	O8-C28-C29-C30
34	9	302	LMG	O7-C10-C11-C12
34	j	101	LMG	O7-C10-C11-C12
38	G	624	SQD	O47-C7-C8-C9
38	m	101	SQD	O47-C7-C8-C9
34	Y	319	LMG	C30-C31-C32-C33
31	S	311	CLA	C2A-CAA-CBA-CGA
31	4	610	CLA	C11-C12-C13-C15
34	6	321	LMG	O6-C5-C6-O5
31	8	612	CLA	C10-C11-C12-C13
31	b	615	CLA	C10-C11-C12-C13
31	n	314	CLA	C10-C11-C12-C13
30	Y	308	CHL	CBA-CGA-O2A-C1
30	q	309	CHL	CBA-CGA-O2A-C1
33	B	624	LHG	O9-C7-C8-C9
33	Y	318	LHG	C8-C7-O7-C5
30	p	608	CHL	CAA-CBA-CGA-O2A
30	q	308	CHL	CAA-CBA-CGA-O2A
30	n	301	CHL	CAA-CBA-CGA-O2A
31	9	306	CLA	CAA-CBA-CGA-O2A
33	A	415	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	R	320	LHG	O7-C7-C8-C9
34	7	301	LMG	C13-C14-C15-C16
34	d	410	LMG	C31-C32-C33-C34
33	N	319	LHG	C27-C28-C29-C30
34	A	418	LMG	C29-C30-C31-C32
34	D	411	LMG	C31-C32-C33-C34
30	7	302	CHL	C10-C11-C12-C13
30	1	607	CHL	C11-C12-C13-C15
30	6	310	CHL	C2-C3-C5-C6
30	Y	309	CHL	C2-C3-C5-C6
30	p	609	CHL	C2-C3-C5-C6
30	y	609	CHL	C2-C3-C5-C6
31	1	611	CLA	C11-C12-C13-C15
31	C	601	CLA	C11-C10-C8-C7
31	8	609	CLA	C6-C7-C8-C10
31	p	602	CLA	C6-C7-C8-C10
31	b	607	CLA	C6-C7-C8-C10
31	b	611	CLA	C6-C7-C8-C10
31	c	601	CLA	C11-C12-C13-C15
31	c	603	CLA	C12-C13-C15-C16
31	c	609	CLA	C11-C10-C8-C7
31	s	312	CLA	C11-C10-C8-C7
33	B	624	LHG	C18-C19-C20-C21
33	c	622	LHG	C26-C27-C28-C29
34	c	621	LMG	O6-C1-O1-C7
30	r	308	CHL	CAA-CBA-CGA-O2A
31	2	612	CLA	CAA-CBA-CGA-O2A
31	6	315	CLA	CAA-CBA-CGA-O2A
31	B	604	CLA	CAA-CBA-CGA-O2A
31	B	614	CLA	CAA-CBA-CGA-O2A
31	B	616	CLA	CAA-CBA-CGA-O2A
33	1	617	LHG	O7-C7-C8-C9
33	t	102	LHG	O8-C23-C24-C25
34	x	202	LMG	O7-C10-C11-C12
30	1	619	CHL	C11-C10-C8-C9
31	1	610	CLA	C11-C12-C13-C14
31	1	610	CLA	C14-C13-C15-C16
31	2	602	CLA	C14-C13-C15-C16
31	6	303	CLA	C11-C12-C13-C14
31	B	603	CLA	C11-C10-C8-C9
31	R	316	CLA	C11-C10-C8-C9
31	S	314	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	7	312	CLA	C11-C12-C13-C14
31	a	406	CLA	C11-C10-C8-C9
31	b	607	CLA	C6-C7-C8-C9
32	p	617	LUT	C13-C14-C15-C35
37	R	318	XAT	C29-C30-C31-C32
43	b	619	BCR	C13-C14-C15-C16
31	6	311	CLA	C15-C16-C17-C18
30	1	607	CHL	C2B-C3B-CAB-CBB
30	5	606	CHL	C2B-C3B-CAB-CBB
30	5	608	CHL	C2B-C3B-CAB-CBB
30	N	308	CHL	C2B-C3B-CAB-CBB
30	N	309	CHL	C2B-C3B-CAB-CBB
30	Y	301	CHL	C2B-C3B-CAB-CBB
30	Y	302	CHL	C2B-C3B-CAB-CBB
30	7	308	CHL	C2B-C3B-CAB-CBB
30	7	321	CHL	C2B-C3B-CAB-CBB
30	8	607	CHL	C2B-C3B-CAB-CBB
30	n	308	CHL	C2B-C3B-CAB-CBB
30	n	309	CHL	C2B-C3B-CAB-CBB
30	y	601	CHL	C2B-C3B-CAB-CBB
31	6	305	CLA	C2B-C3B-CAB-CBB
31	B	611	CLA	C2B-C3B-CAB-CBB
31	R	316	CLA	C2B-C3B-CAB-CBB
31	b	613	CLA	C2B-C3B-CAB-CBB
31	s	315	CLA	C2B-C3B-CAB-CBB
30	5	608	CHL	O2A-C1-C2-C3
30	7	309	CHL	O2A-C1-C2-C3
30	9	310	CHL	O2A-C1-C2-C3
31	b	602	CLA	O2A-C1-C2-C3
30	6	308	CHL	CAA-CBA-CGA-O2A
30	Y	307	CHL	CAA-CBA-CGA-O2A
31	R	316	CLA	CAA-CBA-CGA-O2A
31	b	607	CLA	CAA-CBA-CGA-O2A
33	r	320	LHG	O7-C7-C8-C9
38	a	411	SQD	C5-C6-S-O8
38	a	412	SQD	C4-C5-C6-S
38	g	301	SQD	C4-C5-C6-S
38	s	301	SQD	C4-C5-C6-S
38	x	201	SQD	C4-C5-C6-S
31	g	310	CLA	C16-C17-C18-C20
38	b	627	SQD	C28-C29-C30-C31
34	9	302	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
44	D	406	PL9	C21-C22-C23-C24
44	d	407	PL9	C11-C12-C13-C14
31	C	603	CLA	CAA-CBA-CGA-O1A
33	S	320	LHG	O9-C7-C8-C9
30	N	301	CHL	CAA-CBA-CGA-O2A
34	b	626	LMG	O8-C28-C29-C30
30	s	302	CHL	CAA-CBA-CGA-O2A
31	4	611	CLA	CAA-CBA-CGA-O2A
36	2	616	NEX	C11-C12-C13-C20
34	7	322	LMG	O9-C10-C11-C12
38	6	301	SQD	O10-C23-C24-C25
31	B	615	CLA	C16-C17-C18-C19
31	c	610	CLA	C16-C17-C18-C20
31	y	612	CLA	C16-C17-C18-C19
42	A	408	PHO	C16-C17-C18-C19
33	L	101	LHG	C27-C28-C29-C30
34	w	204	LMG	C33-C34-C35-C36
38	b	627	SQD	C27-C28-C29-C30
30	Y	308	CHL	O1A-CGA-O2A-C1
30	4	609	CHL	C2-C3-C5-C6
30	9	309	CHL	C2-C3-C5-C6
31	G	612	CLA	CAA-CBA-CGA-O1A
33	4	618	LHG	O10-C23-C24-C25
33	d	408	LHG	O9-C7-C8-C9
32	7	318	LUT	C31-C32-C33-C34
38	y	621	SQD	C24-C23-O48-C46
31	B	604	CLA	C13-C15-C16-C17
34	G	621	LMG	C32-C33-C34-C35
31	y	614	CLA	O1D-CGD-O2D-CED
30	3	302	CHL	C1A-C2A-CAA-CBA
30	5	608	CHL	C1A-C2A-CAA-CBA
30	0	605	CHL	C1A-C2A-CAA-CBA
30	7	309	CHL	C1A-C2A-CAA-CBA
30	7	310	CHL	C1A-C2A-CAA-CBA
30	9	309	CHL	C1A-C2A-CAA-CBA
31	1	612	CLA	C1A-C2A-CAA-CBA
31	5	612	CLA	C1A-C2A-CAA-CBA
31	A	405	CLA	C1A-C2A-CAA-CBA
31	C	607	CLA	C1A-C2A-CAA-CBA
31	R	311	CLA	C1A-C2A-CAA-CBA
31	8	612	CLA	C1A-C2A-CAA-CBA
31	9	316	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	p	612	CLA	C1A-C2A-CAA-CBA
31	p	615	CLA	C1A-C2A-CAA-CBA
31	g	312	CLA	C1A-C2A-CAA-CBA
31	n	314	CLA	C1A-C2A-CAA-CBA
31	y	611	CLA	C1A-C2A-CAA-CBA
34	A	414	LMG	C34-C35-C36-C37
34	s	321	LMG	C15-C16-C17-C18
31	0	615	CLA	CAA-CBA-CGA-O1A
31	a	406	CLA	CAA-CBA-CGA-O1A
30	5	608	CHL	CAA-CBA-CGA-O2A
31	8	611	CLA	CAA-CBA-CGA-O1A
34	n	322	LMG	C11-C12-C13-C14
31	B	603	CLA	C2-C1-O2A-CGA
31	0	602	CLA	C2-C1-O2A-CGA
31	b	607	CLA	C5-C6-C7-C8
30	N	308	CHL	CBA-CGA-O2A-C1
31	S	314	CLA	CAA-CBA-CGA-O1A
31	S	316	CLA	CAA-CBA-CGA-O1A
33	p	619	LHG	O10-C23-C24-C25
33	r	320	LHG	O9-C7-C8-C9
34	r	321	LMG	O9-C10-C11-C12
38	M	102	SQD	O49-C7-C8-C9
31	n	313	CLA	CAA-CBA-CGA-O1A
33	p	619	LHG	C4-C5-C6-O8
38	s	301	SQD	O6-C44-C45-C46
30	8	608	CHL	CAA-CBA-CGA-O2A
31	s	314	CLA	CAA-CBA-CGA-O2A
33	2	617	LHG	C19-C20-C21-C22
33	c	622	LHG	C28-C29-C30-C31
34	W	201	LMG	C18-C19-C20-C21
31	R	304	CLA	C8-C10-C11-C12
31	8	604	CLA	C8-C10-C11-C12
31	2	602	CLA	C2A-CAA-CBA-CGA
31	5	615	CLA	C2A-CAA-CBA-CGA
31	s	311	CLA	C2A-CAA-CBA-CGA
31	5	602	CLA	C11-C12-C13-C14
31	g	311	CLA	C11-C12-C13-C14
31	C	605	CLA	CAA-CBA-CGA-O1A
34	9	321	LMG	O10-C28-C29-C30
31	C	609	CLA	C8-C10-C11-C12
31	r	311	CLA	C4C-C3C-CAC-CBC
33	L	101	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
45	c	617	DGD	C4B-C5B-C6B-C7B
30	N	308	CHL	O1A-CGA-O2A-C1
33	0	619	LHG	C24-C25-C26-C27
33	l	101	LHG	C10-C11-C12-C13
30	y	606	CHL	CAA-CBA-CGA-O2A
31	R	312	CLA	CAA-CBA-CGA-O2A
31	b	605	CLA	CAA-CBA-CGA-O2A
34	9	302	LMG	O8-C28-C29-C30
33	F1	301	LHG	C25-C26-C27-C28
34	k	101	LMG	C37-C38-C39-C40
31	3	315	CLA	CAA-CBA-CGA-O1A
31	B	604	CLA	CAA-CBA-CGA-O1A
31	7	314	CLA	CAA-CBA-CGA-O1A
33	S	320	LHG	O10-C23-C24-C25
34	N	320	LMG	O9-C10-C11-C12
34	0	622	LMG	O9-C10-C11-C12
34	k	101	LMG	O9-C10-C11-C12
34	x	202	LMG	O10-C28-C29-C30
31	B	614	CLA	C2-C3-C5-C6
38	a	411	SQD	C29-C30-C31-C32
38	G	624	SQD	C2-C1-O6-C44
31	6	305	CLA	C5-C6-C7-C8
31	B	607	CLA	C5-C6-C7-C8
31	B	615	CLA	C13-C15-C16-C17
34	m	102	LMG	C31-C32-C33-C34
30	4	605	CHL	C4B-C3B-CAB-CBB
30	4	608	CHL	C4B-C3B-CAB-CBB
30	4	609	CHL	C4B-C3B-CAB-CBB
30	5	601	CHL	C4B-C3B-CAB-CBB
30	6	306	CHL	C4B-C3B-CAB-CBB
30	0	608	CHL	C4B-C3B-CAB-CBB
30	9	303	CHL	C4B-C3B-CAB-CBB
30	r	309	CHL	C4B-C3B-CAB-CBB
30	y	609	CHL	C4B-C3B-CAB-CBB
31	G	610	CLA	C4B-C3B-CAB-CBB
31	R	314	CLA	C4B-C3B-CAB-CBB
31	S	312	CLA	C4B-C3B-CAB-CBB
31	r	314	CLA	C4B-C3B-CAB-CBB
33	B	624	LHG	C4-O6-P-O5
33	Y	318	LHG	C4-O6-P-O4
33	0	619	LHG	C3-O3-P-O5
33	d	408	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
34	r	321	LMG	O6-C5-C6-O5
31	B	612	CLA	C16-C17-C18-C19
31	y	613	CLA	C16-C17-C18-C20
34	a	413	LMG	C28-C29-C30-C31
31	1	613	CLA	CAA-CBA-CGA-O1A
31	4	613	CLA	CAA-CBA-CGA-O1A
31	S	303	CLA	CAA-CBA-CGA-O1A
31	0	613	CLA	CAA-CBA-CGA-O1A
31	y	613	CLA	CAA-CBA-CGA-O1A
33	2	617	LHG	O10-C23-C24-C25
33	0	619	LHG	O10-C23-C24-C25
33	F1	301	LHG	O10-C23-C24-C25
34	j	101	LMG	O9-C10-C11-C12
38	m	101	SQD	O49-C7-C8-C9
30	1	608	CHL	O2A-C1-C2-C3
30	N	308	CHL	O2A-C1-C2-C3
31	3	306	CLA	CAA-CBA-CGA-O2A
34	b	624	LMG	O7-C10-C11-C12
38	a	411	SQD	O47-C7-C8-C9
34	D	411	LMG	O6-C1-O1-C7
34	d	410	LMG	O6-C1-O1-C7
31	0	614	CLA	O1A-CGA-O2A-C1
34	c	620	LMG	C29-C30-C31-C32
32	3	318	LUT	C5-C6-C7-C8
33	t	102	LHG	C33-C34-C35-C36
34	I	101	LMG	C11-C12-C13-C14
31	r	311	CLA	C5-C6-C7-C8
31	2	612	CLA	CAA-CBA-CGA-O1A
31	6	316	CLA	CAA-CBA-CGA-O1A
31	B	616	CLA	CAA-CBA-CGA-O1A
31	7	312	CLA	CAA-CBA-CGA-O1A
33	3	320	LHG	O9-C7-C8-C9
34	D	410	LMG	O10-C28-C29-C30
34	9	302	LMG	O9-C10-C11-C12
34	b	626	LMG	O10-C28-C29-C30
38	x	201	SQD	O10-C23-C24-C25
34	n	321	LMG	C34-C35-C36-C37
38	G	617	SQD	C24-C25-C26-C27
38	a	411	SQD	C25-C26-C27-C28
31	2	610	CLA	CAA-CBA-CGA-O2A
31	C	604	CLA	CAA-CBA-CGA-O2A
31	g	313	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
38	M	102	SQD	C13-C14-C15-C16
30	N	306	CHL	CAA-CBA-CGA-O1A
31	Y	313	CLA	CAA-CBA-CGA-O1A
33	1	617	LHG	O9-C7-C8-C9
33	a	415	LHG	O10-C23-C24-C25
34	C	622	LMG	O9-C10-C11-C12
34	7	301	LMG	O9-C10-C11-C12
31	6	315	CLA	C5-C6-C7-C8
33	t	102	LHG	C10-C11-C12-C13
30	n	310	CHL	CAA-CBA-CGA-O2A
31	N	305	CLA	CAA-CBA-CGA-O2A
33	D	407	LHG	O8-C23-C24-C25
33	8	618	LHG	O8-C23-C24-C25
34	C	624	LMG	O7-C10-C11-C12
31	6	303	CLA	C10-C11-C12-C13
31	b	611	CLA	C15-C16-C17-C18
33	l	101	LHG	C17-C18-C19-C20
31	p	614	CLA	CAA-CBA-CGA-O1A
33	y	619	LHG	O10-C23-C24-C25
38	G	624	SQD	O49-C7-C8-C9
31	1	602	CLA	C4-C3-C5-C6
32	4	616	LUT	C13-C14-C15-C35
32	7	318	LUT	C13-C14-C15-C35
34	4	621	LMG	C14-C15-C16-C17
34	J	102	LMG	C31-C32-C33-C34
34	x	202	LMG	C29-C30-C31-C32
30	3	309	CHL	O1D-CGD-O2D-CED
44	D	406	PL9	C11-C12-C13-C14
44	d	407	PL9	C31-C32-C33-C34
34	2	620	LMG	C40-C41-C42-C43
31	4	611	CLA	CAA-CBA-CGA-O1A
30	5	607	CHL	CAD-CBD-CGD-O1D
30	0	605	CHL	CAD-CBD-CGD-O1D
30	y	605	CHL	CAD-CBD-CGD-O1D
31	1	610	CLA	CAD-CBD-CGD-O1D
31	3	301	CLA	CAD-CBD-CGD-O1D
31	N	311	CLA	CAD-CBD-CGD-O1D
31	R	315	CLA	CAD-CBD-CGD-O1D
31	8	610	CLA	CAD-CBD-CGD-O1D
31	8	614	CLA	CAD-CBD-CGD-O1D
31	n	312	CLA	CAD-CBD-CGD-O1D
31	n	316	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	r	315	CLA	CAD-CBD-CGD-O1D
31	y	610	CLA	CAD-CBD-CGD-O1D
31	y	611	CLA	CAD-CBD-CGD-O1D
34	2	621	LMG	C7-C8-O7-C10
34	A	414	LMG	C7-C8-O7-C10
34	p	620	LMG	C9-C8-O7-C10
34	g	322	LMG	C7-C8-O7-C10
38	G	624	SQD	O5-C5-C6-S
38	a	411	SQD	C5-C6-S-O7
45	c	617	DGD	C3G-C2G-O2G-C1B
30	p	607	CHL	CAA-CBA-CGA-O1A
30	p	608	CHL	CAA-CBA-CGA-O1A
30	q	308	CHL	CAA-CBA-CGA-O1A
31	b	609	CLA	CAA-CBA-CGA-O1A
33	3	320	LHG	O10-C23-C24-C25
33	l	101	LHG	O10-C23-C24-C25
34	I	101	LMG	O10-C28-C29-C30
30	1	605	CHL	CAA-CBA-CGA-O2A
30	2	606	CHL	CAA-CBA-CGA-O2A
30	4	606	CHL	CAA-CBA-CGA-O2A
30	R	308	CHL	CAA-CBA-CGA-O2A
30	7	309	CHL	CAA-CBA-CGA-O2A
31	q	315	CLA	CAA-CBA-CGA-O2A
33	n	320	LHG	O8-C23-C24-C25
31	0	611	CLA	C8-C10-C11-C12
31	y	612	CLA	C10-C11-C12-C13
30	1	601	CHL	C14-C13-C15-C16
30	7	306	CHL	C6-C7-C8-C9
30	g	309	CHL	C14-C13-C15-C16
31	1	611	CLA	C11-C12-C13-C14
31	1	612	CLA	C11-C10-C8-C9
31	2	612	CLA	C6-C7-C8-C9
31	C	609	CLA	C11-C12-C13-C14
31	S	305	CLA	C14-C13-C15-C16
31	Y	310	CLA	C6-C7-C8-C9
31	7	303	CLA	C11-C10-C8-C9
31	q	315	CLA	C14-C13-C15-C16
31	b	603	CLA	C11-C12-C13-C14
31	b	604	CLA	C14-C13-C15-C16
31	b	612	CLA	C14-C13-C15-C16
31	b	613	CLA	C11-C10-C8-C9
31	r	305	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	s	312	CLA	C11-C10-C8-C9
38	6	301	SQD	C26-C27-C28-C29
30	8	605	CHL	CBD-CGD-O2D-CED
30	6	306	CHL	CAA-CBA-CGA-O2A
30	s	302	CHL	CAA-CBA-CGA-O1A
30	q	309	CHL	C5-C6-C7-C8
31	1	610	CLA	C13-C15-C16-C17
31	Y	312	CLA	C8-C10-C11-C12
31	c	601	CLA	C10-C11-C12-C13
33	t	102	LHG	O10-C23-C24-C25
33	A	417	LHG	C10-C11-C12-C13
38	B	623	SQD	C24-C25-C26-C27
30	R	309	CHL	CAA-CBA-CGA-O2A
31	Y	311	CLA	CAA-CBA-CGA-O2A
31	Y	314	CLA	CAA-CBA-CGA-O2A
31	0	604	CLA	CAA-CBA-CGA-O2A
31	8	604	CLA	CAA-CBA-CGA-O2A
31	9	316	CLA	CAA-CBA-CGA-O2A
31	b	617	CLA	CAA-CBA-CGA-O2A
31	s	303	CLA	CAA-CBA-CGA-O2A
33	Y	318	LHG	O8-C23-C24-C25
33	7	319	LHG	O8-C23-C24-C25
33	9	320	LHG	O7-C7-C8-C9
33	9	320	LHG	O8-C23-C24-C25
34	1	618	LMG	O7-C10-C11-C12
34	3	321	LMG	O7-C10-C11-C12
34	B	621	LMG	O7-C10-C11-C12
34	b	622	LMG	O7-C10-C11-C12
34	w	204	LMG	O7-C10-C11-C12
38	A	413	SQD	O47-C7-C8-C9
31	6	316	CLA	C4C-C3C-CAC-CBC
38	a	411	SQD	C11-C10-C9-C8
31	3	316	CLA	C5-C6-C7-C8
31	5	611	CLA	C8-C10-C11-C12
31	s	314	CLA	C10-C11-C12-C13
30	n	306	CHL	CBD-CGD-O2D-CED
33	D	408	LHG	C19-C20-C21-C22
38	b	627	SQD	C17-C18-C19-C20
45	c	617	DGD	C4A-C5A-C6A-C7A
45	c	617	DGD	C2B-C3B-C4B-C5B
31	5	613	CLA	CAA-CBA-CGA-O1A
33	L	101	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	4	621	LMG	C12-C13-C14-C15
34	S	321	LMG	C19-C20-C21-C22
31	B	605	CLA	C10-C11-C12-C13
33	A	417	LHG	C34-C35-C36-C37
33	C	623	LHG	C30-C31-C32-C33
30	7	321	CHL	CAA-CBA-CGA-O2A
30	n	308	CHL	CAA-CBA-CGA-O2A
31	2	602	CLA	CAA-CBA-CGA-O2A
31	3	305	CLA	CAA-CBA-CGA-O2A
31	B	608	CLA	CAA-CBA-CGA-O2A
31	D	404	CLA	CAA-CBA-CGA-O2A
31	p	611	CLA	CAA-CBA-CGA-O2A
31	p	613	CLA	CAA-CBA-CGA-O2A
31	q	305	CLA	CAA-CBA-CGA-O2A
31	y	615	CLA	CAA-CBA-CGA-O2A
33	S	322	LHG	O7-C7-C8-C9
33	s	322	LHG	O7-C7-C8-C9
34	J	101	LMG	O7-C10-C11-C12
34	c	621	LMG	O7-C10-C11-C12
34	d	409	LMG	O7-C10-C11-C12
38	a	412	SQD	O47-C7-C8-C9
30	0	607	CHL	C5-C6-C7-C8
31	N	303	CLA	C15-C16-C17-C18
31	b	606	CLA	C10-C11-C12-C13
38	A	413	SQD	C13-C14-C15-C16
30	5	608	CHL	CAA-CBA-CGA-O1A
30	N	301	CHL	CAA-CBA-CGA-O1A
31	6	315	CLA	CAA-CBA-CGA-O1A
31	b	617	CLA	CAA-CBA-CGA-O1A
31	s	303	CLA	CAA-CBA-CGA-O1A
31	b	606	CLA	C16-C17-C18-C20
31	r	311	CLA	C2C-C3C-CAC-CBC
34	2	620	LMG	C11-C12-C13-C14
34	C	619	LMG	C22-C23-C24-C25
31	r	306	CLA	O2A-C1-C2-C3
30	G	605	CHL	C3A-C2A-CAA-CBA
30	0	607	CHL	C3A-C2A-CAA-CBA
30	g	306	CHL	C3A-C2A-CAA-CBA
31	1	604	CLA	C11-C10-C8-C7
31	1	610	CLA	C11-C12-C13-C15
31	3	304	CLA	C11-C10-C8-C7
31	5	611	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	5	614	CLA	C3A-C2A-CAA-CBA
31	B	609	CLA	C12-C13-C15-C16
31	C	609	CLA	C11-C12-C13-C15
31	D	404	CLA	C12-C13-C15-C16
31	G	612	CLA	C11-C10-C8-C7
31	N	310	CLA	C11-C12-C13-C15
31	S	305	CLA	C12-C13-C15-C16
31	7	312	CLA	C11-C12-C13-C15
31	8	604	CLA	C3A-C2A-CAA-CBA
31	q	315	CLA	C12-C13-C15-C16
31	b	606	CLA	C11-C12-C13-C15
31	c	608	CLA	C11-C10-C8-C7
31	d	404	CLA	C11-C12-C13-C15
31	n	311	CLA	C6-C7-C8-C10
31	r	305	CLA	C11-C10-C8-C7
31	s	316	CLA	C3A-C2A-CAA-CBA
42	D	401	PHO	C3A-C2A-CAA-CBA
30	R	309	CHL	CAA-CBA-CGA-O1A
30	Y	307	CHL	CAA-CBA-CGA-O1A
30	7	309	CHL	CAA-CBA-CGA-O1A
30	8	605	CHL	CAA-CBA-CGA-O1A
30	p	601	CHL	CAA-CBA-CGA-O1A
30	n	301	CHL	CAA-CBA-CGA-O1A
30	r	308	CHL	CAA-CBA-CGA-O1A
31	B	614	CLA	CAA-CBA-CGA-O1A
31	N	314	CLA	CAA-CBA-CGA-O1A
31	p	613	CLA	CAA-CBA-CGA-O1A
33	1	617	LHG	O10-C23-C24-C25
33	9	320	LHG	O10-C23-C24-C25
34	I	101	LMG	O9-C10-C11-C12
38	a	412	SQD	O49-C7-C8-C9
34	A	412	LMG	C11-C12-C13-C14
30	0	605	CHL	CAA-CBA-CGA-O2A
31	A	405	CLA	CAA-CBA-CGA-O2A
31	G	610	CLA	CAA-CBA-CGA-O2A
31	9	315	CLA	CAA-CBA-CGA-O2A
31	c	603	CLA	CAA-CBA-CGA-O2A
31	r	303	CLA	CAA-CBA-CGA-O2A
31	y	611	CLA	CAA-CBA-CGA-O2A
33	1	617	LHG	O8-C23-C24-C25
33	D	408	LHG	O8-C23-C24-C25
33	S	322	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
33	b	625	LHG	O8-C23-C24-C25
33	d	408	LHG	O8-C23-C24-C25
34	4	620	LMG	O7-C10-C11-C12
34	J	102	LMG	O7-C10-C11-C12
34	c	624	LMG	O7-C10-C11-C12
38	b	627	SQD	O48-C23-C24-C25
34	3	321	LMG	C11-C12-C13-C14
30	p	608	CHL	O2A-C1-C2-C3
47	e	102	HEM	C3A-C2A-CAA-CBA
32	5	616	LUT	C27-C28-C29-C30
32	9	318	LUT	C31-C32-C33-C34
32	r	317	LUT	C27-C28-C29-C30
30	1	605	CHL	CAA-CBA-CGA-O1A
30	2	606	CHL	CAA-CBA-CGA-O1A
30	6	308	CHL	CAA-CBA-CGA-O1A
30	7	321	CHL	CAA-CBA-CGA-O1A
30	8	608	CHL	CAA-CBA-CGA-O1A
30	n	306	CHL	CAA-CBA-CGA-O1A
30	n	308	CHL	CAA-CBA-CGA-O1A
31	3	306	CLA	CAA-CBA-CGA-O1A
31	R	312	CLA	CAA-CBA-CGA-O1A
31	Y	314	CLA	CAA-CBA-CGA-O1A
31	9	306	CLA	CAA-CBA-CGA-O1A
31	y	615	CLA	CAA-CBA-CGA-O1A
34	B	621	LMG	O9-C10-C11-C12
34	b	601	LMG	O9-C10-C11-C12
34	b	622	LMG	O9-C10-C11-C12
38	A	413	SQD	O49-C7-C8-C9
36	N	318	NEX	C9-C10-C11-C12
33	q	320	LHG	C12-C13-C14-C15
31	5	611	CLA	CAA-CBA-CGA-O2A
31	6	305	CLA	CAA-CBA-CGA-O2A
31	G	613	CLA	CAA-CBA-CGA-O2A
31	q	314	CLA	CAA-CBA-CGA-O2A
31	n	305	CLA	CAA-CBA-CGA-O2A
31	r	312	CLA	CAA-CBA-CGA-O2A
33	e	101	LHG	O7-C7-C8-C9
33	j	102	LHG	O7-C7-C8-C9
33	s	320	LHG	O8-C23-C24-C25
38	M	102	SQD	O48-C23-C24-C25
33	t	102	LHG	C31-C32-C33-C34
45	C	620	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
34	6	323	LMG	O6-C1-O1-C7
30	0	607	CHL	C10-C11-C12-C13
31	S	310	CLA	C8-C10-C11-C12
33	Y	318	LHG	C25-C26-C27-C28
30	4	606	CHL	CAA-CBA-CGA-O1A
30	R	308	CHL	CAA-CBA-CGA-O1A
30	y	606	CHL	CAA-CBA-CGA-O1A
31	2	602	CLA	CAA-CBA-CGA-O1A
31	D	404	CLA	CAA-CBA-CGA-O1A
31	b	607	CLA	CAA-CBA-CGA-O1A
33	6	320	LHG	O9-C7-C8-C9
33	A	415	LHG	O9-C7-C8-C9
33	R	320	LHG	O9-C7-C8-C9
33	Y	318	LHG	O10-C23-C24-C25
34	d	409	LMG	O9-C10-C11-C12
34	w	204	LMG	O9-C10-C11-C12
34	x	202	LMG	O9-C10-C11-C12
38	S	301	SQD	O49-C7-C8-C9
34	a	401	LMG	C14-C15-C16-C17
34	y	620	LMG	C31-C32-C33-C34
45	c	616	DGD	C4D-C5D-C6D-O5D
30	1	619	CHL	CAA-CBA-CGA-O2A
31	3	304	CLA	CAA-CBA-CGA-O2A
31	8	614	CLA	CAA-CBA-CGA-O2A
33	A	417	LHG	O8-C23-C24-C25
34	d	409	LMG	C15-C16-C17-C18
30	8	608	CHL	C10-C11-C12-C13
31	G	610	CLA	CAA-CBA-CGA-O1A
31	R	316	CLA	CAA-CBA-CGA-O1A
31	8	604	CLA	CAA-CBA-CGA-O1A
31	g	313	CLA	CAA-CBA-CGA-O1A
33	S	322	LHG	O9-C7-C8-C9
34	b	624	LMG	O9-C10-C11-C12
31	3	301	CLA	C2A-CAA-CBA-CGA
31	S	310	CLA	C2A-CAA-CBA-CGA
31	c	602	CLA	C2A-CAA-CBA-CGA
31	1	612	CLA	C16-C17-C18-C20
31	c	609	CLA	C8-C10-C11-C12
33	z	102	LHG	C12-C13-C14-C15
38	A	413	SQD	C7-C8-C9-C10
31	3	305	CLA	CAA-CBA-CGA-O1A
31	0	604	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	q	305	CLA	CAA-CBA-CGA-O1A
31	y	611	CLA	CAA-CBA-CGA-O1A
33	7	319	LHG	O10-C23-C24-C25
33	8	618	LHG	O10-C23-C24-C25
34	J	102	LMG	O9-C10-C11-C12
45	c	617	DGD	O1A-C1A-C2A-C3A
31	G	604	CLA	C4-C3-C5-C6
31	c	611	CLA	C4-C3-C5-C6
31	d	405	CLA	C4-C3-C5-C6
33	N	319	LHG	C17-C18-C19-C20
34	B	625	LMG	C32-C33-C34-C35
34	A	418	LMG	O7-C10-C11-C12

There are no ring outliers.

654 monomers are involved in 3749 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	b	619	BCR	4	0
33	9	320	LHG	9	0
35	G	614	RRX	28	0
31	2	611	CLA	9	0
30	9	311	CHL	6	0
31	3	313	CLA	4	0
31	C	607	CLA	5	0
38	a	412	SQD	4	0
32	Y	316	LUT	3	0
34	D	410	LMG	5	0
38	g	318	SQD	9	0
30	4	606	CHL	17	0
31	B	610	CLA	11	0
31	y	610	CLA	14	0
31	3	306	CLA	12	0
32	5	617	LUT	15	0
30	3	308	CHL	11	0
31	r	311	CLA	5	0
31	s	315	CLA	3	0
30	Y	302	CHL	10	0
34	b	629	LMG	5	0
30	G	608	CHL	8	0
34	X	203	LMG	1	0
38	A	413	SQD	3	0
31	9	313	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	613	CLA	8	0
34	3	321	LMG	13	0
43	d	406	BCR	5	0
31	s	314	CLA	4	0
31	C	604	CLA	6	0
32	p	616	LUT	15	0
31	N	312	CLA	5	0
31	c	609	CLA	2	0
38	g	301	SQD	12	0
38	r	322	SQD	4	0
31	G	603	CLA	10	0
31	p	603	CLA	5	0
38	M	102	SQD	3	0
31	3	314	CLA	13	0
31	r	304	CLA	3	0
38	G	617	SQD	9	0
31	2	603	CLA	10	0
43	D	405	BCR	13	0
30	7	310	CHL	6	0
30	2	608	CHL	10	0
31	B	611	CLA	11	0
34	9	301	LMG	14	0
34	D	411	LMG	1	0
31	N	311	CLA	4	0
31	7	305	CLA	13	0
31	Y	310	CLA	13	0
37	r	318	XAT	4	0
31	n	305	CLA	14	0
35	g	315	RRX	3	0
31	B	604	CLA	8	0
31	S	316	CLA	4	0
31	c	610	CLA	6	0
31	p	615	CLA	9	0
33	D	408	LHG	8	0
30	7	302	CHL	4	0
32	S	318	LUT	8	0
31	5	613	CLA	10	0
30	R	309	CHL	9	0
30	0	607	CHL	15	0
31	r	312	CLA	5	0
30	5	608	CHL	11	0
34	c	620	LMG	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	d	410	LMG	5	0
31	6	311	CLA	15	0
34	W	203	LMG	1	0
44	A	416	PL9	5	0
30	6	307	CHL	12	0
30	n	309	CHL	3	0
31	s	310	CLA	3	0
33	8	618	LHG	4	0
34	w	203	LMG	1	0
31	S	304	CLA	4	0
31	n	314	CLA	14	0
31	Y	305	CLA	5	0
31	1	603	CLA	9	0
34	Y	319	LMG	5	0
34	9	302	LMG	11	0
30	3	309	CHL	13	0
31	4	603	CLA	10	0
43	B	617	BCR	7	0
30	0	605	CHL	7	0
31	C	603	CLA	3	0
36	p	618	NEX	2	0
30	s	302	CHL	1	0
31	r	306	CLA	5	0
30	1	606	CHL	13	0
30	7	321	CHL	17	0
34	Q1	101	LMG	14	0
38	6	301	SQD	4	0
31	S	303	CLA	9	0
31	Y	314	CLA	3	0
31	q	313	CLA	8	0
31	5	614	CLA	6	0
31	q	306	CLA	8	0
34	g	320	LMG	4	0
37	2	619	XAT	11	0
31	c	612	CLA	8	0
33	K	102	LHG	6	0
31	1	612	CLA	12	0
30	Y	309	CHL	11	0
34	N	320	LMG	2	0
31	b	614	CLA	13	0
34	B	621	LMG	8	0
43	z	101	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	R	310	CHL	2	0
30	6	308	CHL	11	0
32	S	317	LUT	9	0
31	R	307	CLA	2	0
32	y	616	LUT	11	0
34	6	323	LMG	2	0
36	Y	317	NEX	2	0
30	3	310	CHL	7	0
31	G	613	CLA	1	0
34	b	622	LMG	8	0
31	N	304	CLA	10	0
34	0	622	LMG	5	0
33	d	408	LHG	13	0
43	c	614	BCR	6	0
37	q	321	XAT	16	0
33	N	319	LHG	3	0
31	2	604	CLA	6	0
43	Z	101	BCR	3	0
34	C	621	LMG	9	0
34	x	202	LMG	5	0
31	p	611	CLA	8	0
43	C	615	BCR	3	0
32	4	616	LUT	11	0
42	A	408	PHO	7	0
30	9	308	CHL	9	0
31	b	615	CLA	6	0
31	5	602	CLA	9	0
43	C	614	BCR	3	0
45	c	619	DGD	26	0
31	b	613	CLA	9	0
30	N	307	CHL	13	0
31	b	611	CLA	10	0
34	p	620	LMG	5	0
30	Y	307	CHL	8	0
42	d	402	PHO	5	0
31	B	602	CLA	4	0
31	8	614	CLA	12	0
36	R	319	NEX	8	0
34	a	401	LMG	5	0
31	N	315	CLA	9	0
30	R	308	CHL	5	0
31	c	608	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	n	322	LMG	14	0
31	8	611	CLA	4	0
31	g	314	CLA	4	0
33	t	102	LHG	1	0
32	N	317	LUT	8	0
32	6	318	LUT	10	0
33	y	619	LHG	11	0
31	0	615	CLA	5	0
37	G	620	XAT	22	0
30	s	309	CHL	3	0
30	p	606	CHL	8	0
36	y	618	NEX	5	0
34	w	204	LMG	1	0
31	6	315	CLA	10	0
30	G	607	CHL	3	0
30	g	302	CHL	7	0
34	n	321	LMG	6	0
36	g	317	NEX	2	0
30	q	307	CHL	9	0
31	A	405	CLA	7	0
31	5	610	CLA	27	0
30	7	309	CHL	3	0
33	S	320	LHG	6	0
31	5	603	CLA	12	0
35	q	317	RRX	20	0
30	p	609	CHL	7	0
33	C	623	LHG	7	0
30	n	310	CHL	9	0
31	G	610	CLA	8	0
30	7	307	CHL	10	0
34	2	618	LMG	7	0
31	b	609	CLA	7	0
30	Y	308	CHL	5	0
34	2	621	LMG	5	0
33	6	320	LHG	2	0
30	8	606	CHL	9	0
31	C	611	CLA	5	0
31	B	601	CLA	2	0
32	Y	315	LUT	9	0
33	G	618	LHG	15	0
31	2	610	CLA	7	0
34	J	102	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	413	LMG	4	0
32	3	318	LUT	13	0
30	p	605	CHL	7	0
32	7	318	LUT	5	0
31	q	305	CLA	7	0
33	3	320	LHG	7	0
31	g	310	CLA	5	0
31	c	605	CLA	6	0
30	N	309	CHL	14	0
30	9	310	CHL	11	0
38	X	201	SQD	1	0
31	2	609	CLA	16	0
38	b	627	SQD	9	0
31	6	313	CLA	3	0
33	A	417	LHG	4	0
30	3	307	CHL	16	0
34	6	321	LMG	10	0
30	6	306	CHL	6	0
30	s	307	CHL	9	0
31	3	316	CLA	10	0
30	S	309	CHL	3	0
31	2	602	CLA	8	0
33	1	617	LHG	5	0
31	s	313	CLA	9	0
33	S	322	LHG	5	0
31	C	606	CLA	8	0
34	c	624	LMG	7	0
30	4	607	CHL	18	0
30	8	601	CHL	10	0
31	c	602	CLA	6	0
43	B	618	BCR	5	0
31	8	603	CLA	12	0
31	b	610	CLA	10	0
31	6	316	CLA	4	0
33	7	319	LHG	3	0
31	G	602	CLA	5	0
34	k	101	LMG	3	0
38	s	301	SQD	6	0
33	2	617	LHG	4	0
32	R	317	LUT	3	0
31	3	315	CLA	7	0
33	r	320	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	0	613	CLA	2	0
31	5	604	CLA	4	0
31	C	605	CLA	6	0
31	Y	304	CLA	15	0
30	p	601	CHL	2	0
31	R	304	CLA	7	0
32	3	317	LUT	11	0
34	r	321	LMG	5	0
31	p	610	CLA	19	0
30	y	606	CHL	10	0
31	0	611	CLA	5	0
34	q	302	LMG	6	0
31	6	304	CLA	7	0
36	s	319	NEX	4	0
37	4	619	XAT	9	0
31	R	313	CLA	2	0
31	p	612	CLA	8	0
31	9	314	CLA	9	0
31	y	614	CLA	5	0
33	q	320	LHG	12	0
30	3	302	CHL	15	0
33	B	624	LHG	6	0
33	5	619	LHG	9	0
31	8	610	CLA	3	0
30	4	601	CHL	6	0
32	G	615	LUT	8	0
30	N	301	CHL	10	0
33	L	101	LHG	4	0
34	B	622	LMG	3	0
34	s	321	LMG	4	0
32	r	317	LUT	4	0
31	b	606	CLA	5	0
37	R	318	XAT	7	0
31	R	312	CLA	5	0
30	S	308	CHL	5	0
31	b	607	CLA	3	0
31	g	305	CLA	7	0
34	f	101	LMG	1	0
31	b	616	CLA	4	0
47	E	101	HEM	10	0
31	4	613	CLA	5	0
31	7	303	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	8	612	CLA	13	0
31	9	305	CLA	9	0
34	7	322	LMG	4	0
44	D	406	PL9	7	0
33	b	625	LHG	8	0
33	0	619	LHG	3	0
31	b	608	CLA	7	0
31	r	316	CLA	4	0
36	S	319	NEX	4	0
30	G	605	CHL	7	0
34	C	622	LMG	2	0
31	R	316	CLA	6	0
32	q	318	LUT	12	0
31	y	611	CLA	7	0
31	4	604	CLA	16	0
31	d	405	CLA	6	0
36	0	618	NEX	10	0
36	r	301	NEX	6	0
30	g	309	CHL	5	0
31	b	603	CLA	7	0
31	S	314	CLA	4	0
30	9	309	CHL	13	0
45	C	618	DGD	6	0
31	C	601	CLA	4	0
32	5	616	LUT	23	0
34	G	621	LMG	10	0
33	c	622	LHG	8	0
30	9	307	CHL	6	0
31	c	607	CLA	5	0
33	e	101	LHG	7	0
30	p	608	CHL	10	0
34	A	414	LMG	2	0
31	Y	312	CLA	8	0
31	C	612	CLA	5	0
31	s	303	CLA	12	0
38	A	411	SQD	1	0
34	b	626	LMG	2	0
31	6	312	CLA	4	0
43	b	620	BCR	1	0
34	w	205	LMG	6	0
33	4	618	LHG	5	0
30	2	601	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	4	612	CLA	5	0
33	Y	318	LHG	4	0
34	W	202	LMG	1	0
34	4	620	LMG	13	0
38	Y	320	SQD	5	0
31	G	609	CLA	10	0
34	7	301	LMG	6	0
30	7	308	CHL	11	0
31	B	607	CLA	5	0
30	y	601	CHL	8	0
31	B	612	CLA	9	0
30	q	310	CHL	14	0
34	S	321	LMG	2	0
34	G	622	LMG	12	0
31	G	604	CLA	7	0
31	7	315	CLA	3	0
31	q	315	CLA	7	0
31	3	311	CLA	8	0
31	y	615	CLA	11	0
31	S	310	CLA	2	0
30	5	605	CHL	11	0
32	n	318	LUT	8	0
31	4	610	CLA	18	0
43	t	101	BCR	13	0
33	a	415	LHG	4	0
33	g	319	LHG	12	0
33	b	628	LHG	13	0
36	r	319	NEX	3	0
32	1	616	LUT	3	0
31	N	313	CLA	15	0
31	R	305	CLA	7	0
33	l	101	LHG	11	0
30	s	308	CHL	8	0
36	5	618	NEX	16	0
32	0	617	LUT	6	0
31	B	606	CLA	6	0
31	r	303	CLA	3	0
34	W	201	LMG	13	0
30	8	608	CHL	8	0
38	a	411	SQD	4	0
31	7	316	CLA	11	0
34	q1	101	LMG	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	T	101	BCR	6	0
36	4	617	NEX	8	0
31	p	614	CLA	11	0
31	c	611	CLA	5	0
33	M	101	LHG	1	0
31	4	611	CLA	4	0
32	y	617	LUT	5	0
31	q	304	CLA	7	0
30	0	606	CHL	5	0
31	R	303	CLA	1	0
31	N	314	CLA	17	0
30	n	307	CHL	8	0
34	1	618	LMG	2	0
31	0	614	CLA	7	0
31	3	312	CLA	4	0
30	2	605	CHL	9	0
38	x	201	SQD	3	0
36	N	318	NEX	7	0
31	R	306	CLA	9	0
36	9	319	NEX	9	0
30	y	608	CHL	4	0
30	1	601	CHL	7	0
30	1	619	CHL	8	0
30	q	303	CHL	8	0
32	7	317	LUT	11	0
31	g	303	CLA	4	0
35	2	614	RRX	12	0
30	q	311	CHL	6	0
31	a	406	CLA	3	0
31	s	316	CLA	5	0
30	9	303	CHL	8	0
31	y	603	CLA	9	0
32	8	615	LUT	9	0
31	3	301	CLA	10	0
31	6	314	CLA	9	0
30	1	607	CHL	12	0
31	S	313	CLA	9	0
31	c	606	CLA	14	0
42	D	401	PHO	9	0
32	6	317	LUT	9	0
30	r	310	CHL	3	0
45	C	620	DGD	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	2	607	CHL	10	0
30	6	309	CHL	8	0
43	h	101	BCR	4	0
30	1	605	CHL	6	0
32	s	318	LUT	12	0
30	4	605	CHL	12	0
30	0	609	CHL	7	0
31	S	305	CLA	10	0
34	j	101	LMG	4	0
31	3	304	CLA	5	0
34	5	620	LMG	11	0
31	p	604	CLA	4	0
32	g	316	LUT	8	0
34	D	409	LMG	8	0
31	B	614	CLA	6	0
31	7	304	CLA	10	0
30	Y	306	CHL	2	0
36	3	319	NEX	10	0
32	N	316	LUT	14	0
31	7	313	CLA	3	0
43	H	101	BCR	4	0
31	B	615	CLA	6	0
30	5	607	CHL	11	0
37	g	321	XAT	20	0
31	0	604	CLA	2	0
34	c	621	LMG	1	0
30	3	303	CHL	8	0
31	1	610	CLA	15	0
30	4	609	CHL	9	0
33	s	322	LHG	6	0
31	p	613	CLA	25	0
31	d	404	CLA	6	0
34	J	101	LMG	4	0
30	5	606	CHL	12	0
34	4	621	LMG	12	0
31	g	311	CLA	5	0
31	C	609	CLA	2	0
43	c	615	BCR	9	0
30	g	308	CHL	6	0
31	a	409	CLA	14	0
30	6	310	CHL	7	0
30	1	608	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	7	312	CLA	7	0
37	9	322	XAT	3	0
32	8	616	LUT	9	0
45	C	617	DGD	9	0
48	r	302	LMU	11	0
31	s	304	CLA	4	0
33	R	320	LHG	1	0
32	s	317	LUT	12	0
30	p	607	CHL	13	0
31	R	311	CLA	5	0
38	B	623	SQD	7	0
30	0	601	CHL	4	0
34	A	412	LMG	4	0
30	7	306	CHL	5	0
31	8	613	CLA	15	0
34	d	409	LMG	4	0
30	6	302	CHL	6	0
38	R	322	SQD	6	0
43	a	410	BCR	4	0
33	n	320	LHG	3	0
31	r	315	CLA	7	0
31	G	611	CLA	3	0
31	1	611	CLA	14	0
30	n	308	CHL	15	0
30	N	308	CHL	4	0
31	2	613	CLA	7	0
34	I	101	LMG	5	0
31	N	310	CLA	16	0
31	c	604	CLA	2	0
31	N	321	CLA	14	0
31	A	406	CLA	8	0
31	8	604	CLA	9	0
34	D	412	LMG	2	0
30	8	607	CHL	3	0
31	n	311	CLA	14	0
31	r	305	CLA	8	0
31	s	312	CLA	6	0
30	G	623	CHL	14	0
36	2	616	NEX	6	0
31	R	315	CLA	2	0
43	b	618	BCR	11	0
47	e	102	HEM	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	409	CLA	7	0
31	c	601	CLA	4	0
30	y	609	CHL	11	0
31	n	315	CLA	16	0
31	b	612	CLA	14	0
30	r	309	CHL	9	0
34	a	416	LMG	3	0
30	5	609	CHL	9	0
32	n	317	LUT	10	0
31	Y	311	CLA	8	0
31	C	613	CLA	7	0
31	s	306	CLA	11	0
33	D	407	LHG	4	0
30	4	608	CHL	9	0
31	S	306	CLA	14	0
31	N	305	CLA	13	0
30	n	302	CHL	8	0
31	S	315	CLA	5	0
31	r	314	CLA	1	0
48	R	302	LMU	8	0
38	0	621	SQD	2	0
30	2	606	CHL	11	0
31	y	602	CLA	1	0
34	g	322	LMG	6	0
38	S	301	SQD	4	0
31	n	316	CLA	11	0
36	R	301	NEX	7	0
31	5	611	CLA	8	0
31	C	610	CLA	5	0
31	y	612	CLA	9	0
31	B	608	CLA	5	0
31	N	303	CLA	2	0
34	7	320	LMG	2	0
36	8	617	NEX	4	0
31	Y	313	CLA	2	0
30	n	306	CHL	10	0
35	9	317	RRX	13	0
31	a	407	CLA	3	0
32	p	617	LUT	9	0
31	p	602	CLA	9	0
31	6	305	CLA	12	0
30	S	302	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	S	312	CLA	6	0
34	m	102	LMG	5	0
30	5	601	CHL	7	0
31	y	613	CLA	8	0
30	S	307	CHL	6	0
34	G	619	LMG	3	0
35	4	615	RRX	17	0
31	B	616	CLA	9	0
32	1	615	LUT	9	0
31	5	612	CLA	6	0
31	6	303	CLA	4	0
31	9	316	CLA	1	0
31	4	602	CLA	10	0
31	5	615	CLA	10	0
34	6	322	LMG	11	0
30	G	606	CHL	10	0
31	3	305	CLA	14	0
31	C	608	CLA	9	0
30	q	308	CHL	7	0
31	g	304	CLA	4	0
31	1	614	CLA	4	0
30	y	607	CHL	12	0
31	8	602	CLA	8	0
34	d	411	LMG	2	0
31	9	304	CLA	9	0
30	1	609	CHL	6	0
31	1	613	CLA	2	0
32	9	318	LUT	15	0
48	c	623	LMU	3	0
30	0	608	CHL	7	0
31	r	307	CLA	5	0
31	c	603	CLA	5	0
34	A	418	LMG	3	0
31	0	612	CLA	3	0
33	A	415	LHG	4	0
34	k	102	LMG	2	0
48	K	101	LMU	1	0
34	X	202	LMG	5	0
34	0	620	LMG	8	0
33	s	320	LHG	5	0
36	q	319	NEX	4	0
31	s	311	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	y	605	CHL	2	0
31	g	312	CLA	6	0
31	n	304	CLA	11	0
34	q	301	LMG	4	0
30	q	309	CHL	19	0
34	C	624	LMG	6	0
31	9	312	CLA	15	0
44	d	407	PL9	9	0
30	G	601	CHL	11	0
31	s	305	CLA	9	0
31	q	314	CLA	8	0
31	C	602	CLA	4	0
31	n	313	CLA	4	0
31	0	603	CLA	5	0
36	n	319	NEX	2	0
43	B	619	BCR	8	0
31	1	602	CLA	5	0
38	y	621	SQD	3	0
31	g	313	CLA	12	0
30	g	306	CHL	7	0
31	D	403	CLA	8	0
31	9	306	CLA	10	0
31	7	314	CLA	4	0
30	N	306	CHL	10	0
31	0	610	CLA	15	0
31	n	303	CLA	8	0
32	0	616	LUT	6	0
34	B	625	LMG	5	0
38	B	620	SQD	7	0
39	A	401	OEX	1	0
45	c	616	DGD	13	0
33	z	102	LHG	3	0
31	n	312	CLA	3	0
30	r	308	CHL	6	0
31	B	609	CLA	7	0
34	2	620	LMG	2	0
44	a	414	PL9	9	0
31	9	315	CLA	8	0
36	G	616	NEX	1	0
31	D	404	CLA	8	0
30	8	605	CHL	5	0
31	B	613	CLA	10	0

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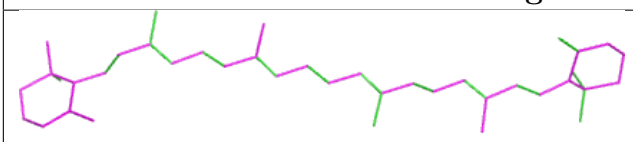
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	b	621	SQD	2	0
30	n	301	CHL	8	0
31	b	617	CLA	7	0
33	j	102	LHG	5	0
31	S	311	CLA	6	0
30	N	302	CHL	3	0
34	9	321	LMG	7	0
33	p	619	LHG	3	0
34	b	624	LMG	2	0
45	c	618	DGD	5	0
31	1	604	CLA	8	0
43	v	101	BCR	3	0
30	g	307	CHL	9	0
31	b	602	CLA	3	0
42	a	408	PHO	3	0
31	B	603	CLA	3	0
34	w	202	LMG	20	0
38	m	101	SQD	2	0
31	y	604	CLA	8	0
31	Y	303	CLA	5	0
36	6	319	NEX	11	0
30	Y	301	CHL	18	0
33	F1	301	LHG	1	0
34	w	201	LMG	7	0
31	G	612	CLA	12	0
31	4	614	CLA	3	0
43	A	410	BCR	3	0
43	V	101	BCR	1	0
32	2	615	LUT	8	0
31	7	311	CLA	17	0
31	b	605	CLA	6	0
31	8	609	CLA	11	0
38	G	624	SQD	4	0
31	0	602	CLA	4	0
31	r	313	CLA	4	0
31	b	604	CLA	3	0
31	B	605	CLA	7	0
34	b	601	LMG	4	0
34	y	620	LMG	4	0
31	q	312	CLA	22	0
45	c	617	DGD	9	0

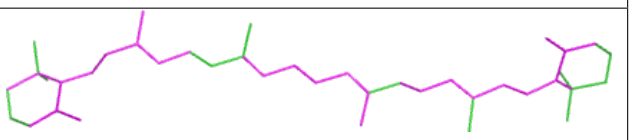
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

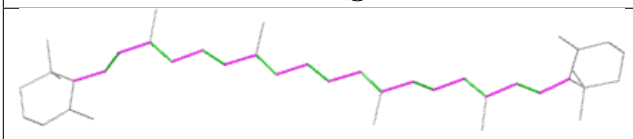
Ligand BCR b 619



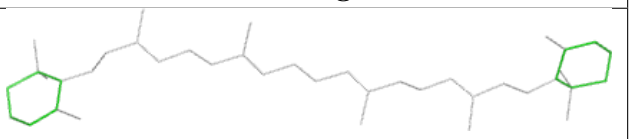
Bond lengths



Bond angles

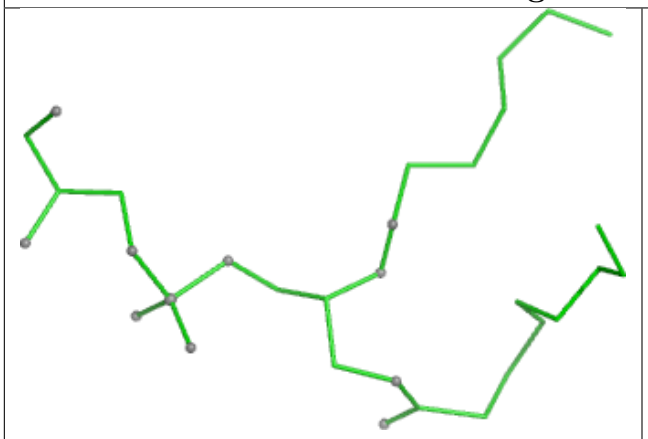


Torsions

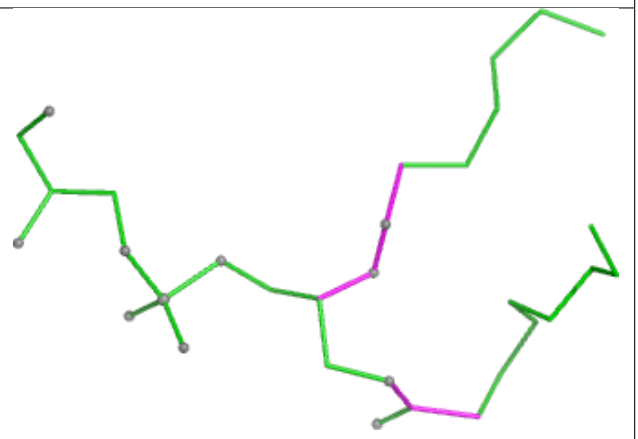


Rings

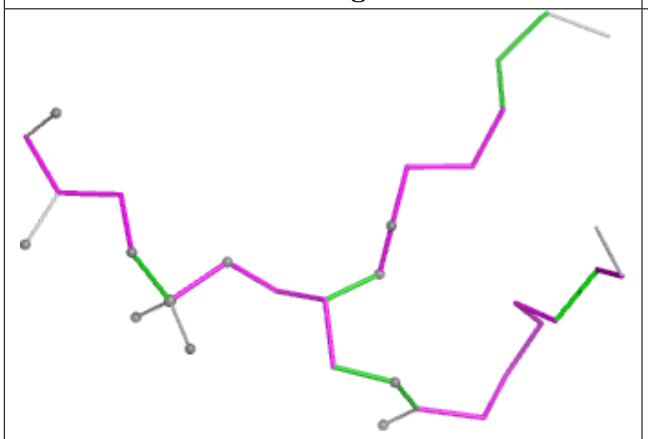
Ligand LHG 9 320



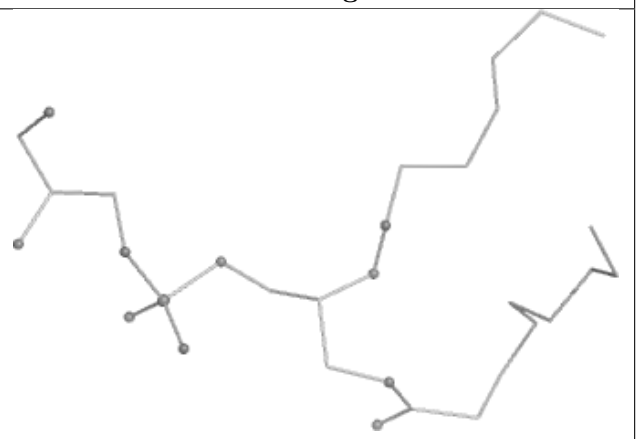
Bond lengths



Bond angles

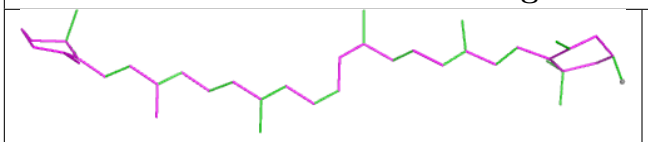


Torsions

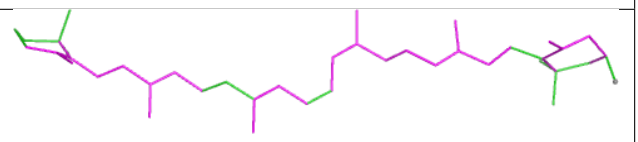


Rings

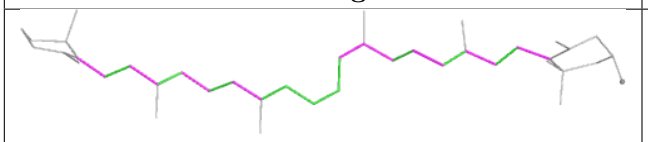
Ligand RRX G 614



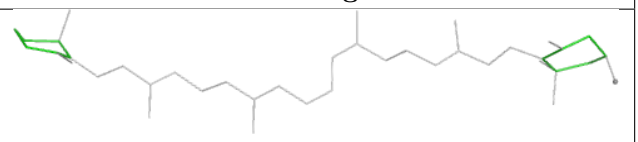
Bond lengths



Bond angles

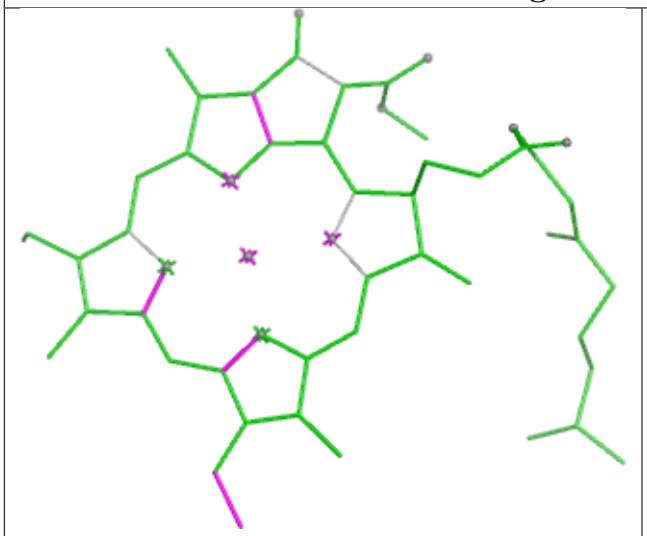


Torsions

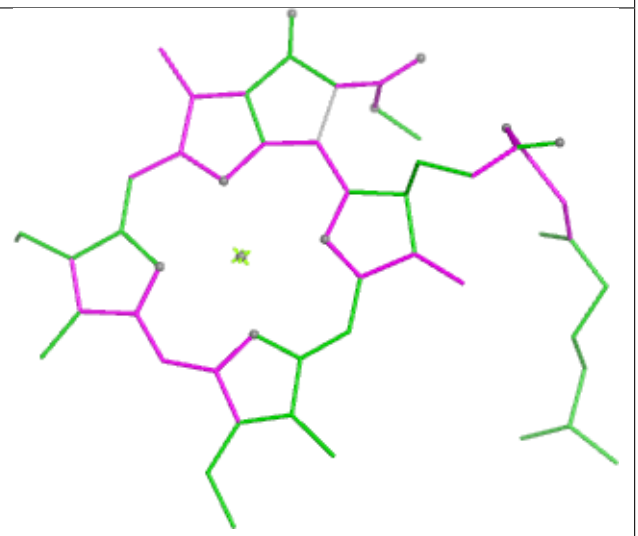


Rings

Ligand CLA 2 611



Bond lengths



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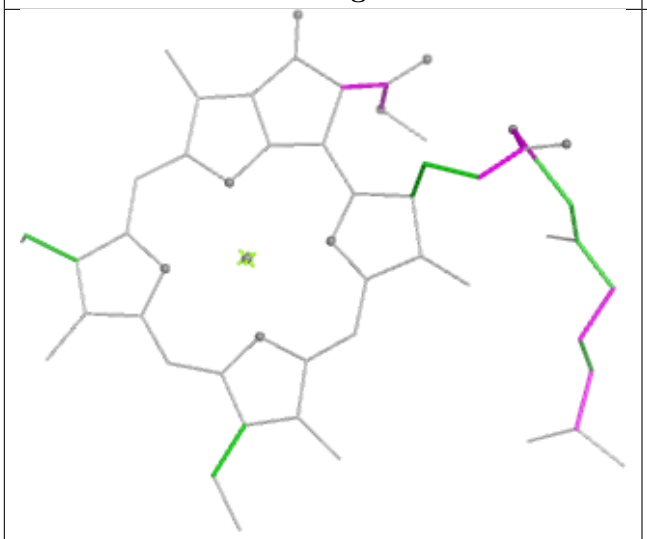

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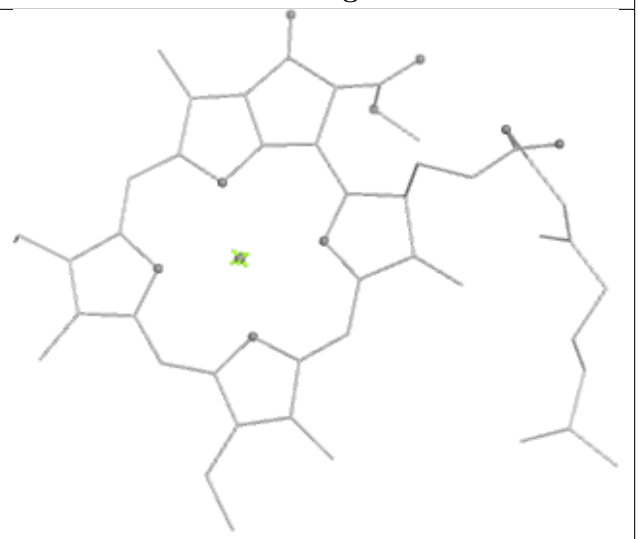
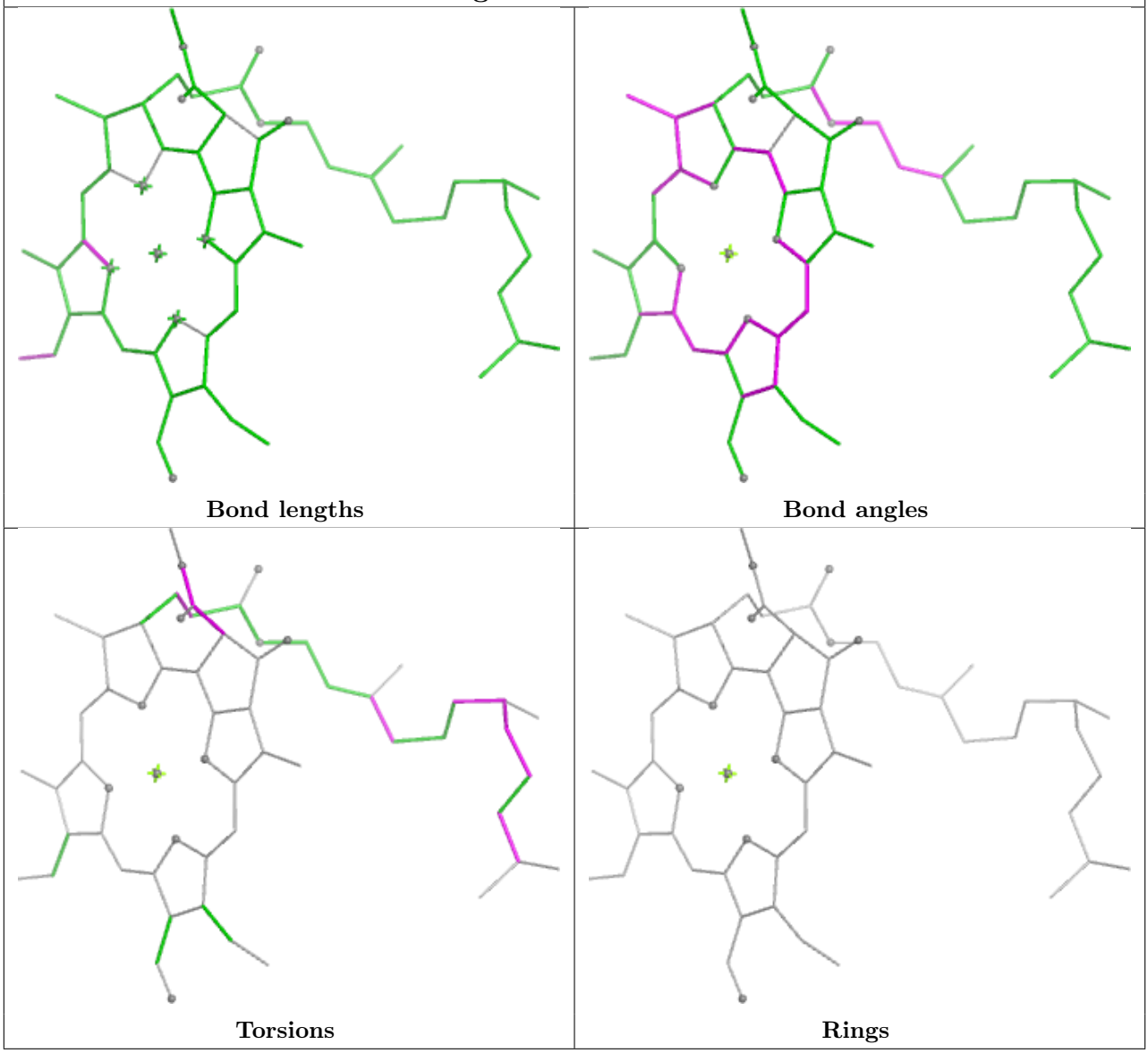
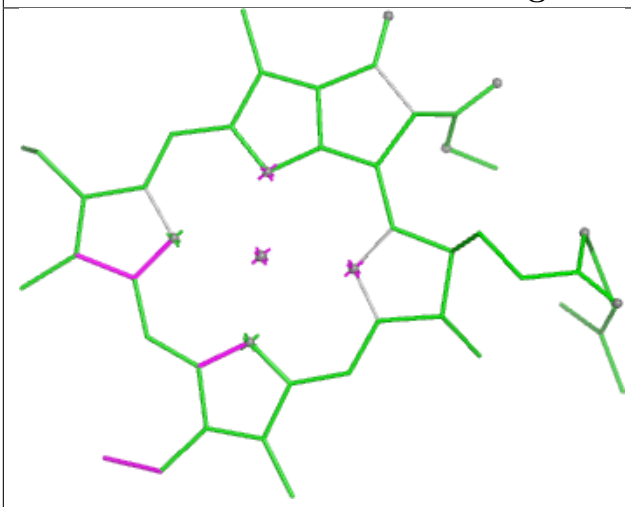


Rings

Ligand CHL 9 311



Ligand CLA 3 313



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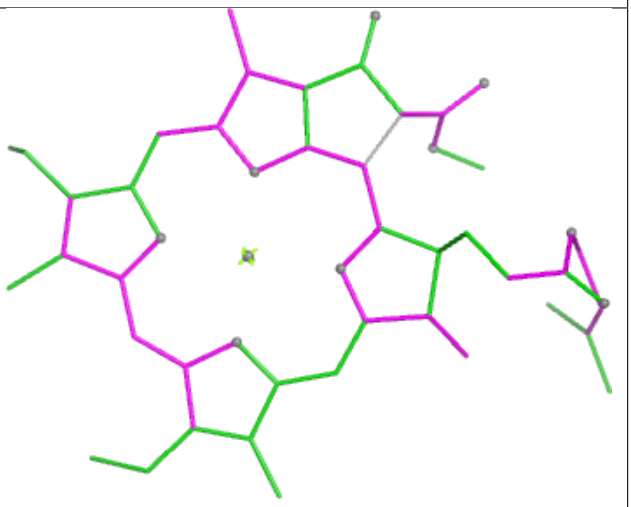
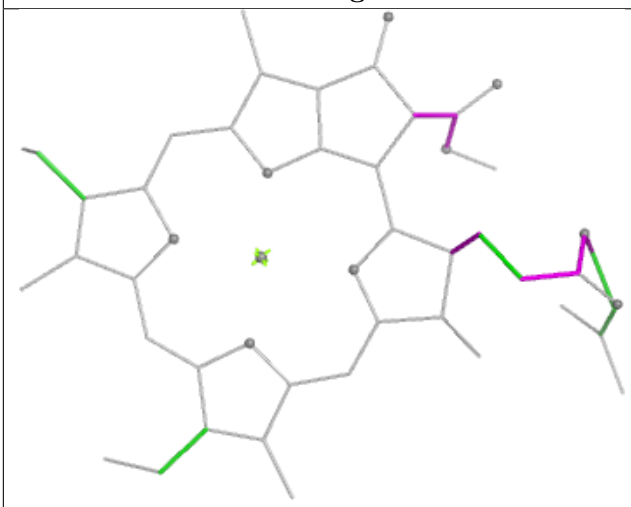


Bond angles



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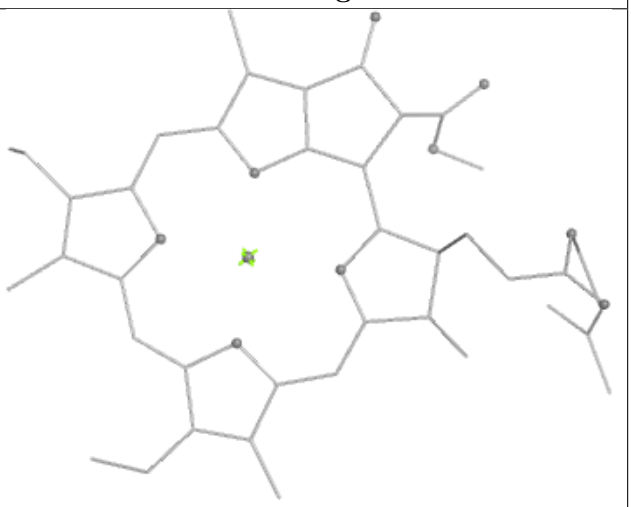
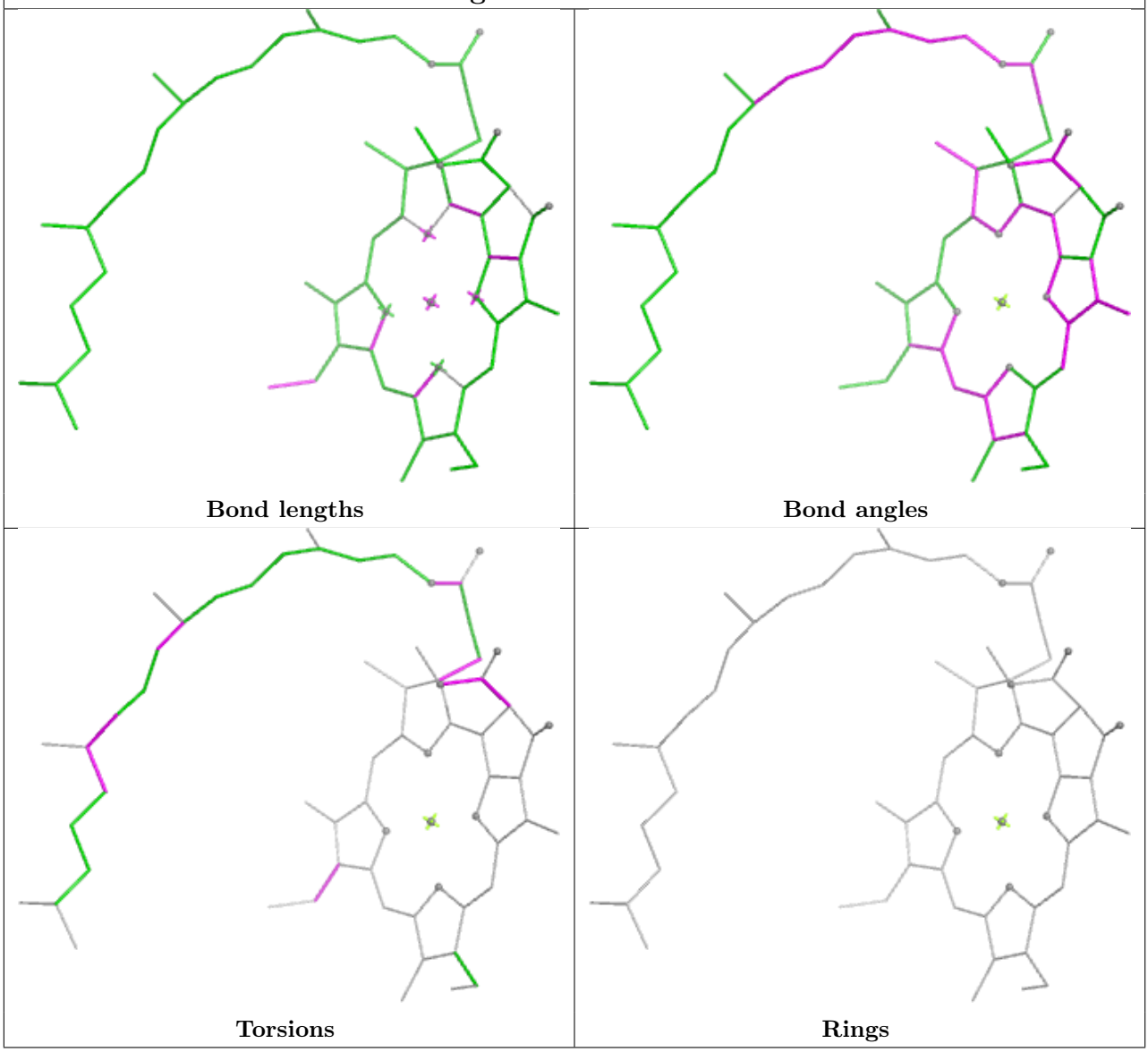
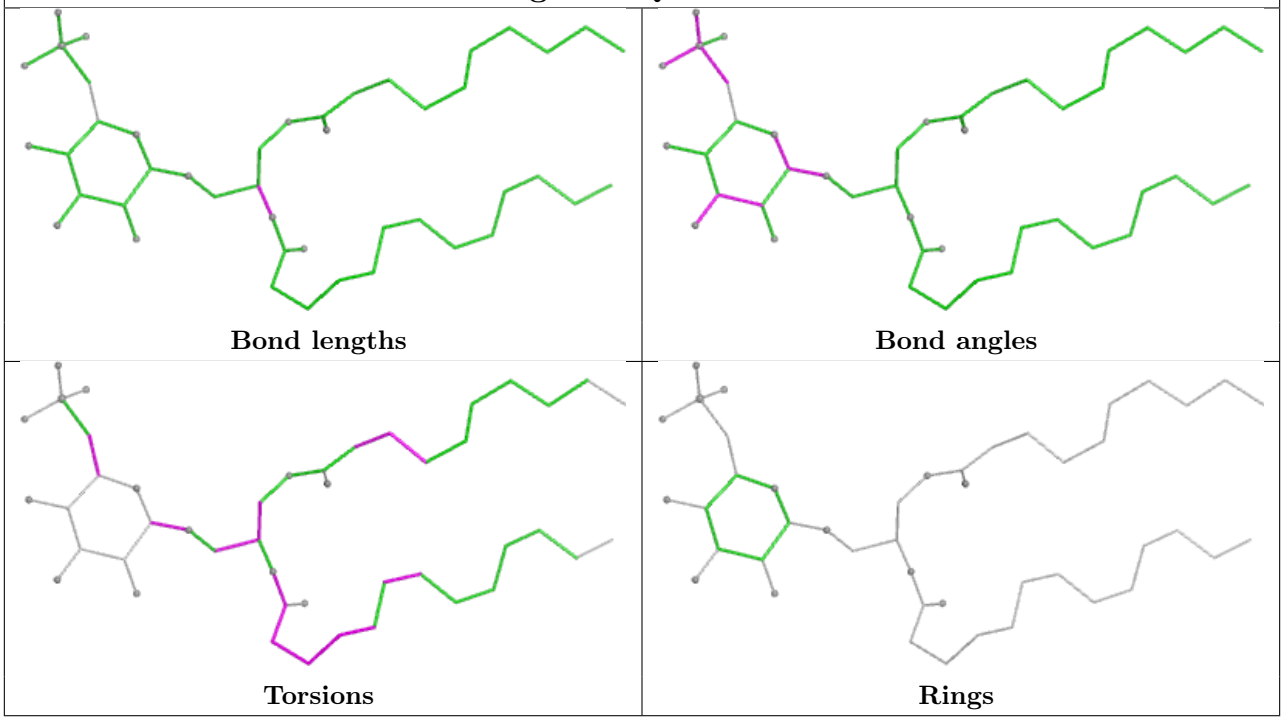


Rings

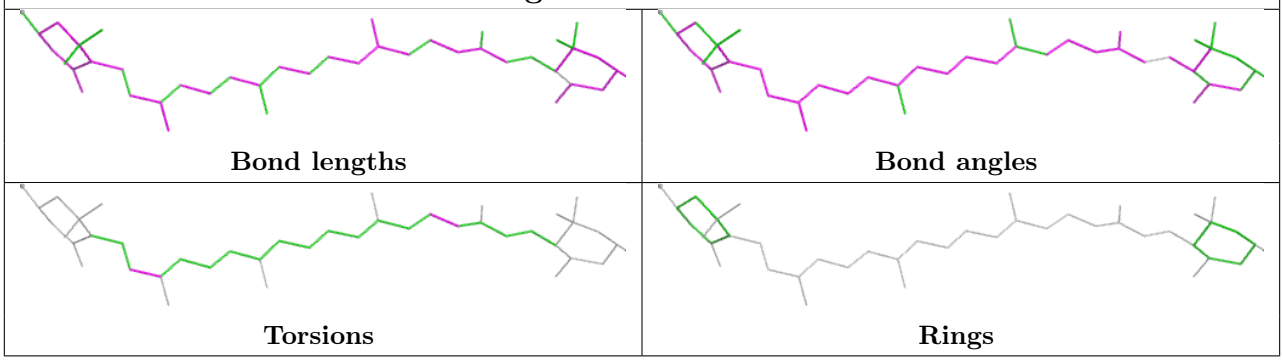
Ligand CLA C 607



Ligand SQD a 412



Ligand LUT Y 316



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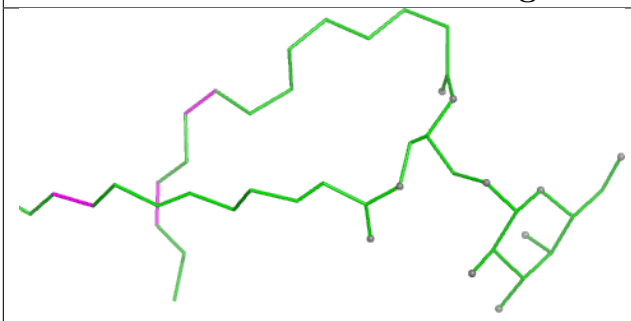
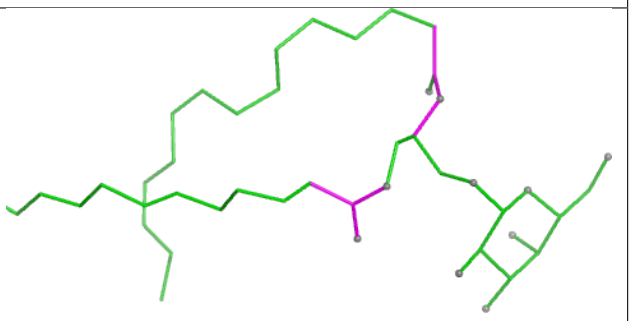
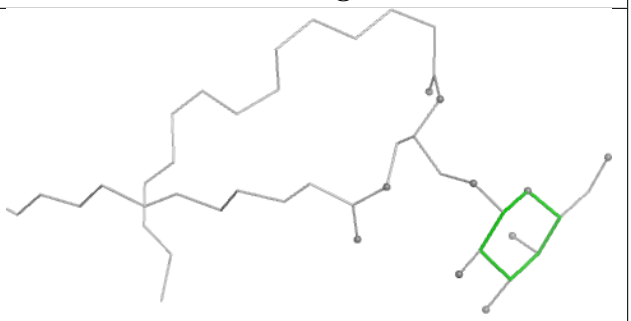
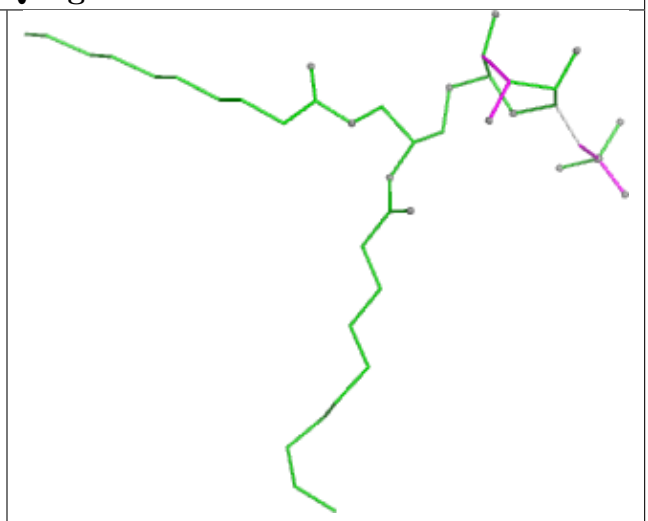
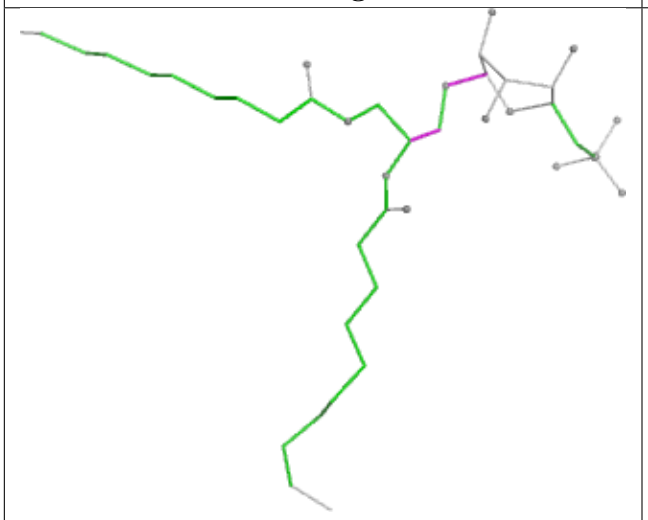
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand SQD g 318

Bond lengths



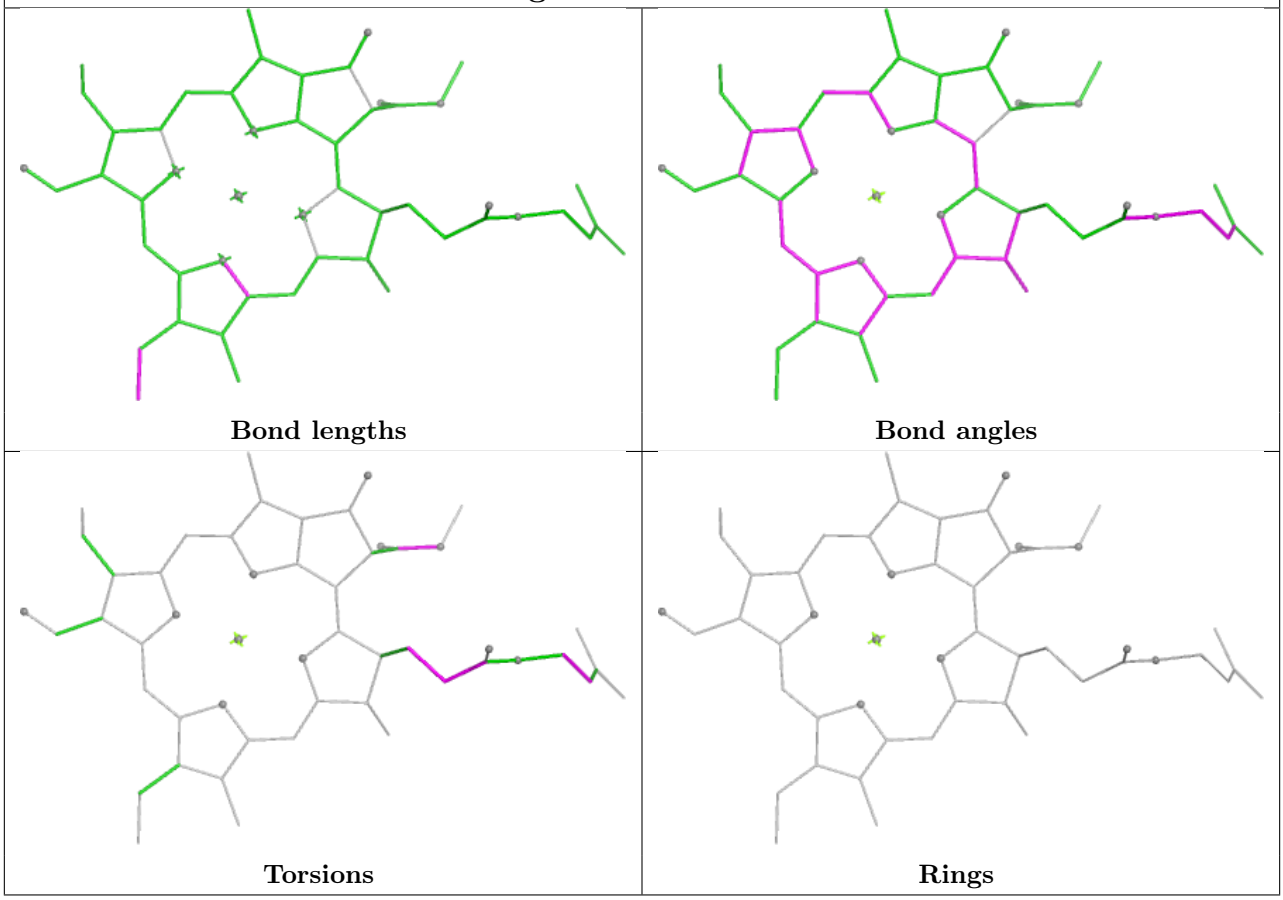
Bond angles

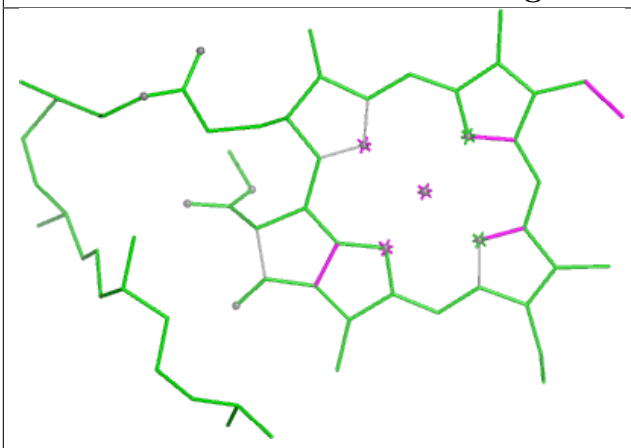
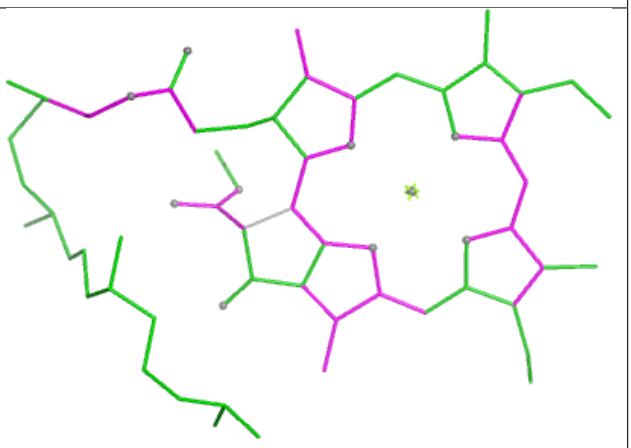
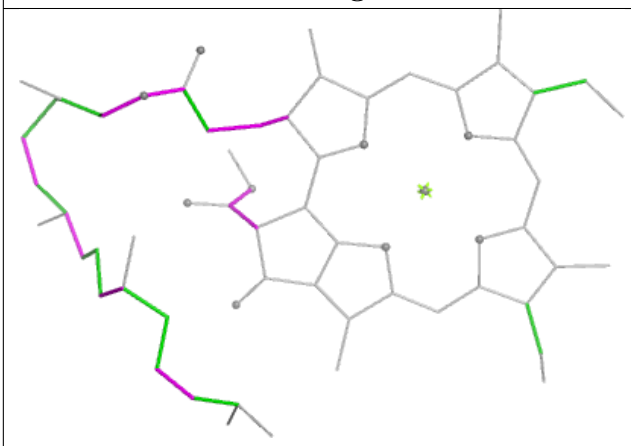
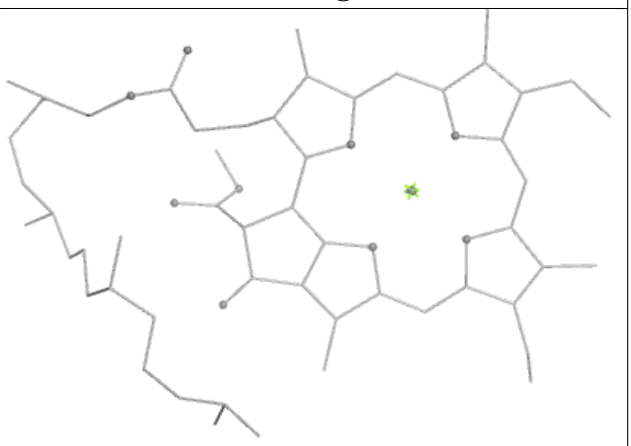


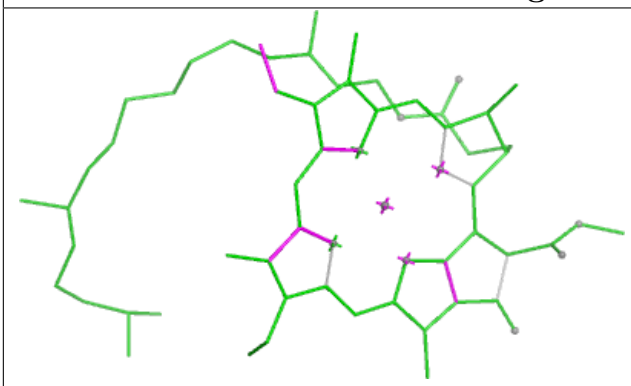
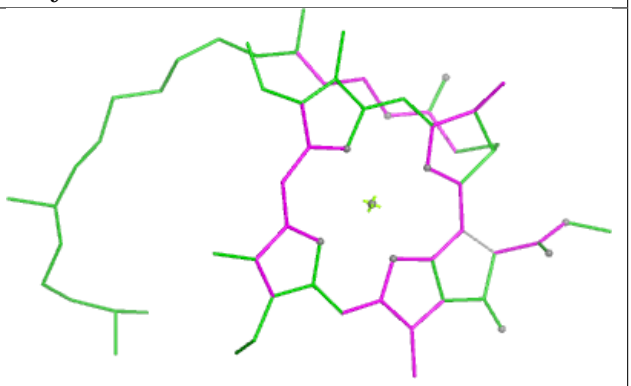
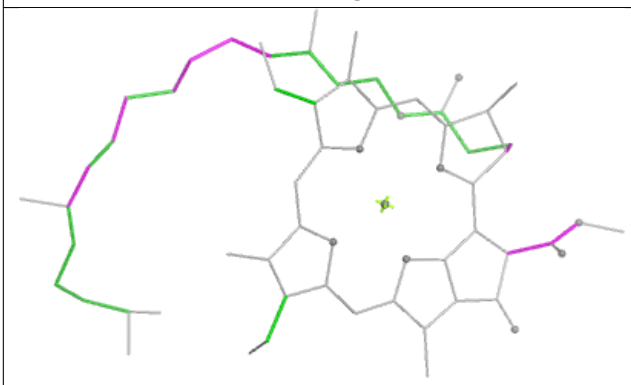
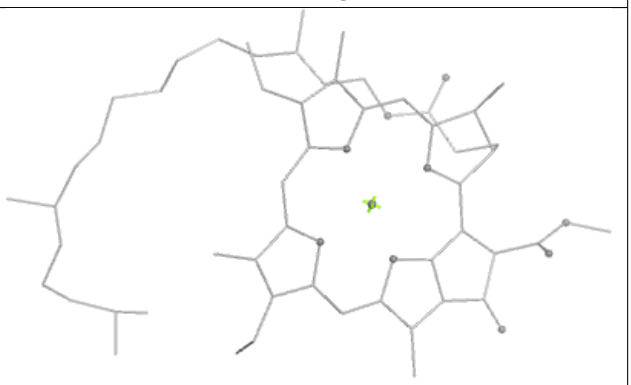
Torsions

Rings

Ligand CHL 4 606

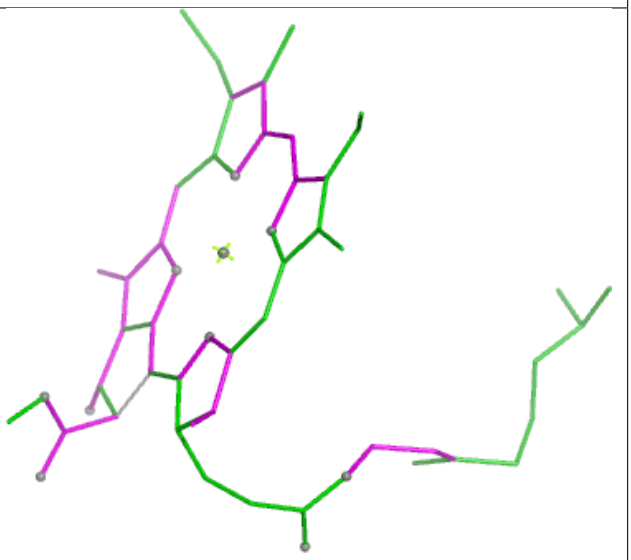


Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

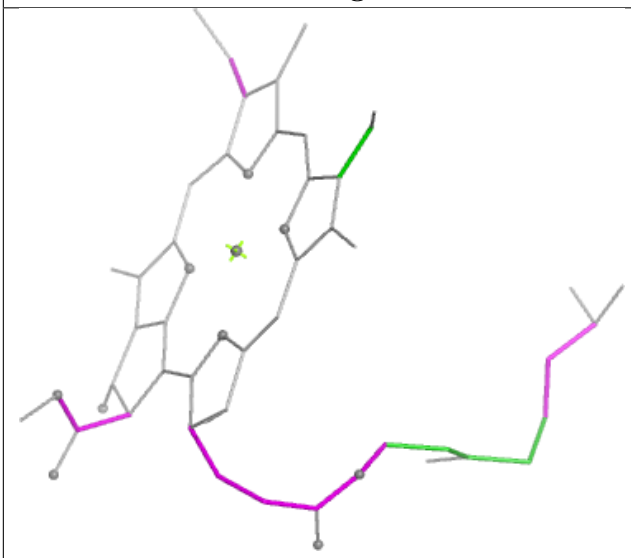
Ligand CLA y 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 306

Bond lengths



Bond angles



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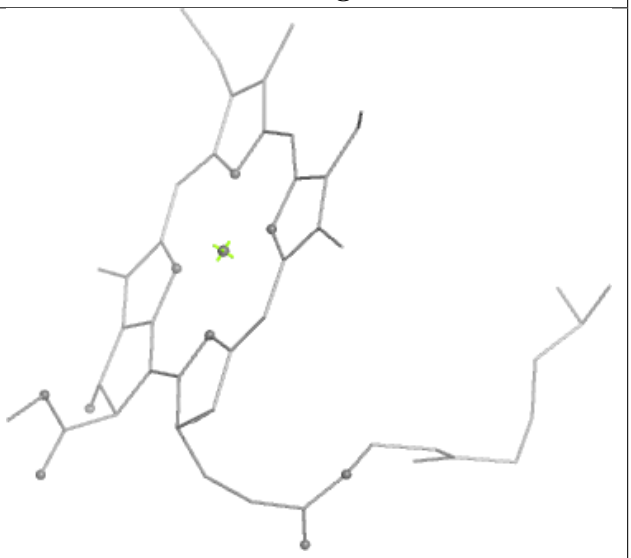
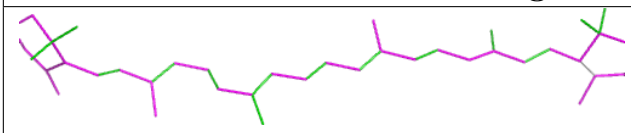
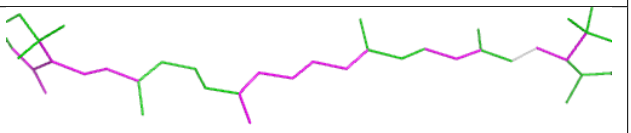


Rings

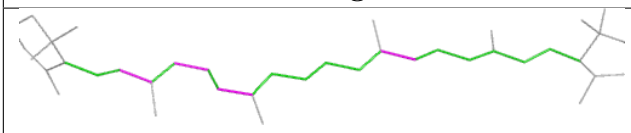
Ligand LUT 5 617



Bond lengths



Bond angles



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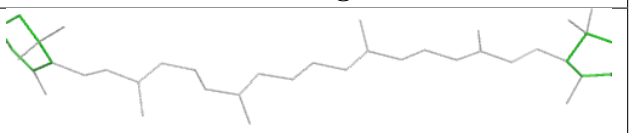
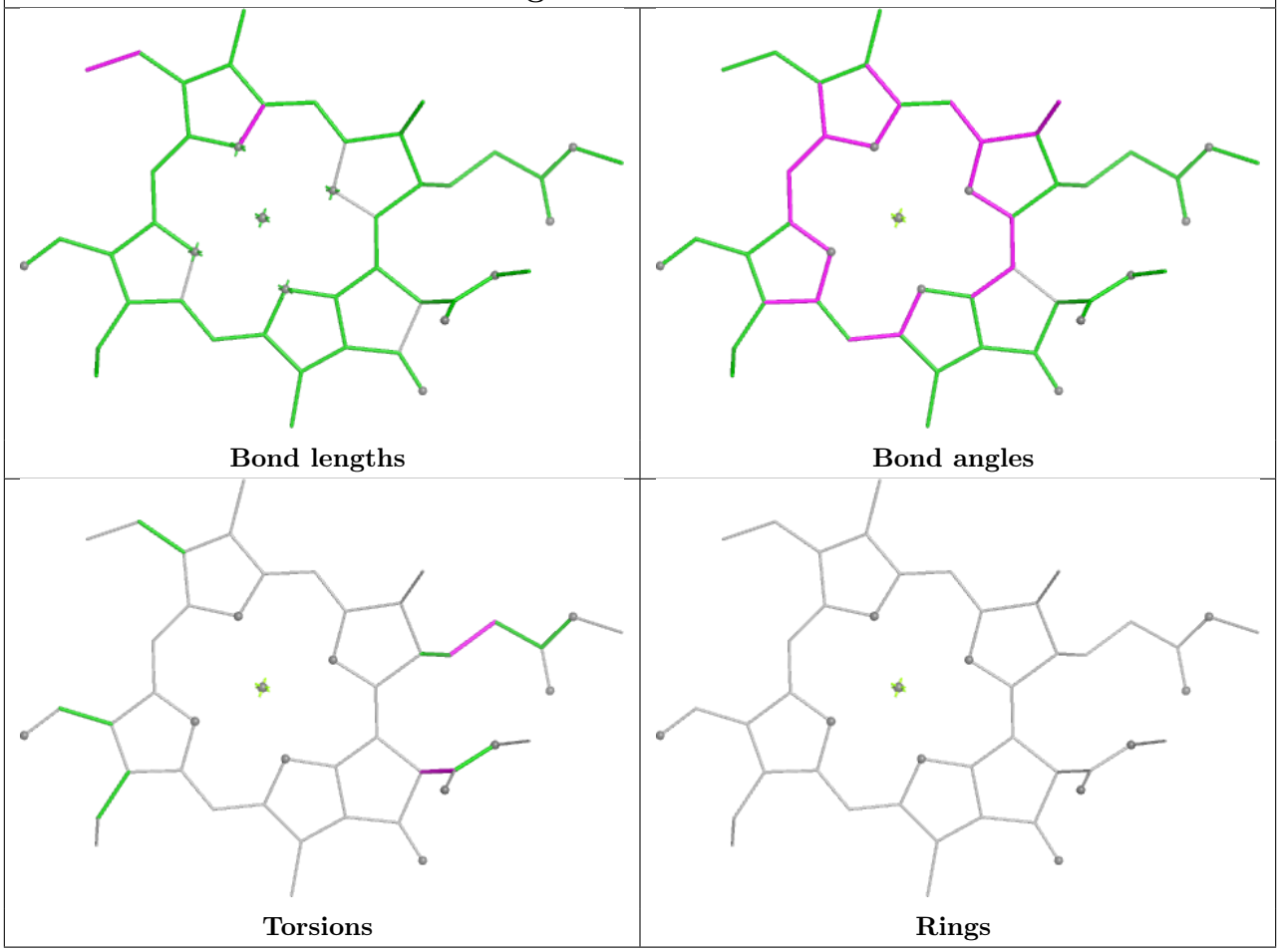
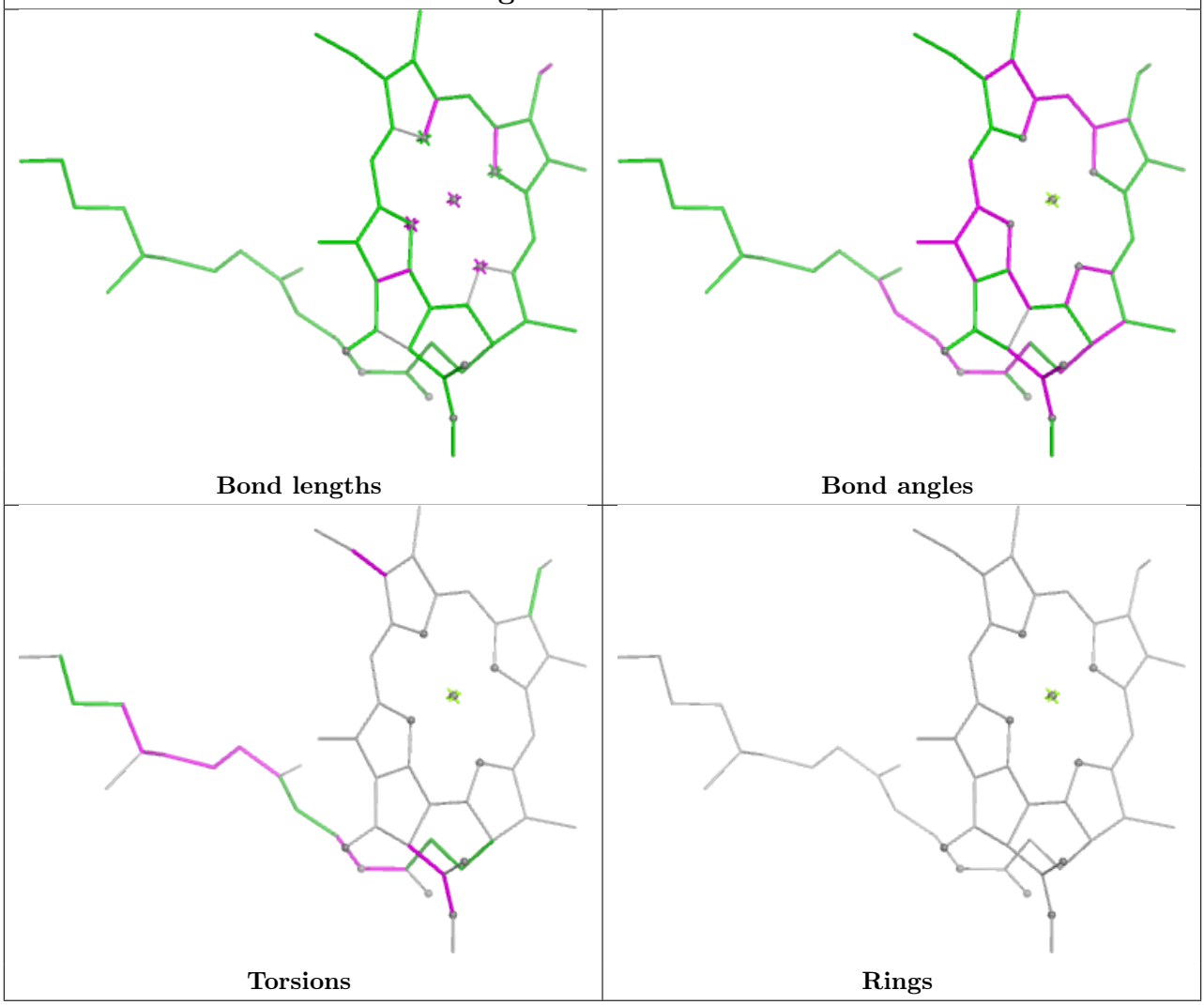


Rings

Ligand CHL 3 308



Ligand CLA r 311



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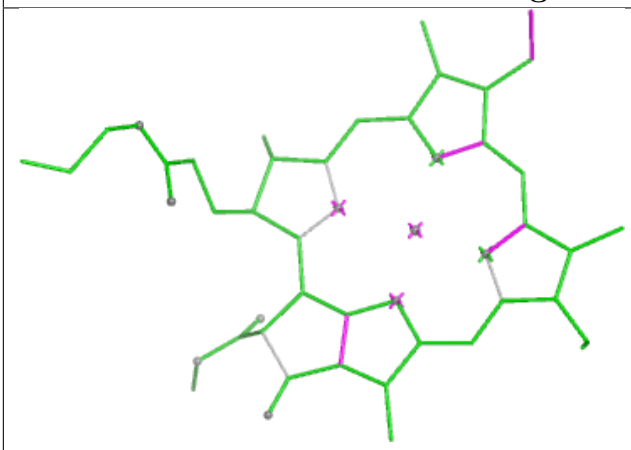

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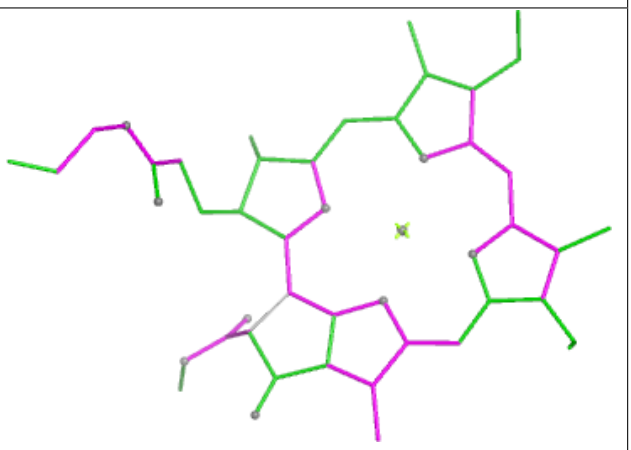
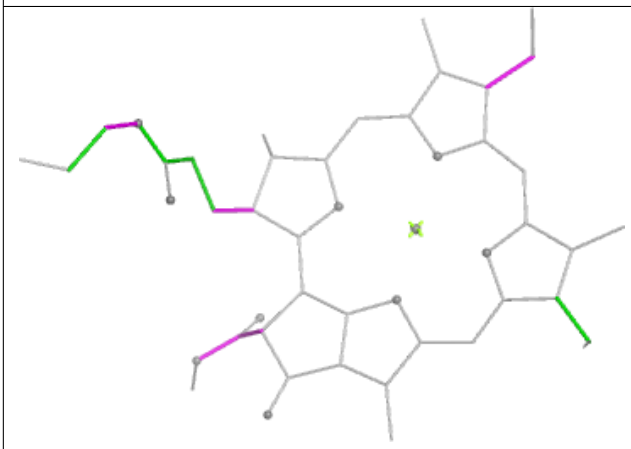


Bond angles



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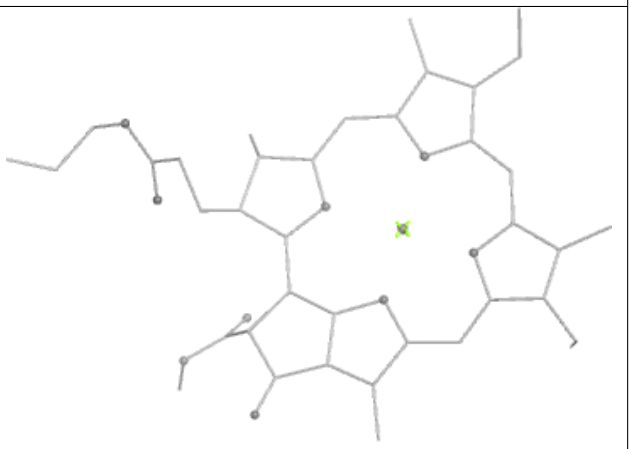
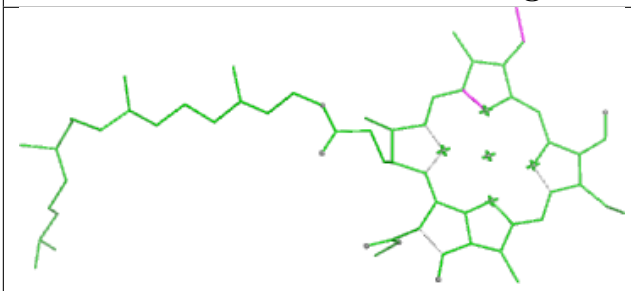


Rings

Ligand CHL Y 302



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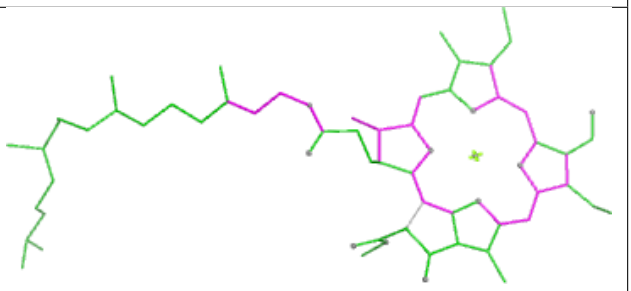
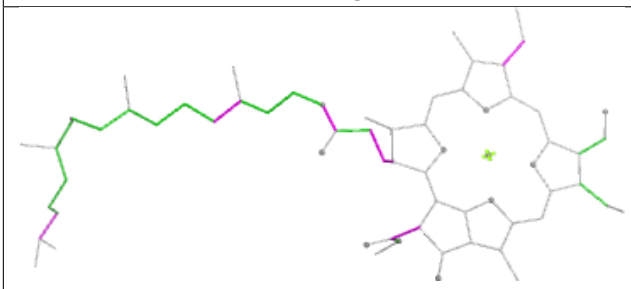


Bond angles



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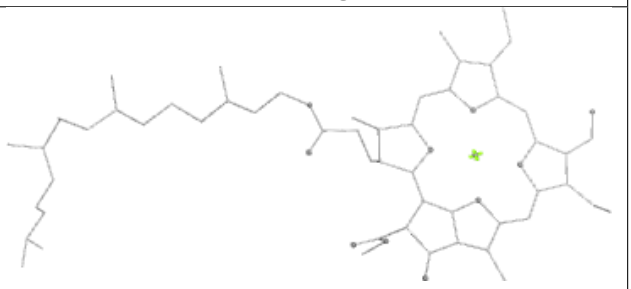
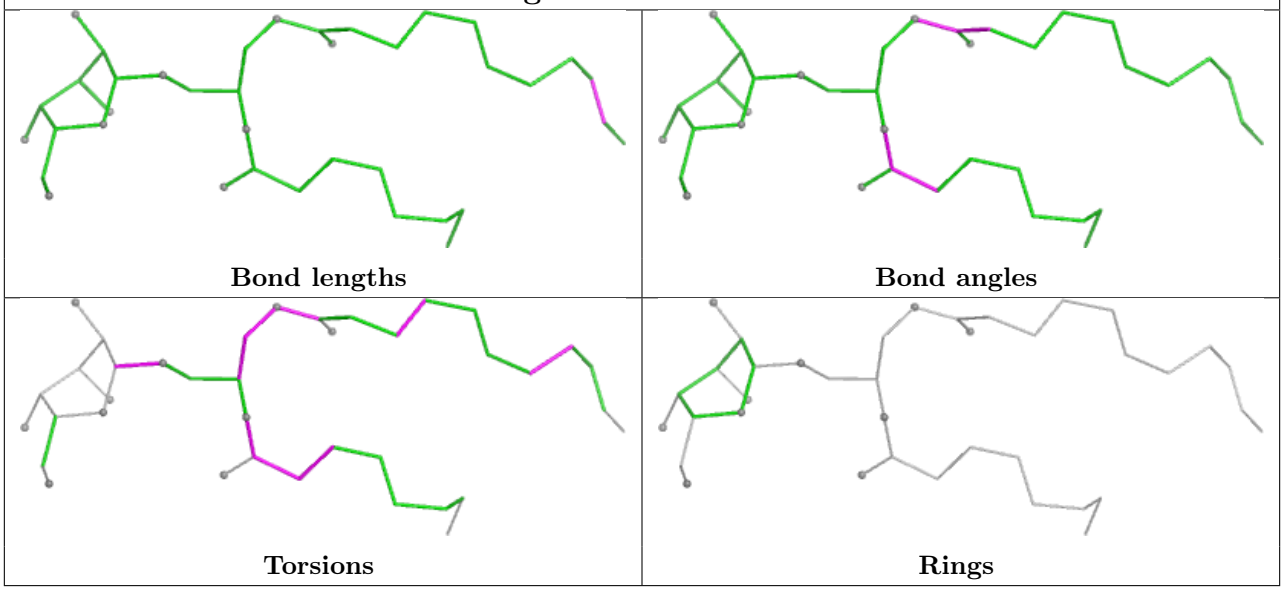
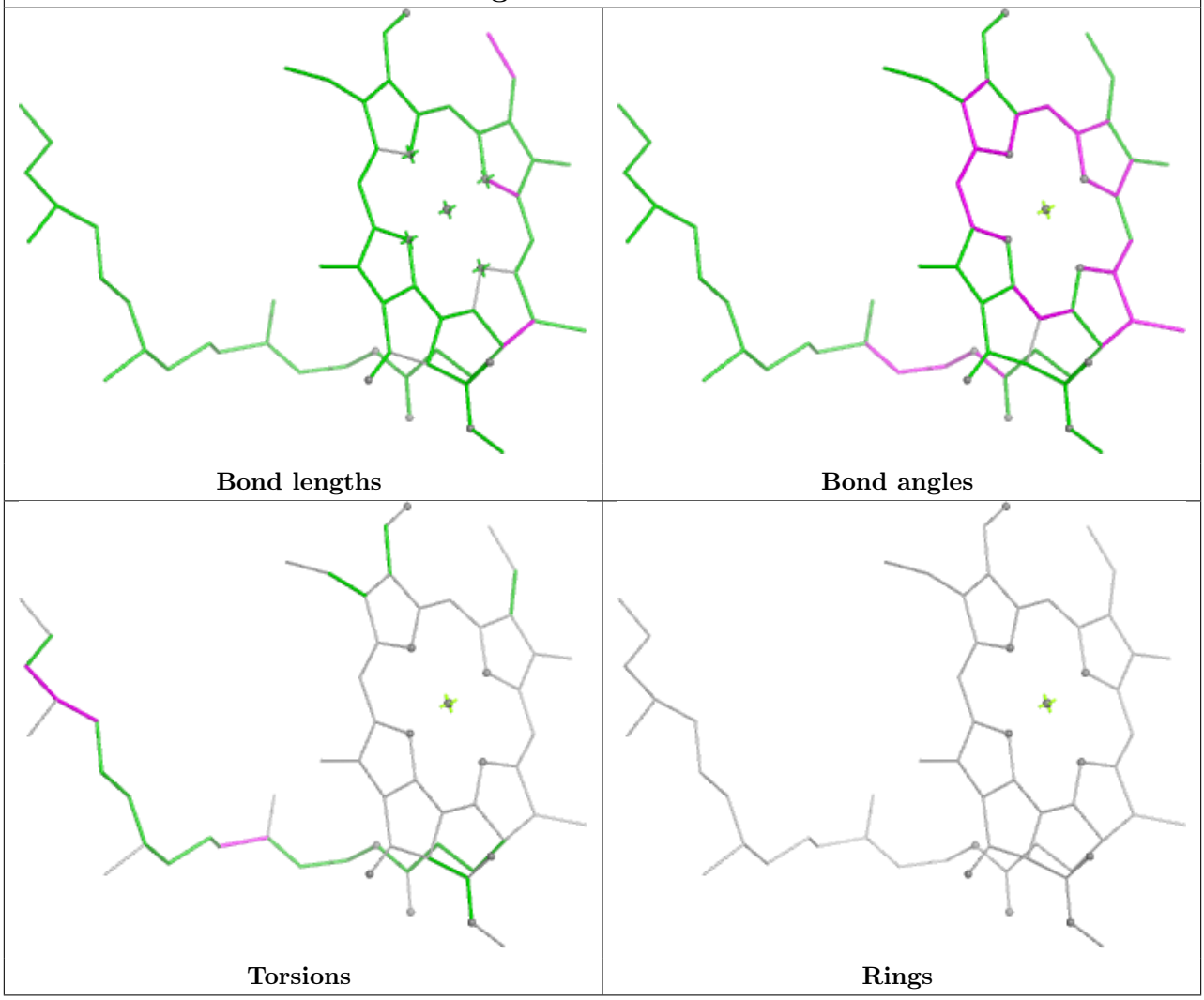


Rings

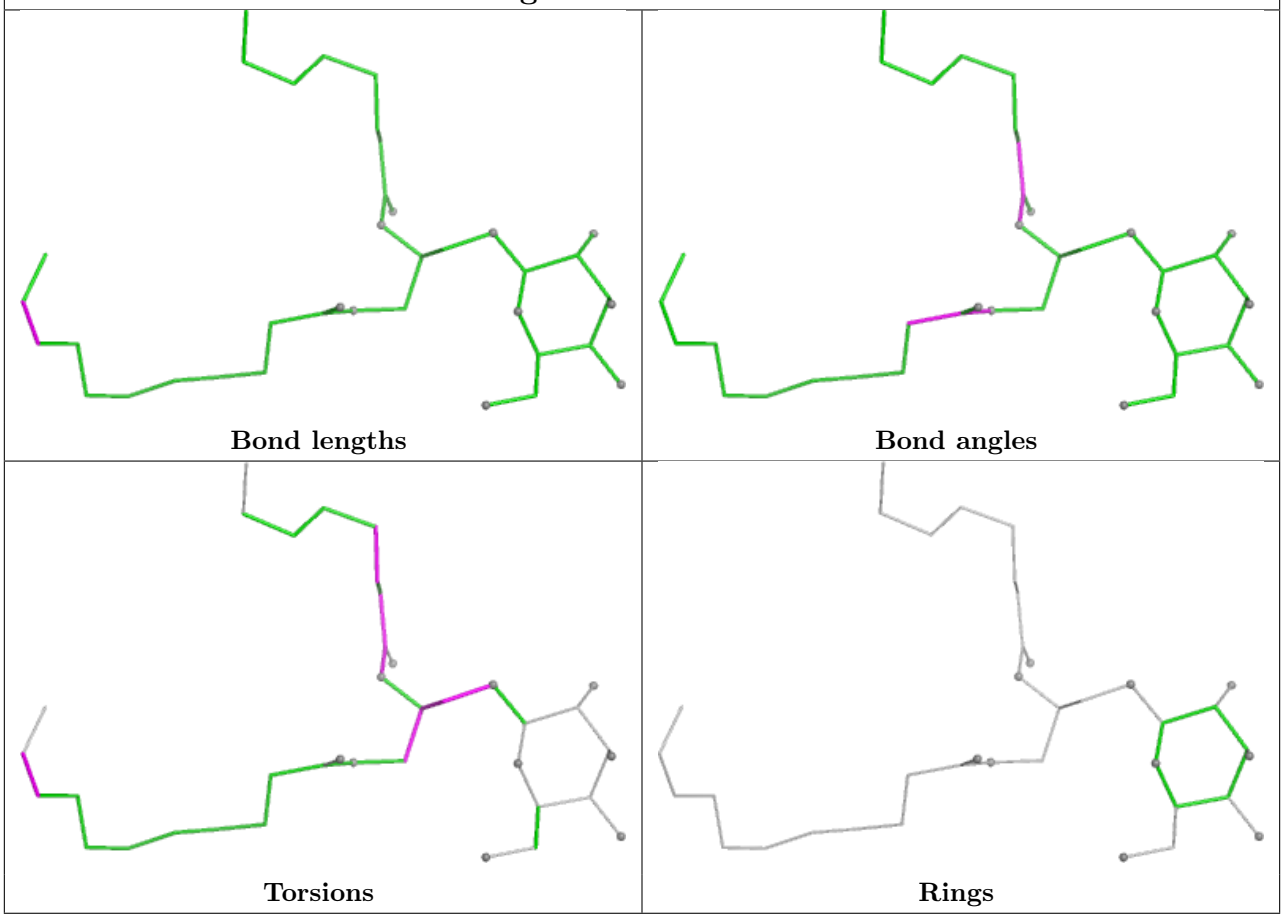
Ligand LMG b 629



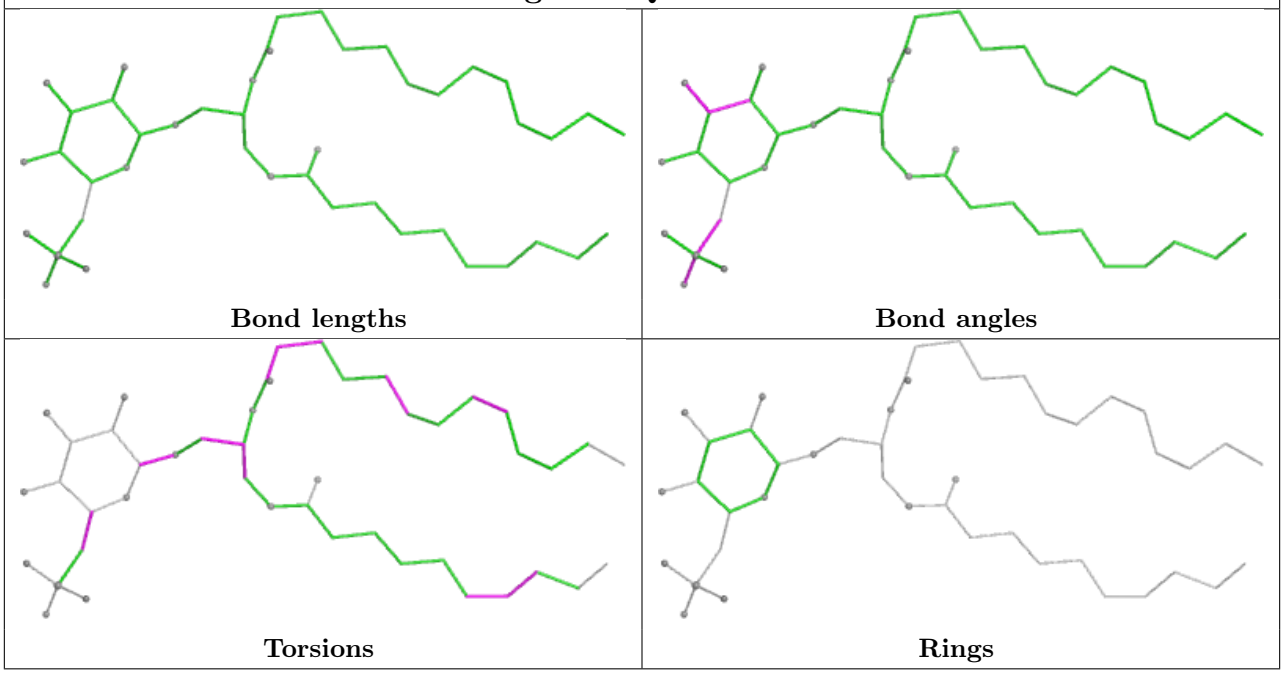
Ligand CHL G 608



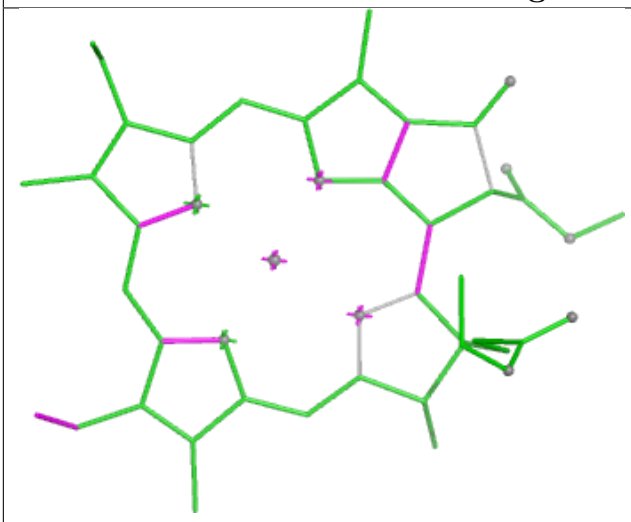
Ligand LMG X 203



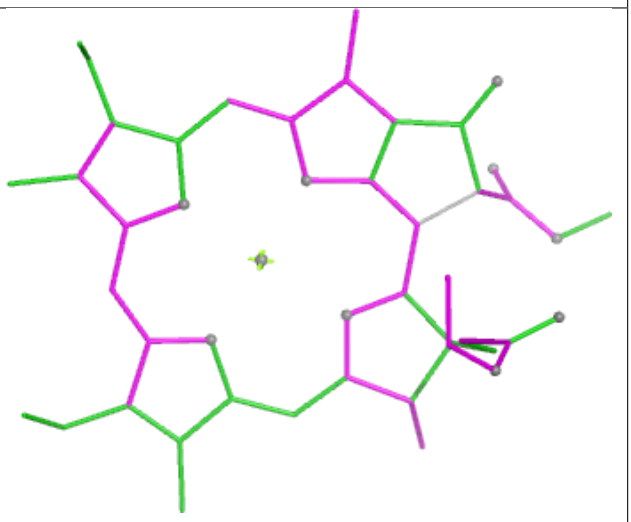
Ligand SQD A 413



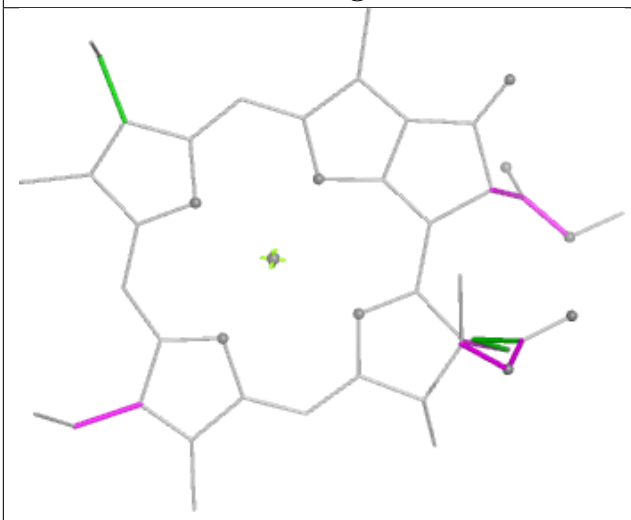
Ligand CLA 9 313



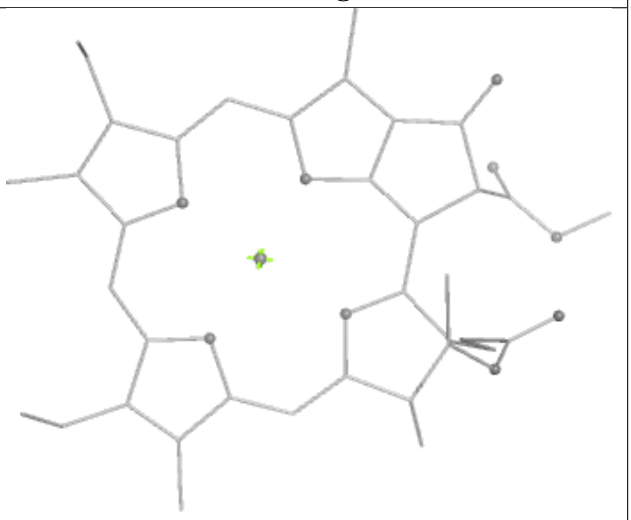
Bond lengths



Bond angles

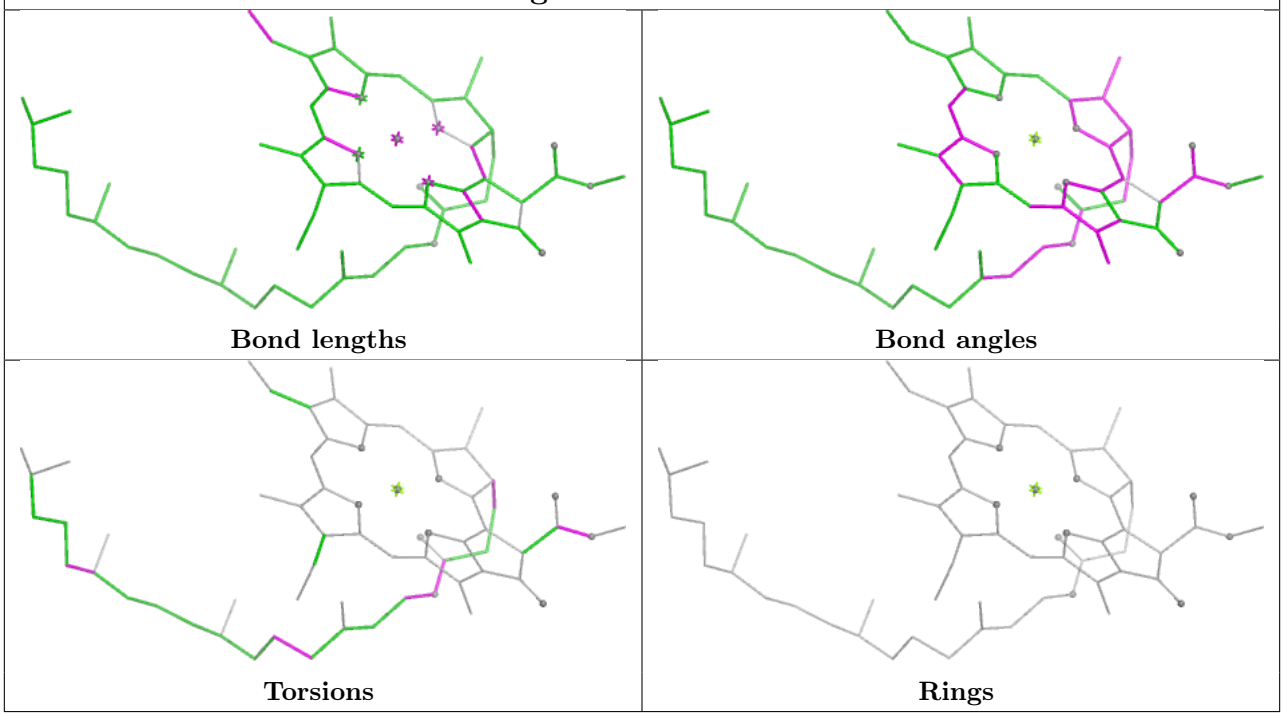


Torsions

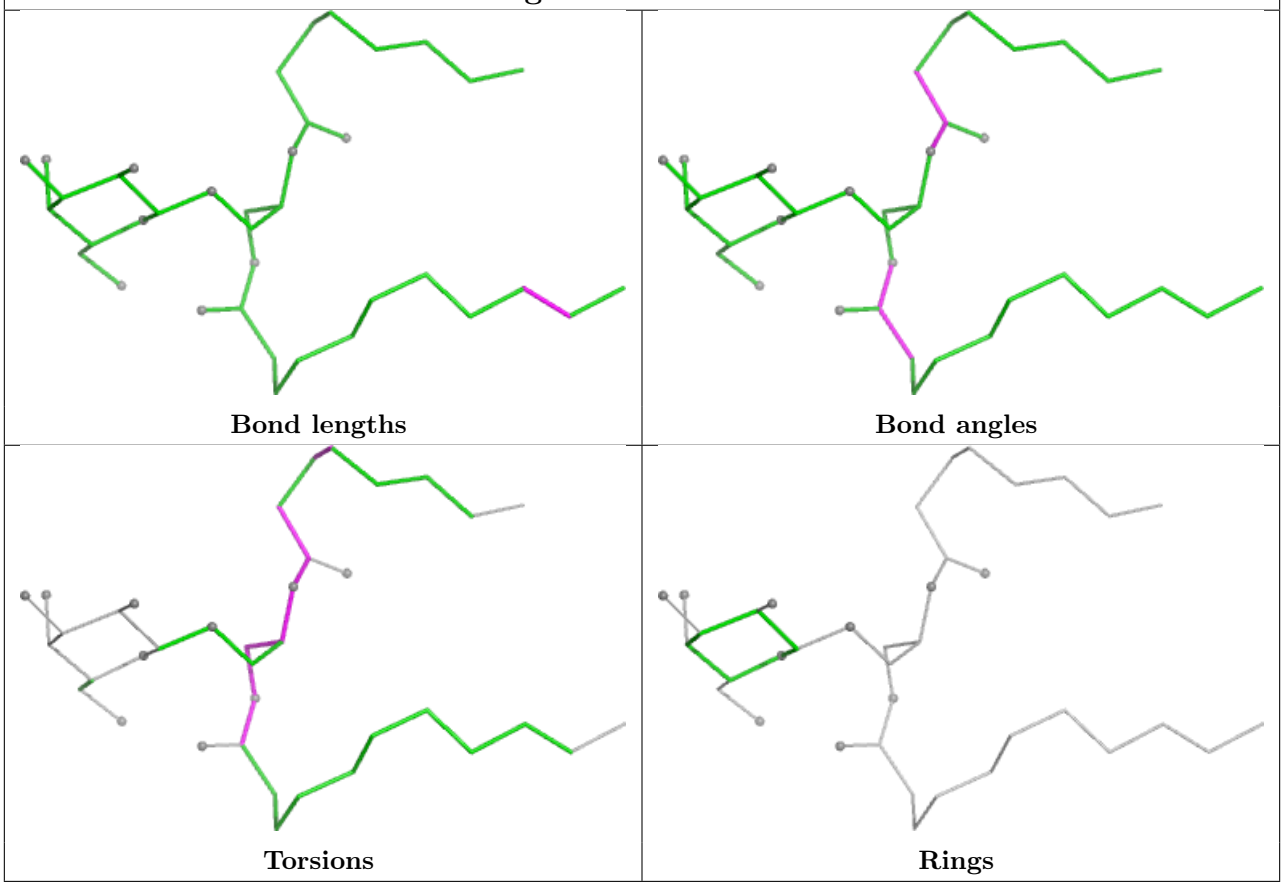


Rings

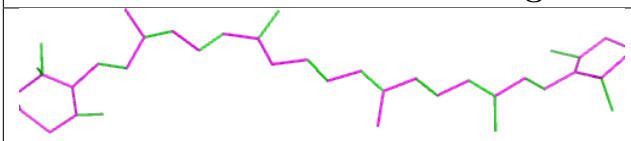
Ligand CLA c 613



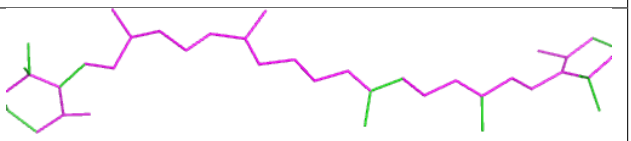
Ligand LMG 3 321



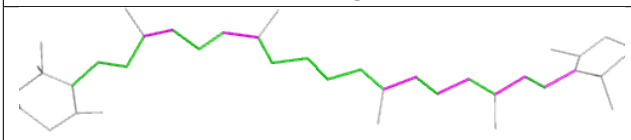
Ligand BCR d 406



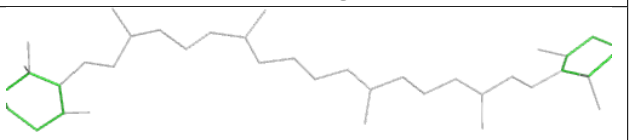
Bond lengths



Bond angles

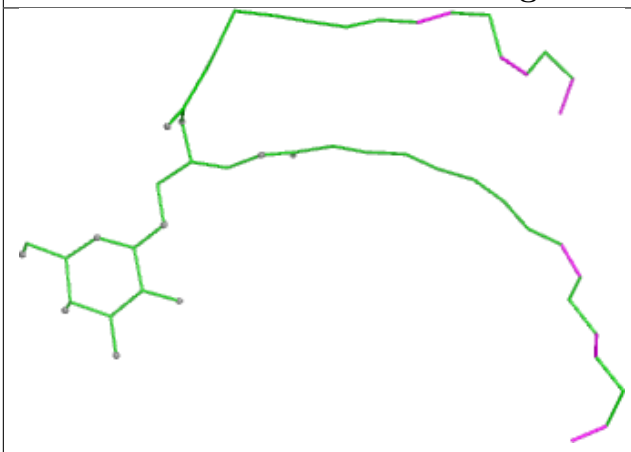


Torsions

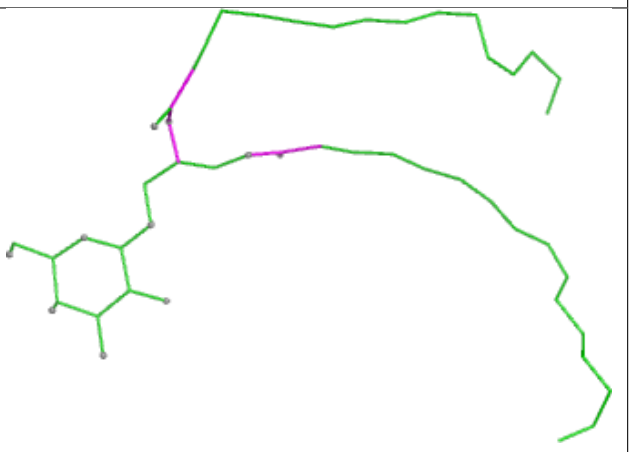


Rings

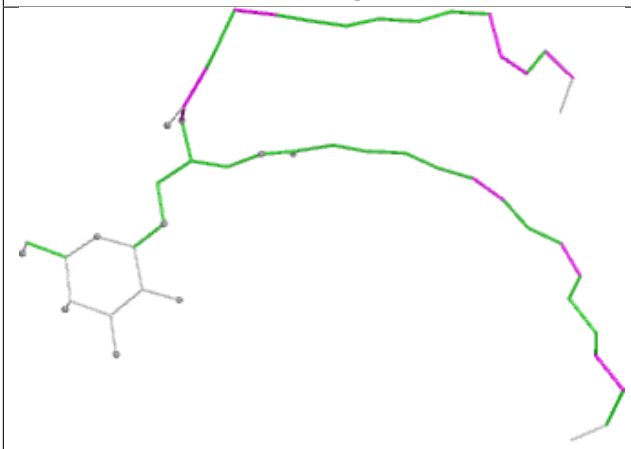
Ligand LMG C 619



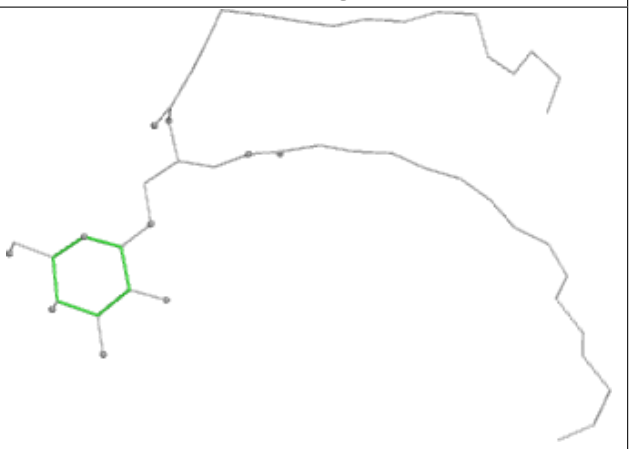
Bond lengths



Bond angles

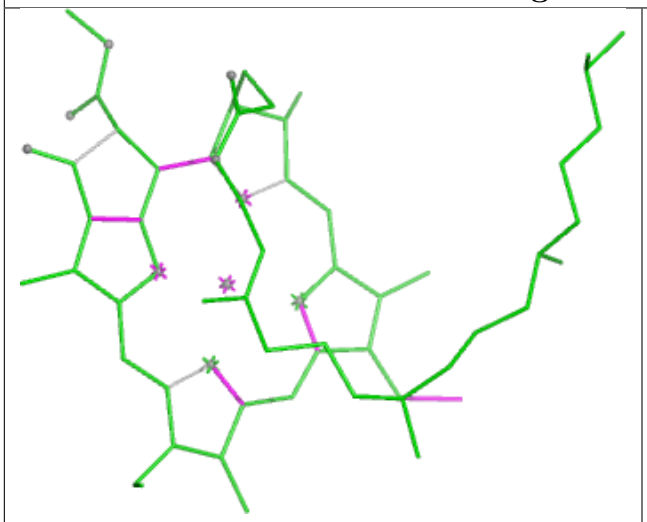


Torsions

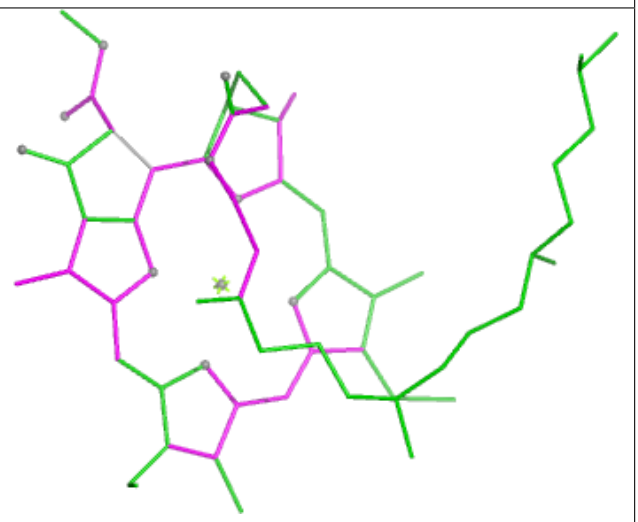


Rings

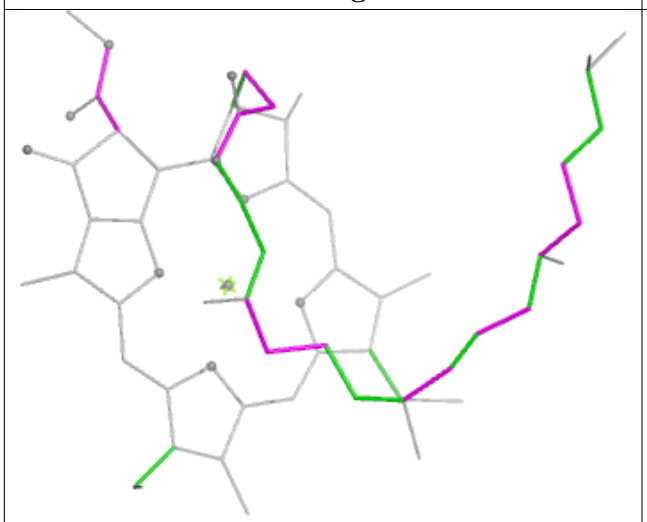
Ligand CLA s 314



Bond lengths



Bond angles



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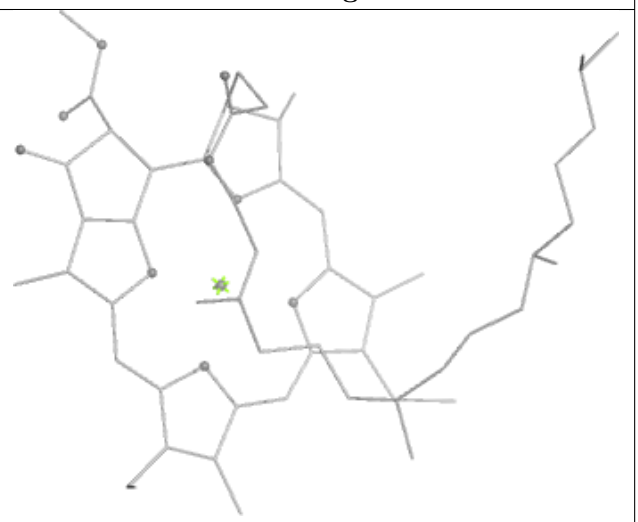
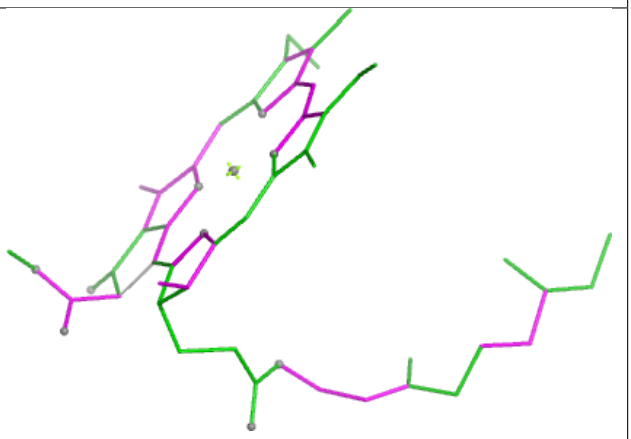
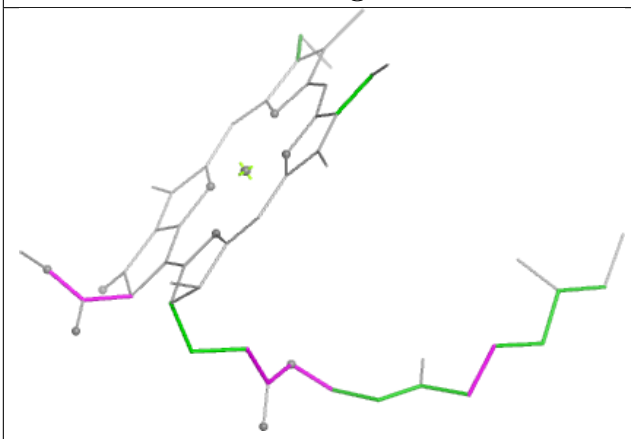
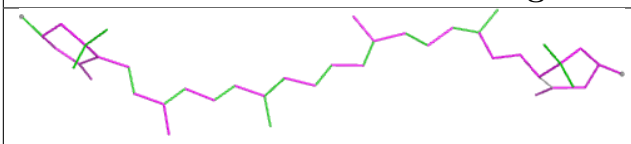
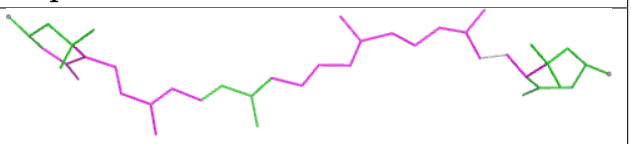
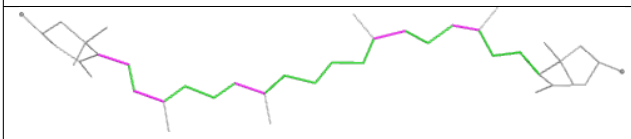
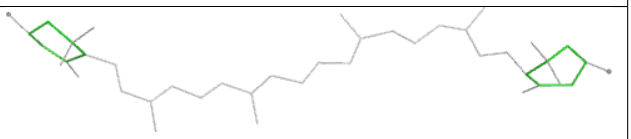
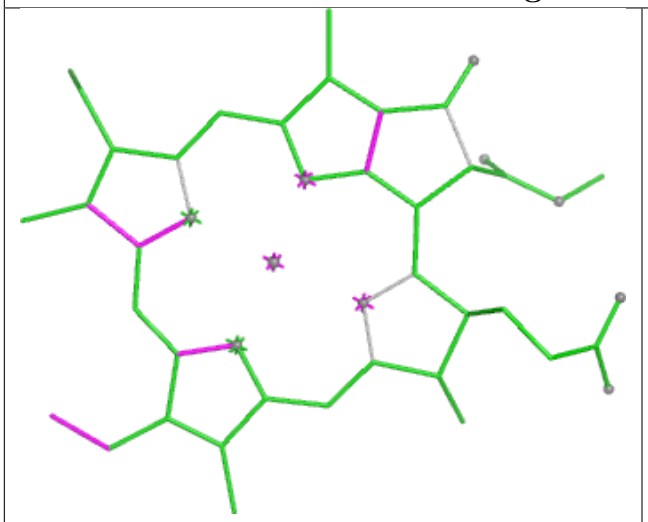


Rings

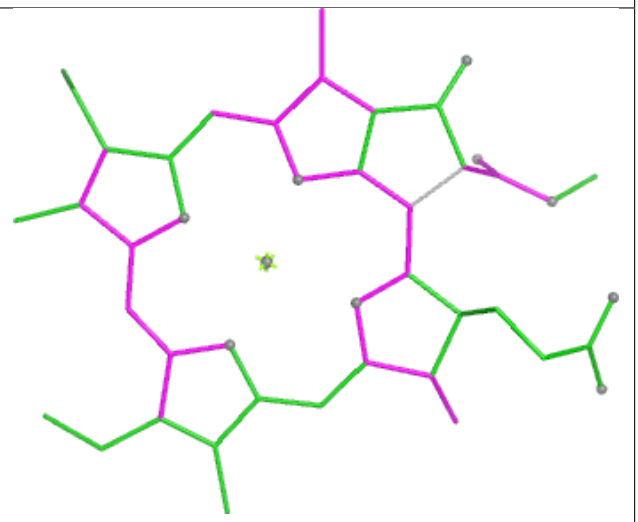
Ligand CLA C 604	
Bond lengths	 Bond angles
 Torsions	Rings

Ligand LUT p 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

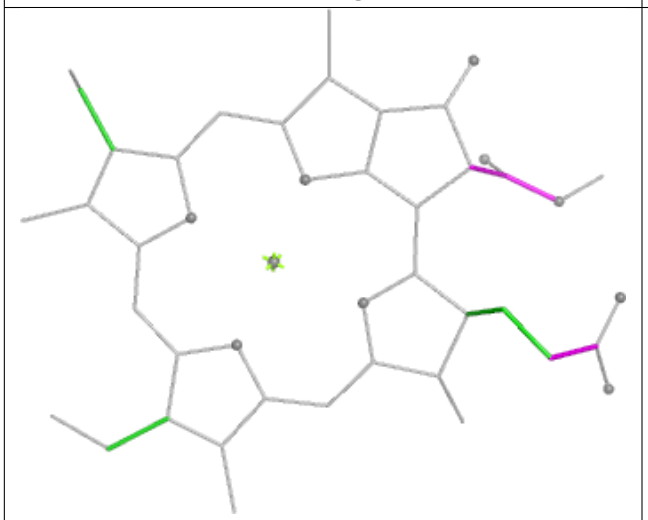
Ligand CLA N 312



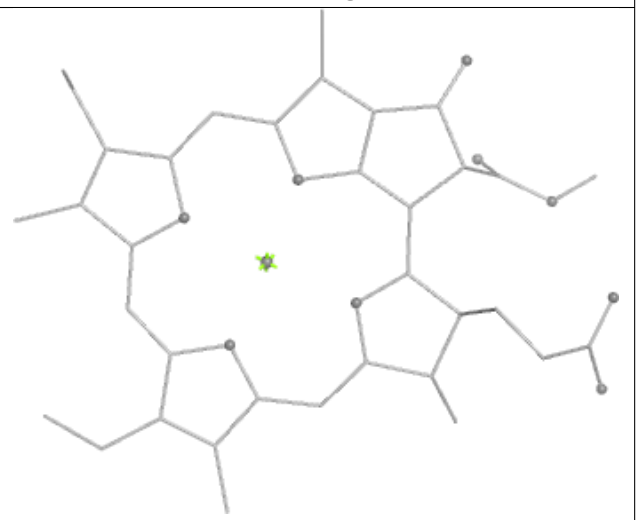
Bond lengths



Bond angles

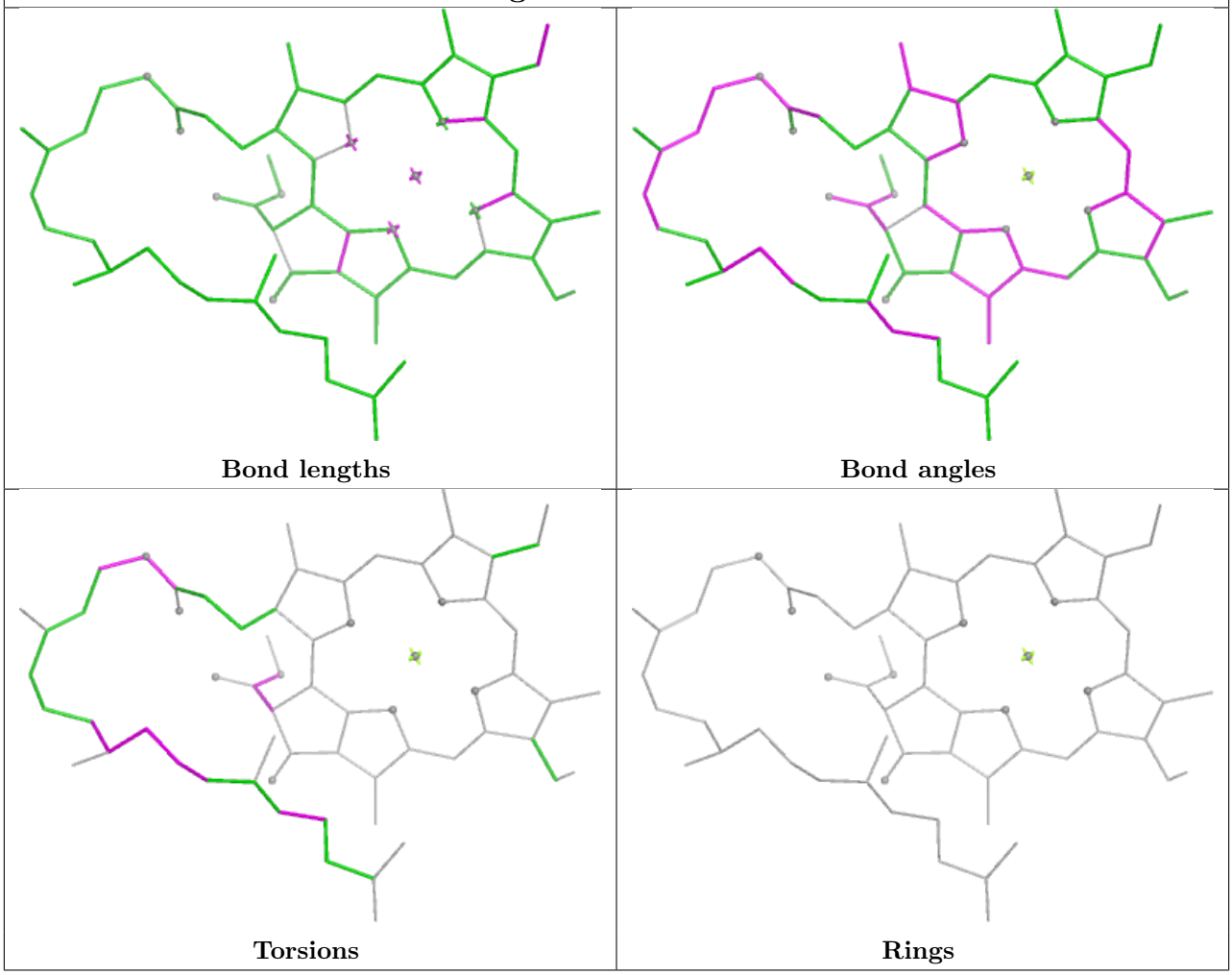


Torsions

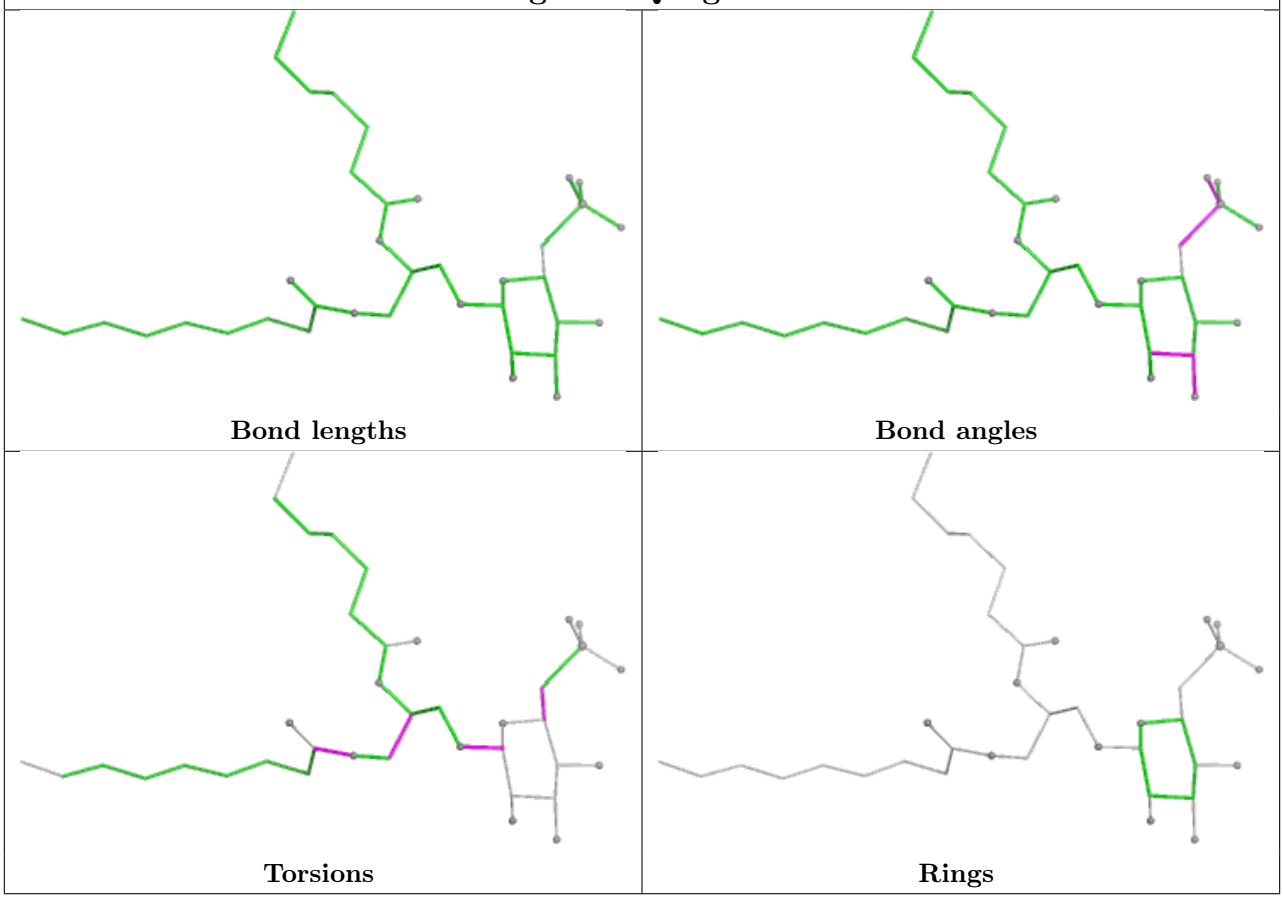


Rings

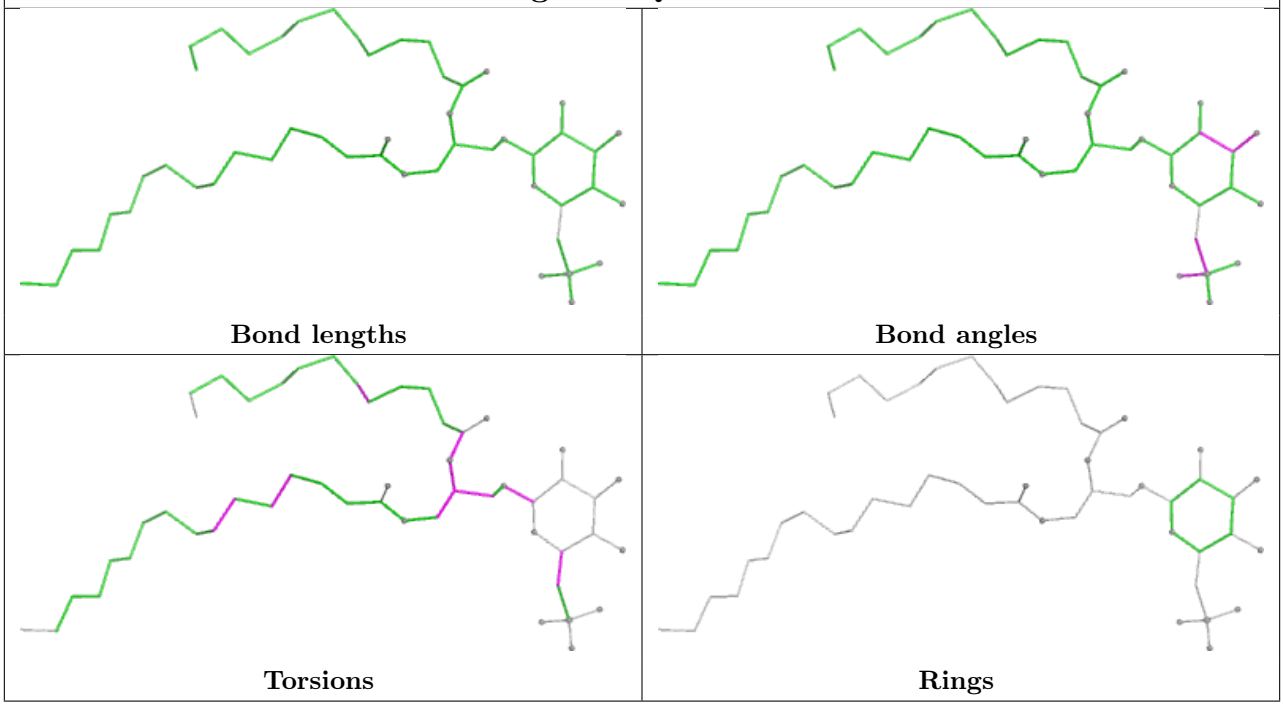
Ligand CLA c 609



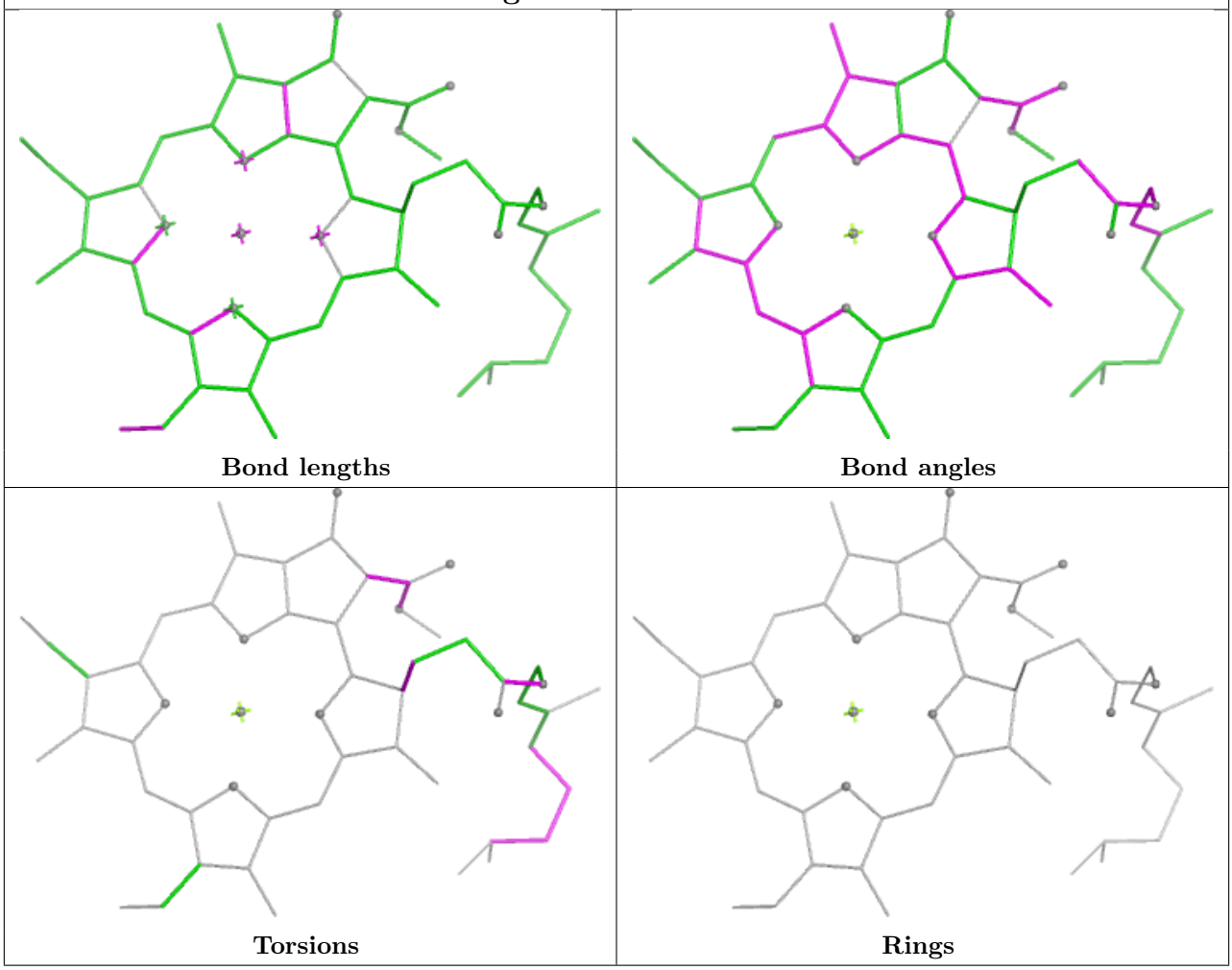
Ligand SQD g 301



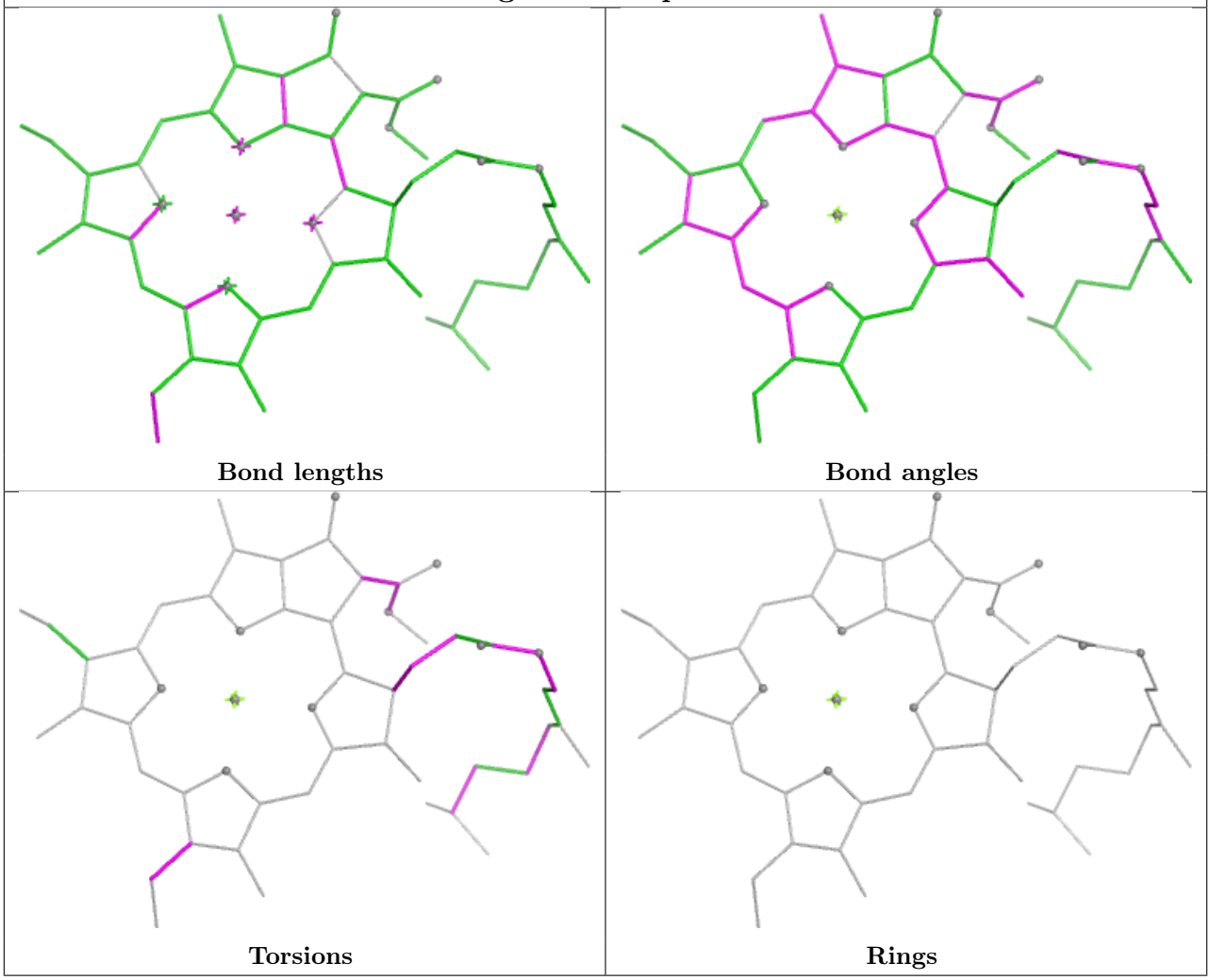
Ligand SQD r 322



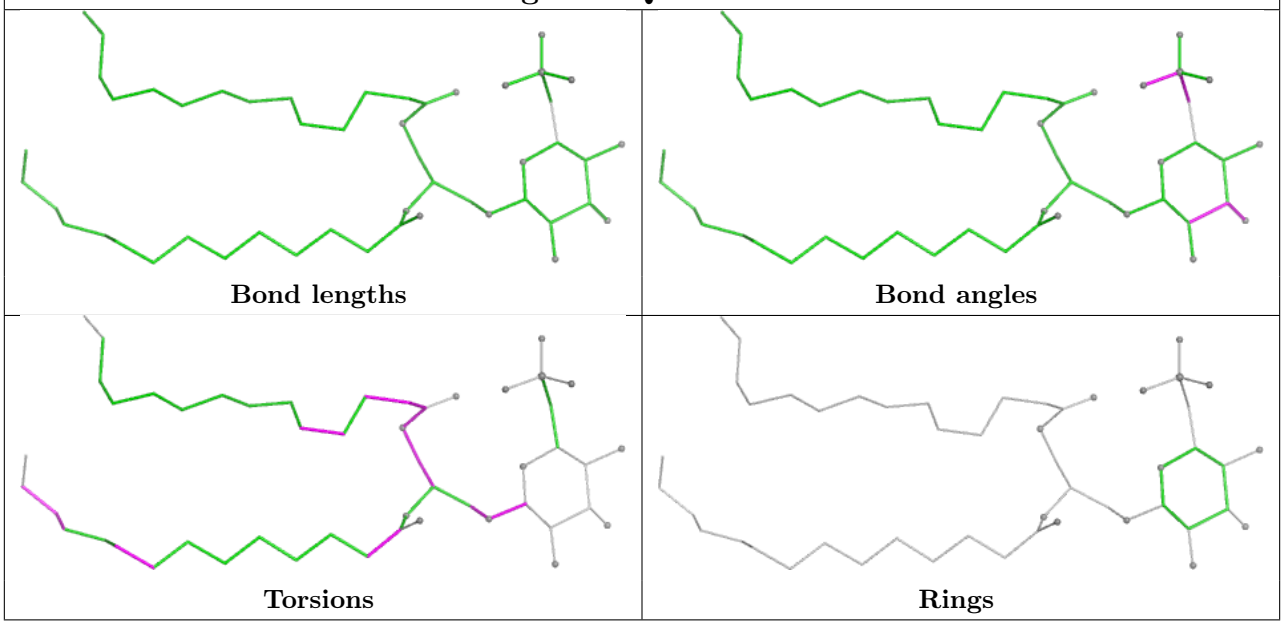
Ligand CLA G 603



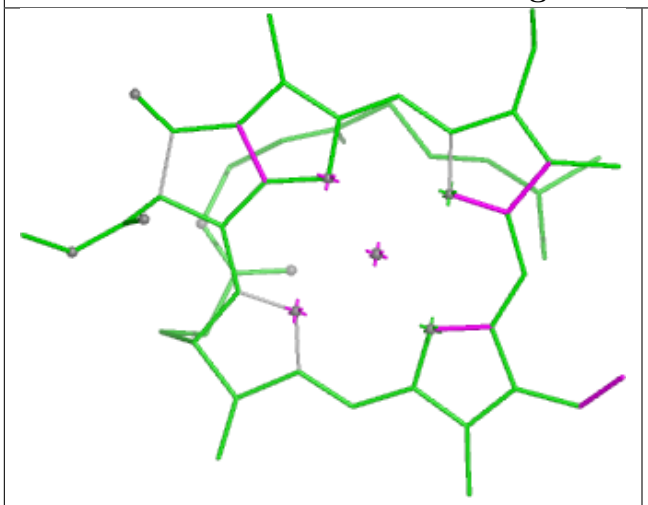
Ligand CLA p 603



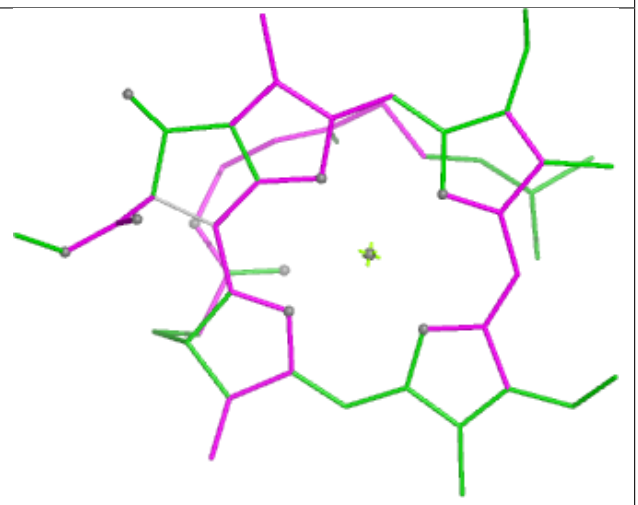
Ligand SQD M 102



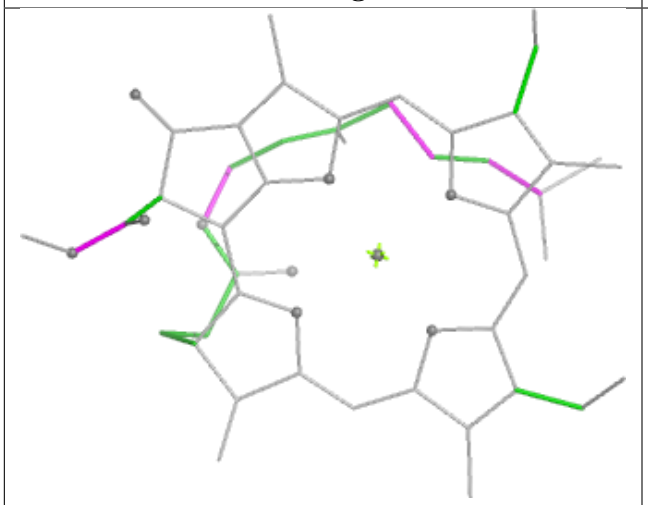
Ligand CLA 3 314



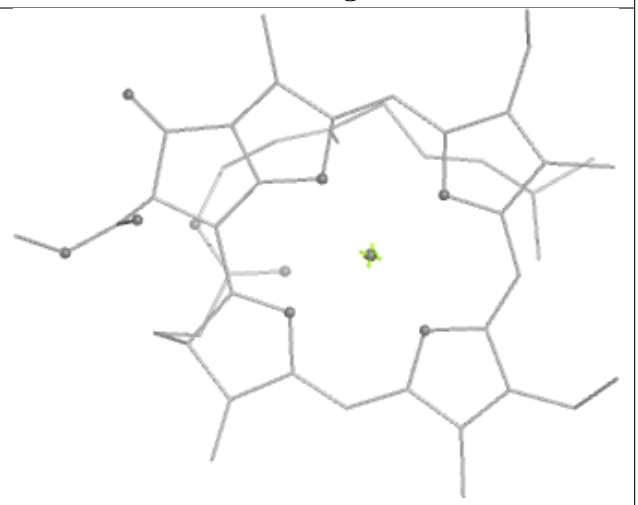
Bond lengths



Bond angles

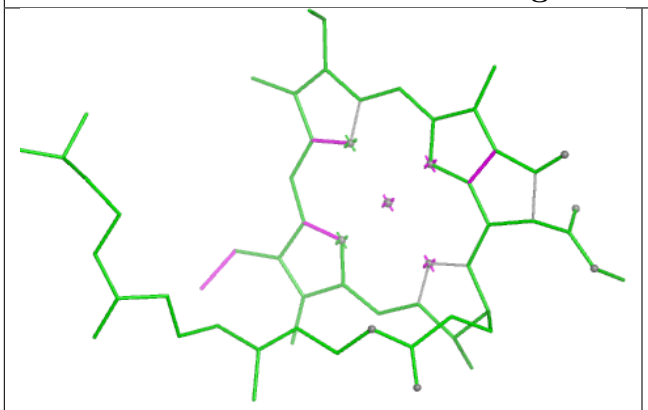


Torsions



Rings

Ligand CLA r 304



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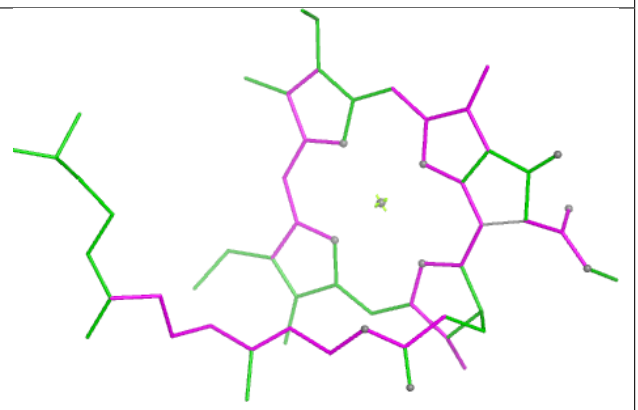
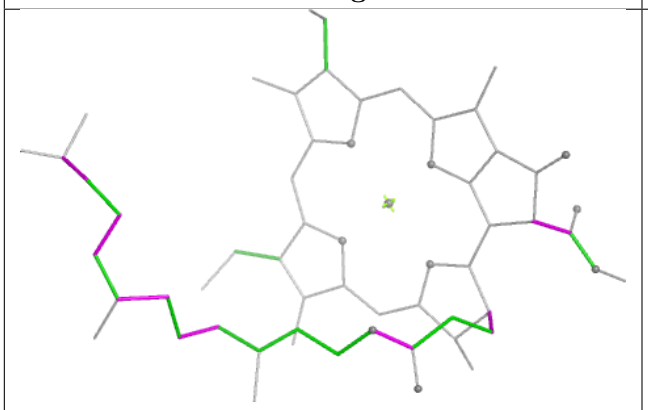


Bond angles



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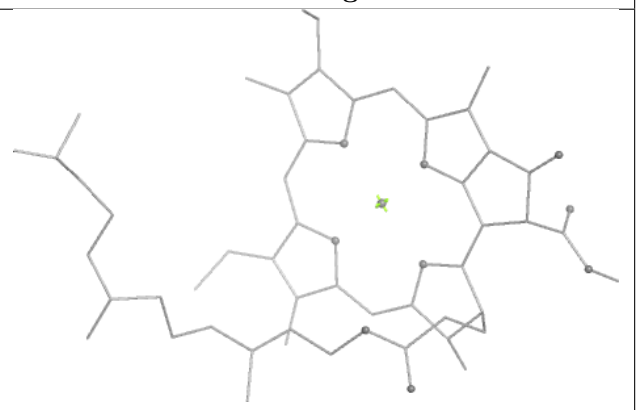
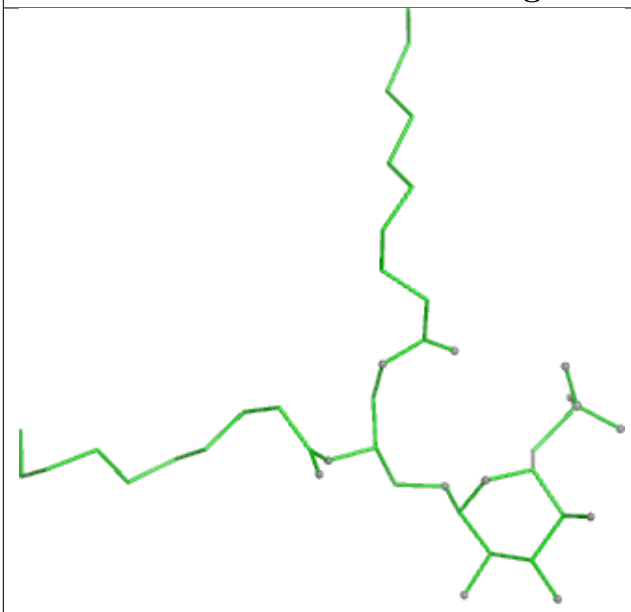
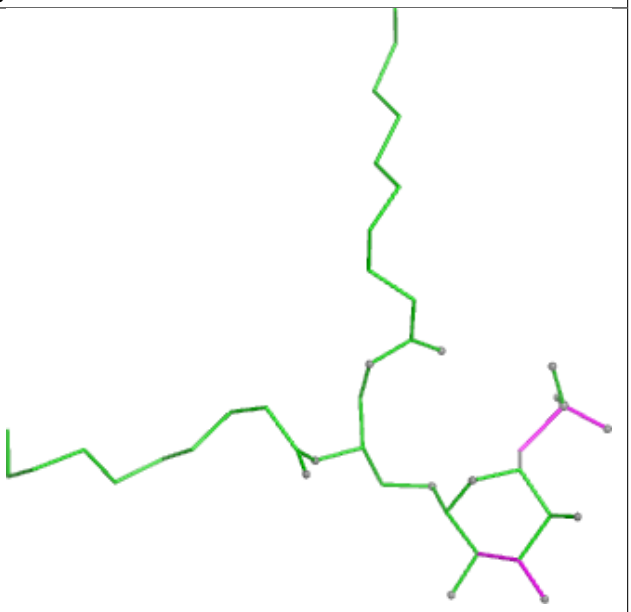


Rings

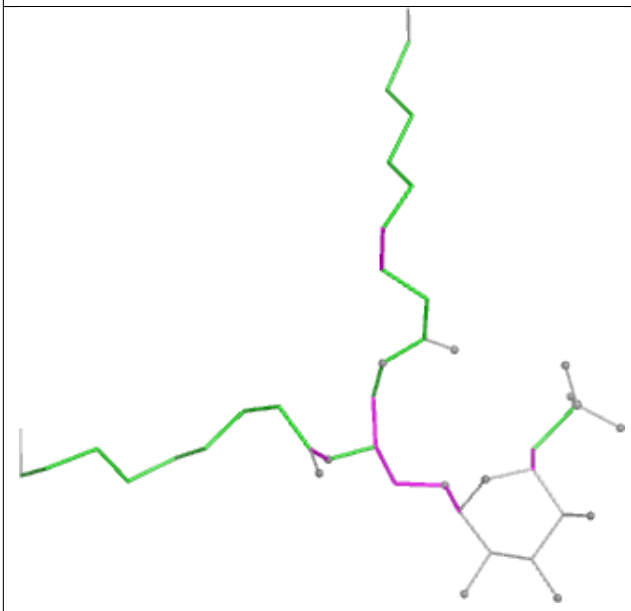
Ligand SQD G 617



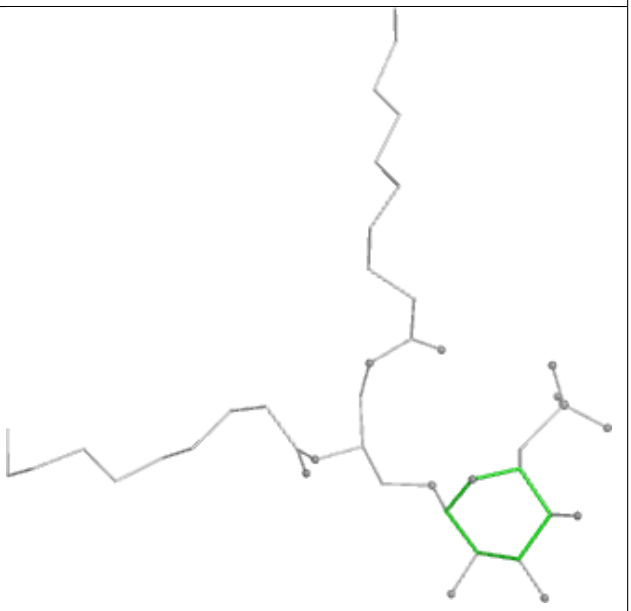
Bond lengths



Bond angles

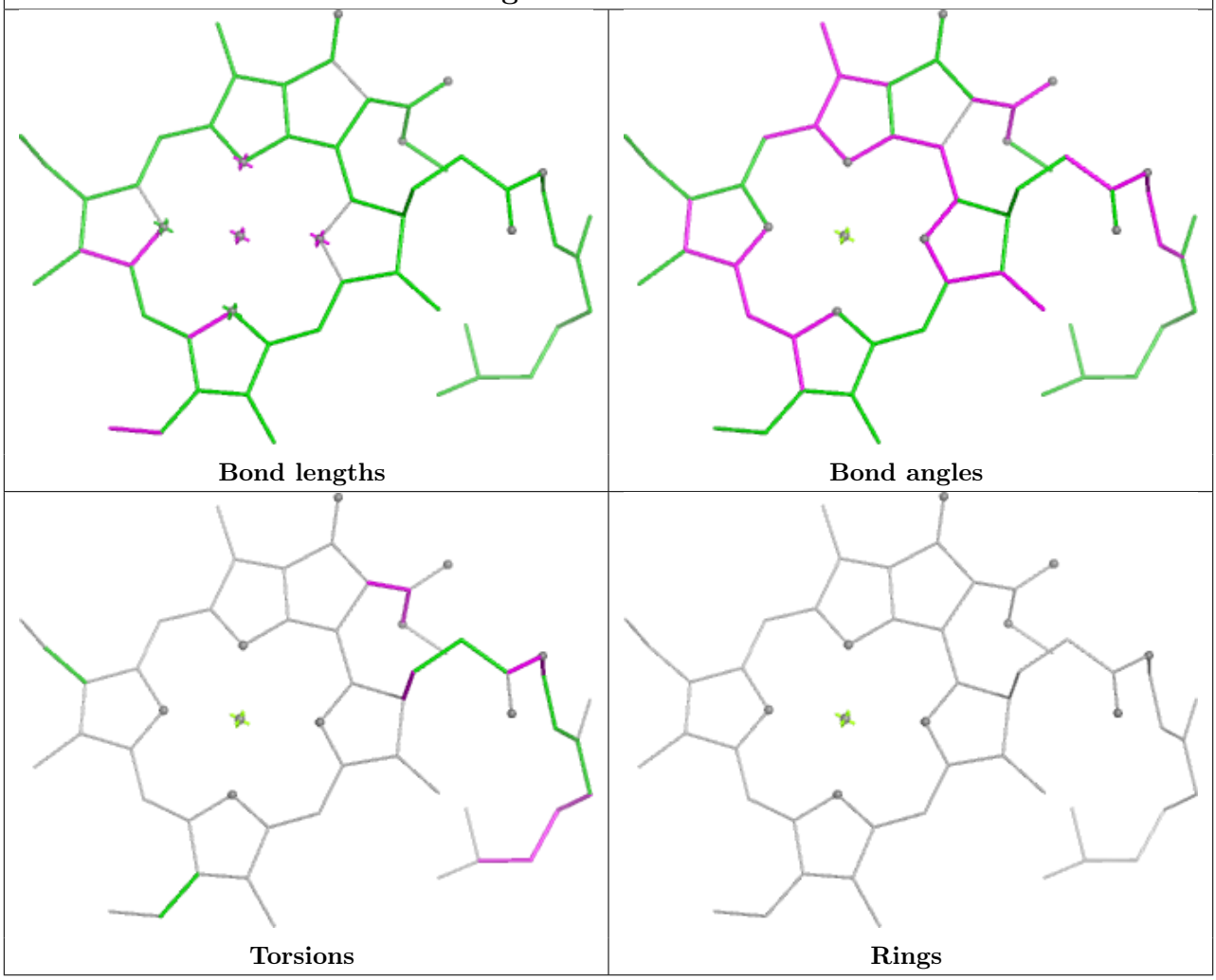


Torsions

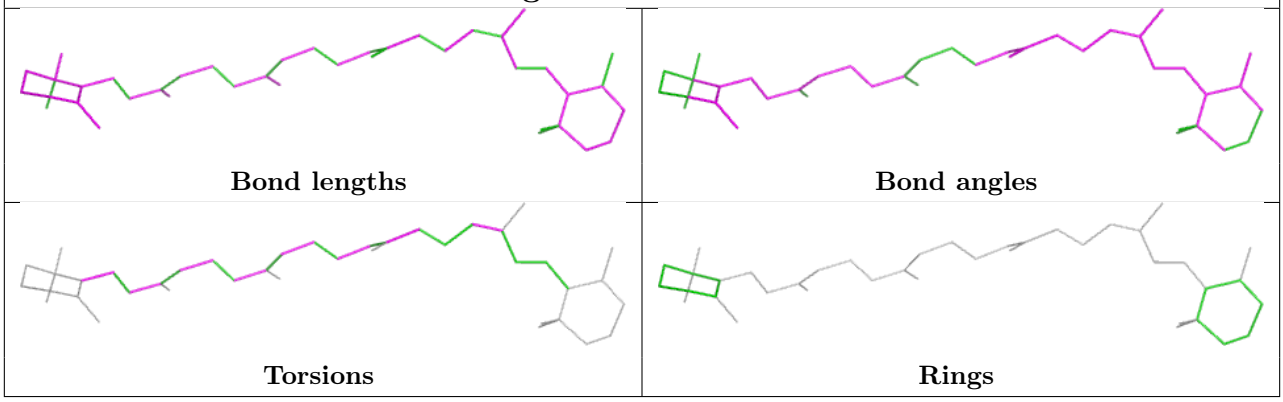


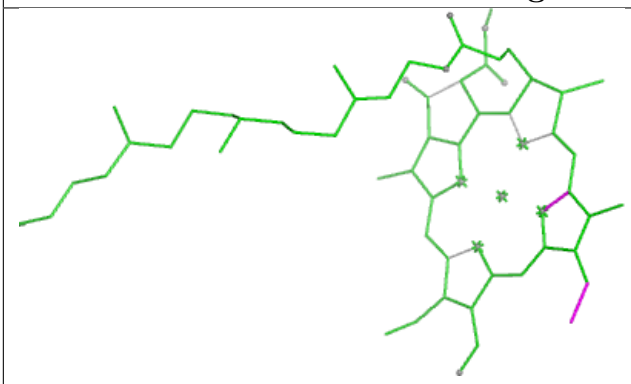
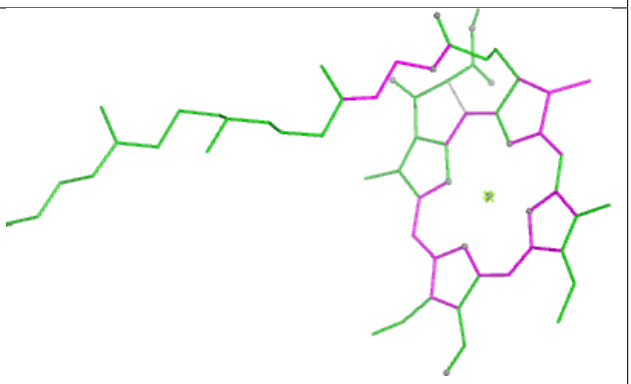
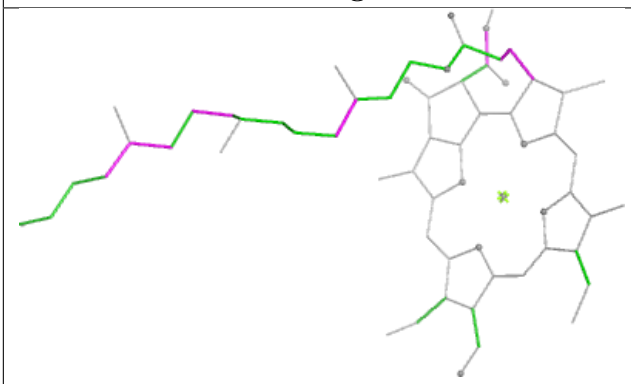
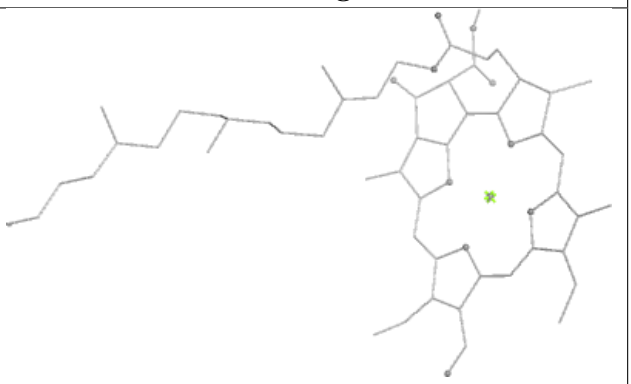
Rings

Ligand CLA 2 603

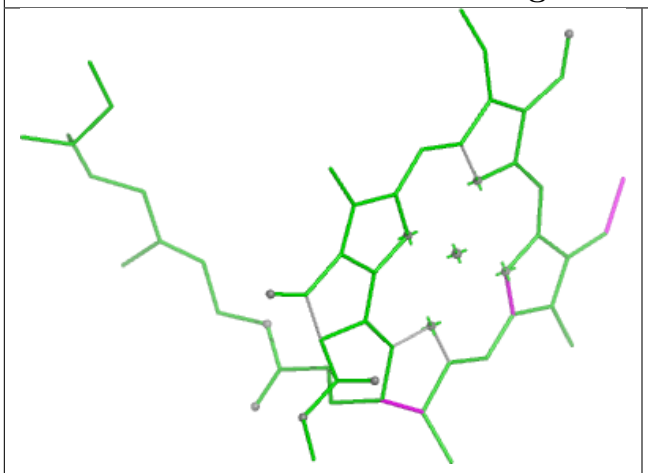


Ligand BCR D 405

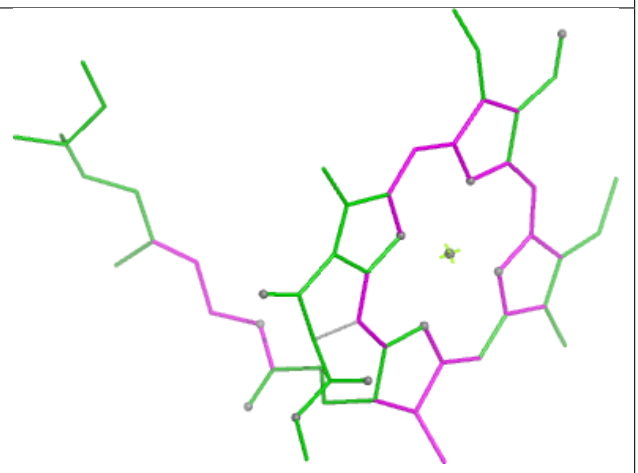


Ligand CHL 7 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

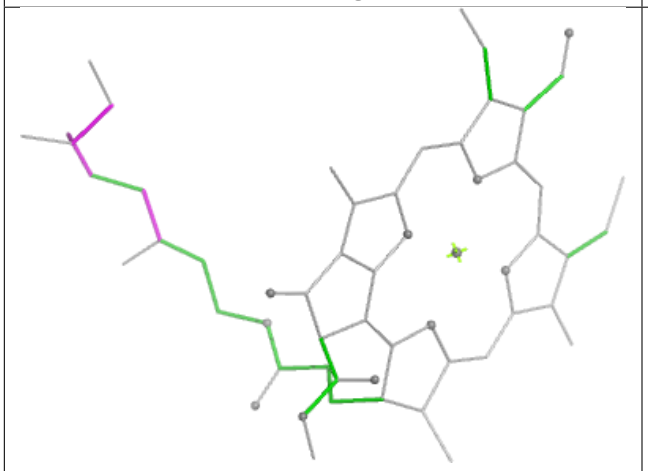
Ligand CHL 2 608



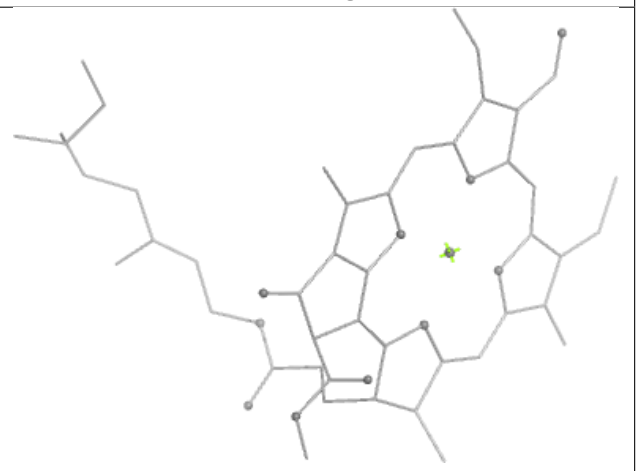
Bond lengths



Bond angles

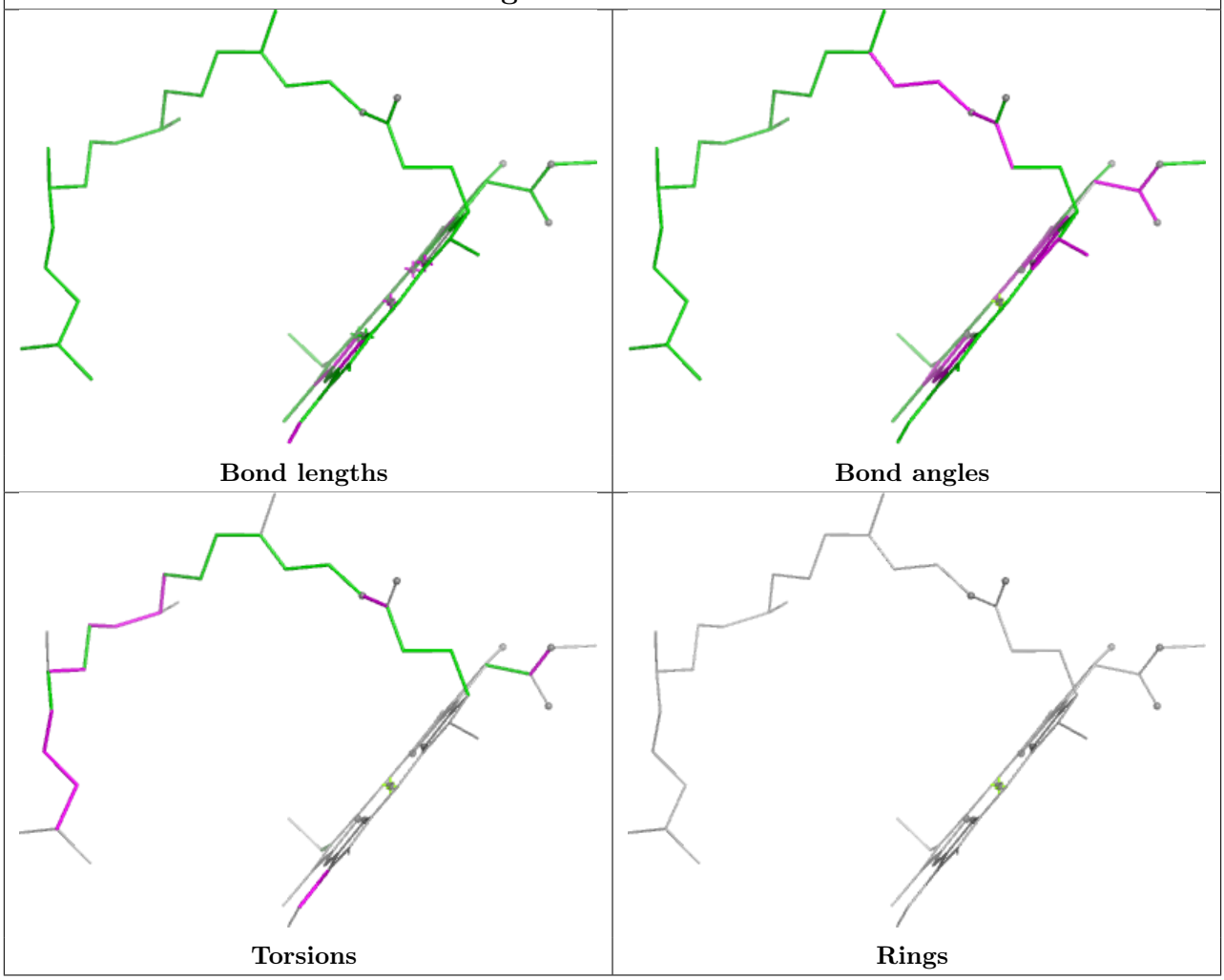


Torsions



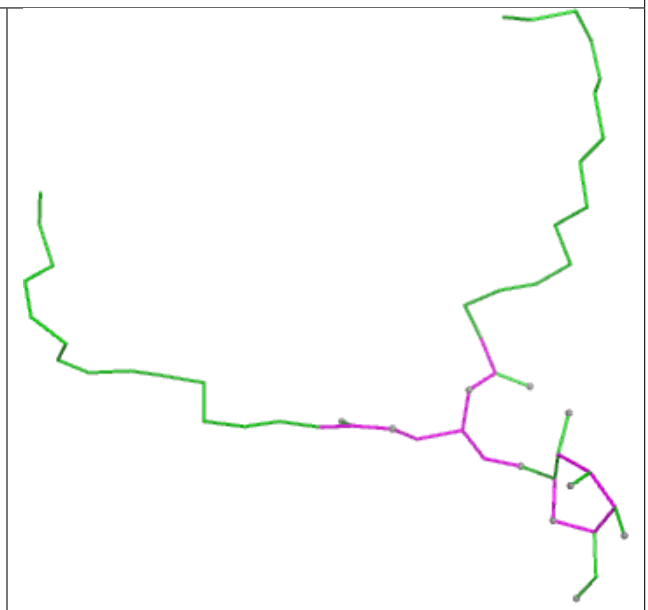
Rings

Ligand CLA B 611



Ligand LMG 9 301

Bond lengths

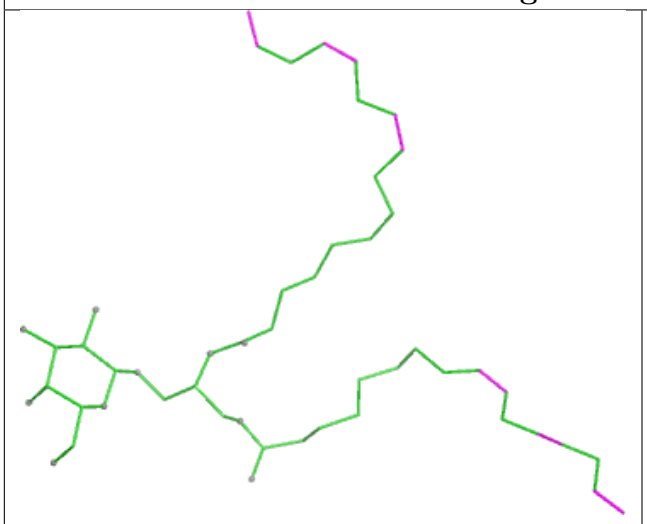


Bond angles

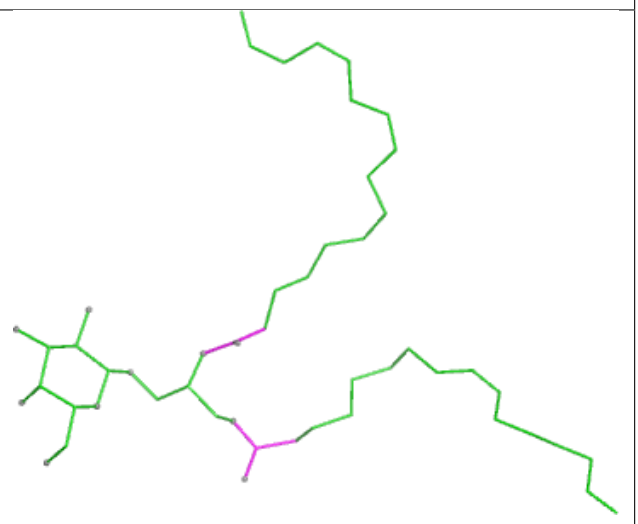
Torsions

Rings

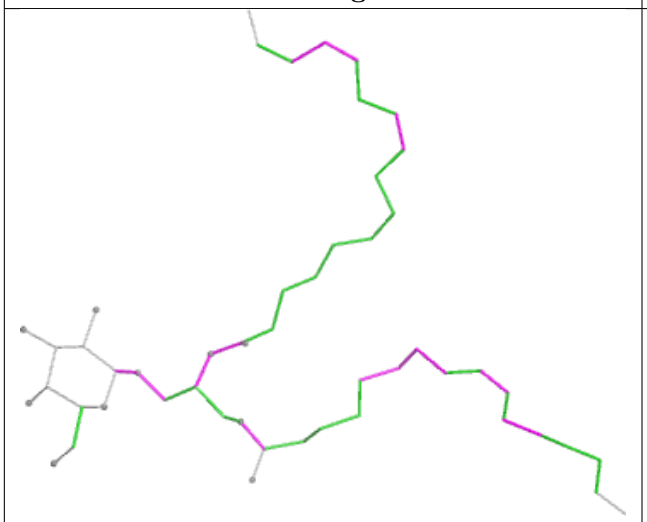
Ligand LMG D 411



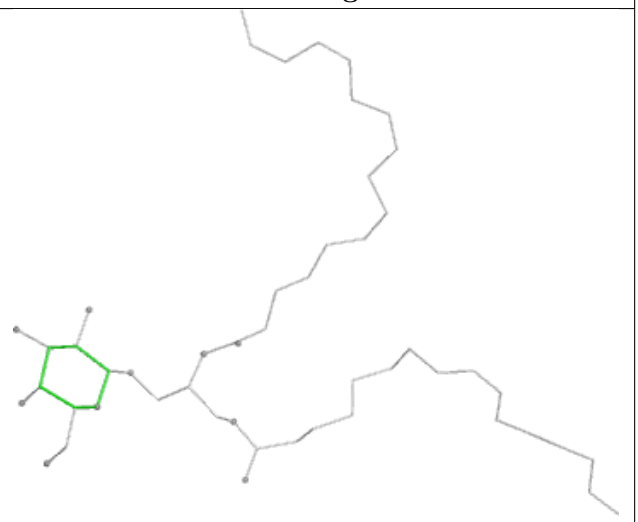
Bond lengths



Bond angles

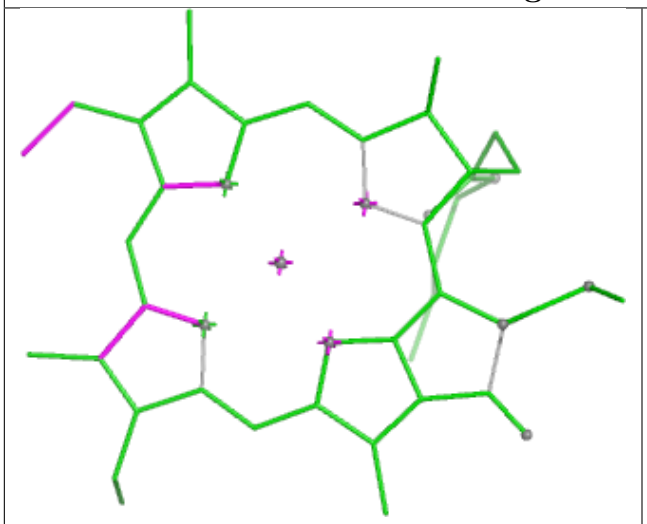


Torsions

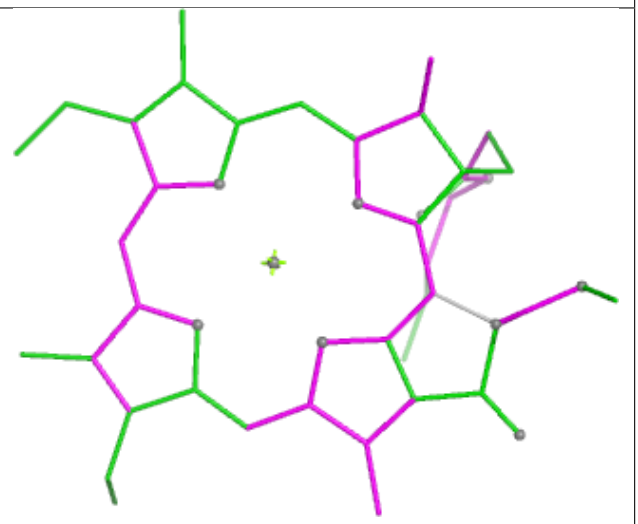


Rings

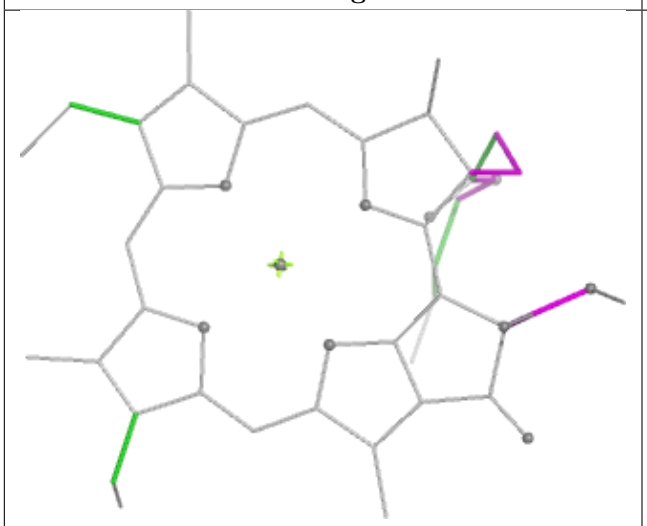
Ligand CLA N 311



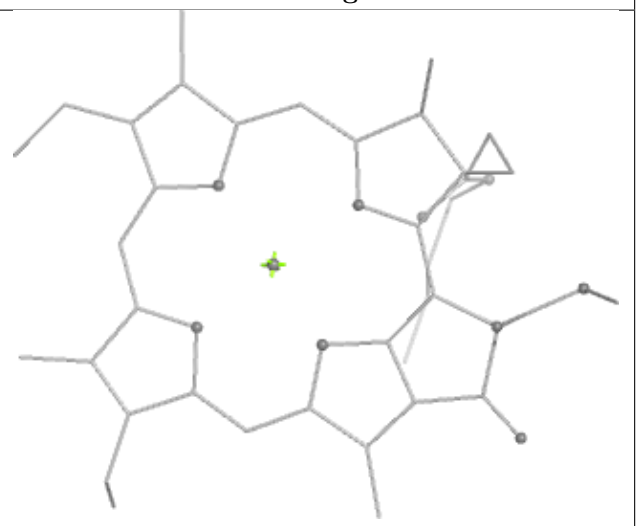
Bond lengths



Bond angles

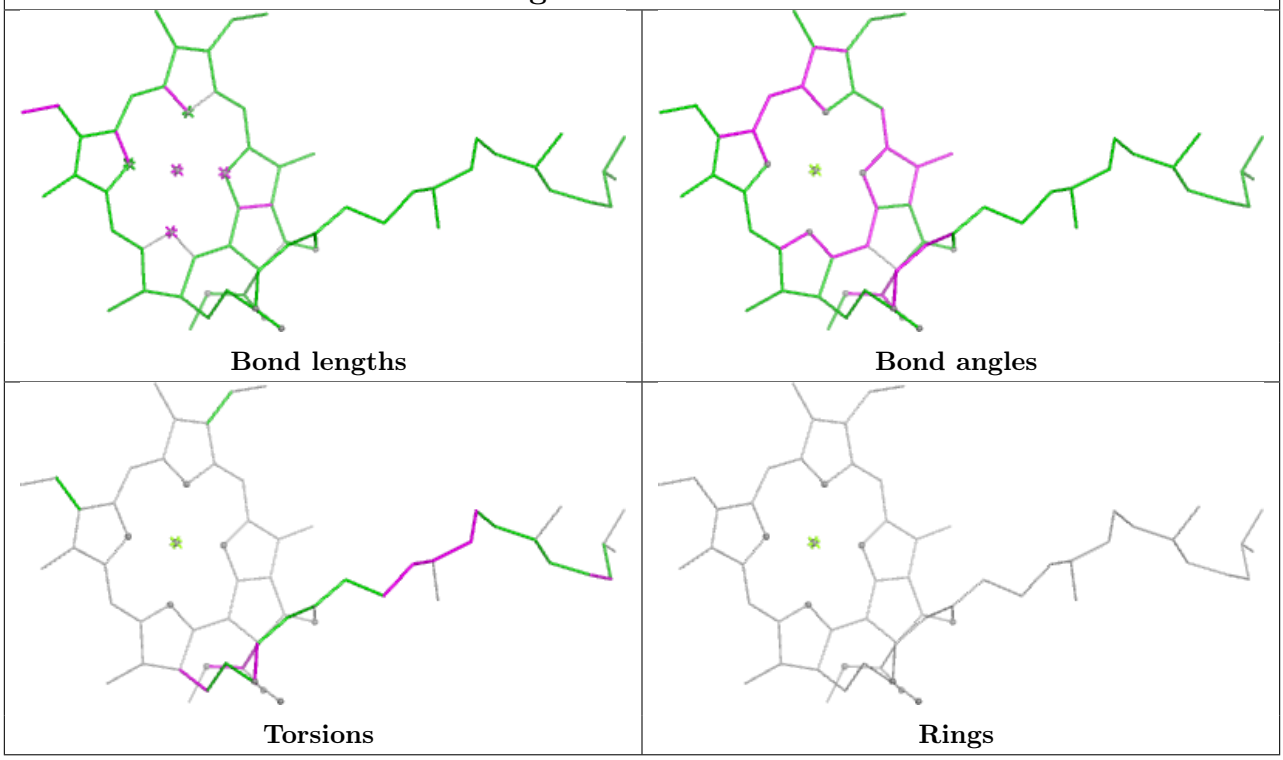


Torsions



Rings

Ligand CLA 7 305



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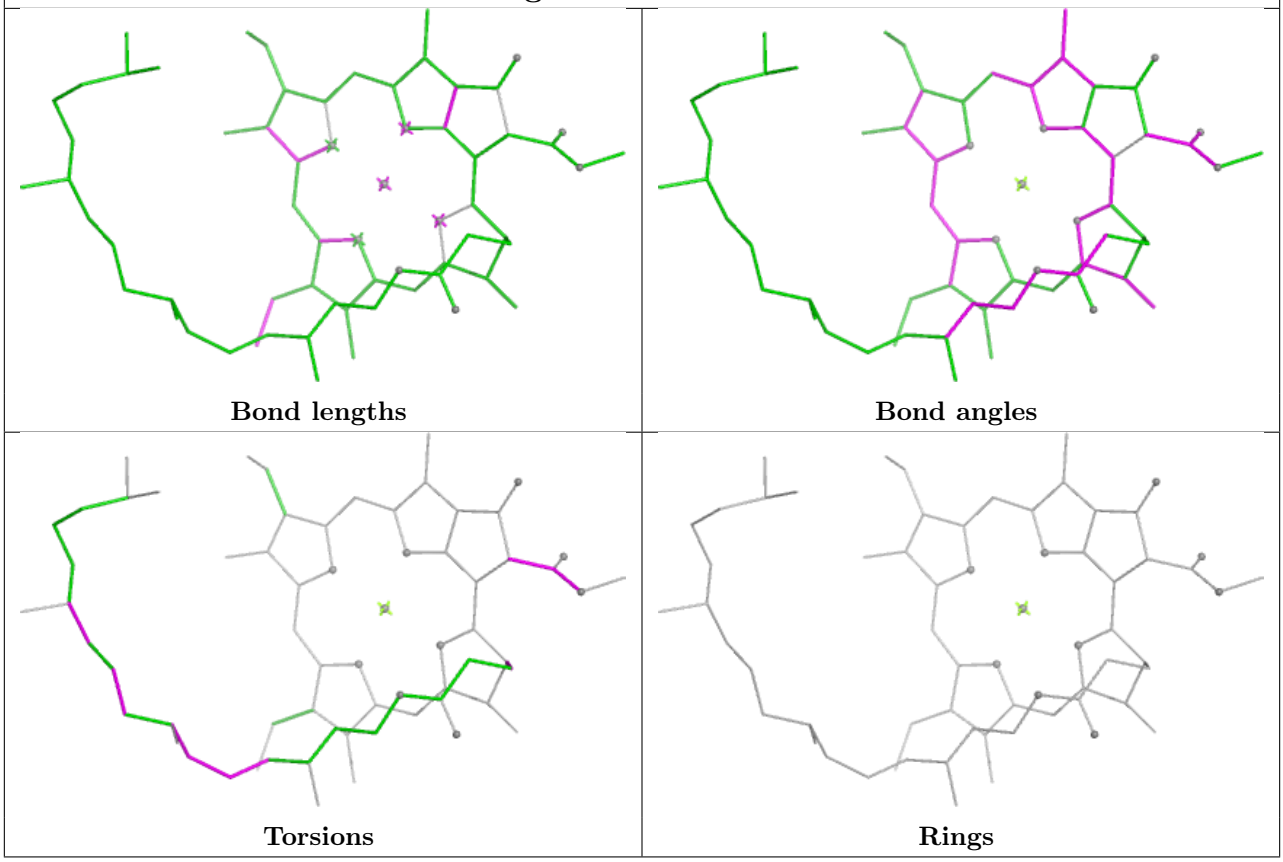
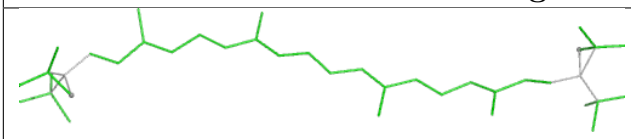


Ligand XAT r 318



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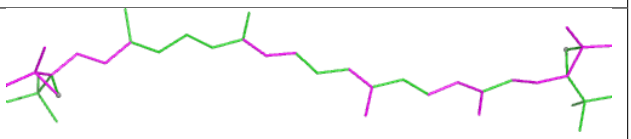

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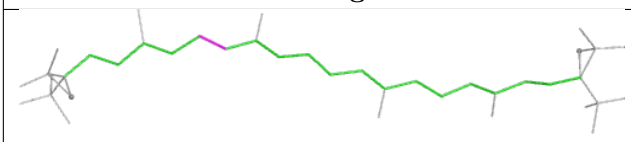

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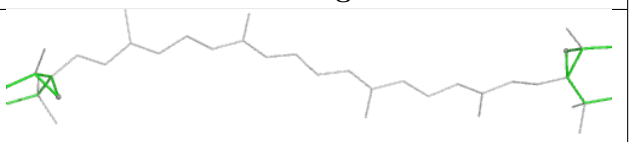
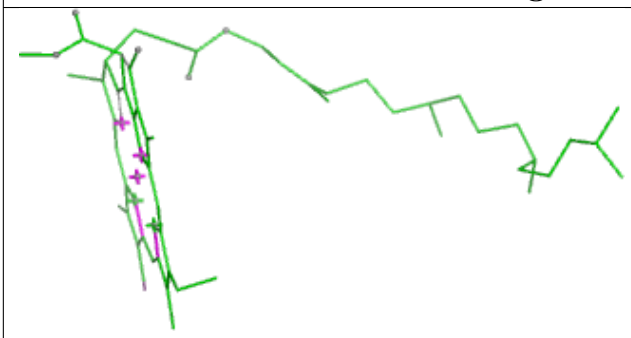


Rings

Ligand CLA n 305



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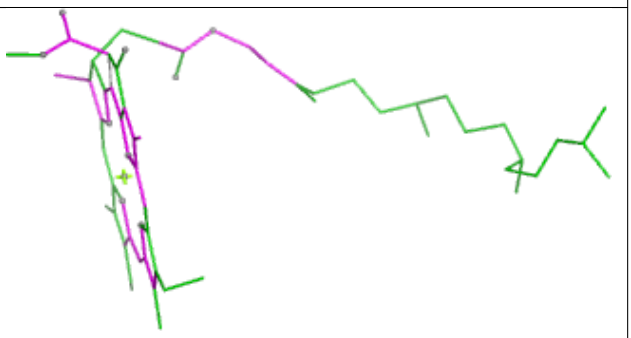

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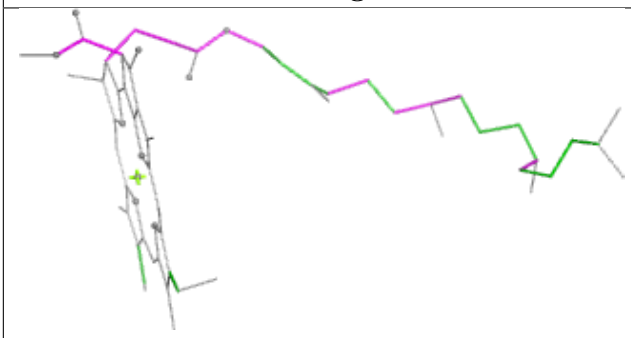

Torsions

Rings

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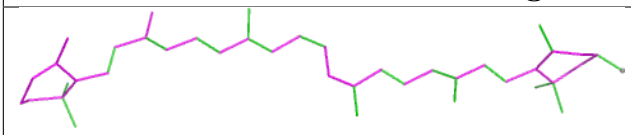

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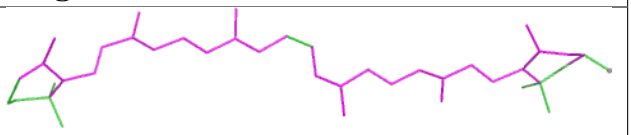

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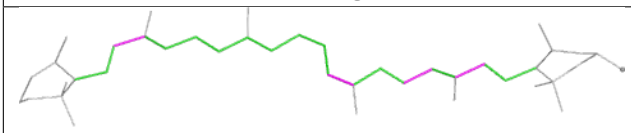

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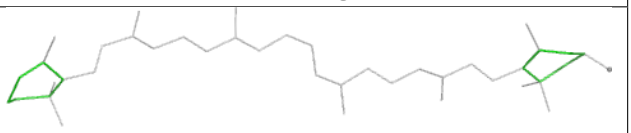

Rings

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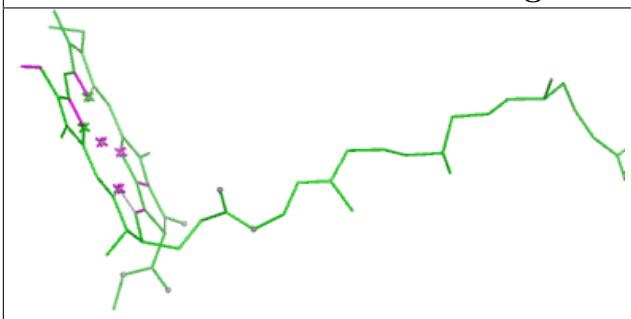
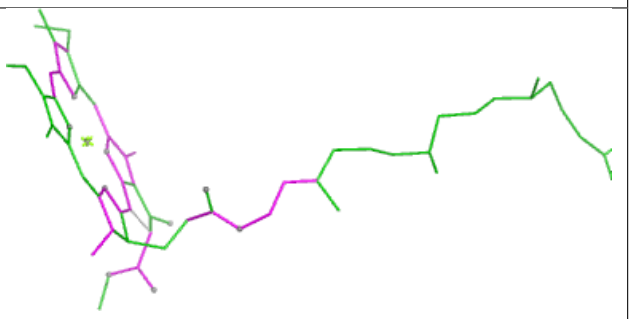
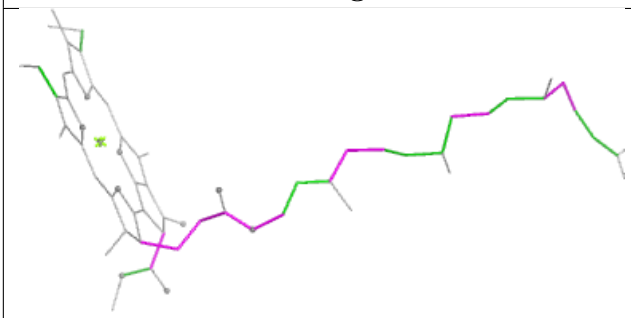
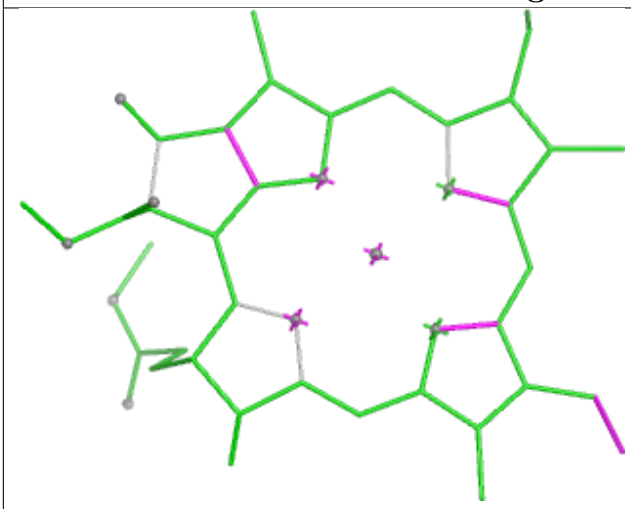
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA S 316



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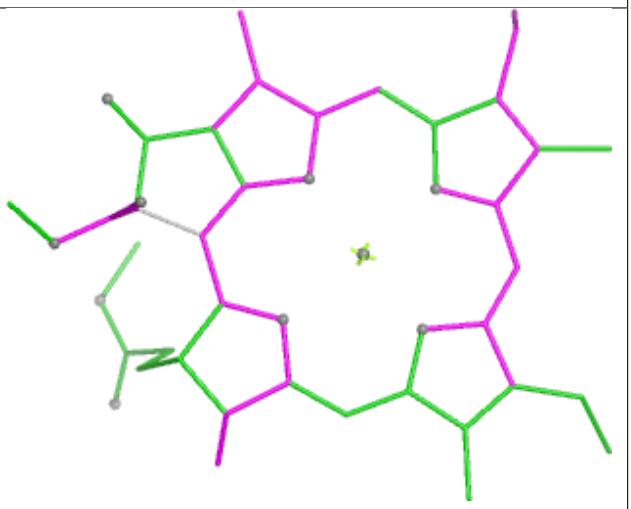
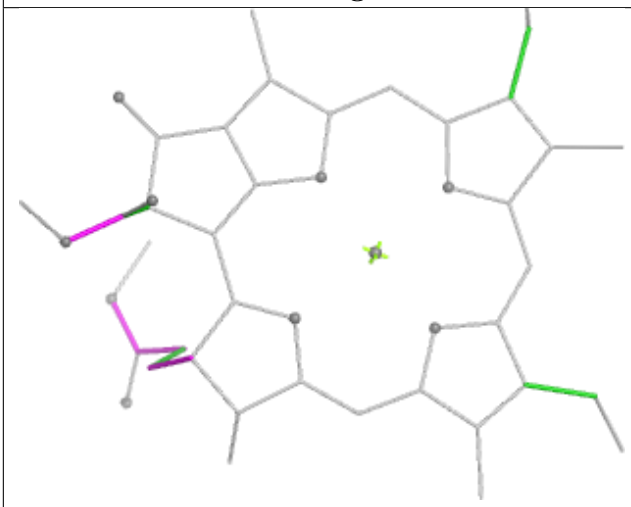


Bond angles



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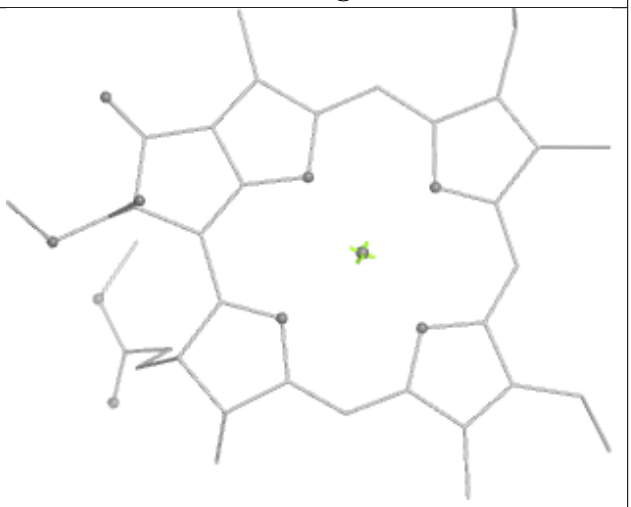
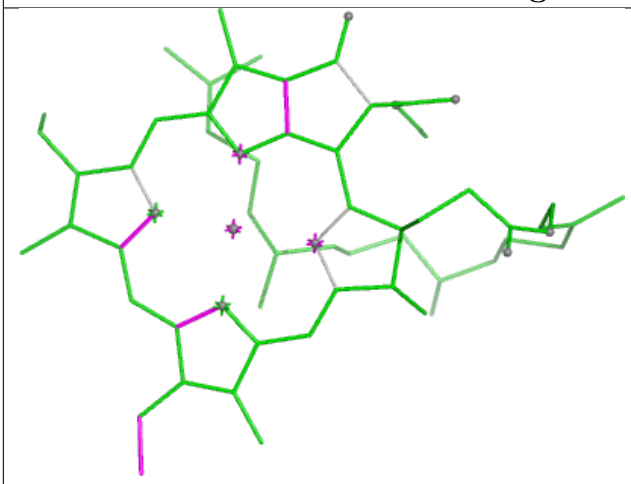


Rings

Ligand CLA c 610



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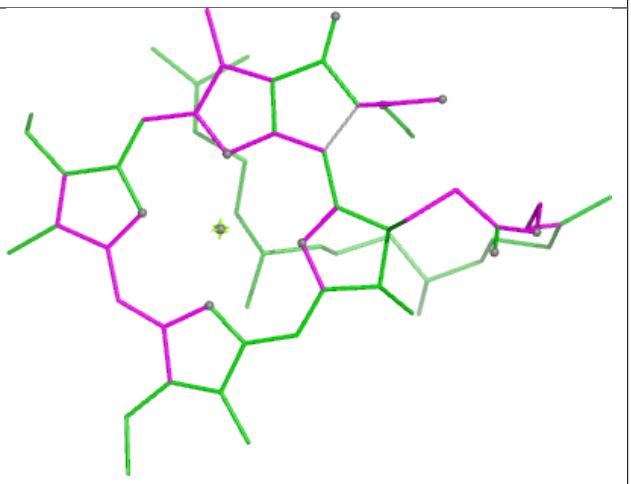

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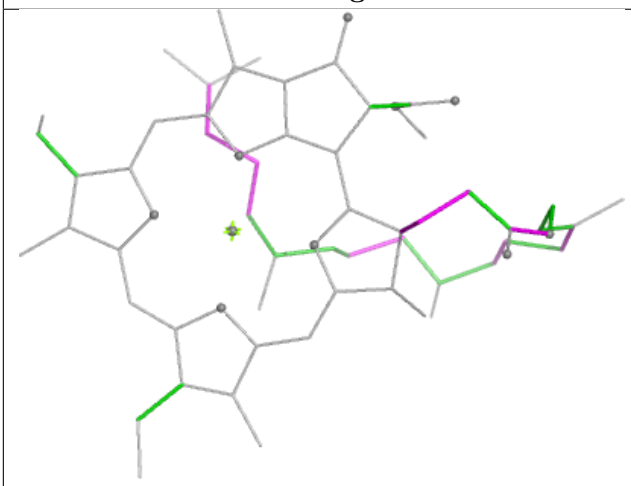

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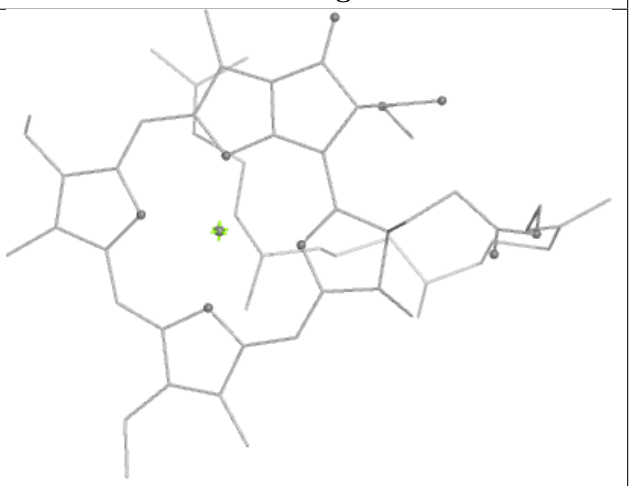
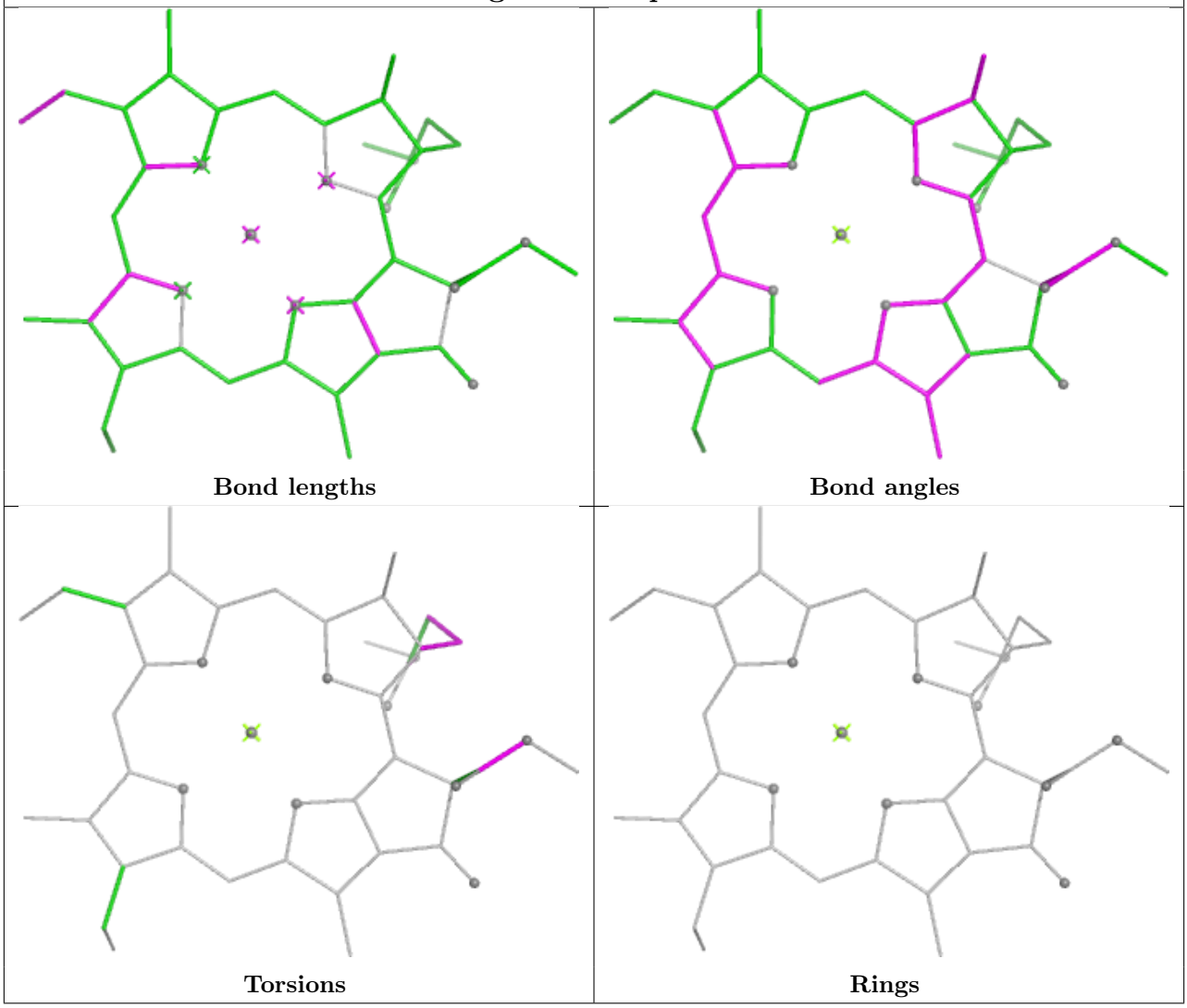
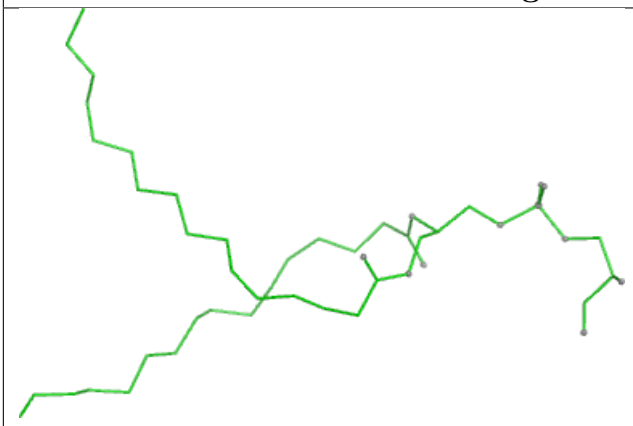


Rings

Ligand CLA p 615



Ligand LHG D 408



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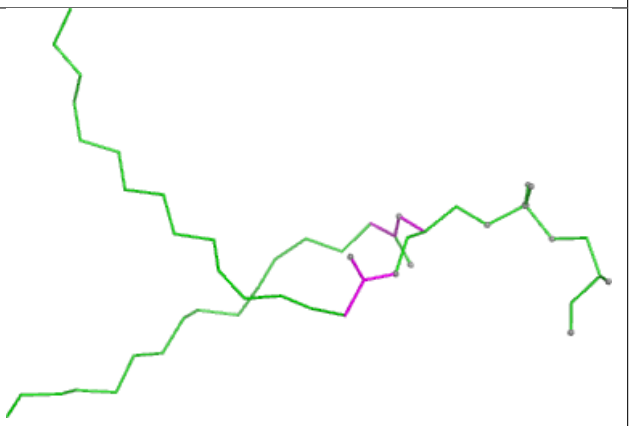

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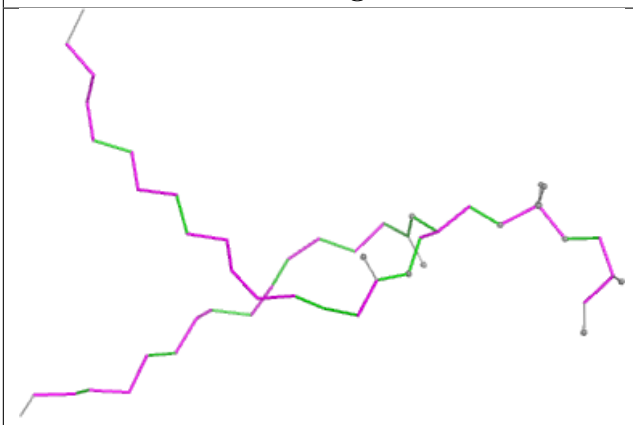

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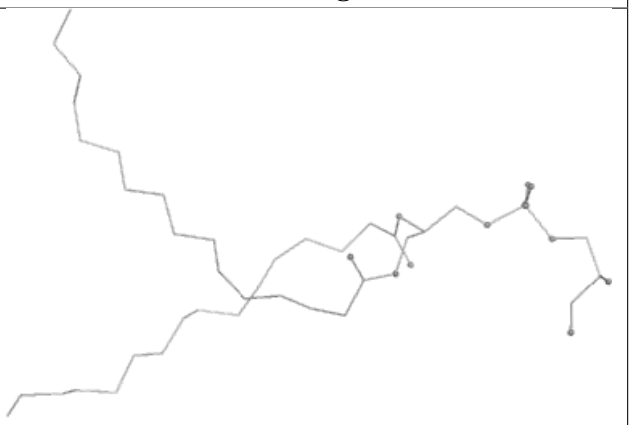
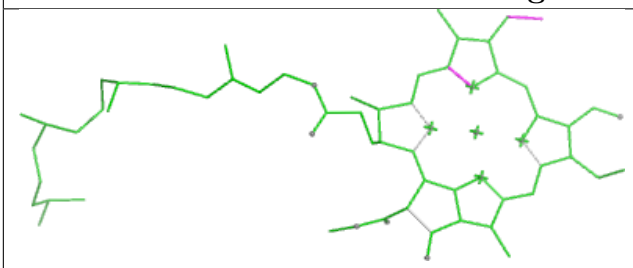


Rings

Ligand CHL 7 302



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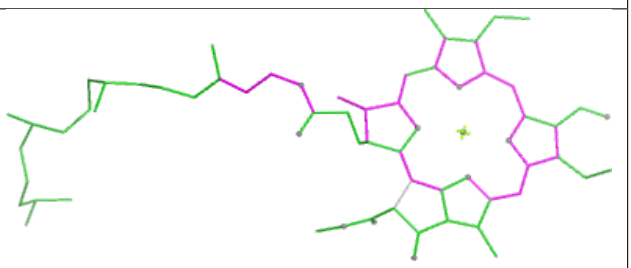

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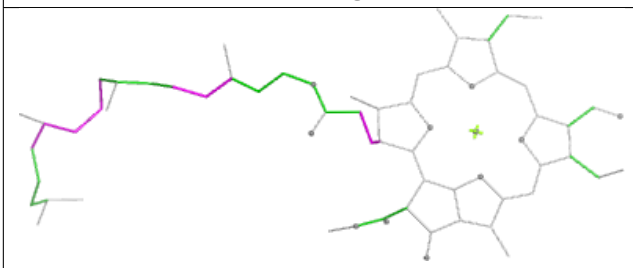

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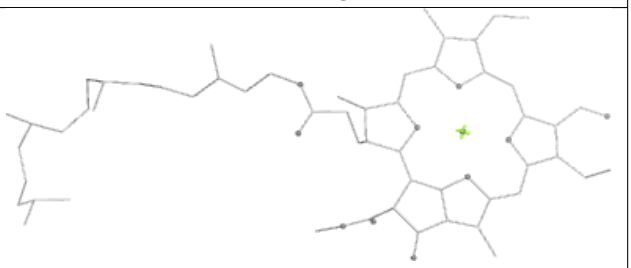
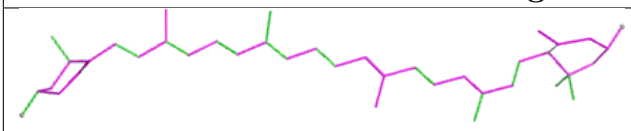


Rings

Ligand LUT S 318



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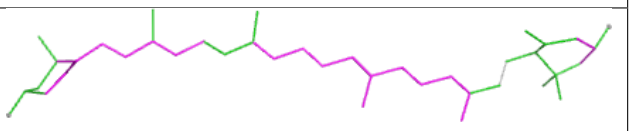

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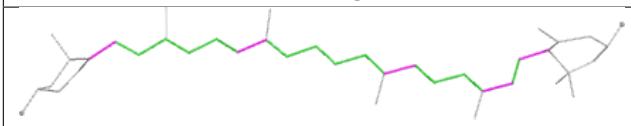

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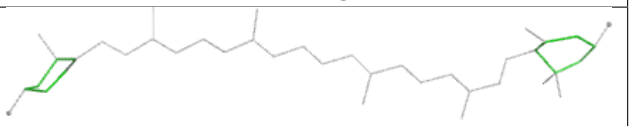
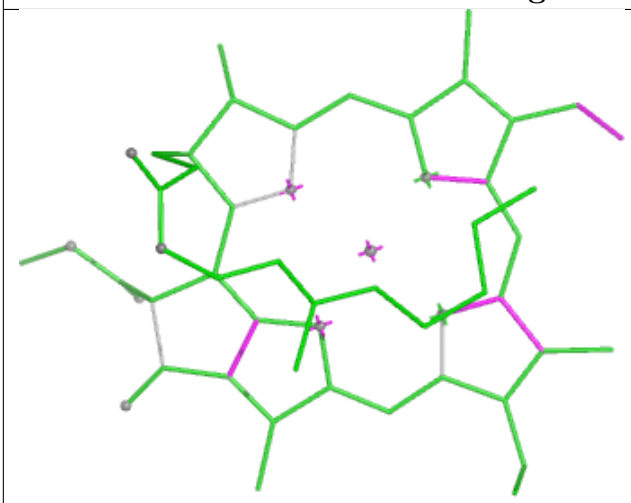


Rings

Ligand CLA 5 613



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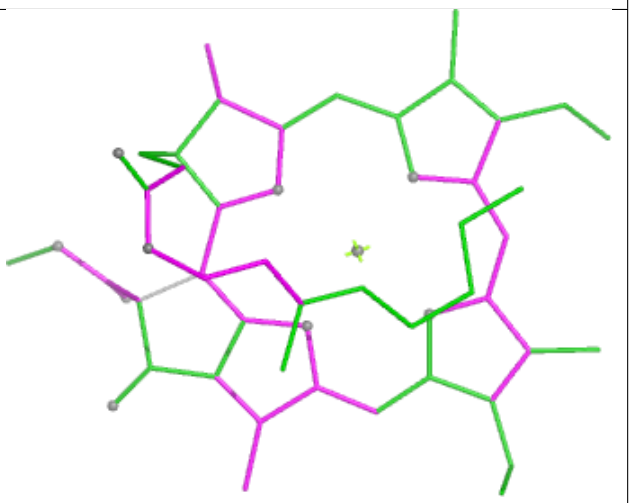
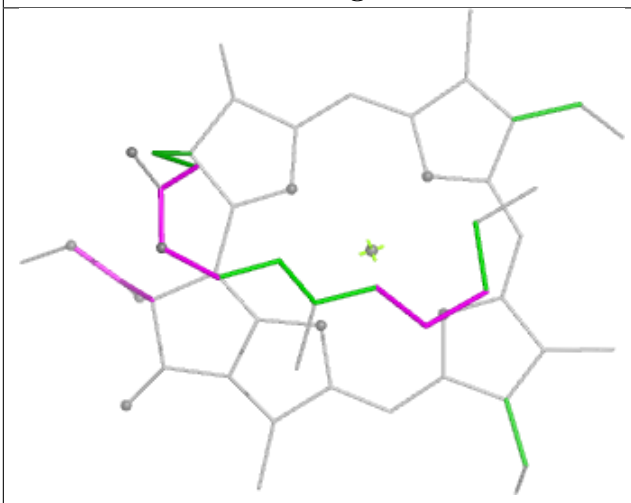


Bond angles



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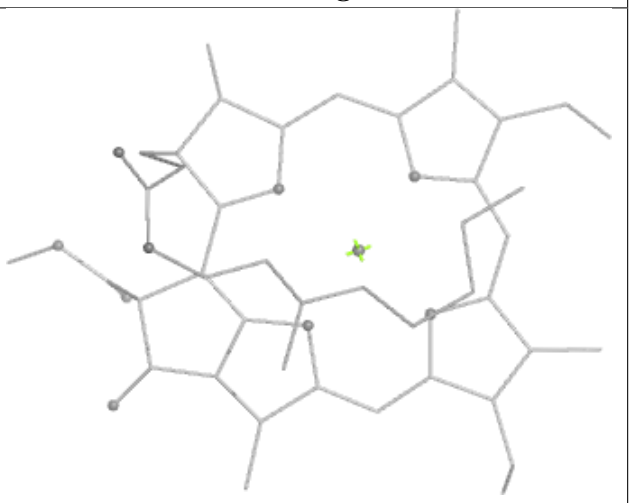
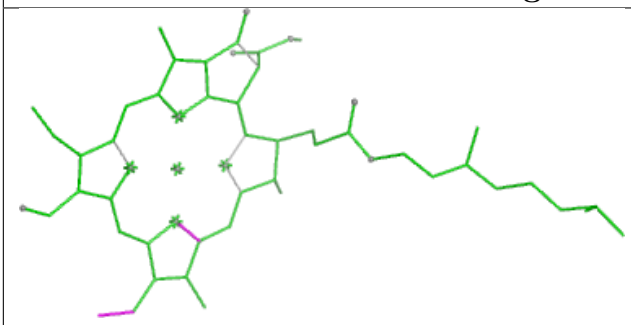
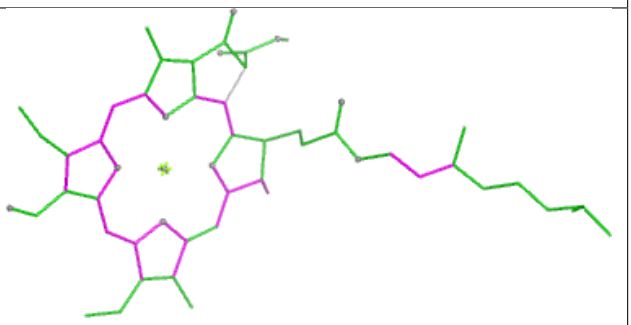
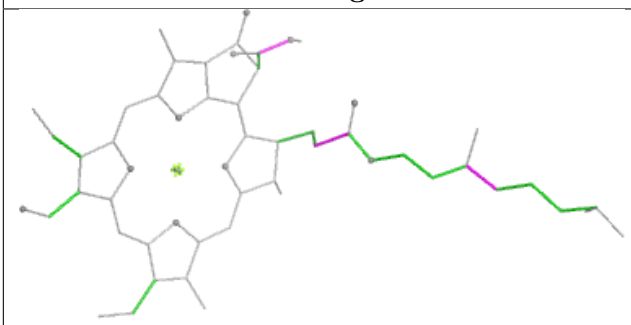
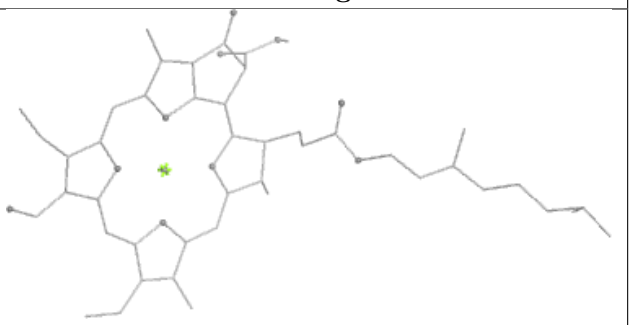
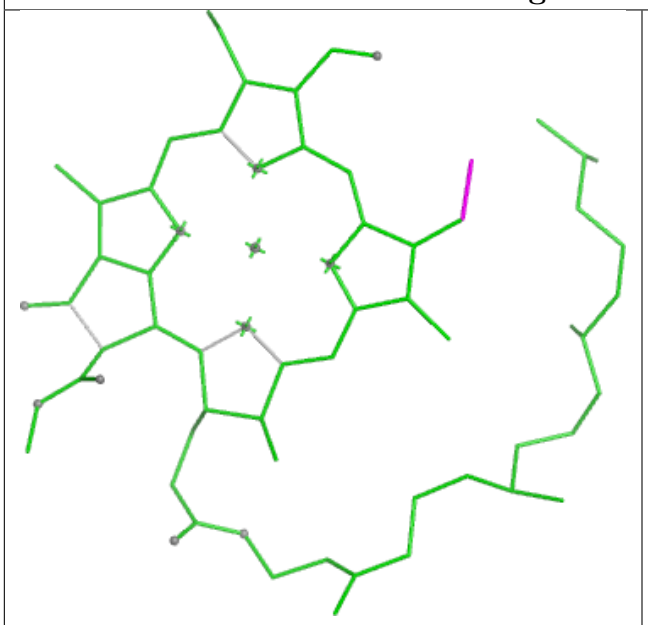


Rings

Ligand CHL R 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 0 607



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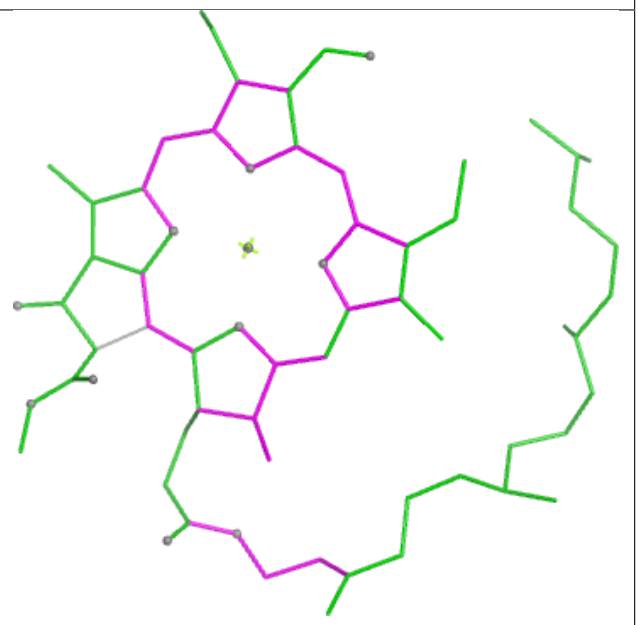
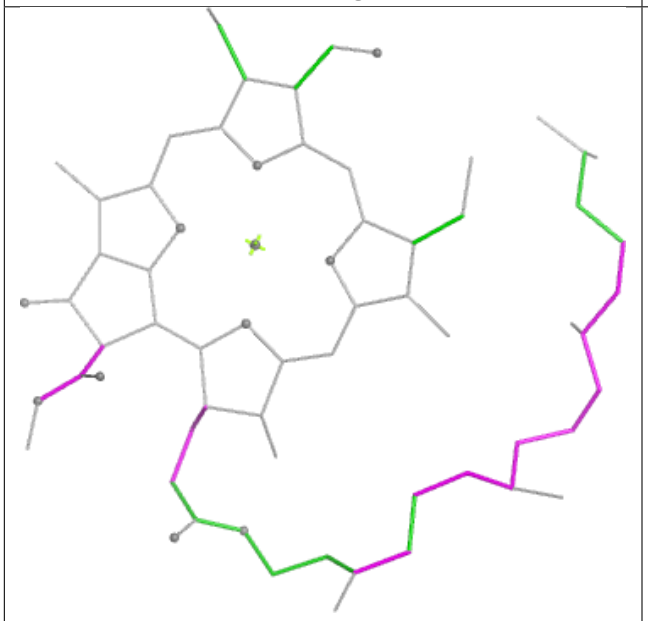


Bond angles



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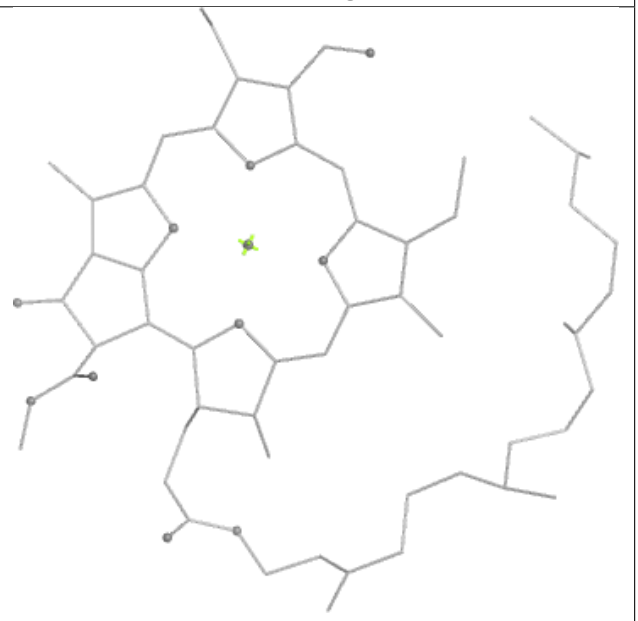
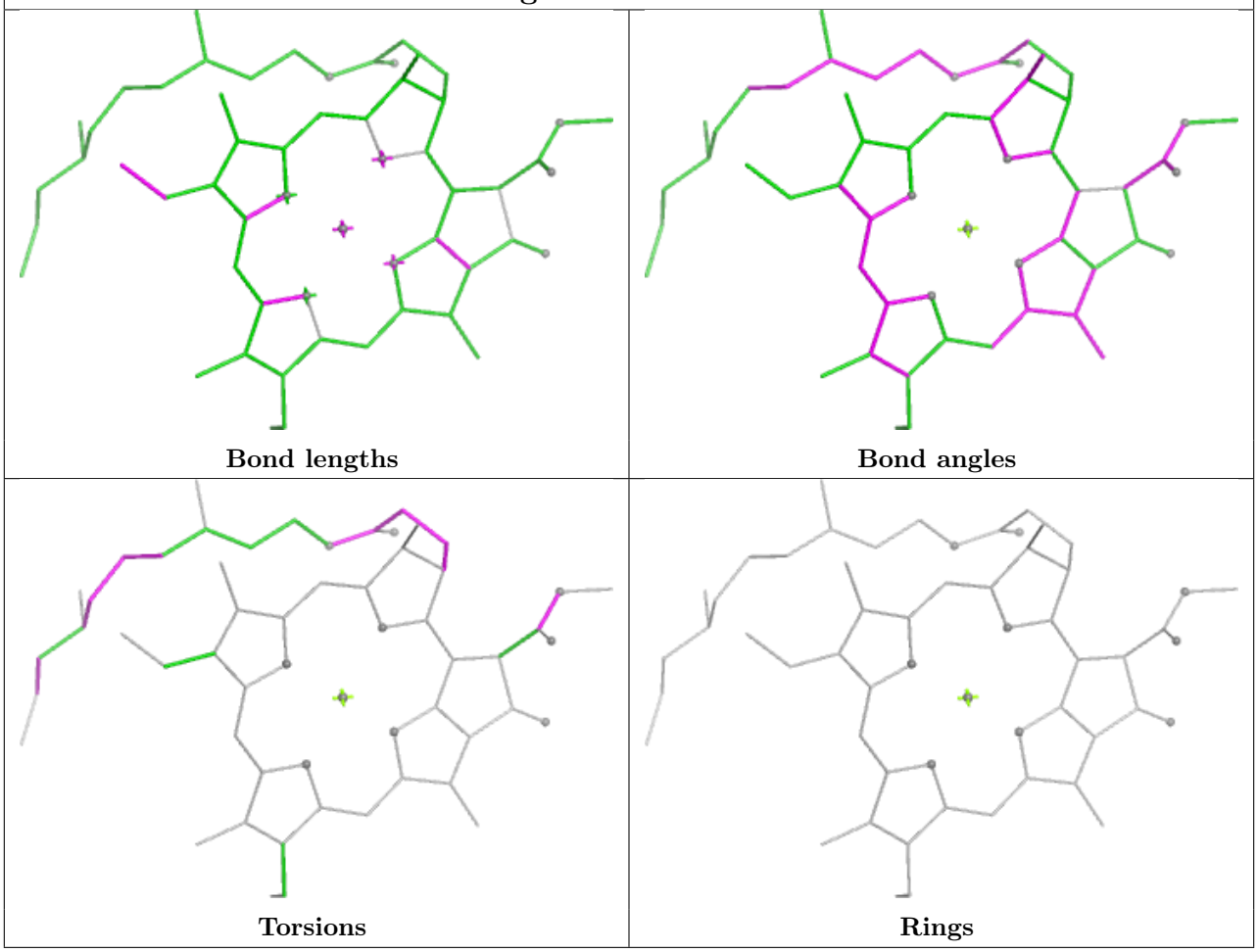
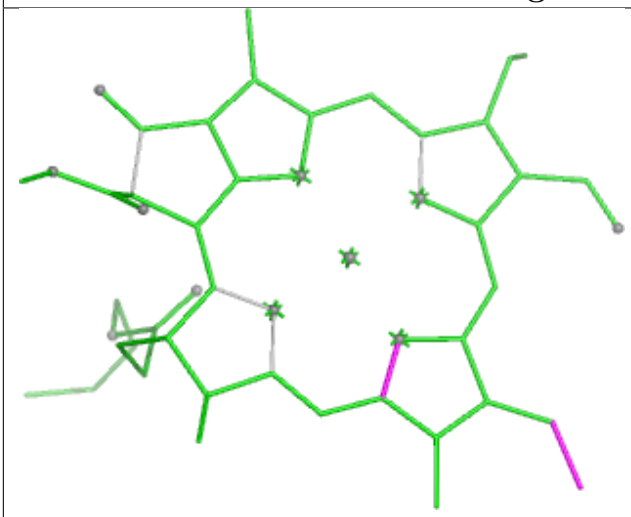


Rings

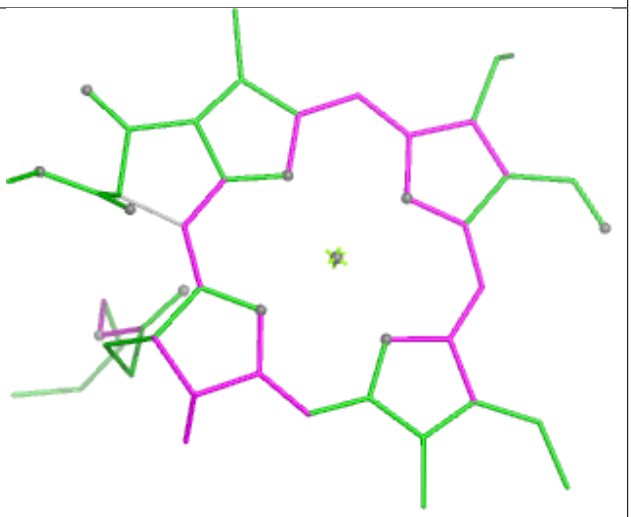
Ligand CLA r 312



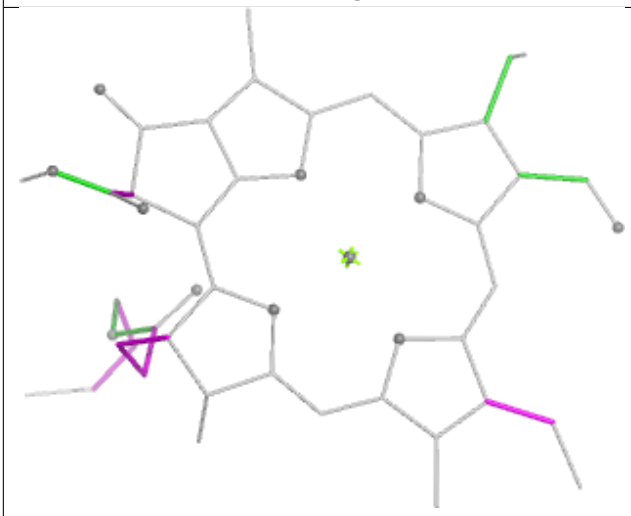
Ligand CHL 5 608



Bond lengths



Bond angles



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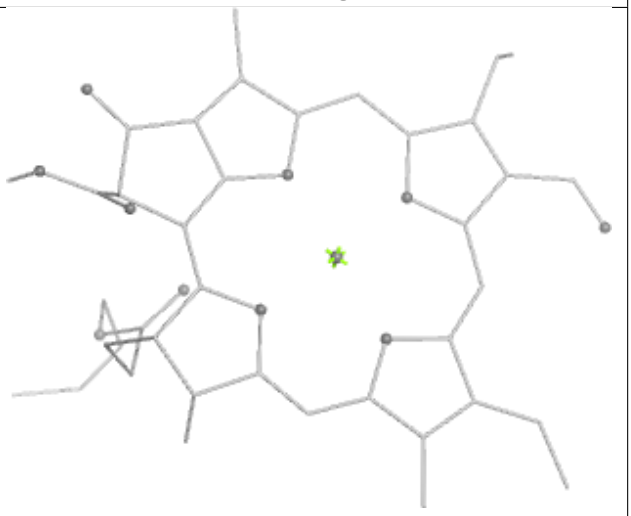

Rings

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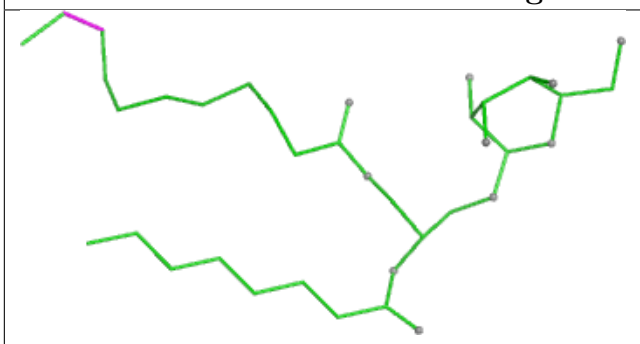
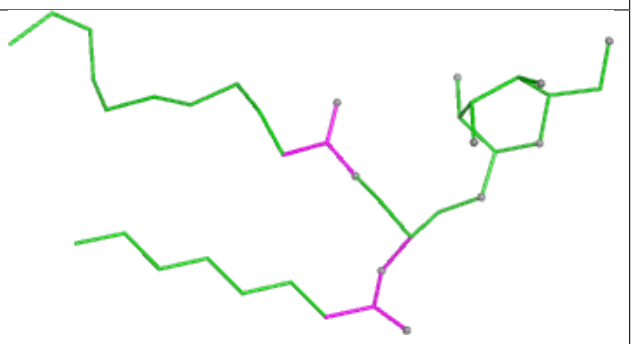
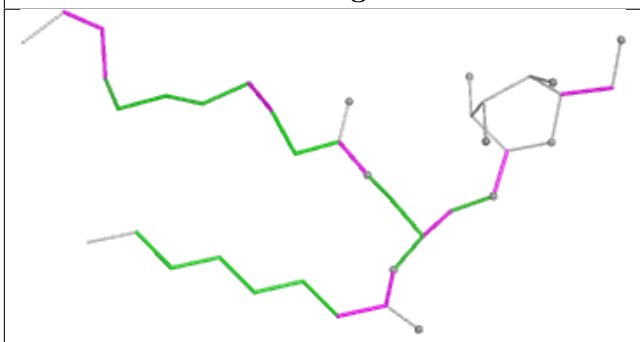
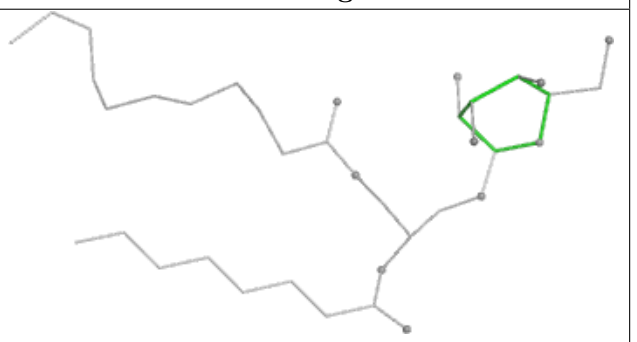
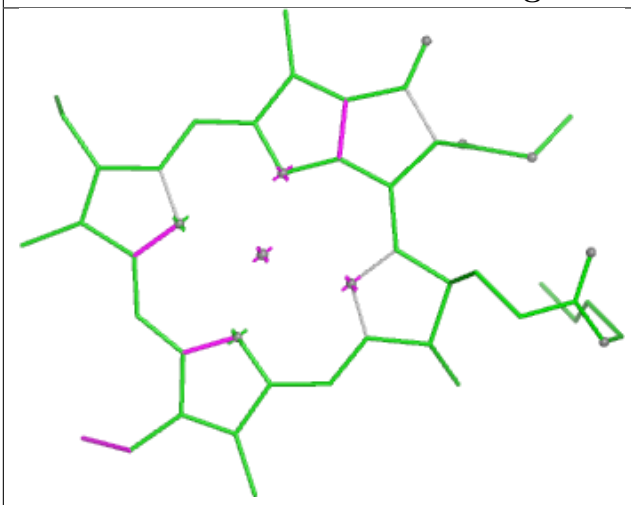
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 314



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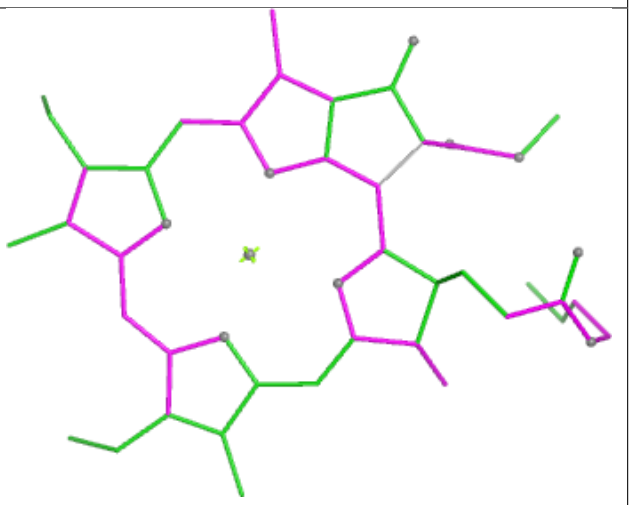

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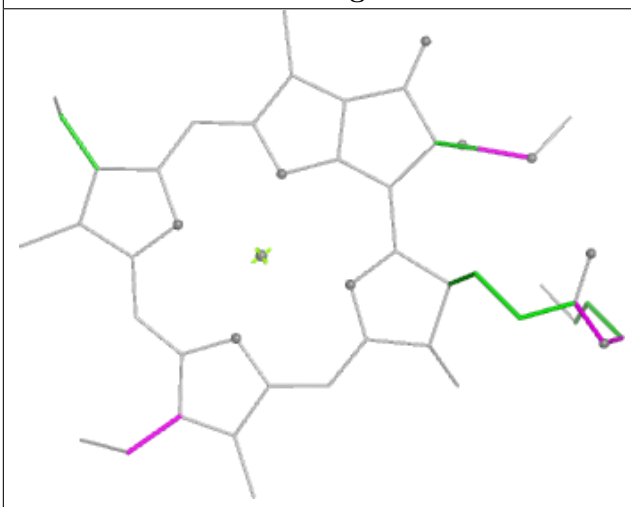

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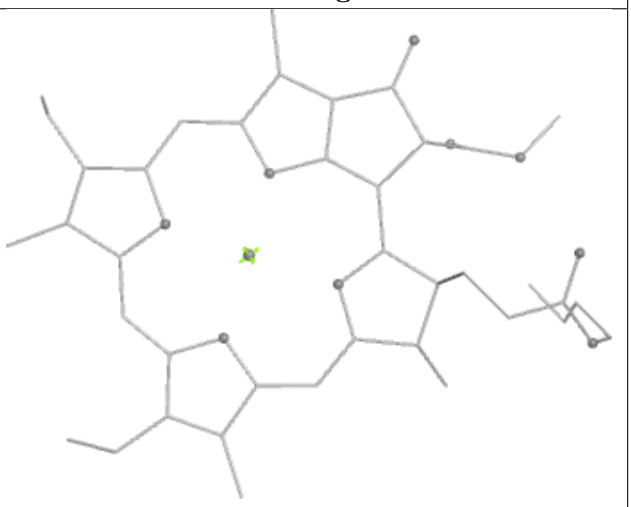
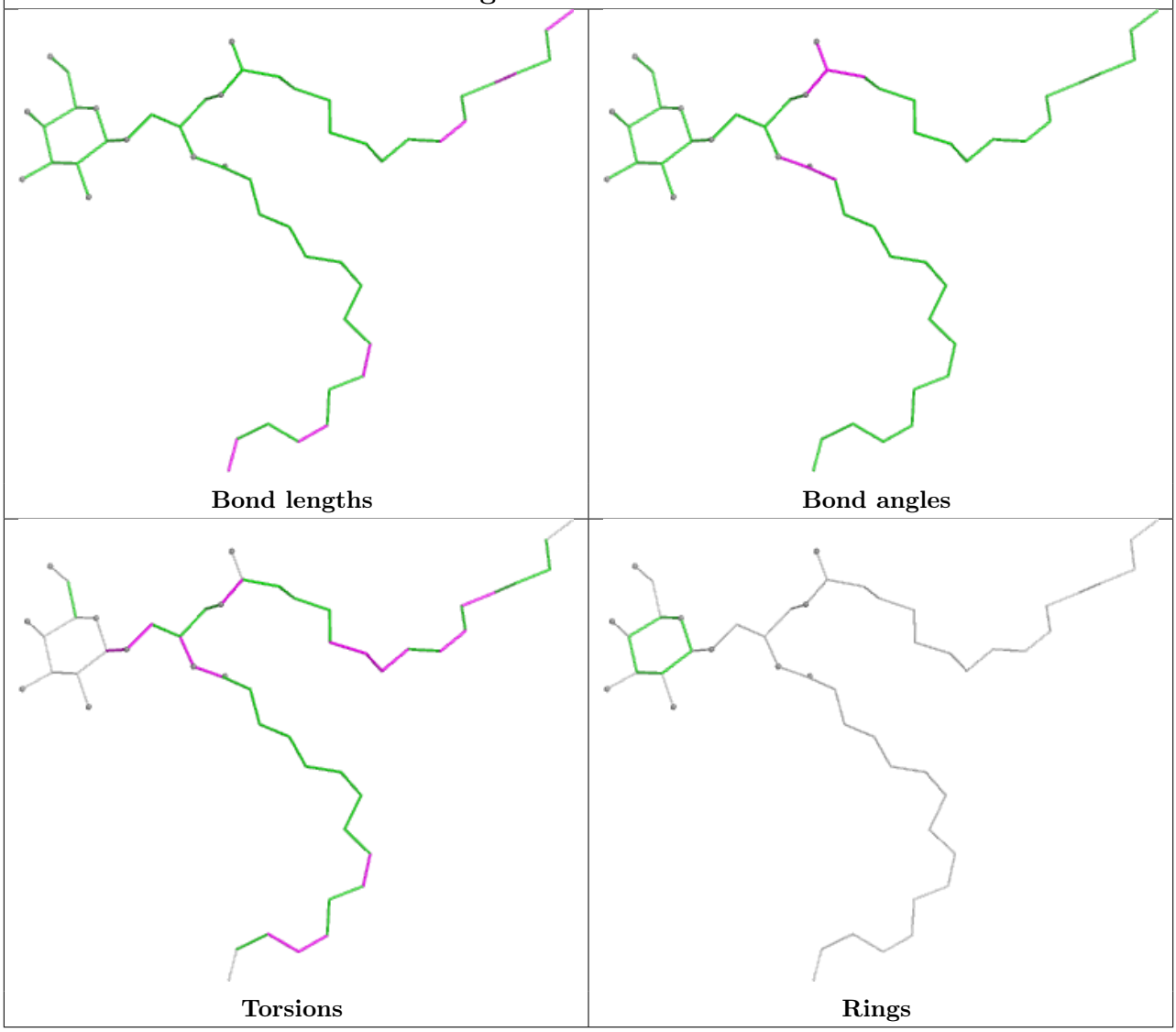
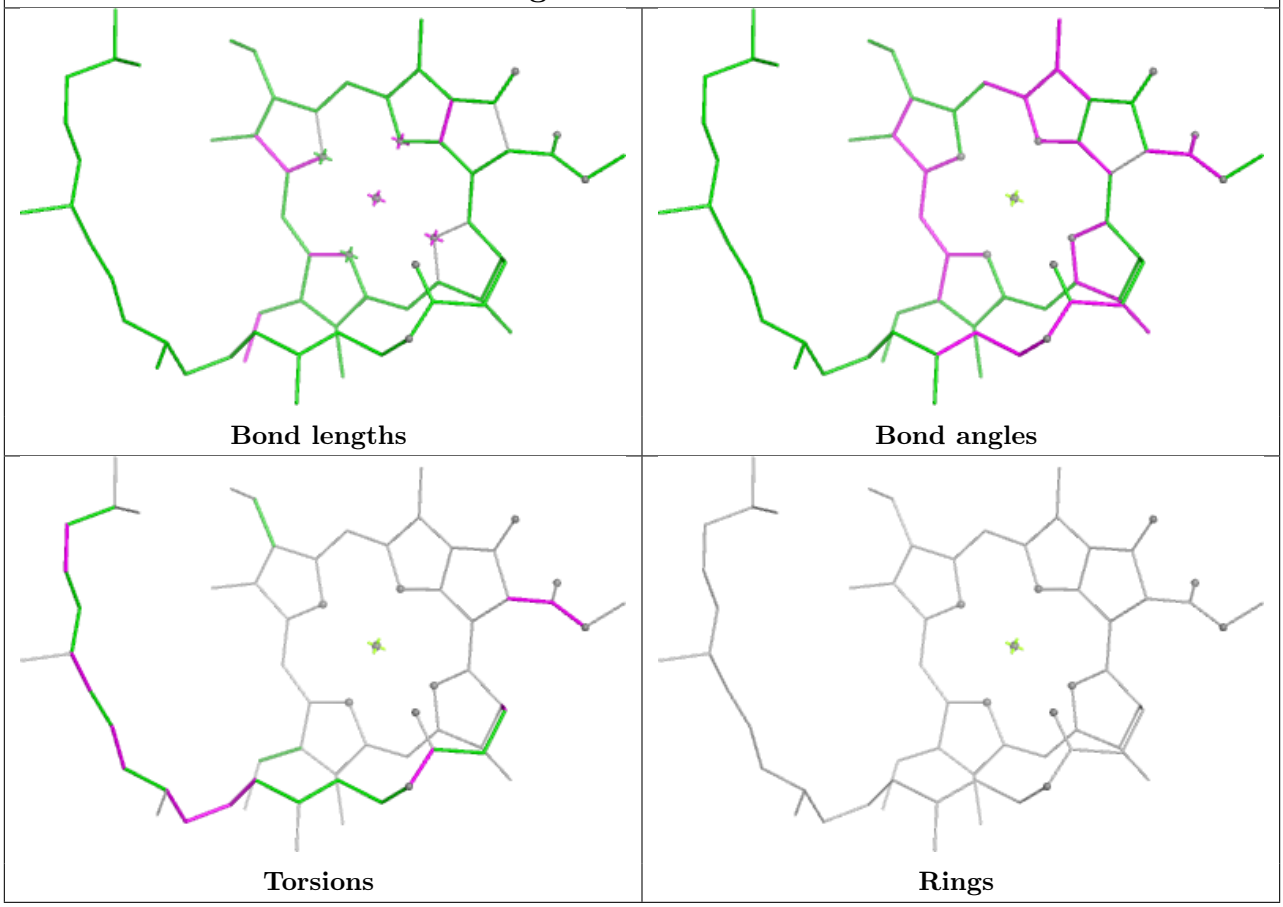


Rings

Ligand LMG d 410



Ligand CLA 6 311



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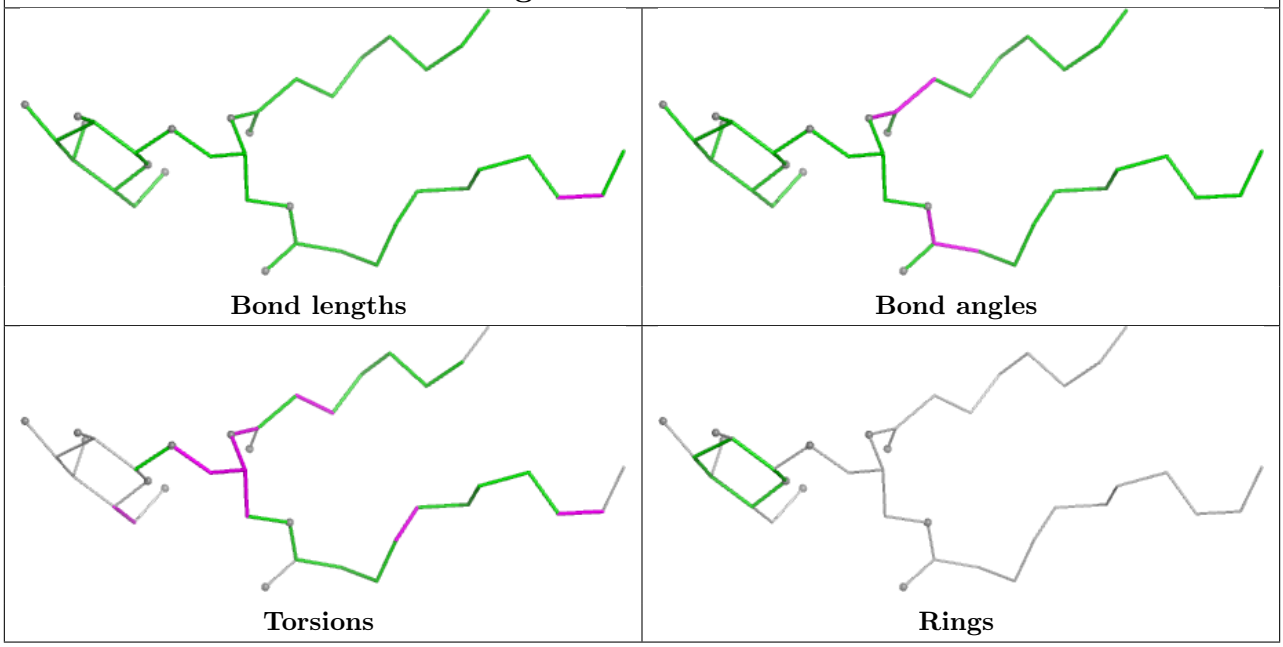
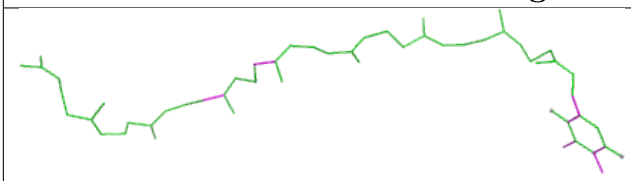


Ligand PL9 A 416



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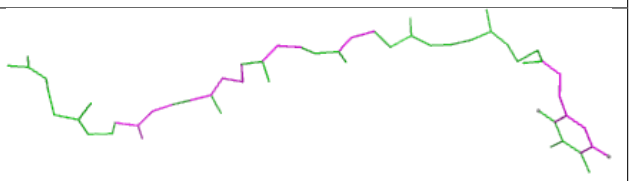
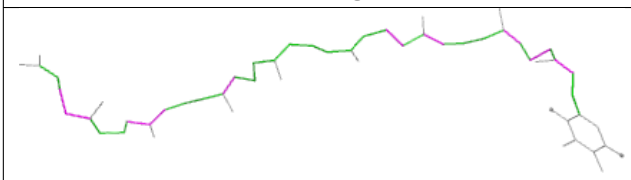


Bond angles



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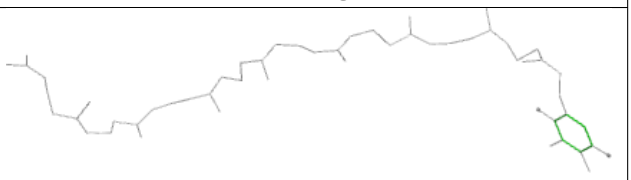
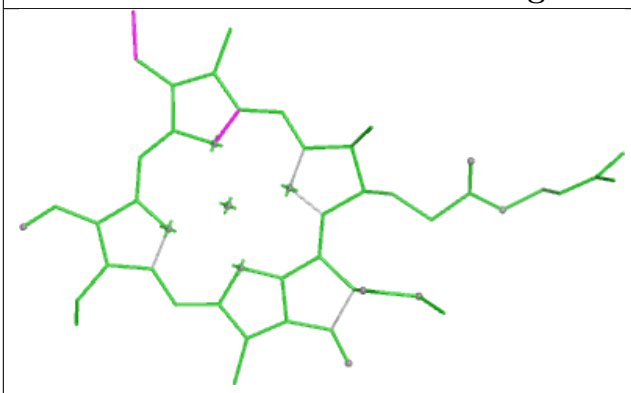


Rings

Ligand CHL 6 307



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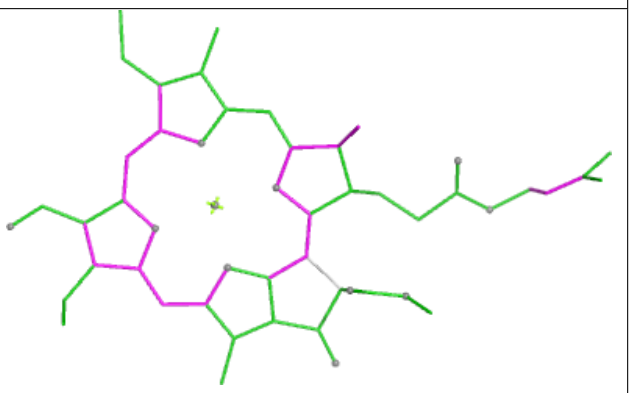
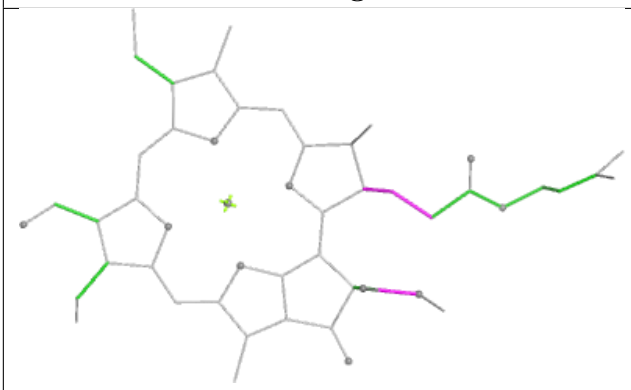


Bond angles



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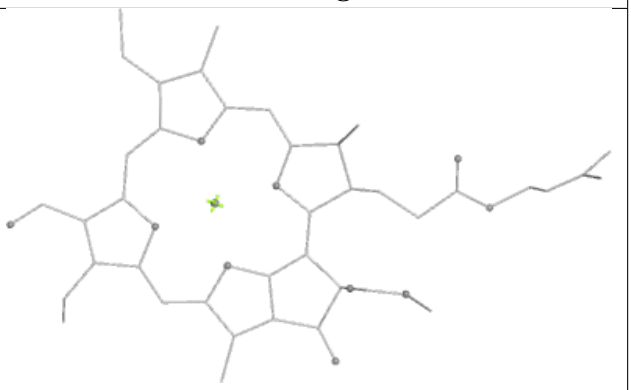
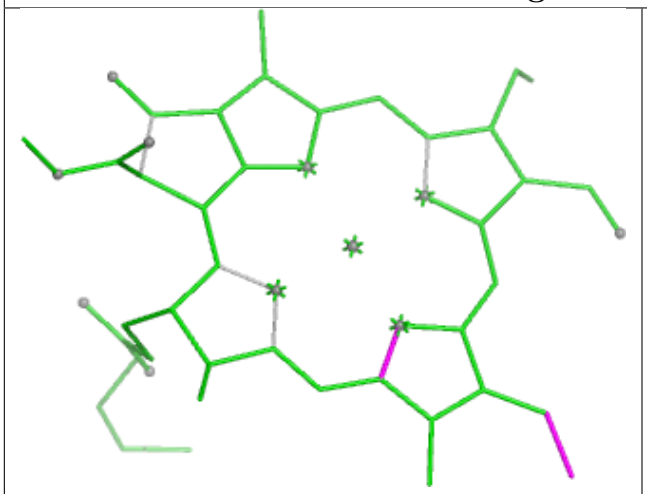


Rings

Ligand CHL n 309



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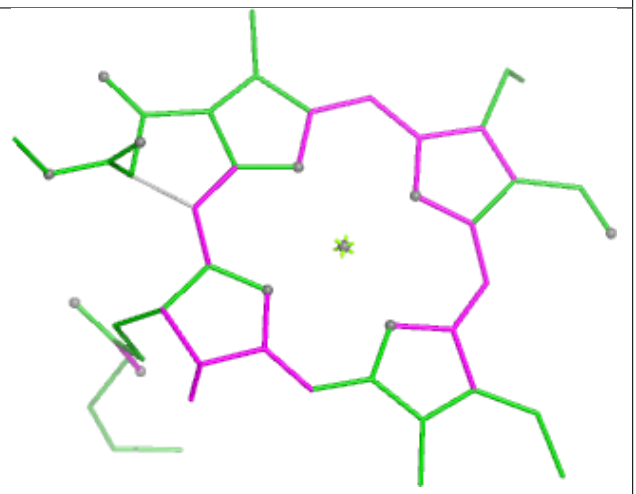

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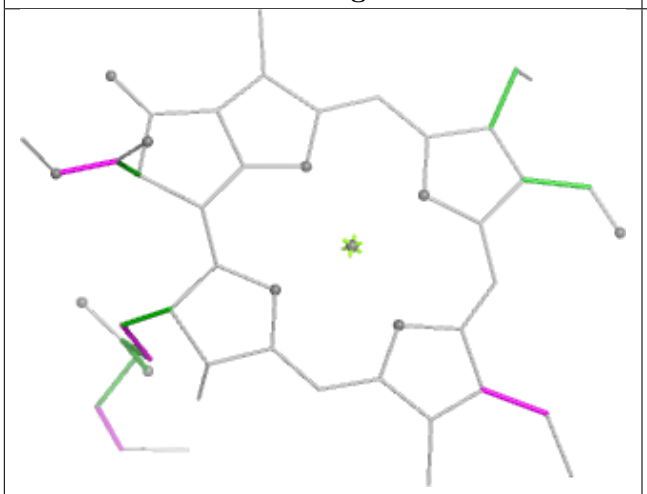

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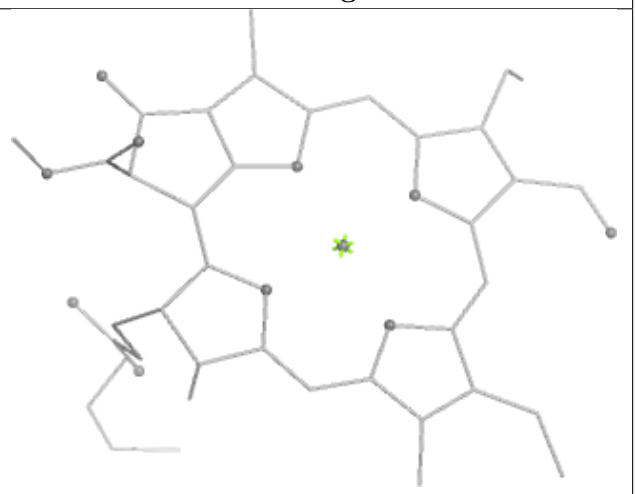
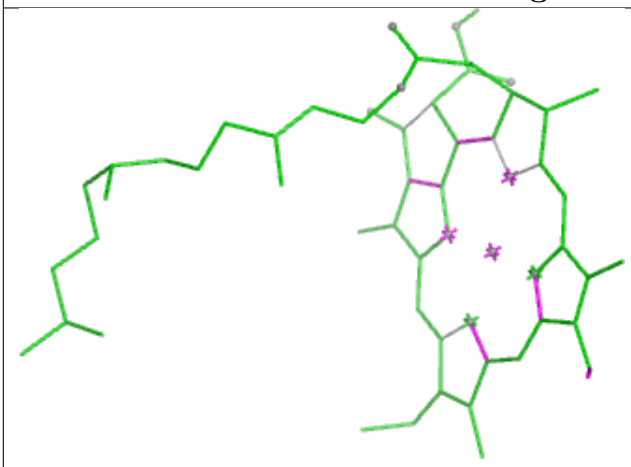
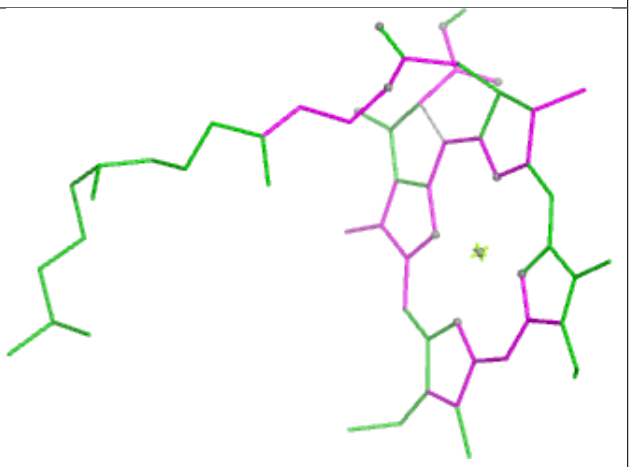
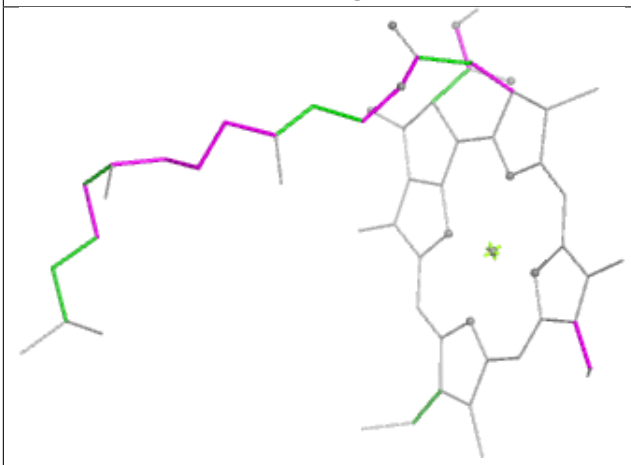
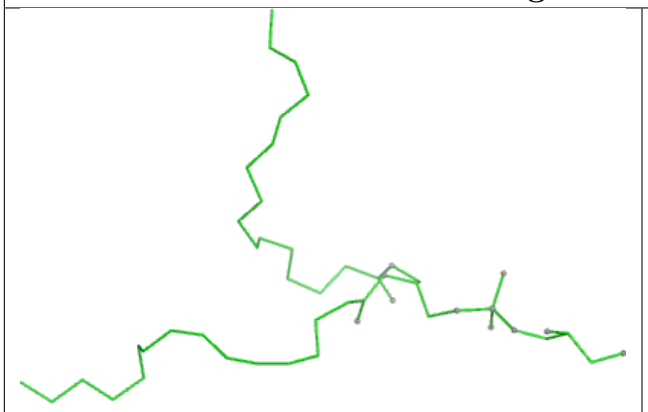


Rings

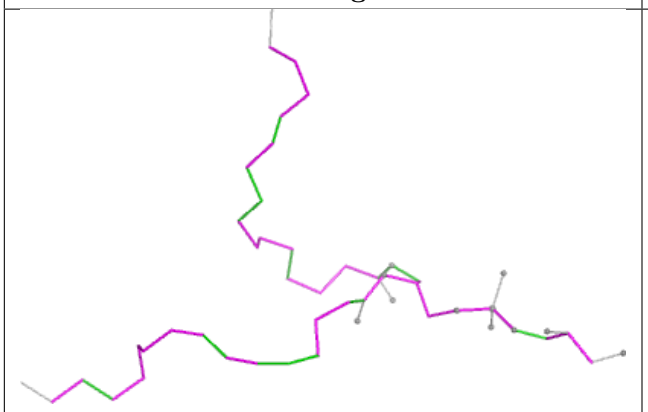
Ligand CLA s 310	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LHG 8 618



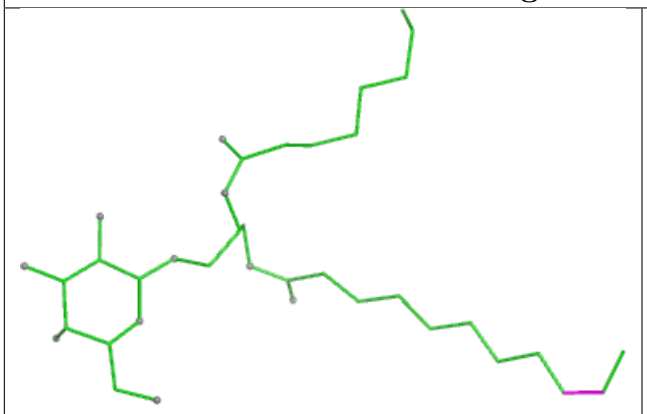
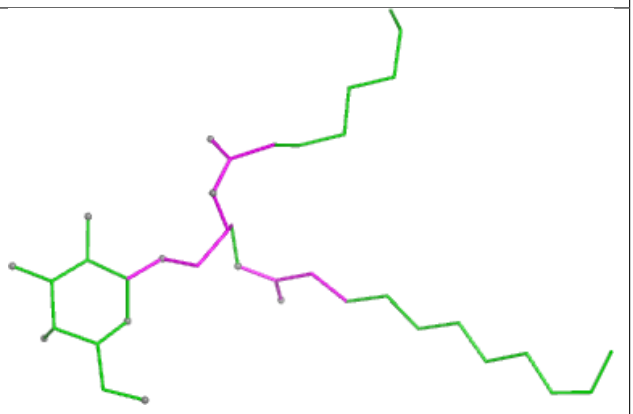
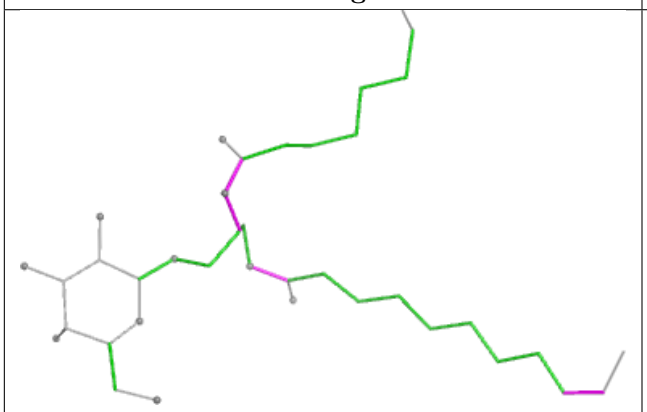
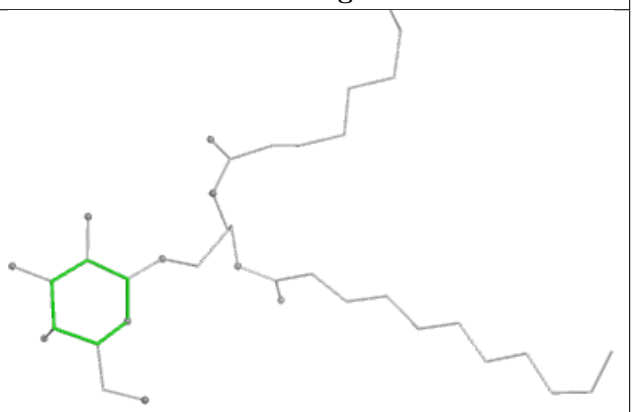
Bond lengths

Bond angles

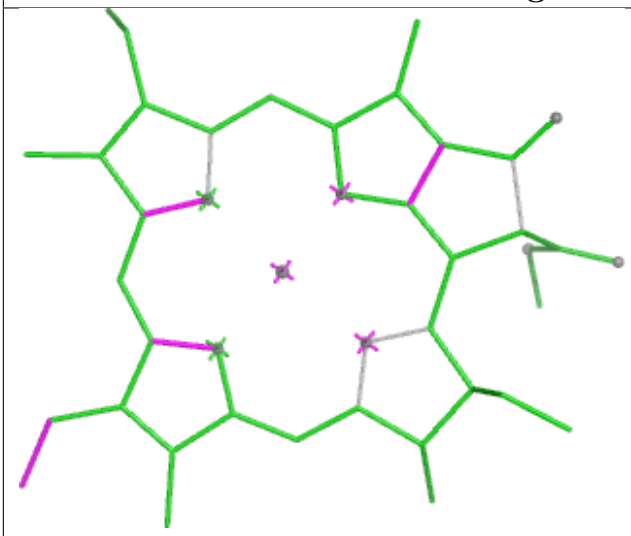


Torsions

Rings

Ligand LMG w 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 304



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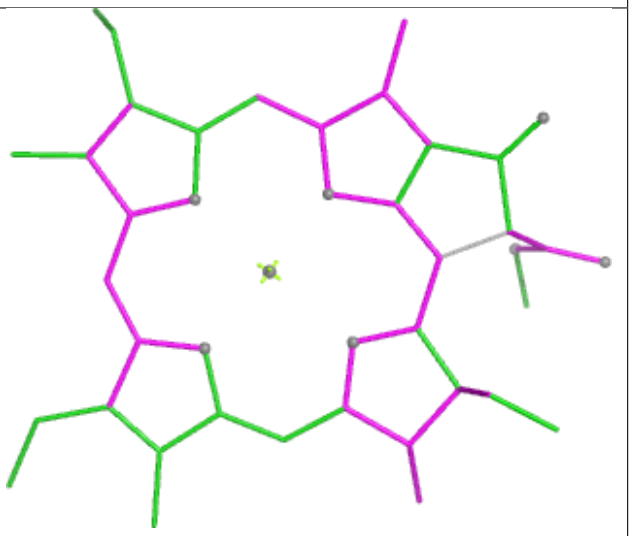
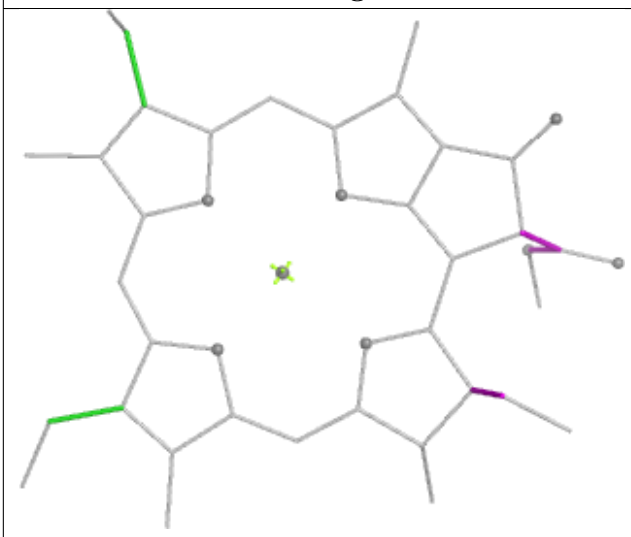


Bond angles



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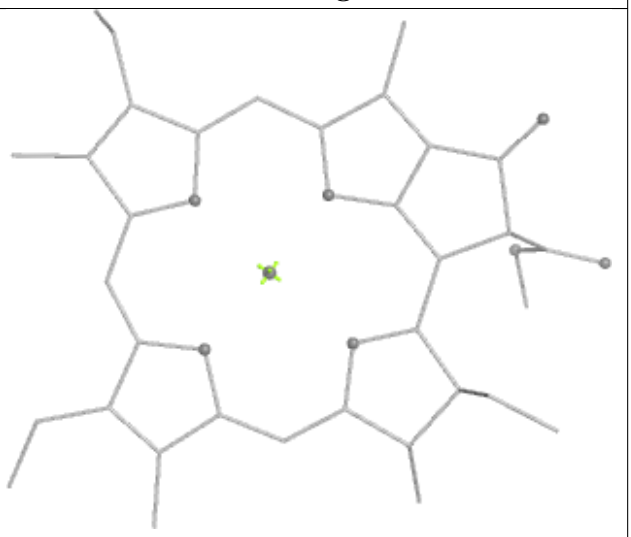
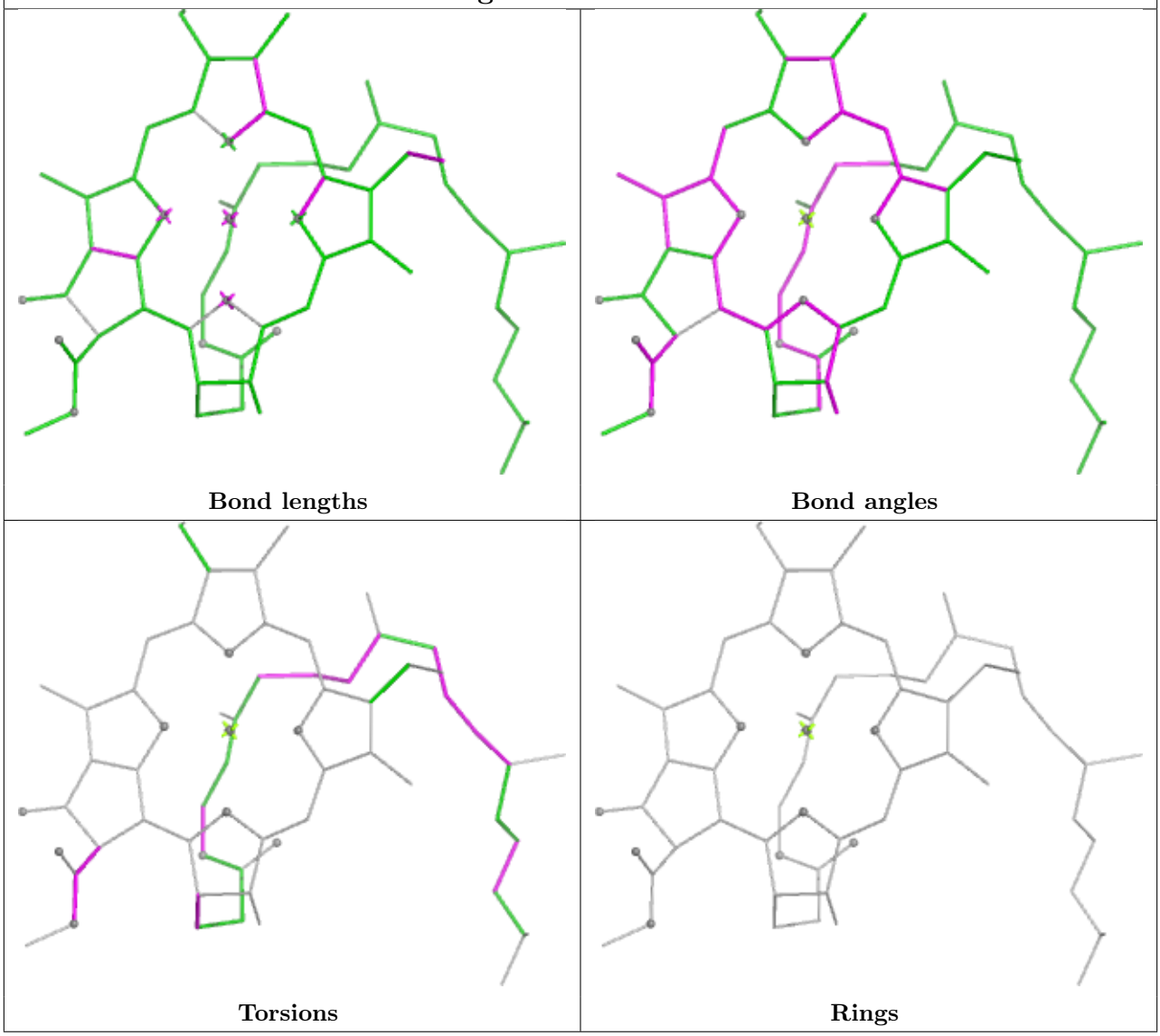
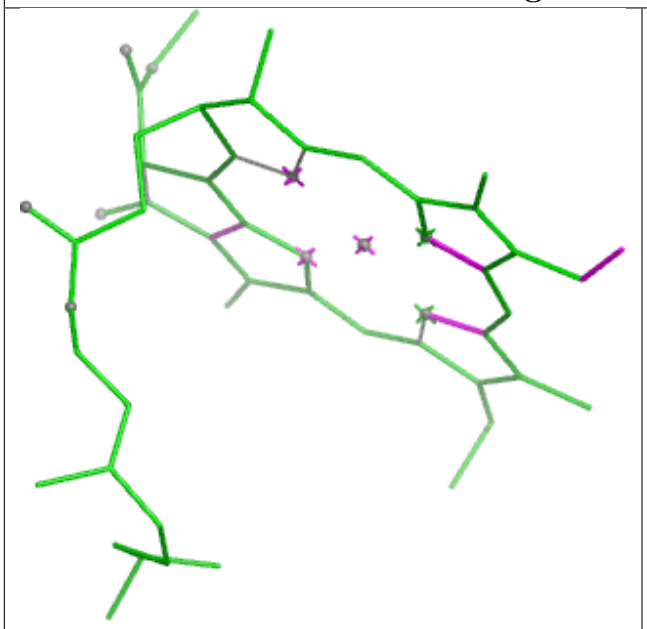


Rings

Ligand CLA n 314



Ligand CLA Y 305



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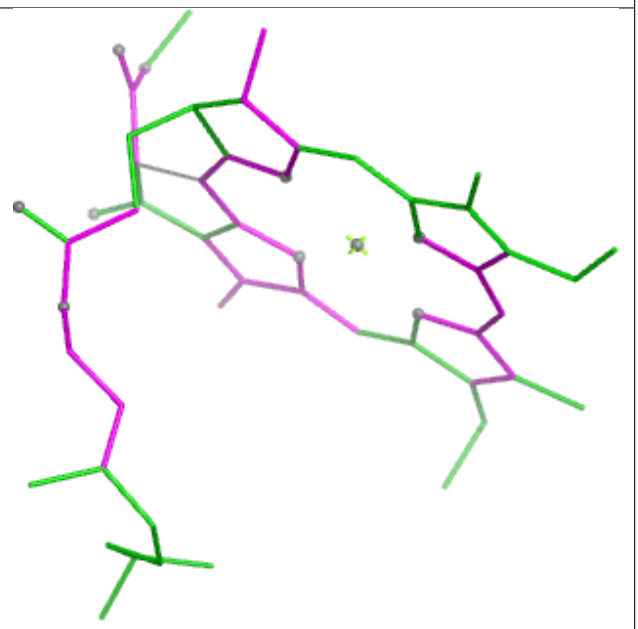
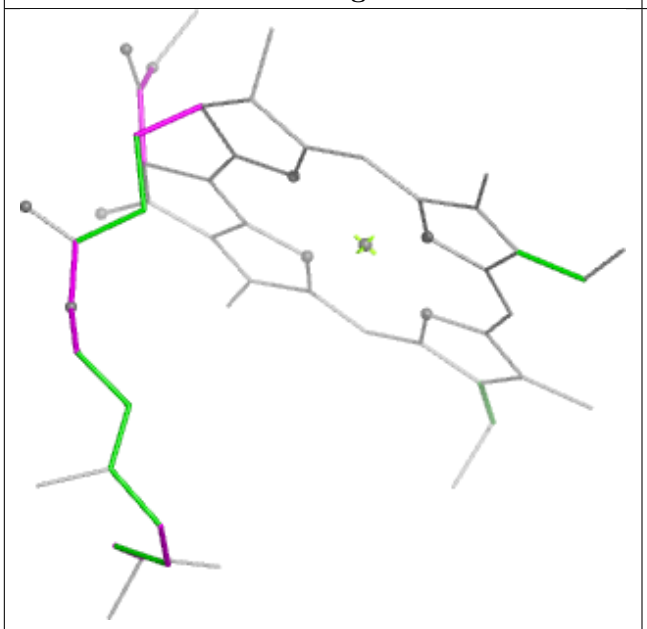
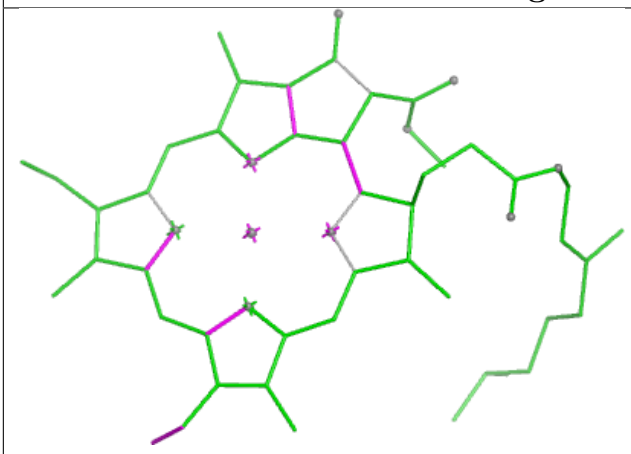
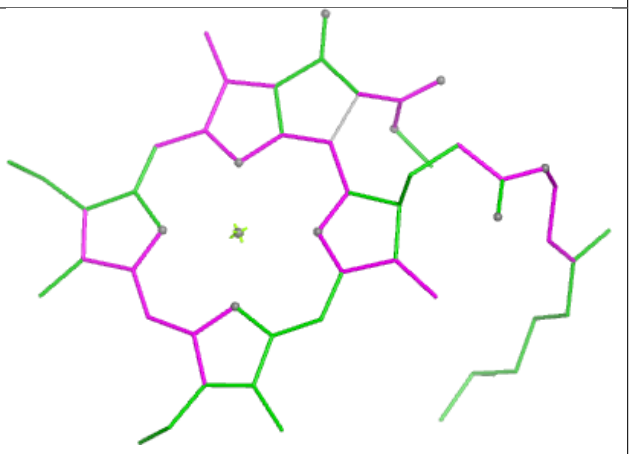
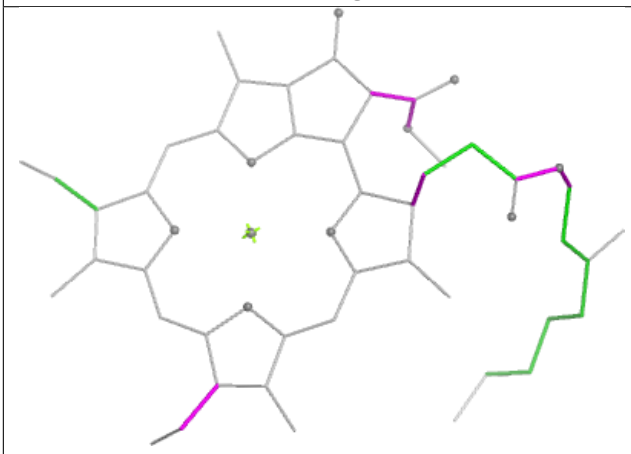
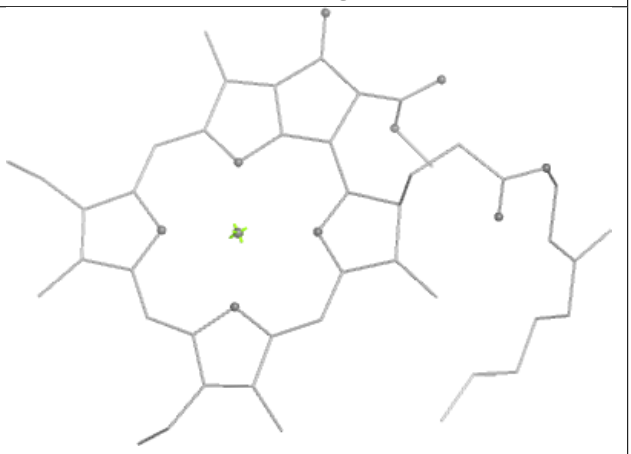


Bond angles

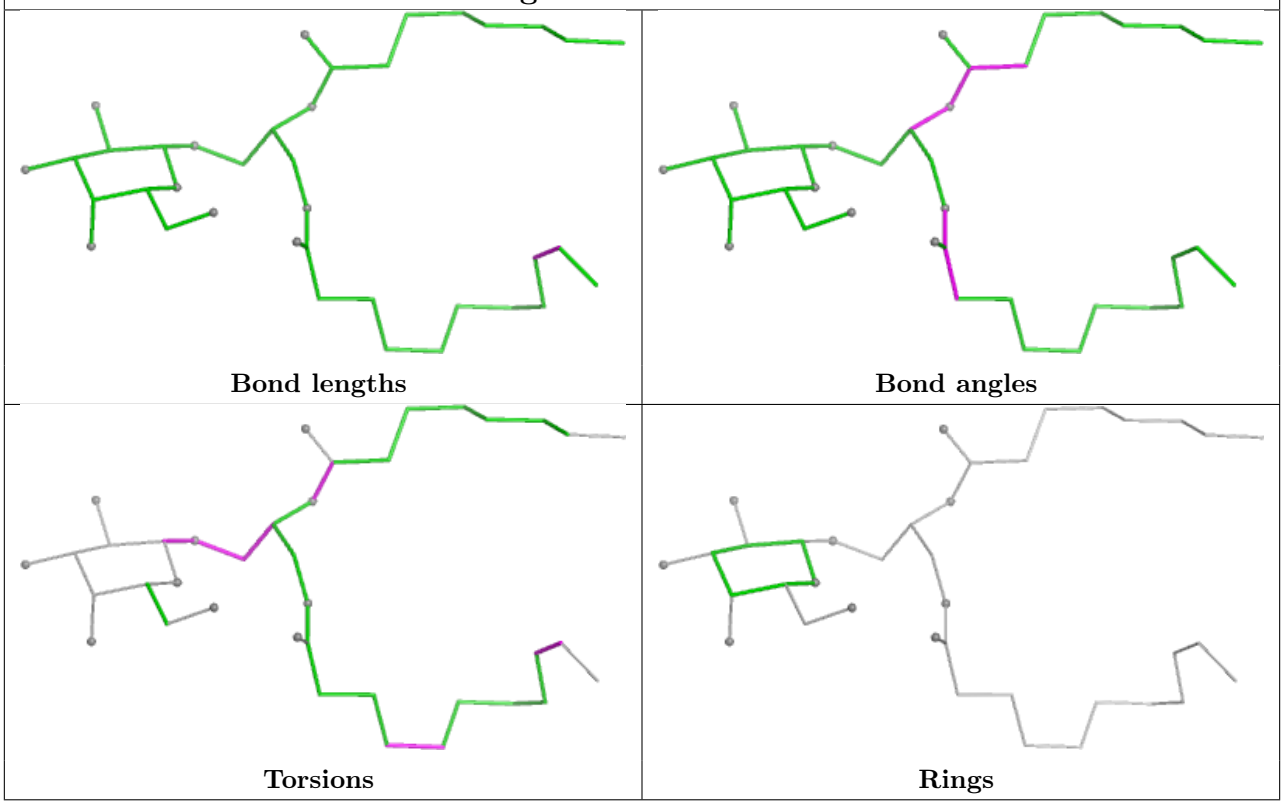


Torsions

Rings

Ligand CLA 1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG Y 319



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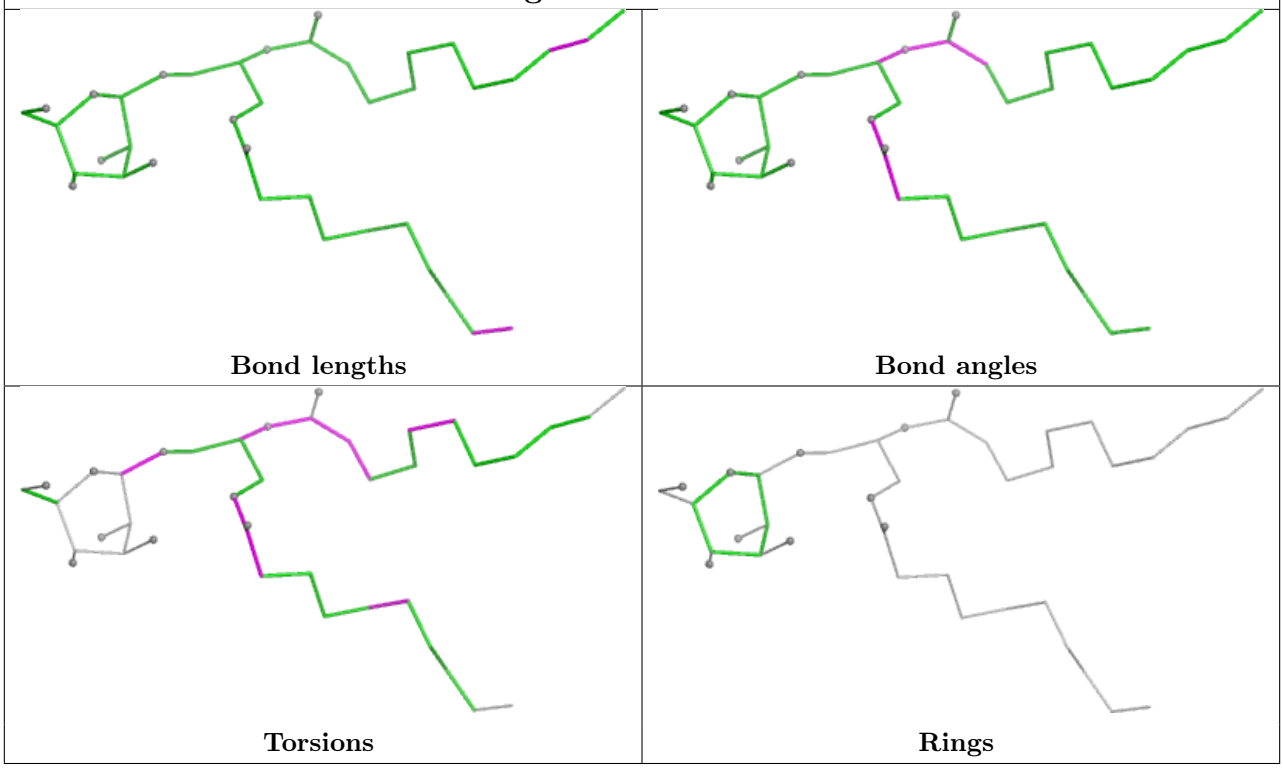
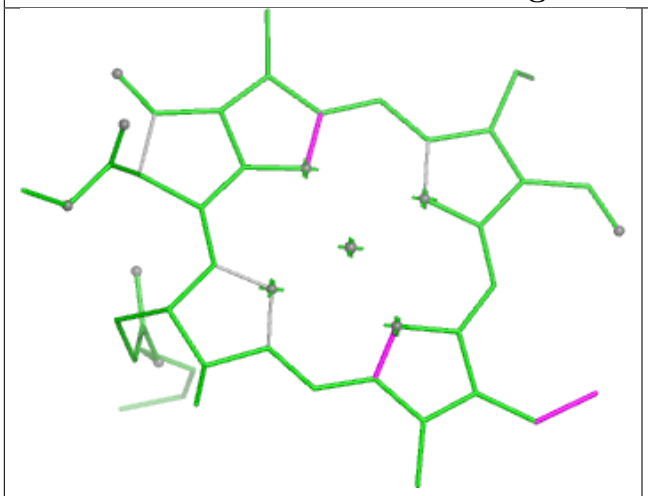
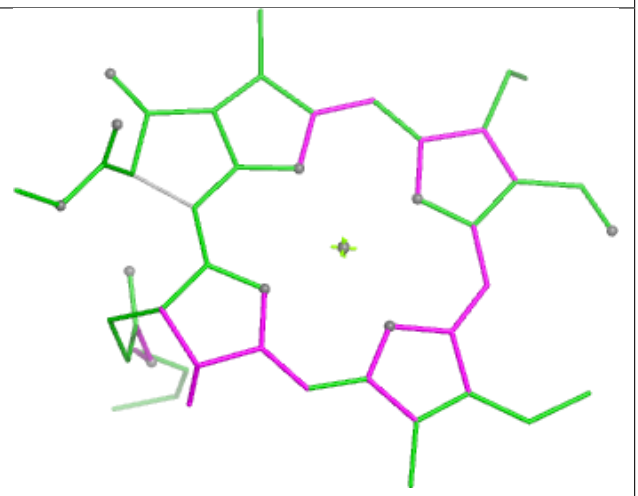


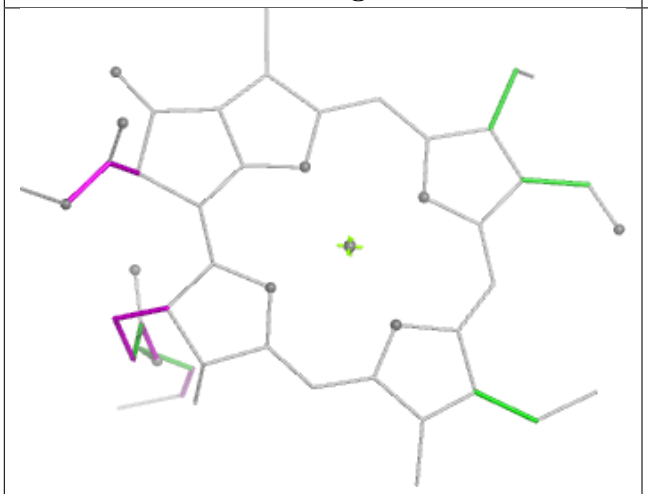
Ligand CHL 3 309



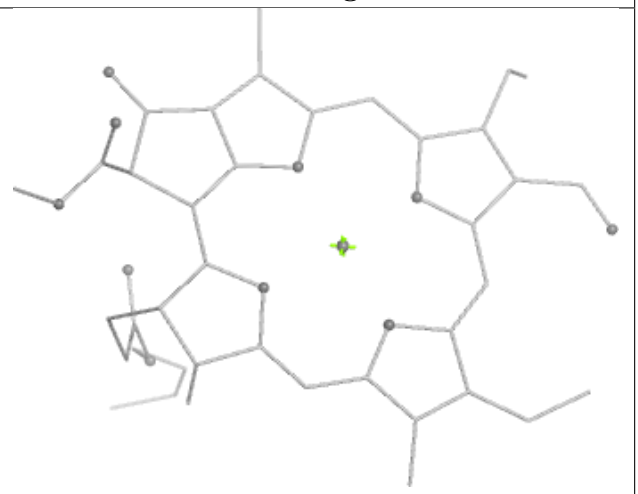
Bond lengths



Bond angles

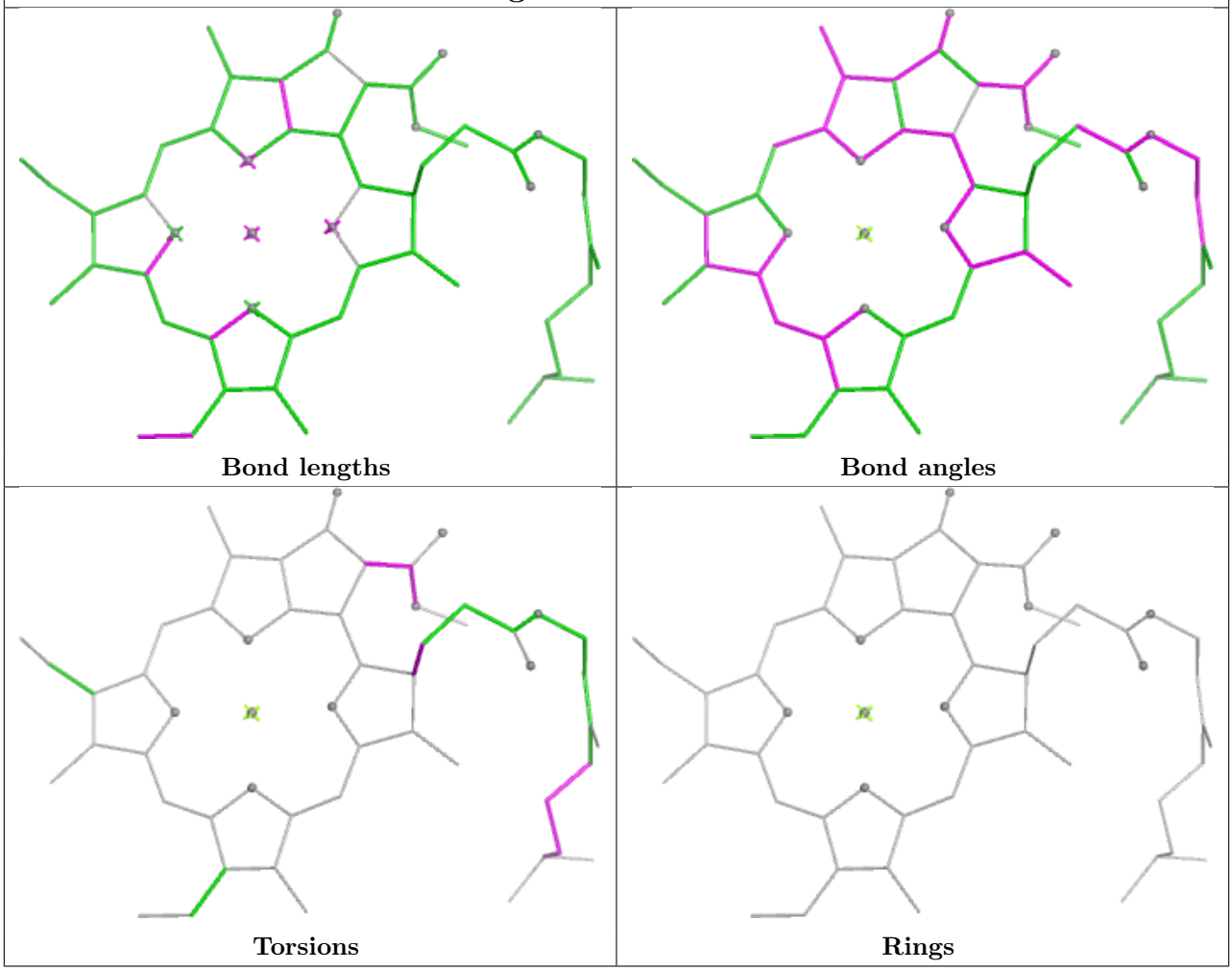


Torsions

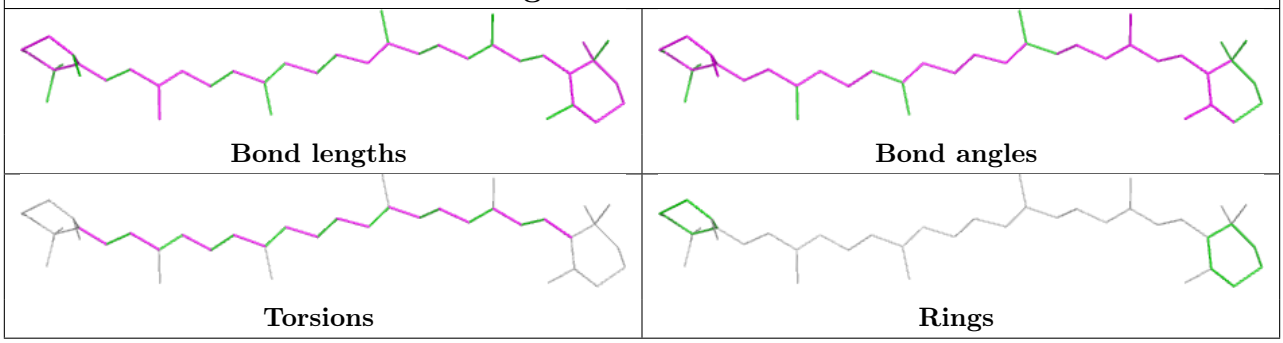


Rings

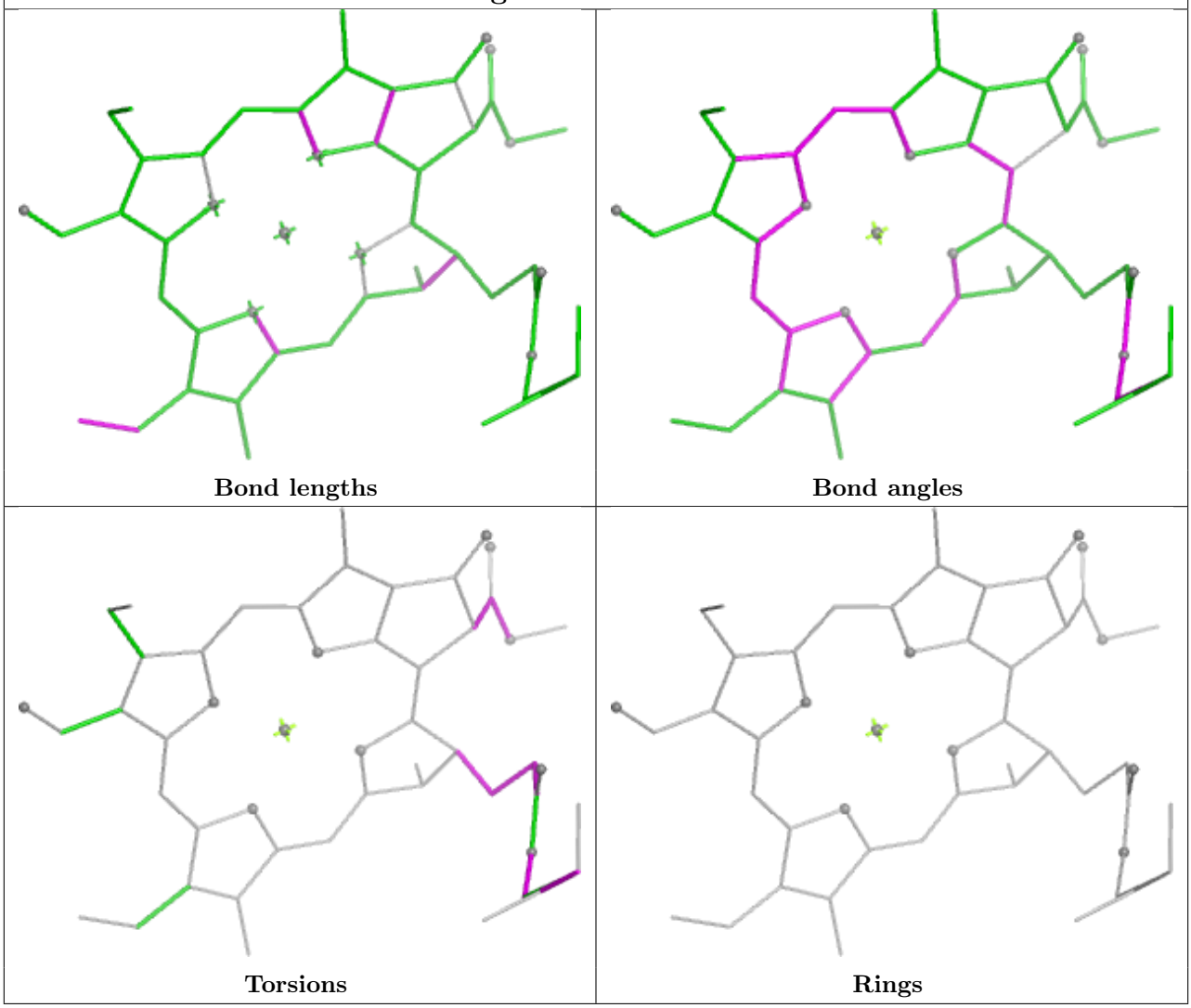
Ligand CLA 4 603



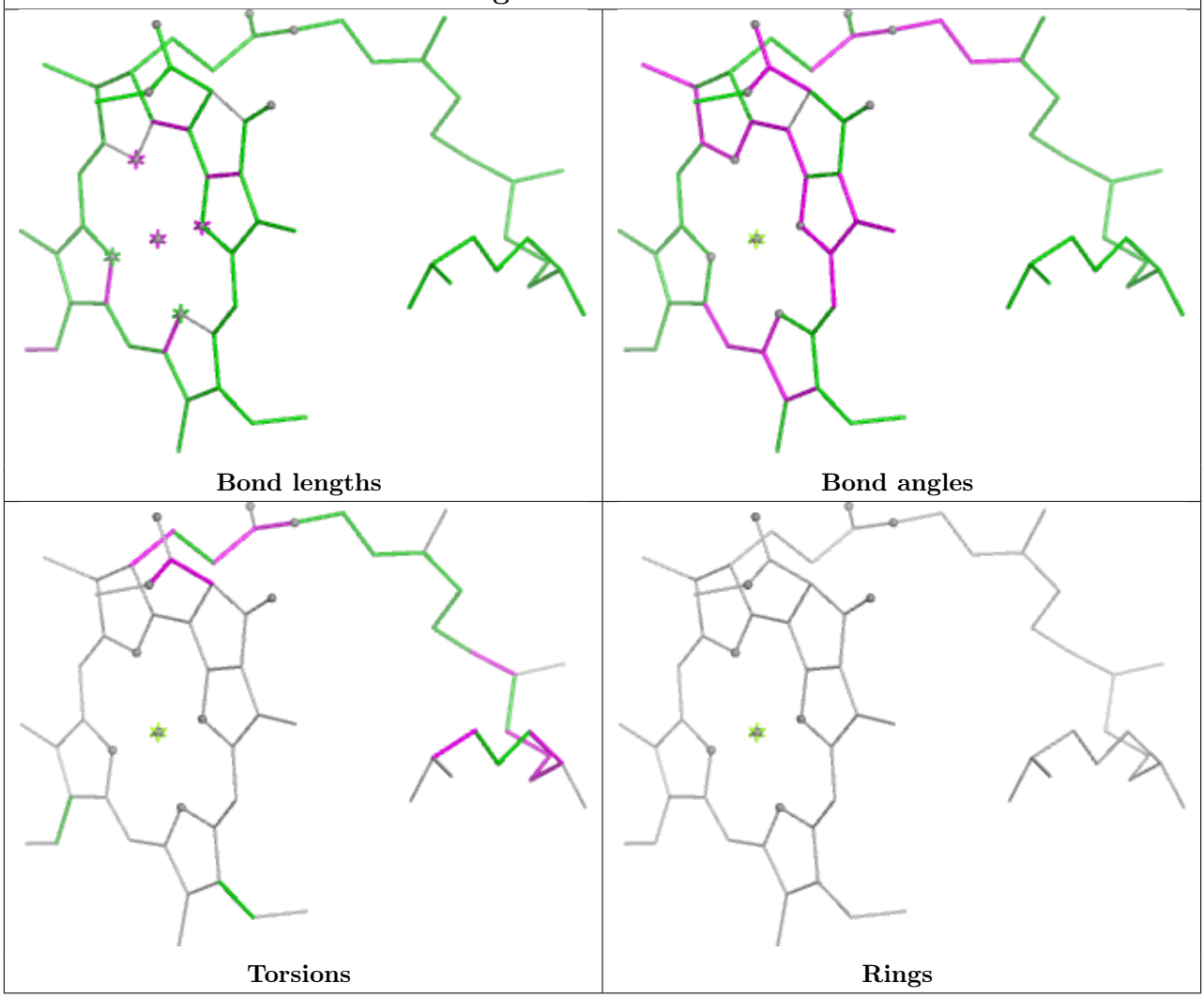
Ligand BCR B 617



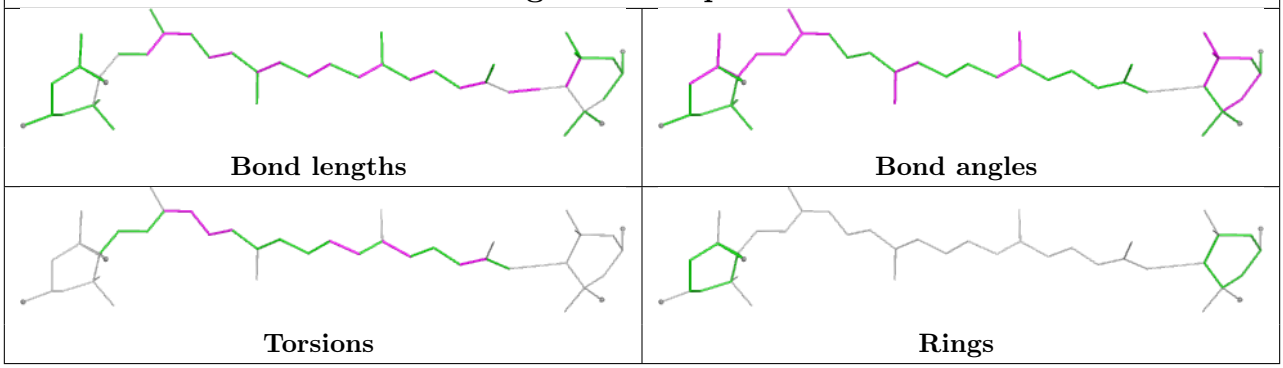
Ligand CHL 0 605

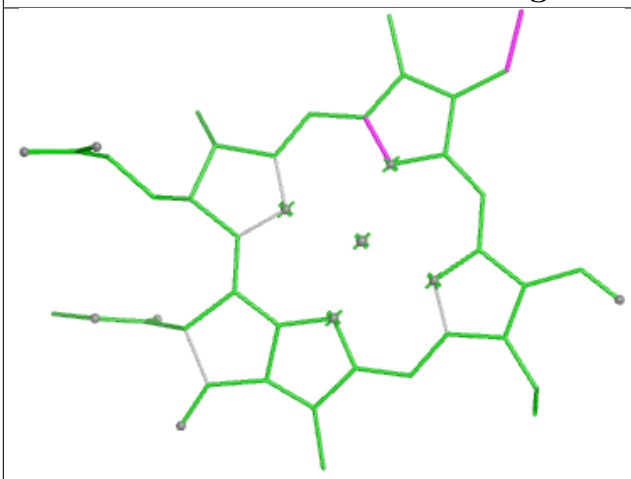
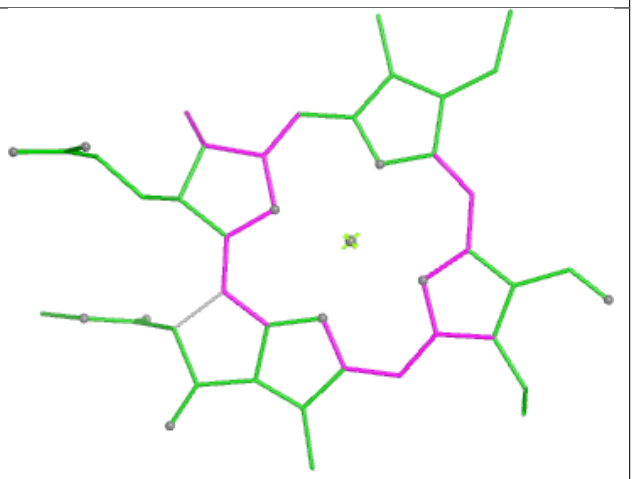
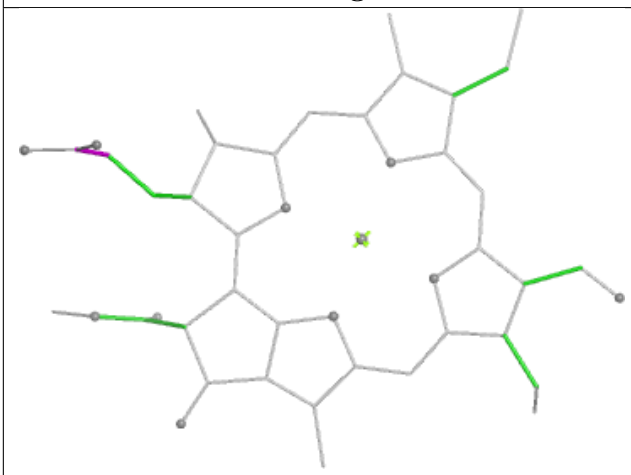
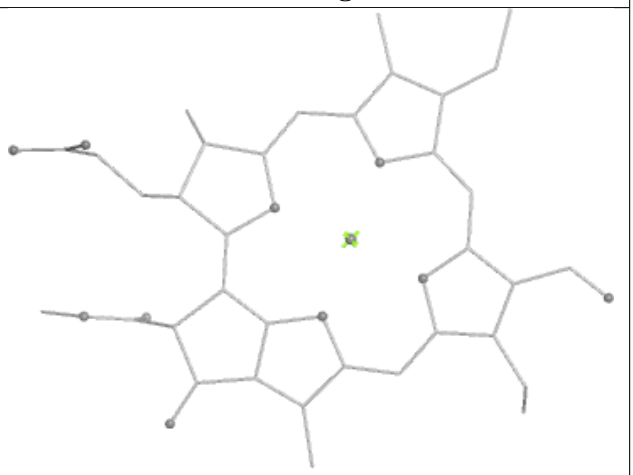


Ligand CLA C 603



Ligand NEX p 618



Ligand CHL s 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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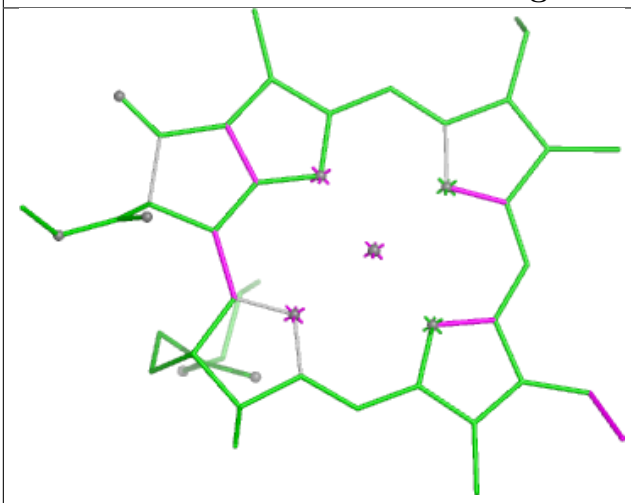	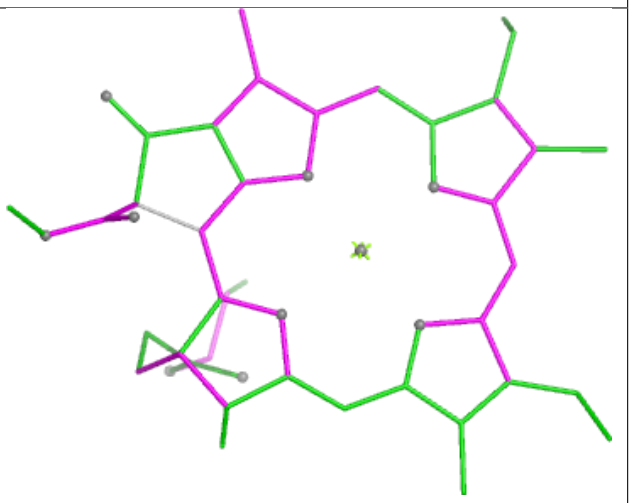
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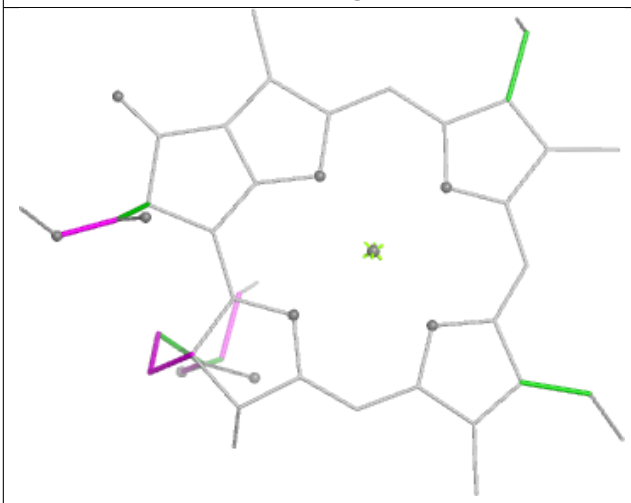
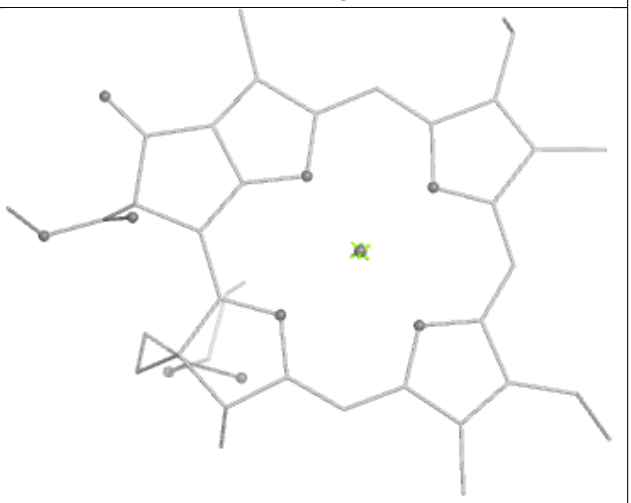
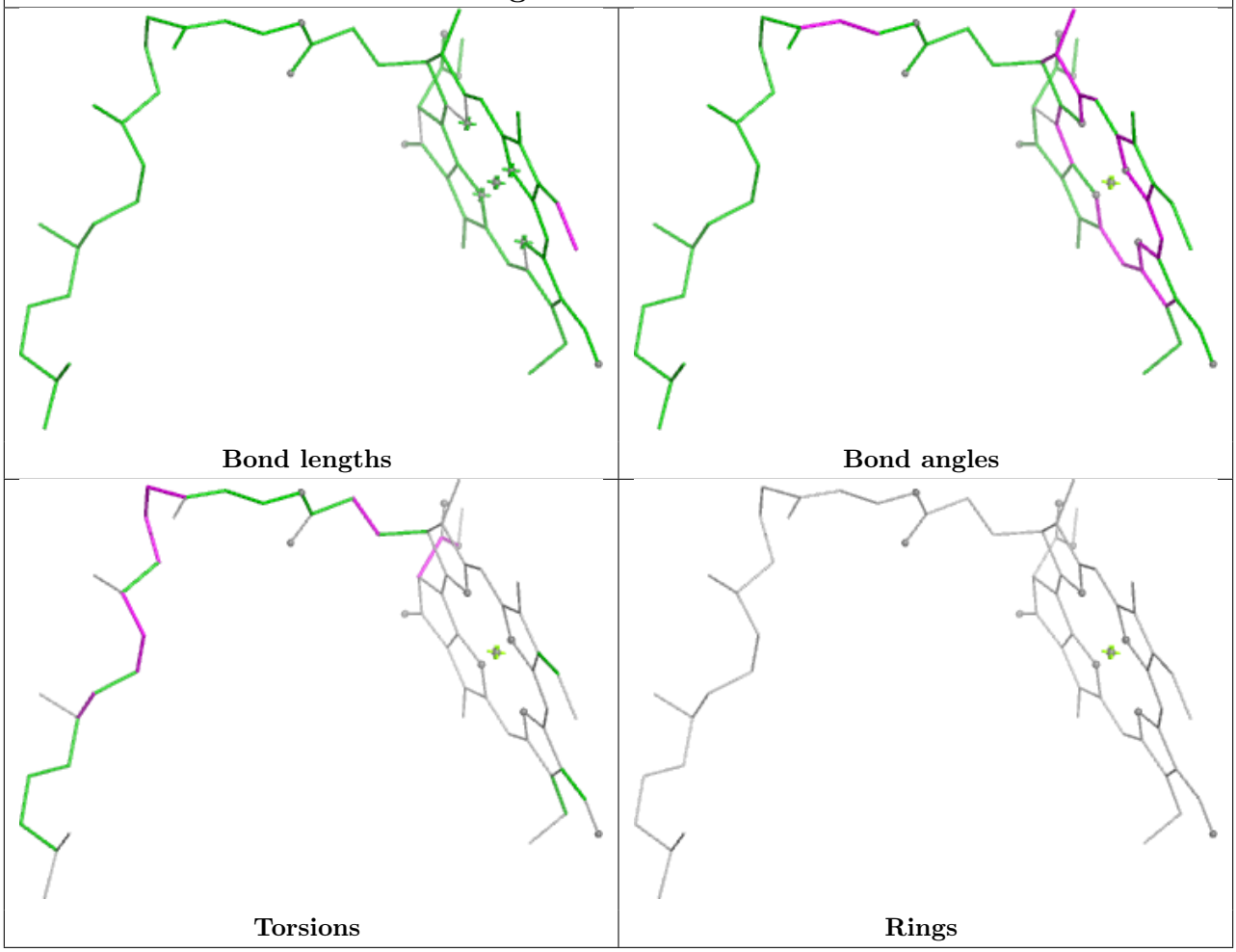
	
Torsions	**Rings**

Ligand CHL 1 606



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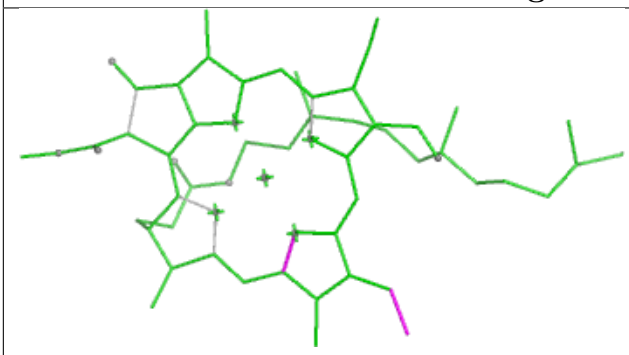	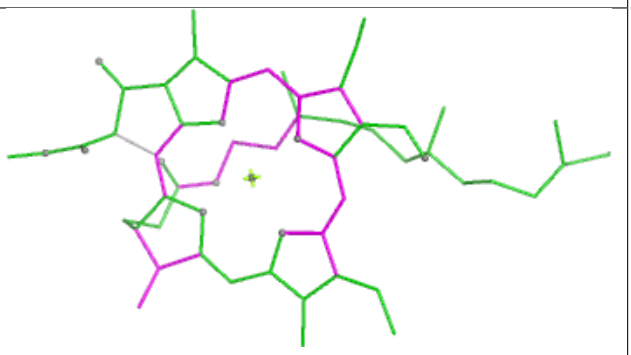
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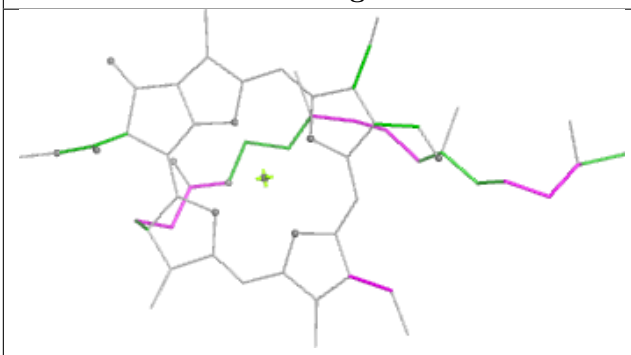
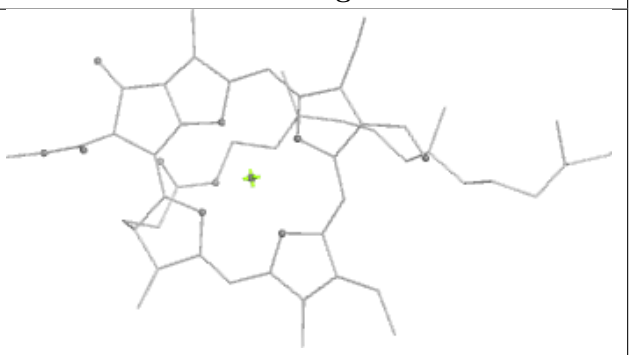
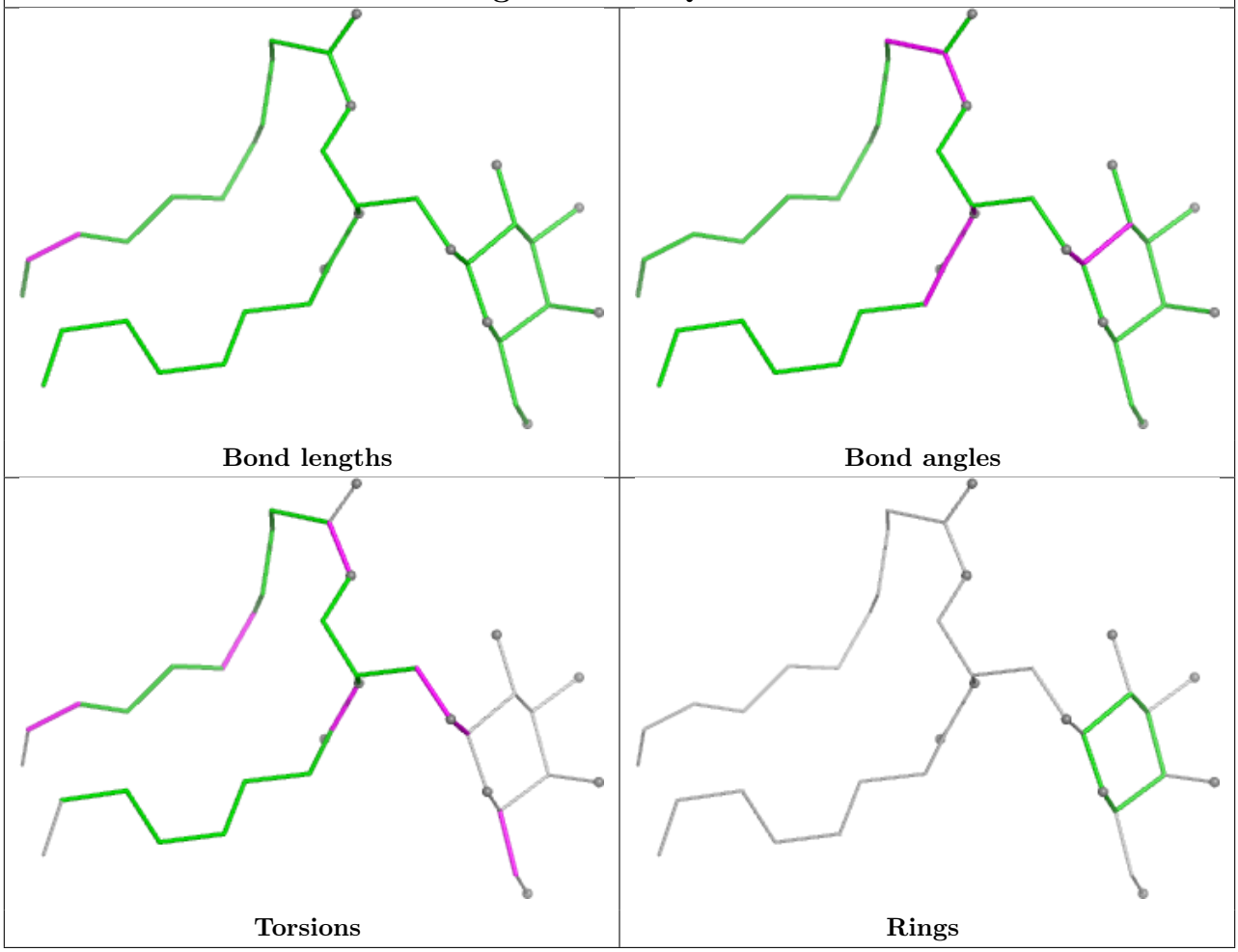
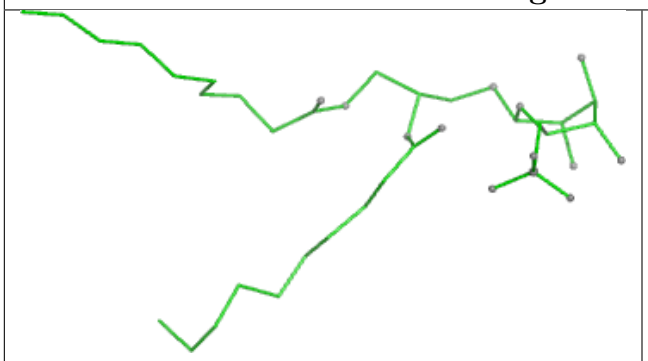
	
Torsions	**Rings**

Ligand LMG Q1 101



Ligand SQD 6 301



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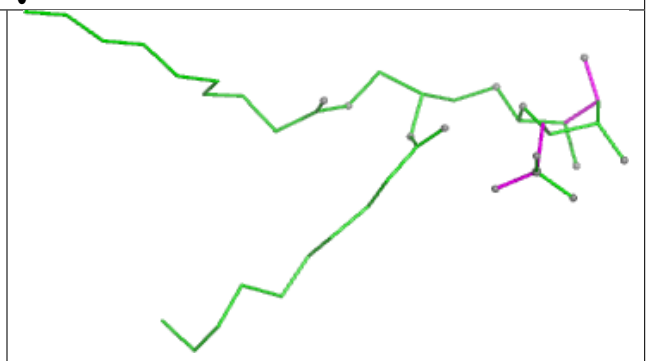

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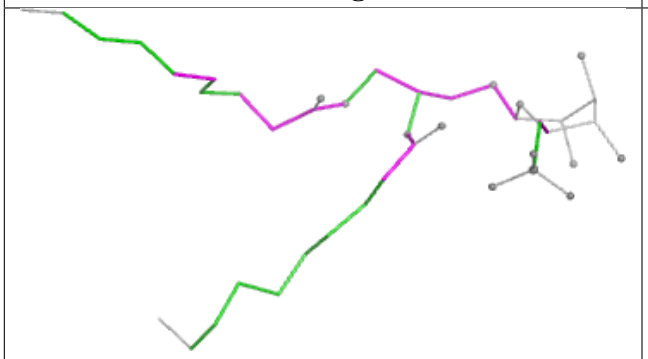

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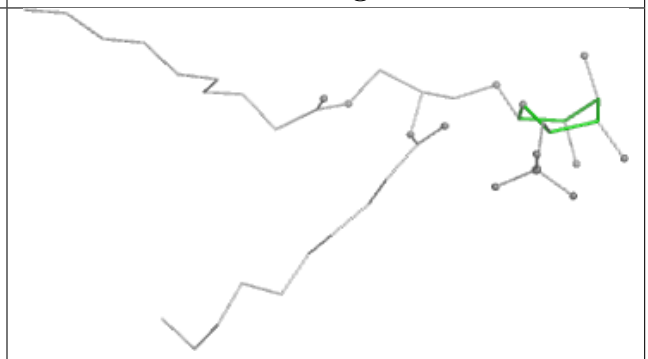
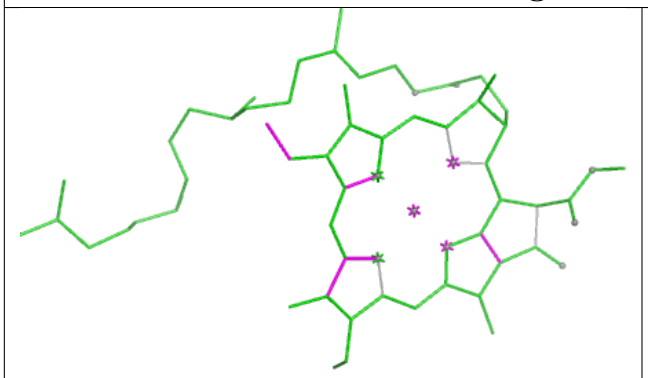


Rings

Ligand CLA S 303



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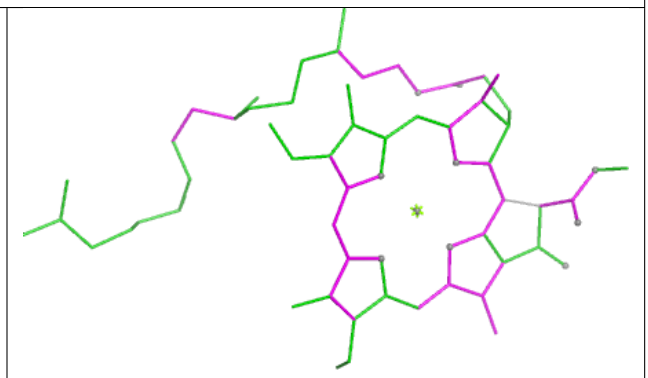

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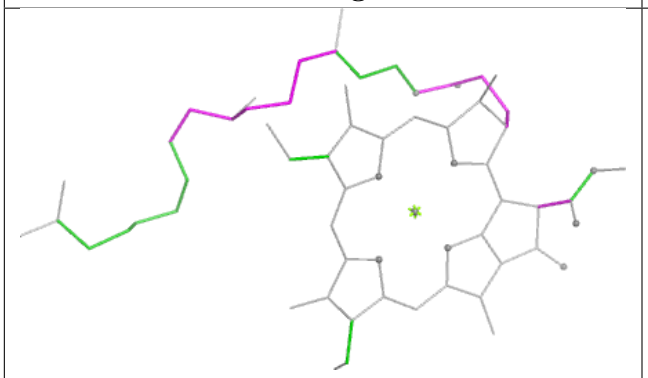

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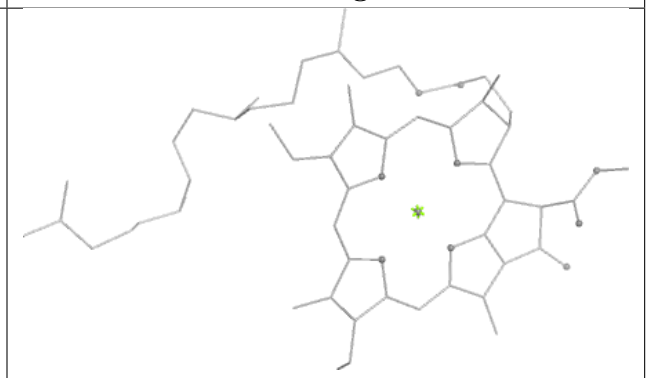
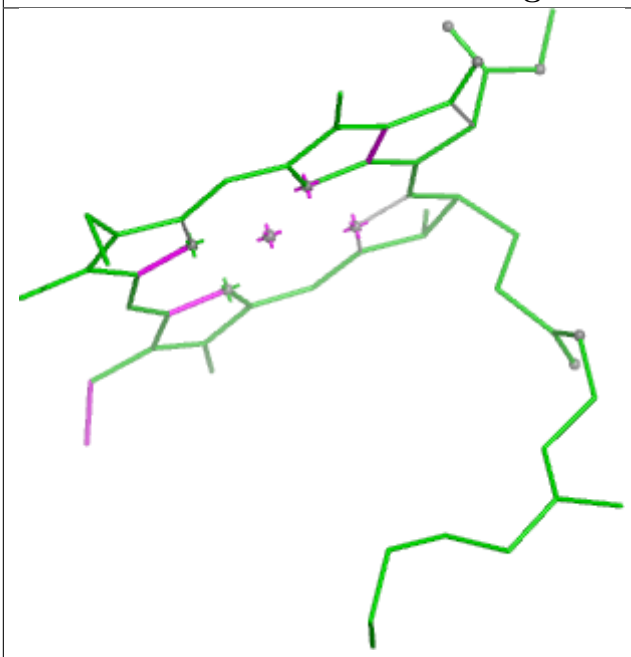


Rings

Ligand CLA Y 314



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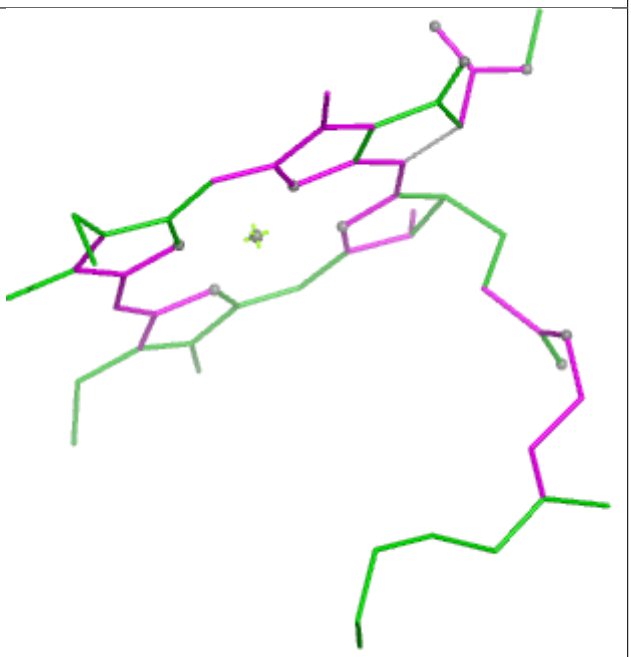

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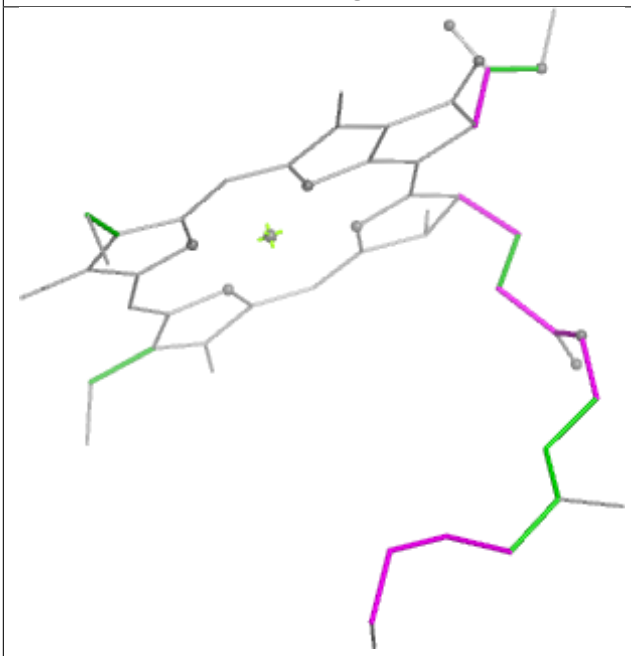

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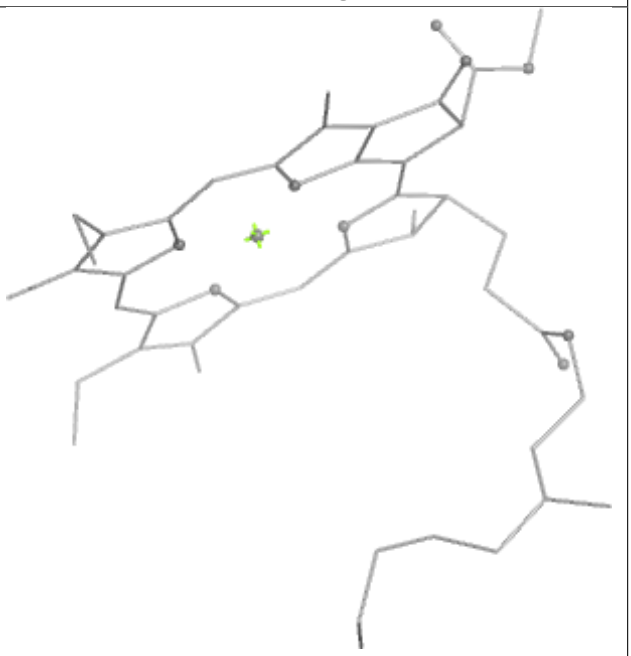

Rings

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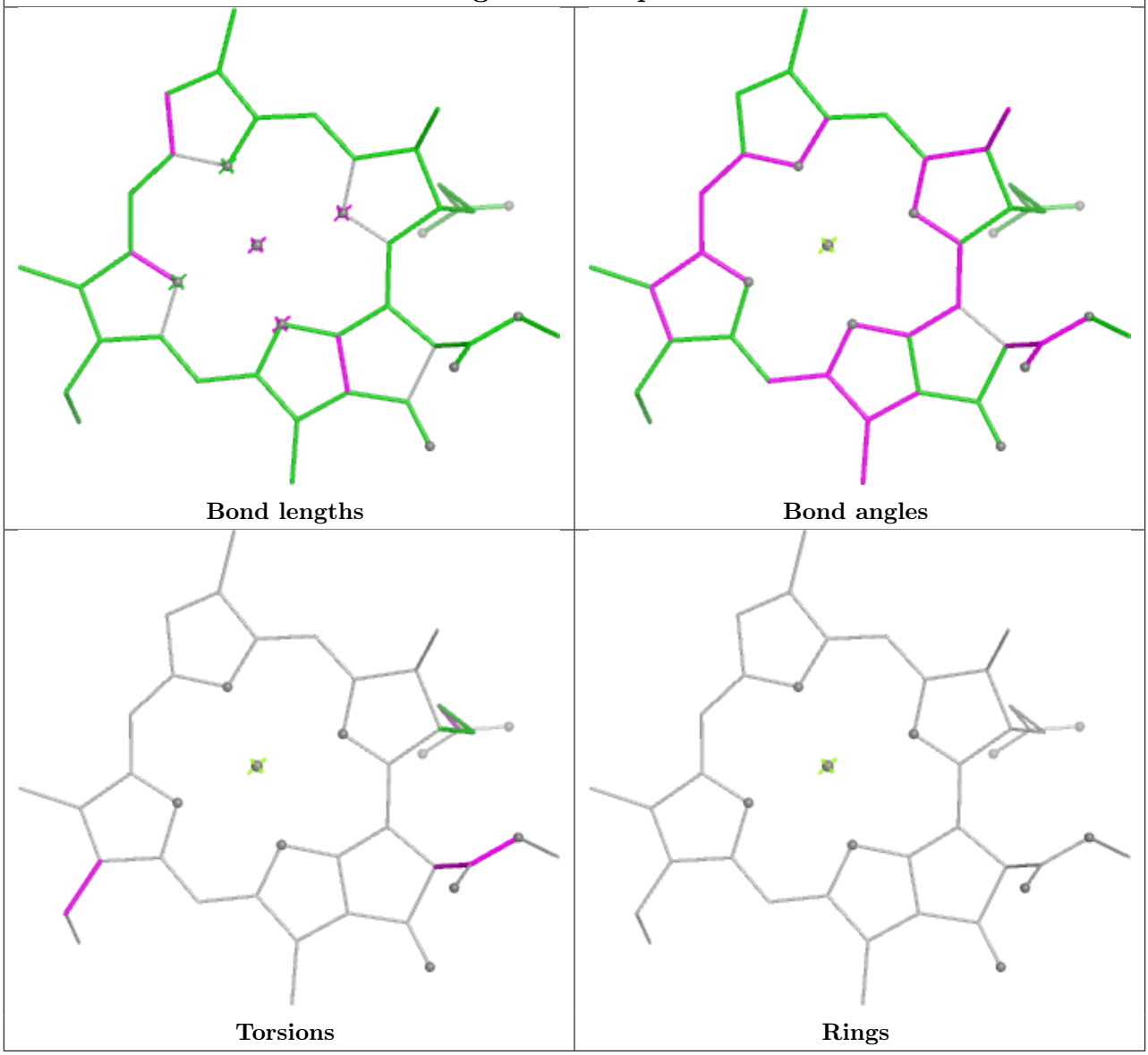
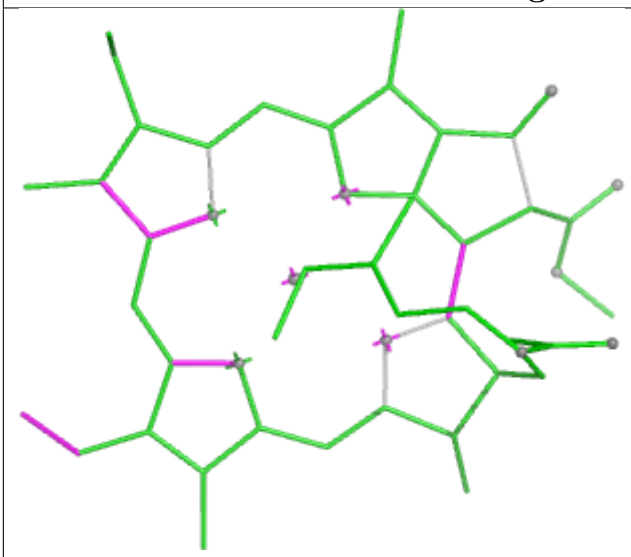


Ligand CLA 5 614



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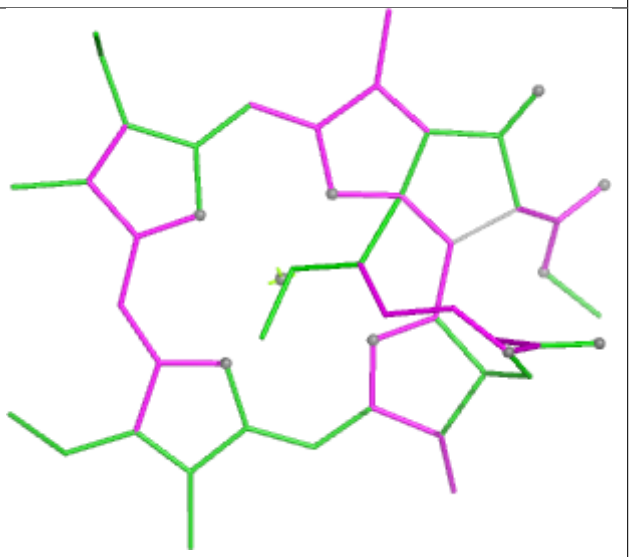

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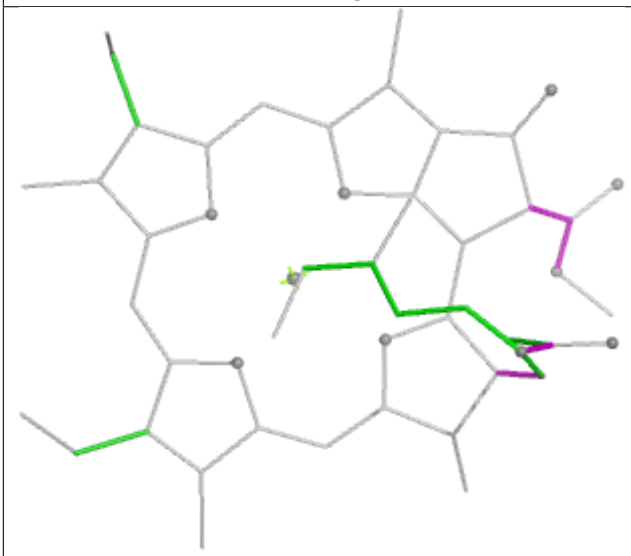

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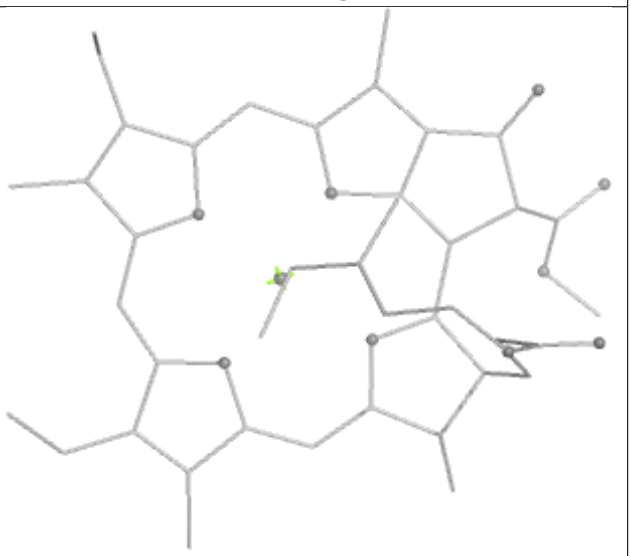

Rings

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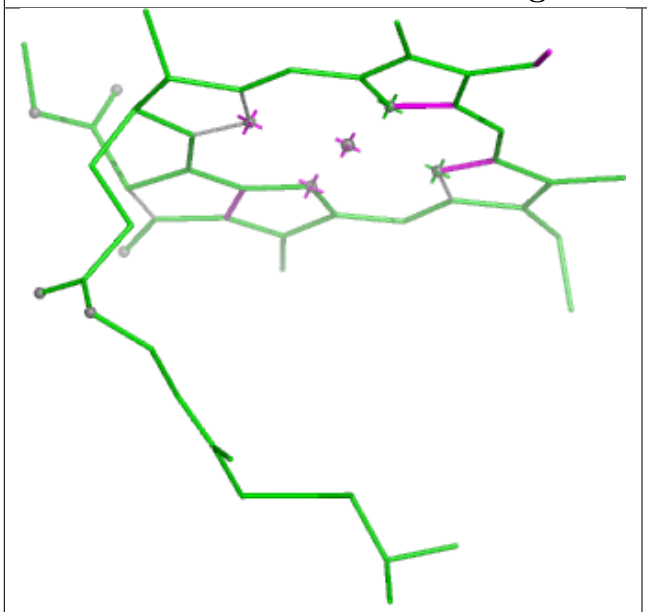

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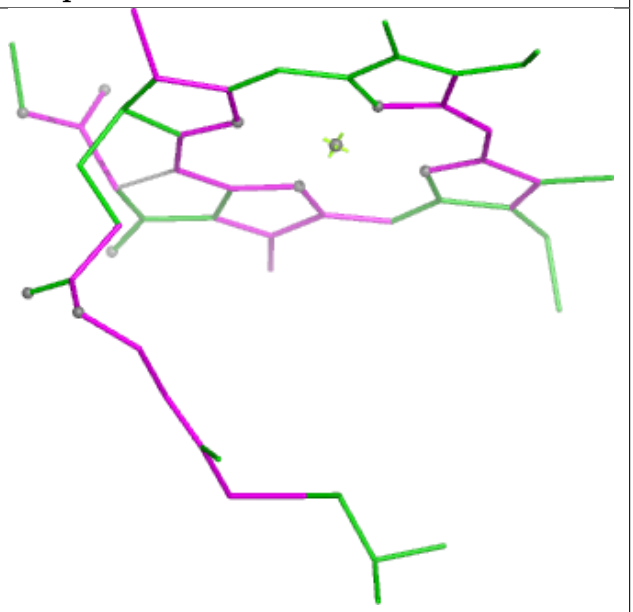

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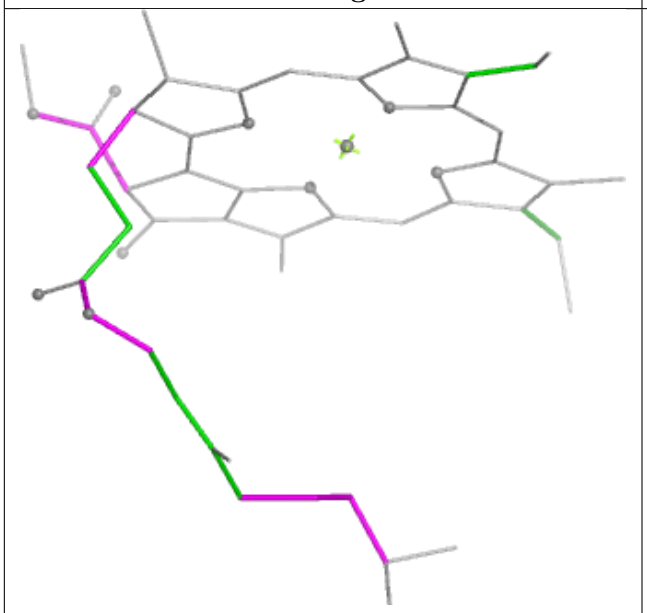

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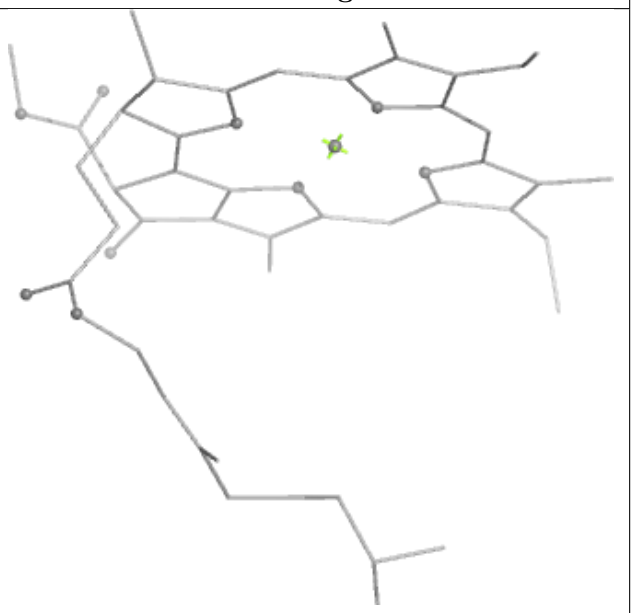
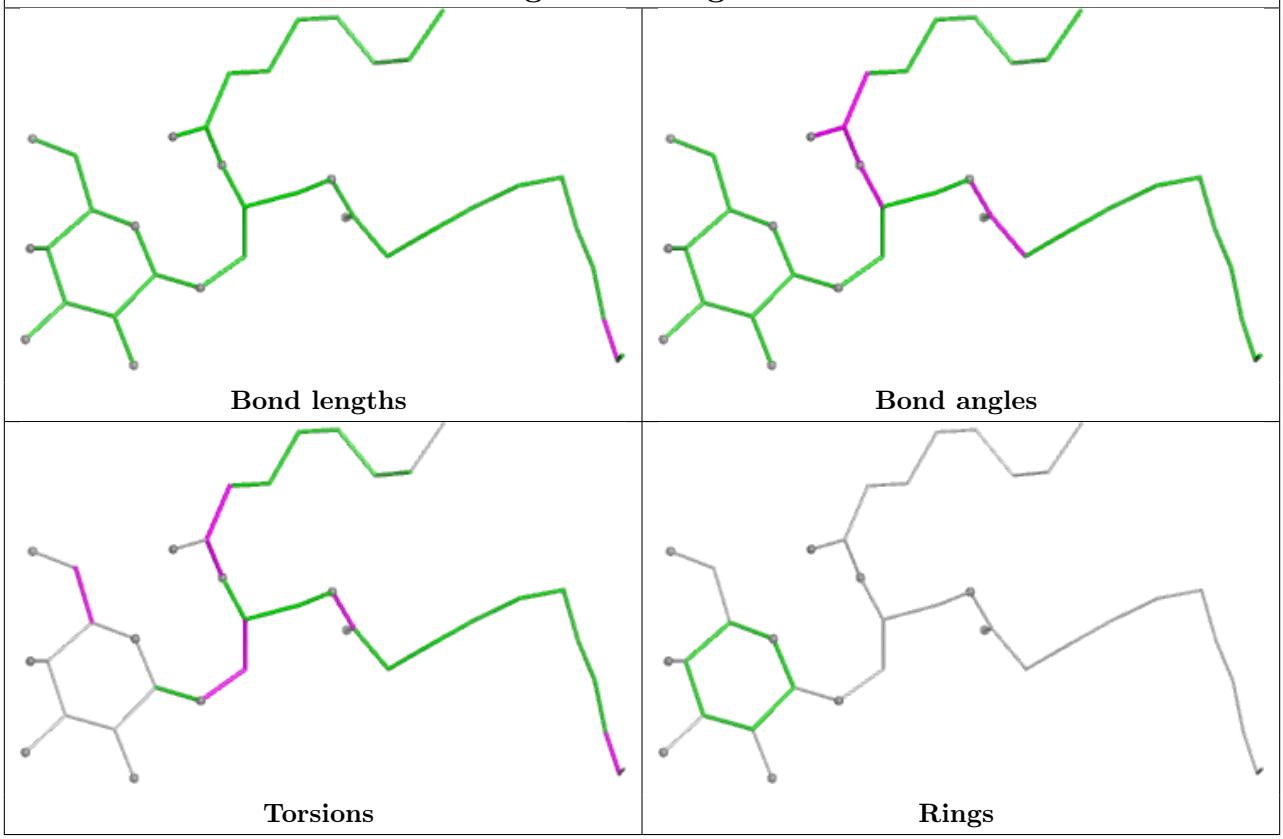


Rings

Ligand LMG g 320



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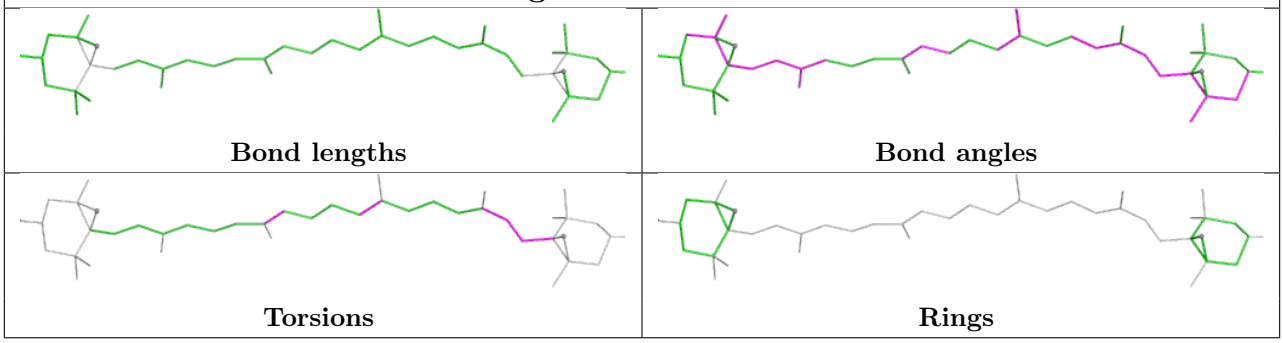

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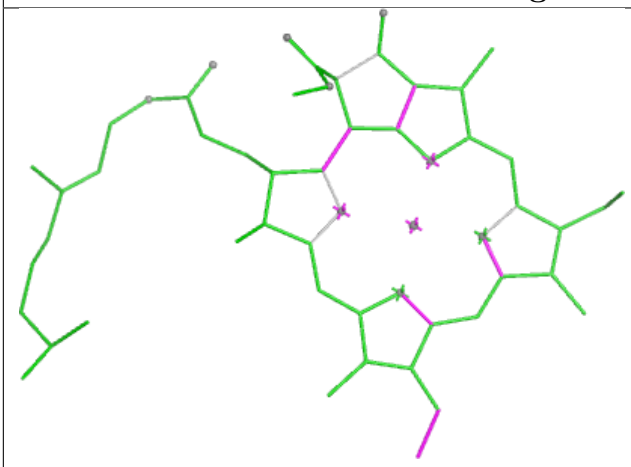

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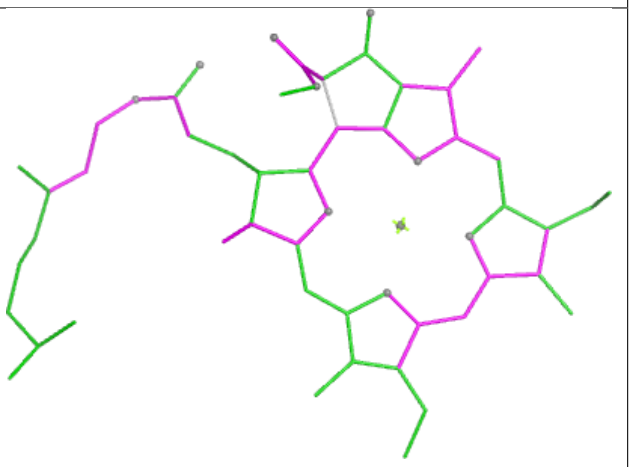
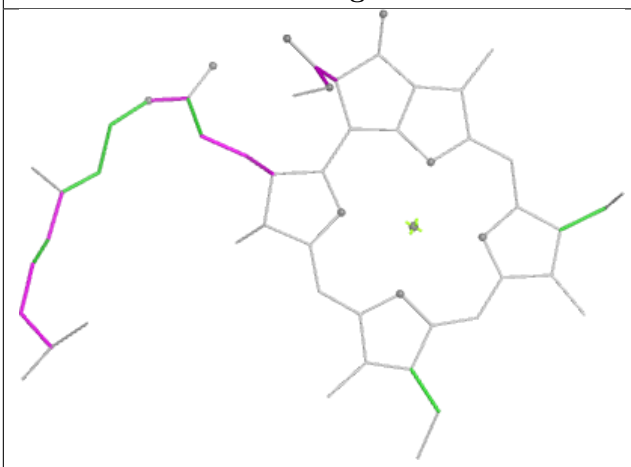


Bond angles



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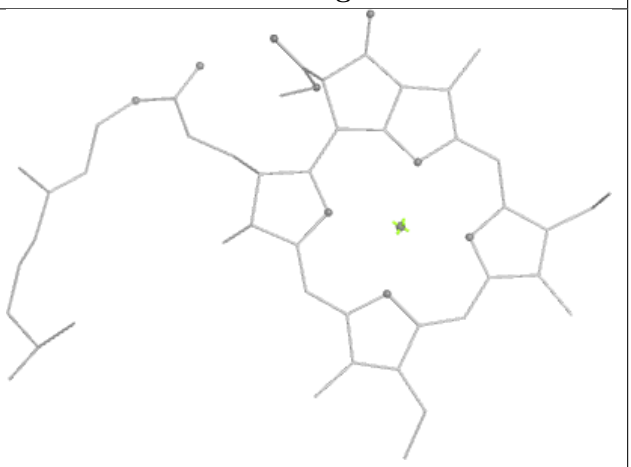
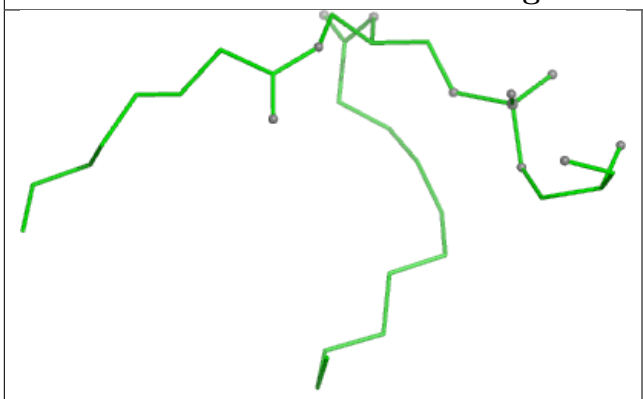
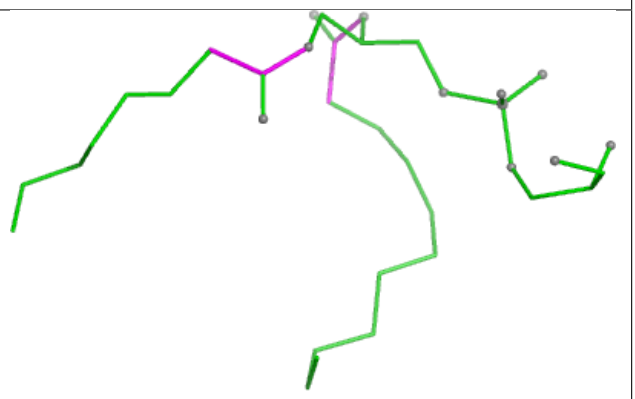
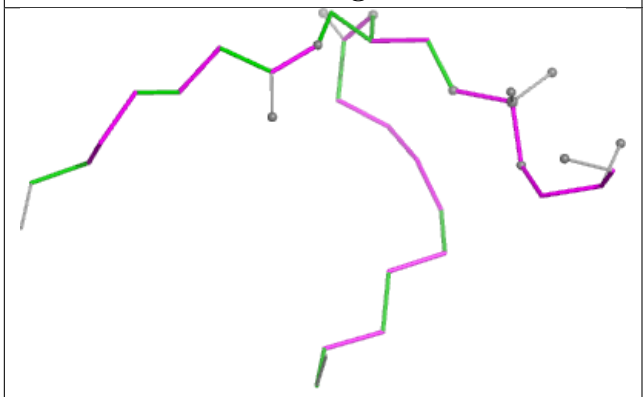
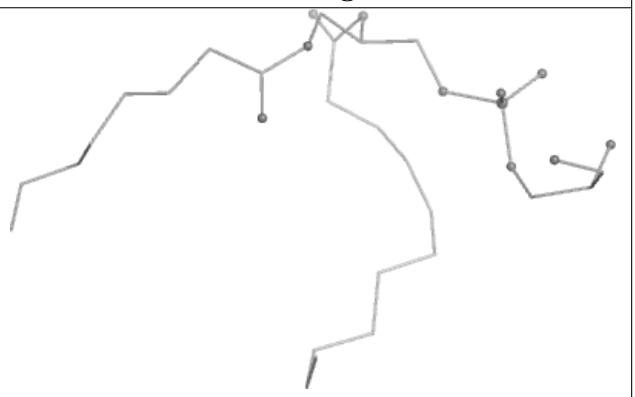
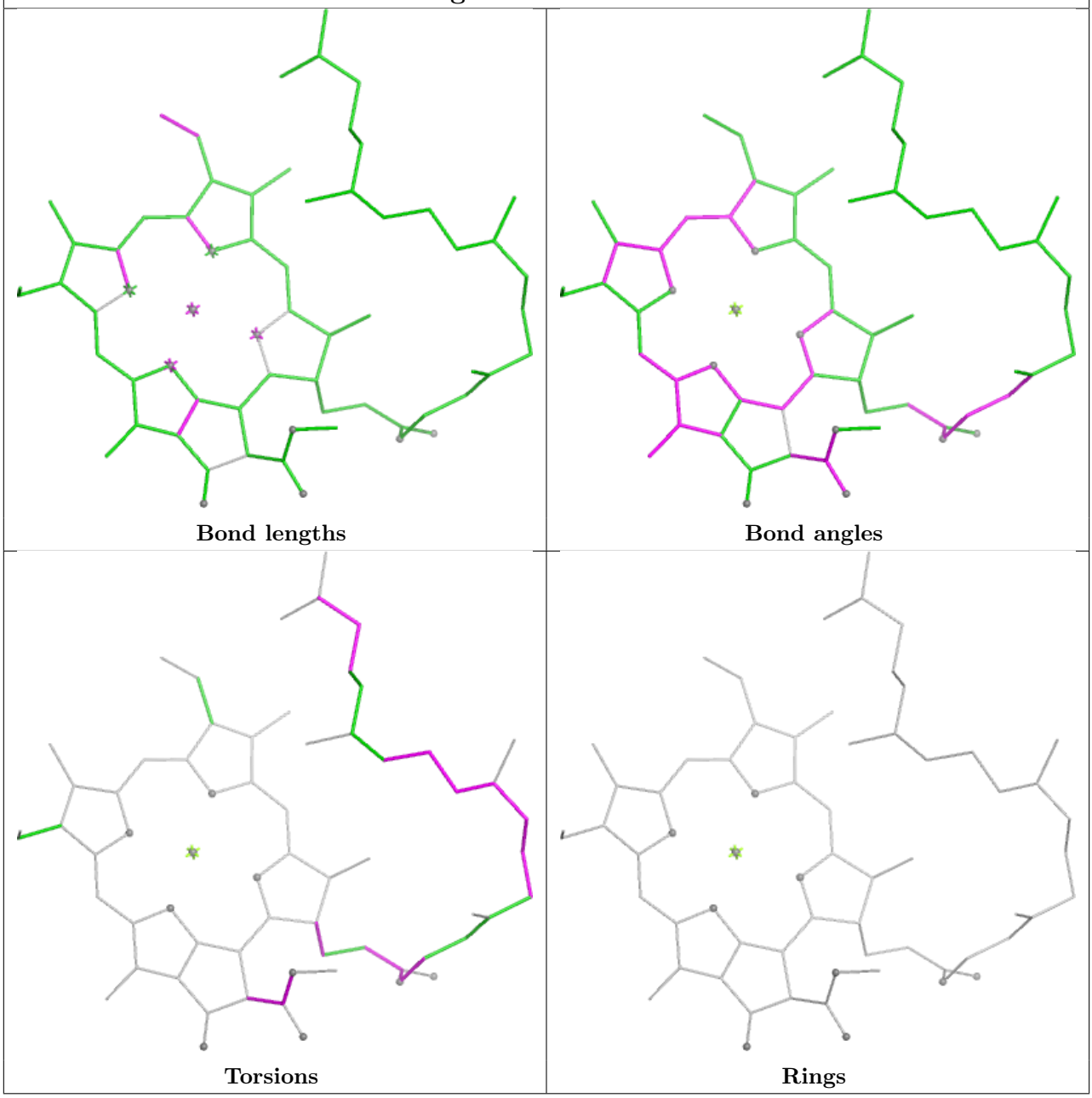


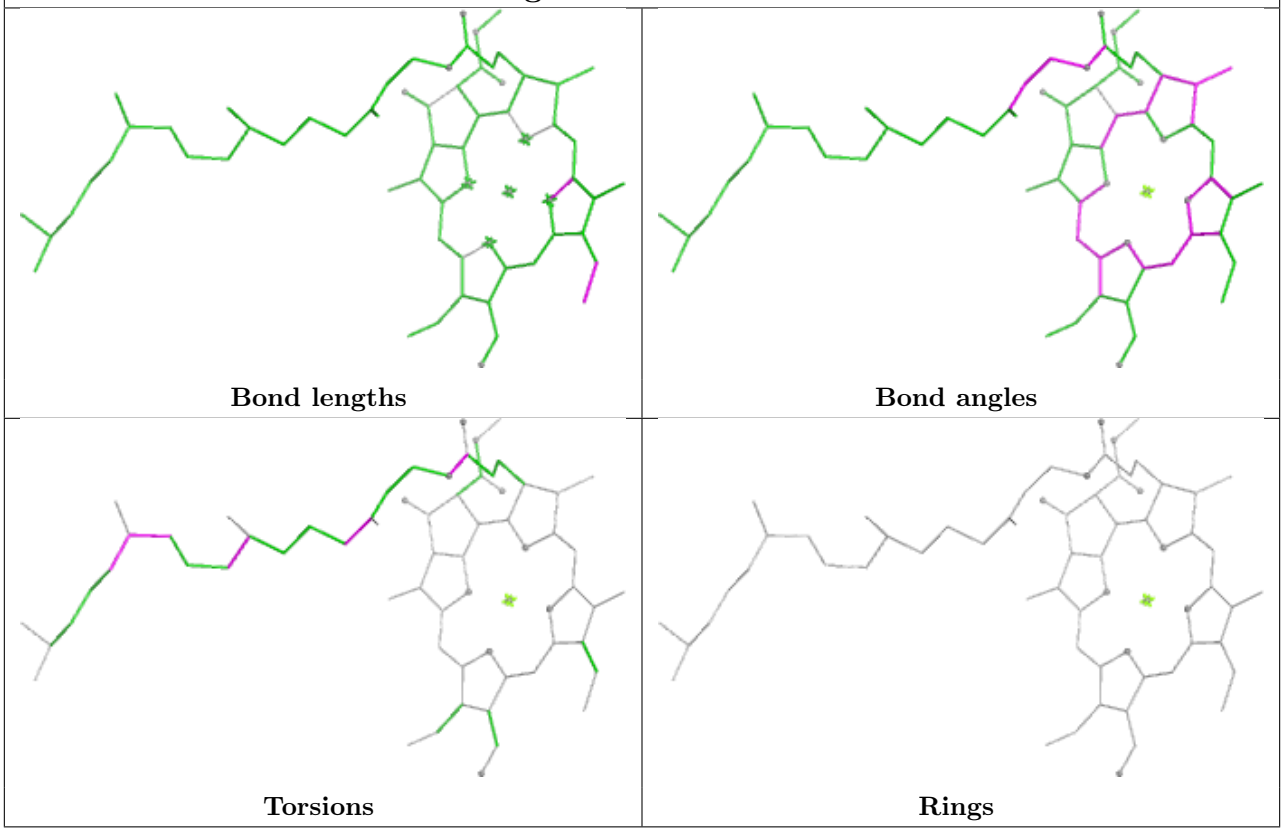
Rings

Ligand LHG K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 612



Ligand CHL Y 309



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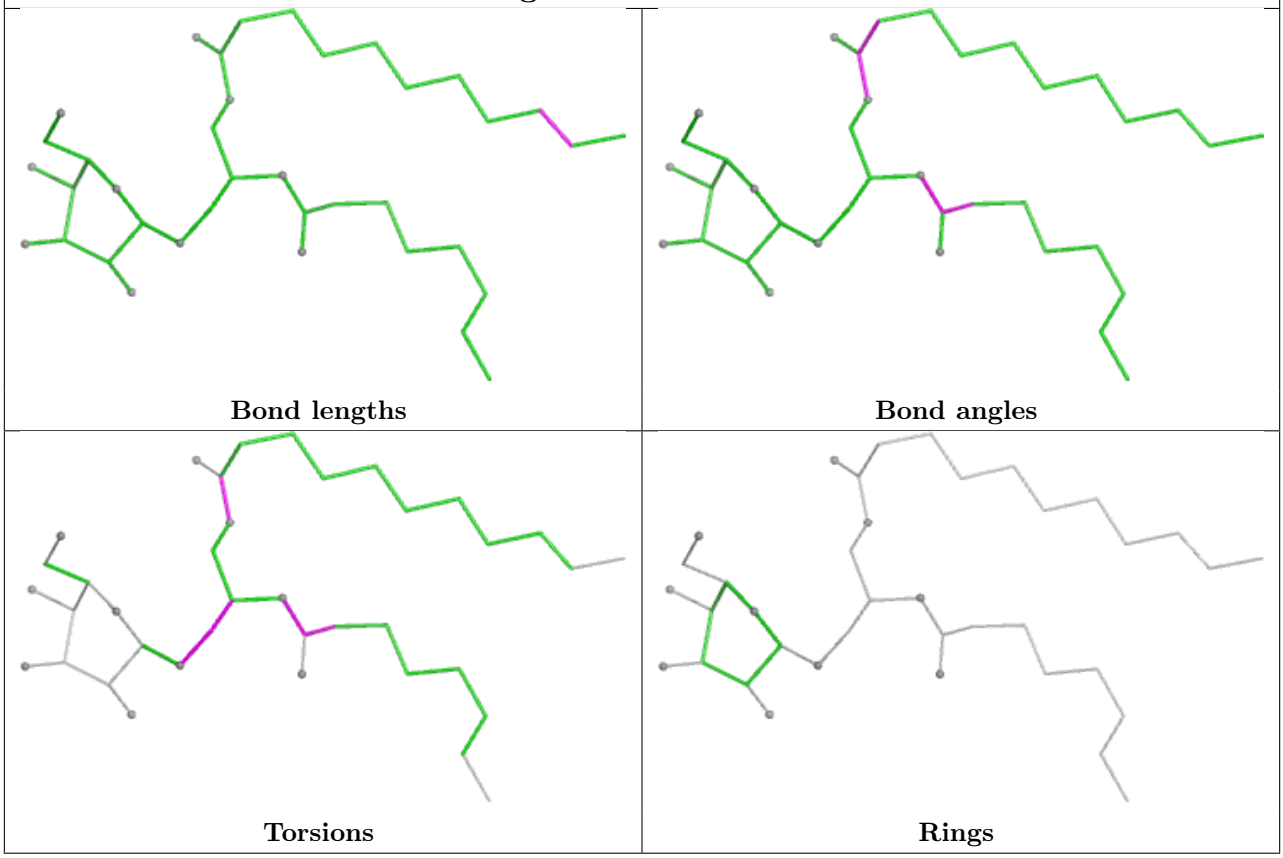
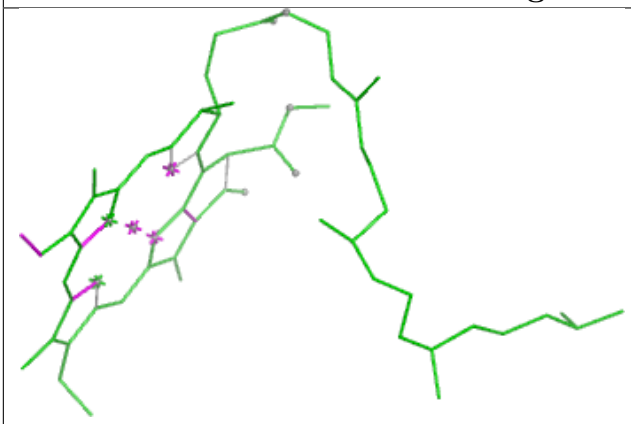
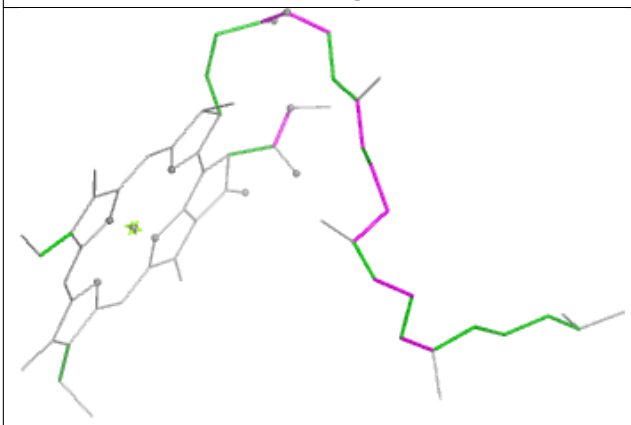


Ligand CLA b 614



Bond lengths

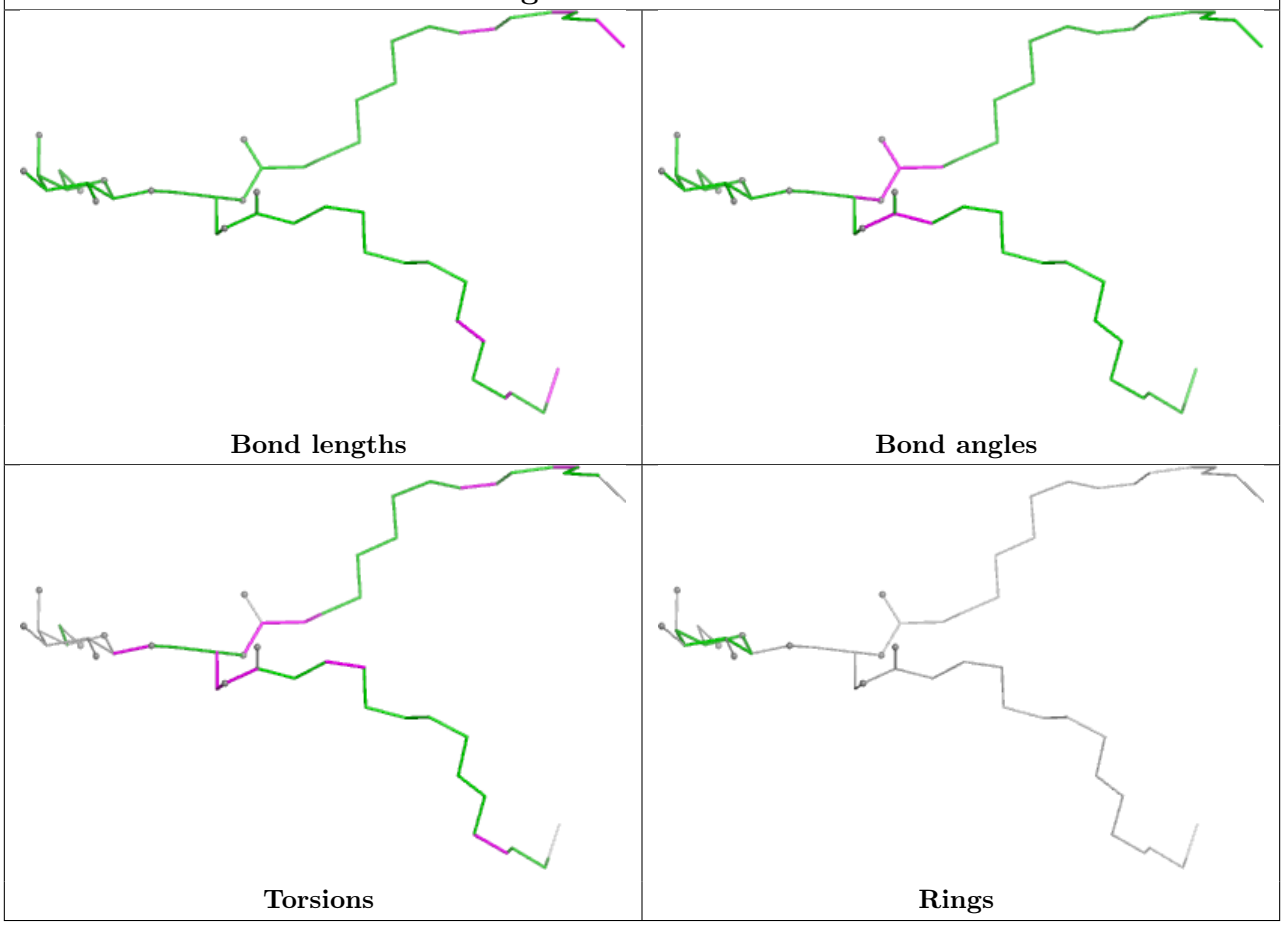
Bond angles



Torsions

Rings

Ligand LMG B 621



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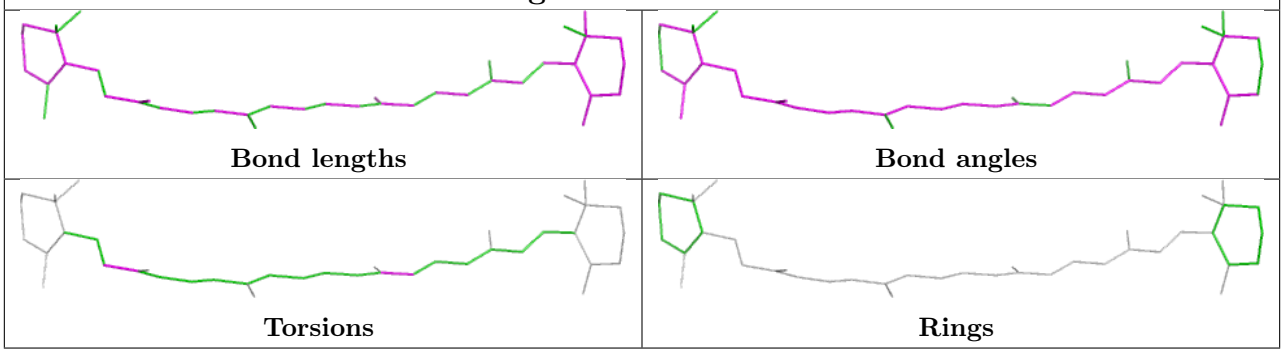

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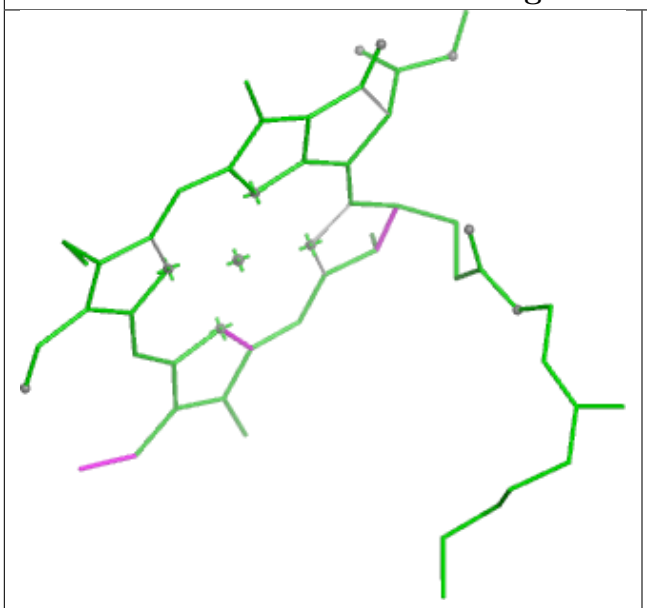
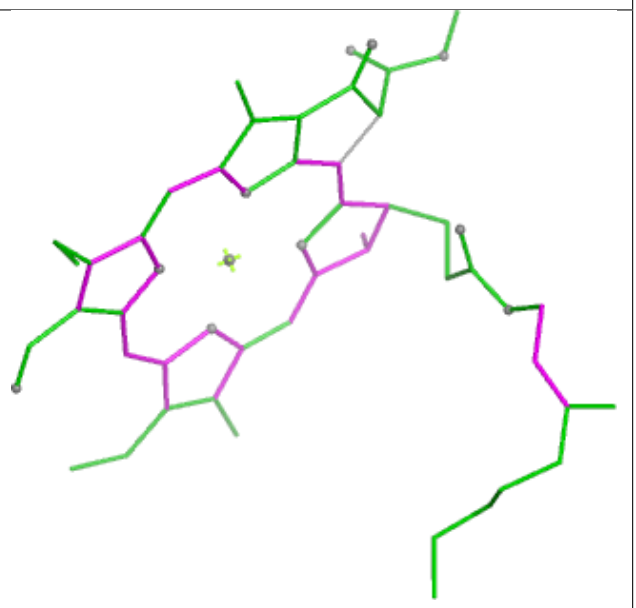


Bond lengths



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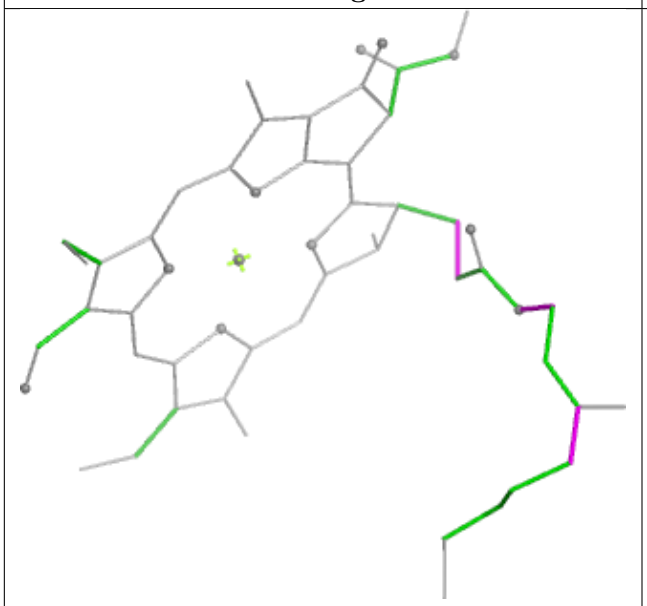

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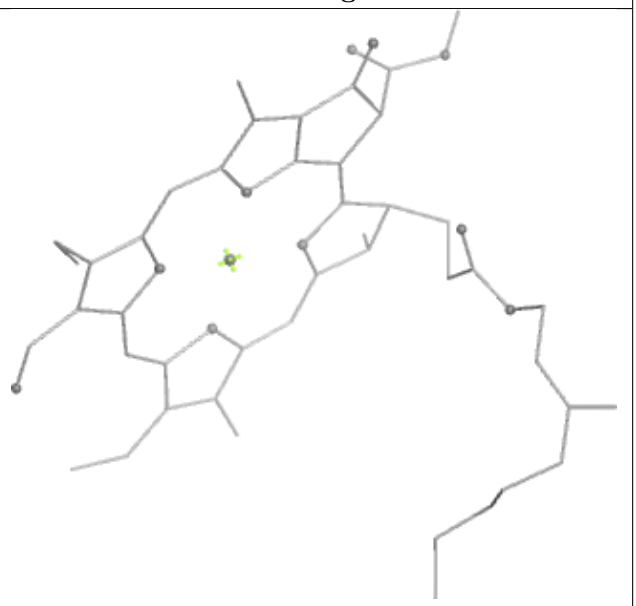
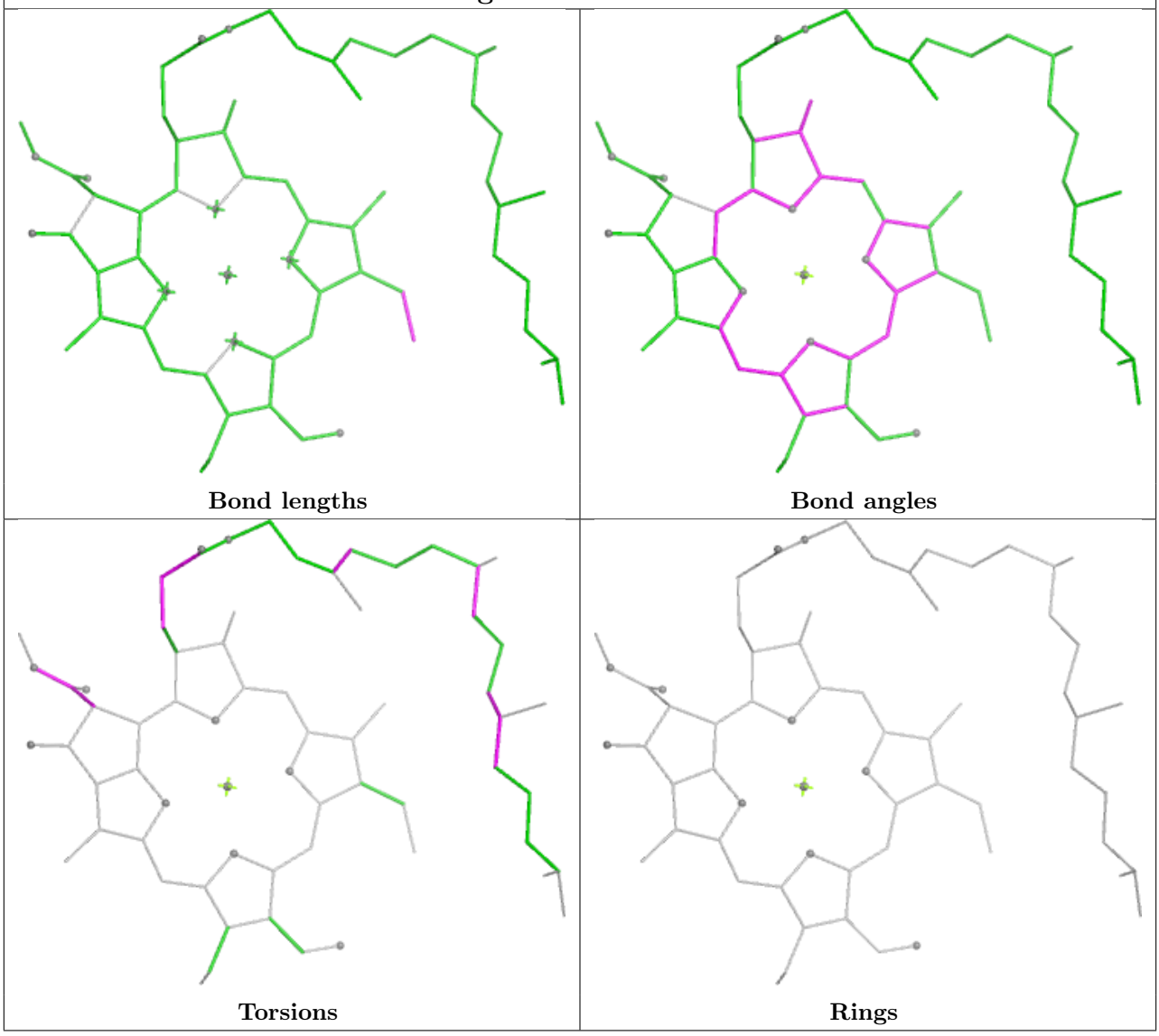
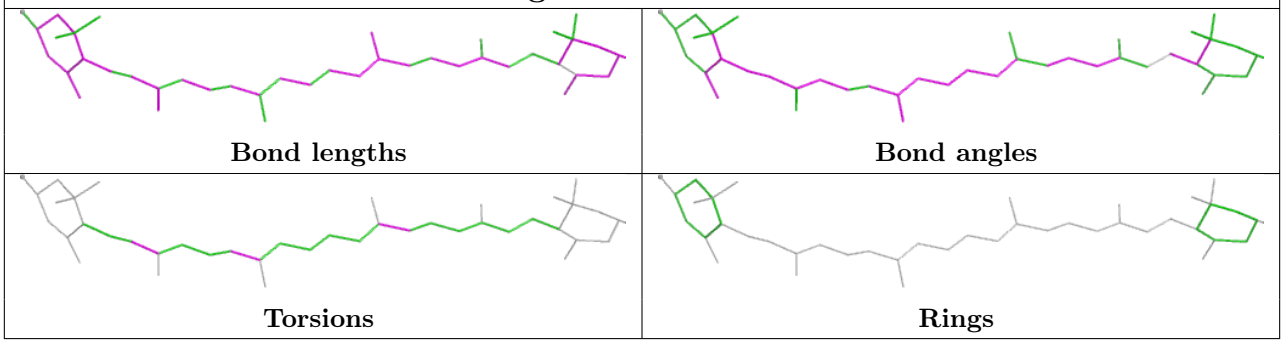


Rings

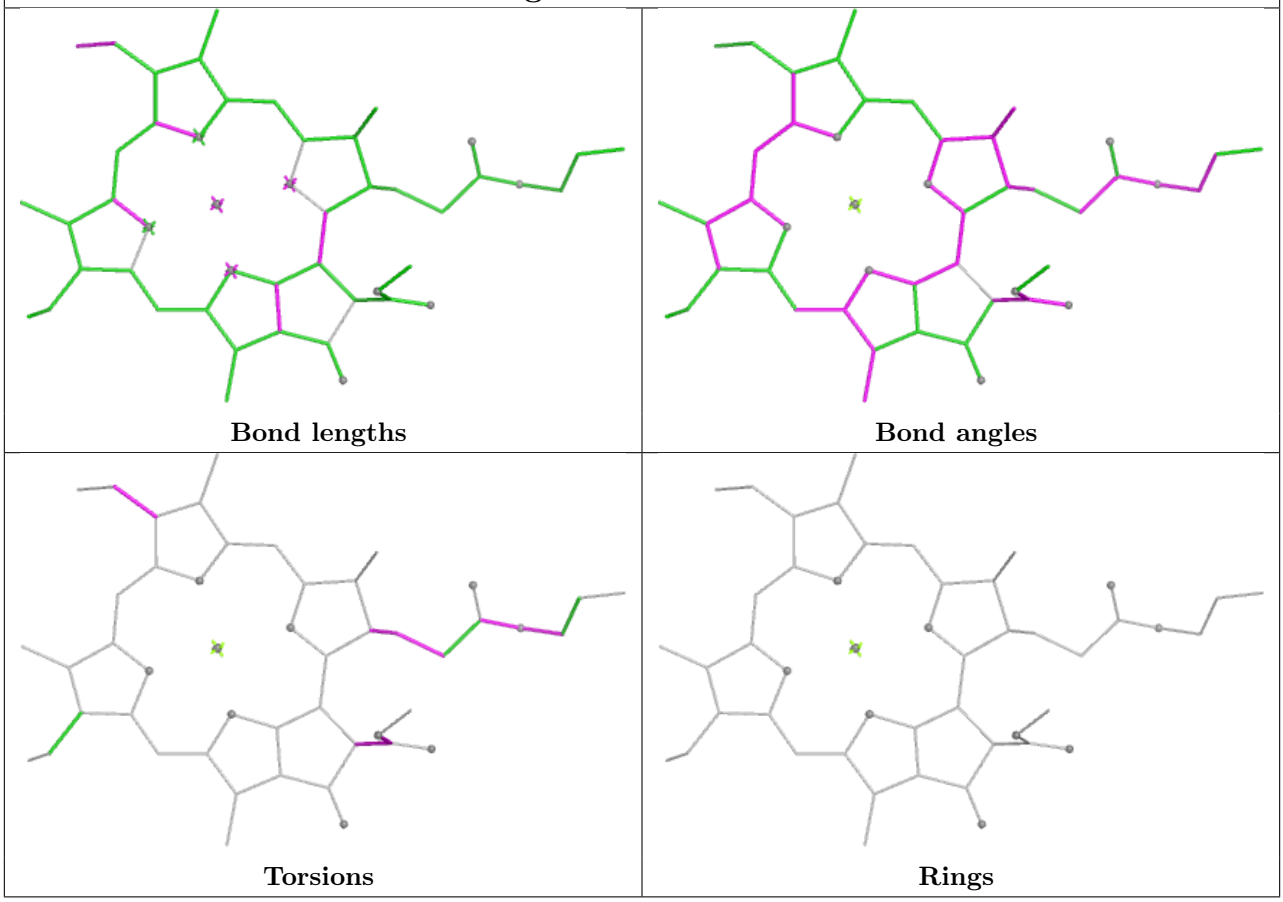
Ligand CHL 6 308



Ligand LUT S 317



Ligand CLA R 307



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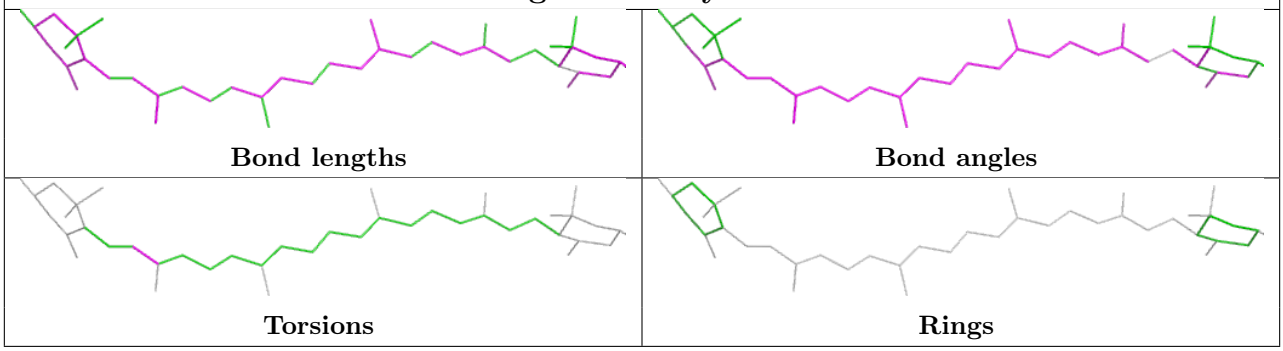

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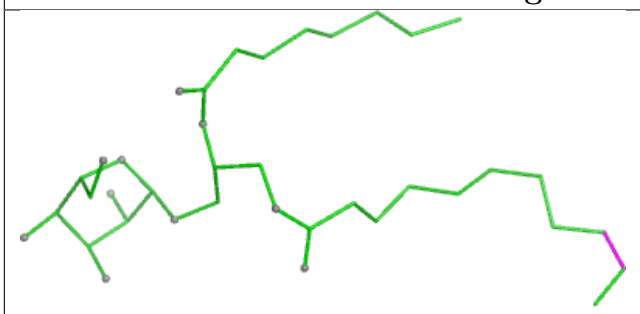
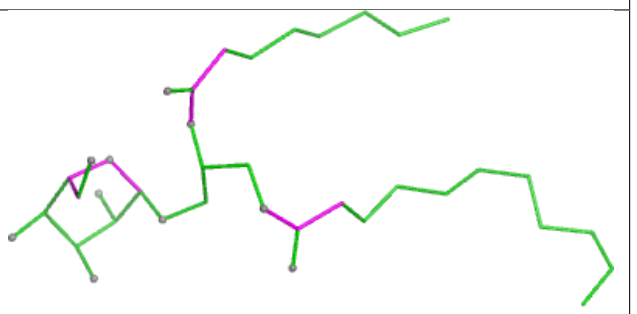
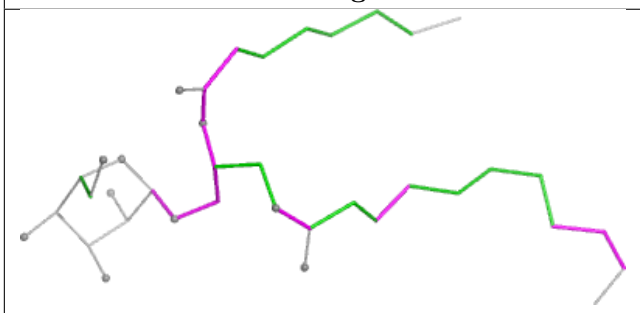
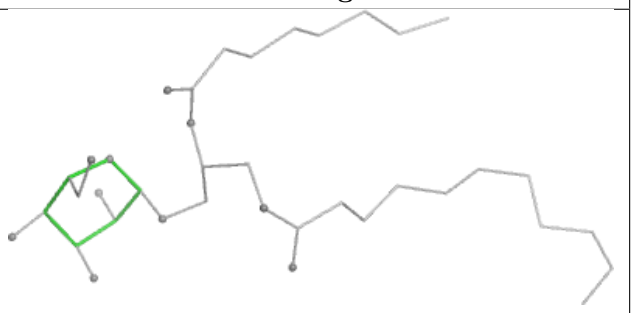
 Bond lengths	 Bond angles
 Torsions	 Rings

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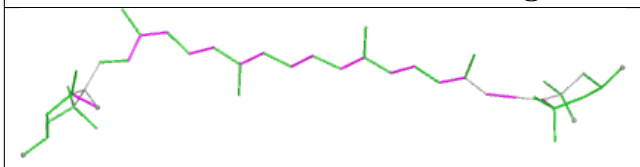
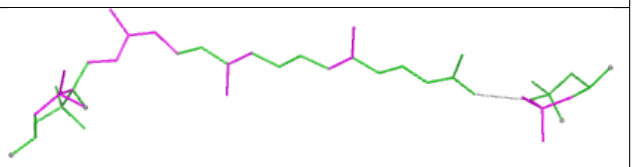
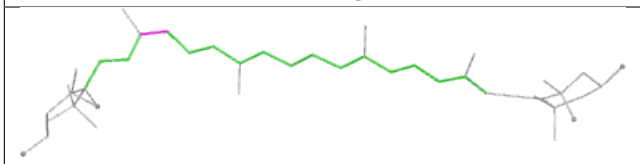
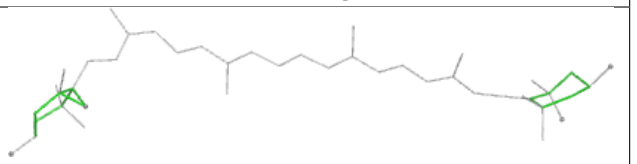
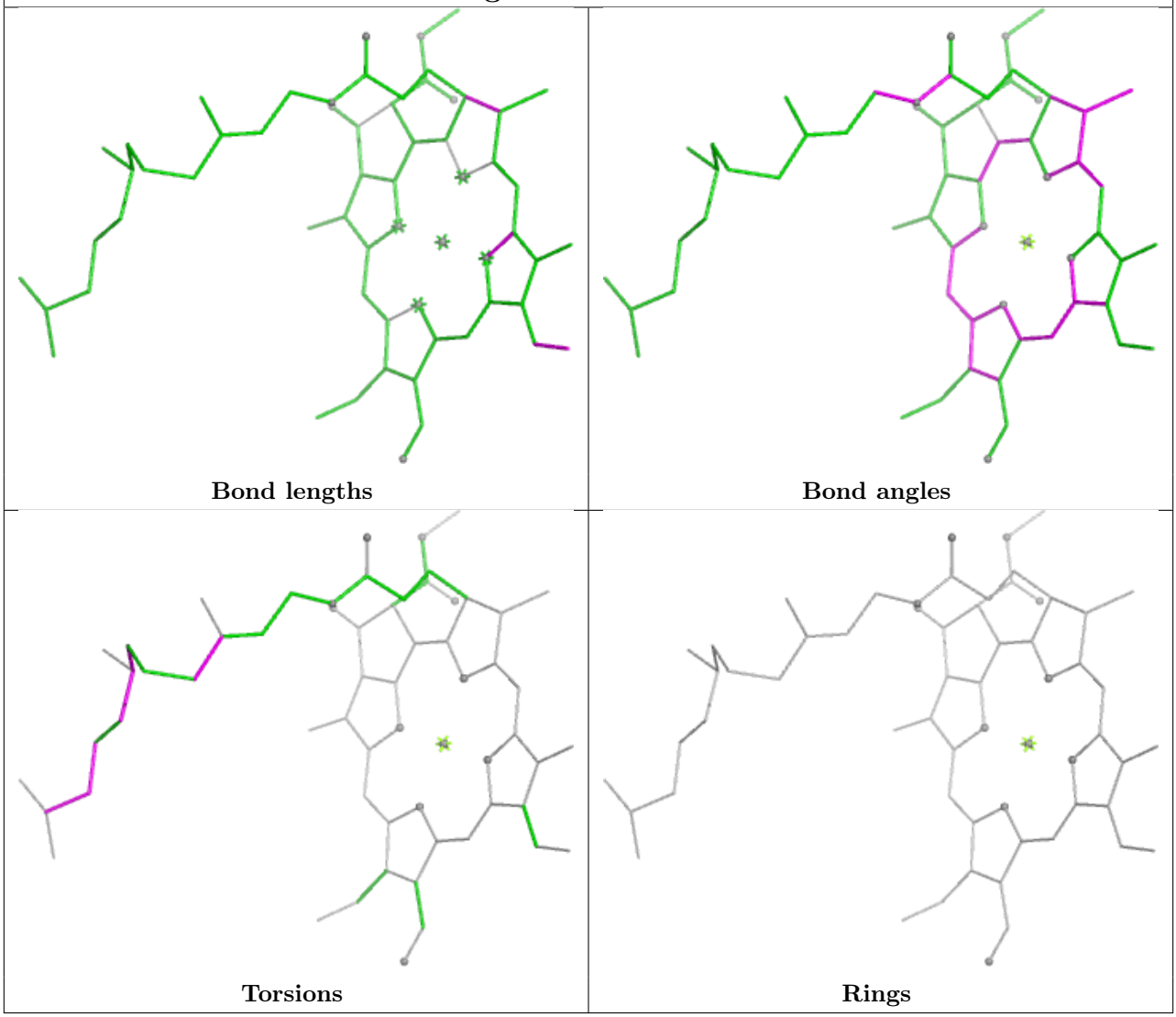
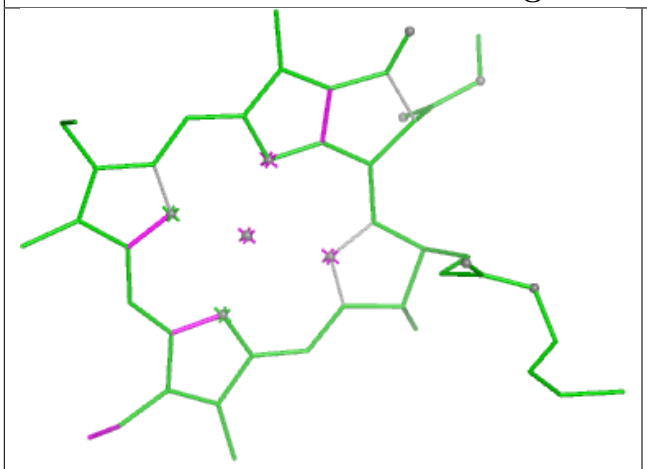
 Bond lengths	 Bond angles
 Torsions	 Rings

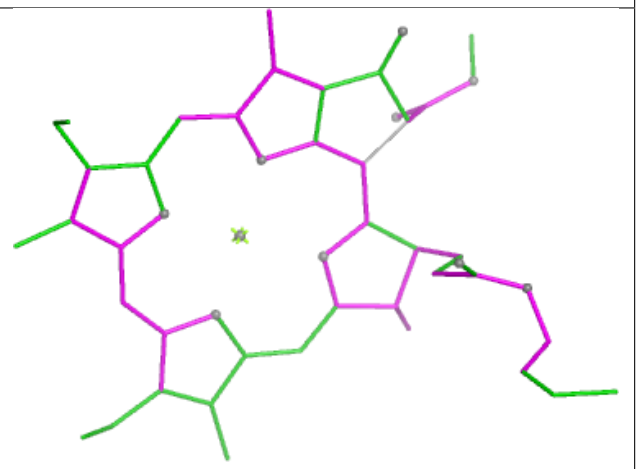
Ligand CHL 3 310



Ligand CLA G 613



Bond lengths



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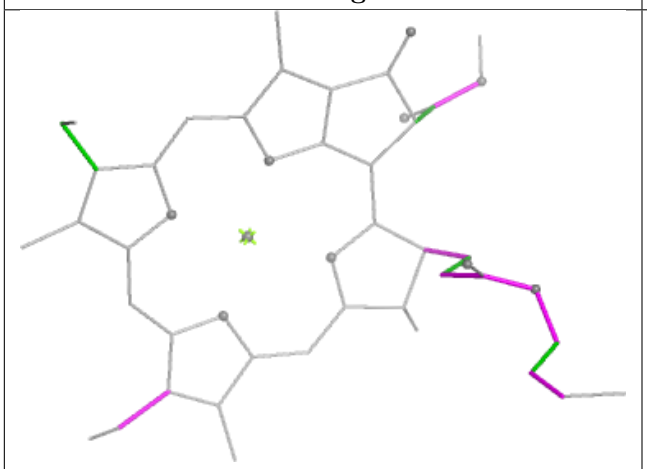

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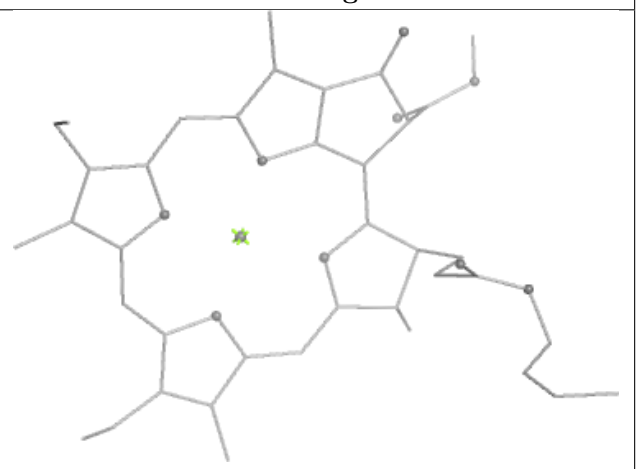
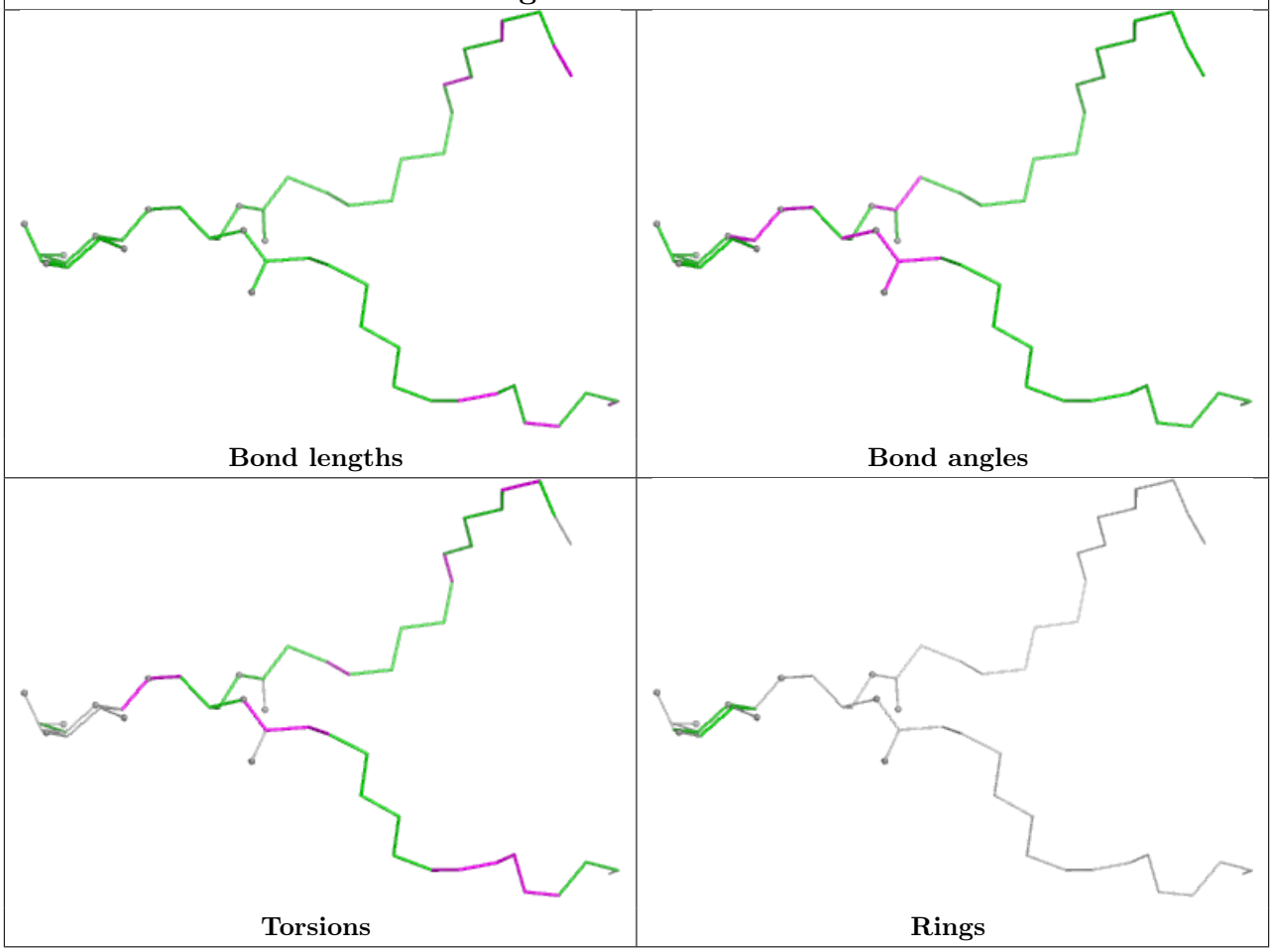
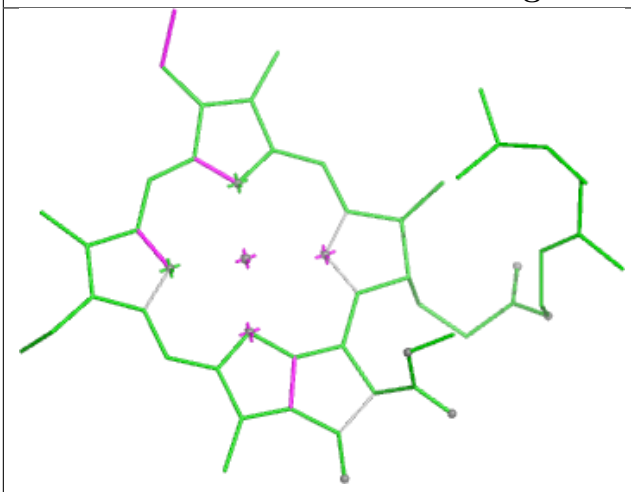


Rings

Ligand LMG b 622



Ligand CLA N 304



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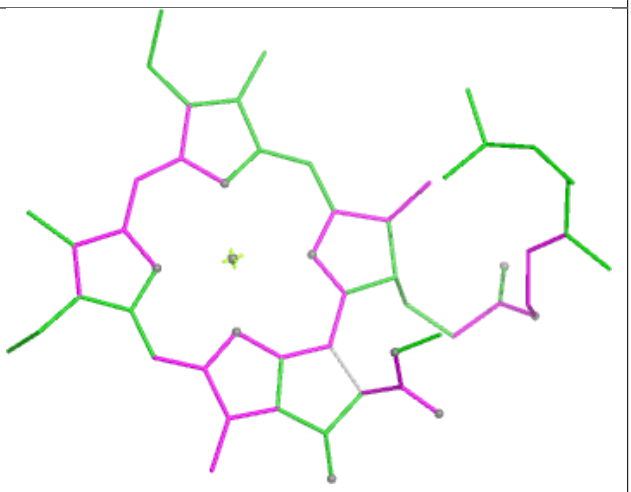

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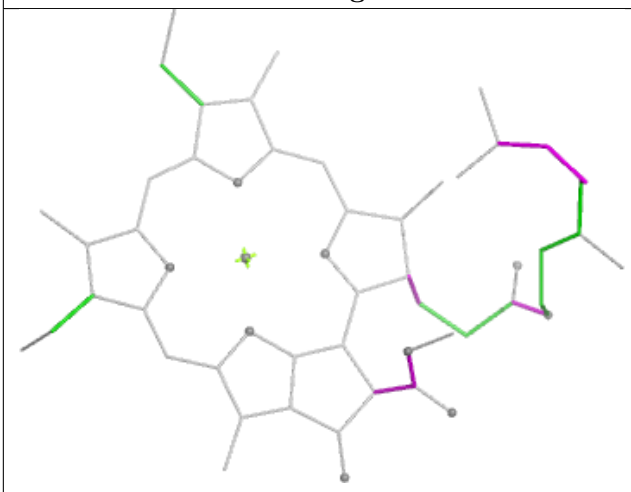

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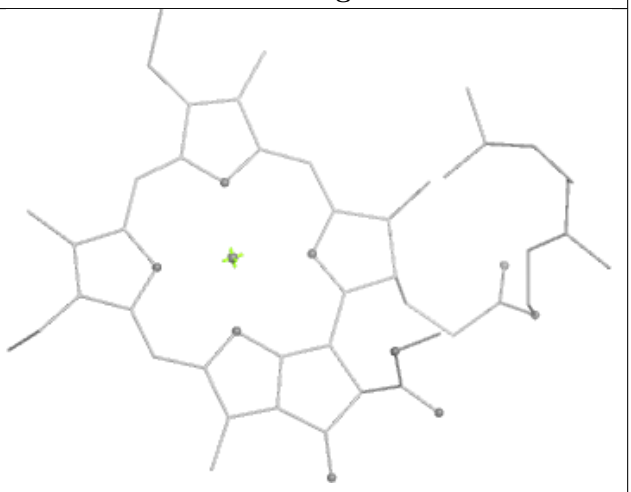
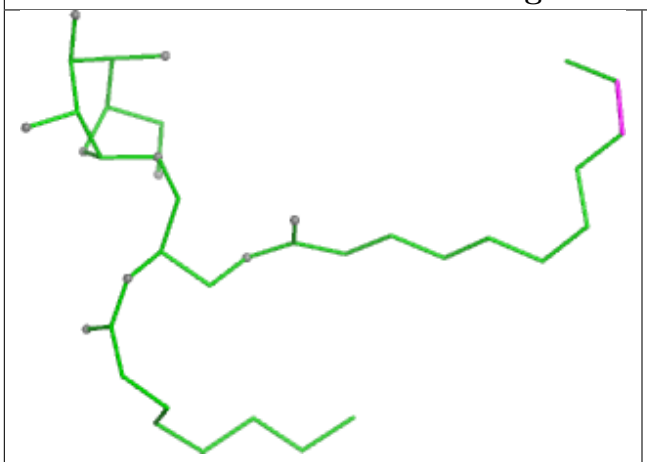


Rings

Ligand LMG 0 622



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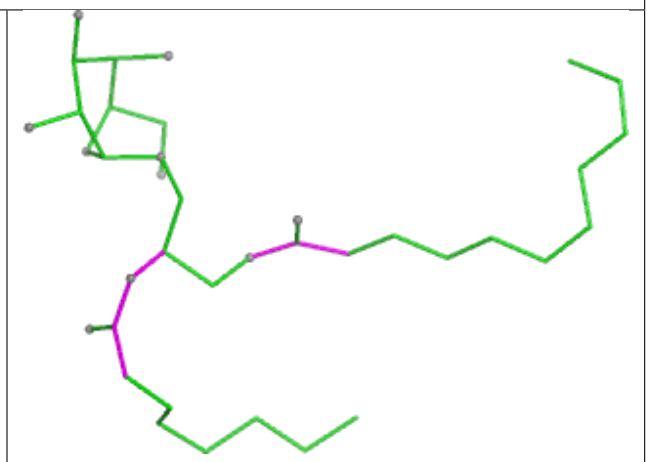

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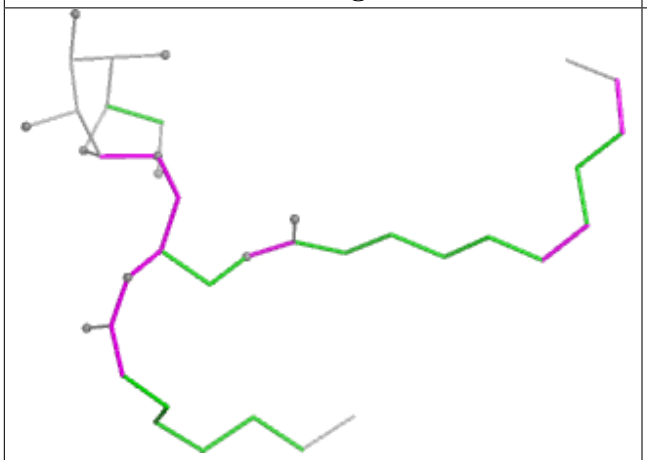

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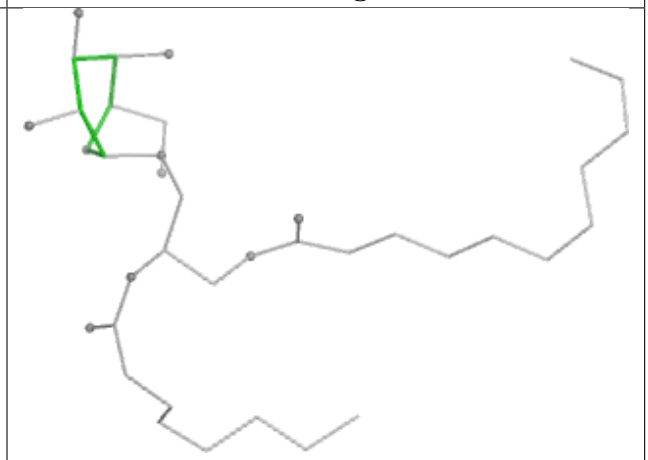
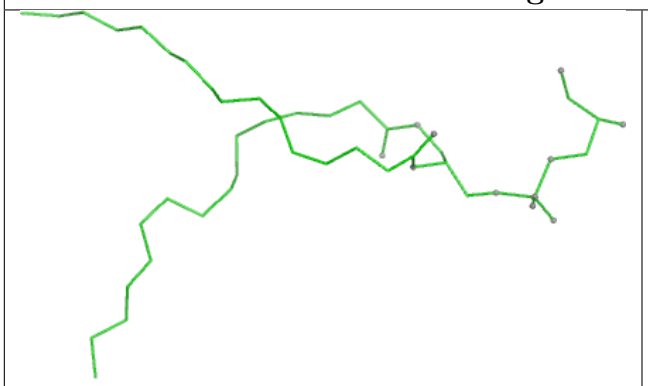


Rings

Ligand LHG d 408



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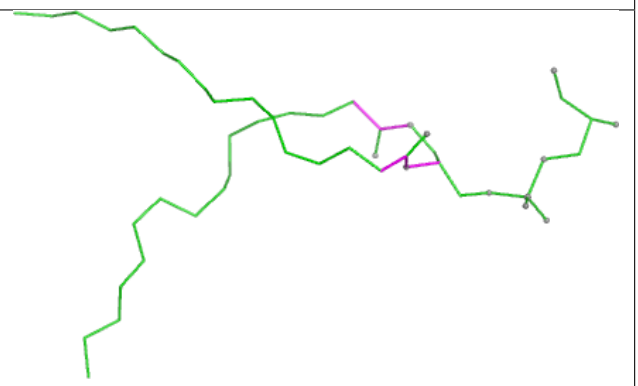
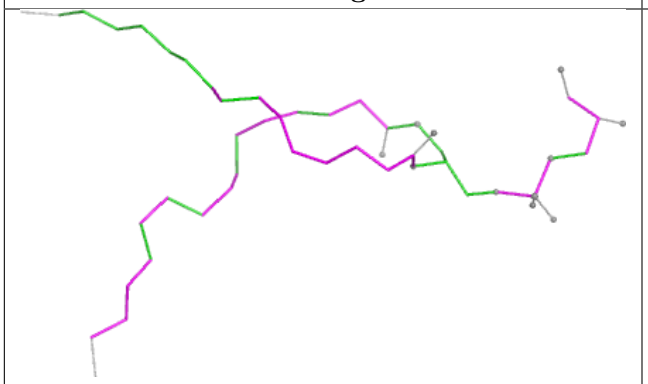


Bond angles



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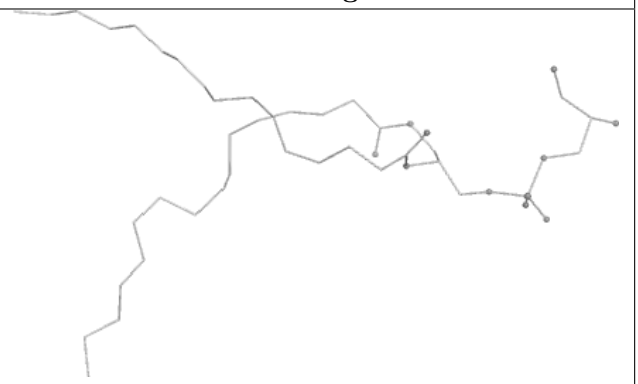
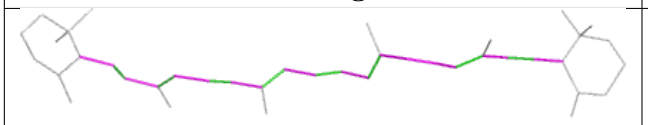


Rings

Ligand BCR c 614

Bond lengths

Bond angles



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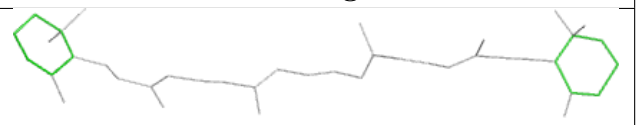
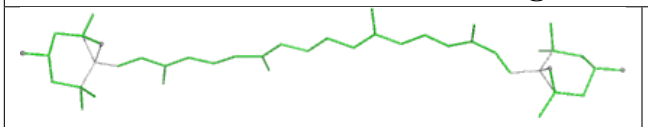


Rings

Ligand XAT q 321



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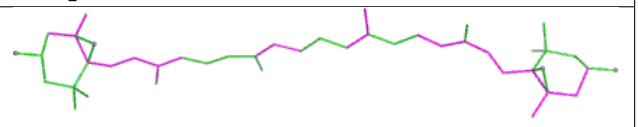

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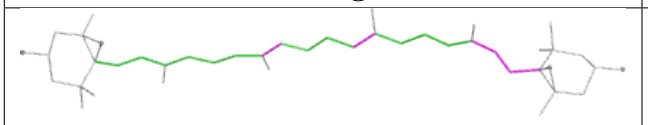

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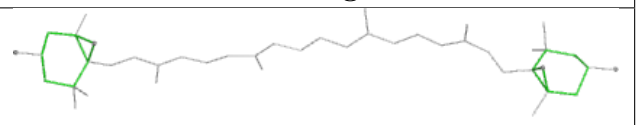
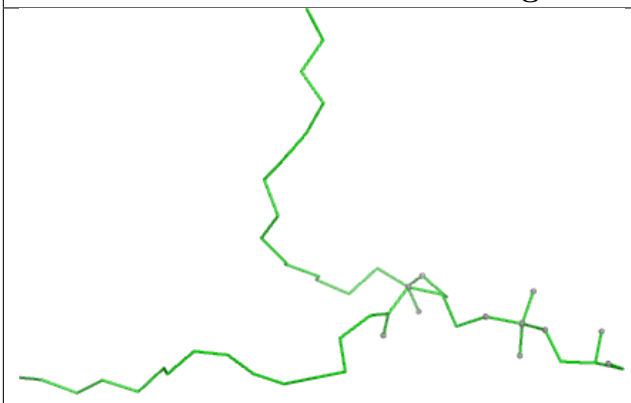


Rings

Ligand LHG N 319



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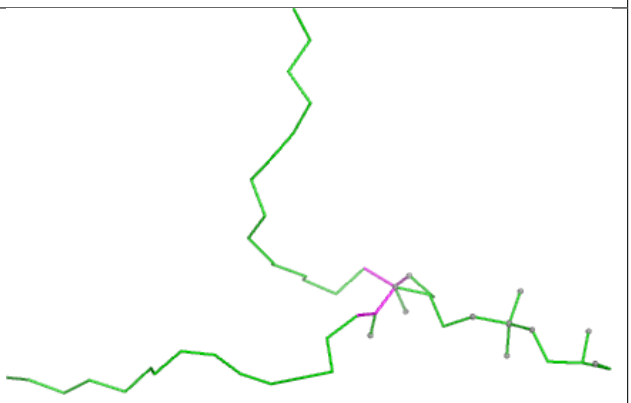

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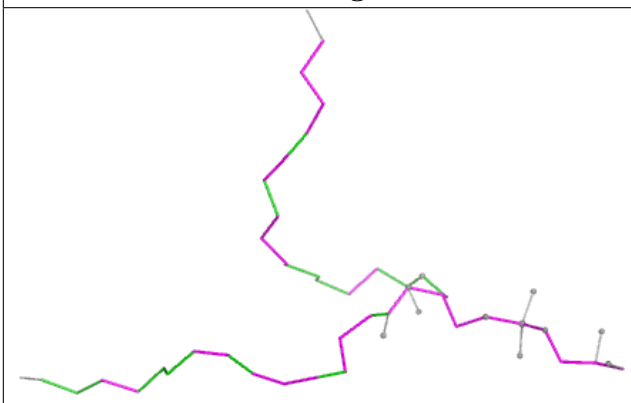
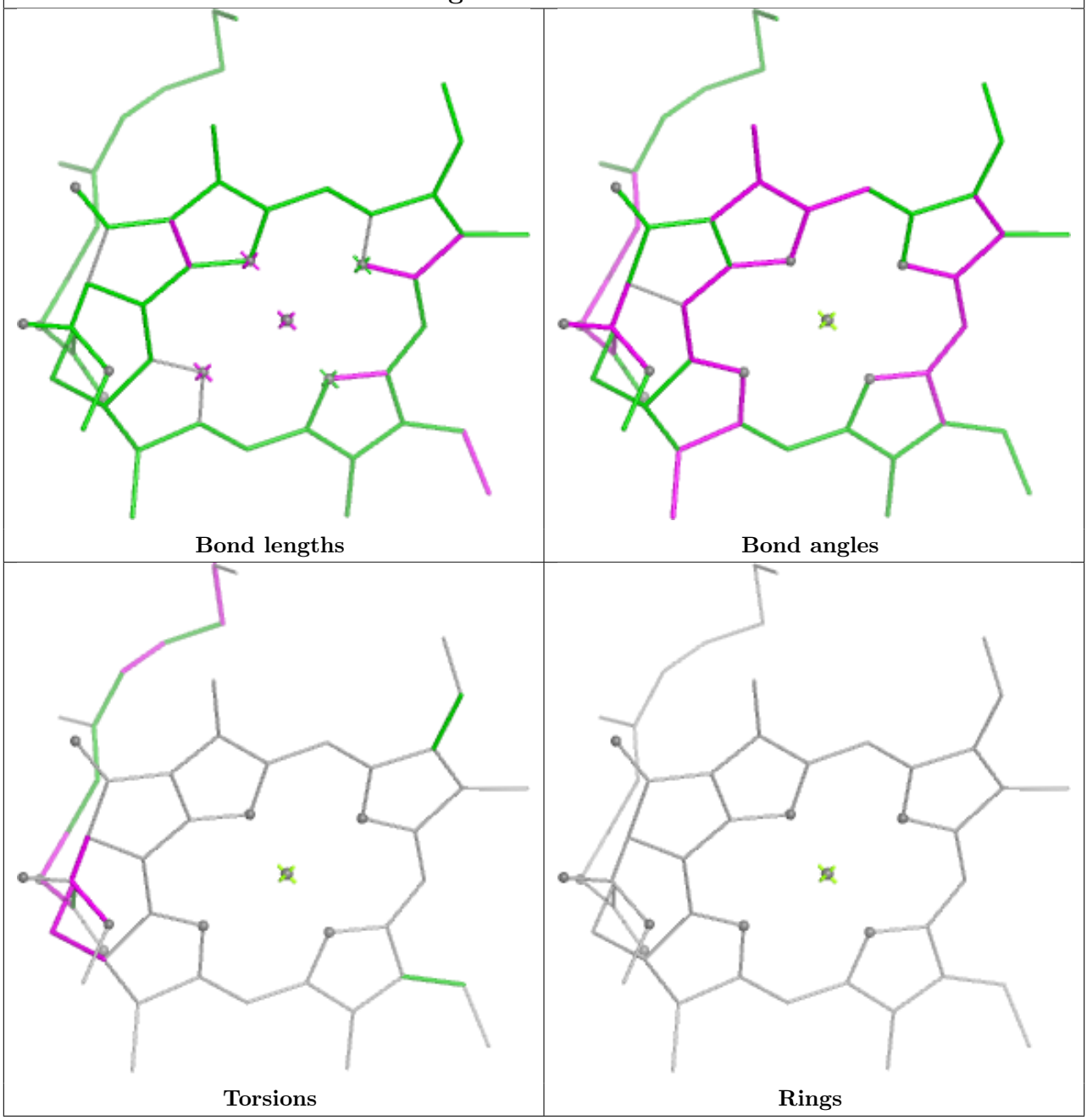


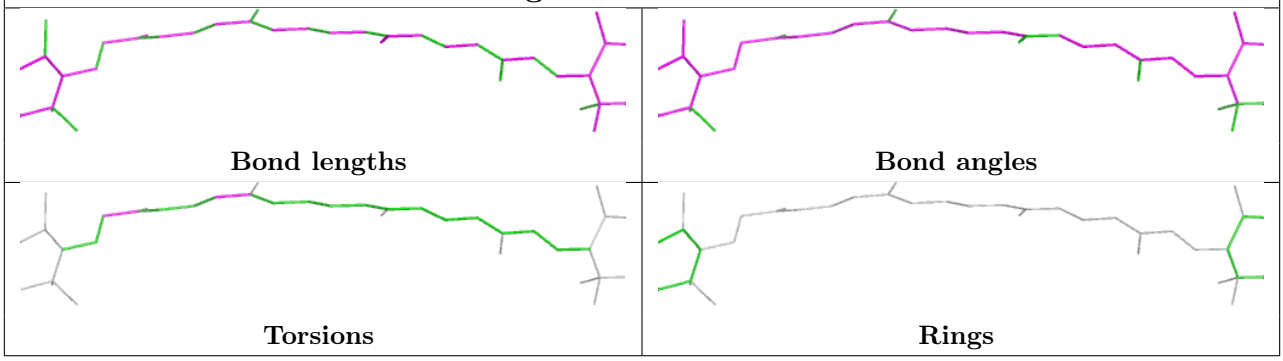
Torsions

Rings

Ligand CLA 2 604



Ligand BCR Z 101



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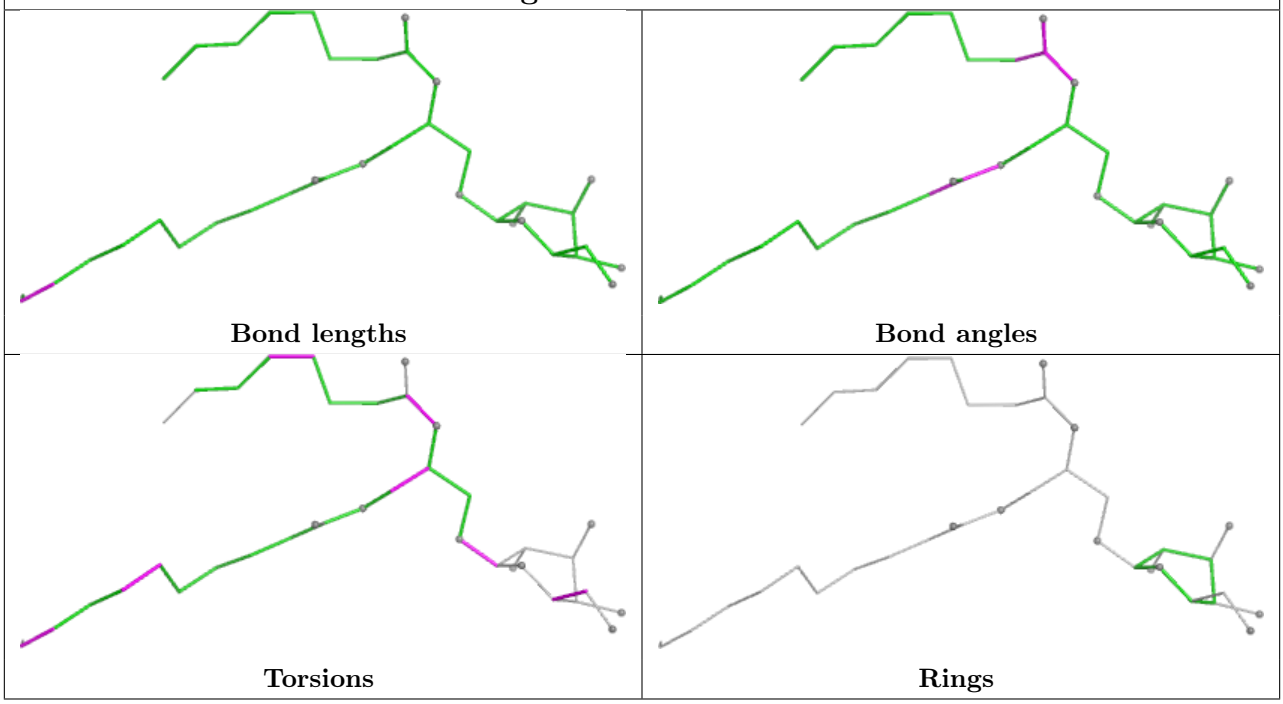
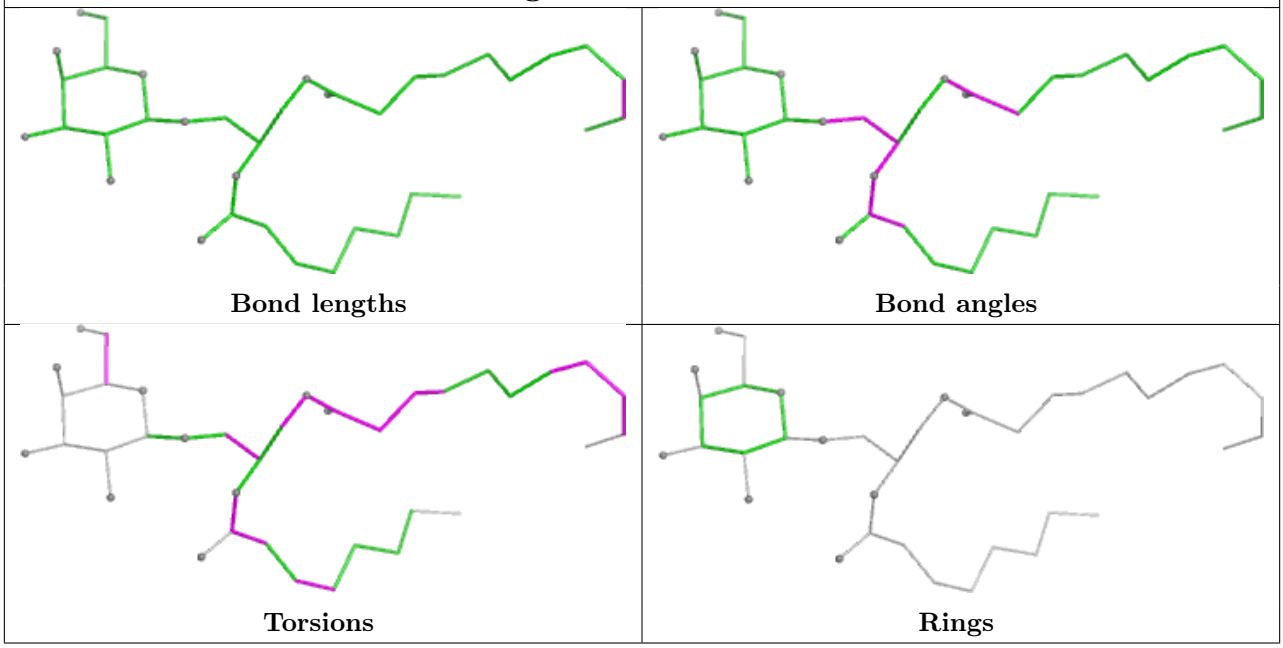
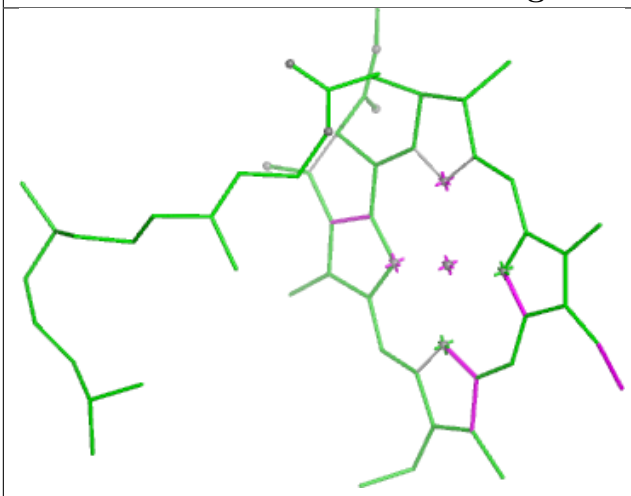


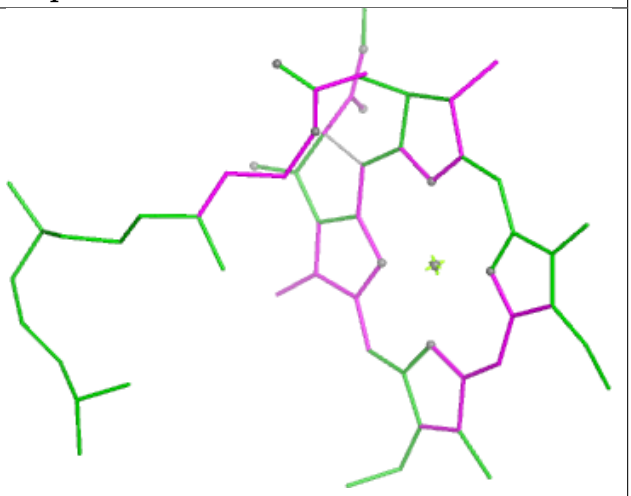
Ligand LMG x 202



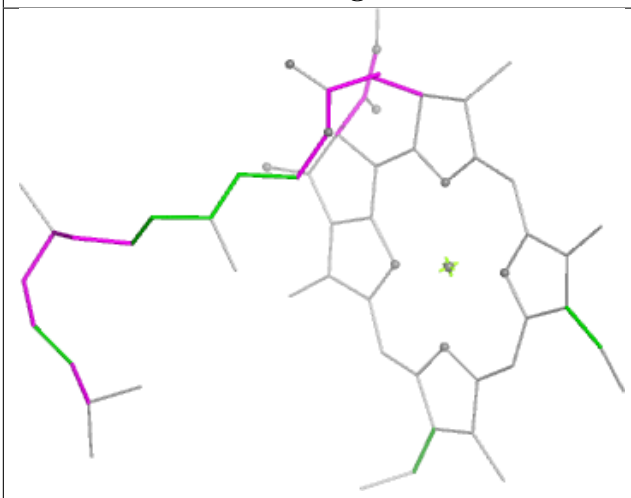
Ligand CLA p 611



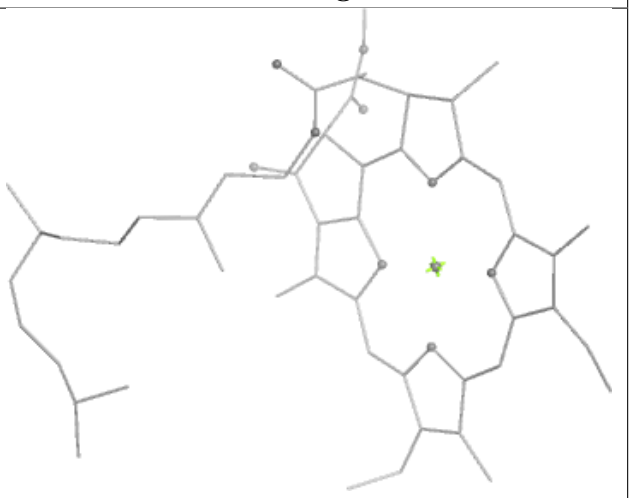
Bond lengths



Bond angles

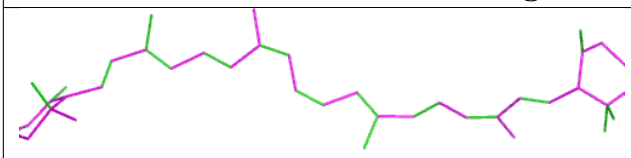


Torsions



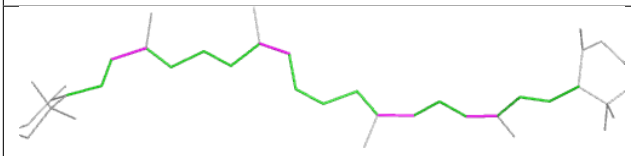
Rings

Ligand BCR C 615



Bond lengths

Bond angles



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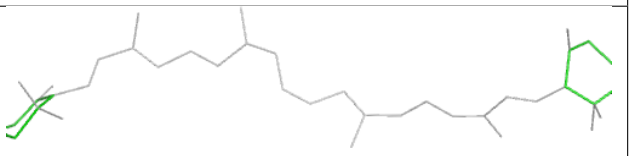
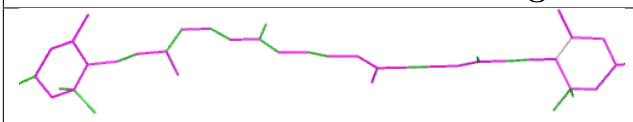


Rings

Ligand LUT 4 616



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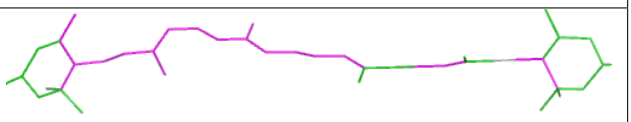

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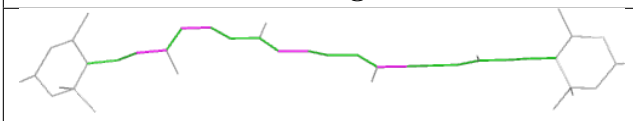
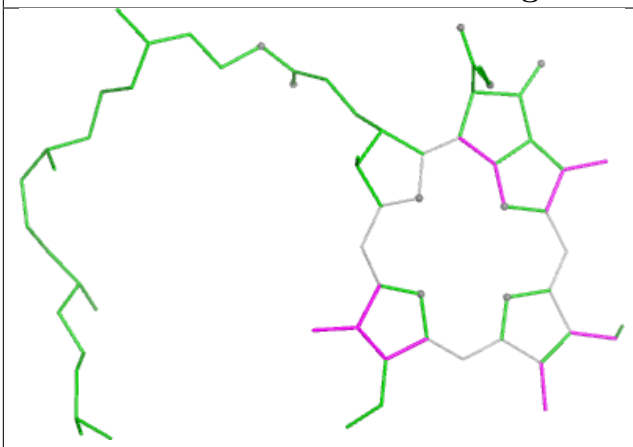


Torsions

Rings

Ligand PHO A 408



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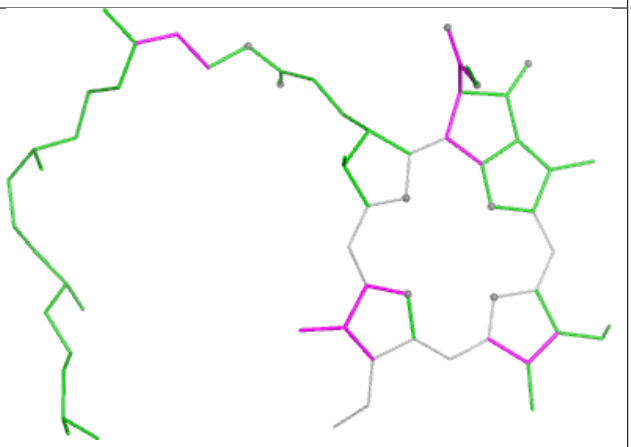

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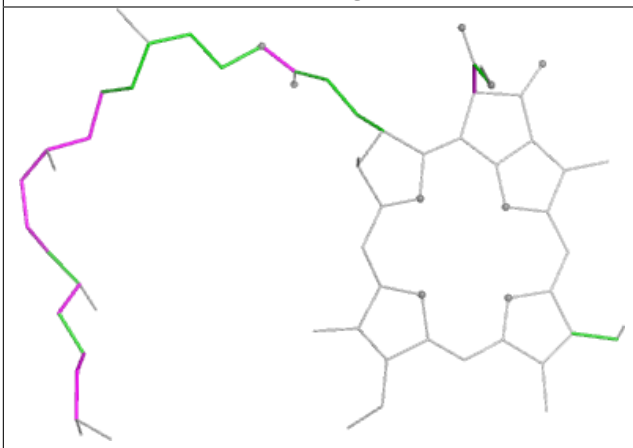

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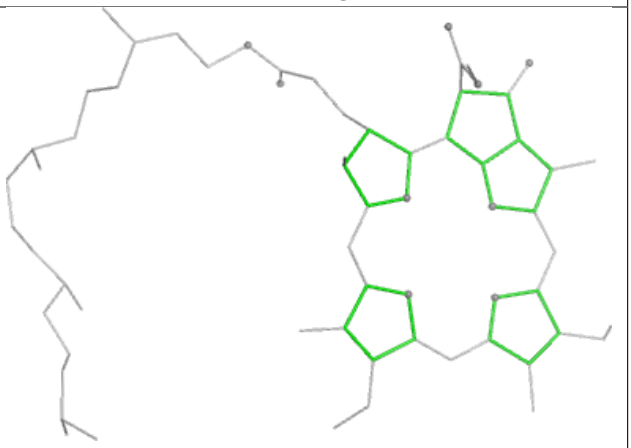
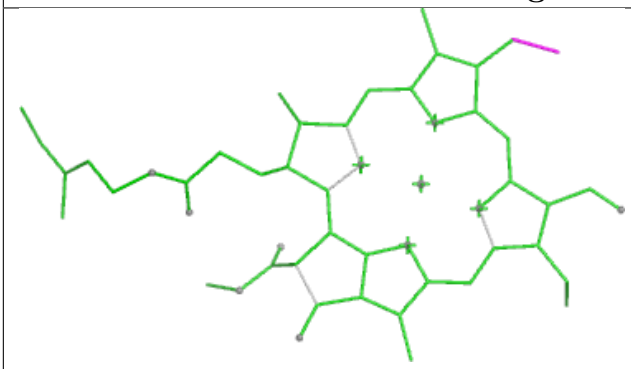
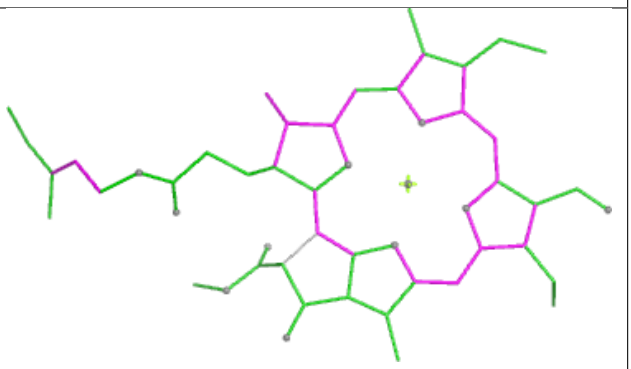
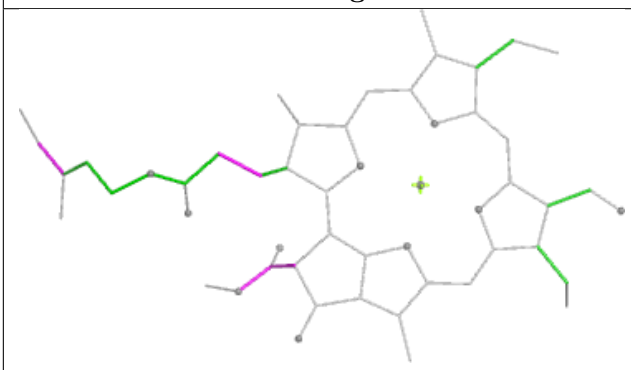
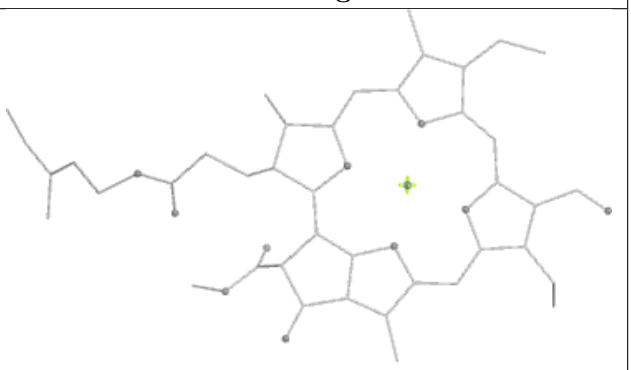
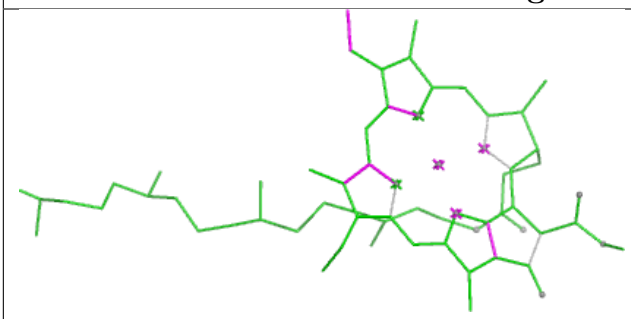
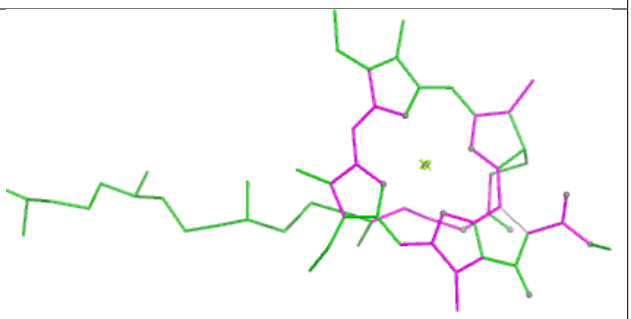
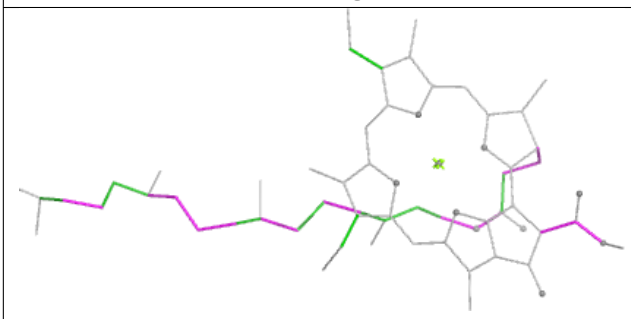
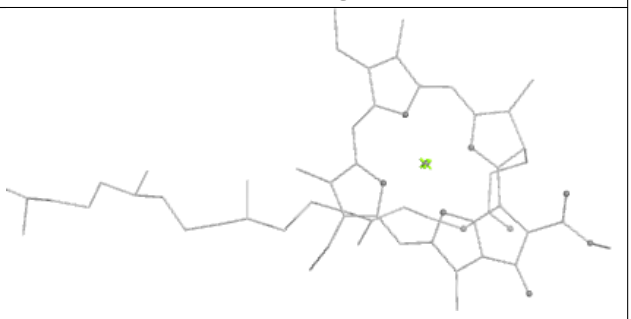
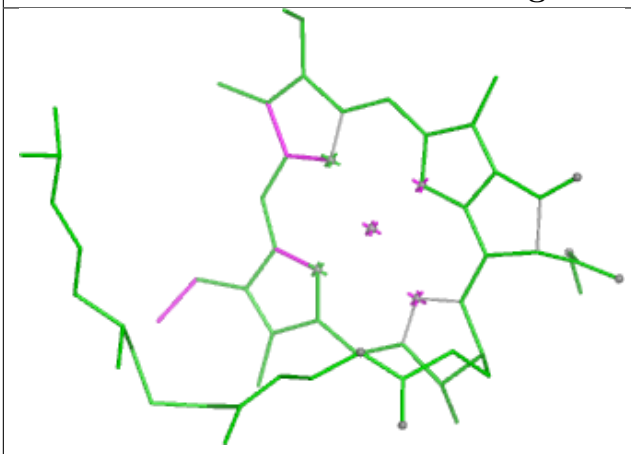


Rings

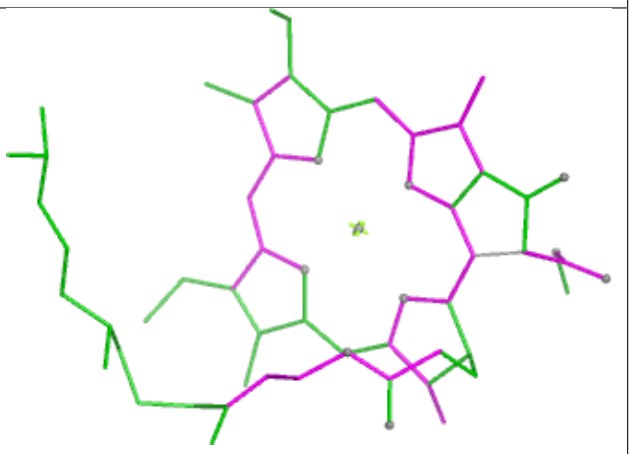
Ligand CHL 9 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 602



Bond lengths



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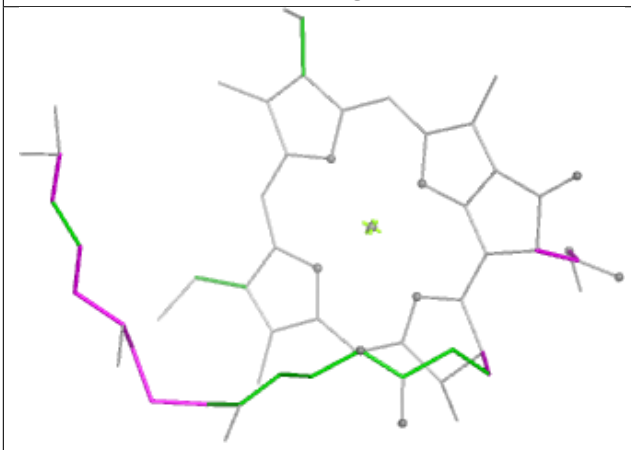

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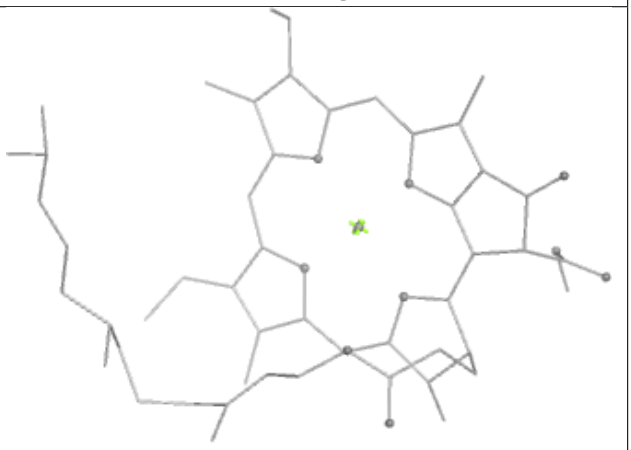
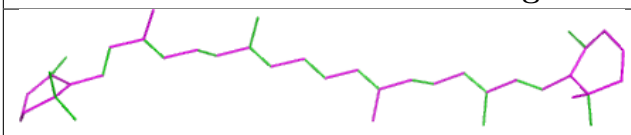


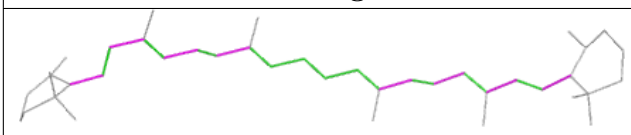
Rings

Ligand BCR C 614



Bond lengths

Bond angles



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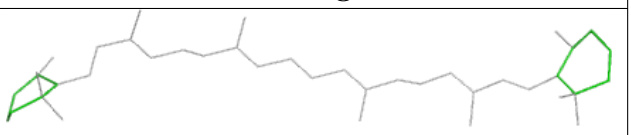
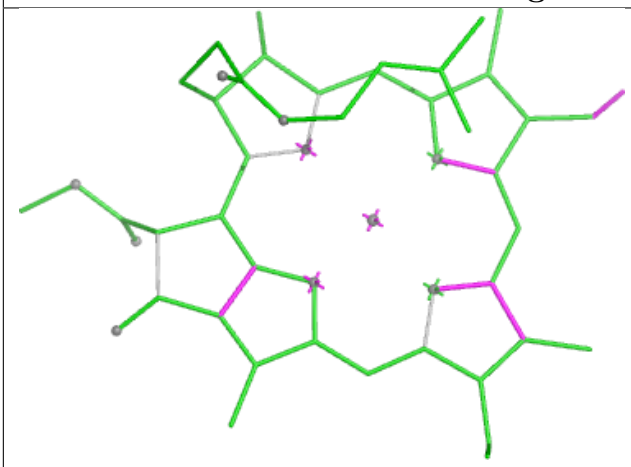


Rings

Ligand CLA q 316



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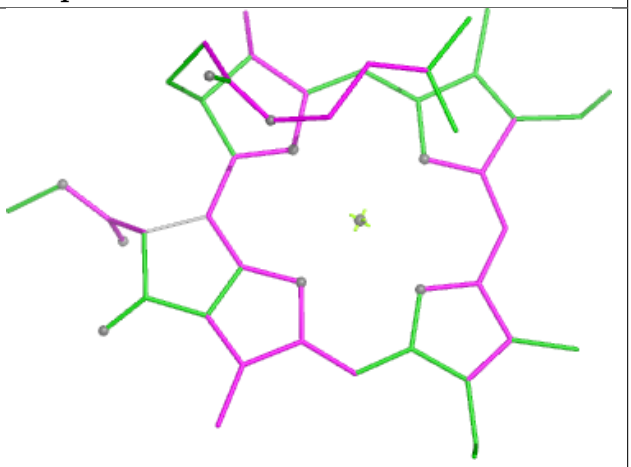
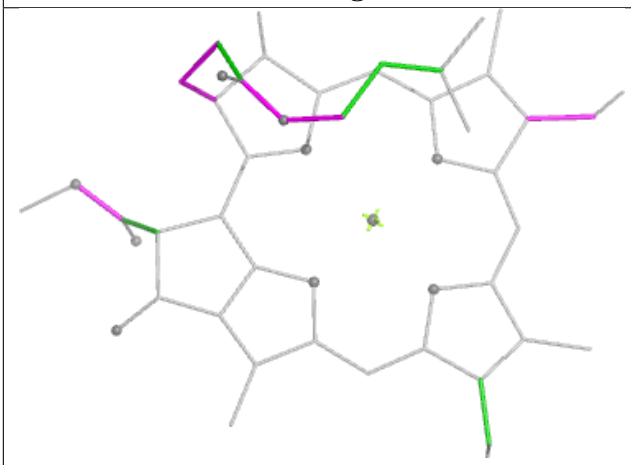


Bond angles



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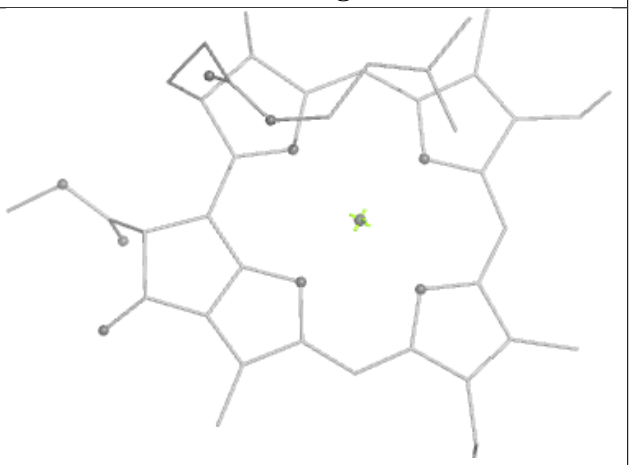
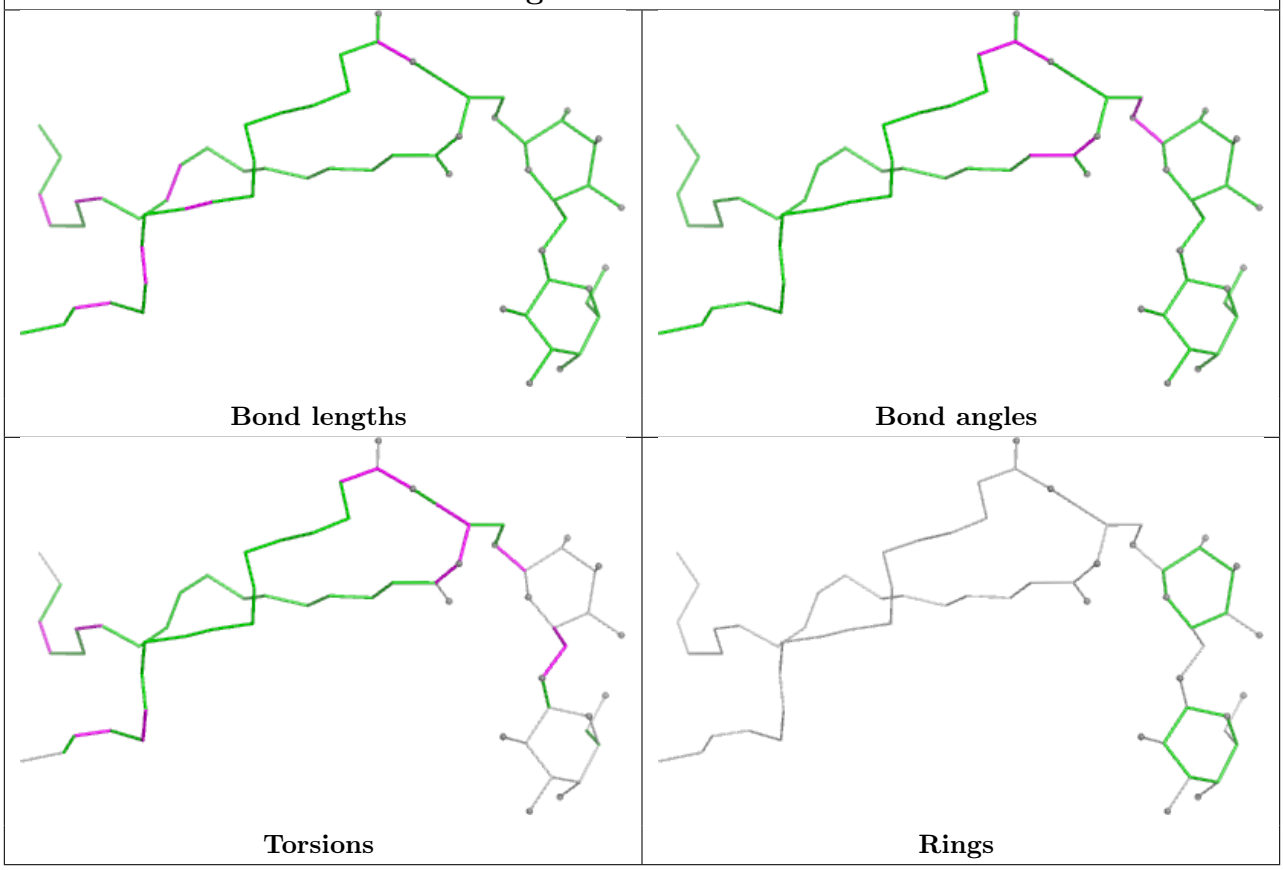


Rings

Ligand DGD c 619



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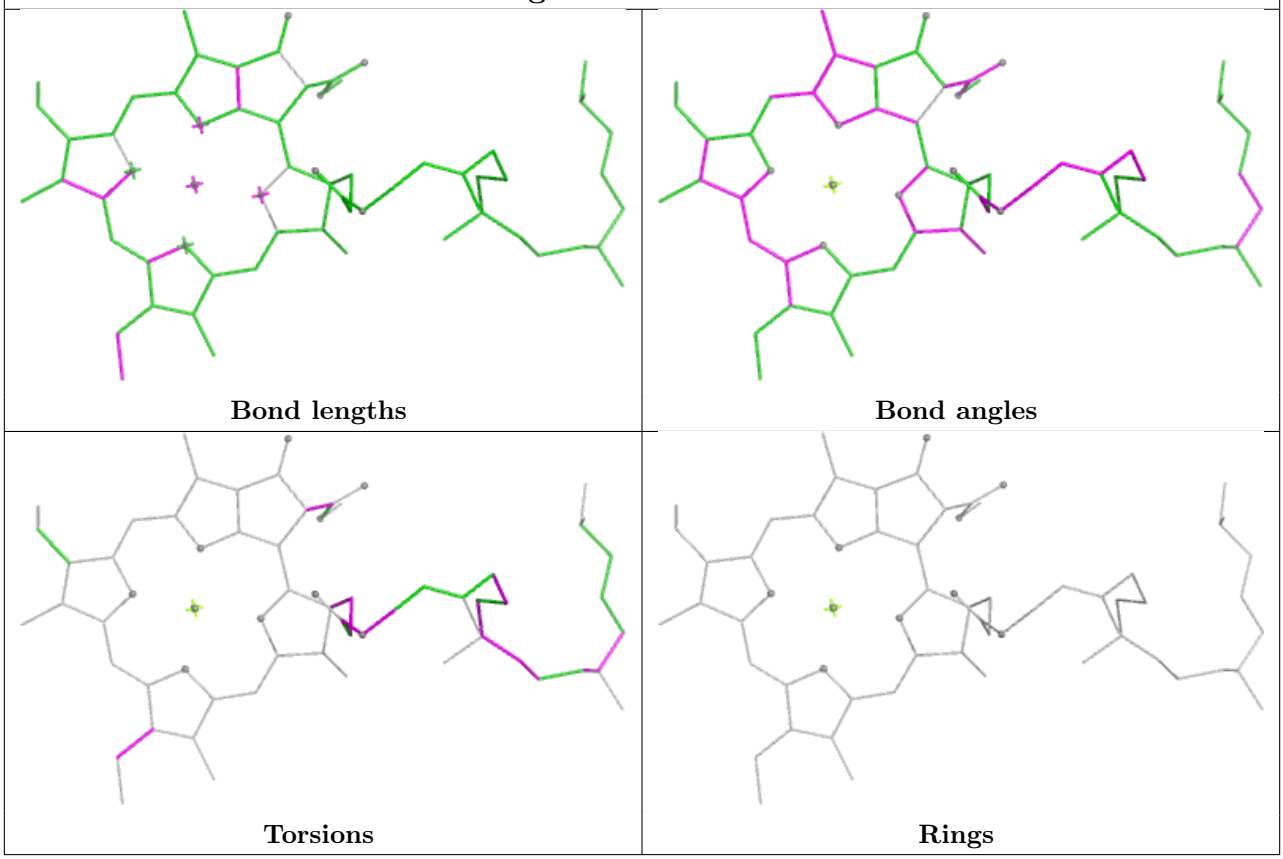

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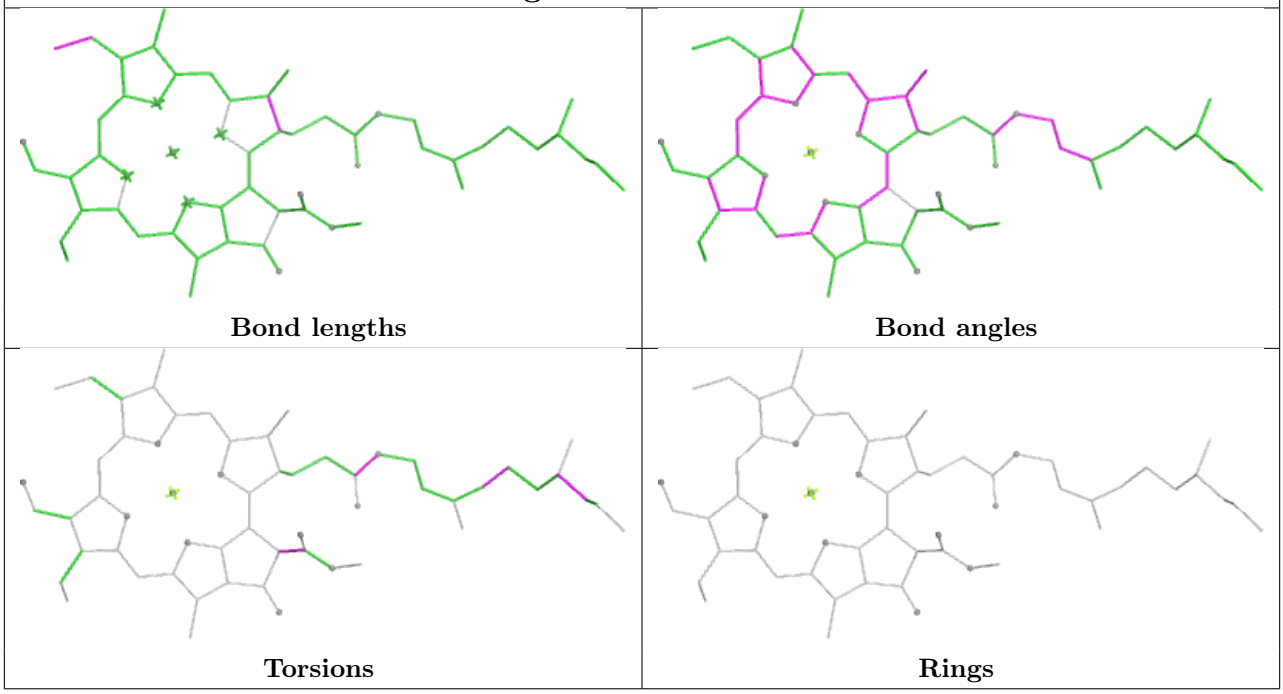

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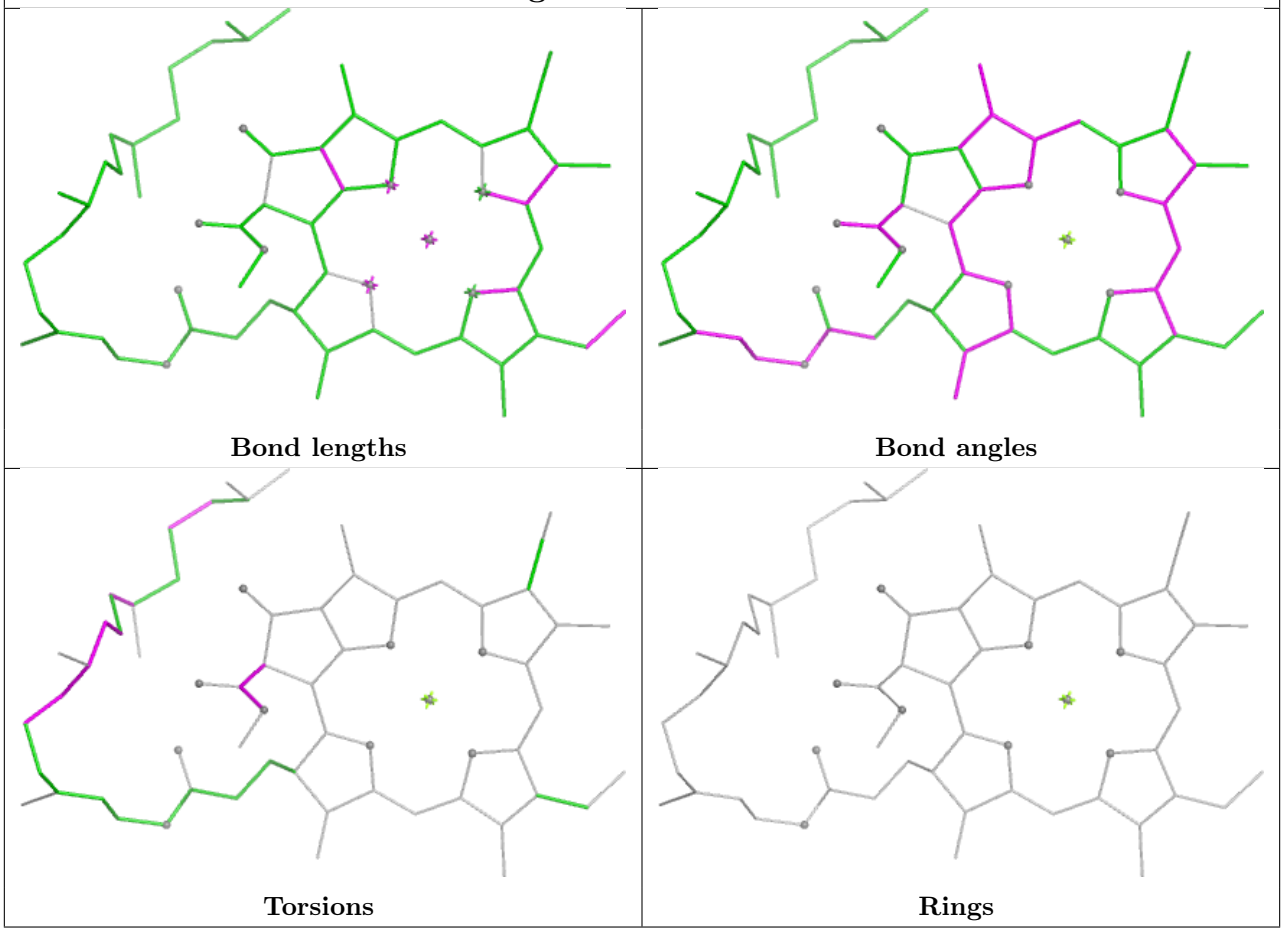
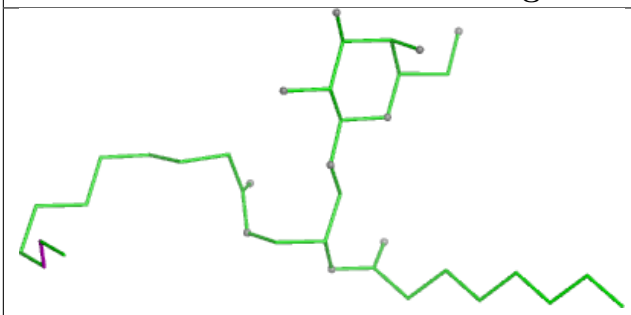
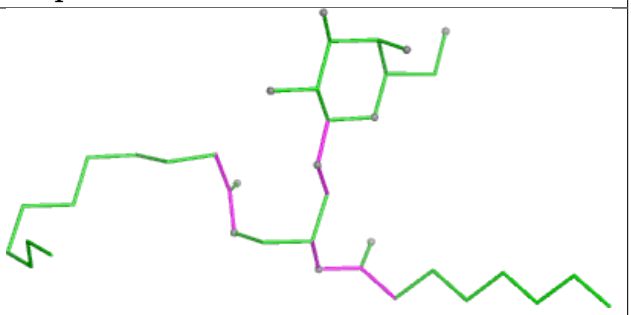
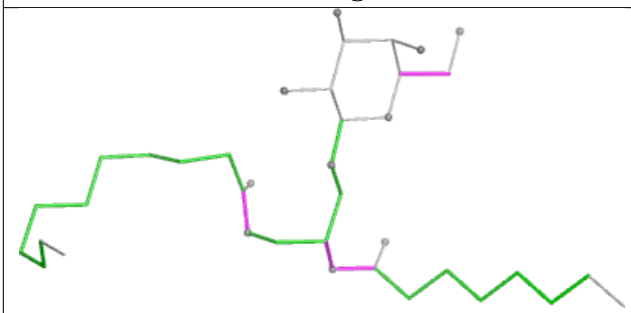
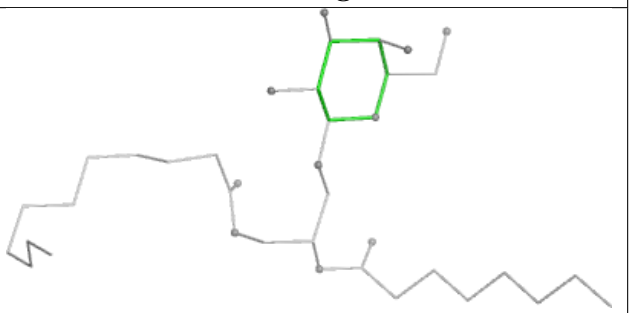
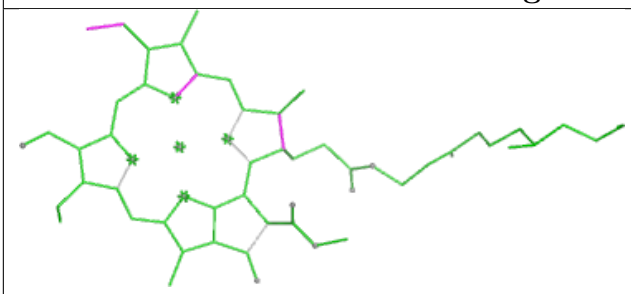
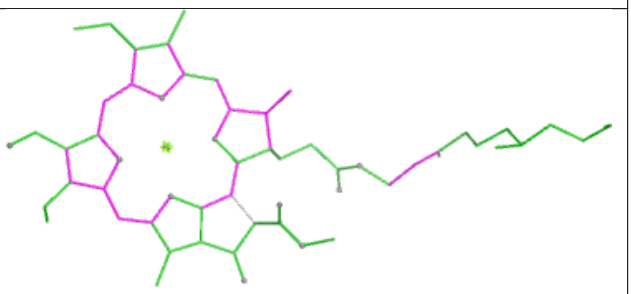
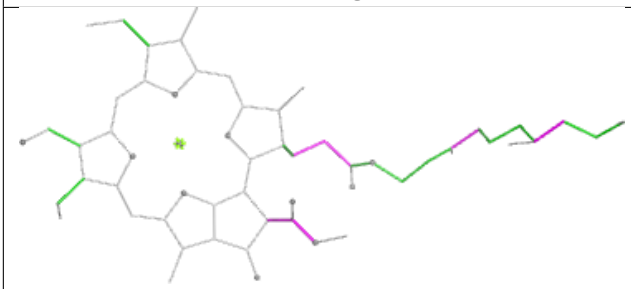
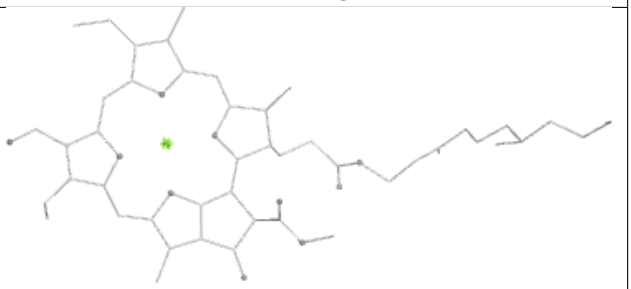
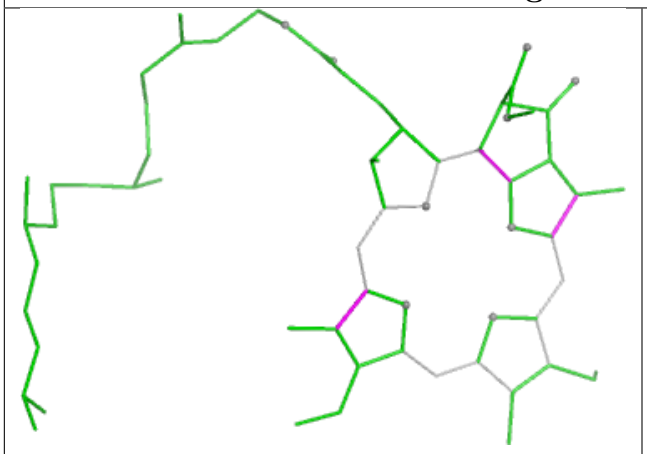


Ligand LMG p 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Y 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO d 402



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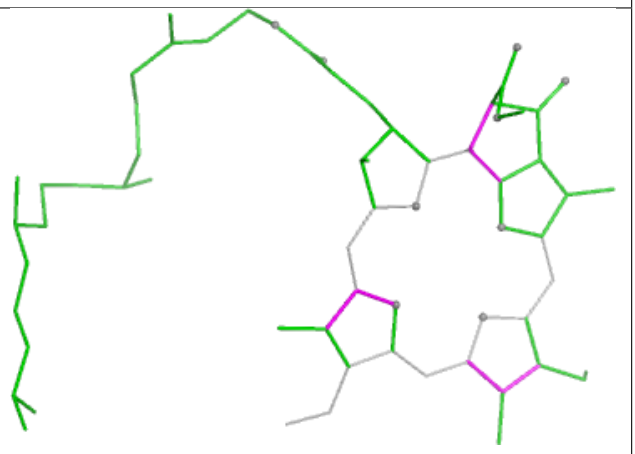

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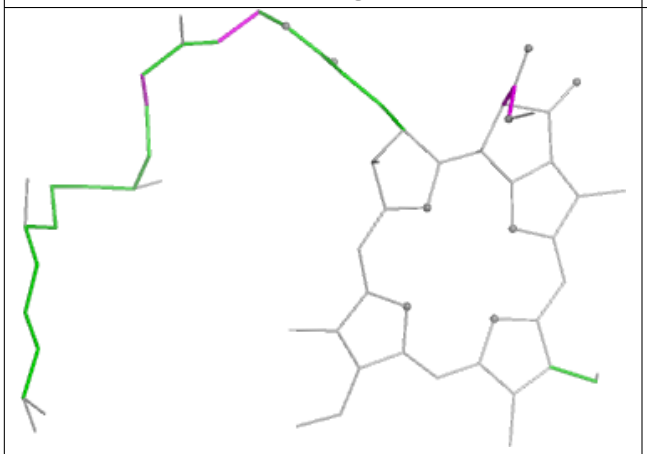
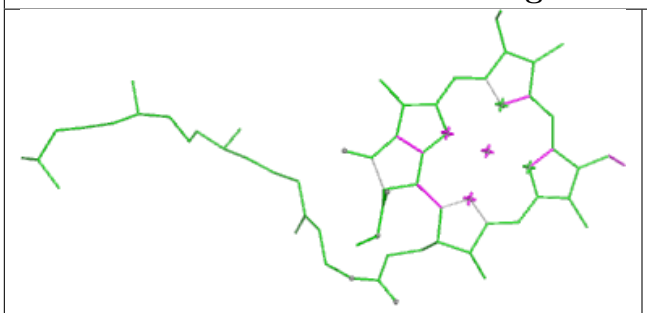


Torsions

Rings

Ligand CLA B 602



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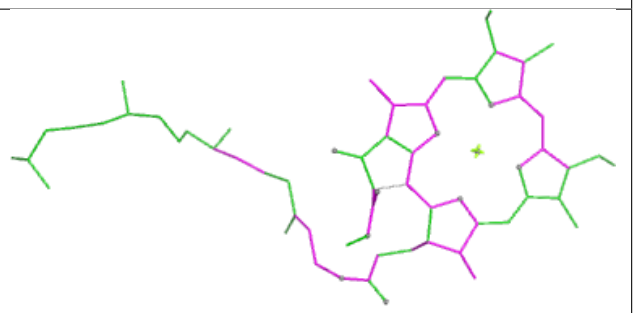
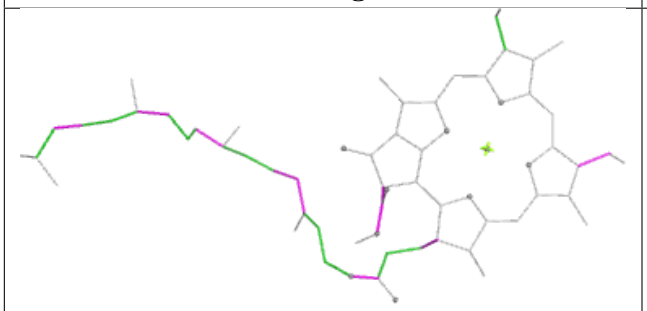


Bond angles



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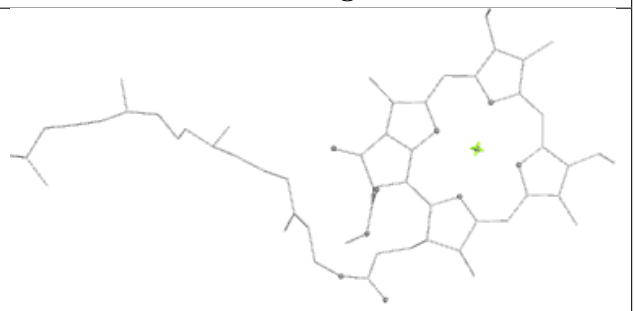
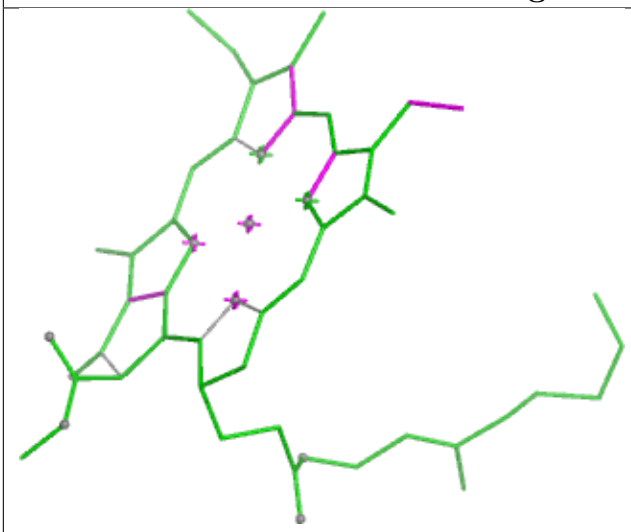


Rings

Ligand CLA 8 614



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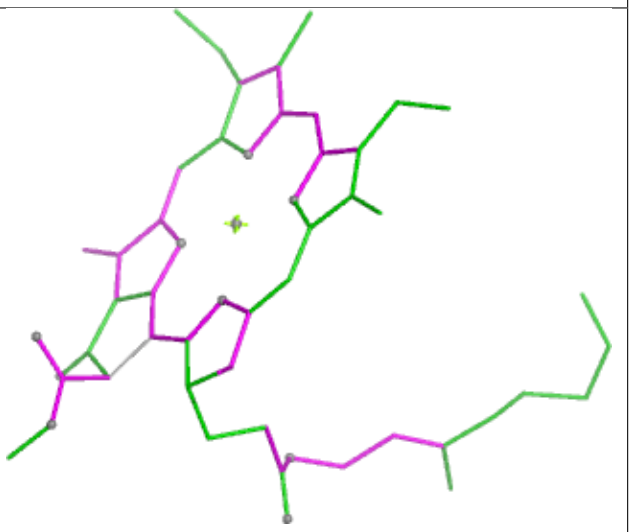

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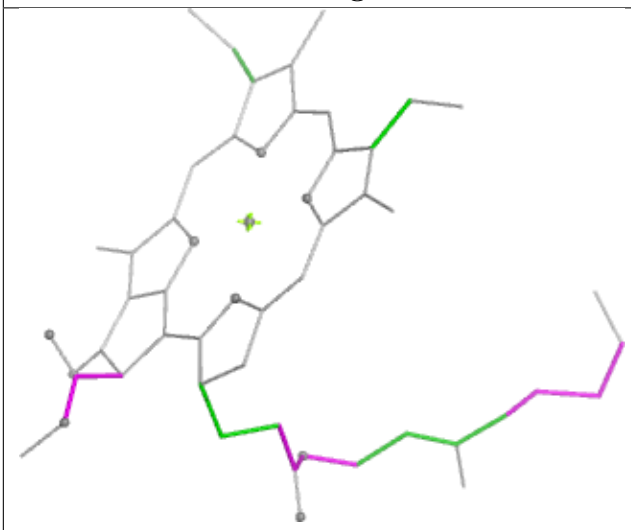

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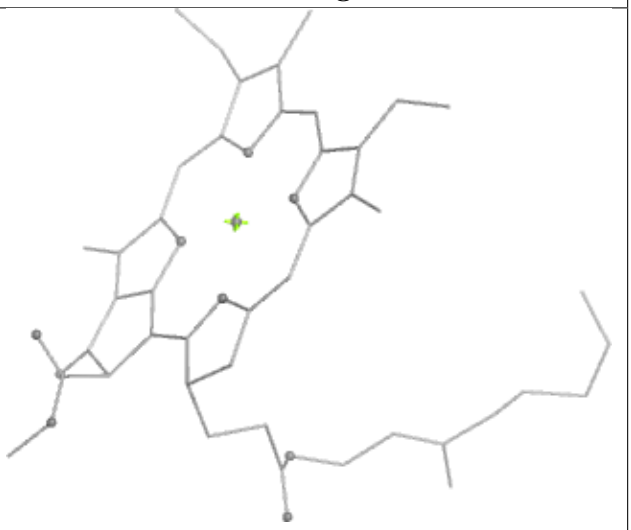
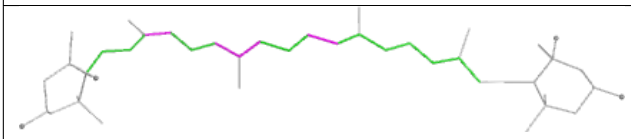


Rings

Ligand NEX R 319

Bond lengths

Bond angles



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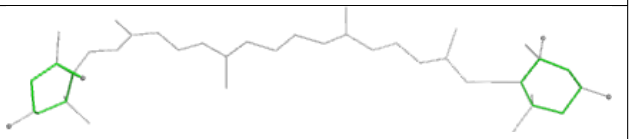
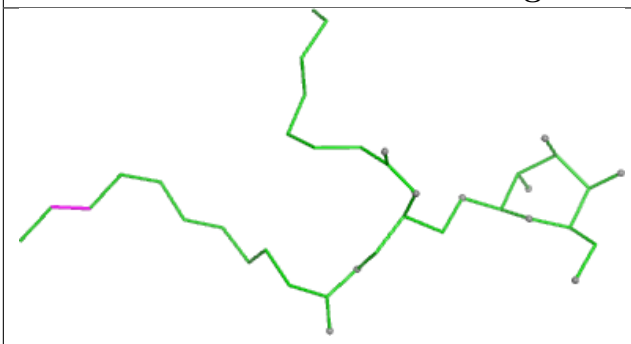
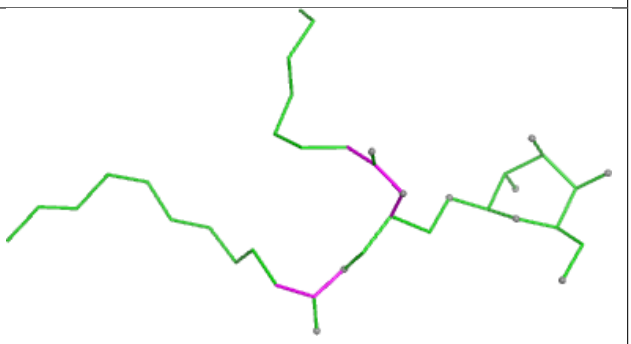
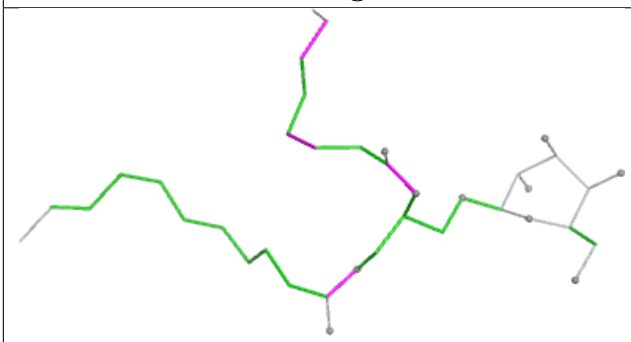
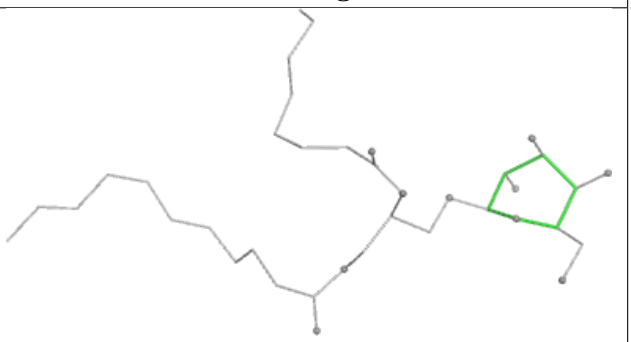
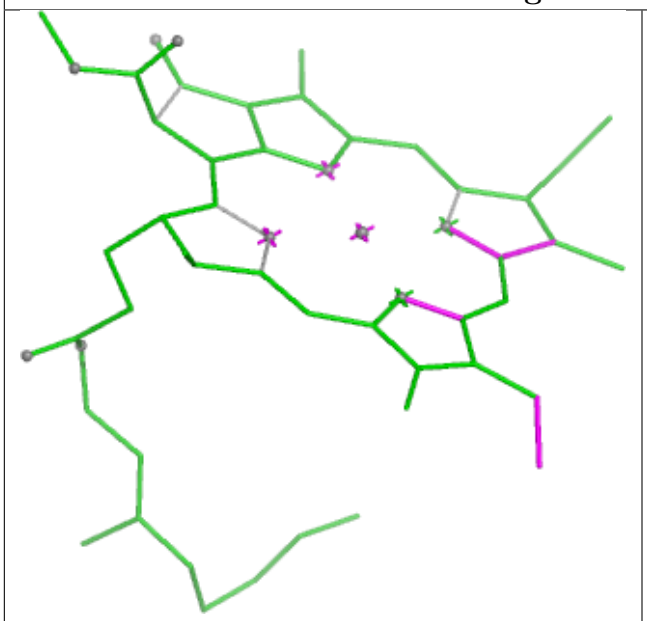


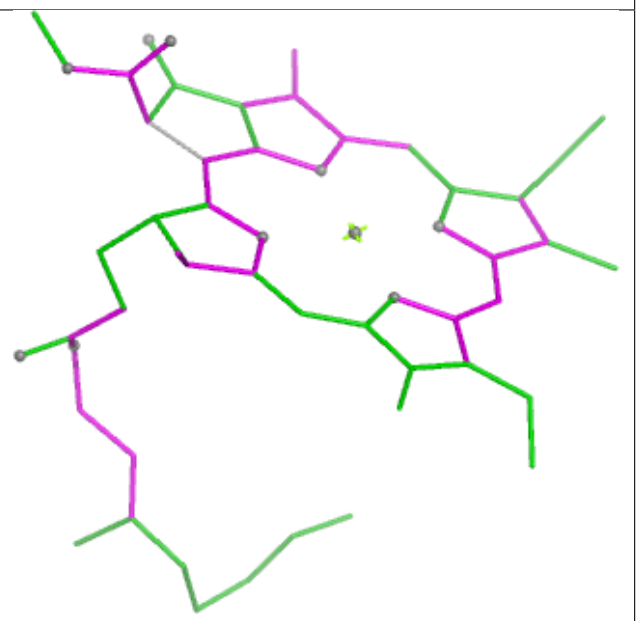
Rings

Ligand LMG a 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

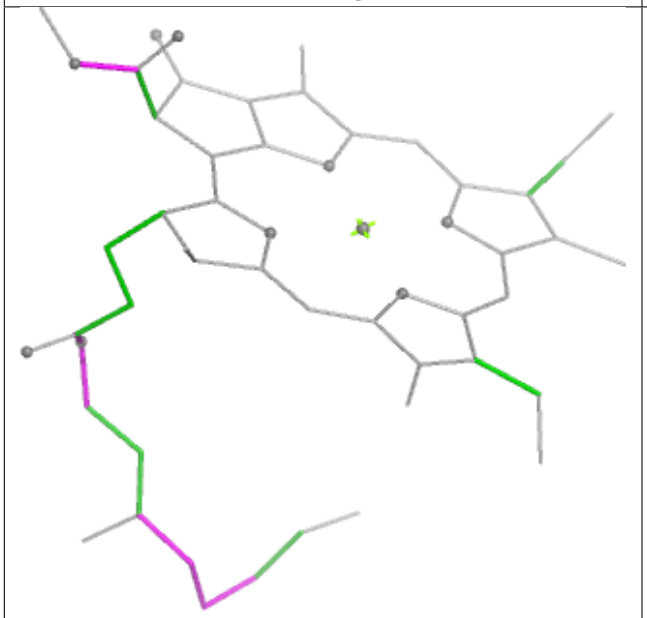
Ligand CLA N 315



Bond lengths



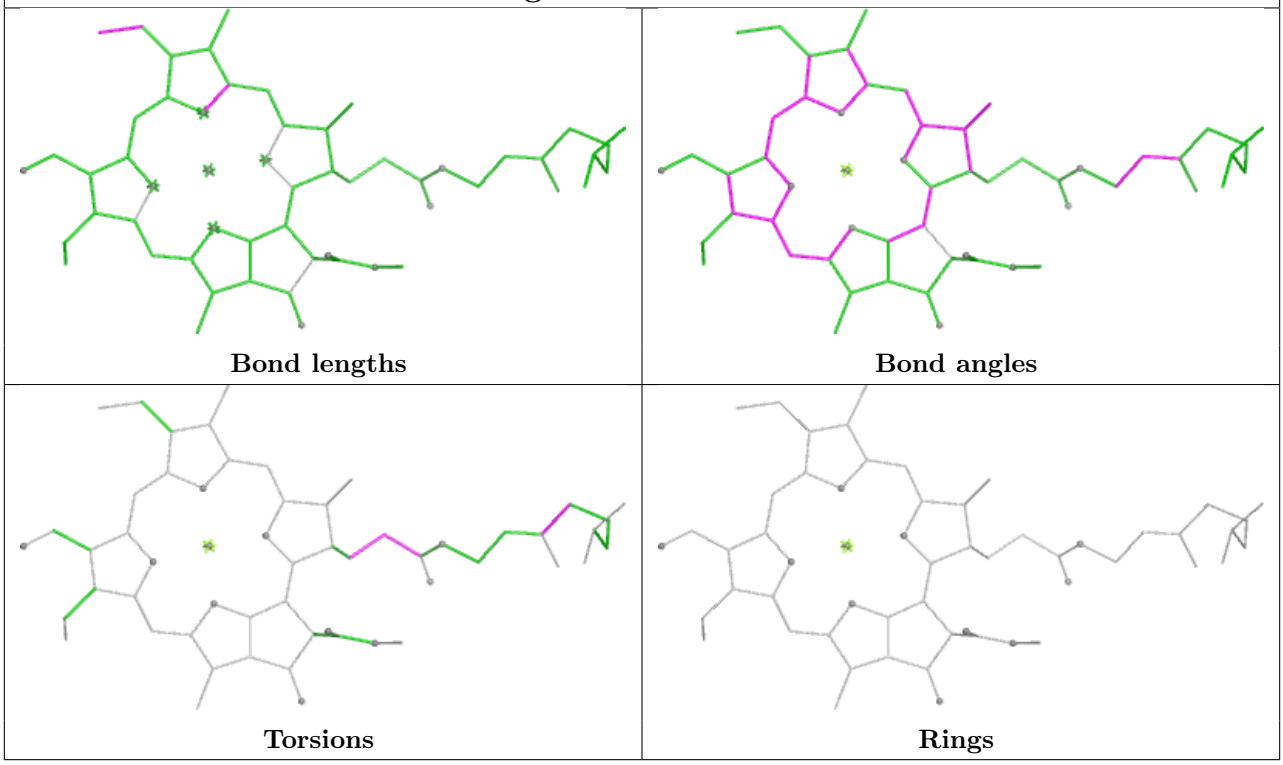
Bond angles



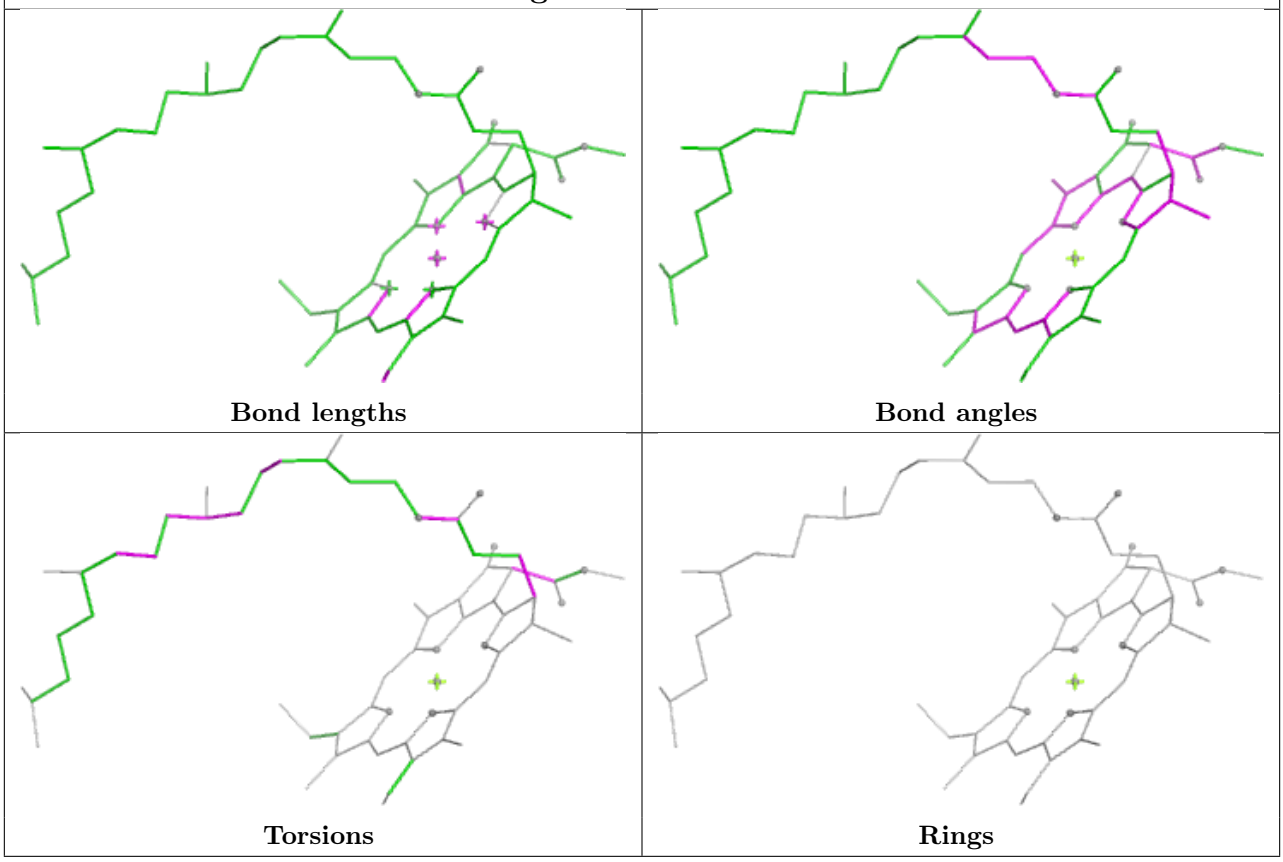
Torsions

Rings

Ligand CHL R 308



Ligand CLA c 608



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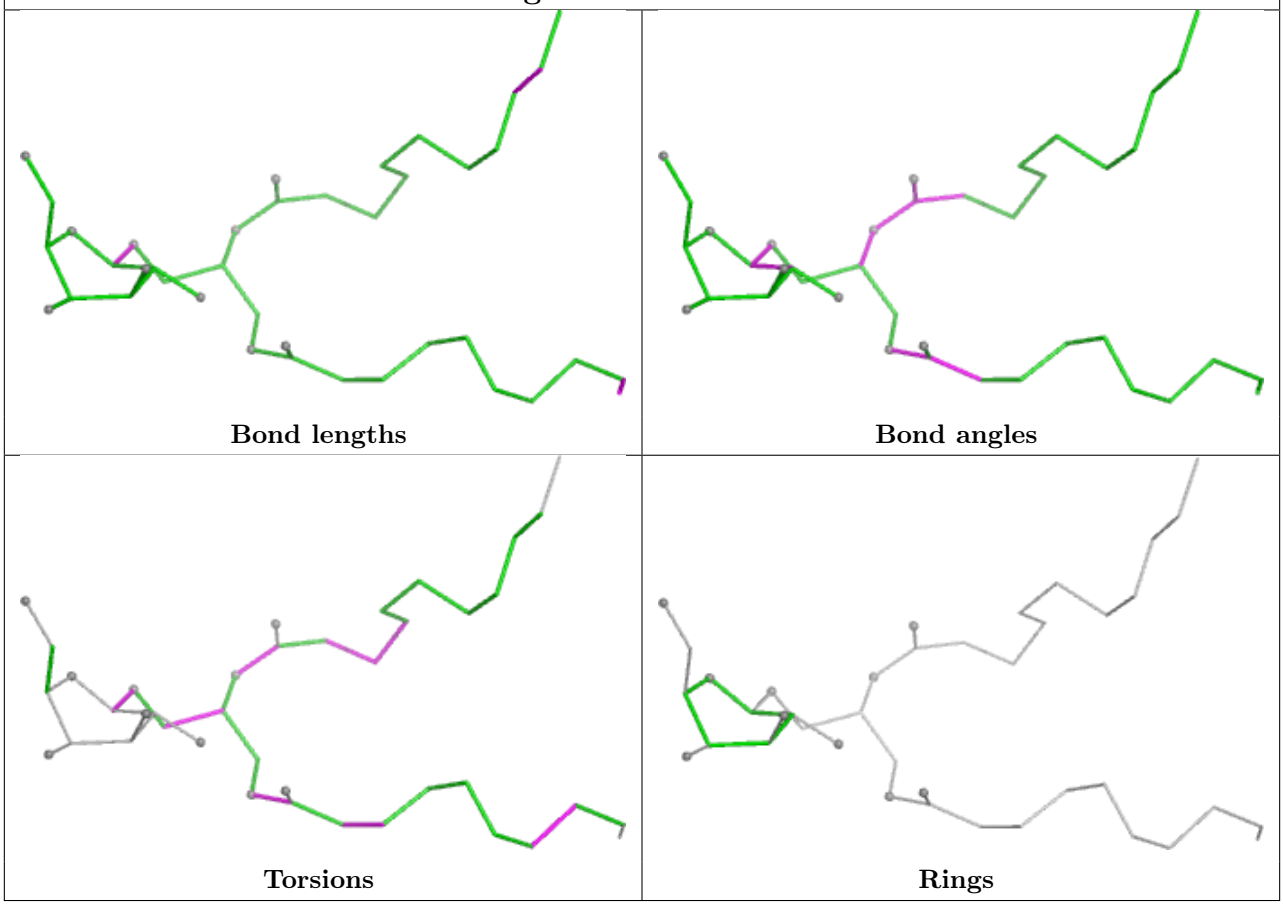
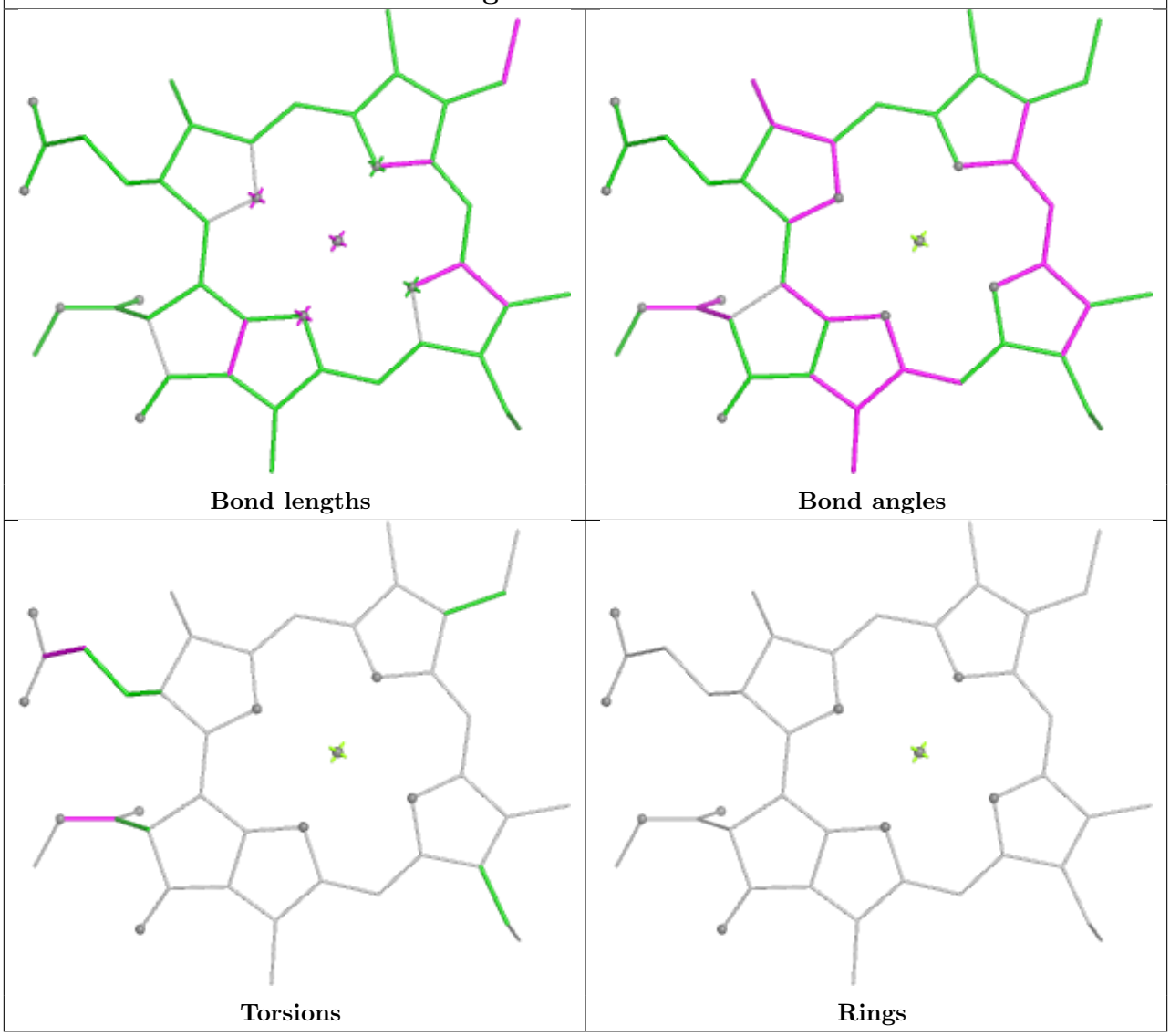
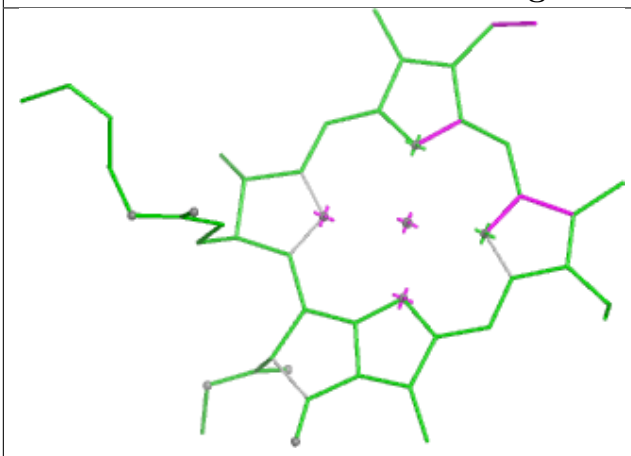


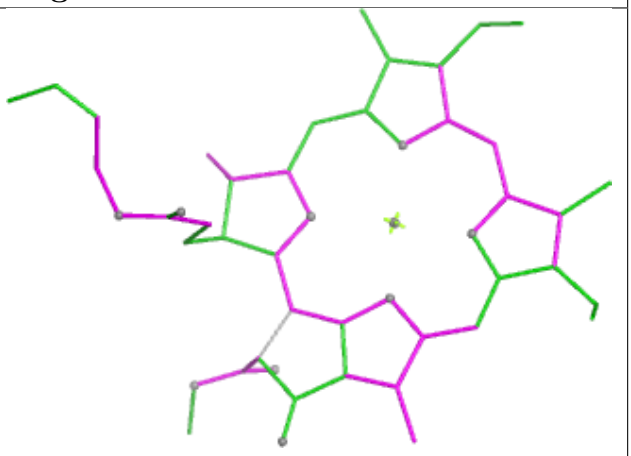
Ligand CLA 8 611



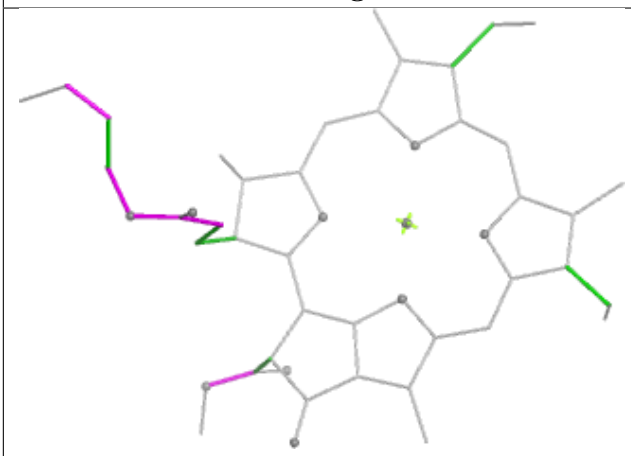
Ligand CLA g 314



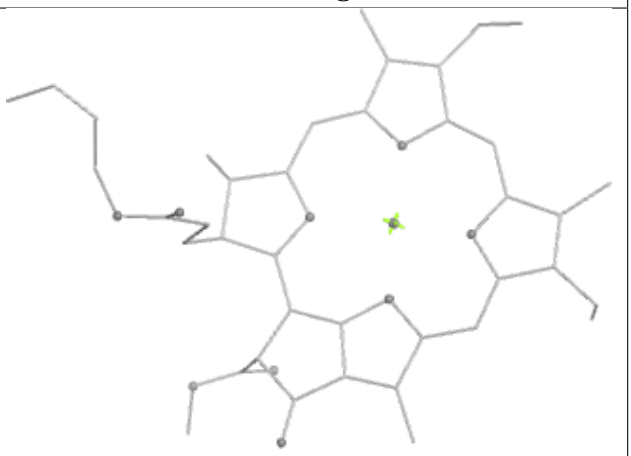
Bond lengths



Bond angles

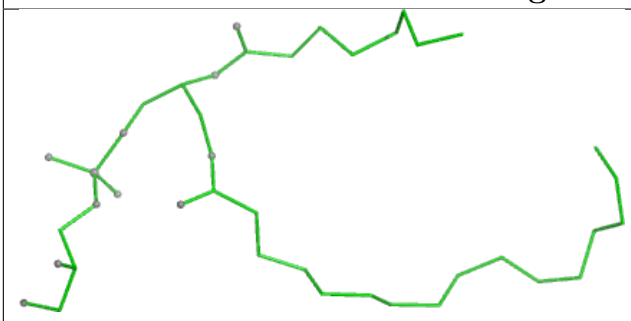


Torsions



Rings

Ligand LHG t 102



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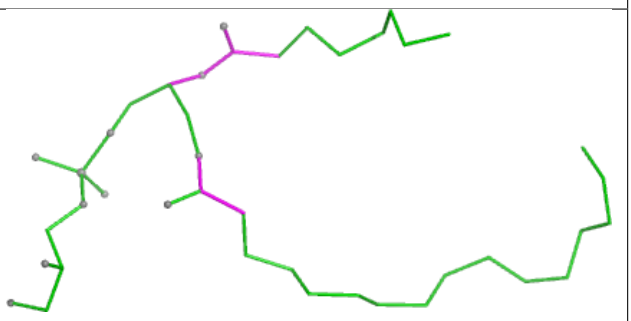
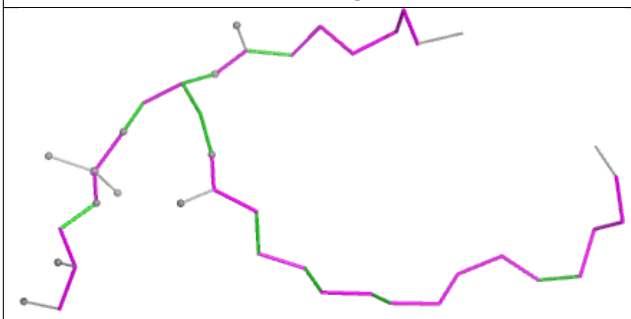


Bond angles



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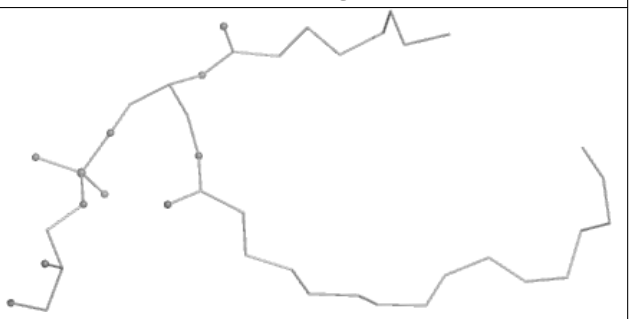
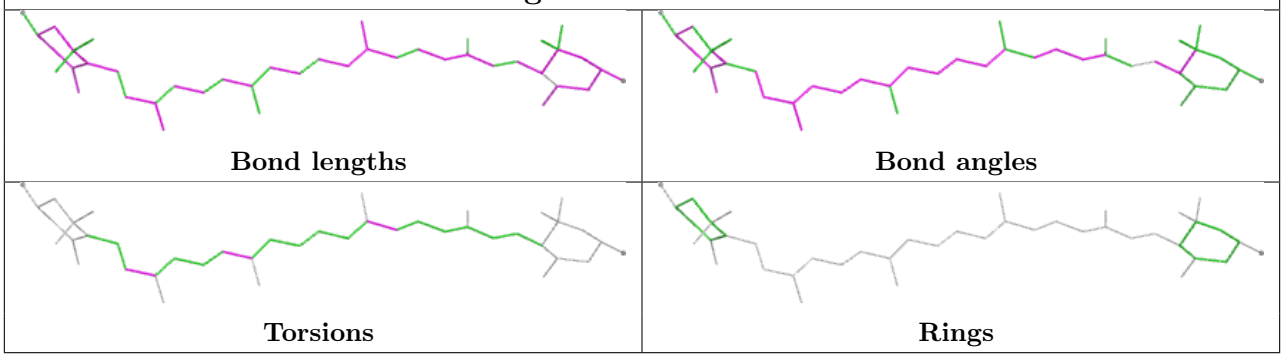


Rings

Ligand LUT N 317



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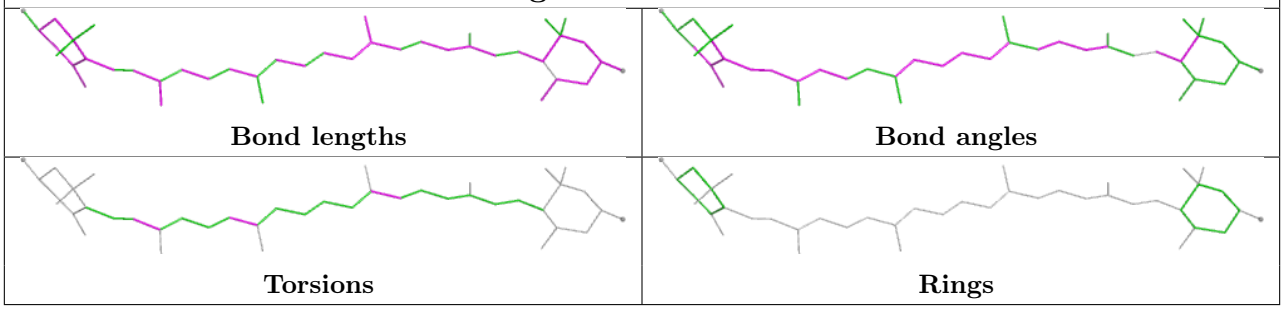
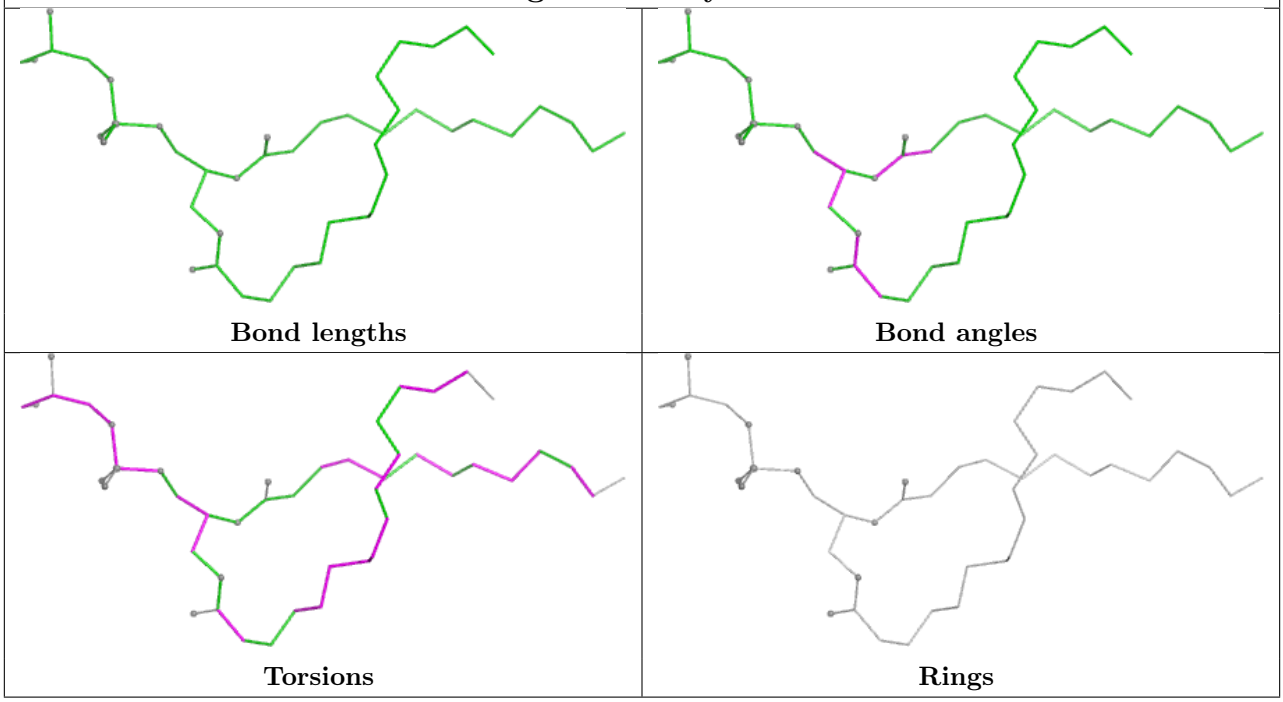
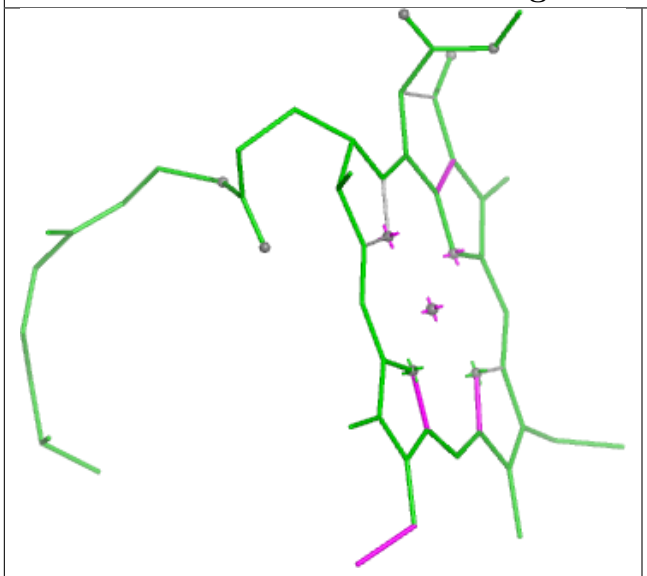


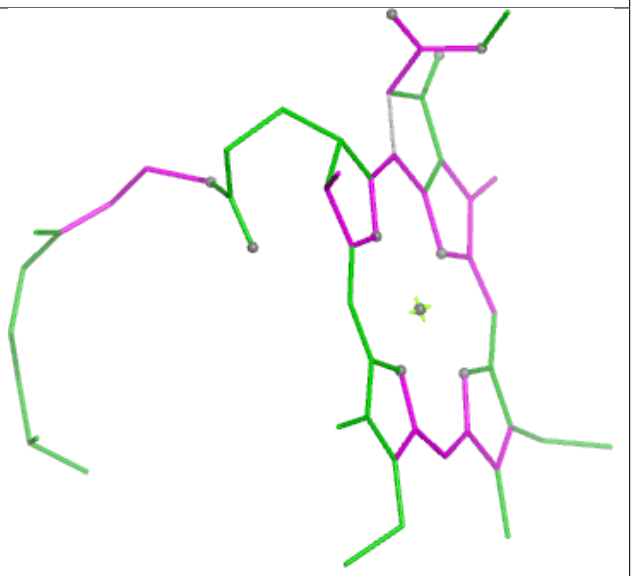
Ligand LHG y 619



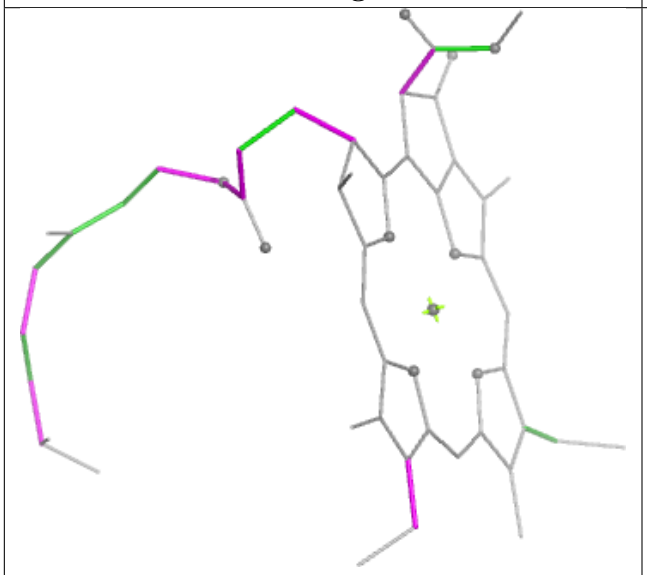
Ligand CLA 0 615



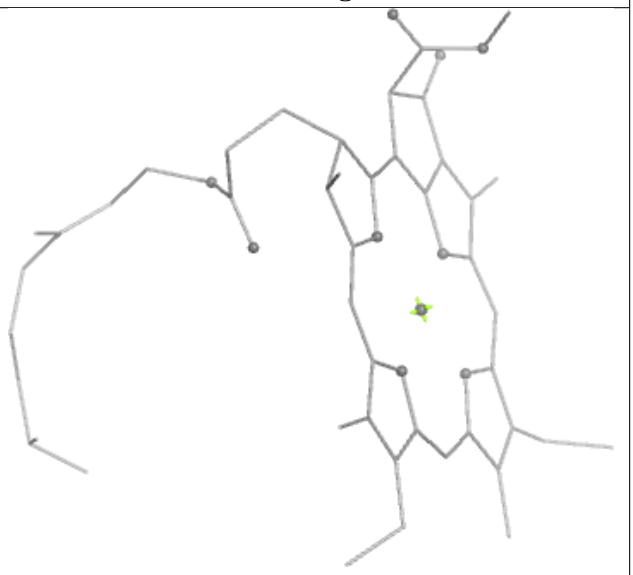
Bond lengths



Bond angles

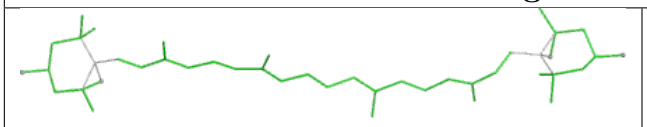


Torsions



Rings

Ligand XAT G 620



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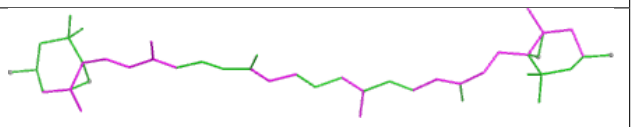
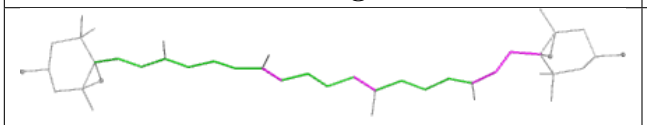


Bond angles



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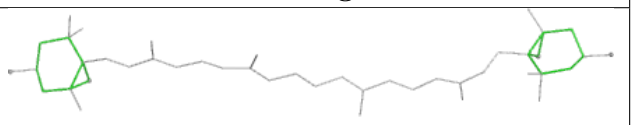
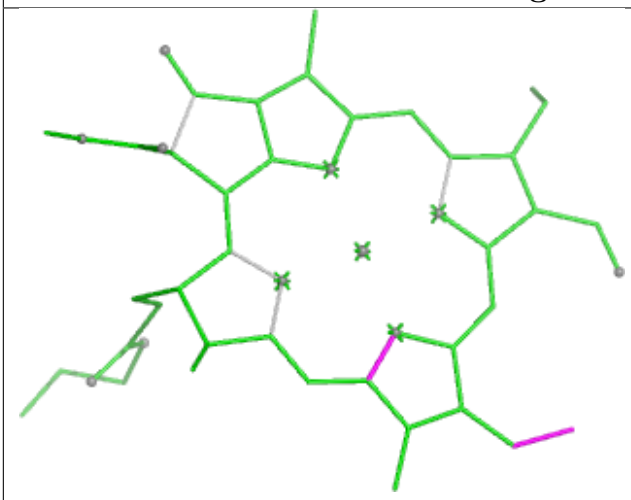


Rings

Ligand CHL s 309



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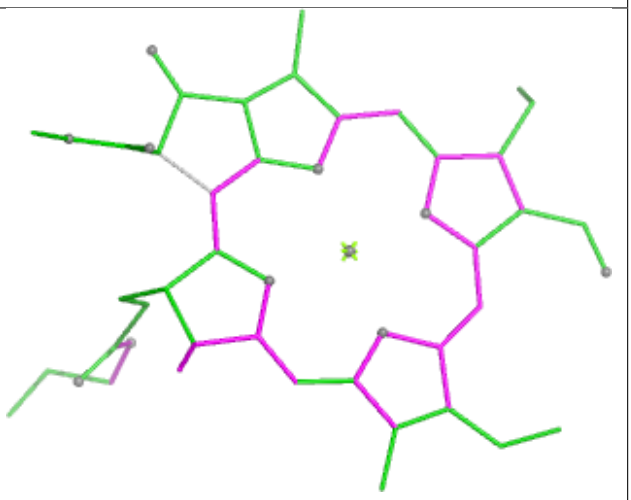
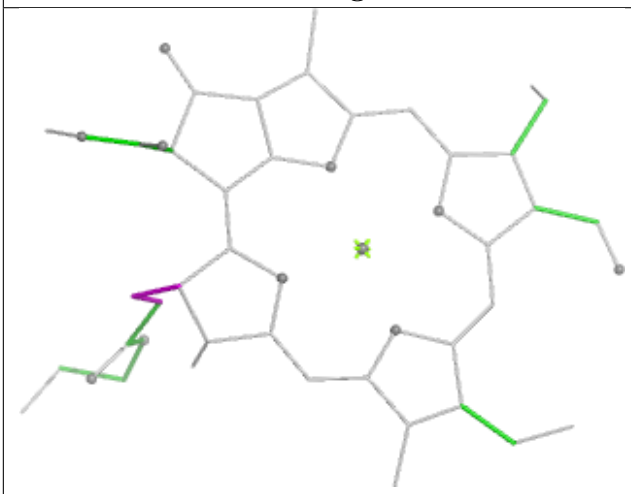


Bond angles



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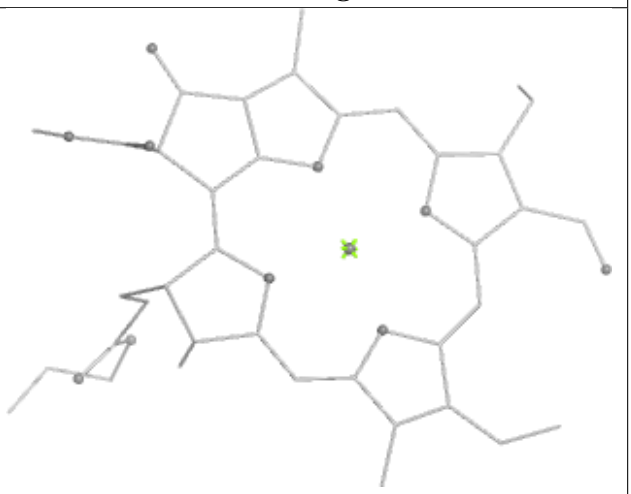
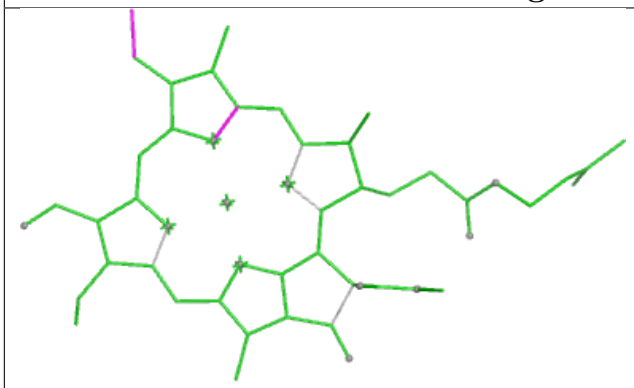
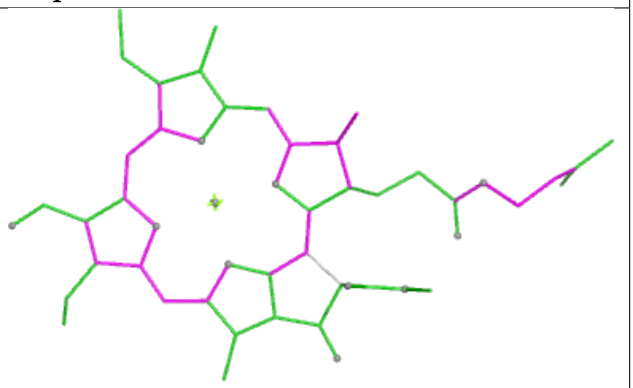
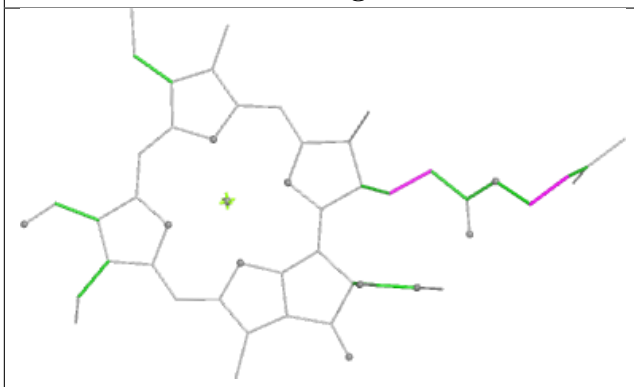
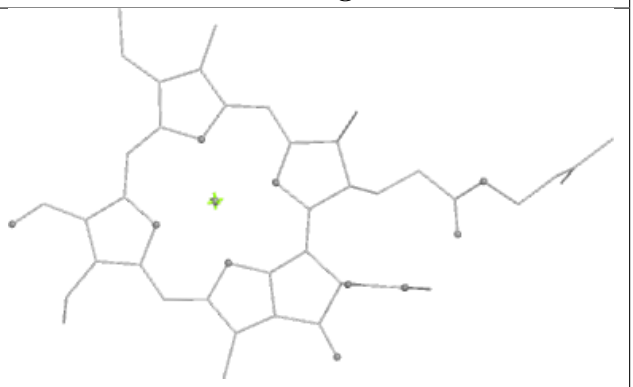


Rings

Ligand CHL p 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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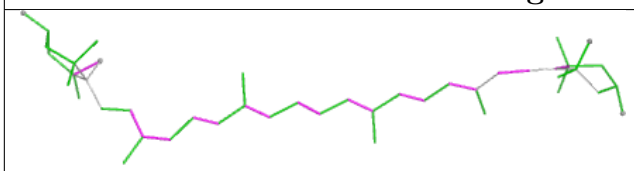
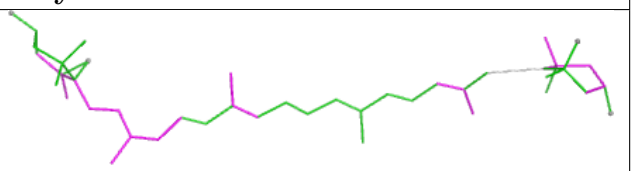
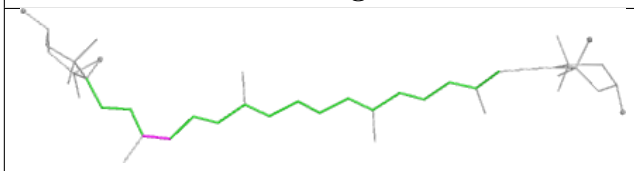
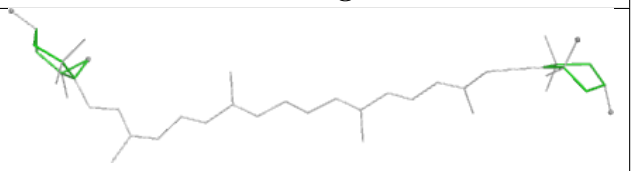
 Bond lengths	 Bond angles
 Torsions	 Rings

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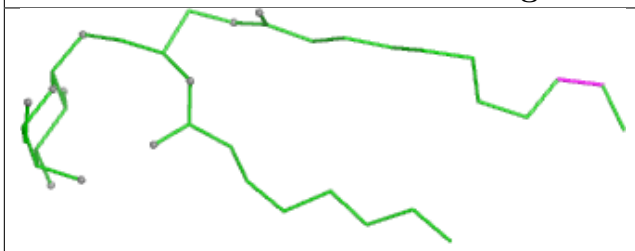
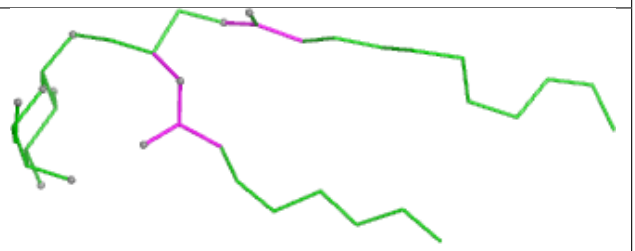
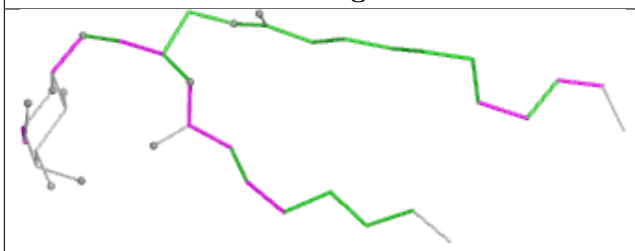
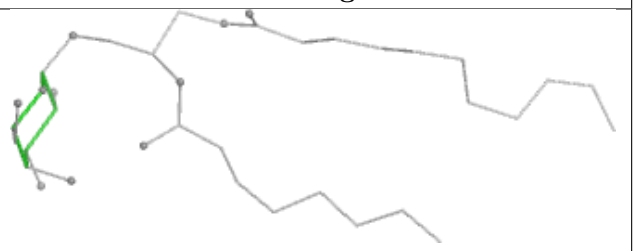
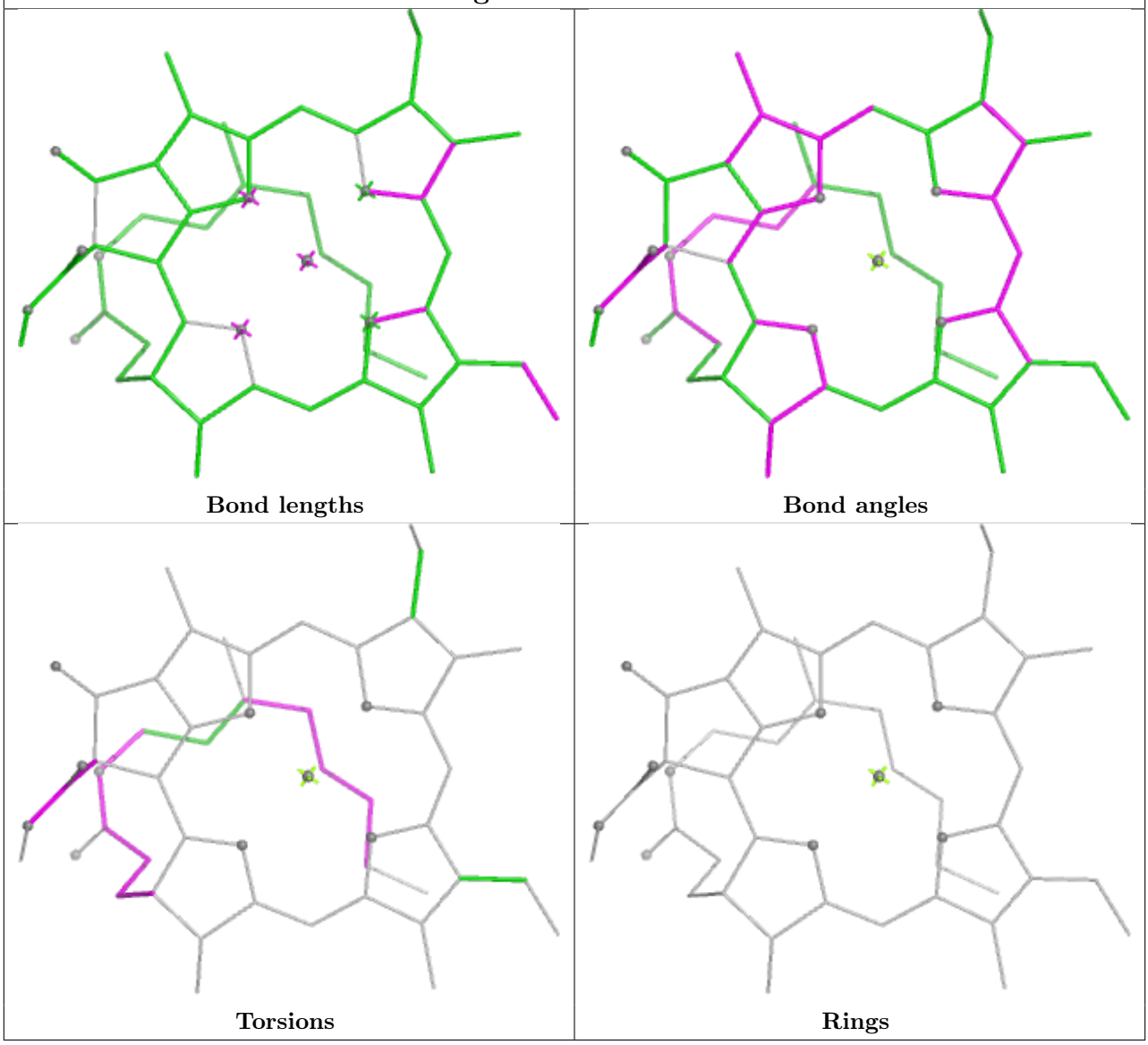
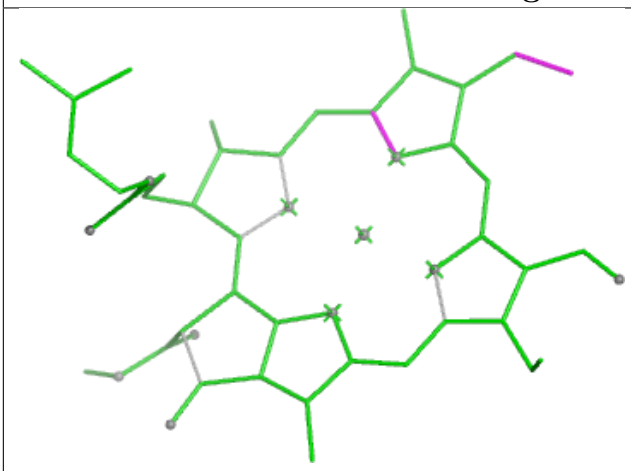
 Bond lengths	 Bond angles
 Torsions	 Rings

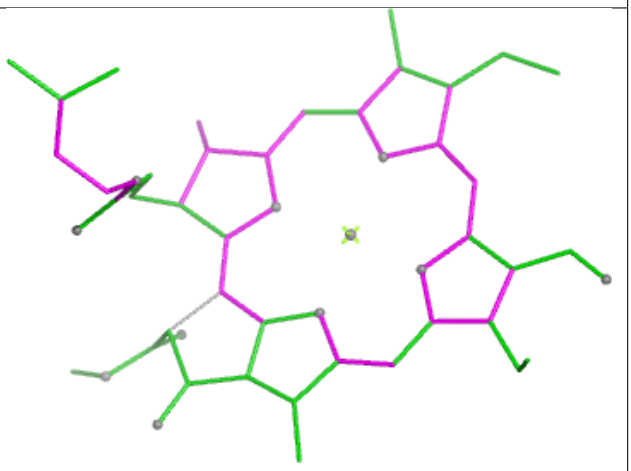
Ligand CLA 6 315



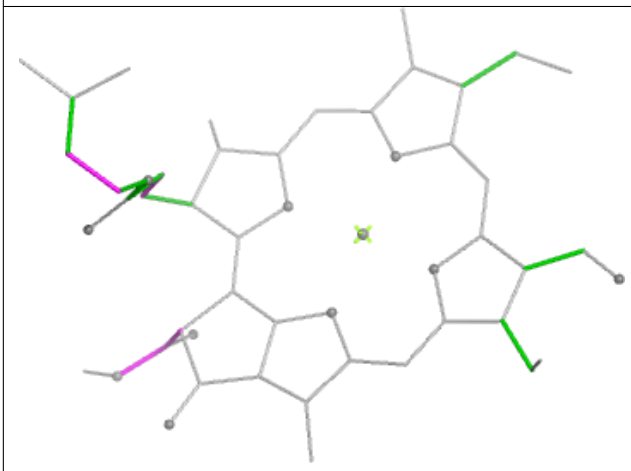
Ligand CHL G 607



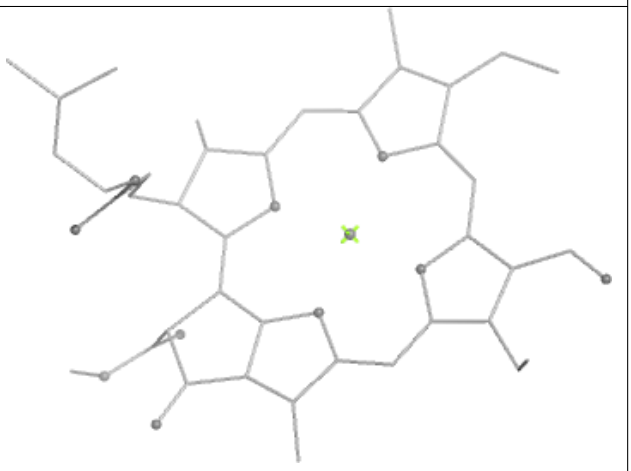
Bond lengths



Bond angles

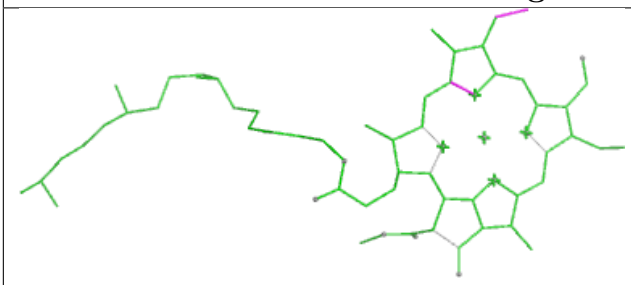


Torsions



Rings

Ligand CHL g 302



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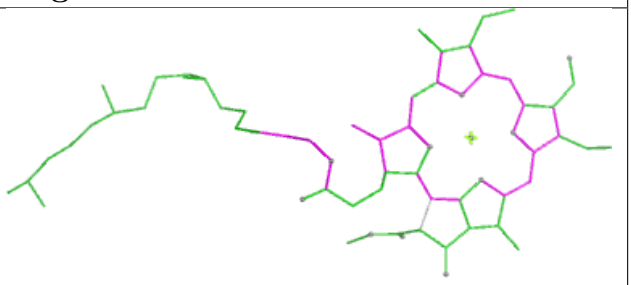
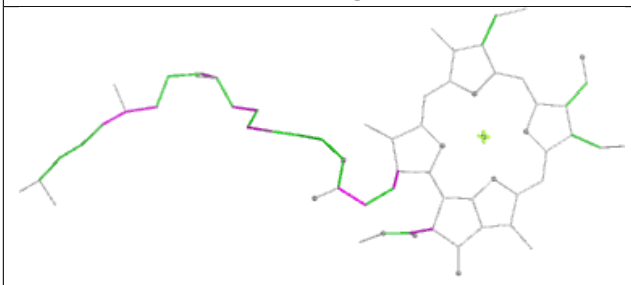


Bond angles



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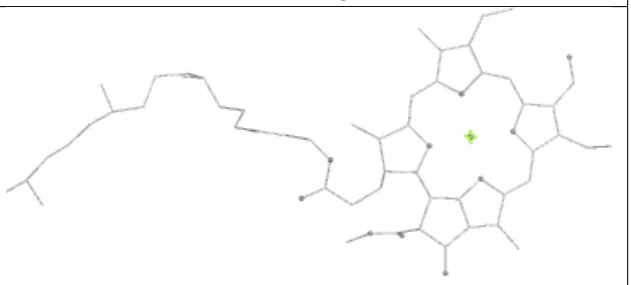
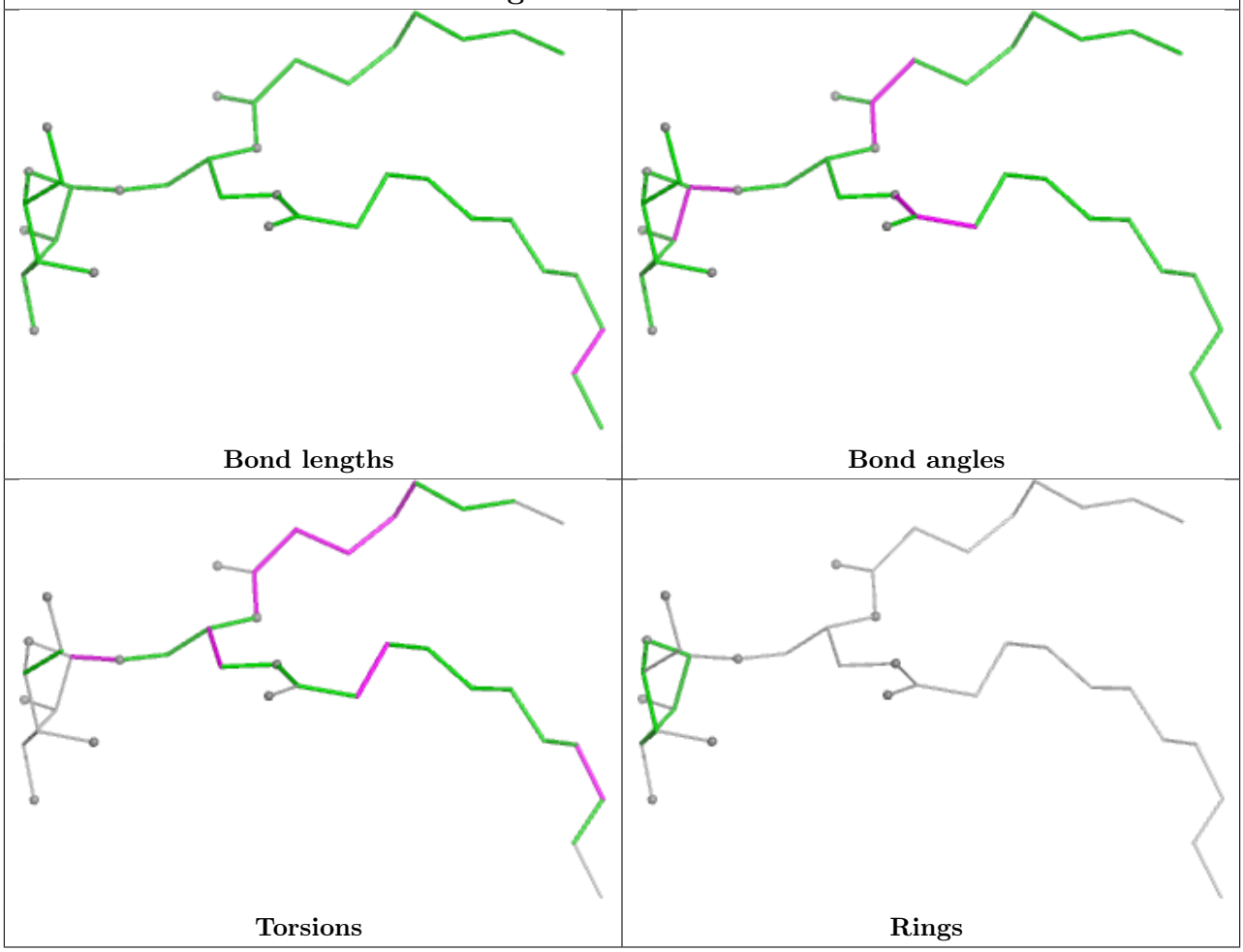
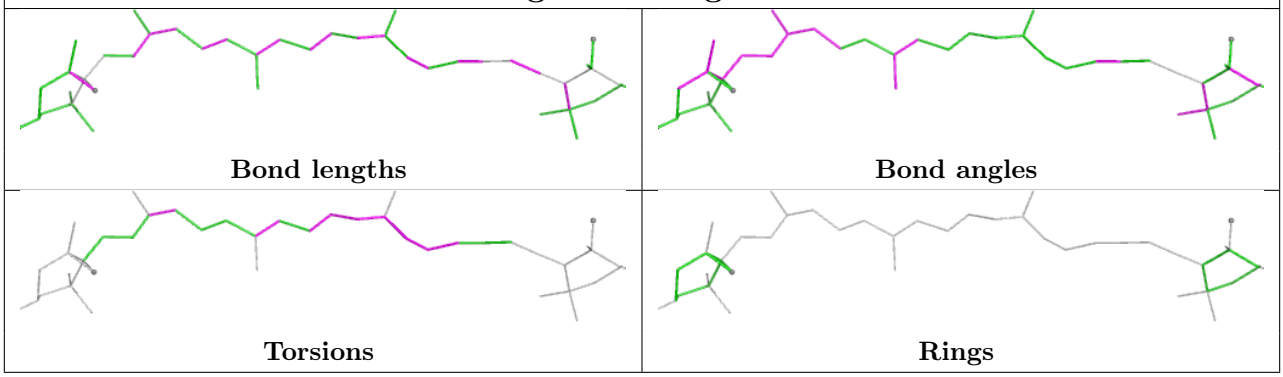


Rings

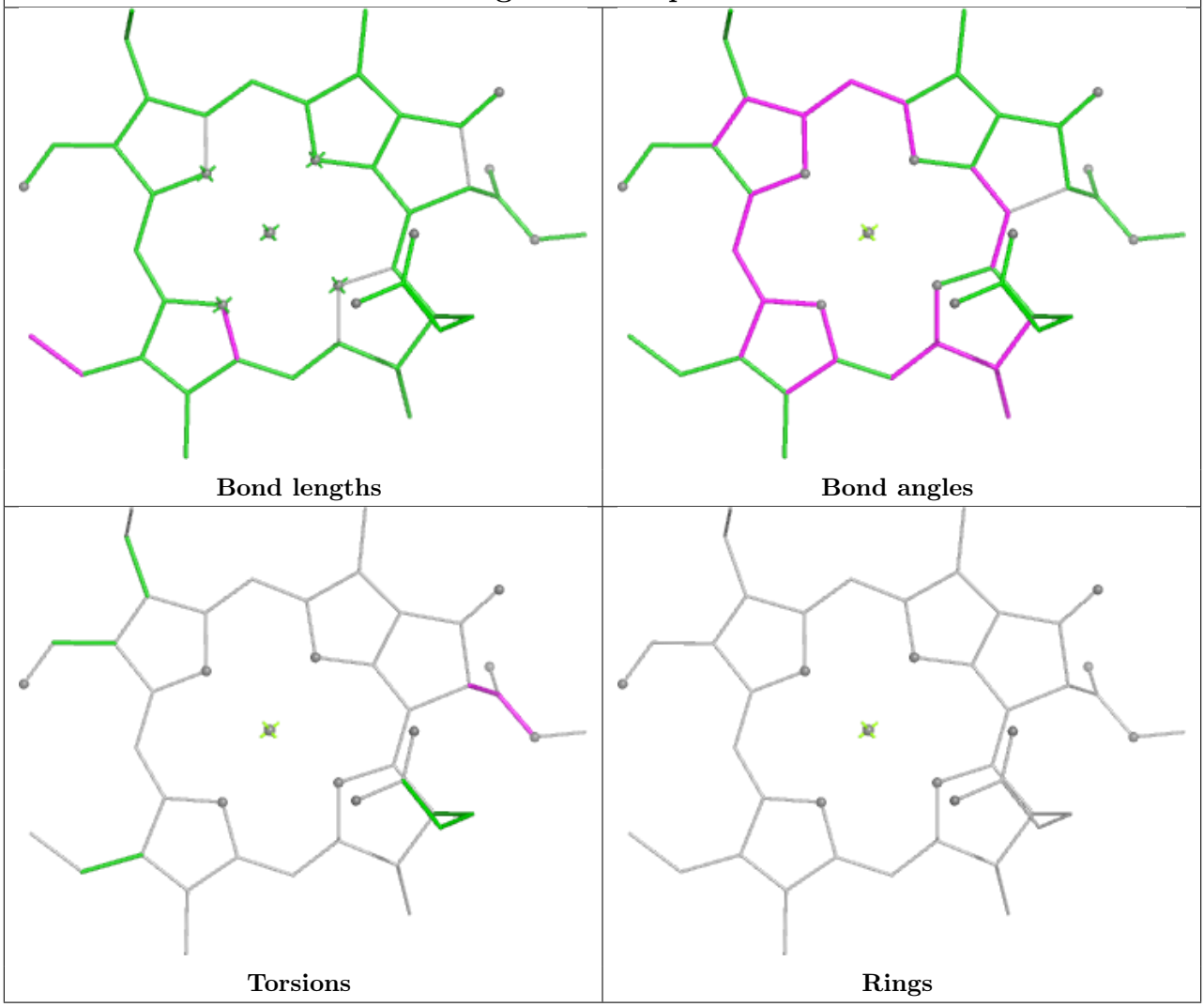
Ligand LMG n 321

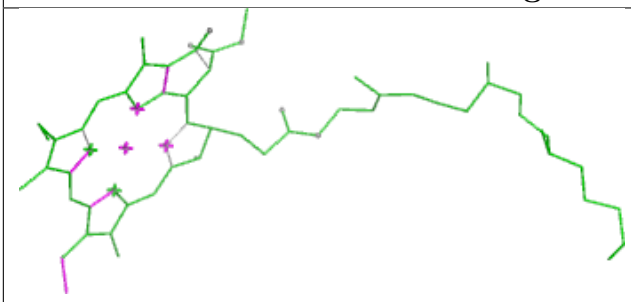
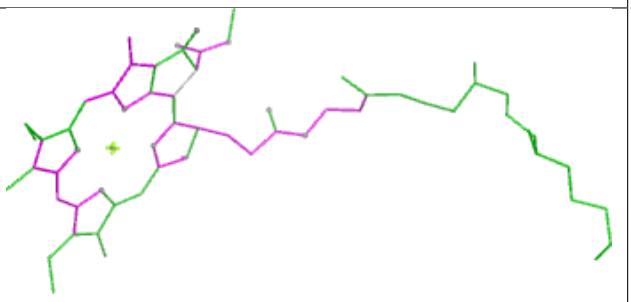
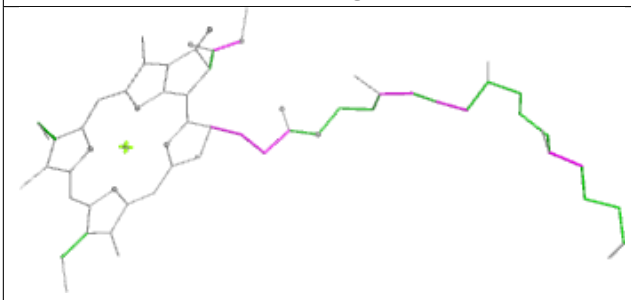
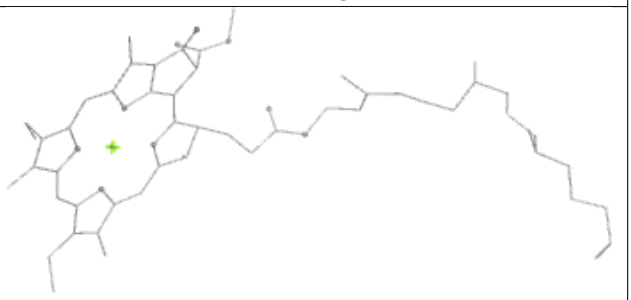


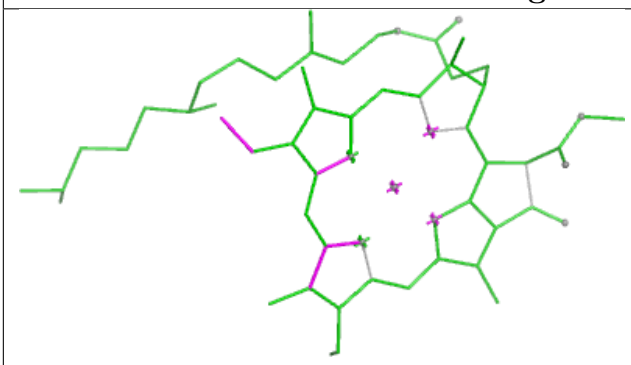
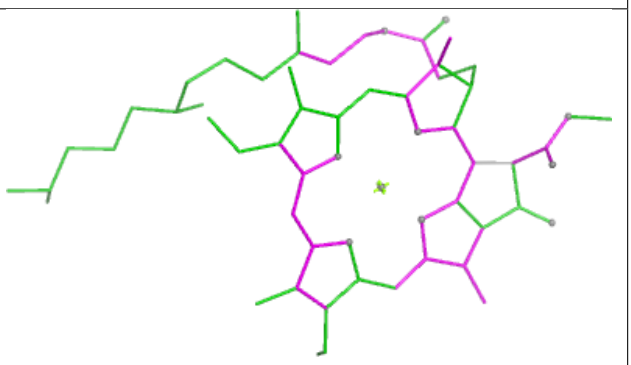
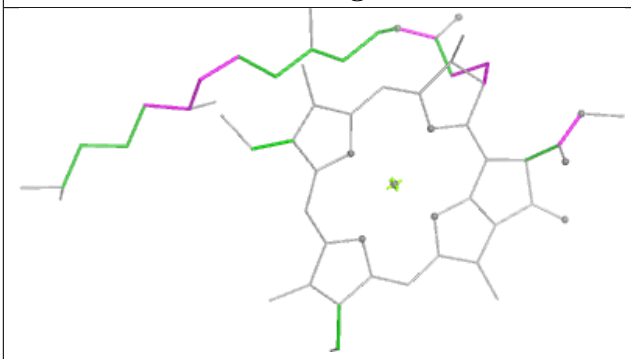
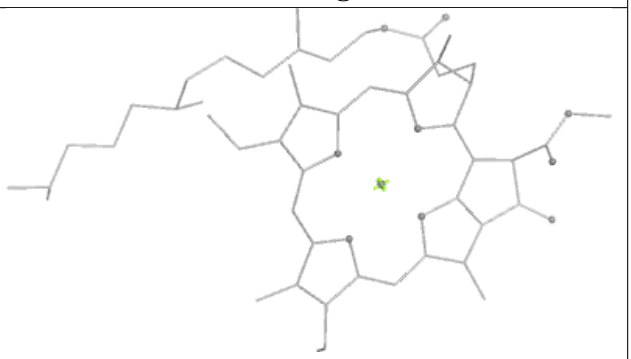
Ligand NEX g 317



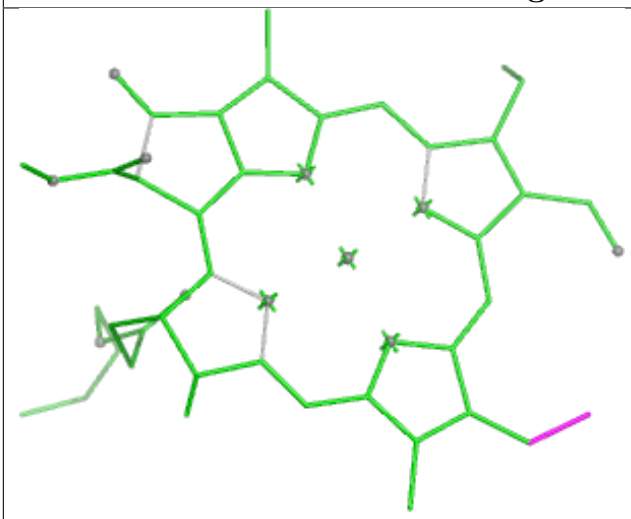
Ligand CHL q 307



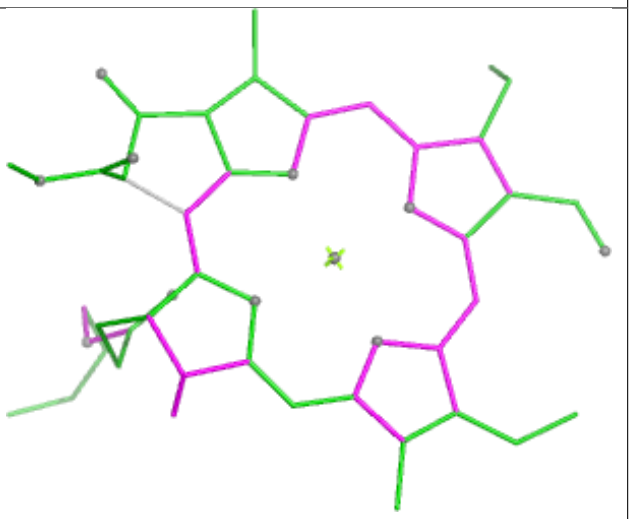
Ligand CLA A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

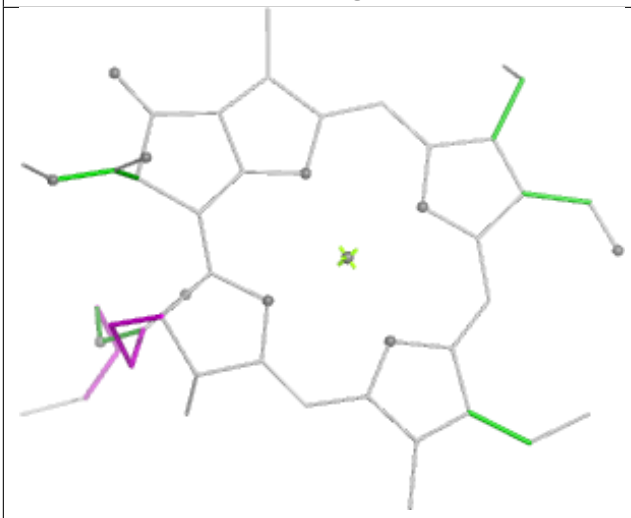
Ligand CHL 7 309



Bond lengths



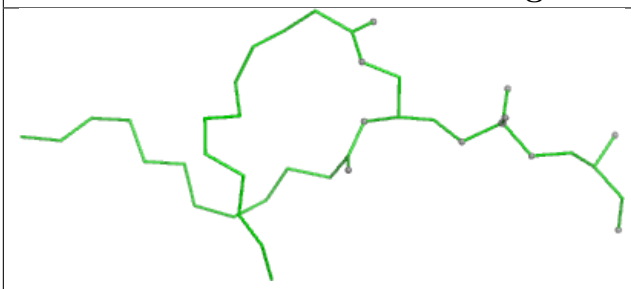
Bond angles



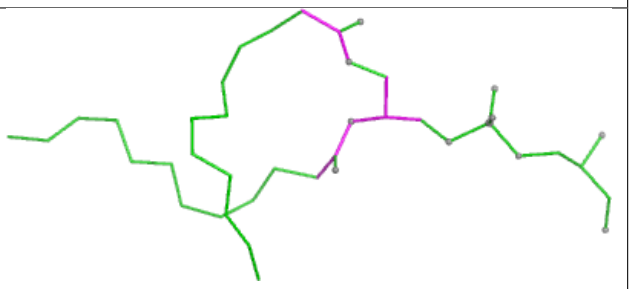
Torsions

Rings

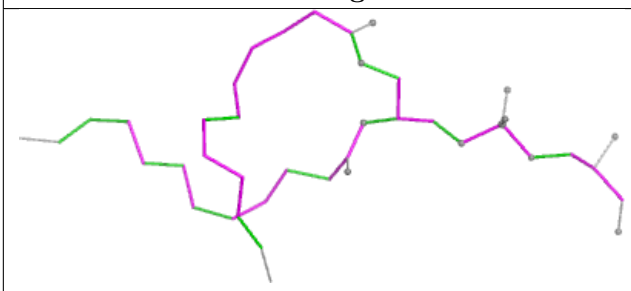
Ligand LHG S 320



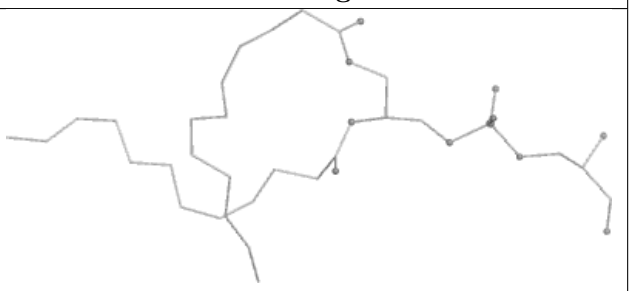
Bond lengths



Bond angles

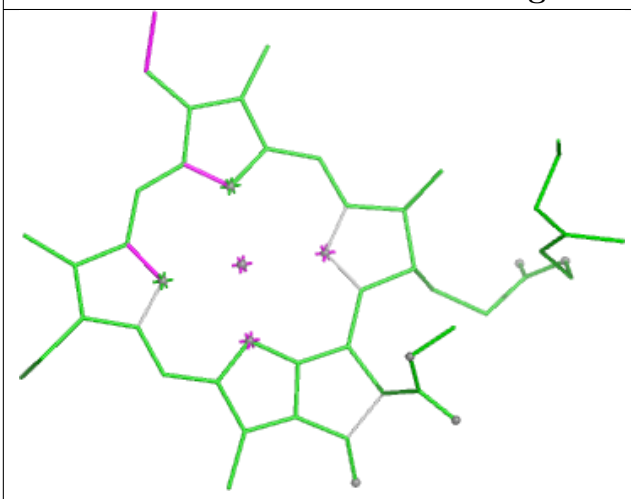


Torsions

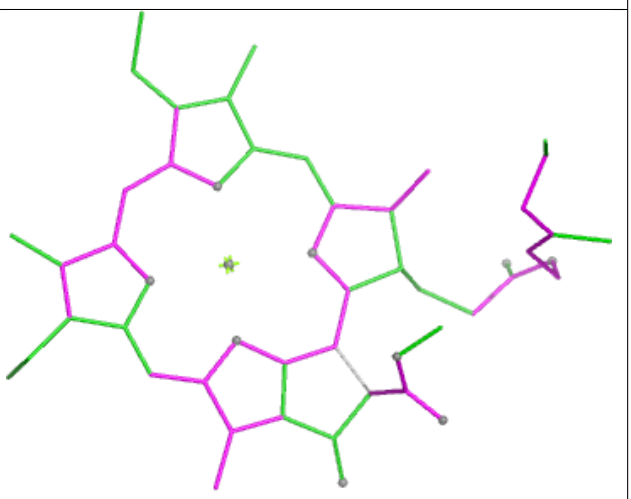


Rings

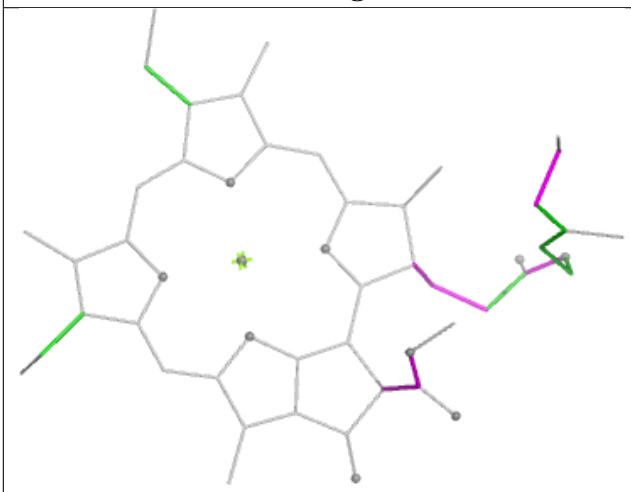
Ligand CLA 5 603



Bond lengths



Bond angles



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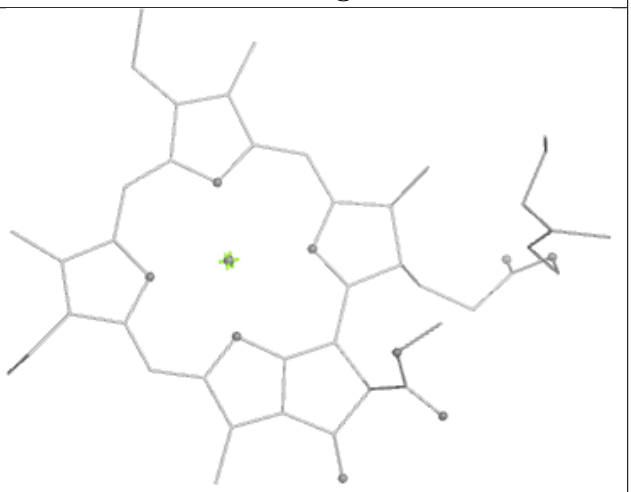
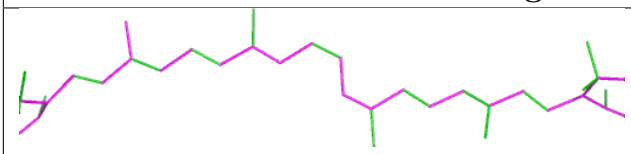
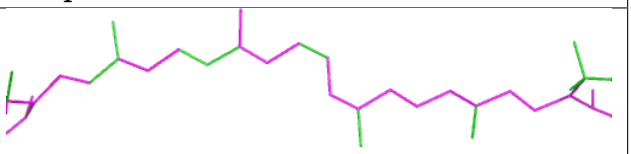


Rings

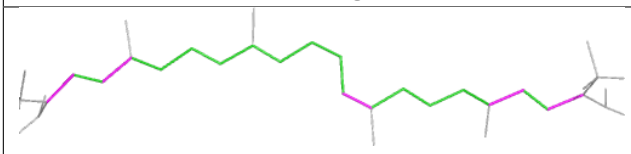
Ligand RRX q 317



Bond lengths



Bond angles



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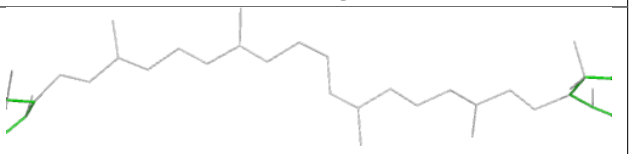
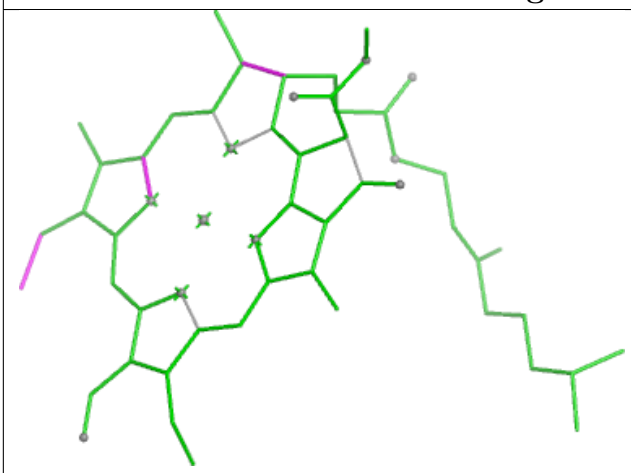


Rings

Ligand CHL p 609



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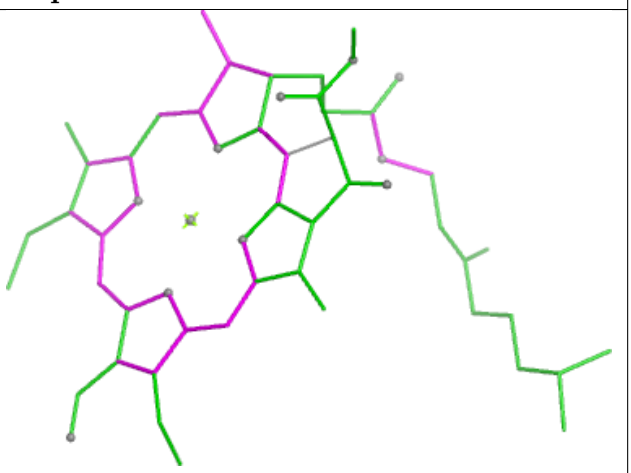
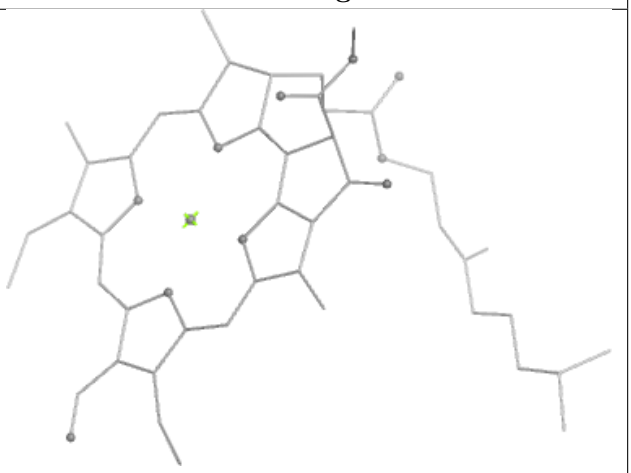


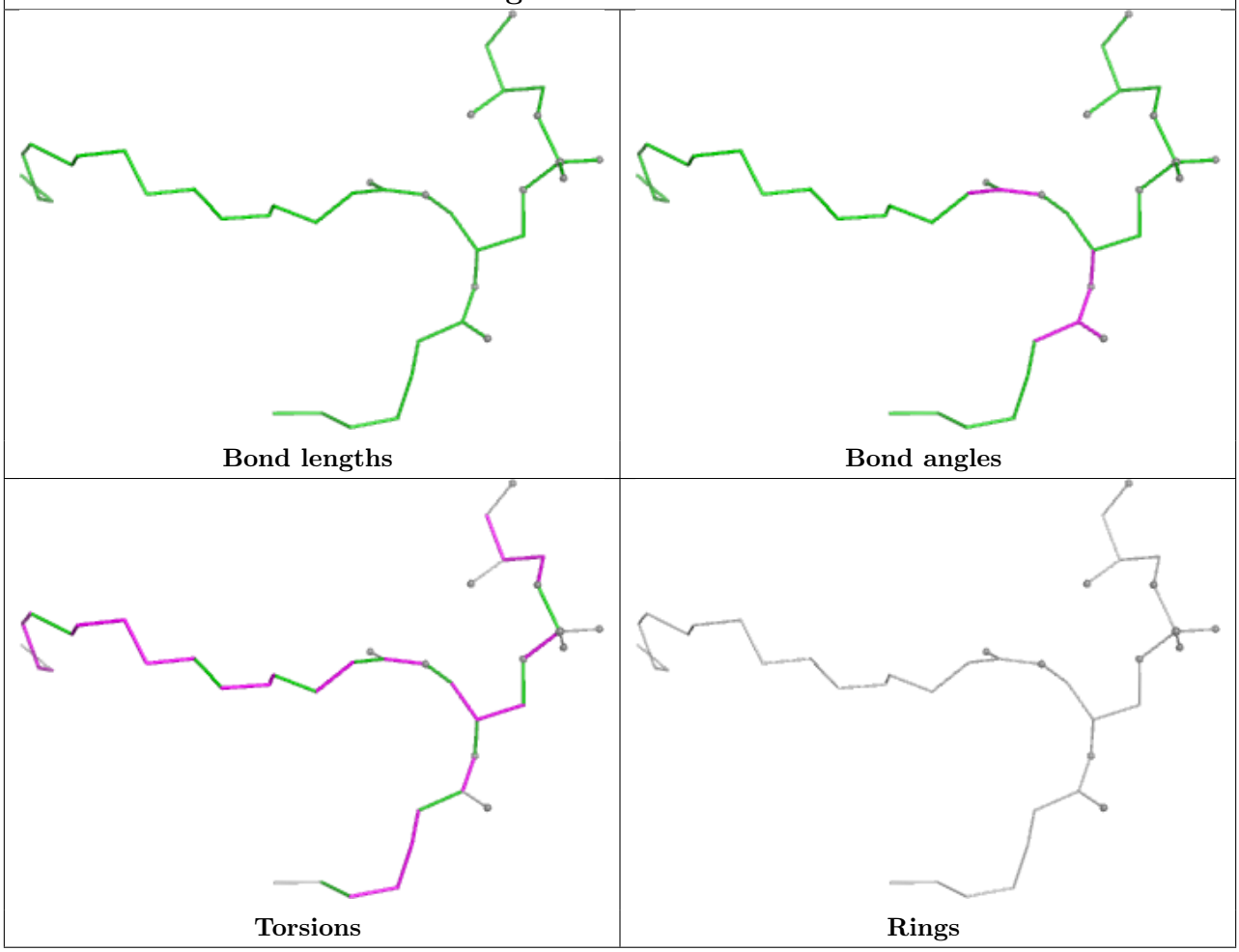
Bond angles

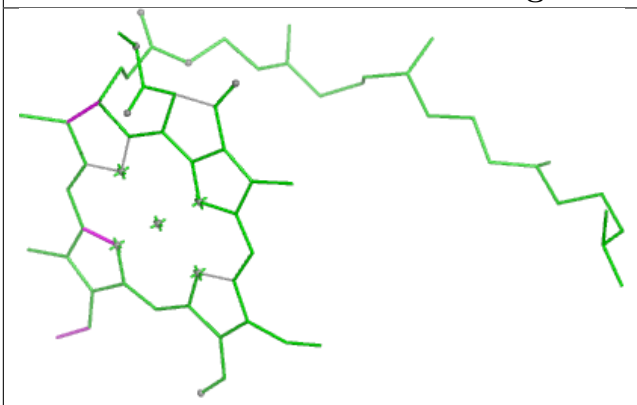
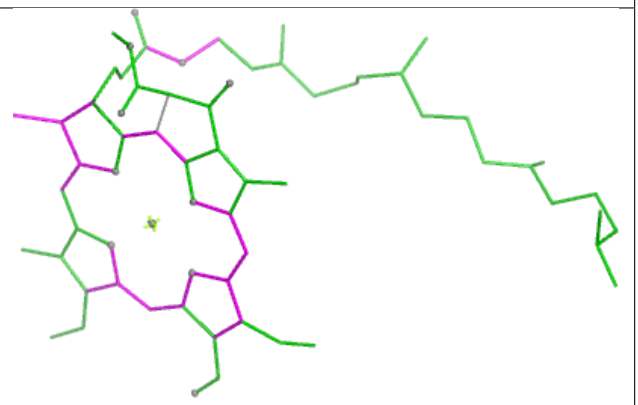
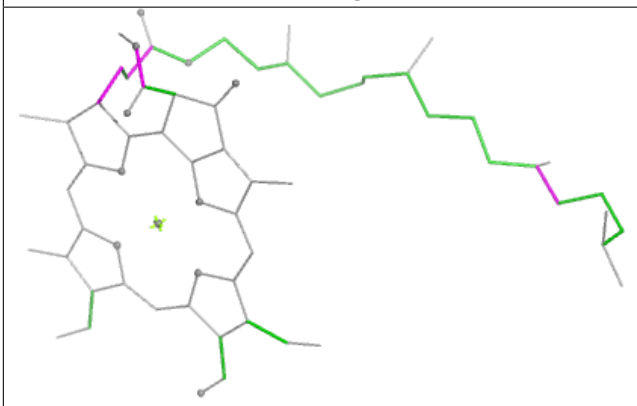
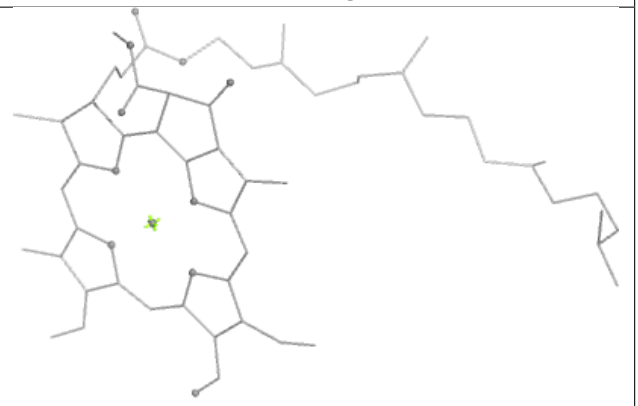
Torsions

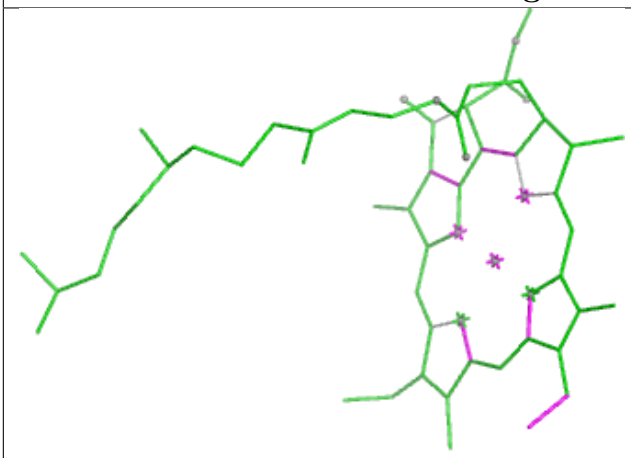
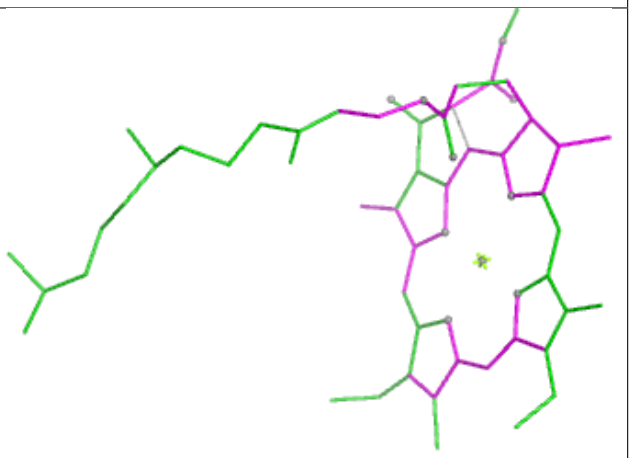
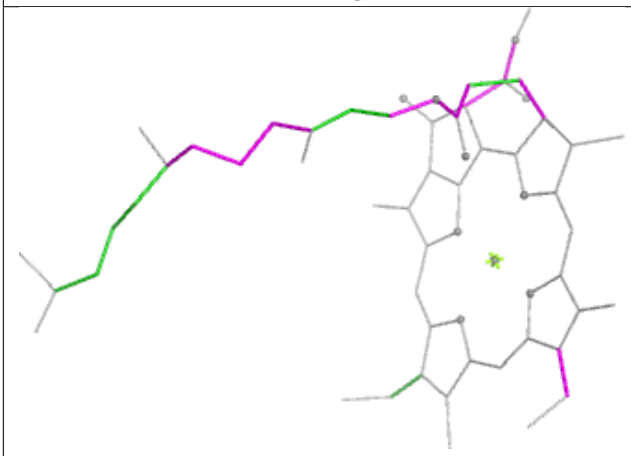


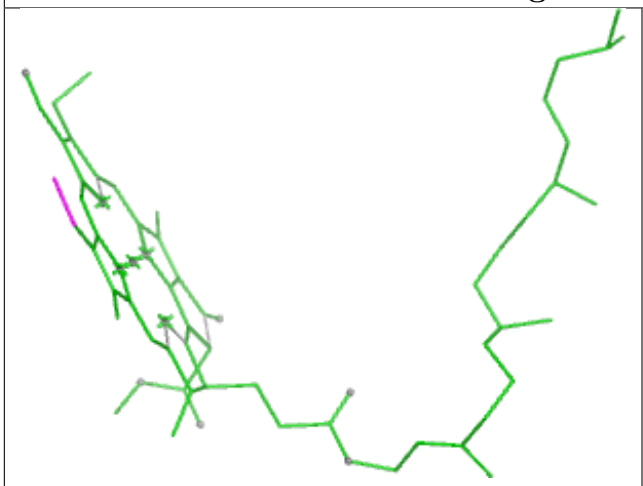
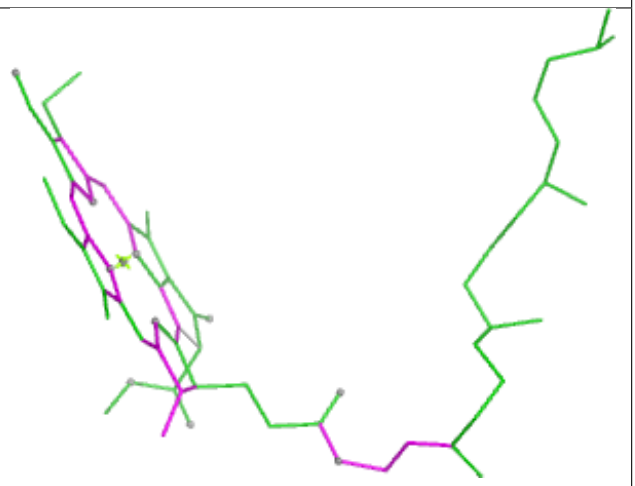
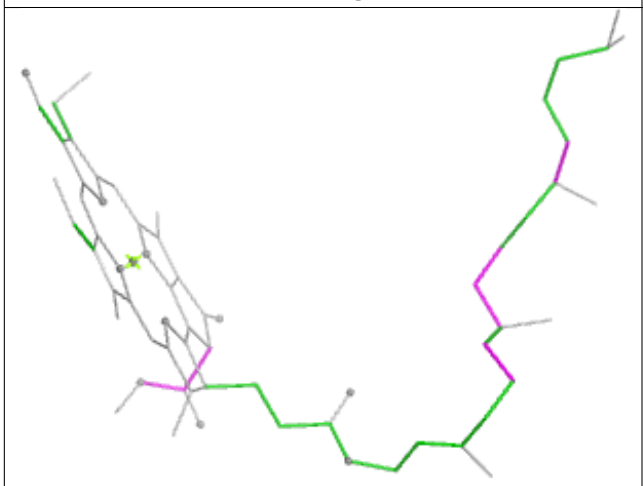
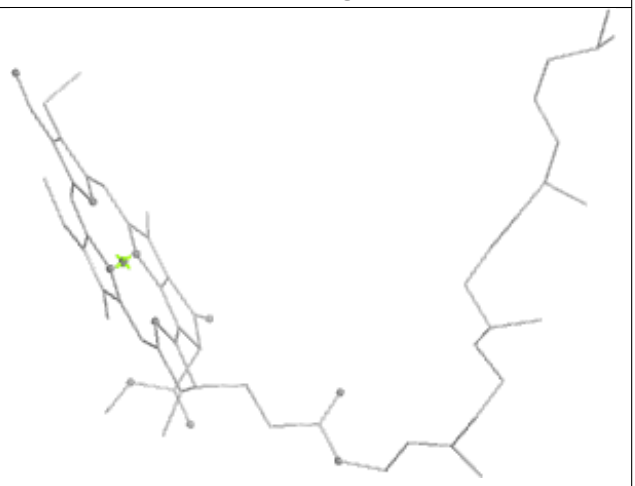
Rings

Ligand LHG C 623

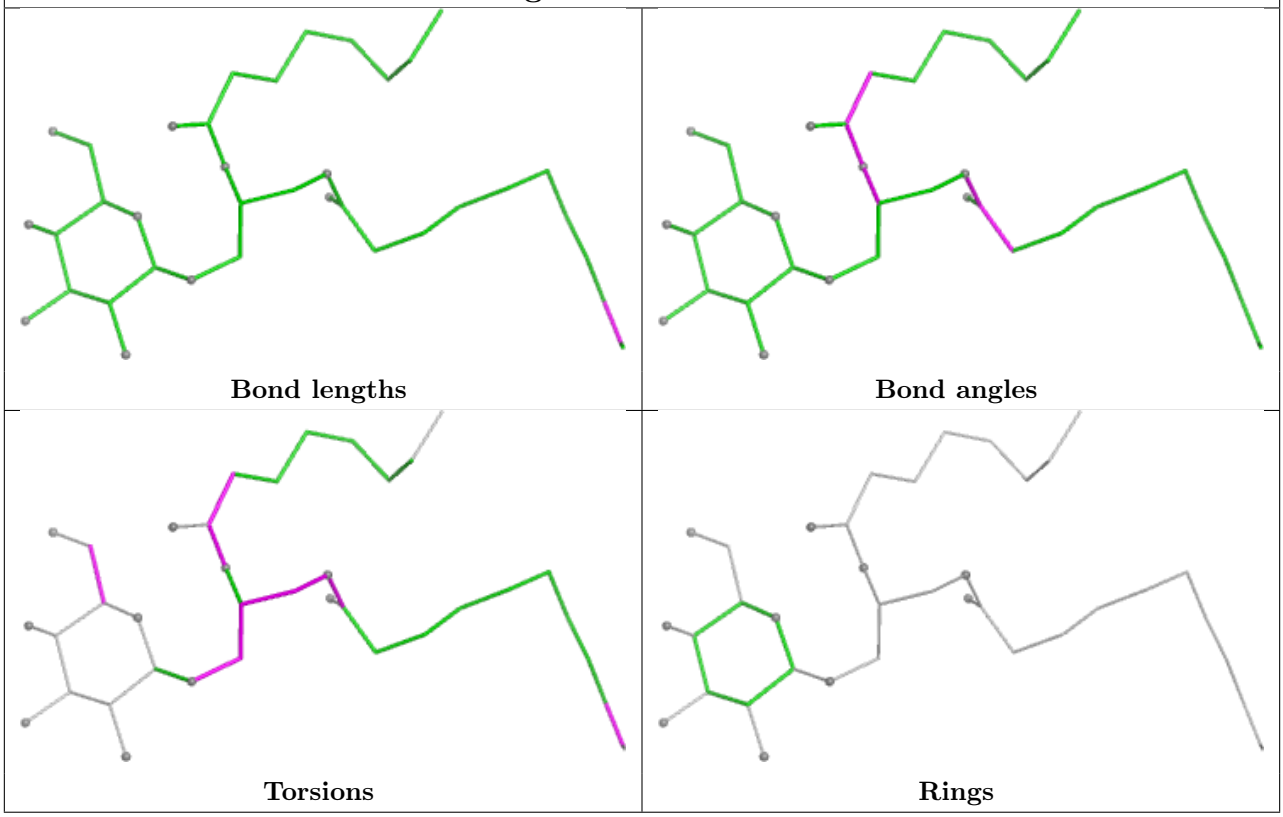


Ligand CHL n 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

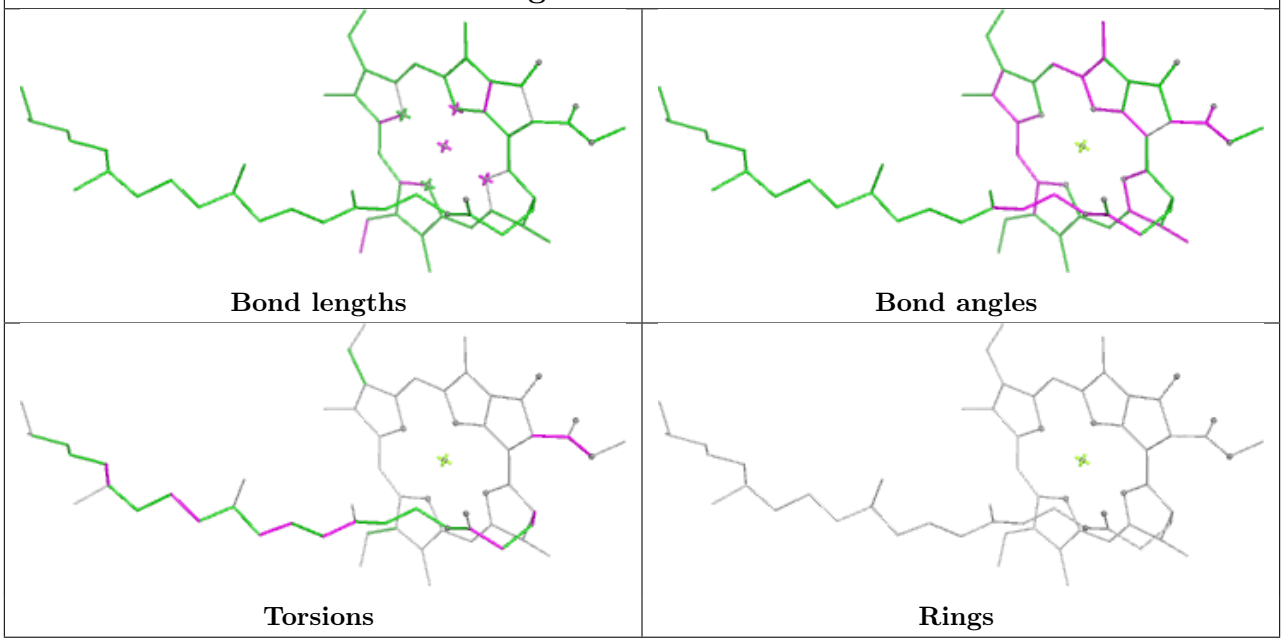
Ligand CLA G 610	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CHL 7 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG 2 618



Ligand CLA b 609



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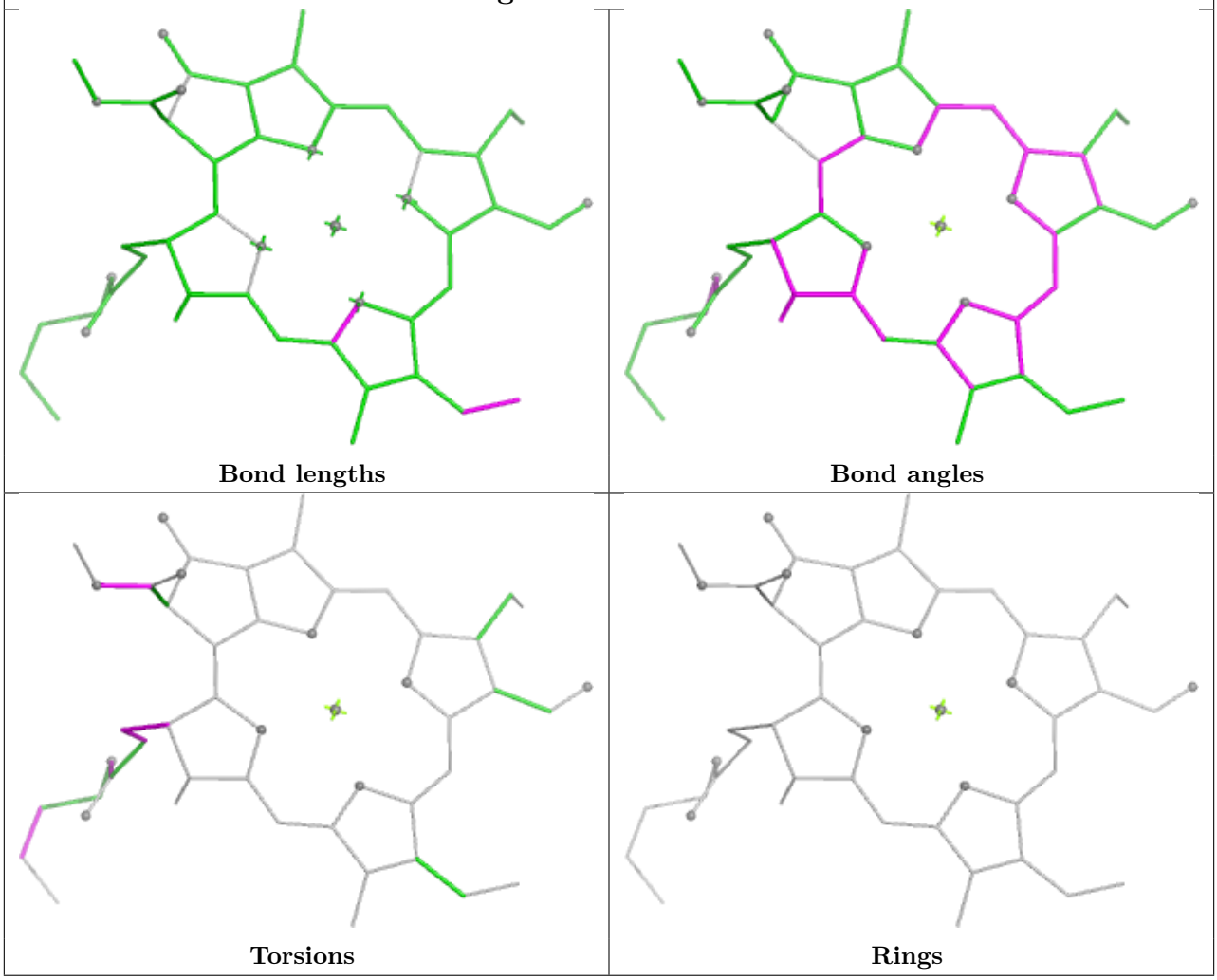

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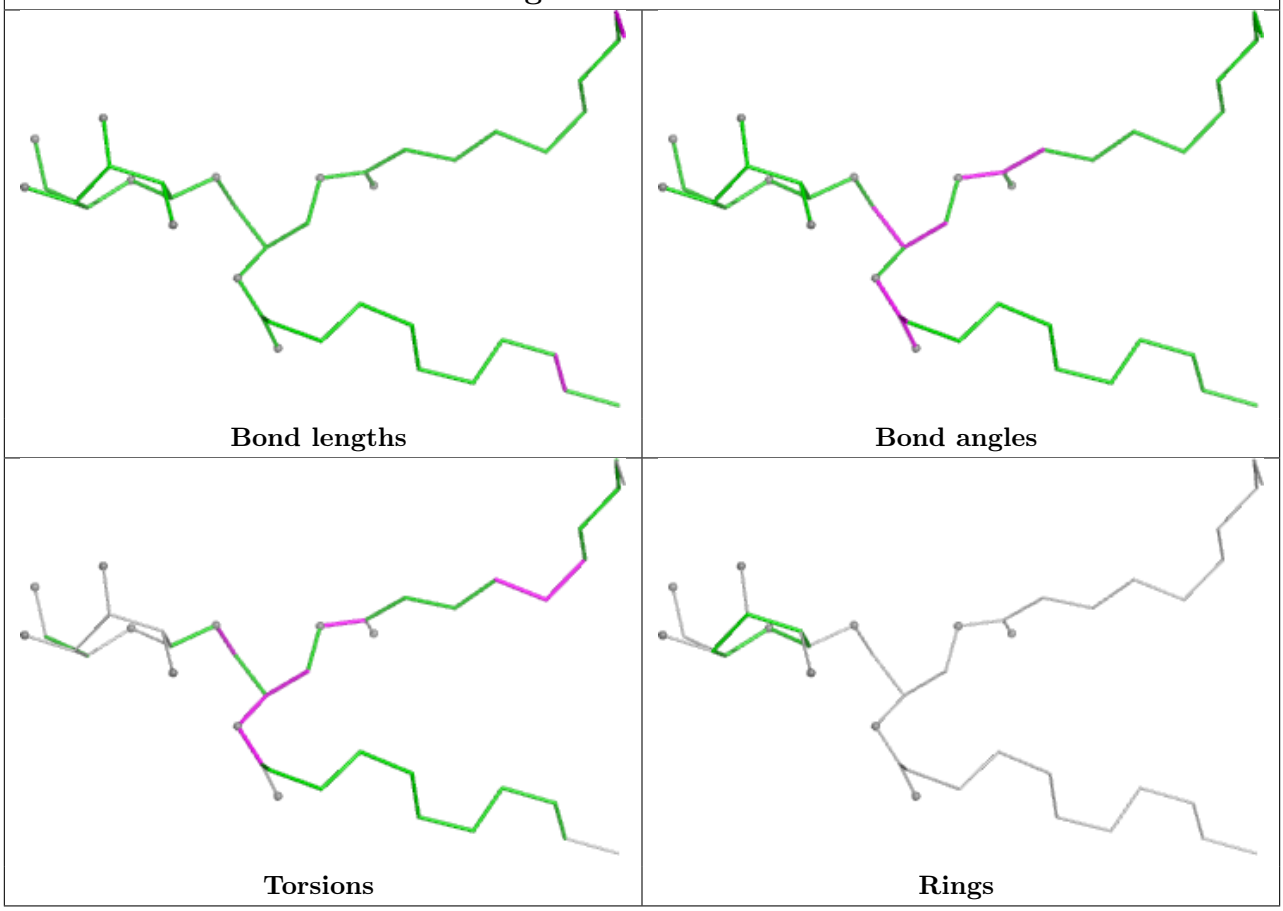
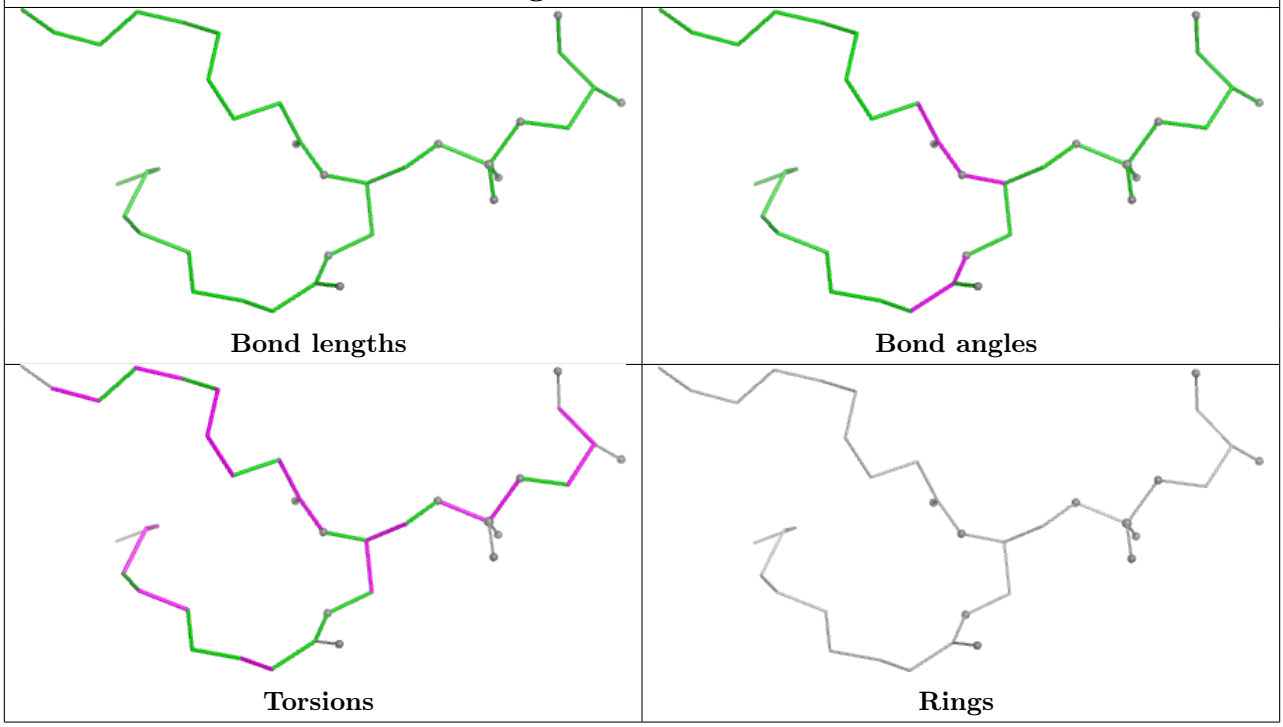


Ligand LHG 6 320



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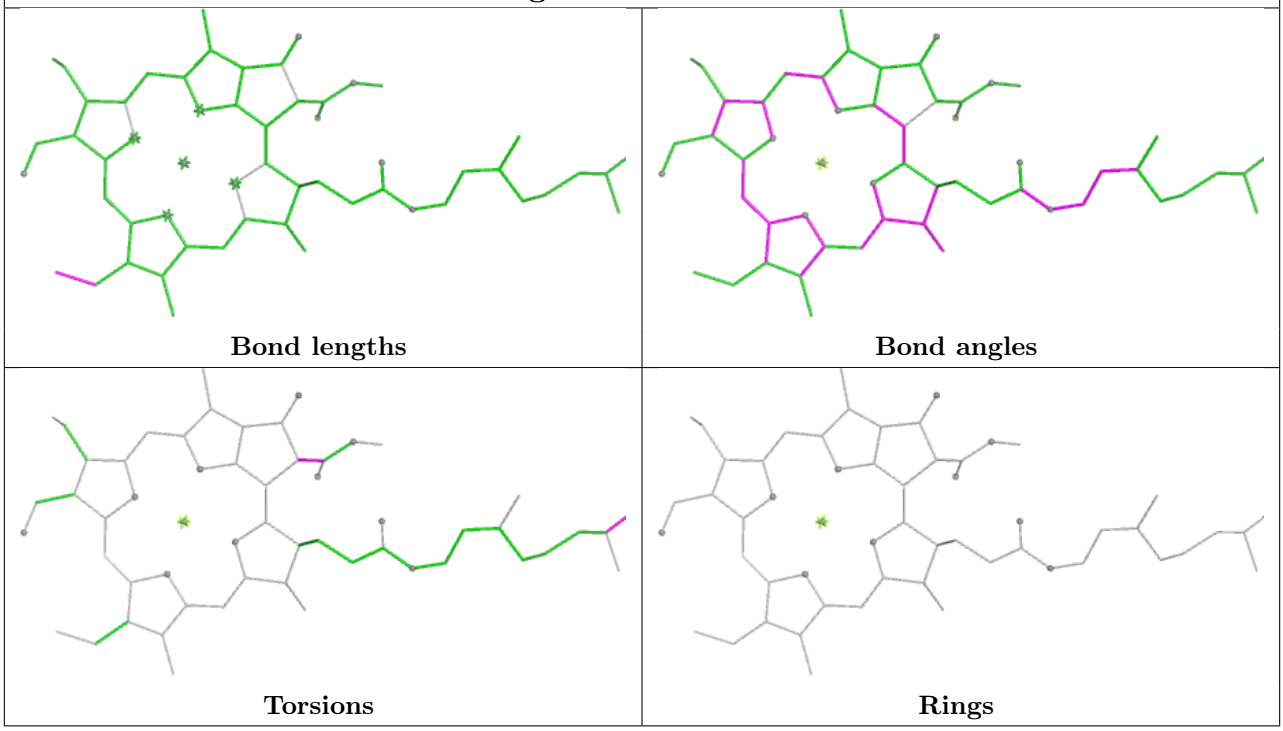
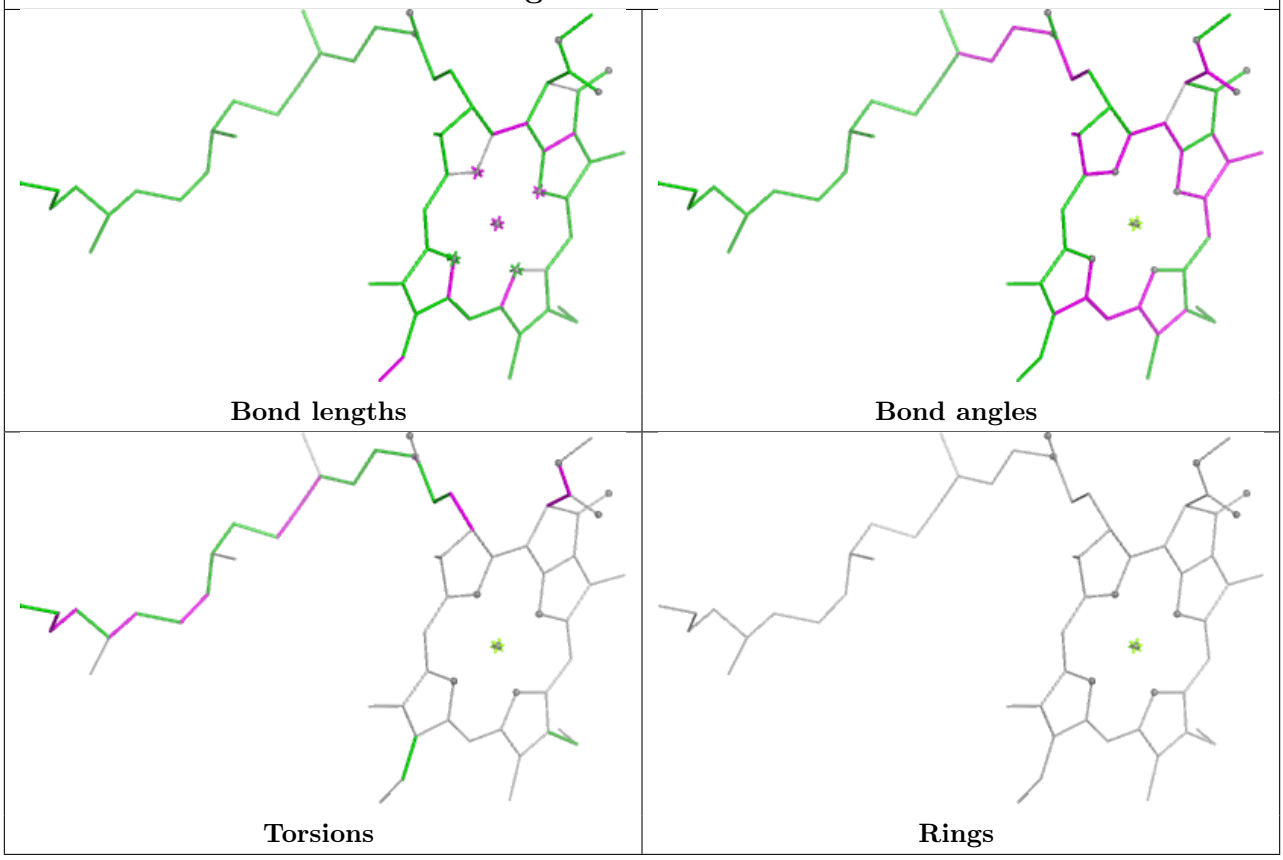


Ligand CLA C 611



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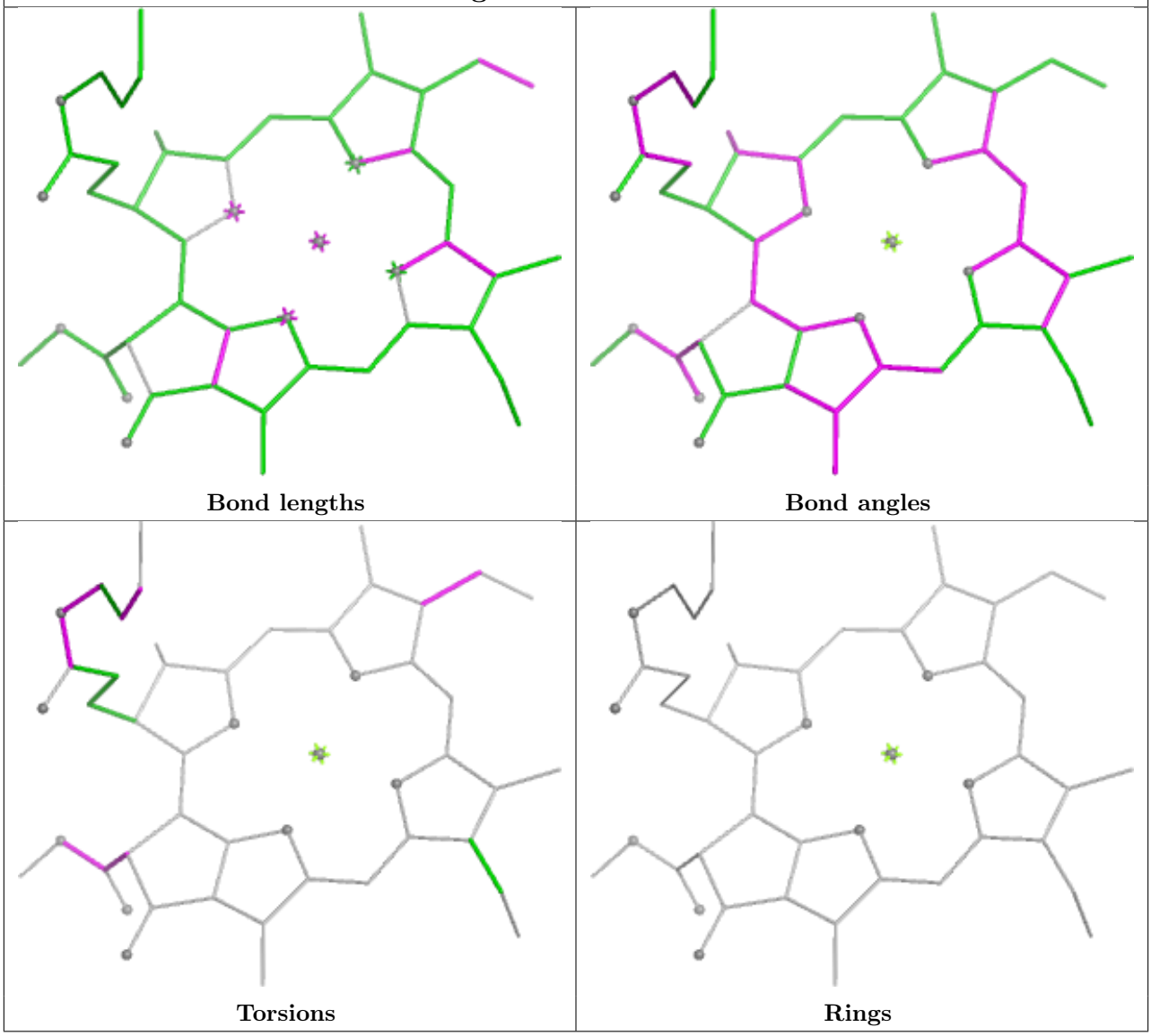
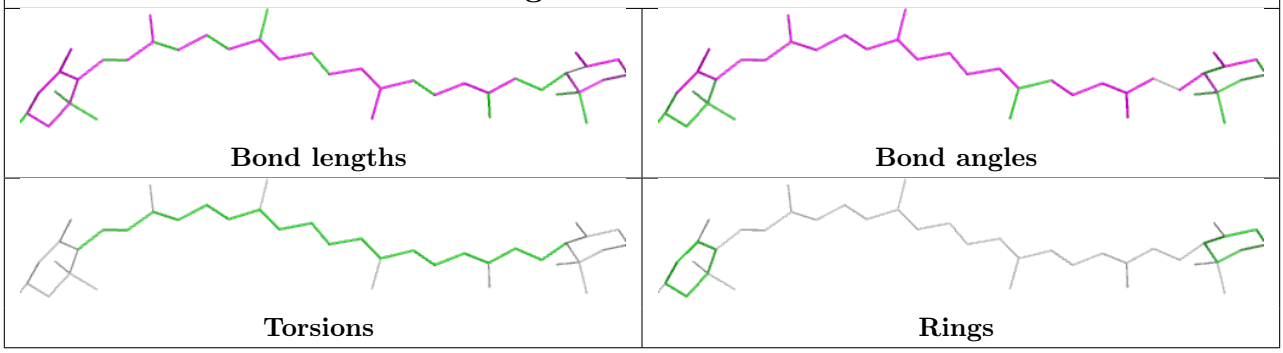


Ligand LUT Y 315



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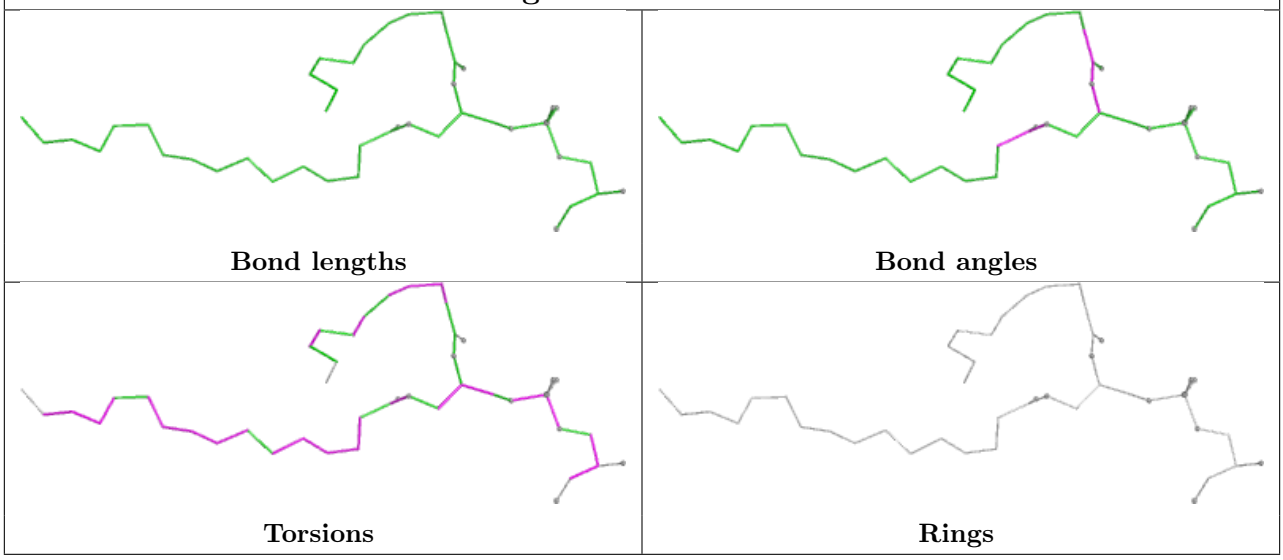

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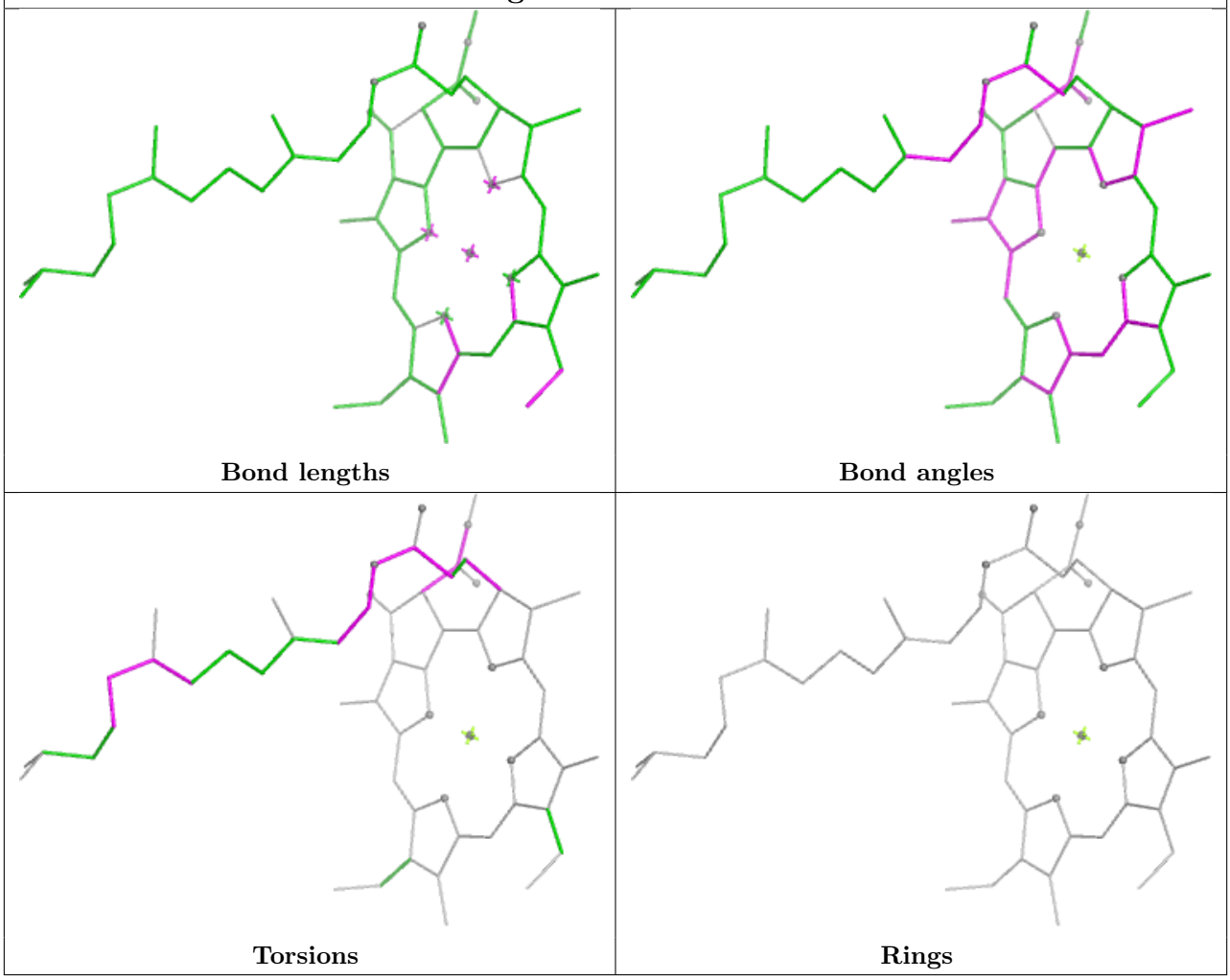

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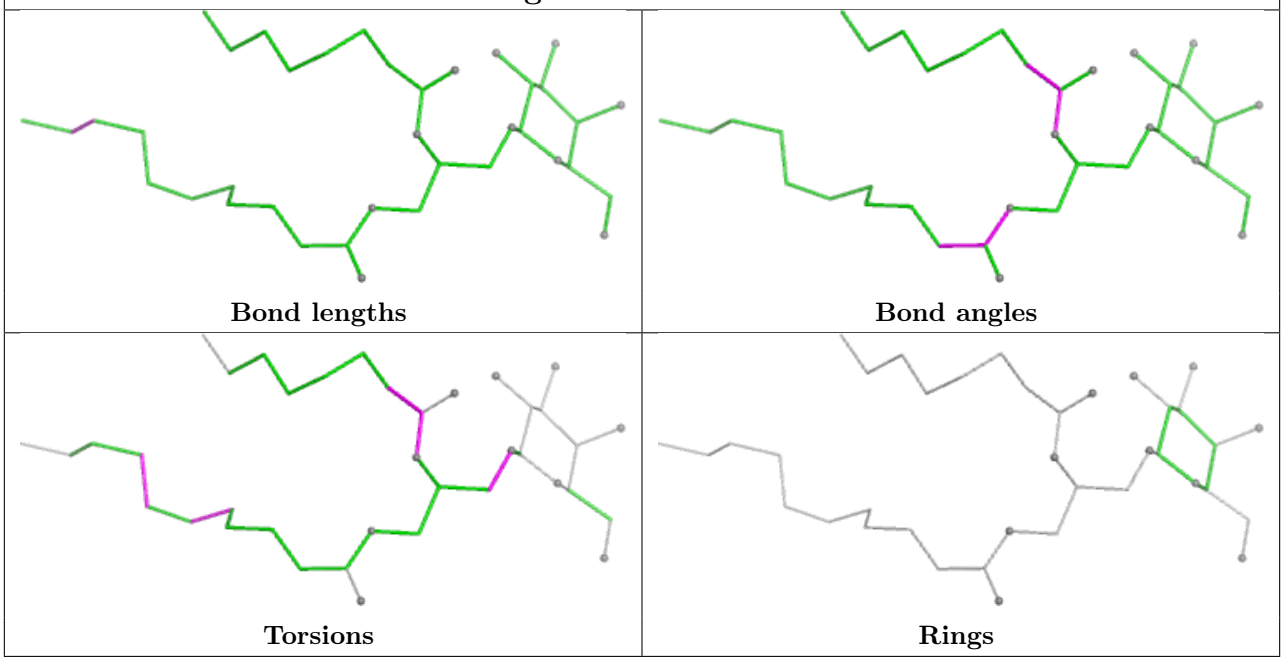

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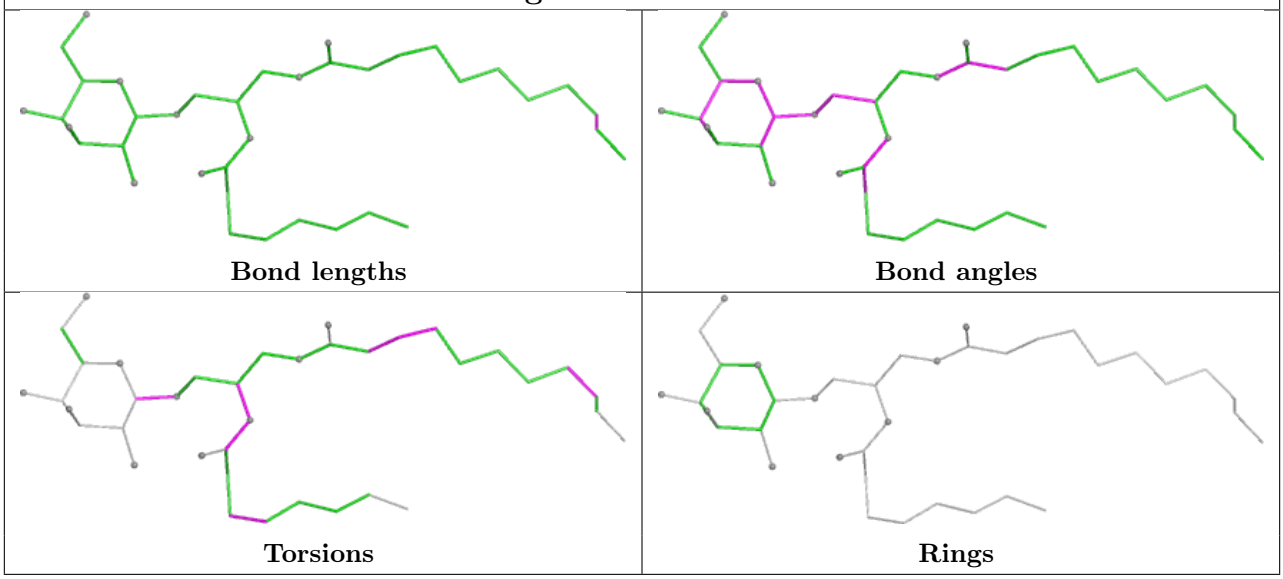
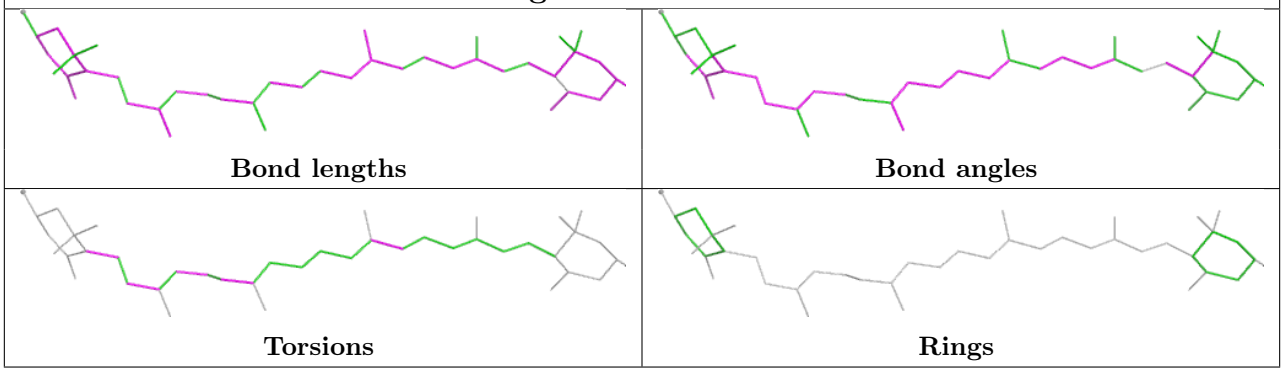
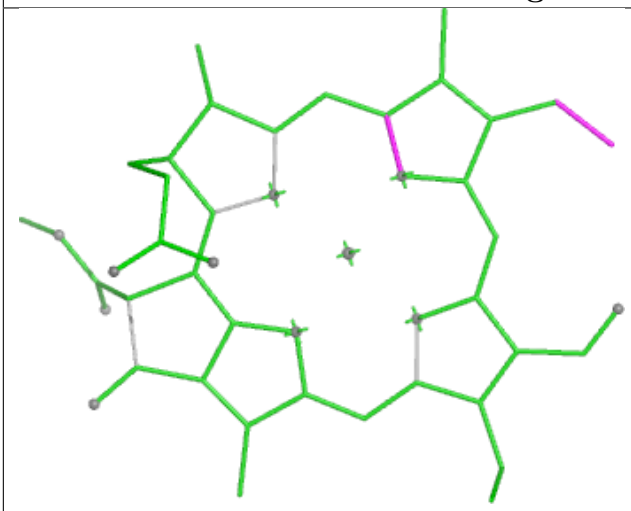


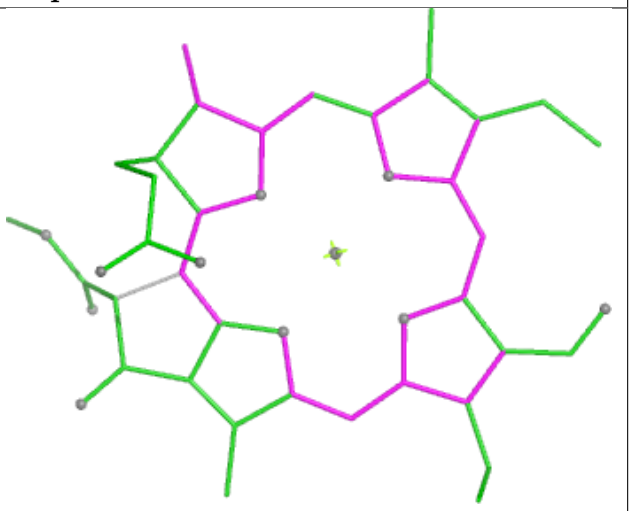
Ligand LUT 3 318



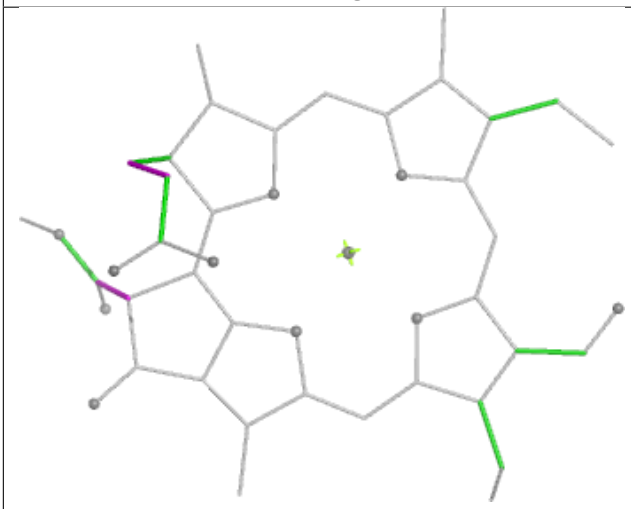
Ligand CHL p 605



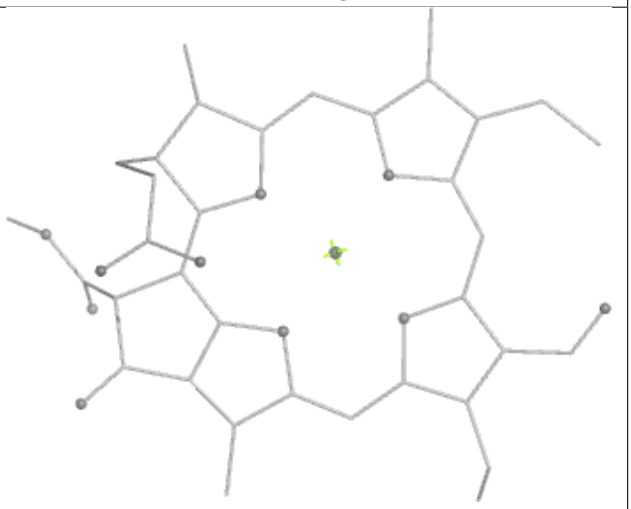
Bond lengths



Bond angles

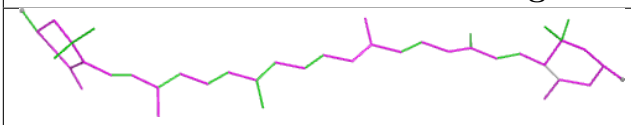


Torsions



Rings

Ligand LUT 7 318



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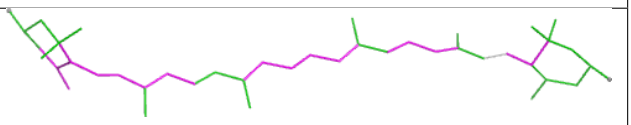
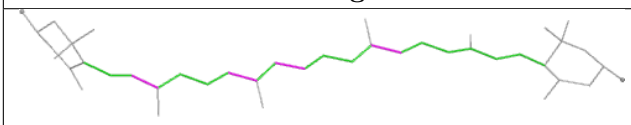
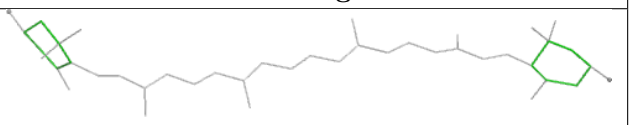


Bond angles

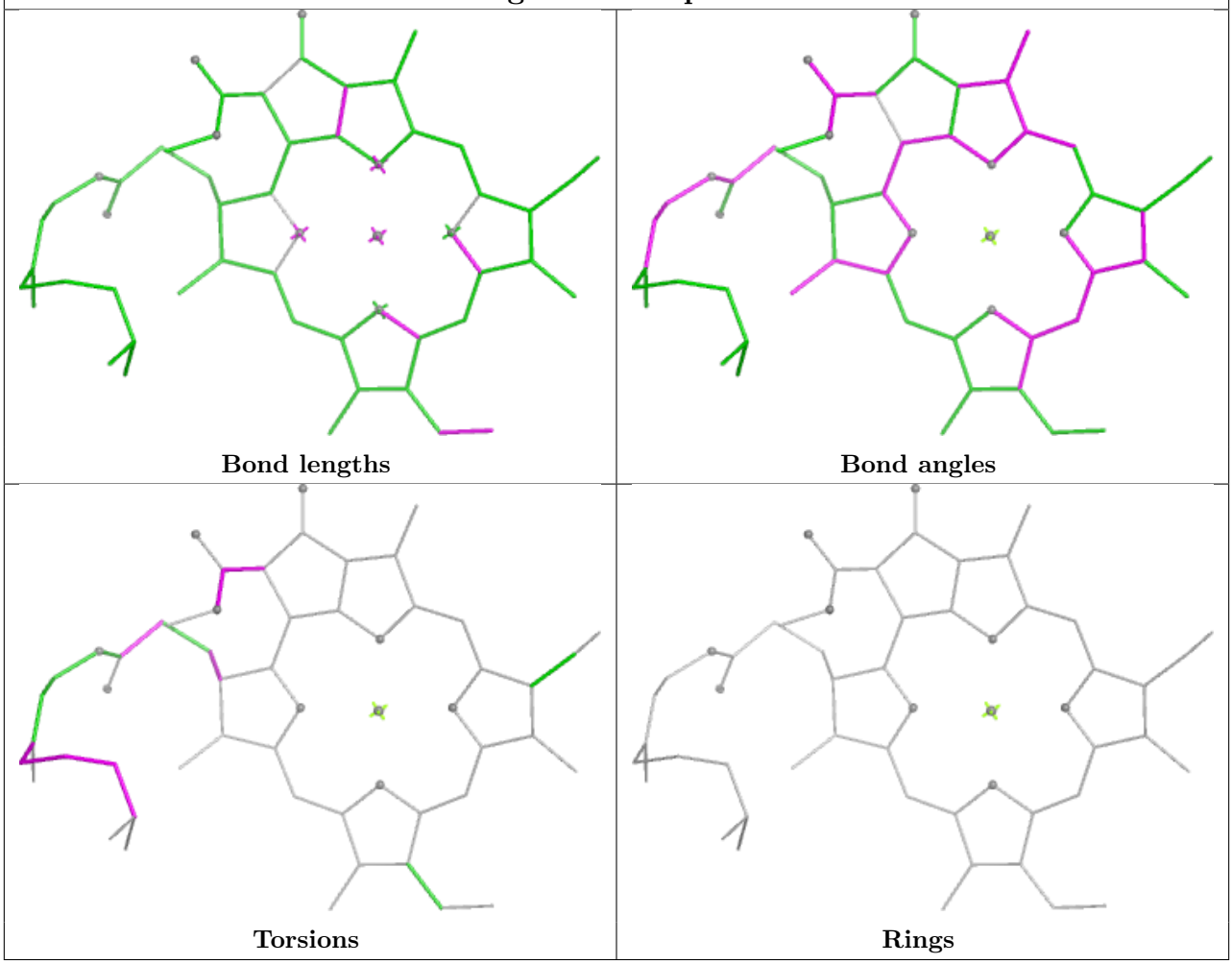


Torsions

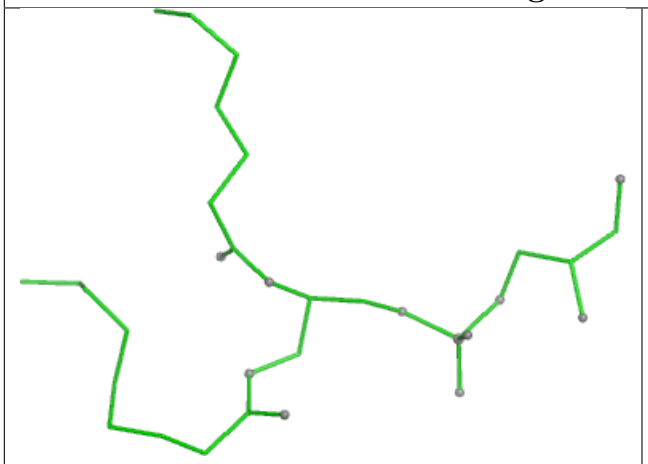


Rings

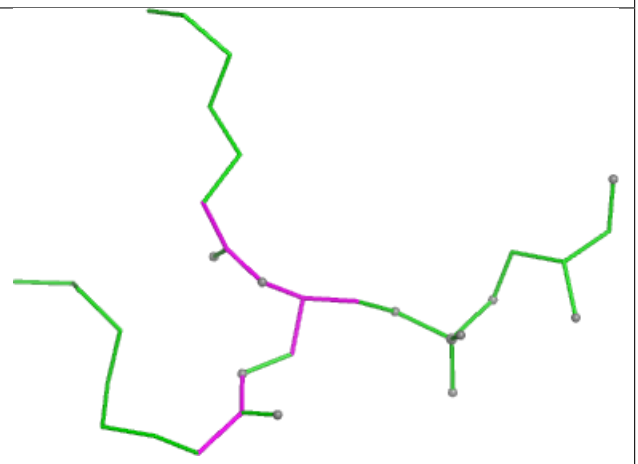
Ligand CLA q 305



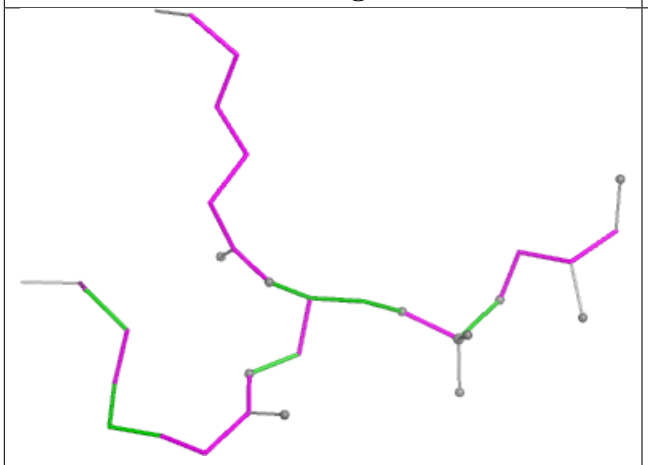
Ligand LHG 3 320



Bond lengths



Bond angles



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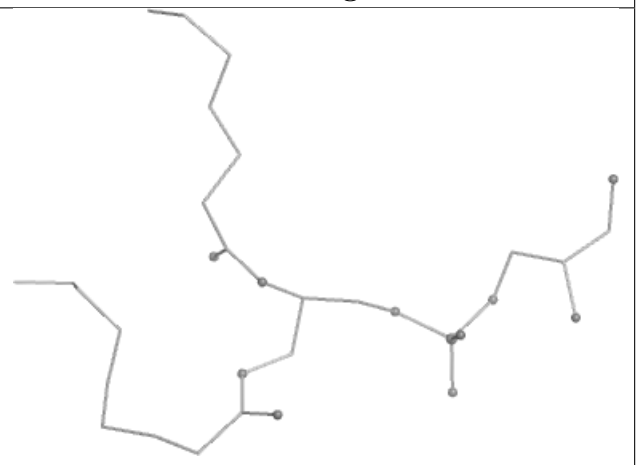
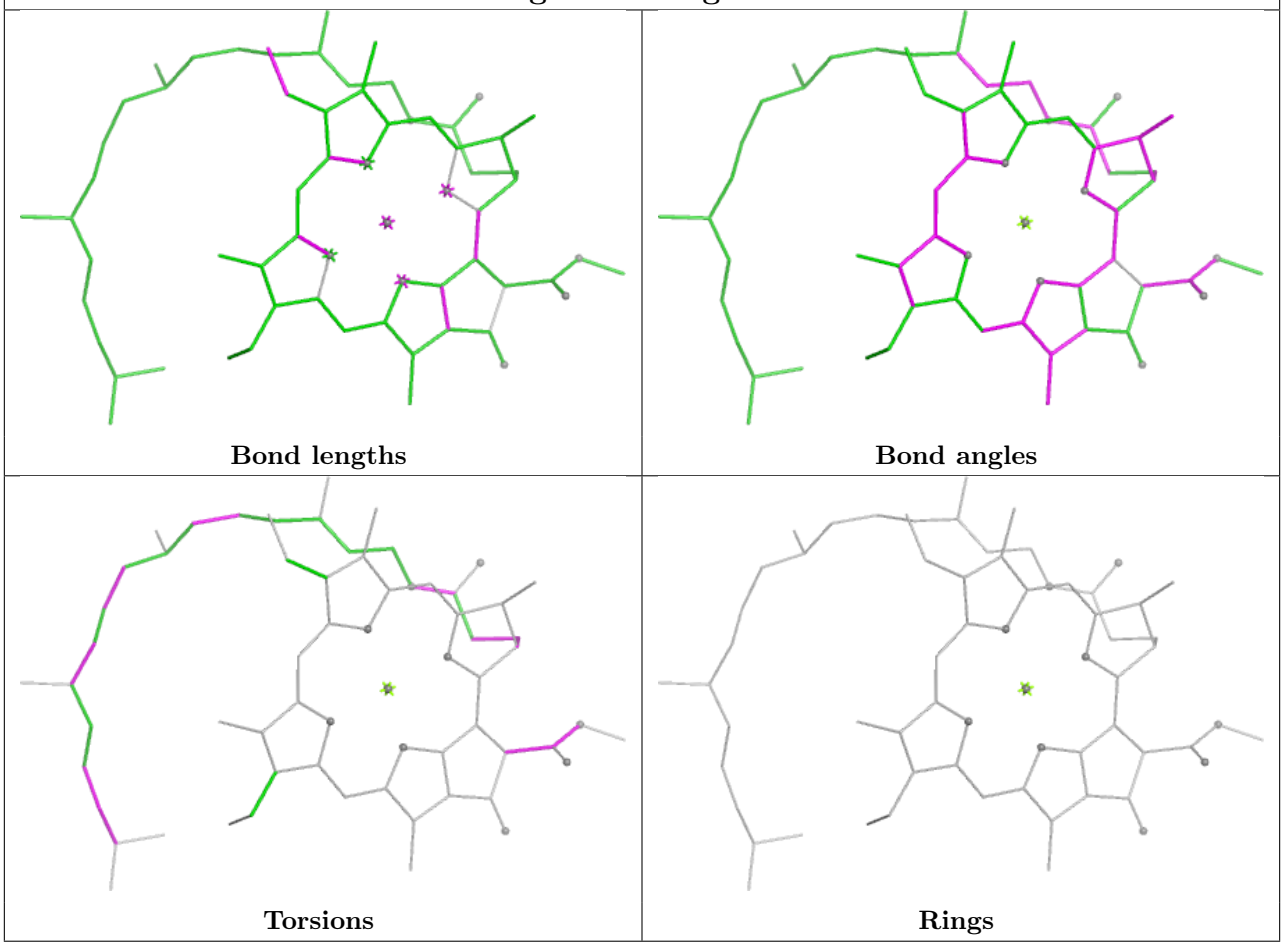
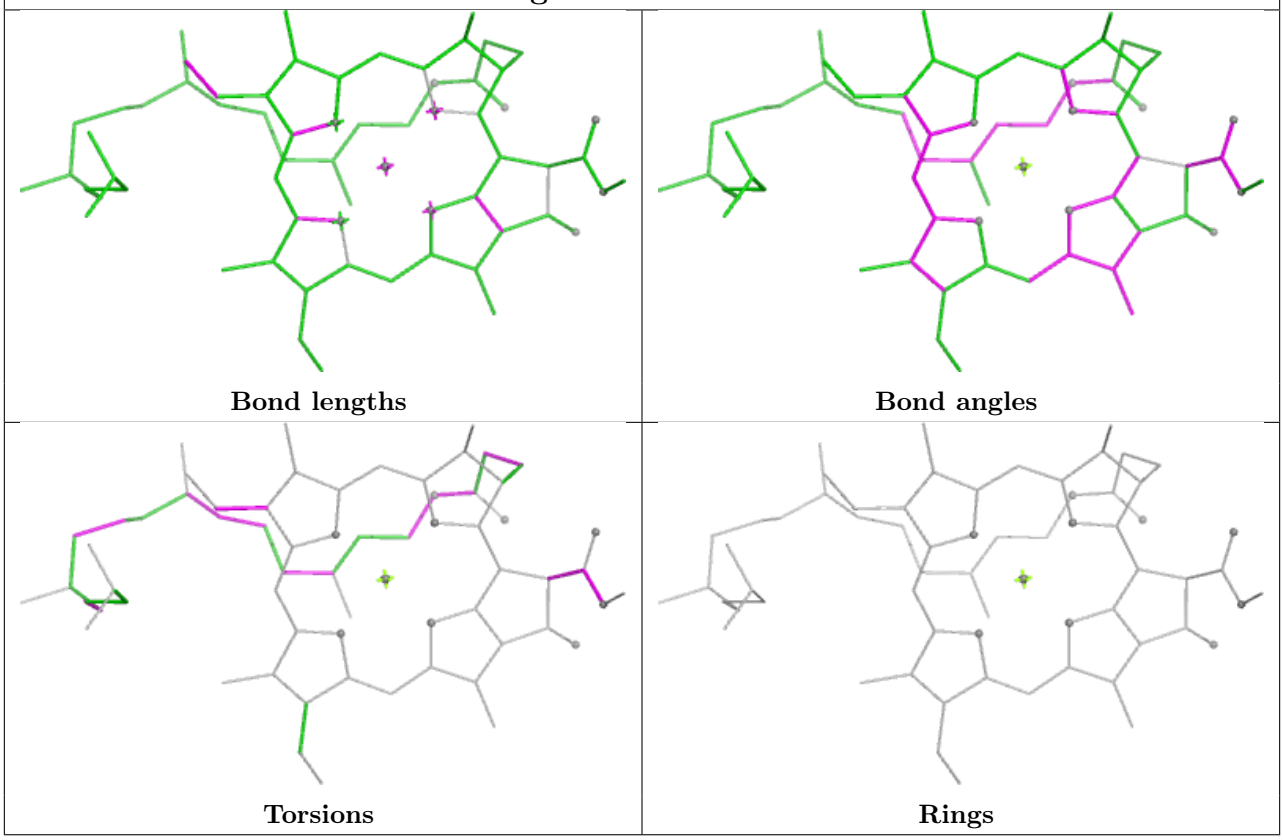


Rings

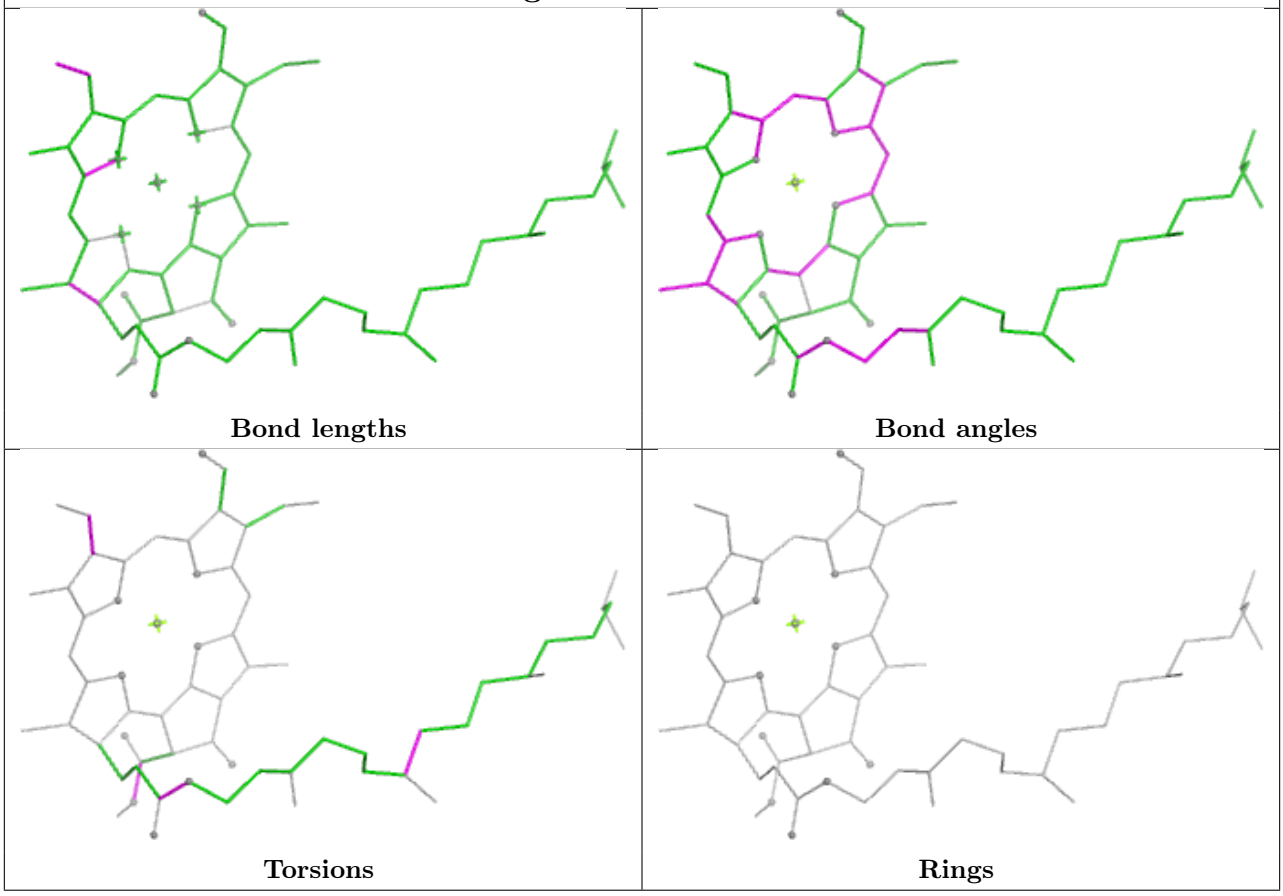
Ligand CLA g 310



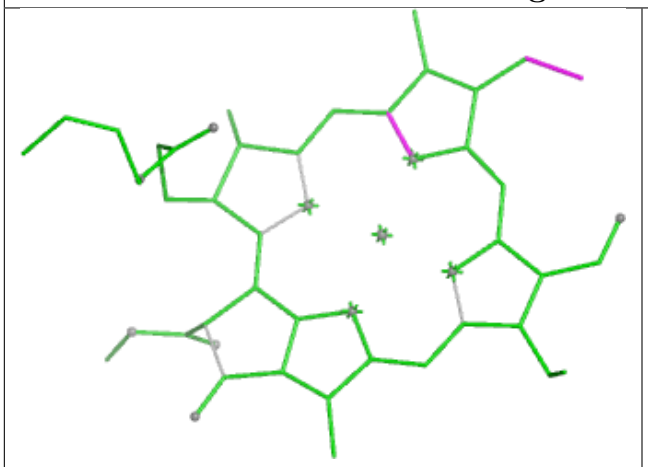
Ligand CLA c 605



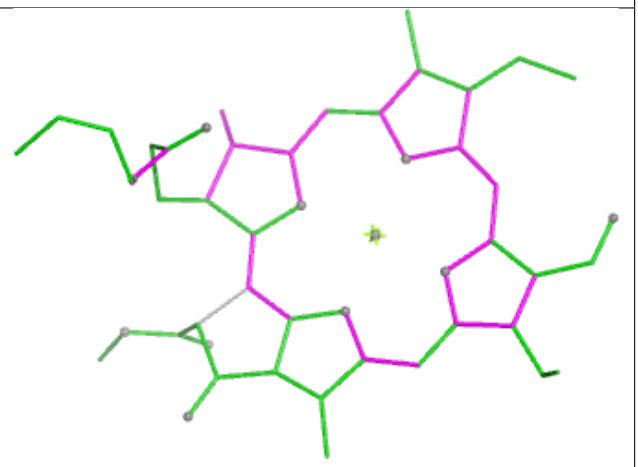
Ligand CHL N 309



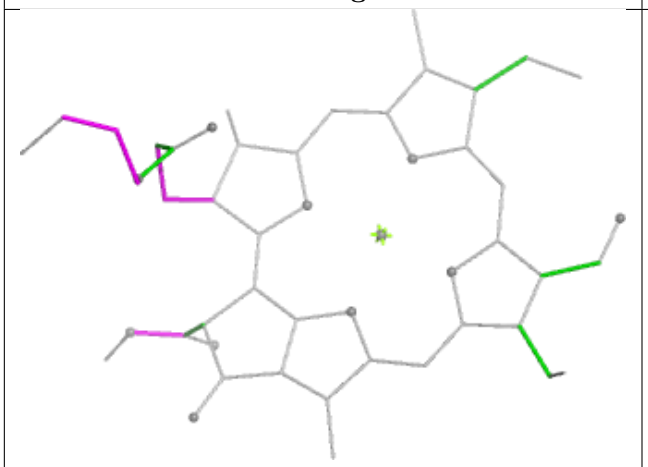
Ligand CHL 9 310



Bond lengths



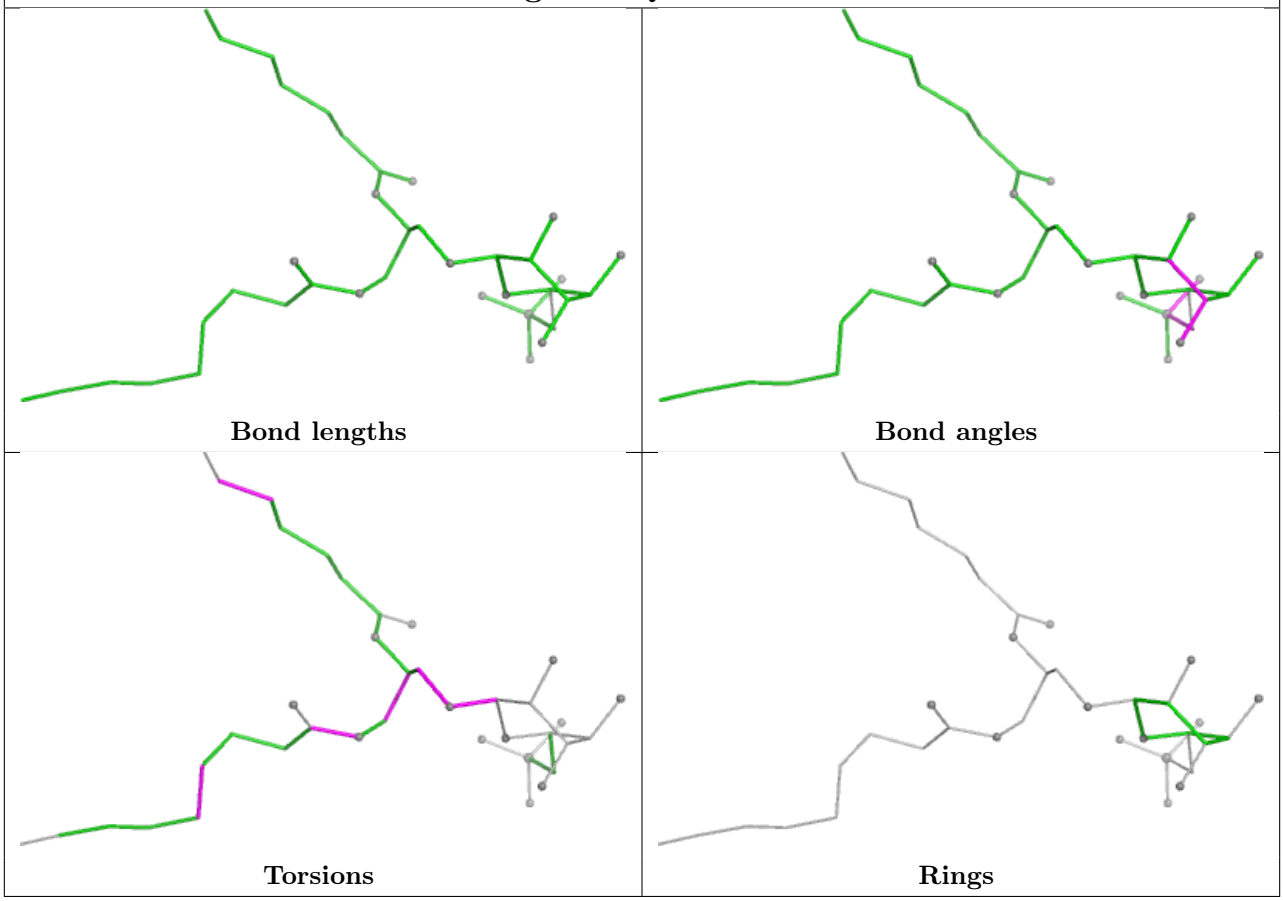
Bond angles



Torsions

Rings

Ligand SQD X 201



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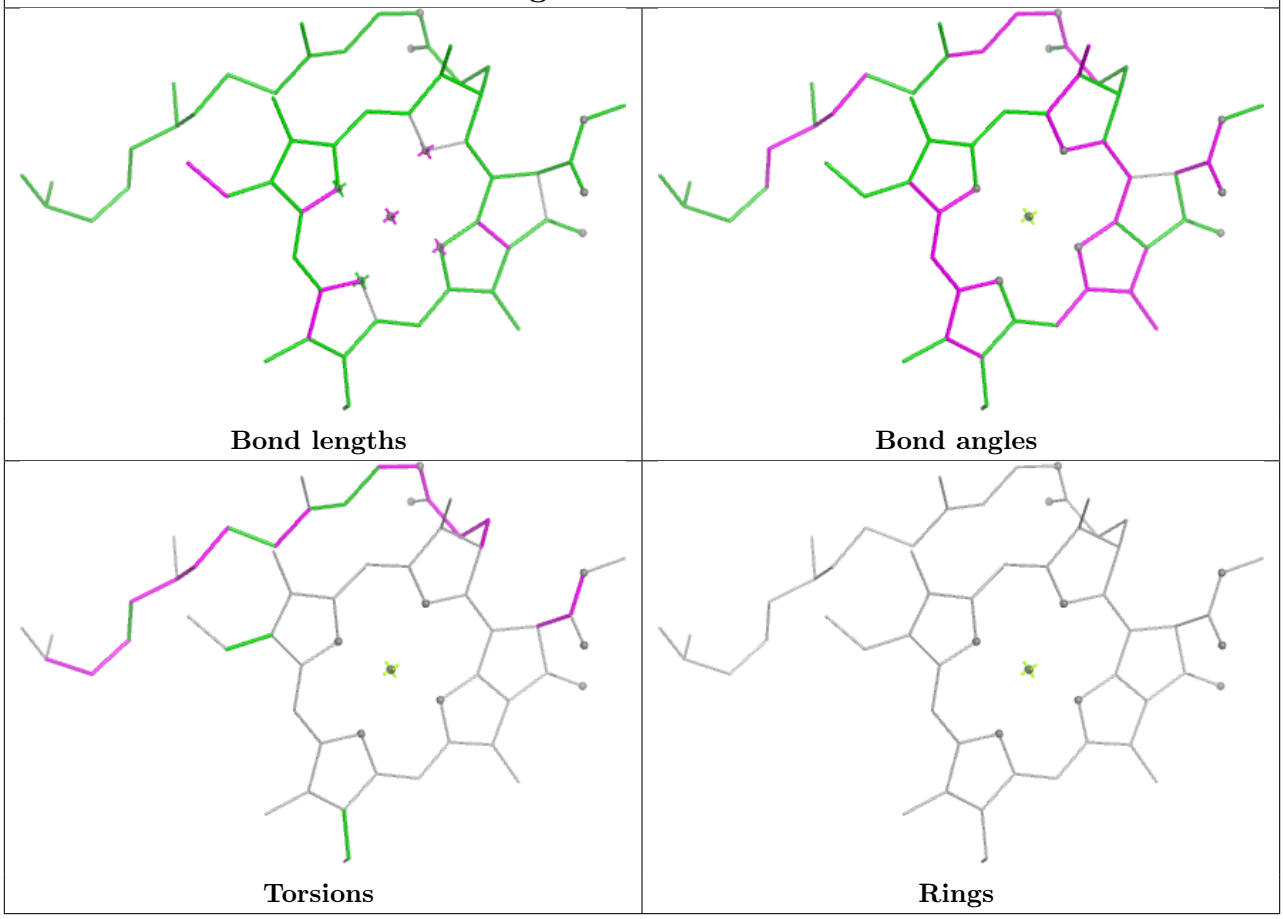

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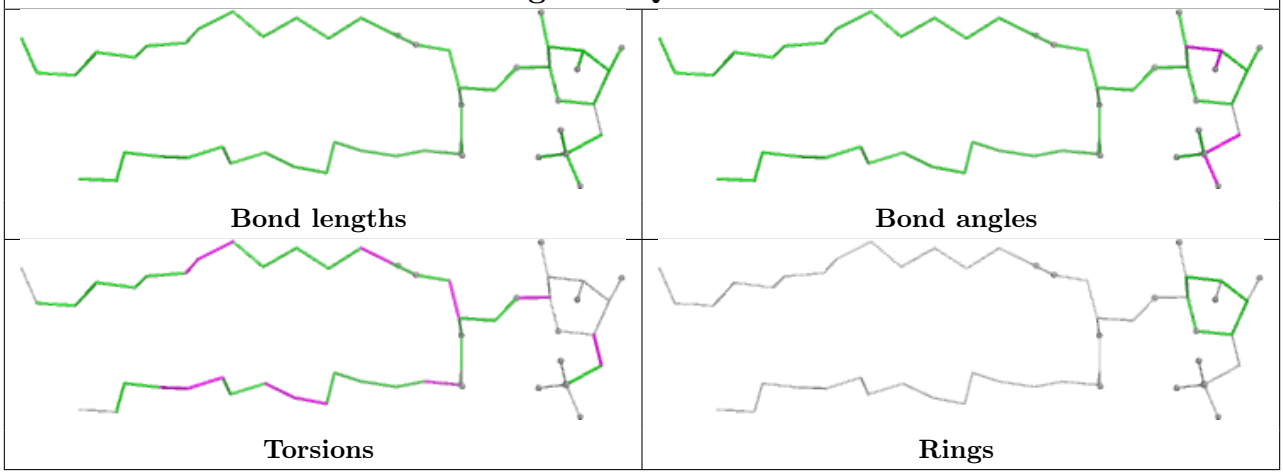

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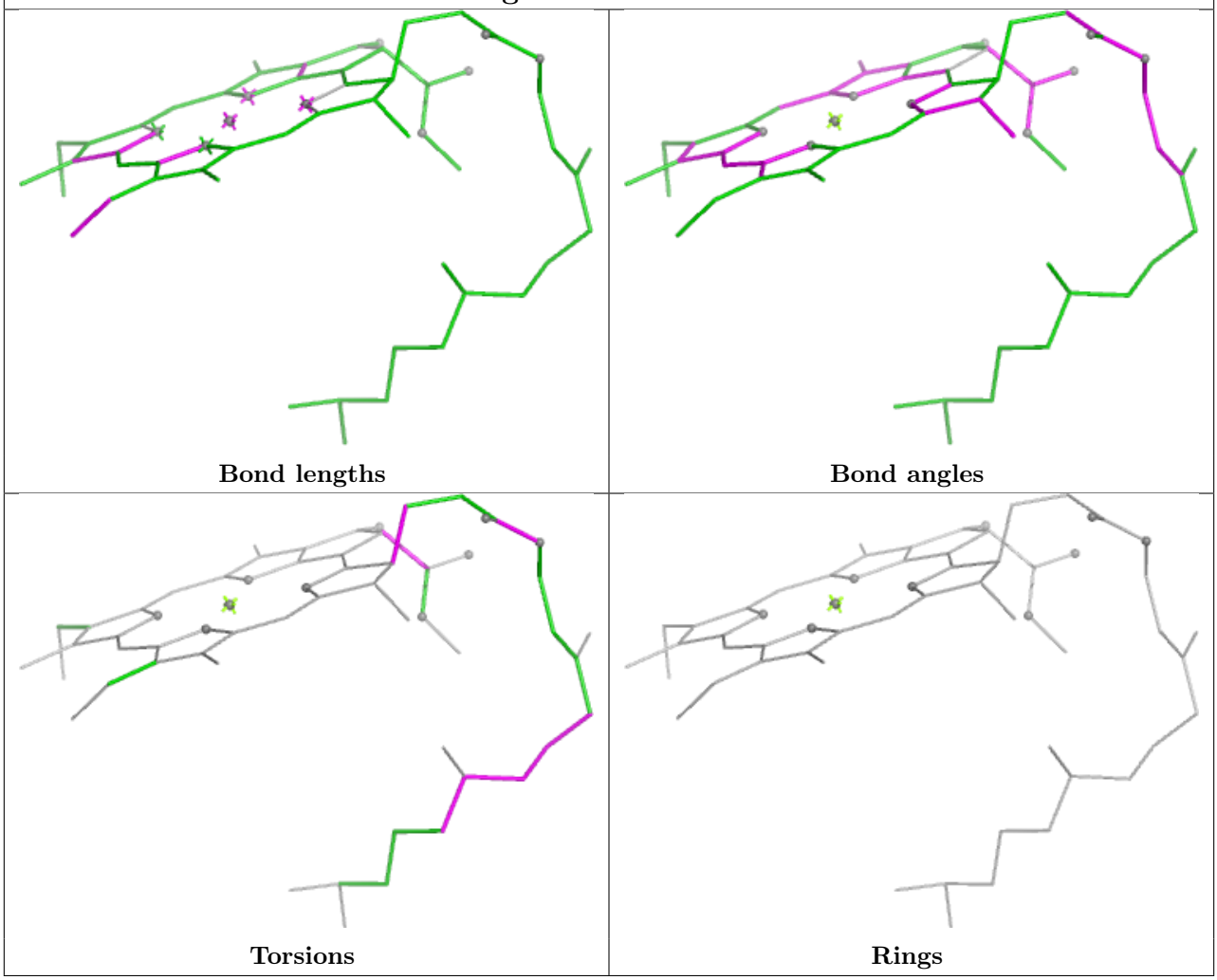

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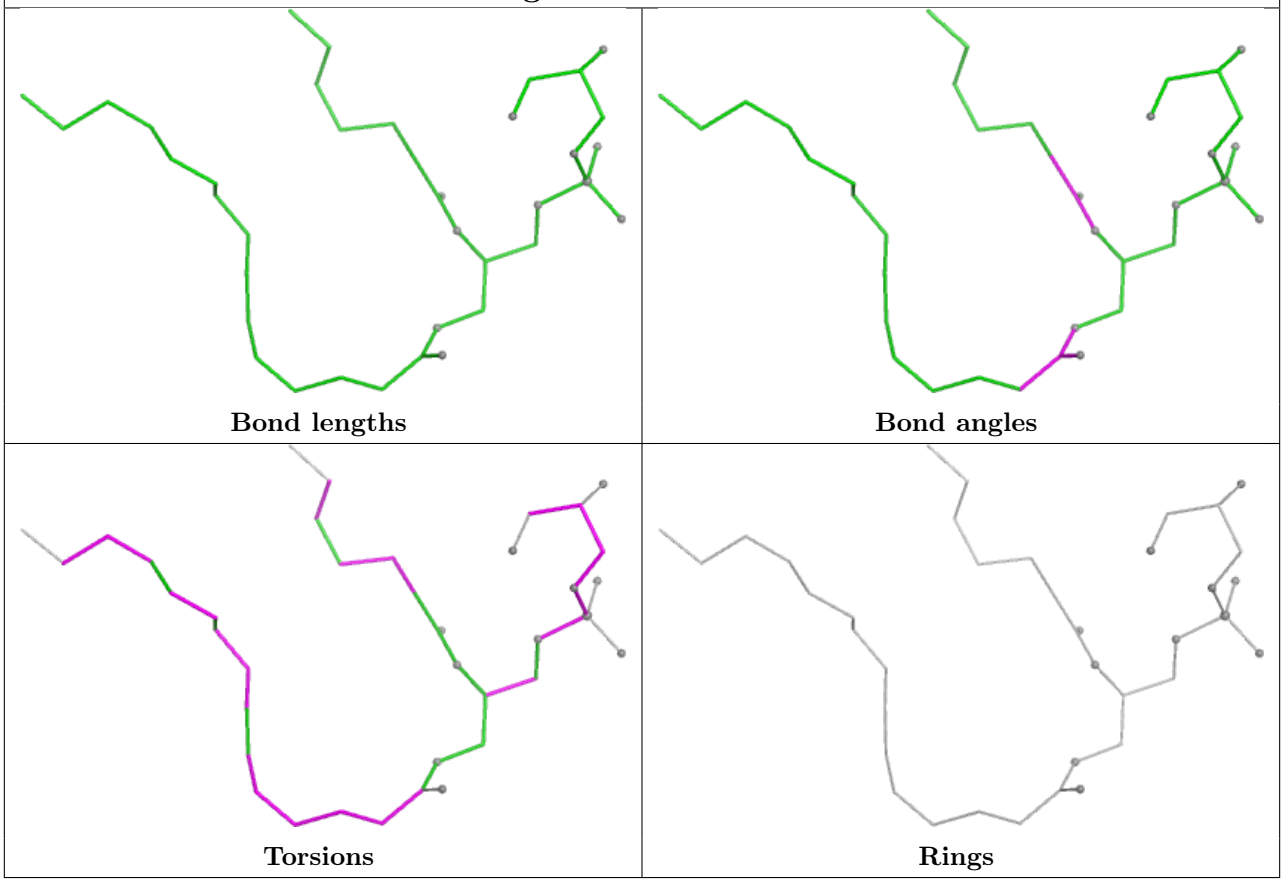
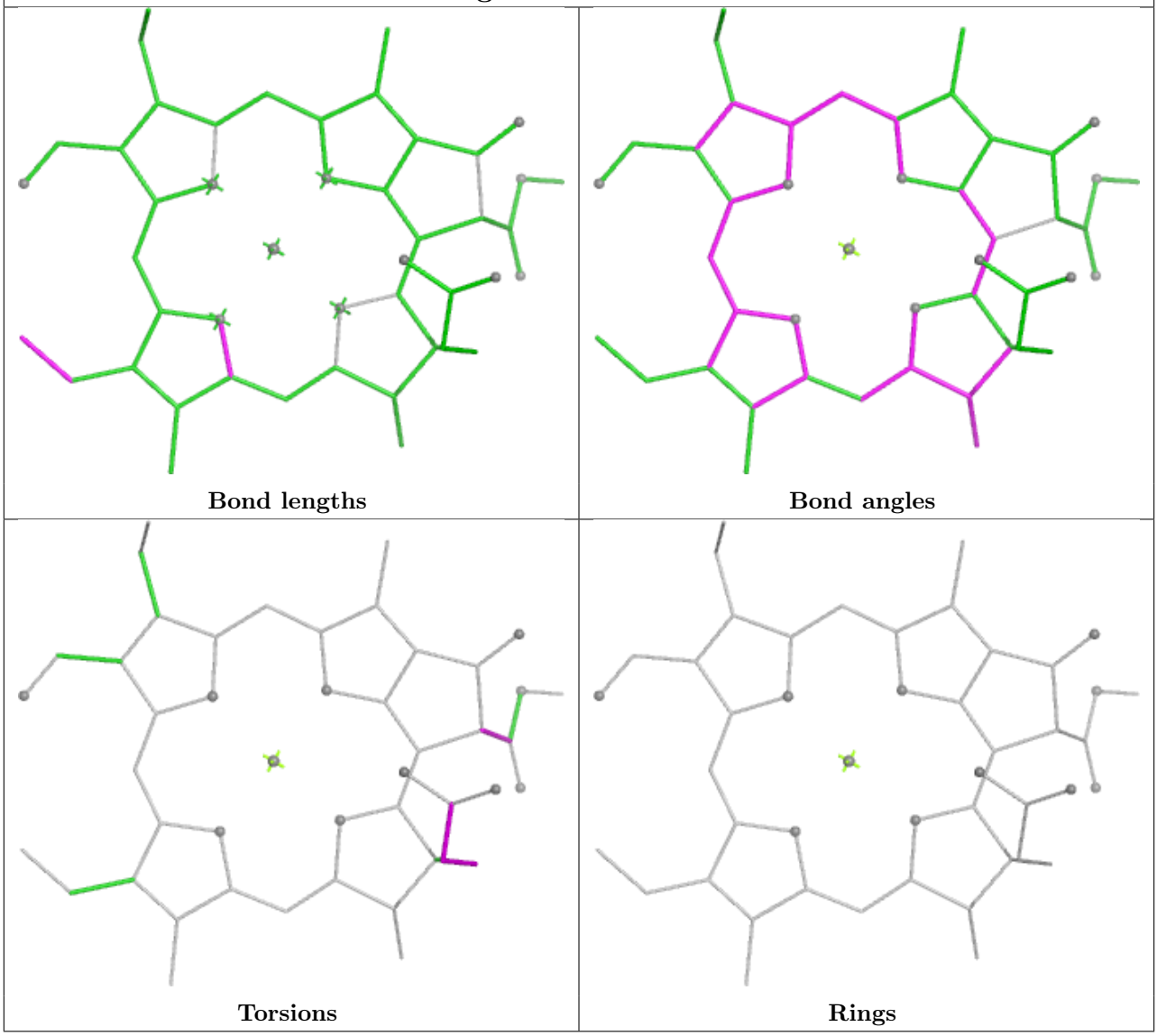


Ligand CHL 3 307



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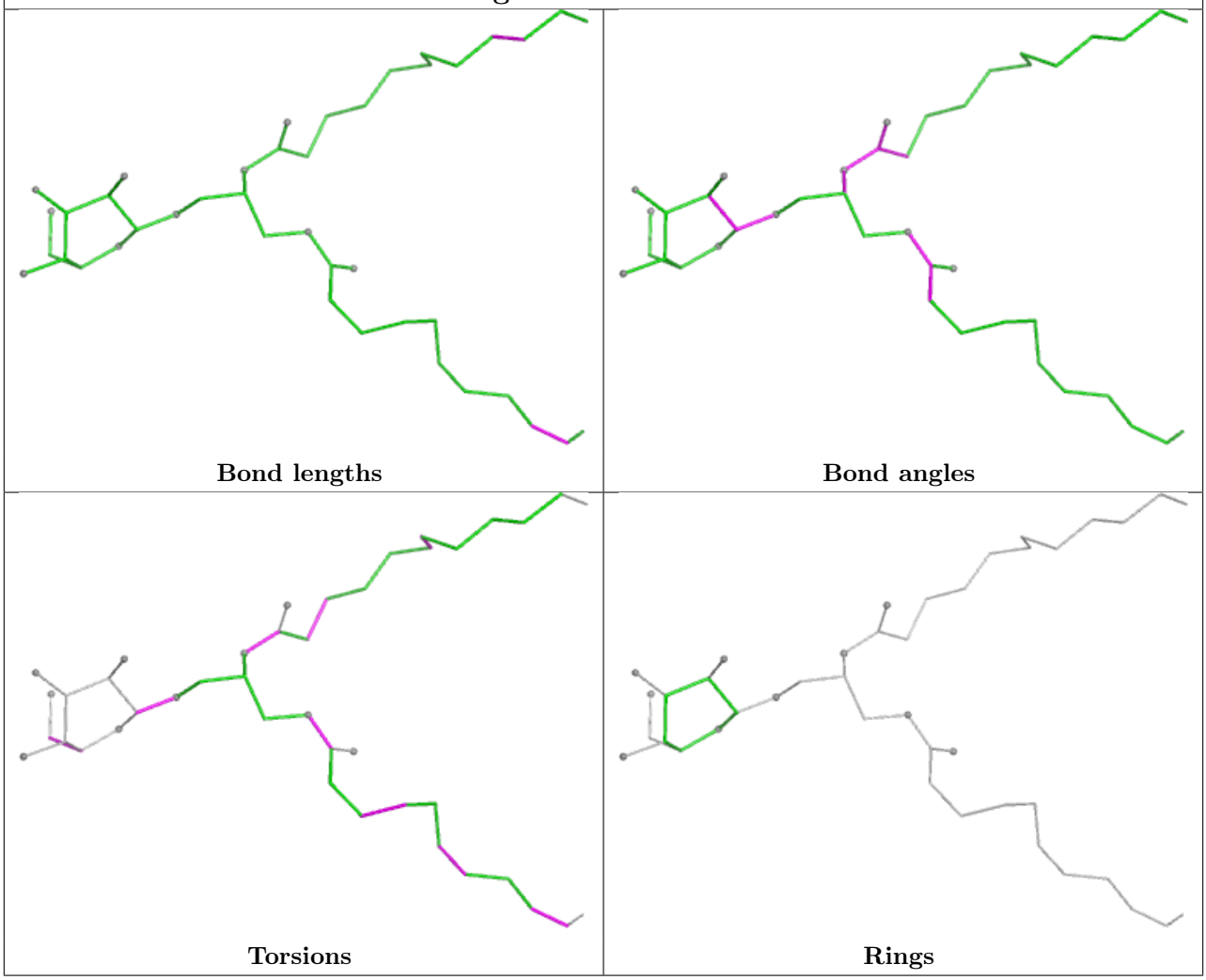

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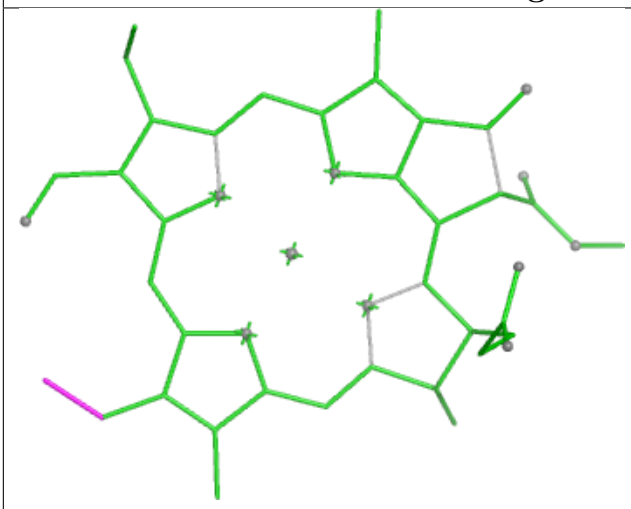
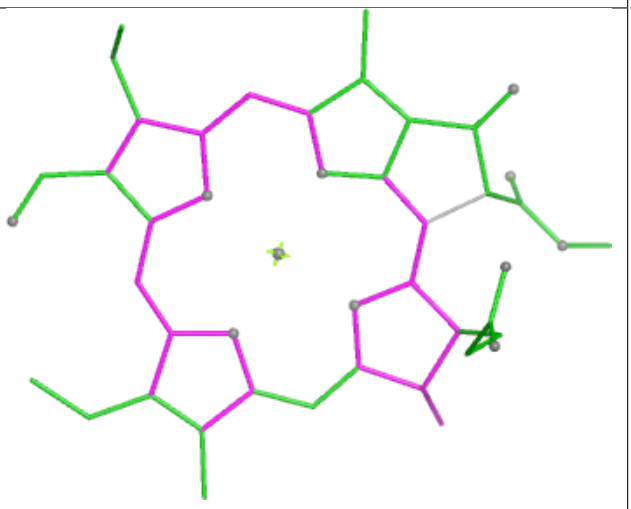
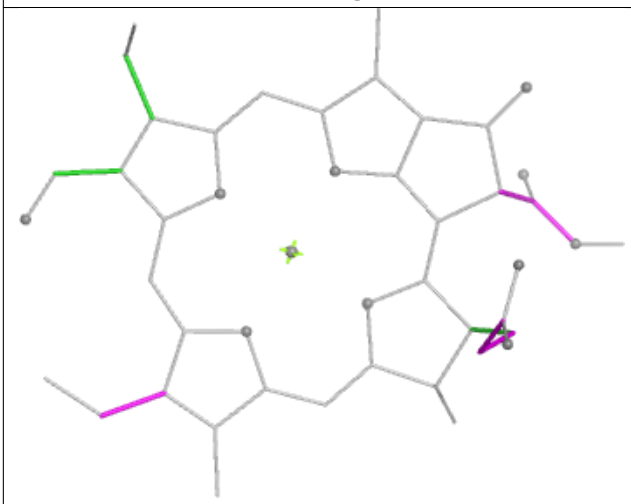
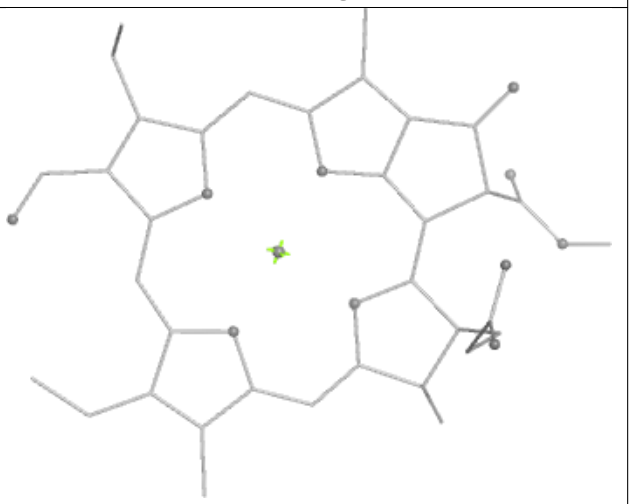
 Bond lengths	 Bond angles
 Torsions	 Rings

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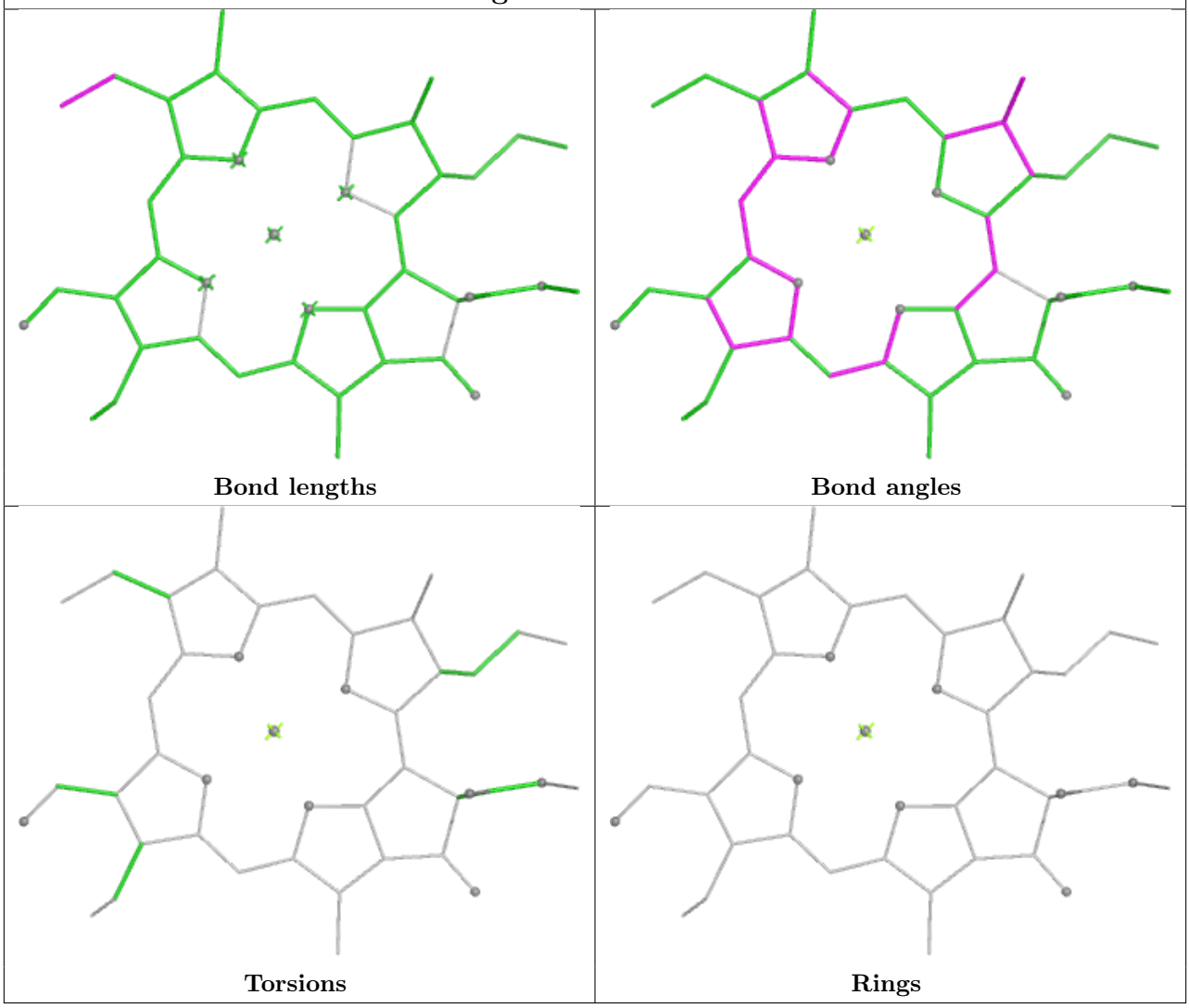


Ligand CLA 3 316

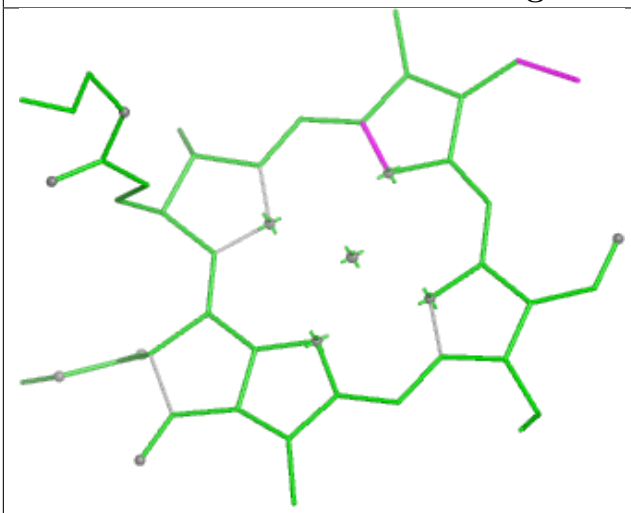
Bond lengths

Bond angles

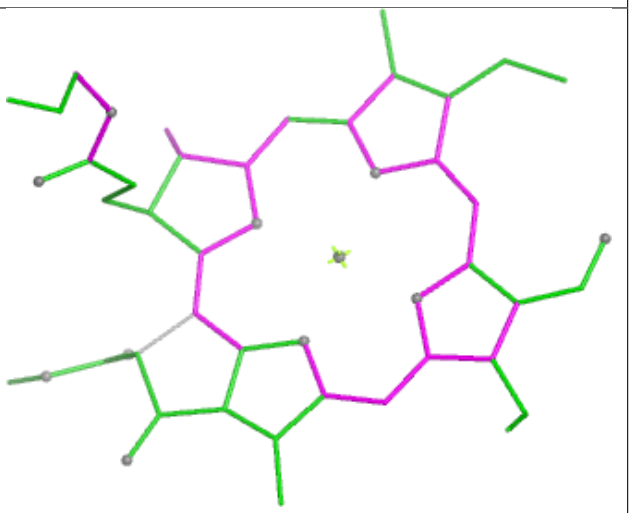
Torsions

Rings

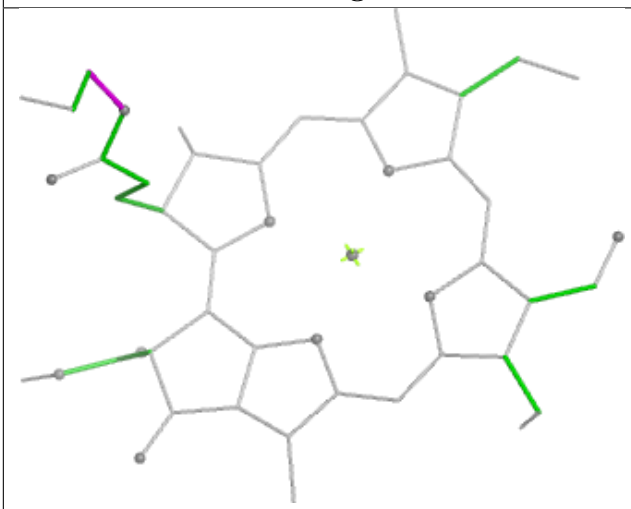
Ligand CHL S 309



Bond lengths



Bond angles



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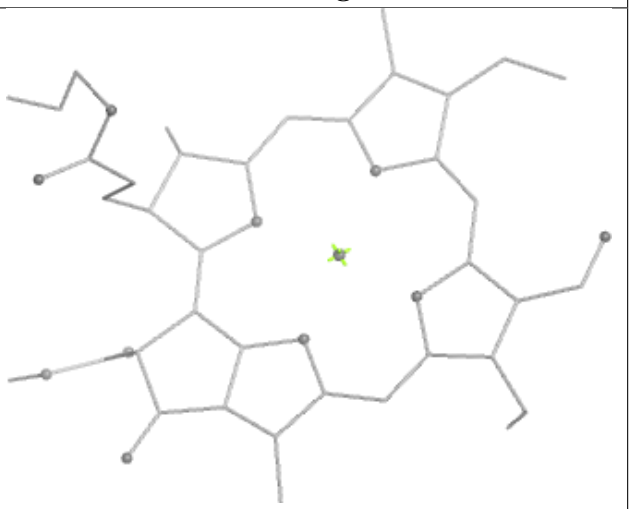
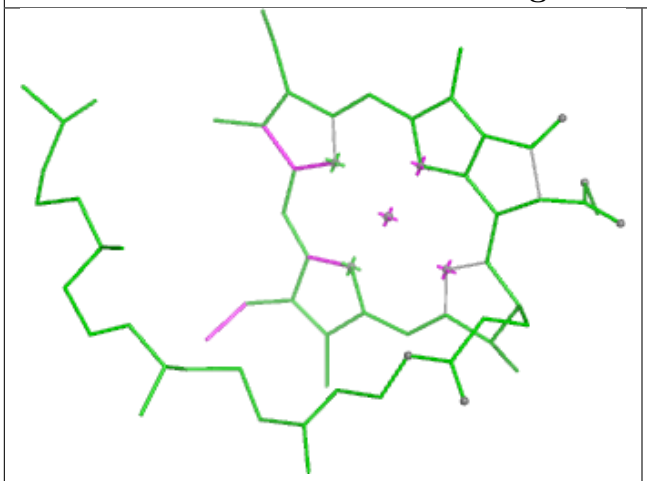


Rings

Ligand CLA 2 602



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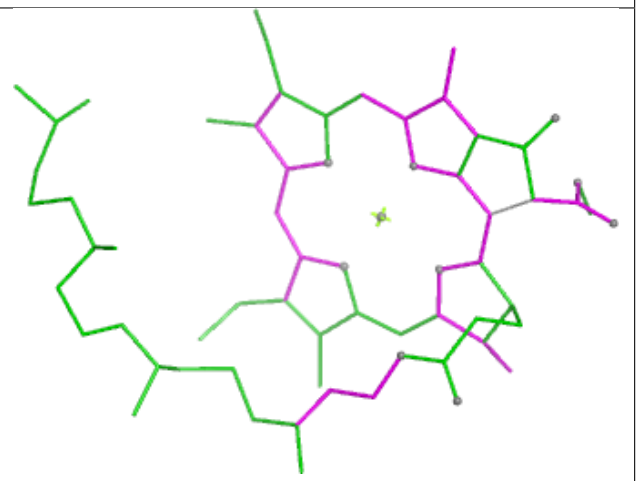

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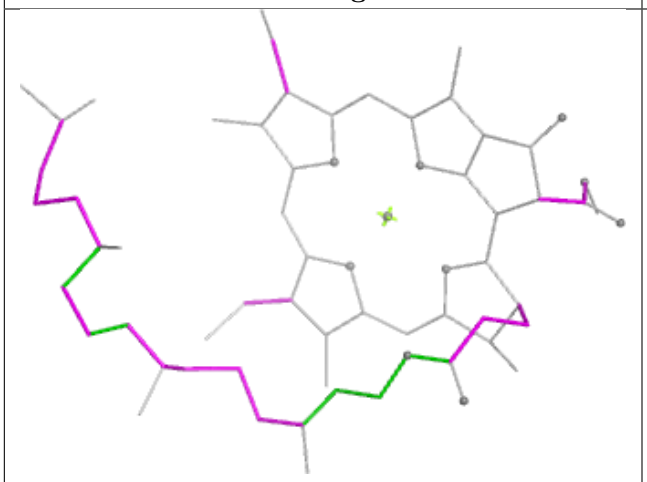

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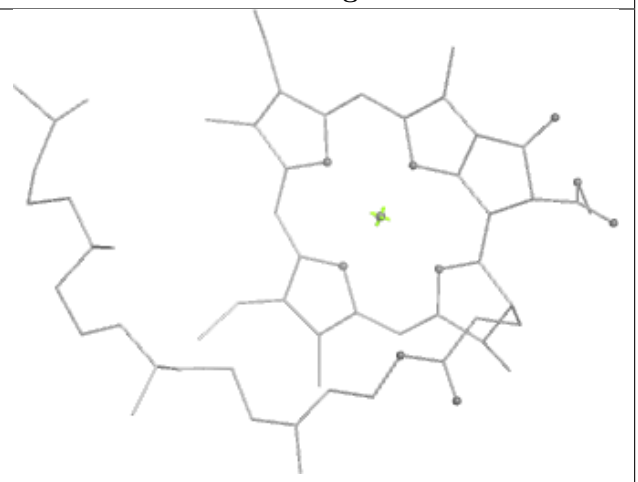
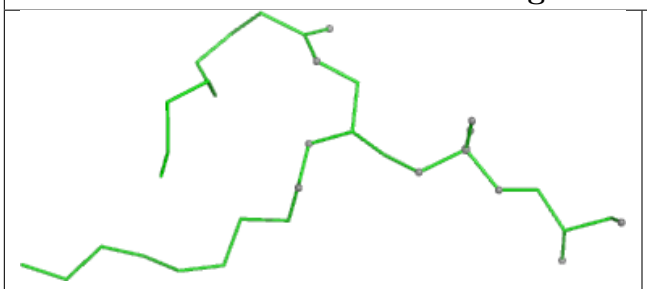


Rings

Ligand LHG 1 617



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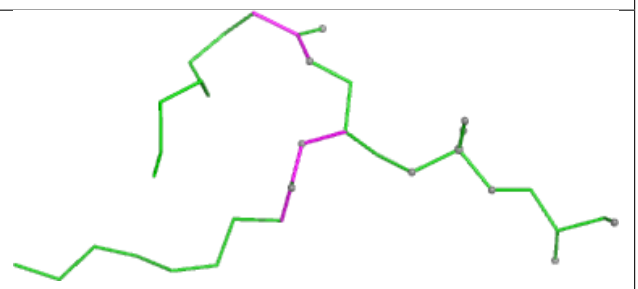

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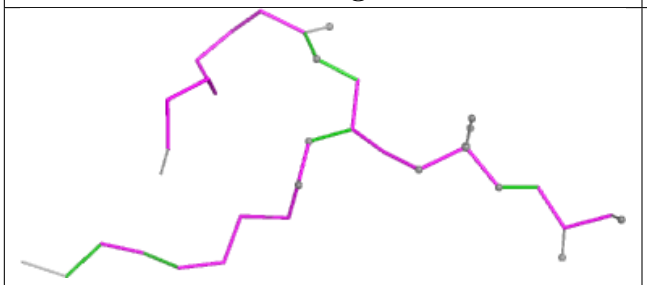

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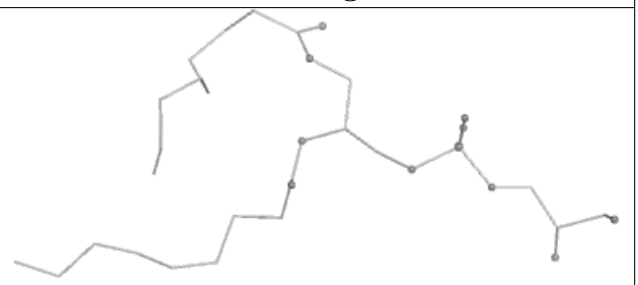
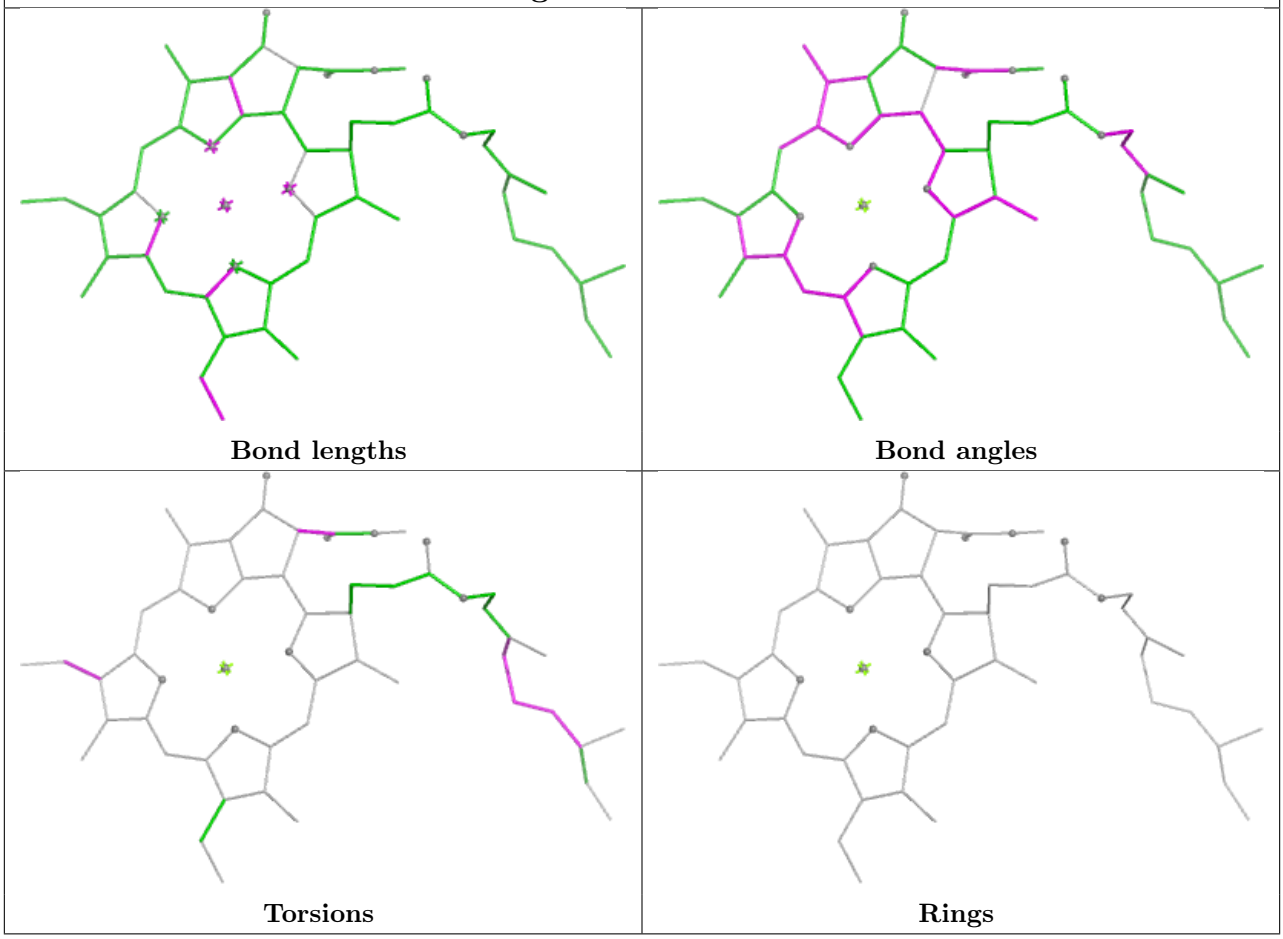


Rings

Ligand CLA s 313



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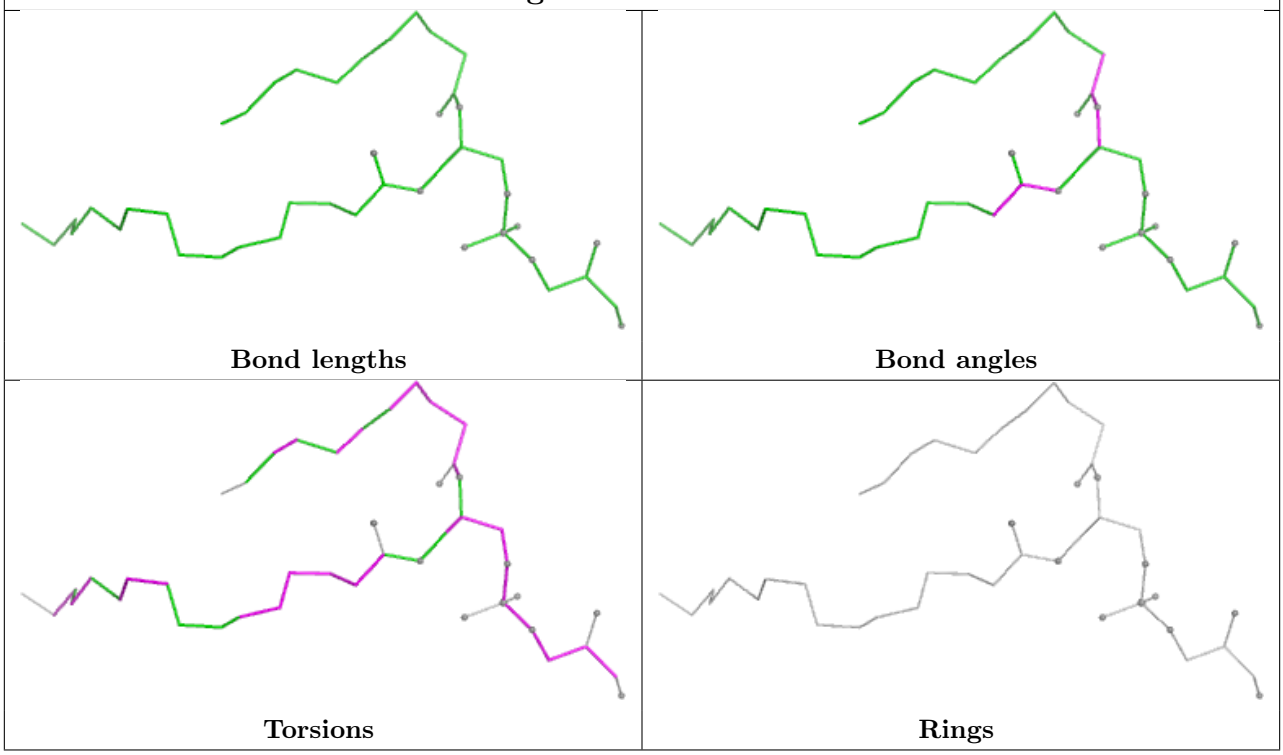

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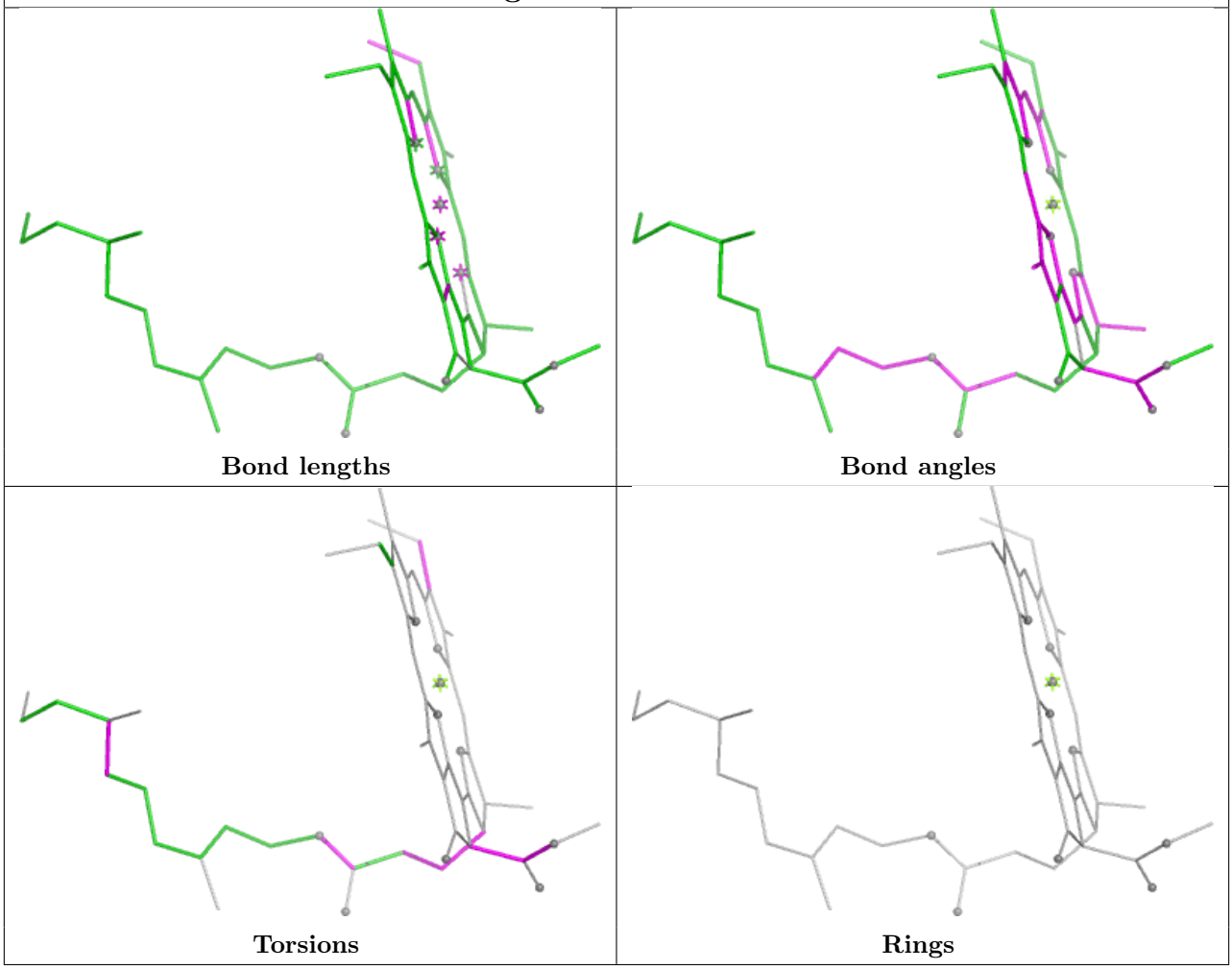

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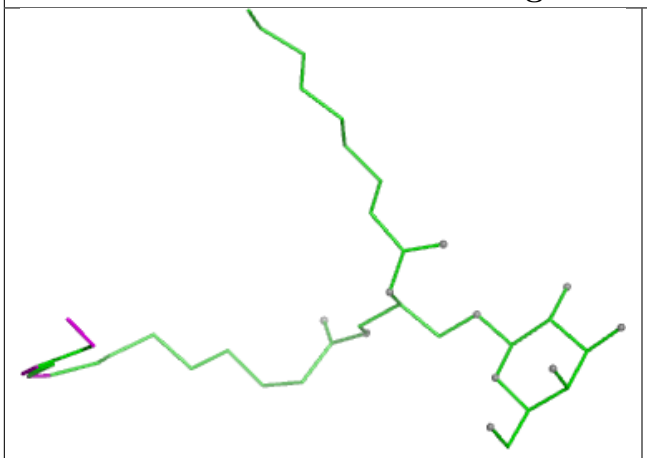
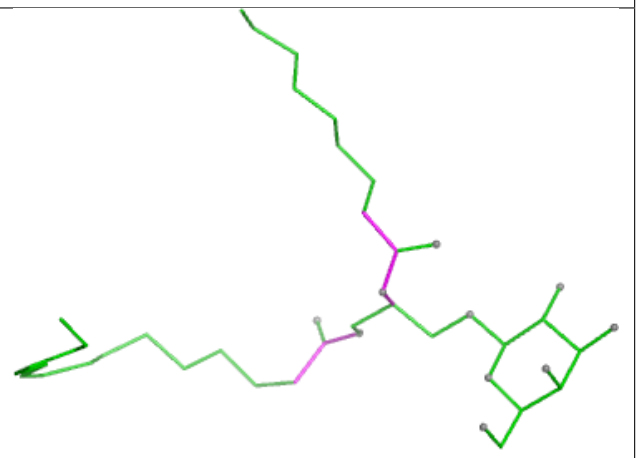
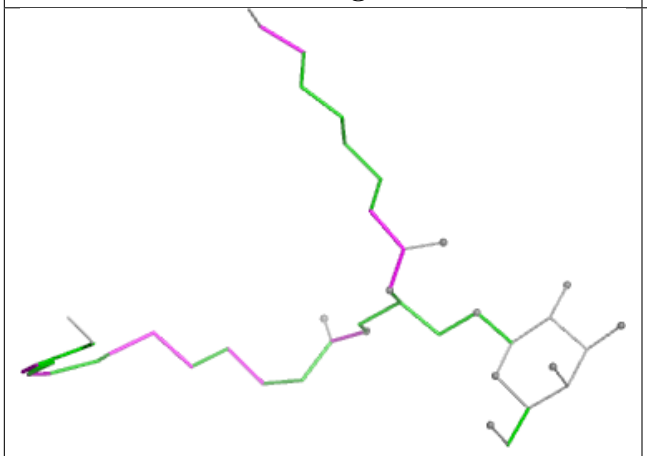


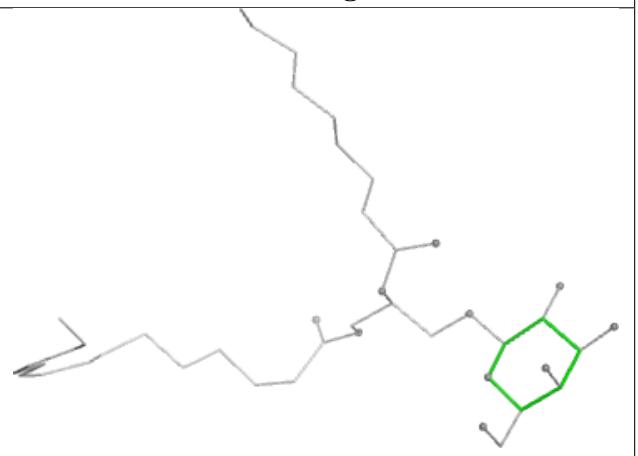
Bond lengths



Bond angles

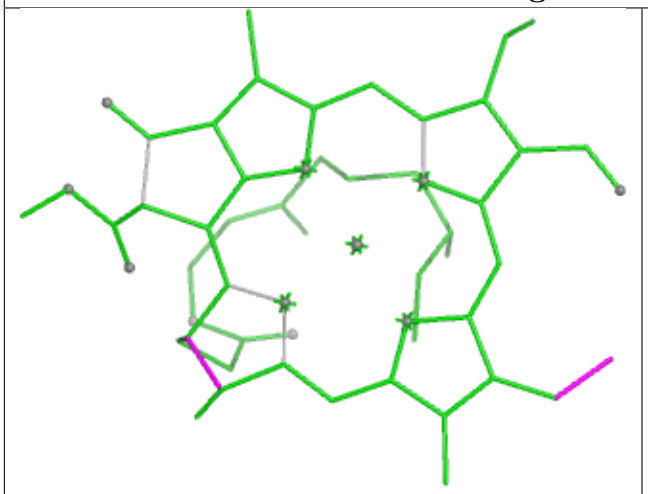


Torsions



Rings

Ligand CHL 4 607



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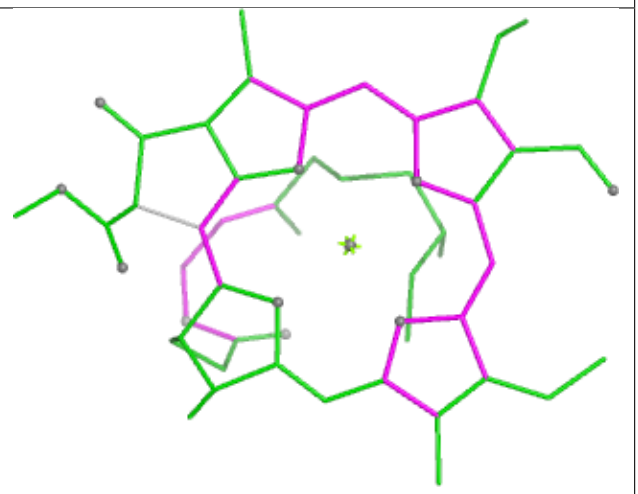
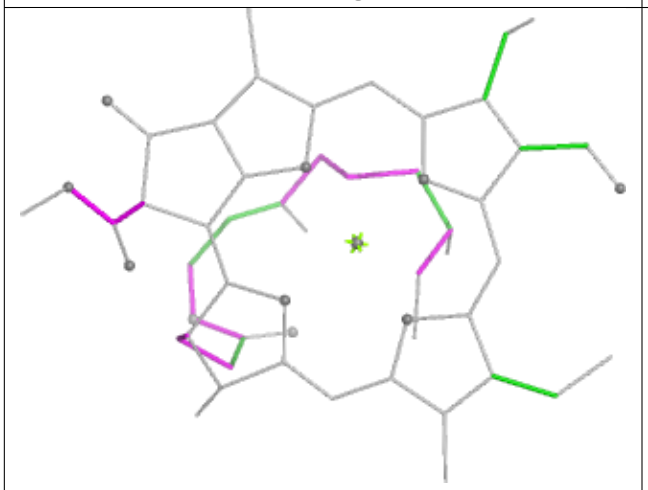


Bond angles



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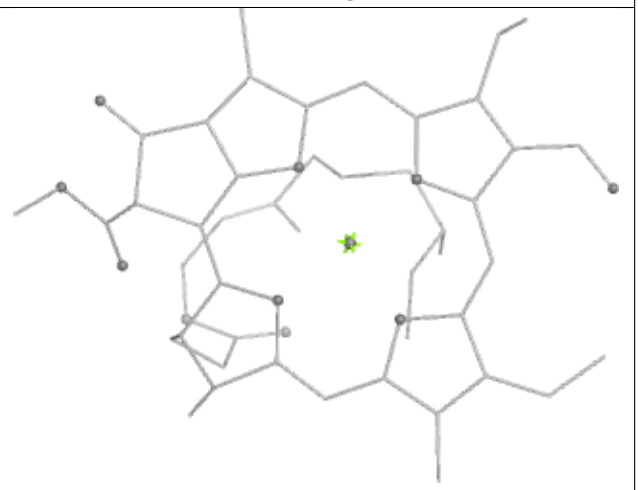
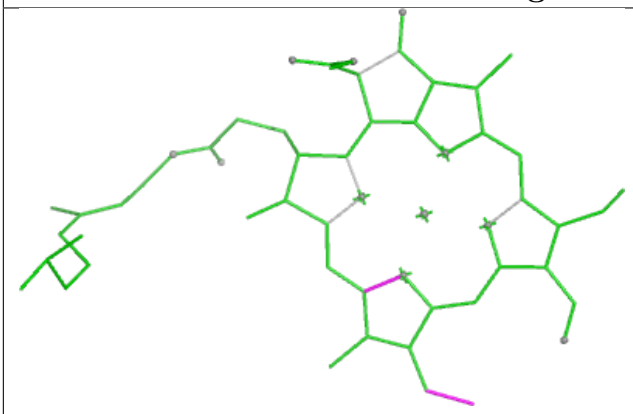


Rings

Ligand CHL 8 601



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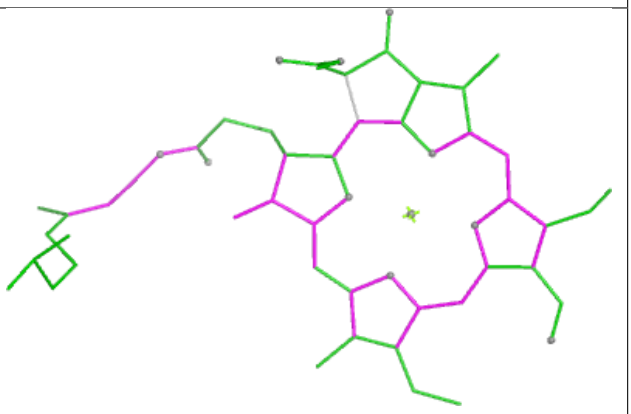
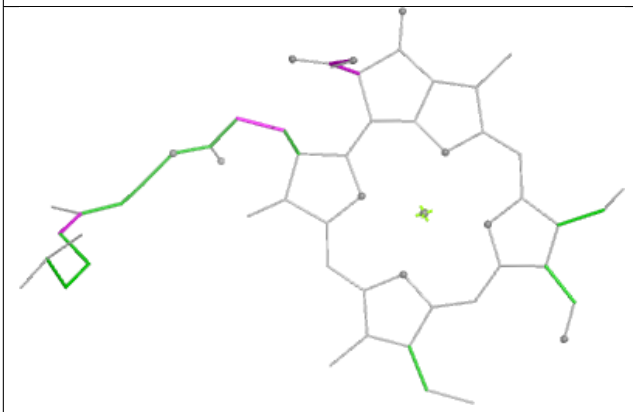


Bond angles



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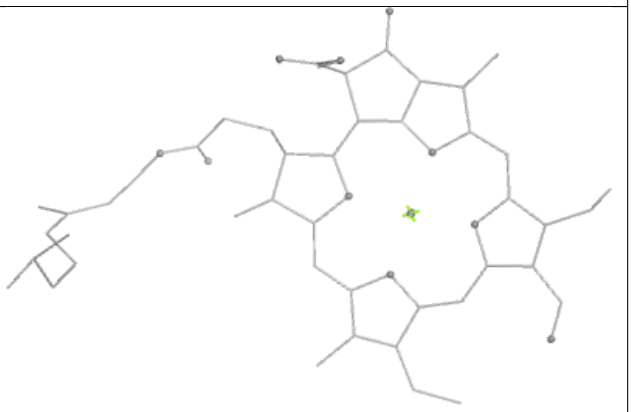
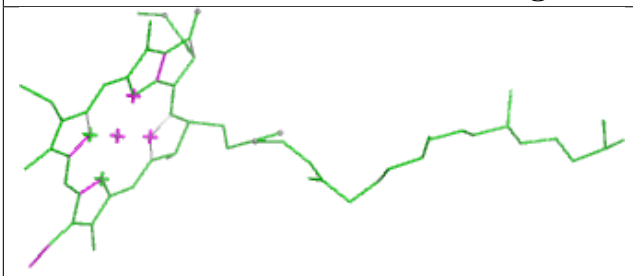


Rings

Ligand CLA c 602



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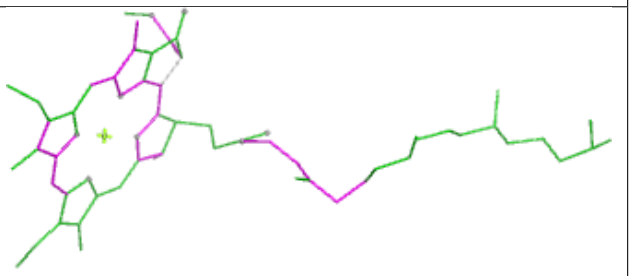

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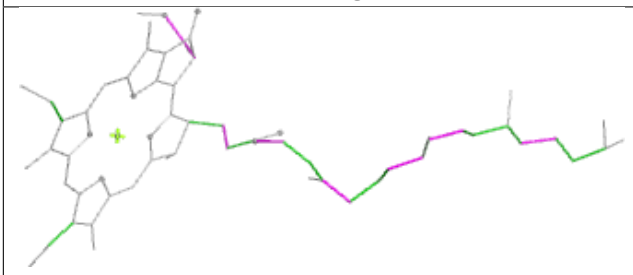
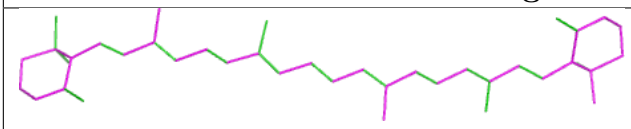


Torsions

Rings

Ligand BCR B 618



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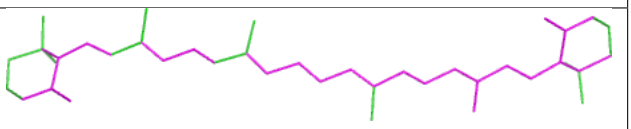
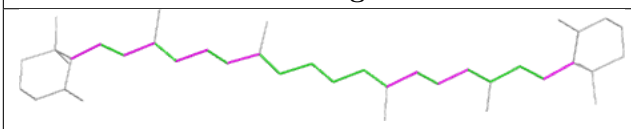


Bond angles



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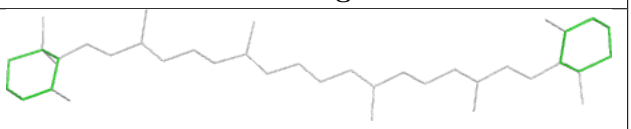
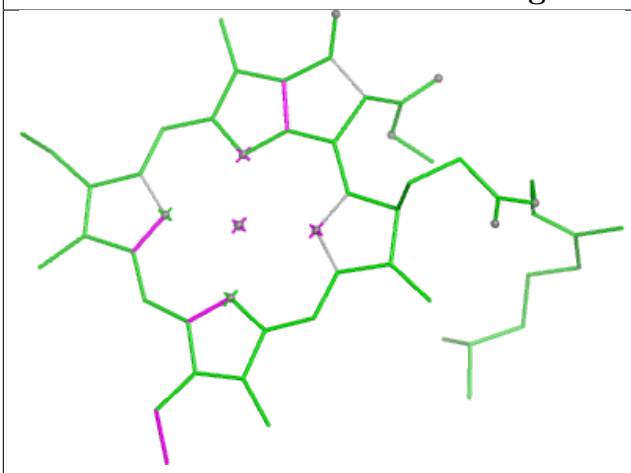


Rings

Ligand CLA 8 603



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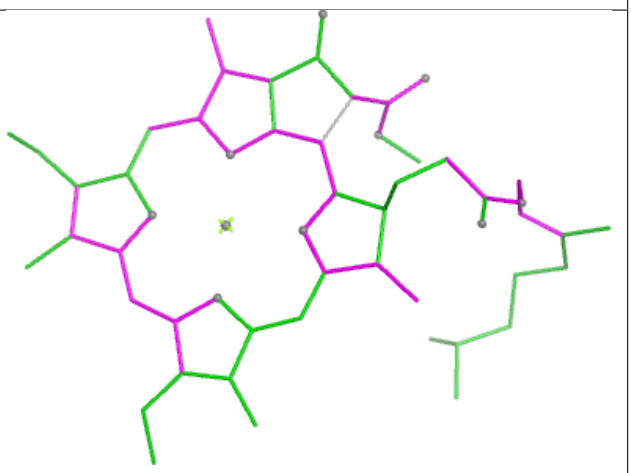
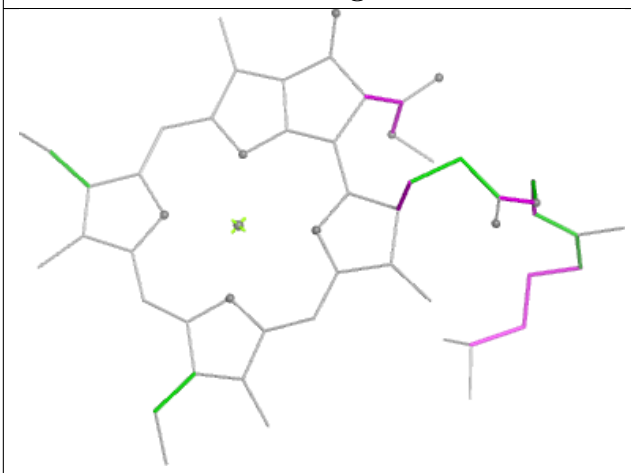


Bond angles



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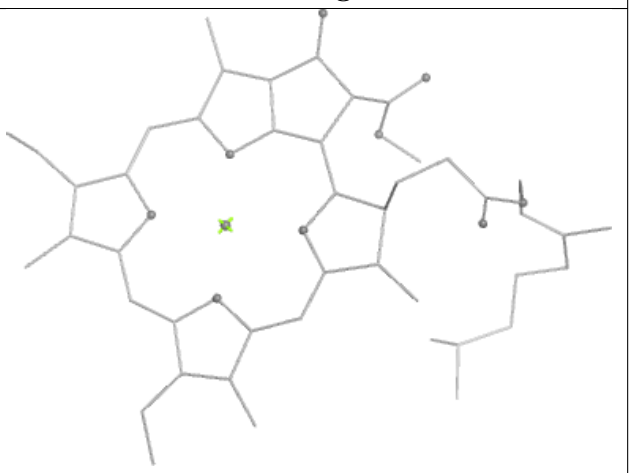
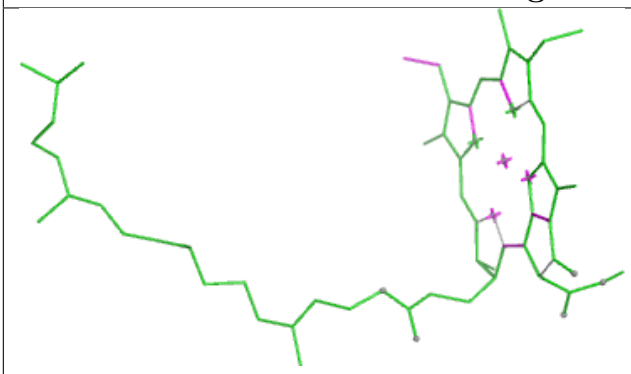
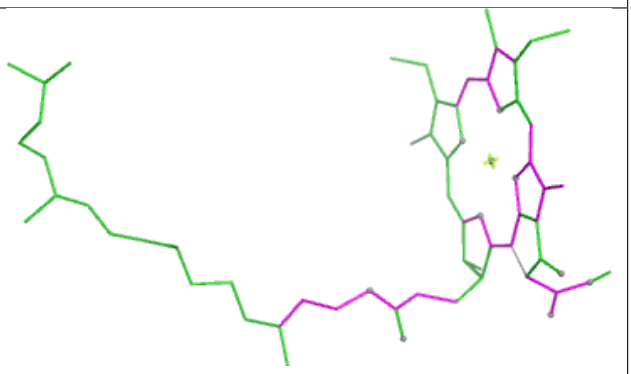
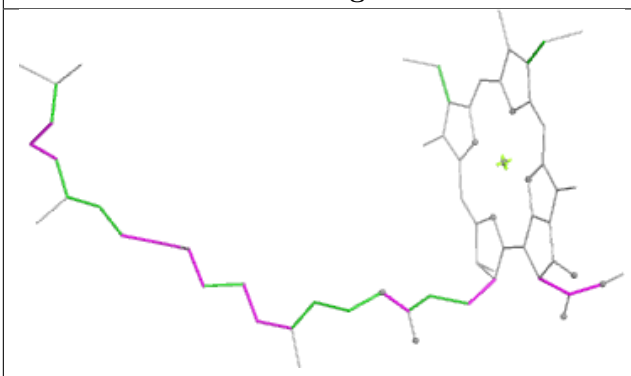
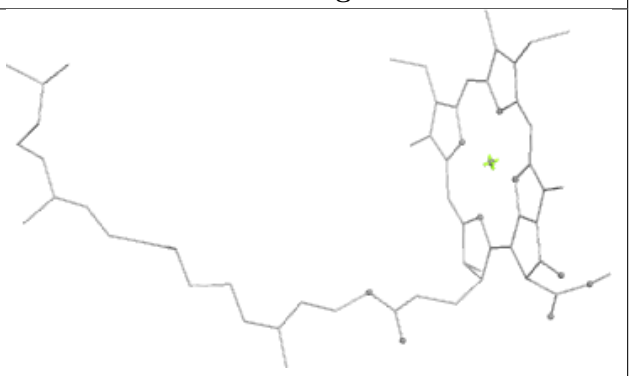
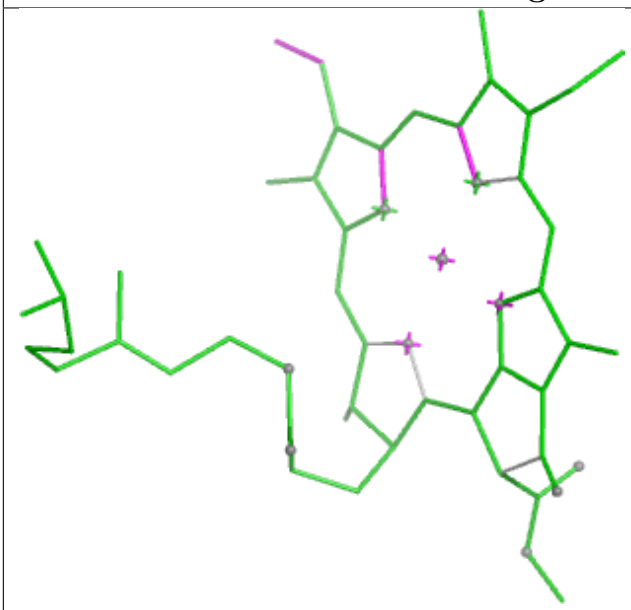


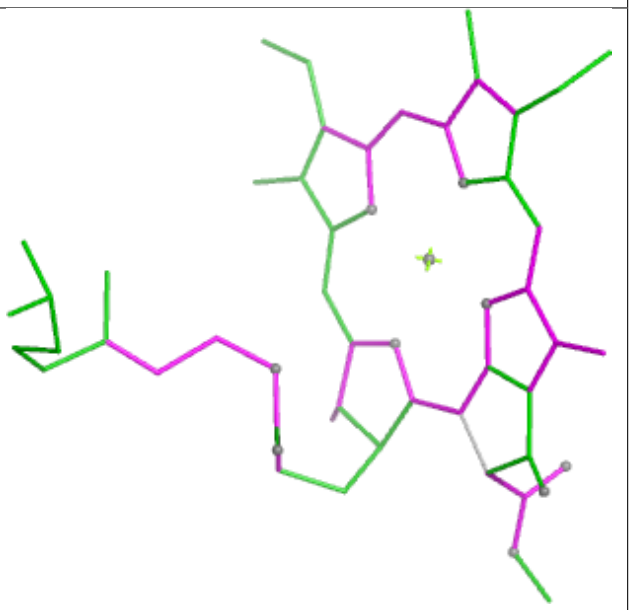
Rings

Ligand CLA b 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

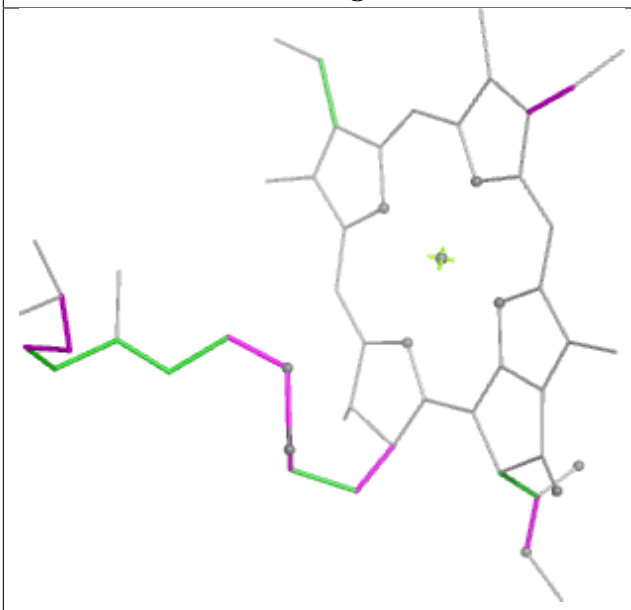
Ligand CLA 6 316



Bond lengths



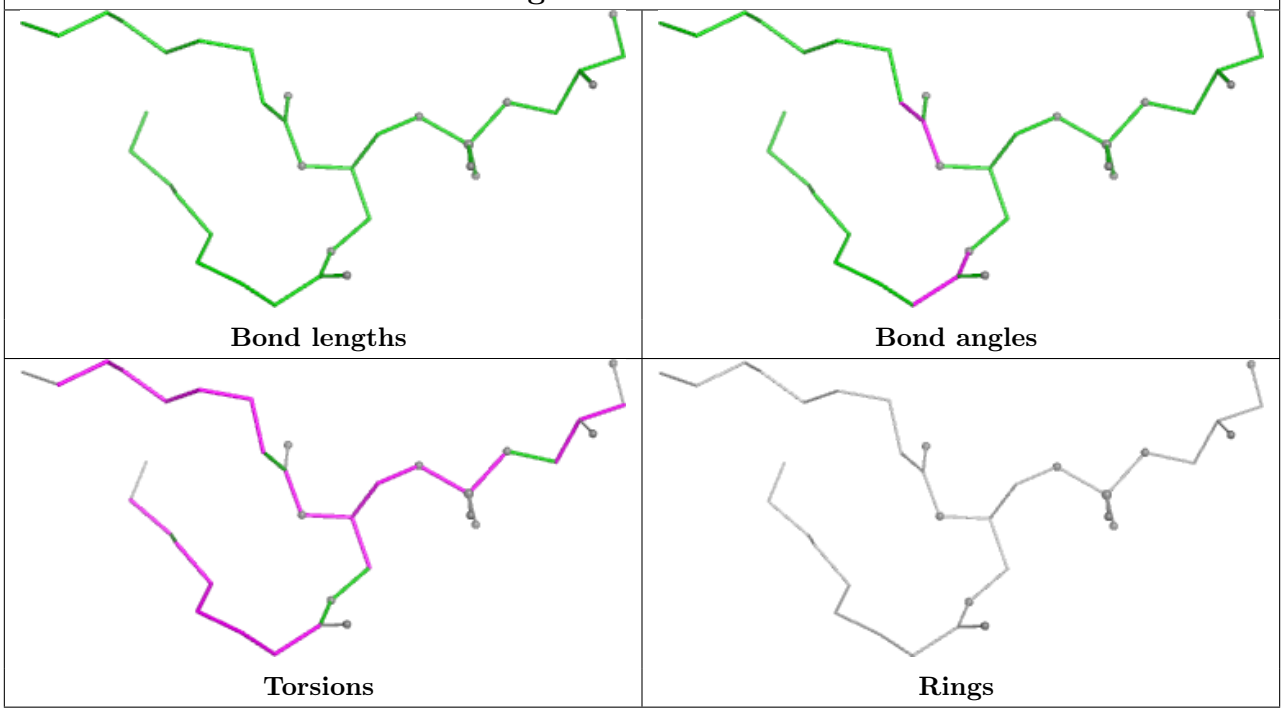
Bond angles



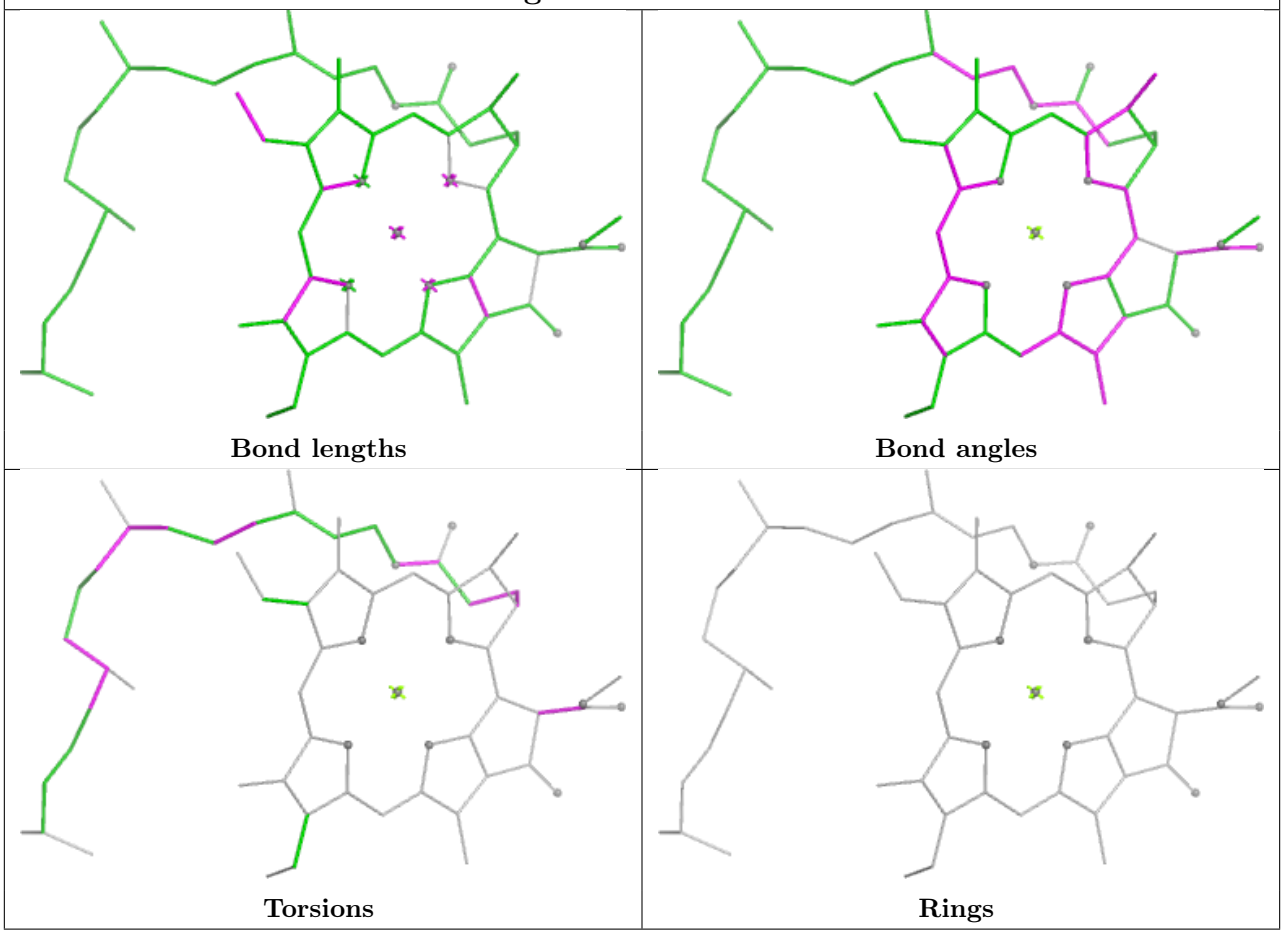
Torsions

Rings

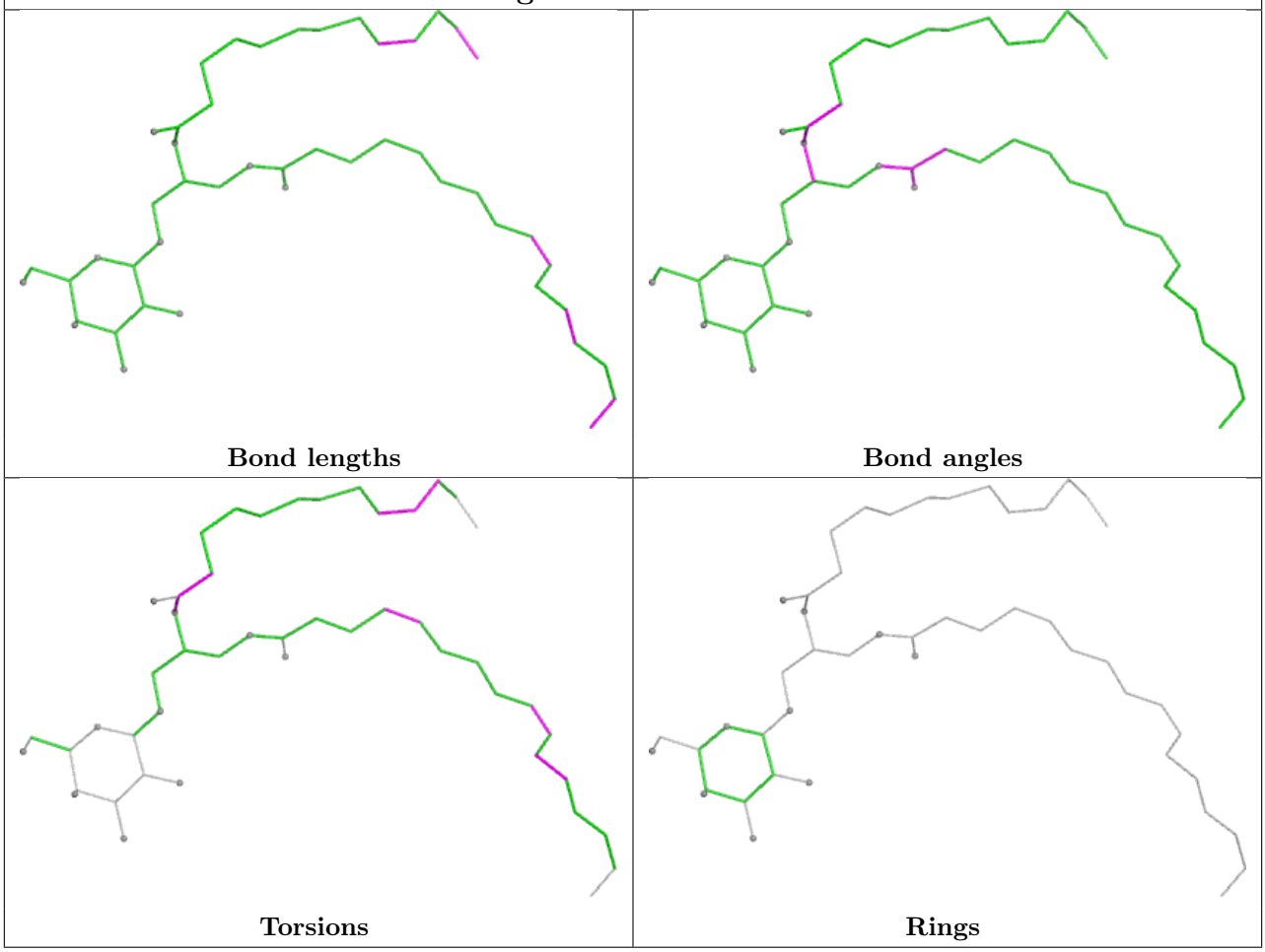
Ligand LHG 7 319



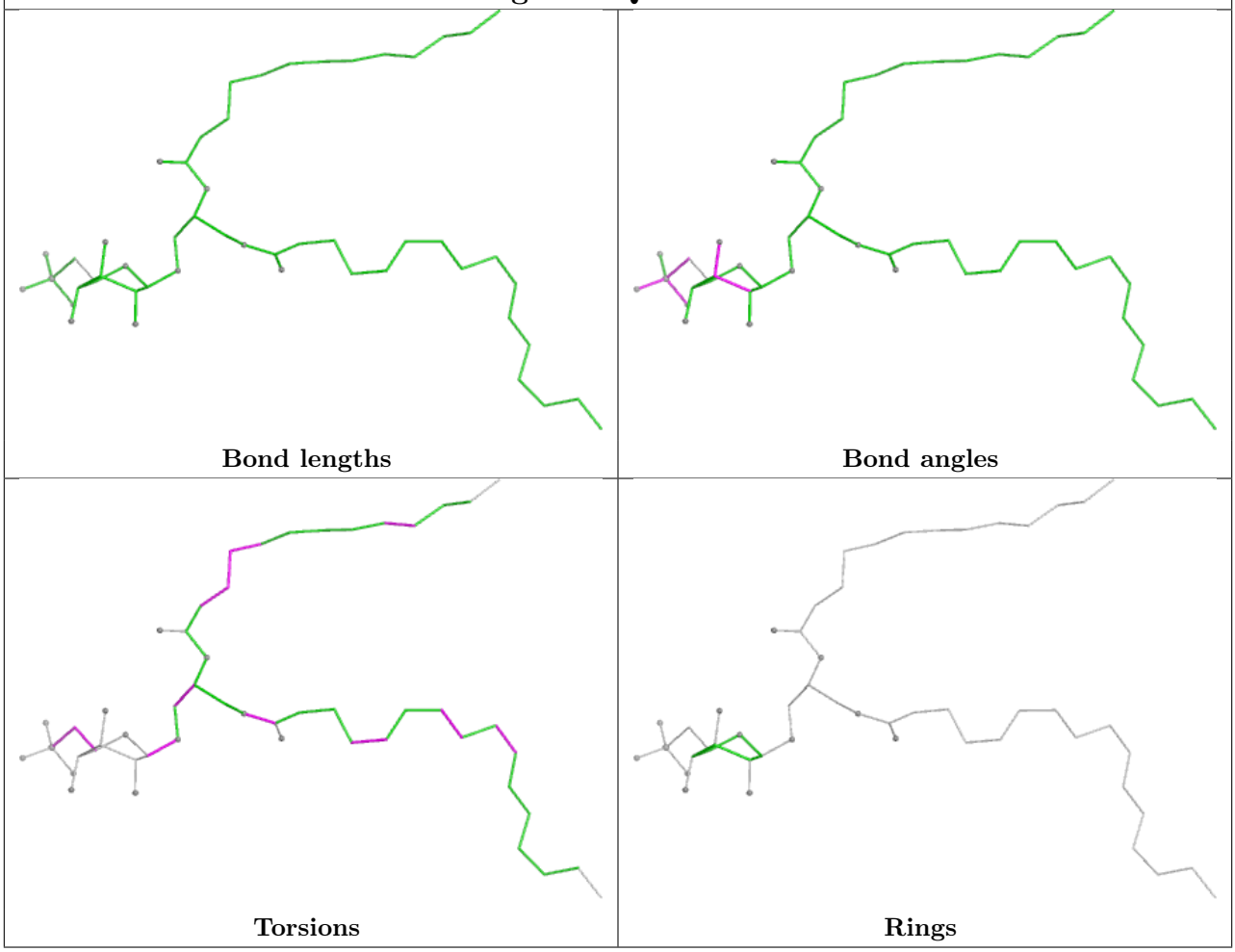
Ligand CLA G 602



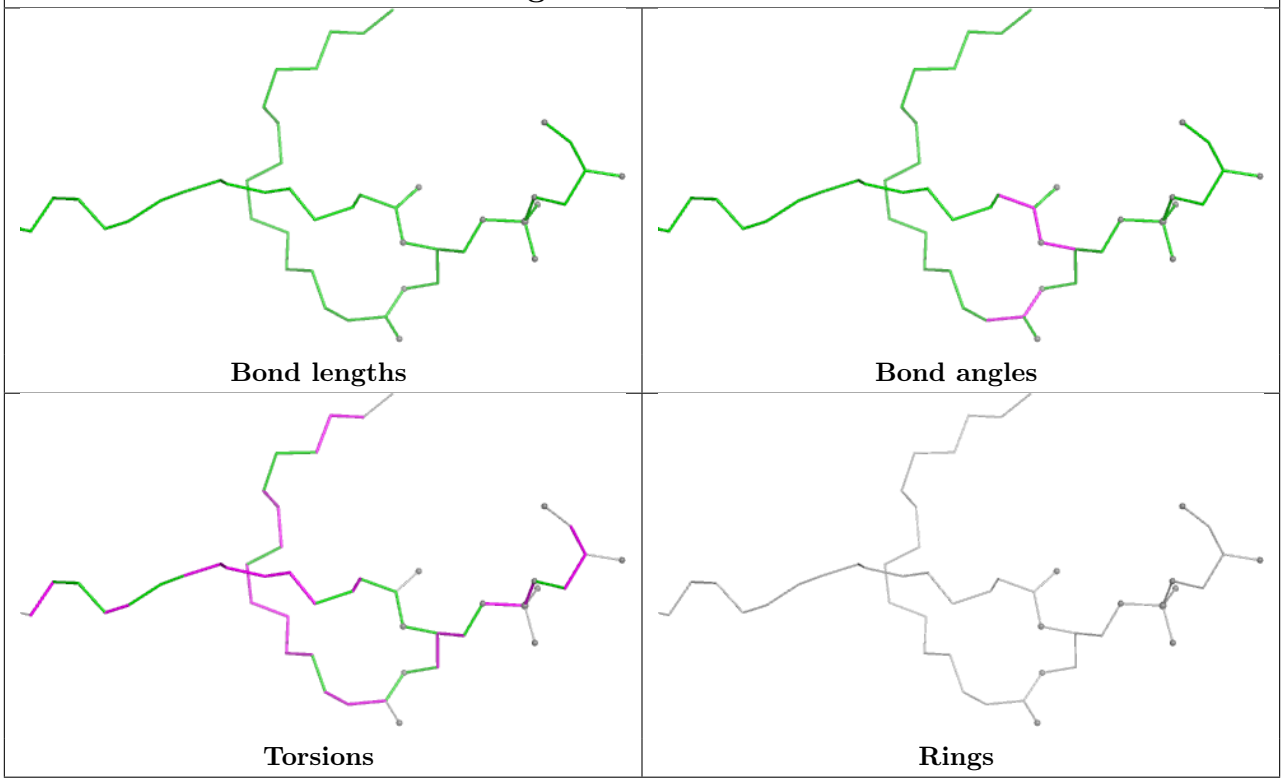
Ligand LMG k 101



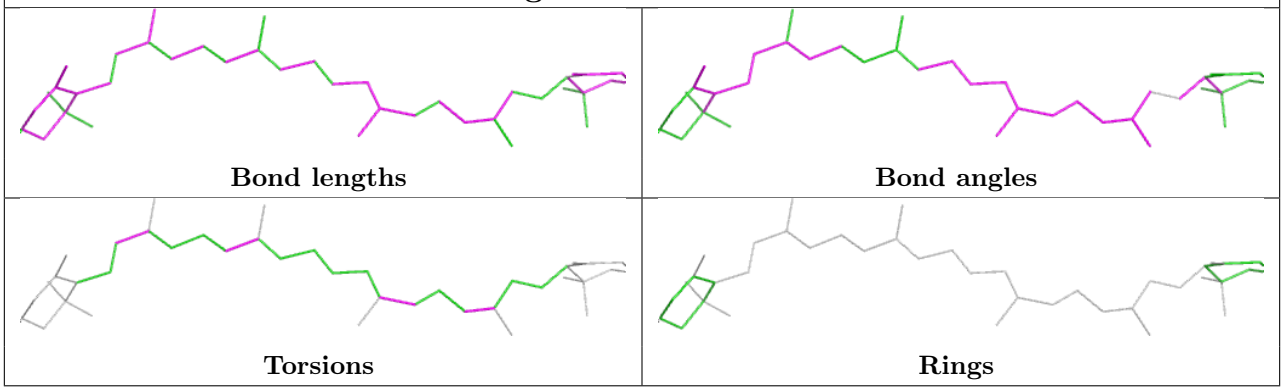
Ligand SQD s 301



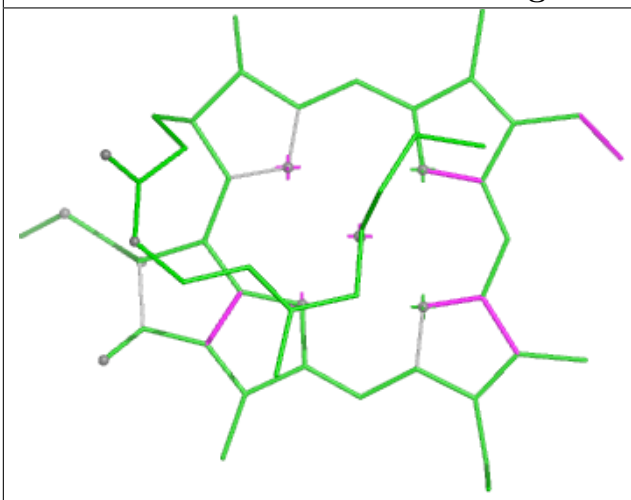
Ligand LHG 2 617



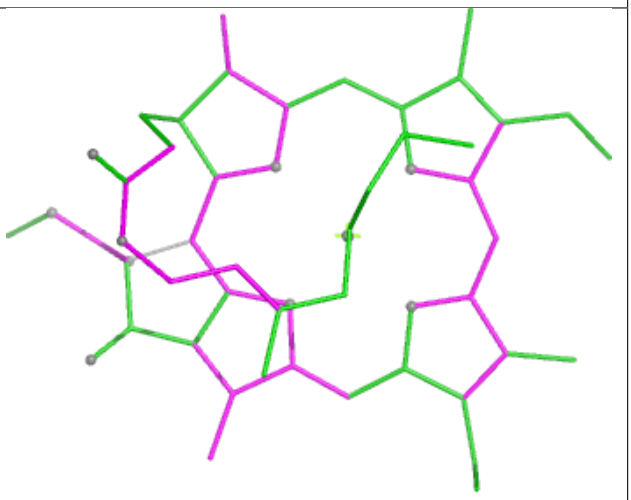
Ligand LUT R 317



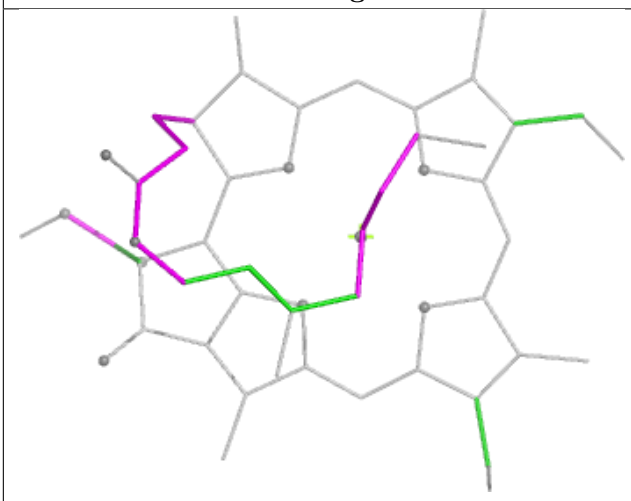
Ligand CLA 3 315



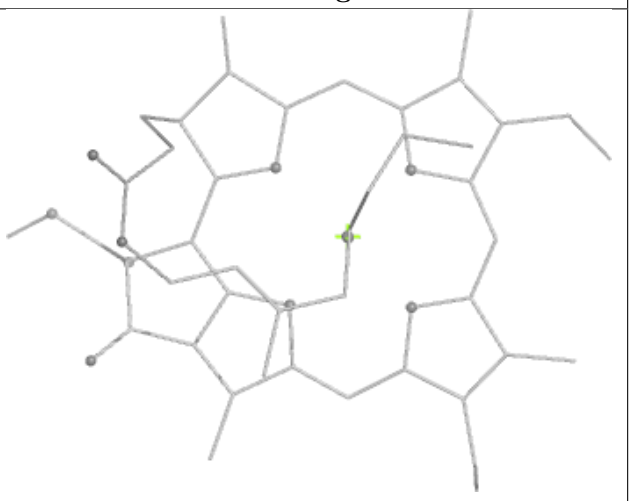
Bond lengths



Bond angles



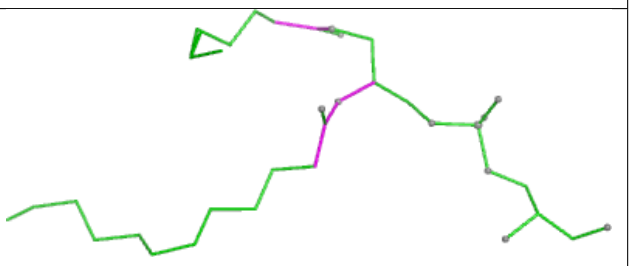
Torsions



Rings

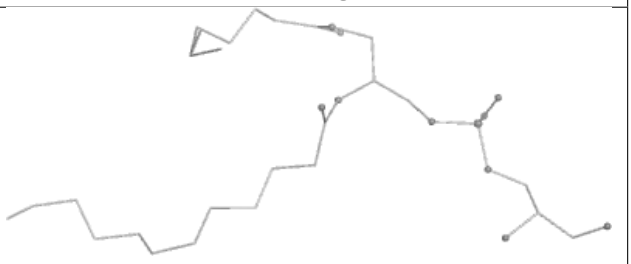
Ligand LHG r 320

Bond lengths



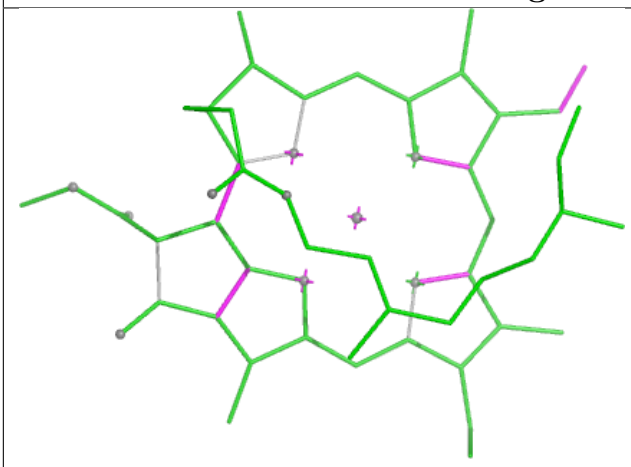
Bond angles

Torsions

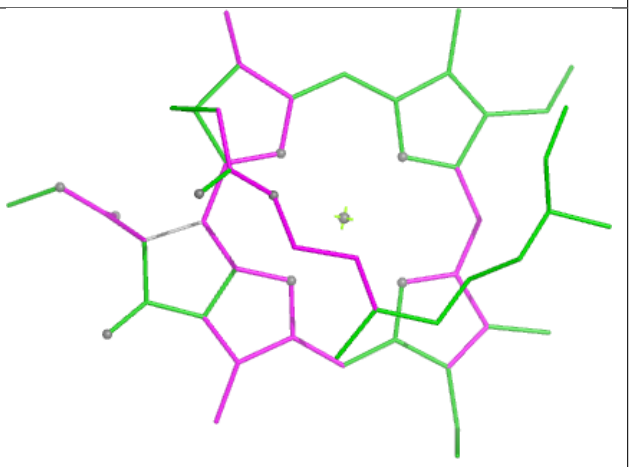


Rings

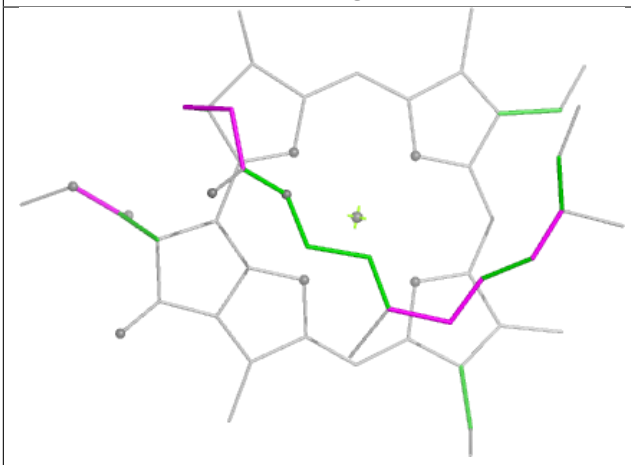
Ligand CLA 0 613



Bond lengths



Bond angles



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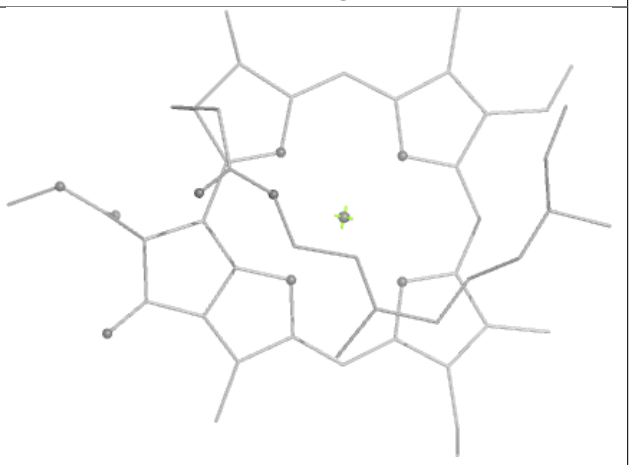
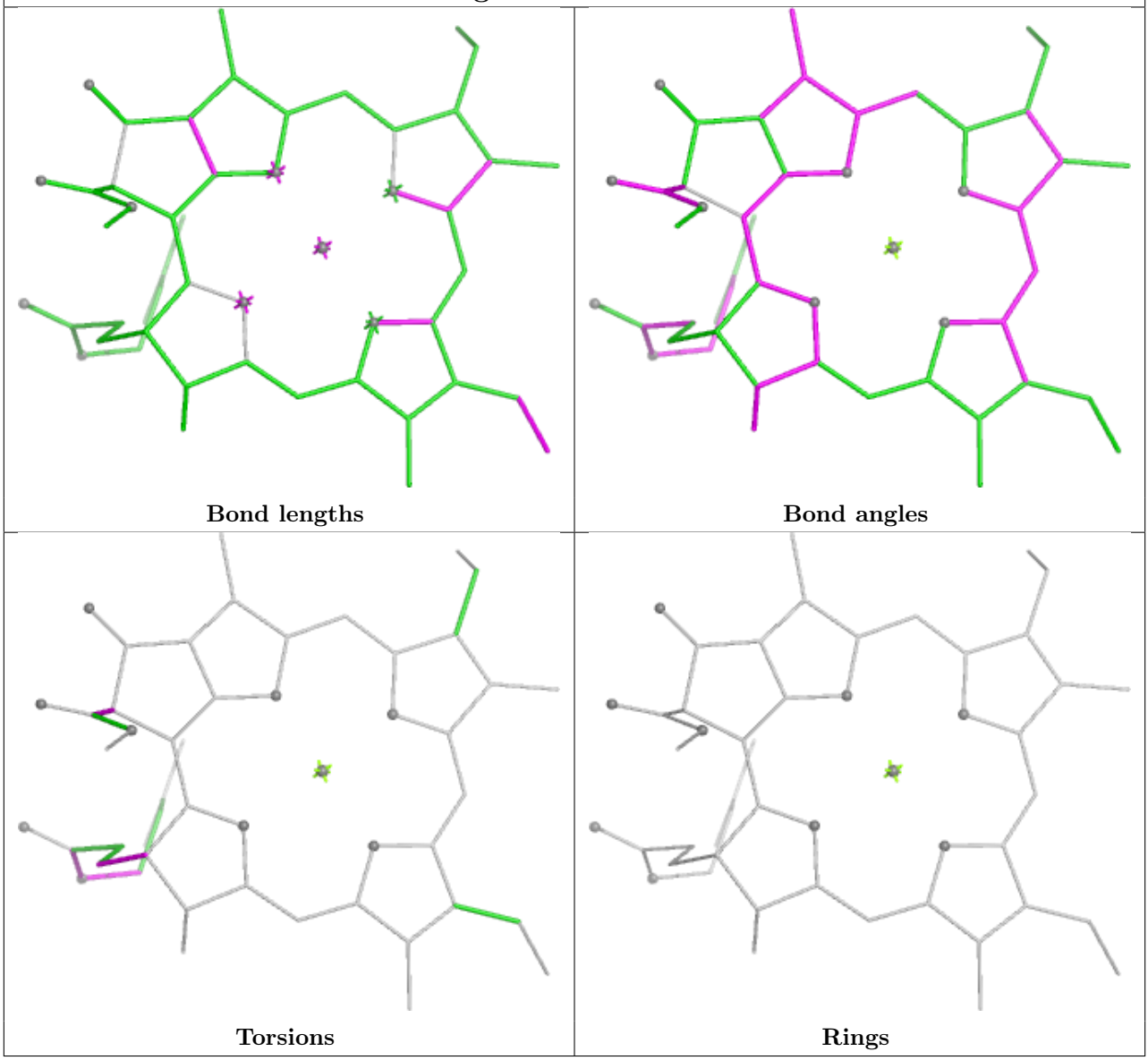
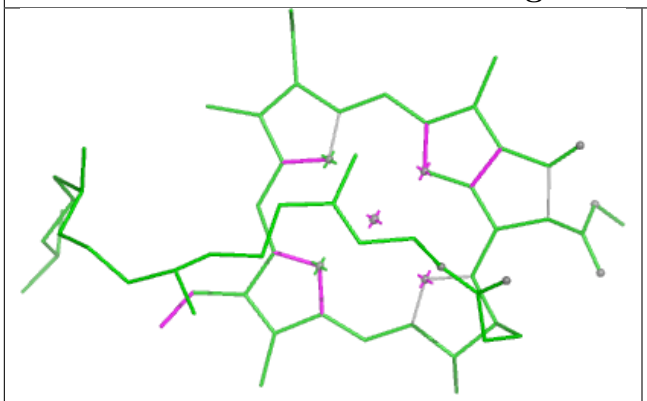


Rings

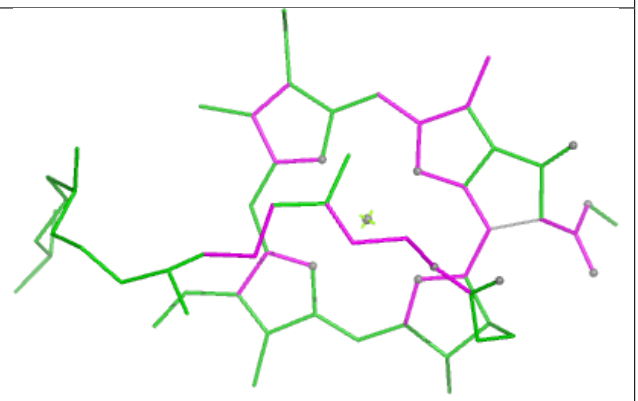
Ligand CLA 5 604



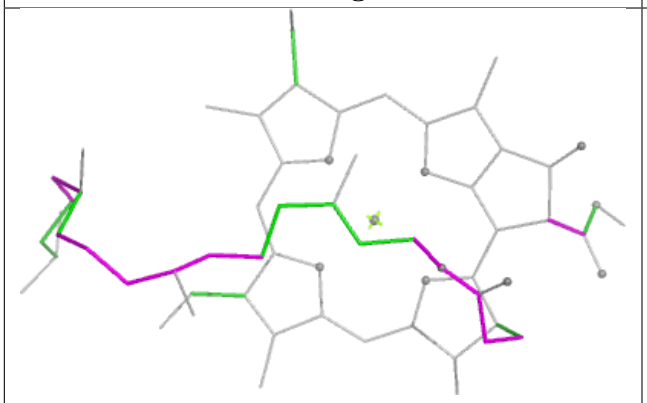
Ligand CLA C 605



Bond lengths



Bond angles



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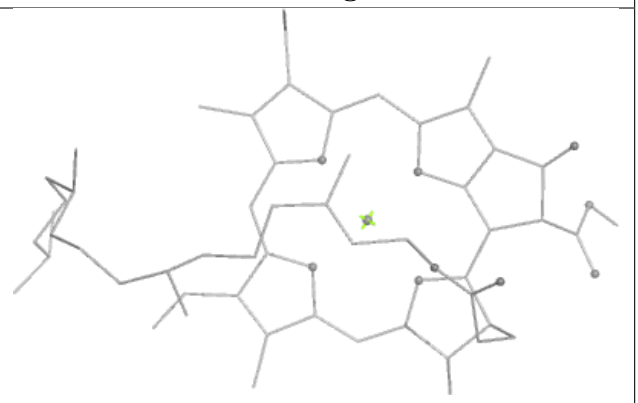
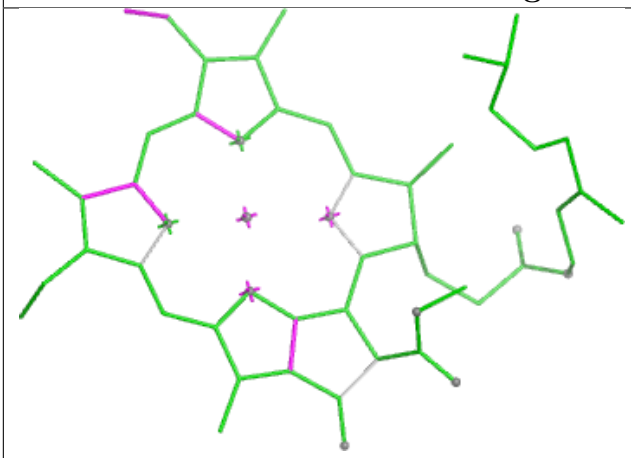
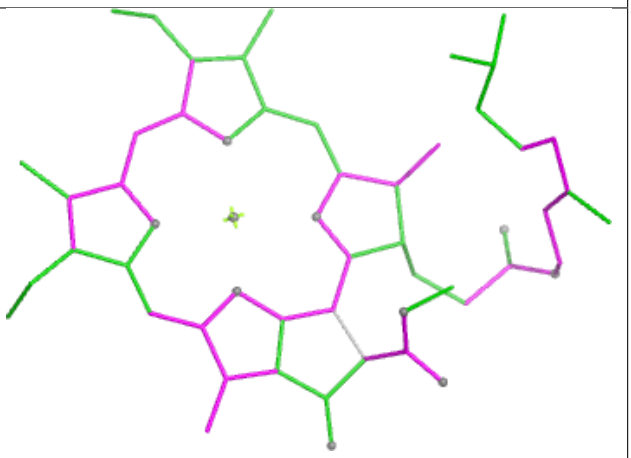
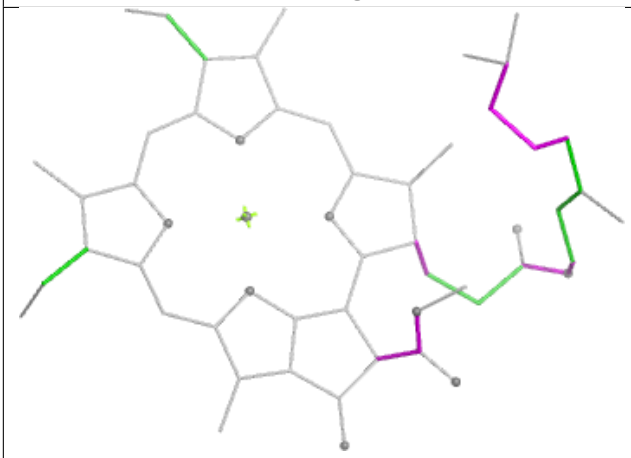
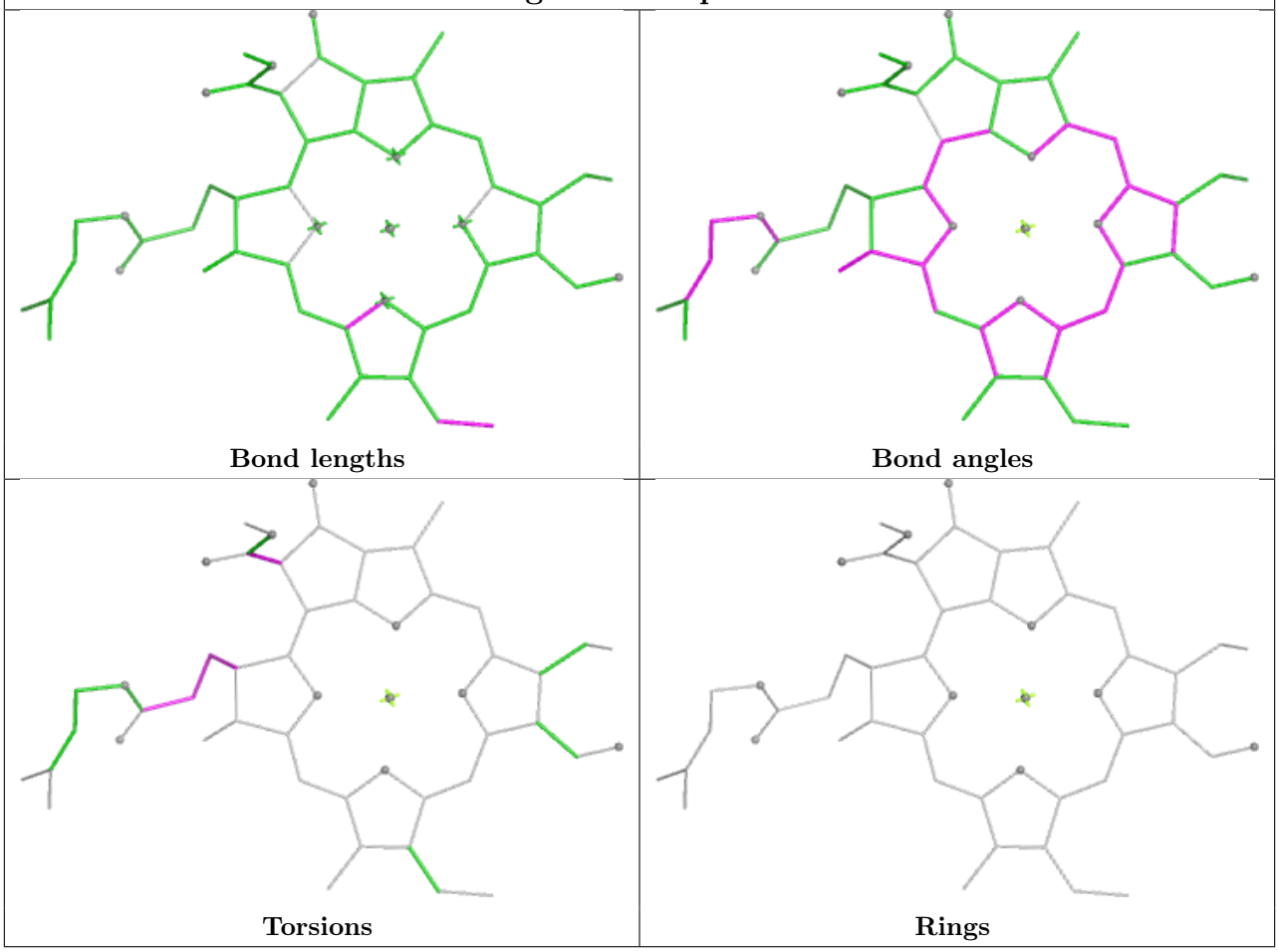
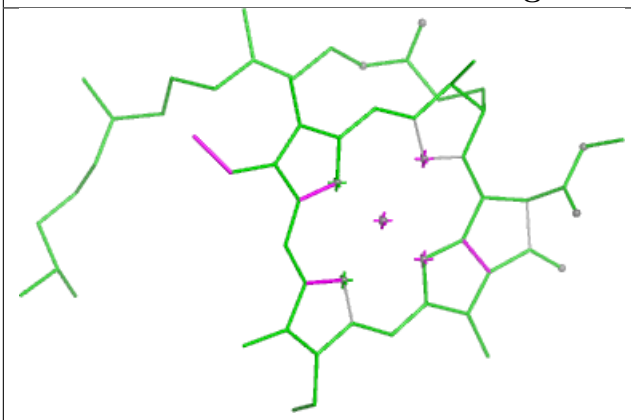
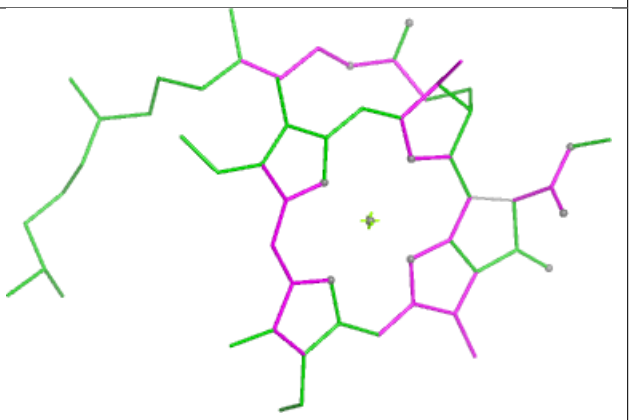
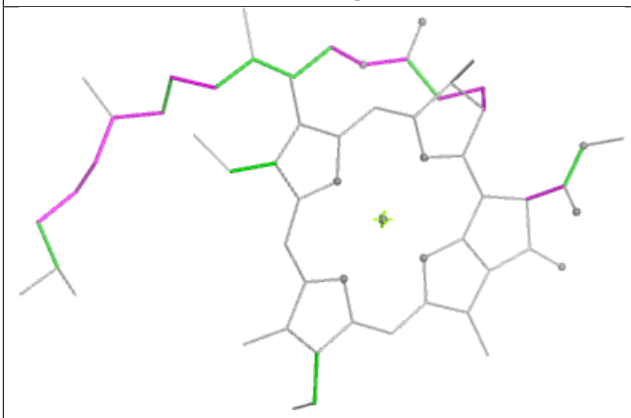
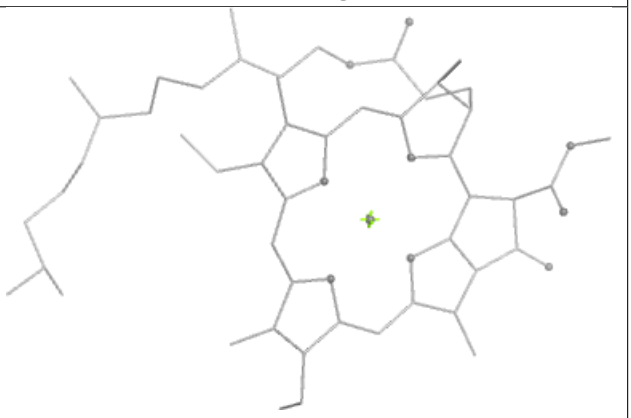


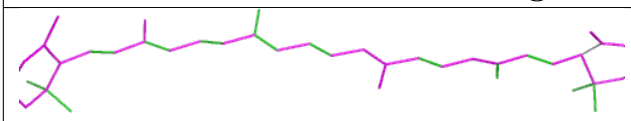
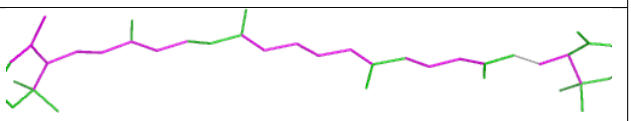
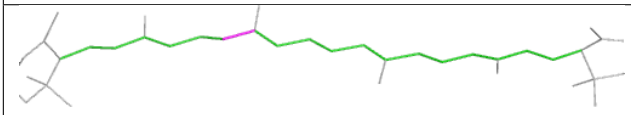
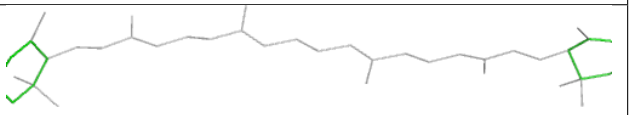
Rings

Ligand CLA Y 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

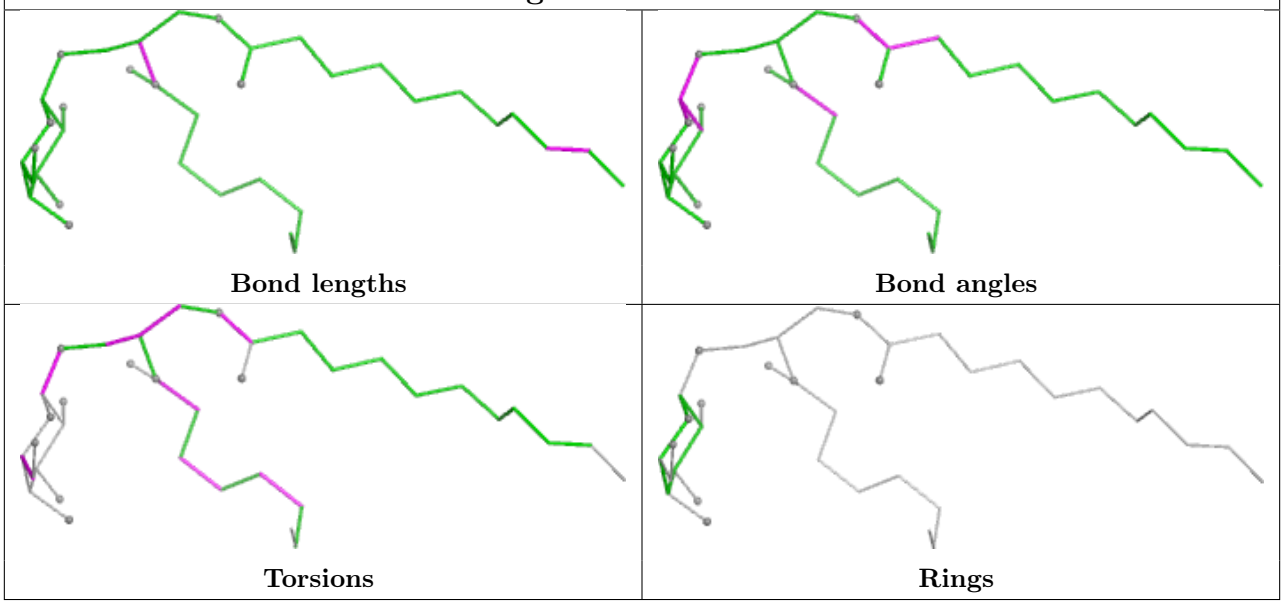
Ligand CHL p 601



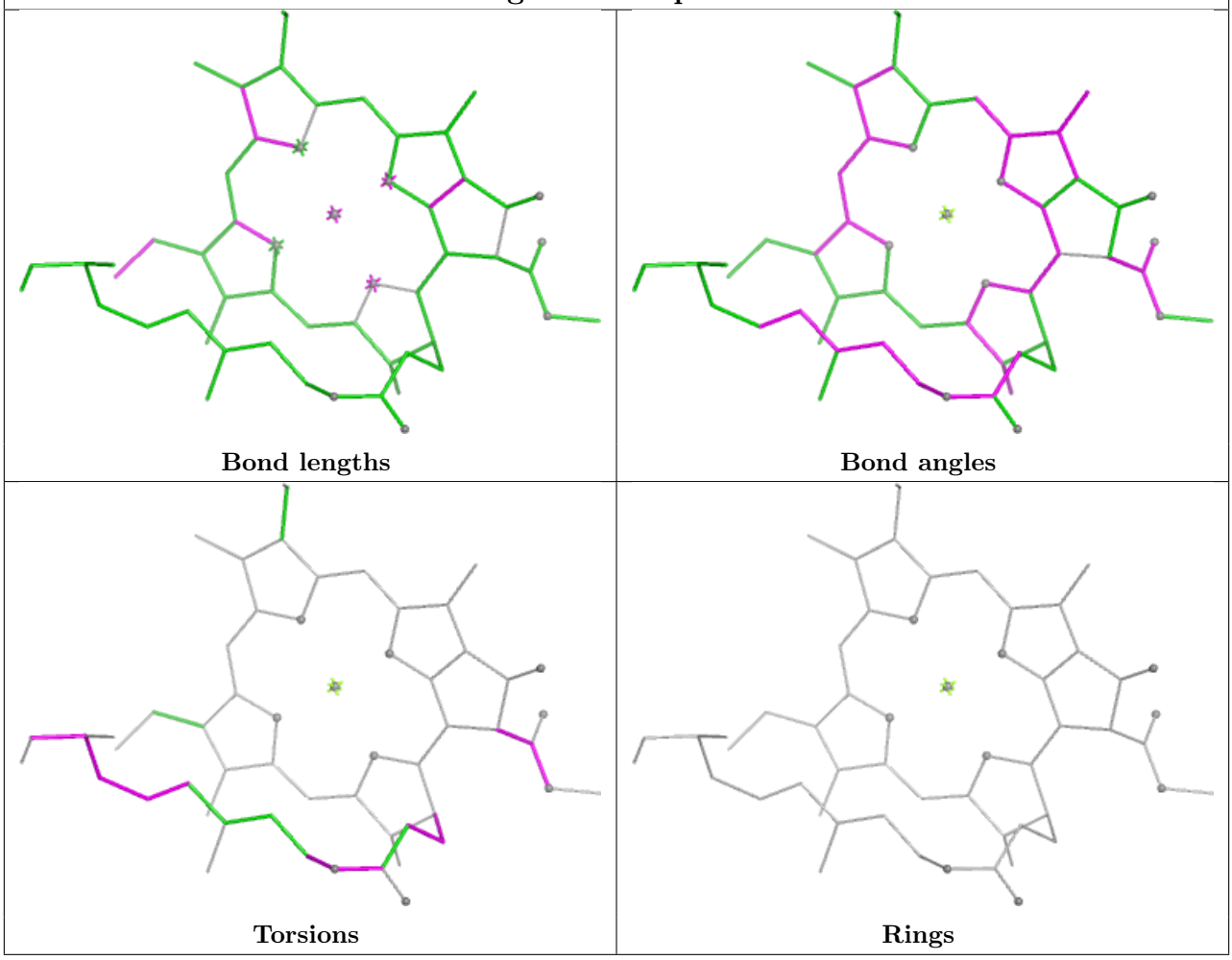
Ligand CLA R 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

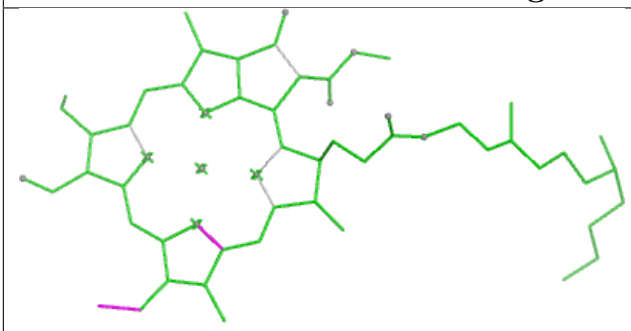
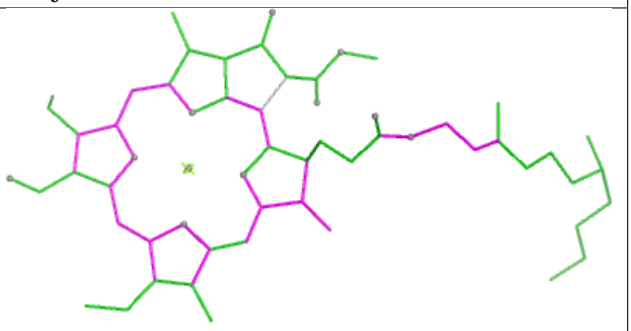
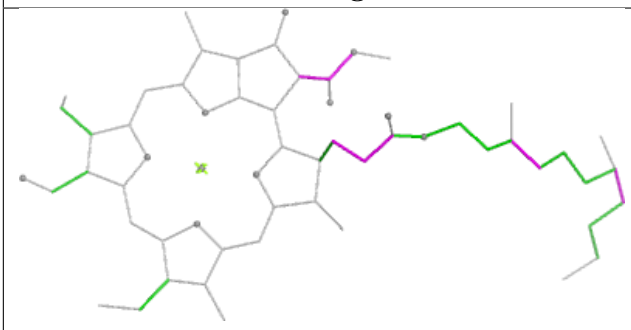
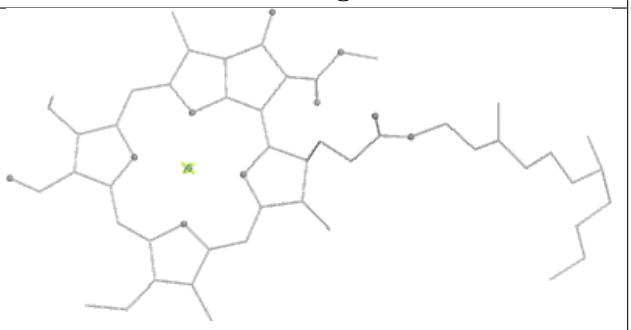
Ligand LUT 3 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG r 321

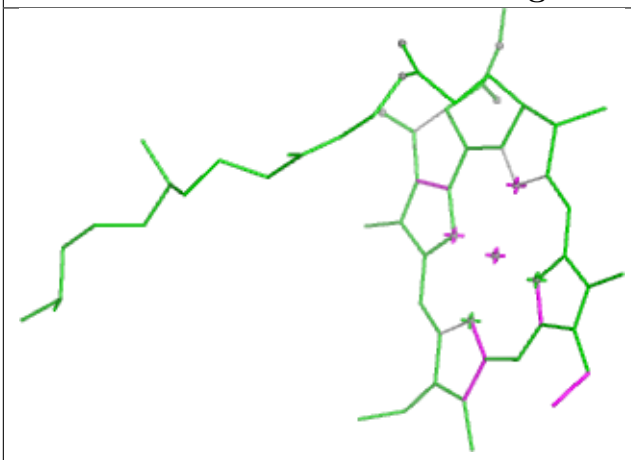


Ligand CLA p 610

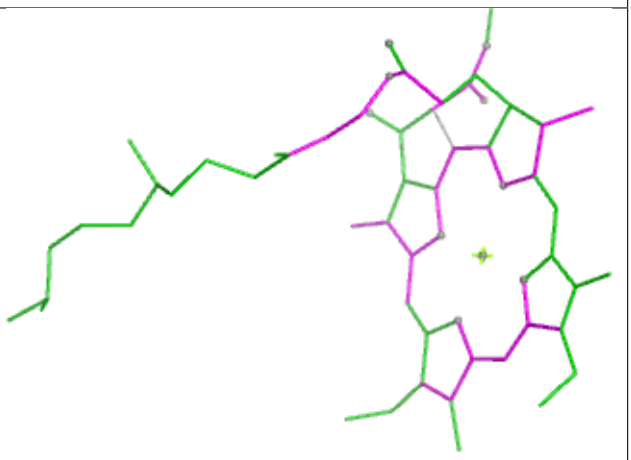


Ligand CHL y 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

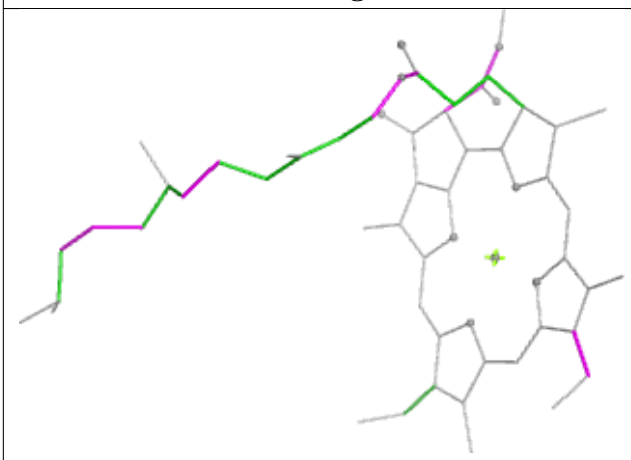
Ligand CLA 0 611



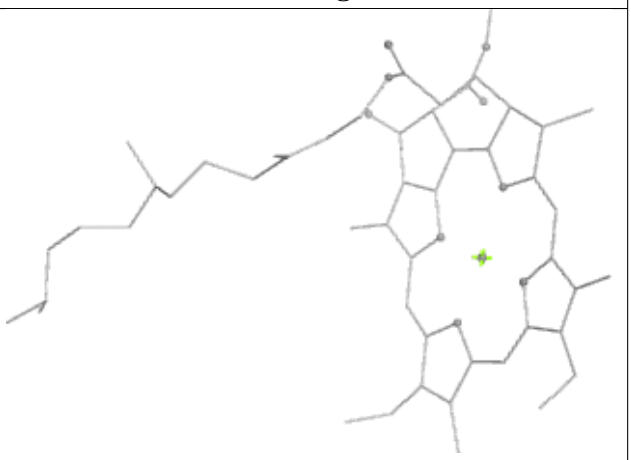
Bond lengths



Bond angles

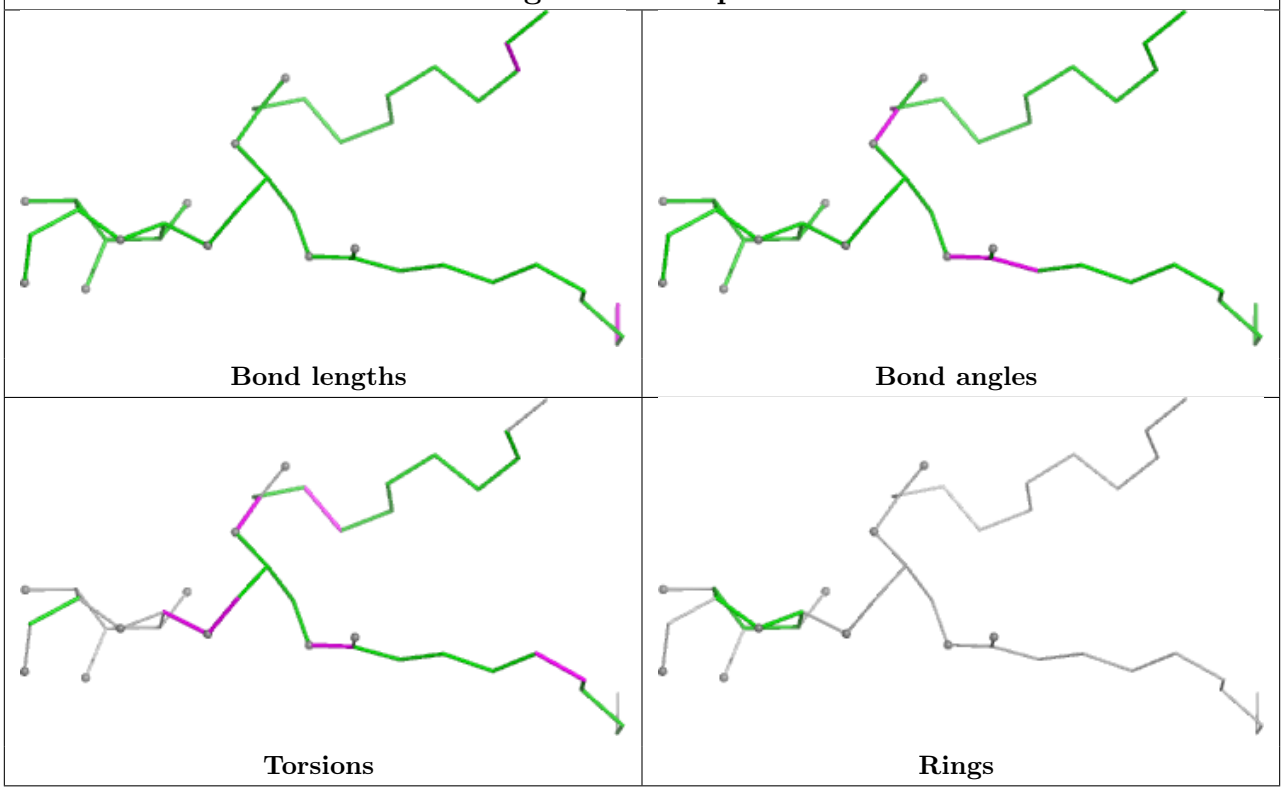


Torsions

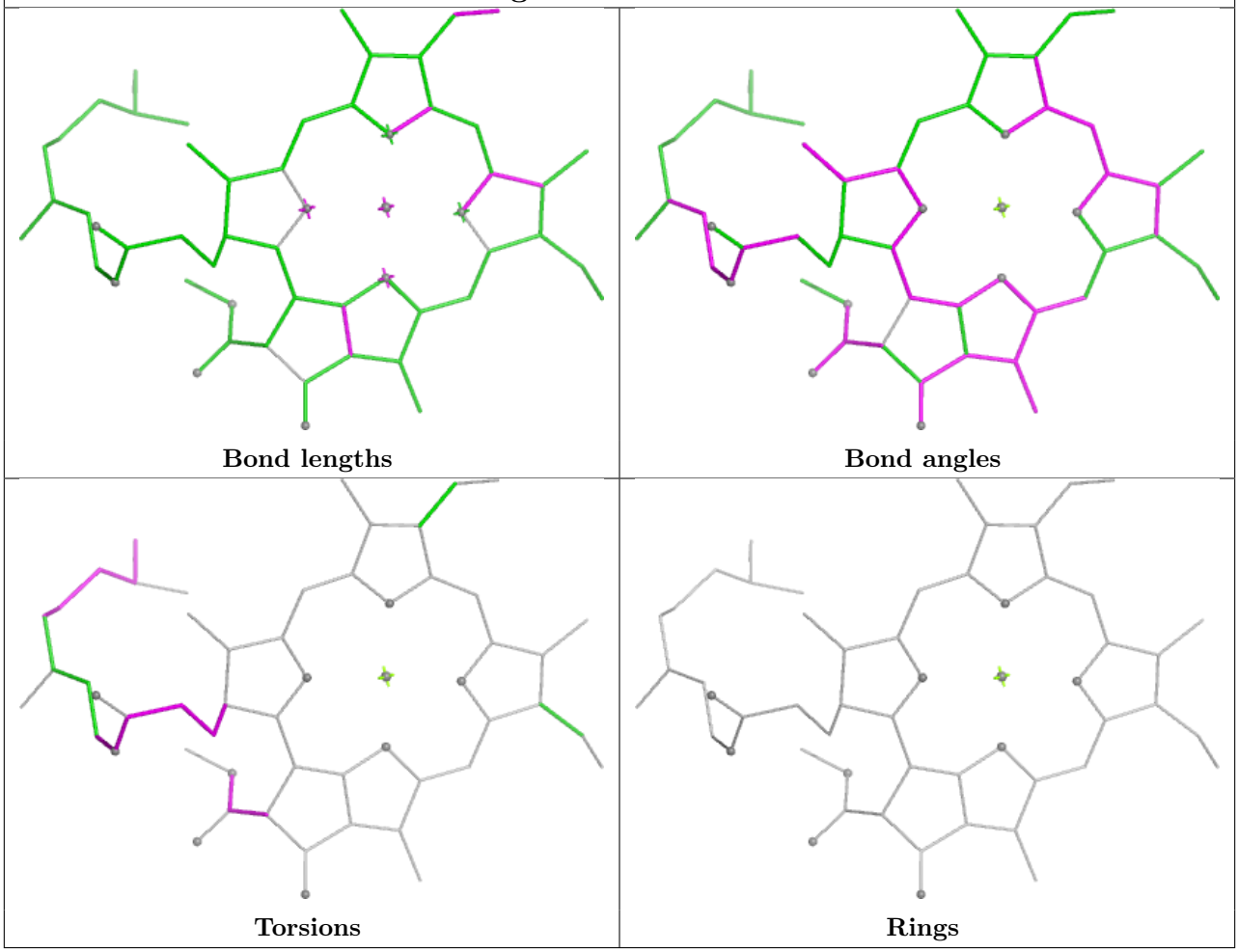


Rings

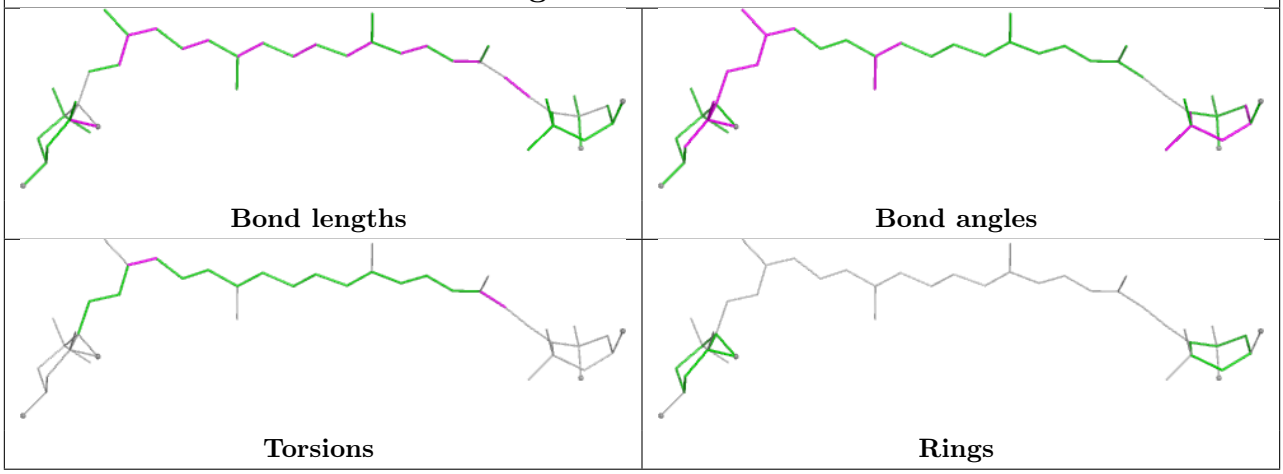
Ligand LMG q 302



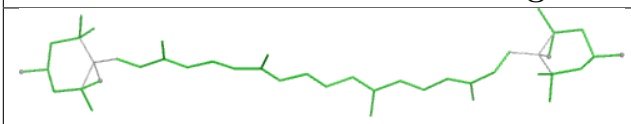
Ligand CLA 6 304



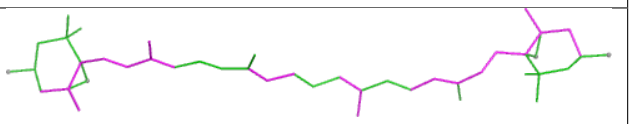
Ligand NEX s 319



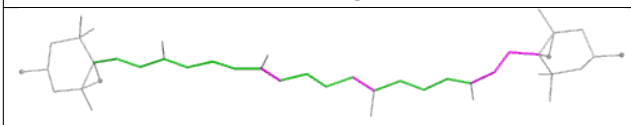
Ligand XAT 4 619



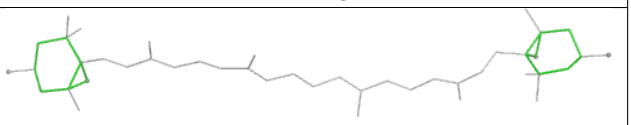
Bond lengths



Bond angles

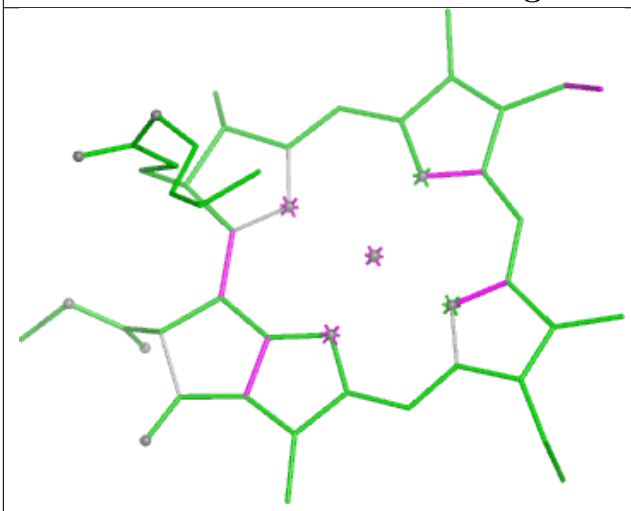


Torsions

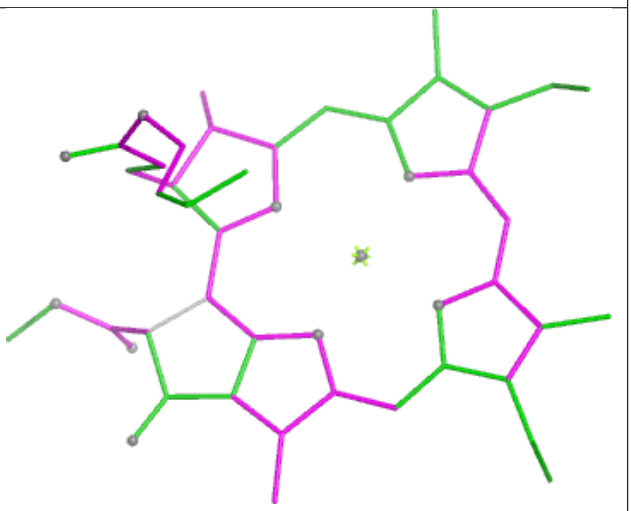


Rings

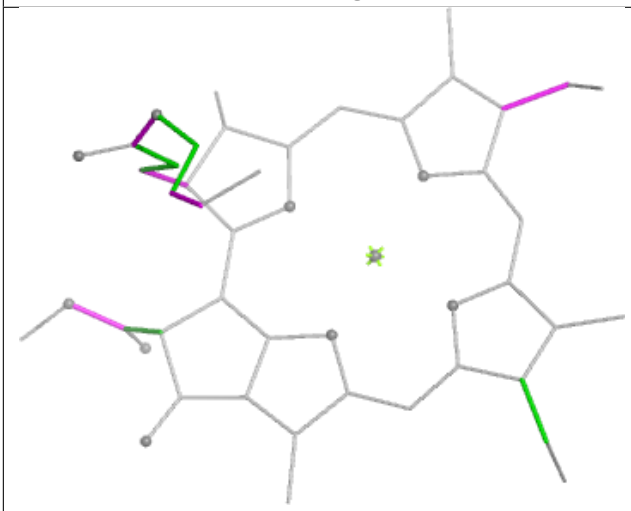
Ligand CLA R 313



Bond lengths



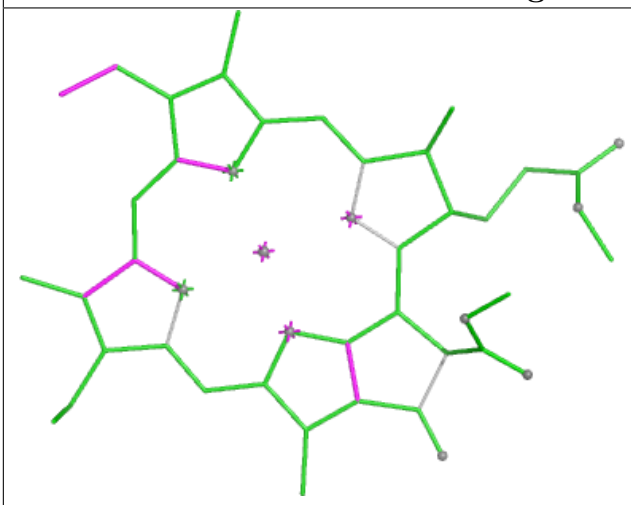
Bond angles



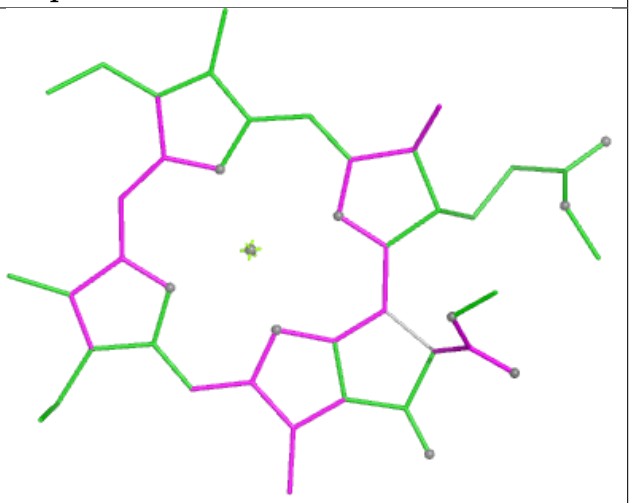
Torsions

Rings

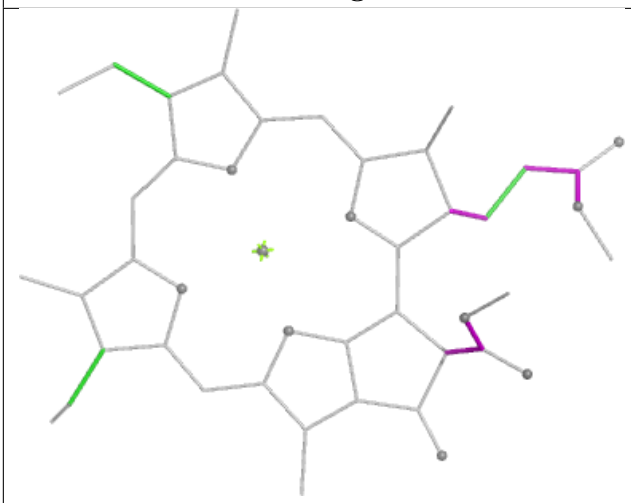
Ligand CLA p 612



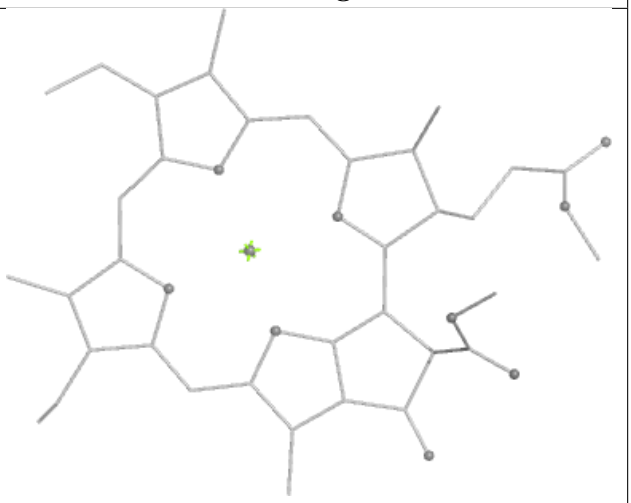
Bond lengths



Bond angles

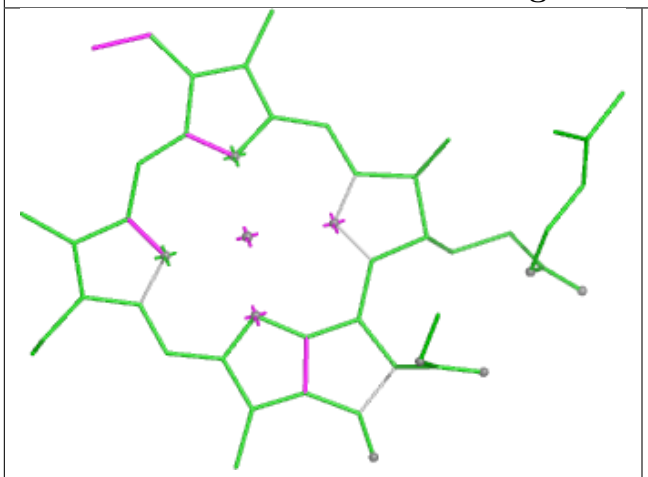


Torsions



Rings

Ligand CLA 9 314



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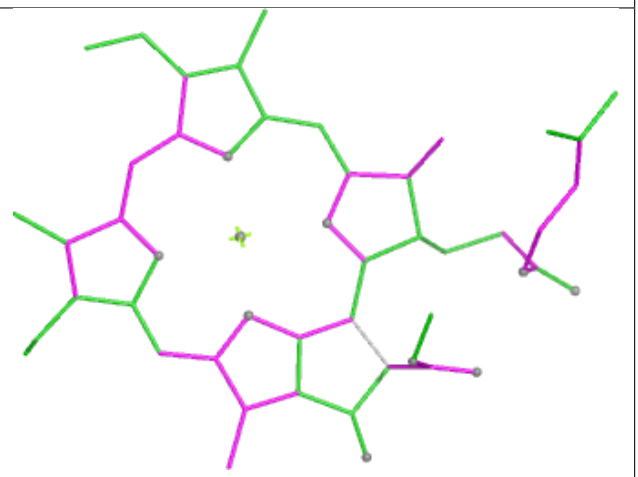
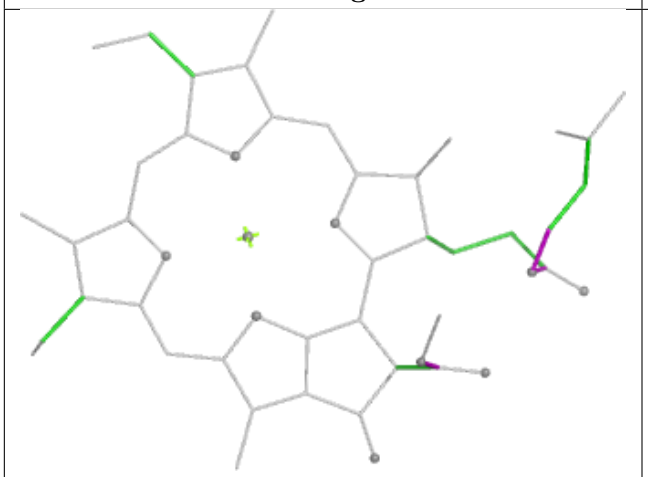


Bond angles



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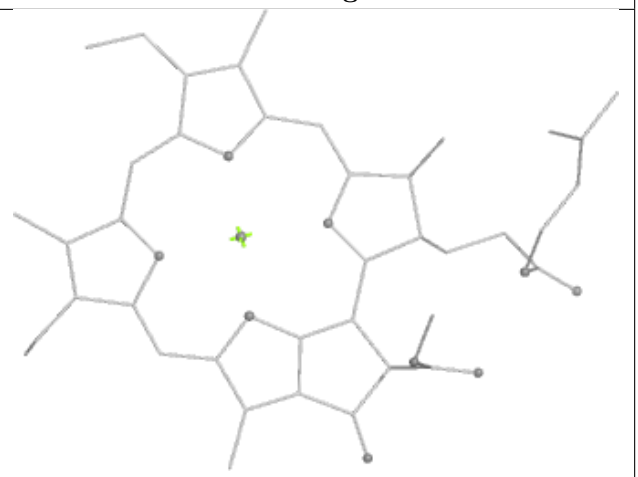
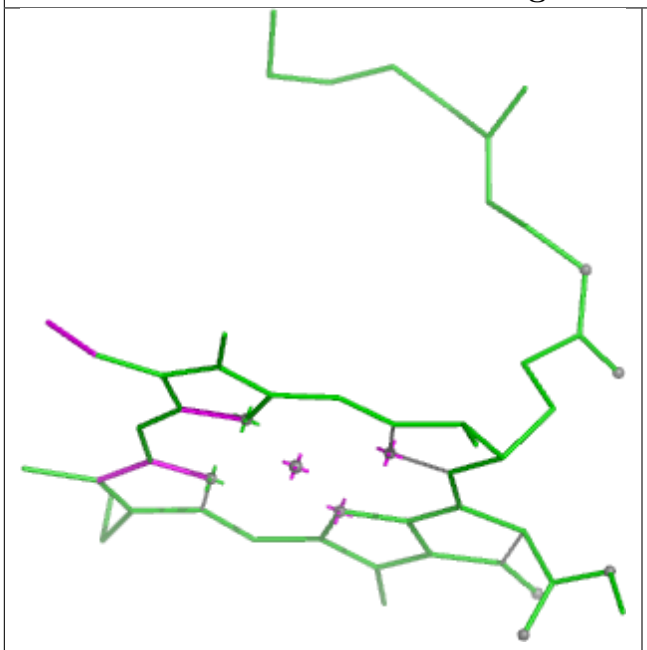


Rings

Ligand CLA y 614



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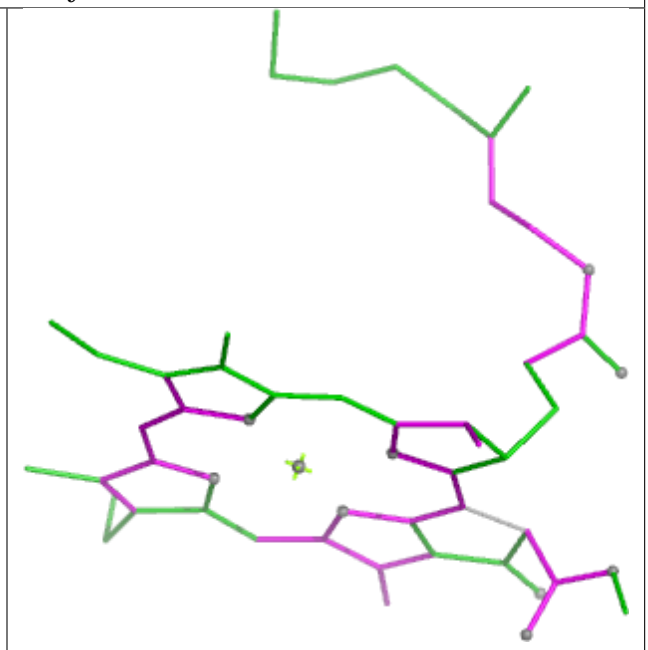
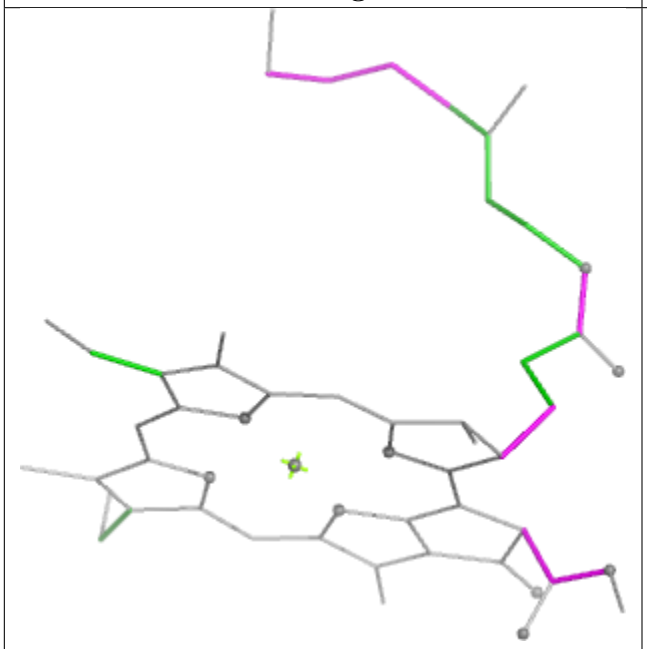


Bond angles



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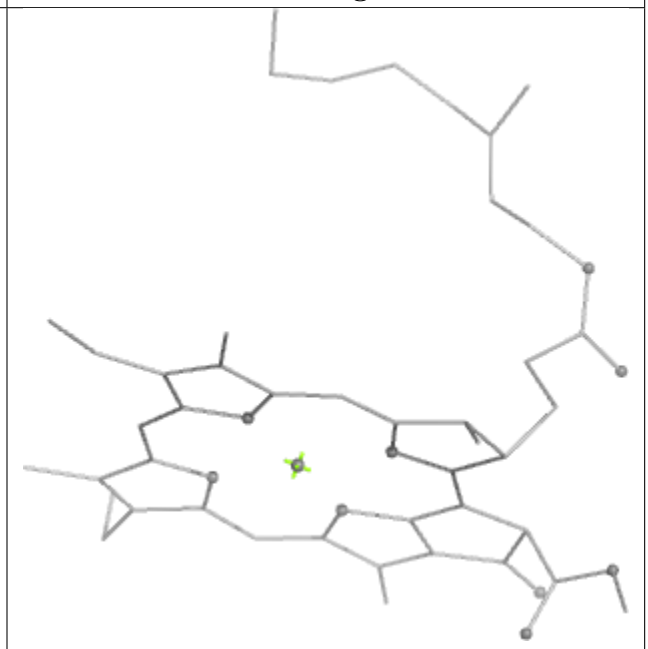
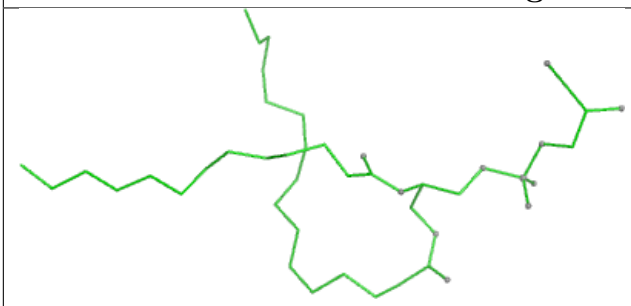
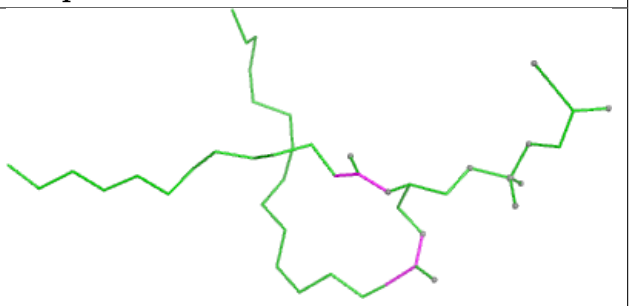
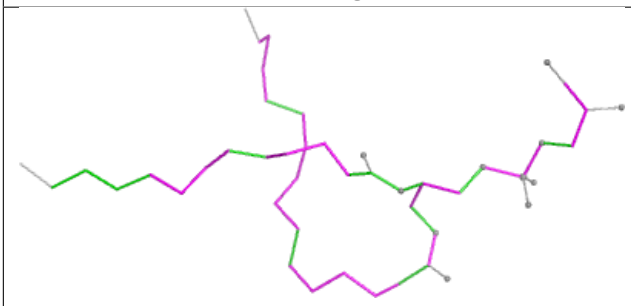
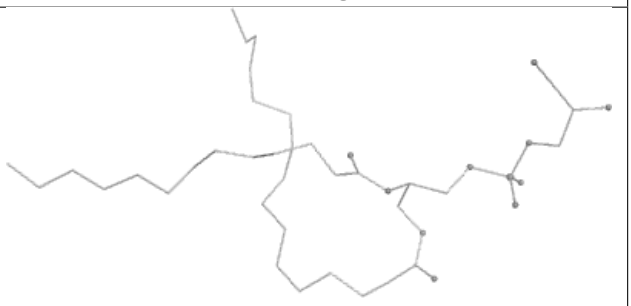
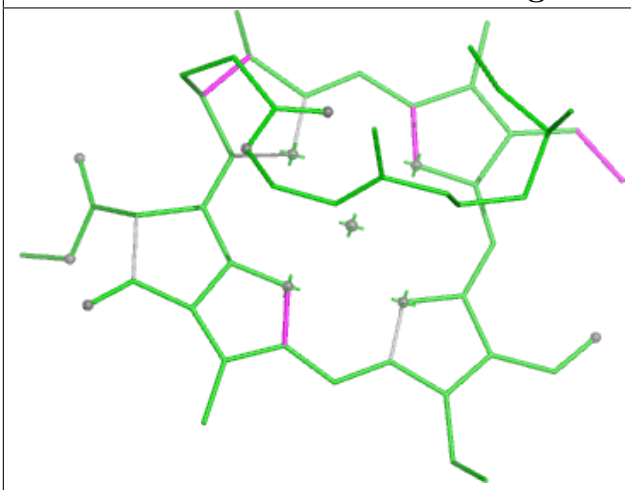


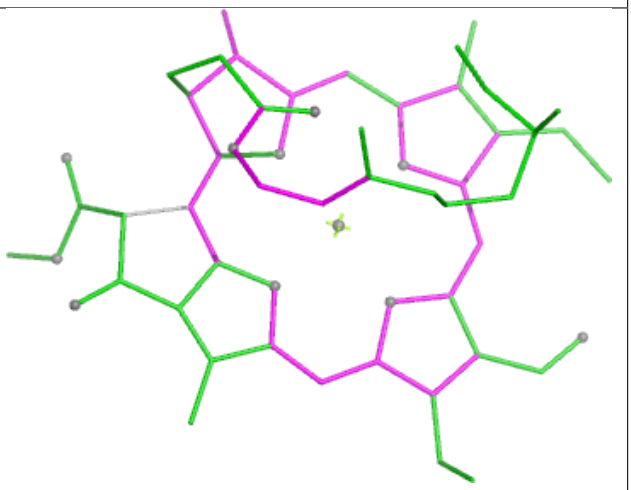
Rings

Ligand LHG q 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

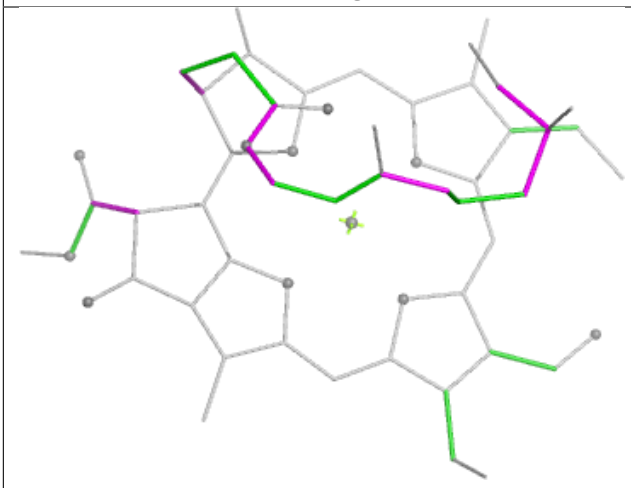
Ligand CHL 3 302



Bond lengths



Bond angles



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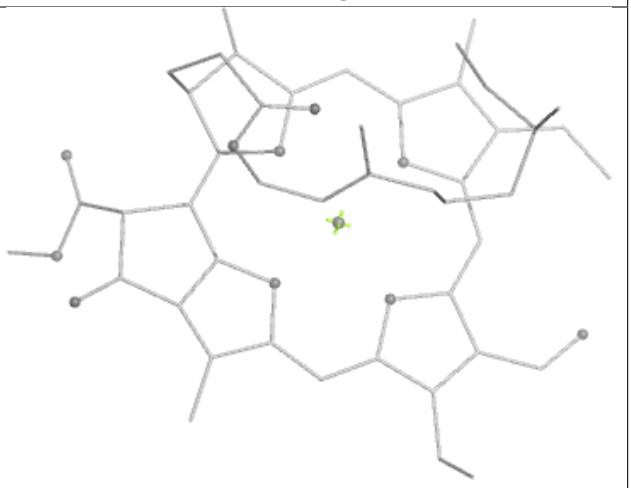
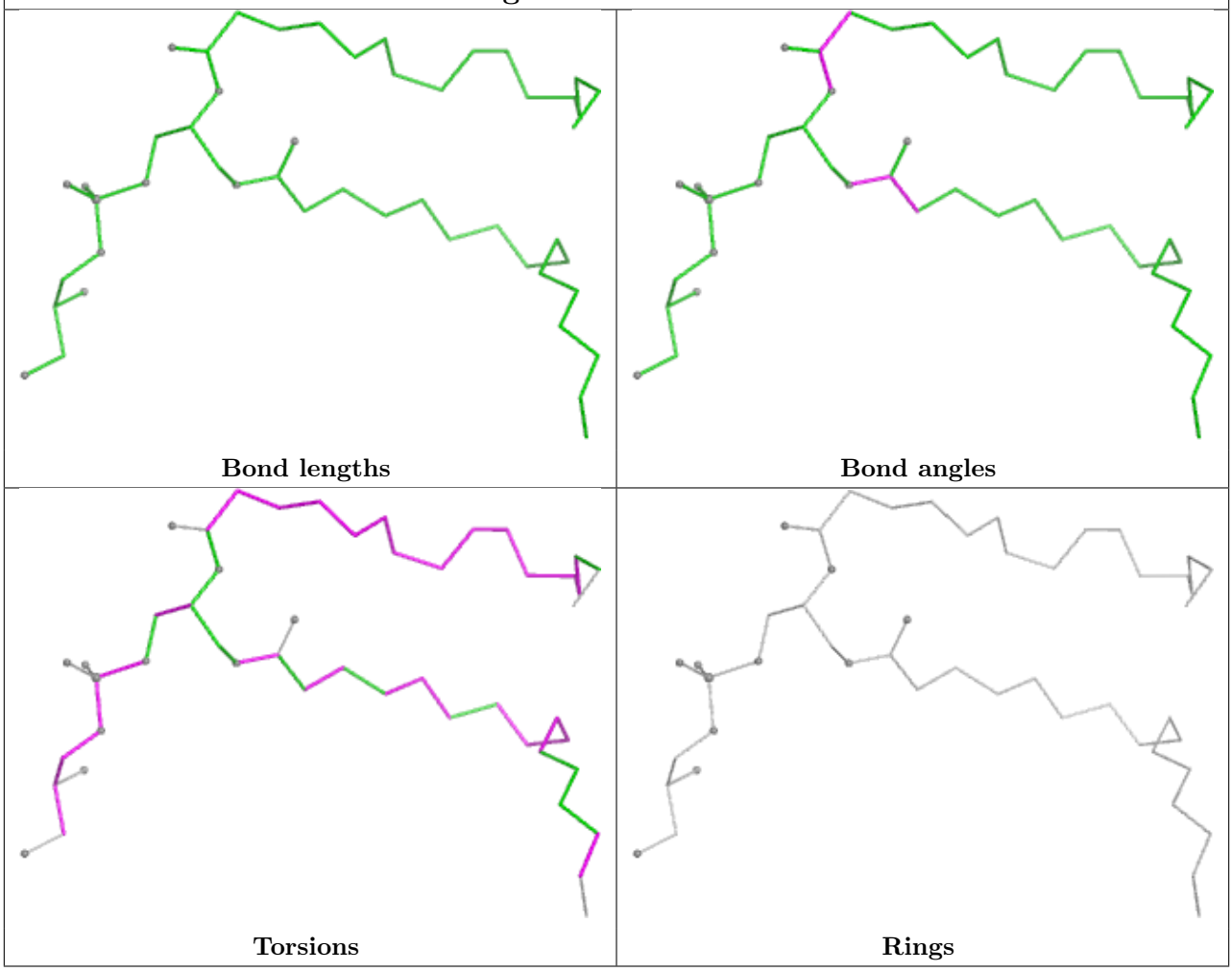
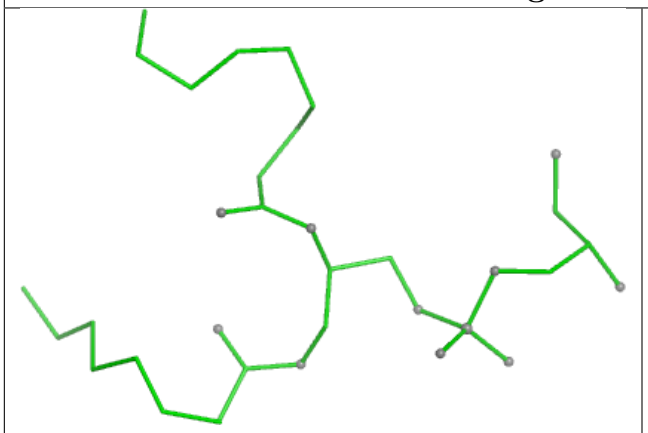


Rings

Ligand LHG B 624



Ligand LHG 5 619



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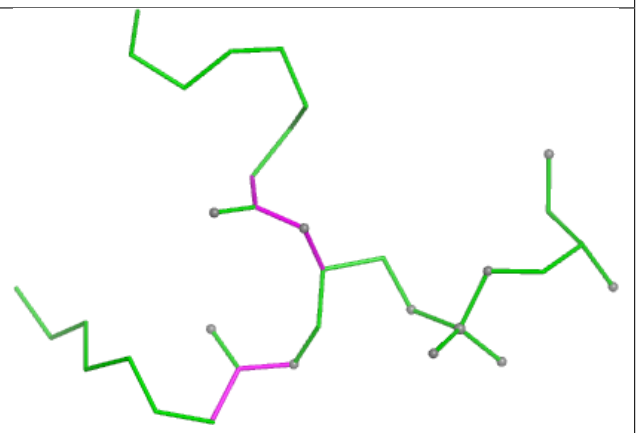
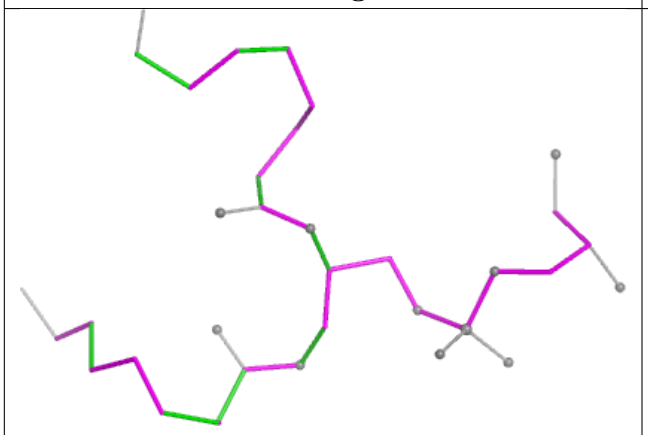


Bond angles



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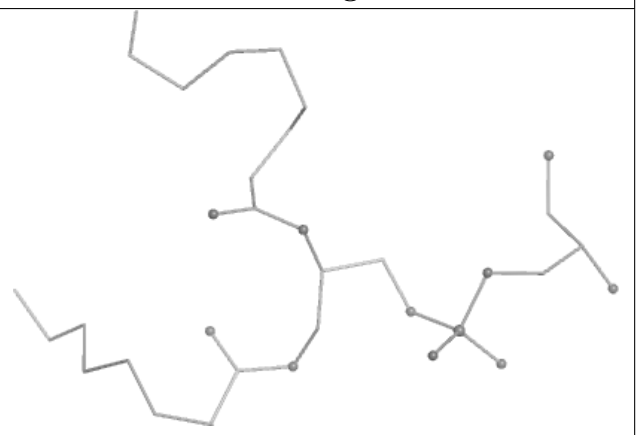
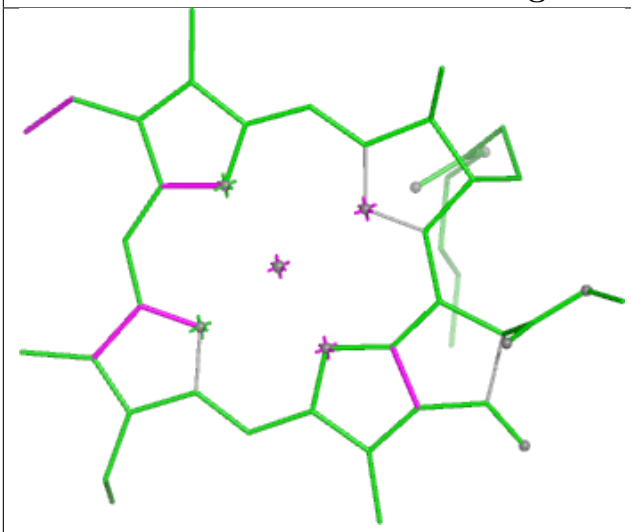


Rings

Ligand CLA 8 610



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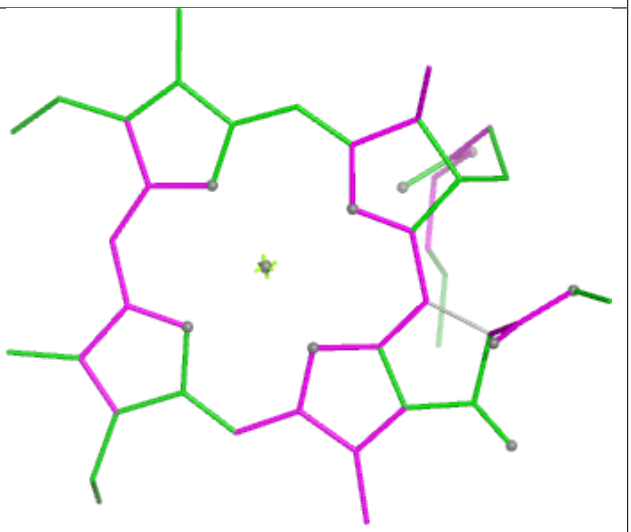
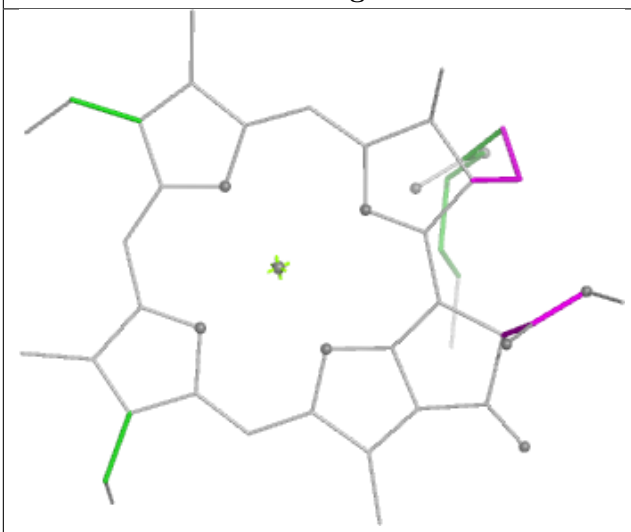


Bond angles



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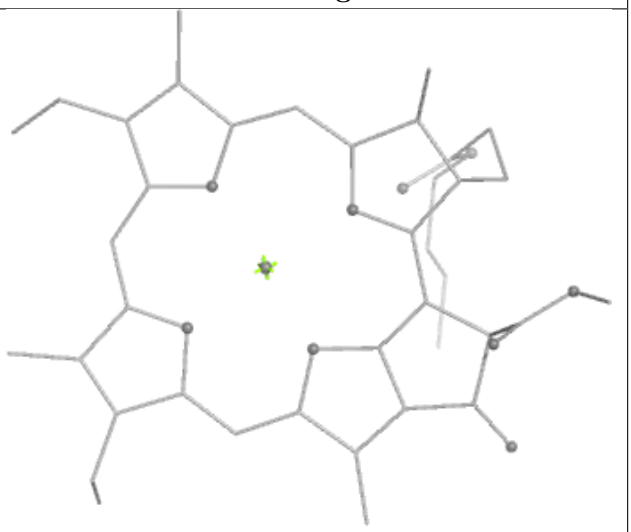
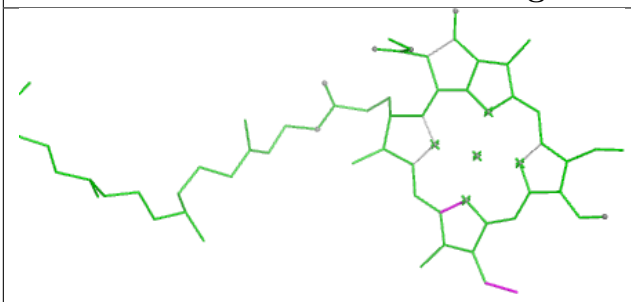
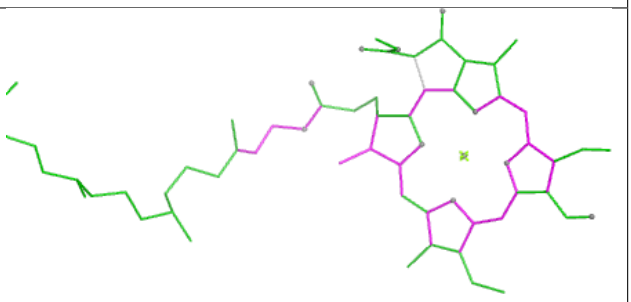
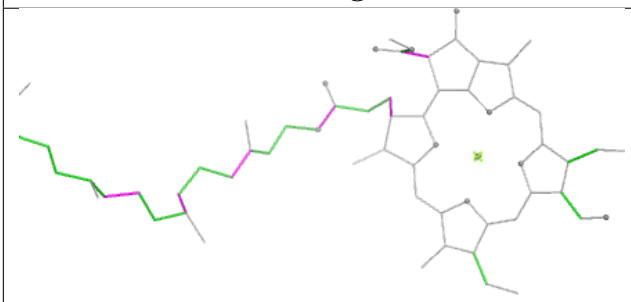
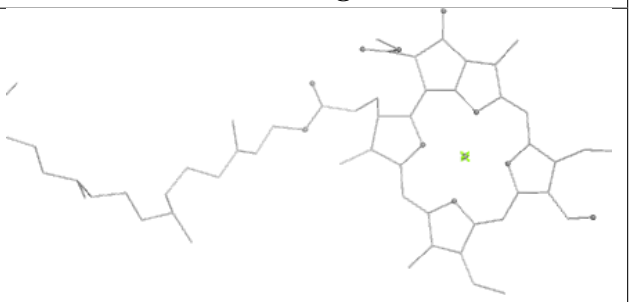
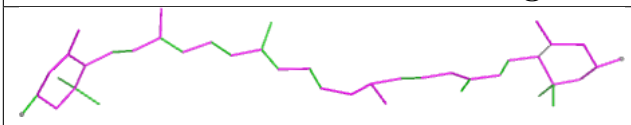
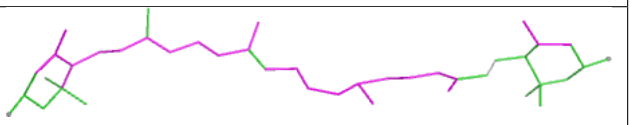
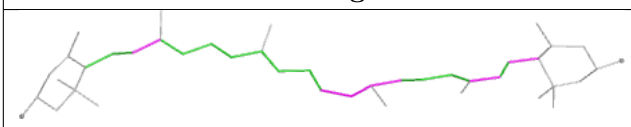
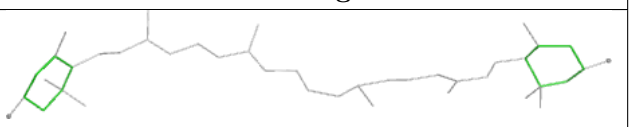
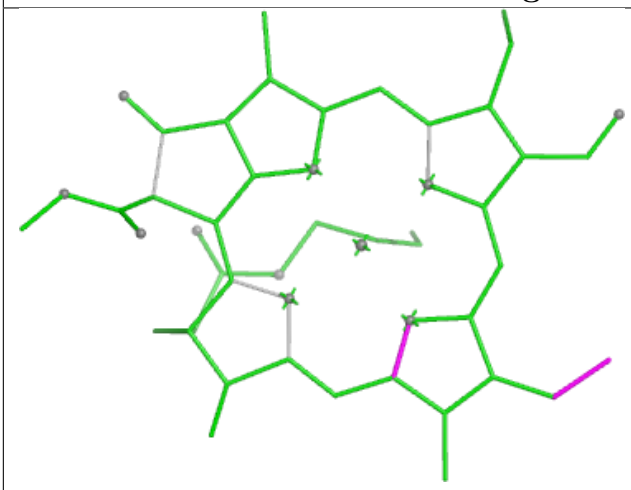


Rings

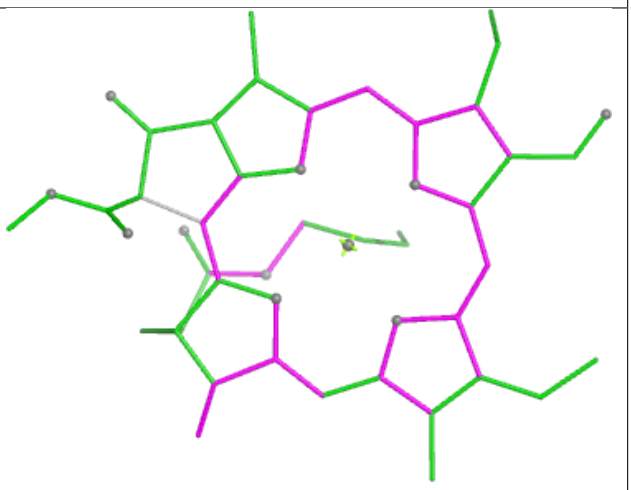
Ligand CHL 4 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT G 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

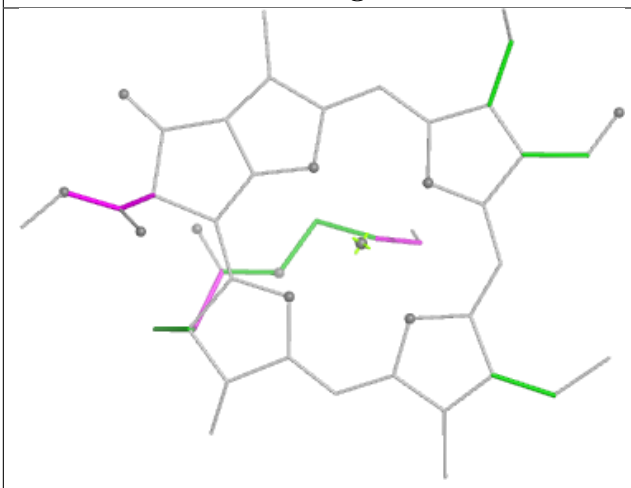
Ligand CHL N 301



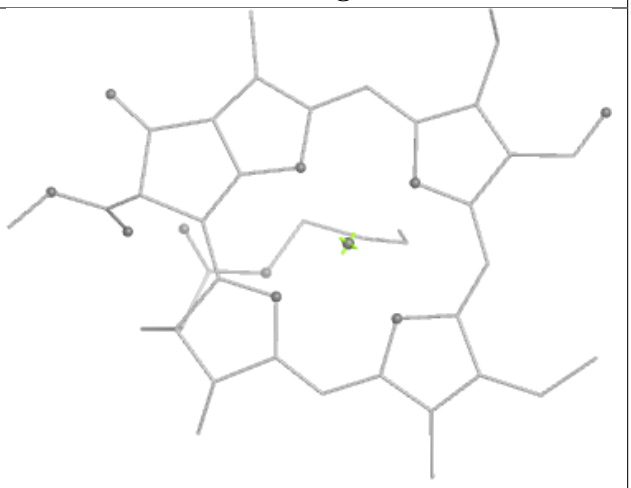
Bond lengths



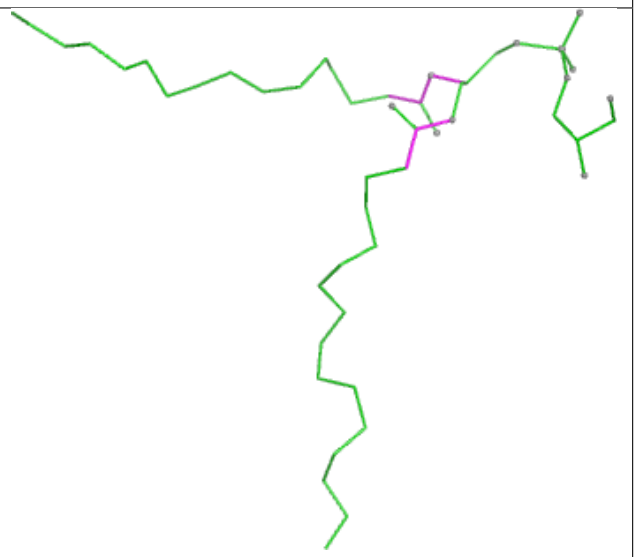
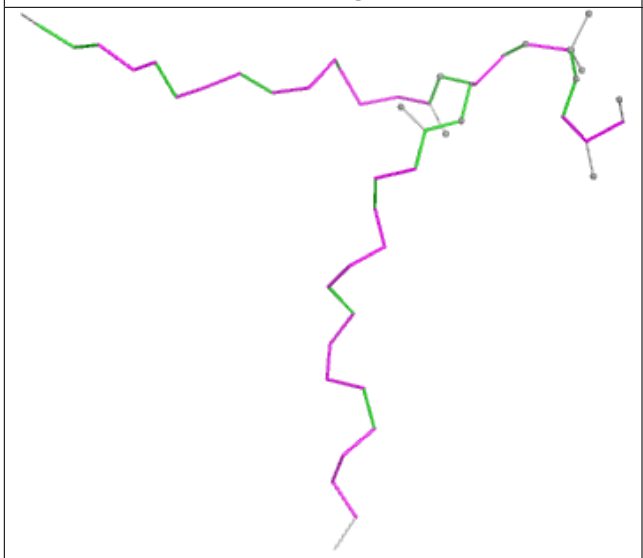
Bond angles



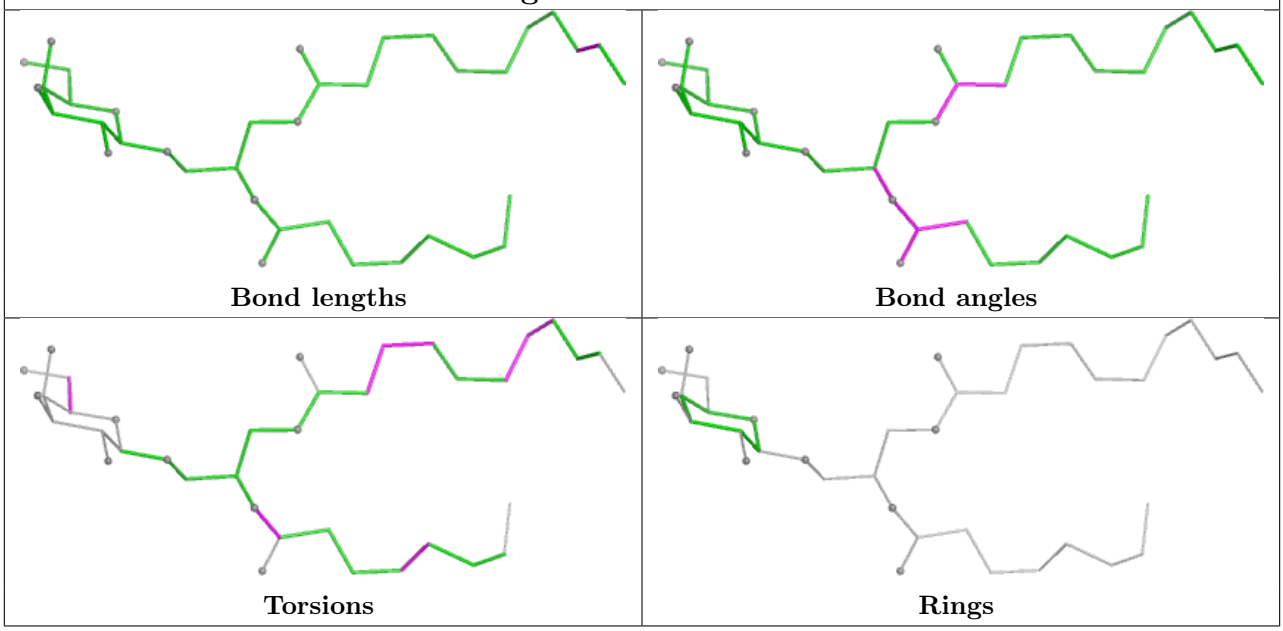
Torsions



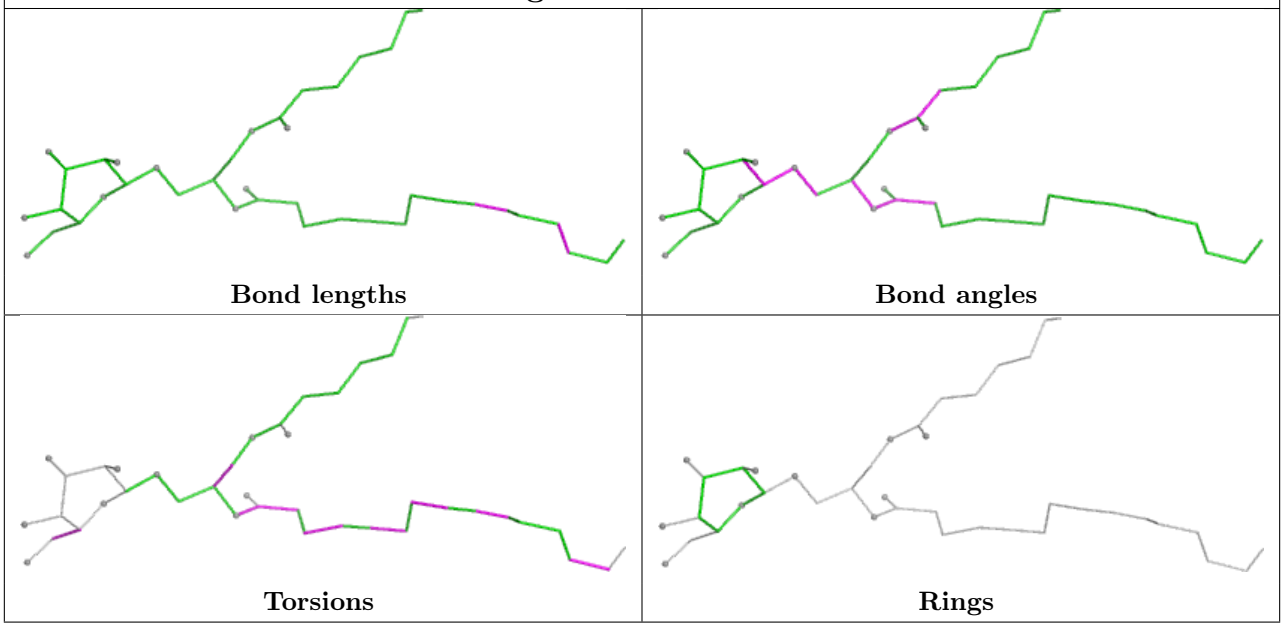
Rings

Ligand LHG L 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

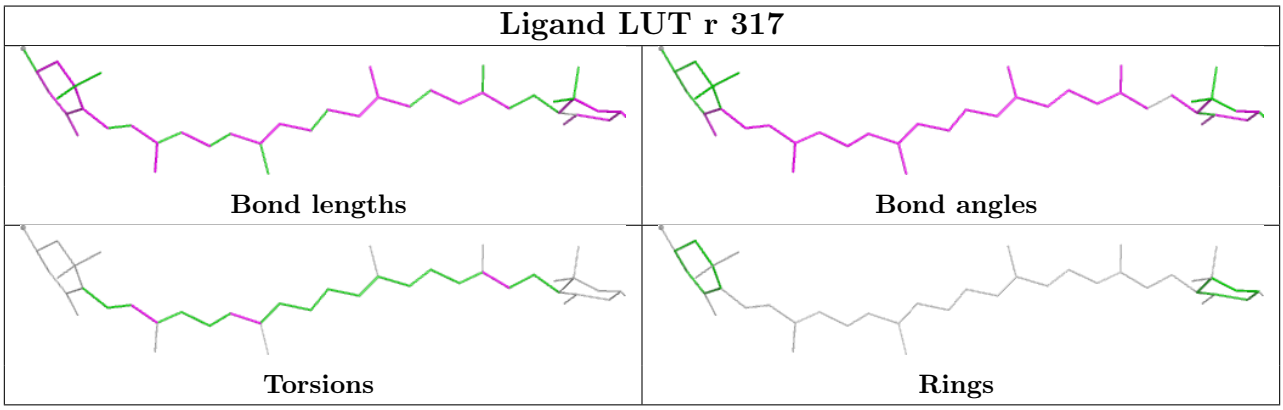
Ligand LMG B 622

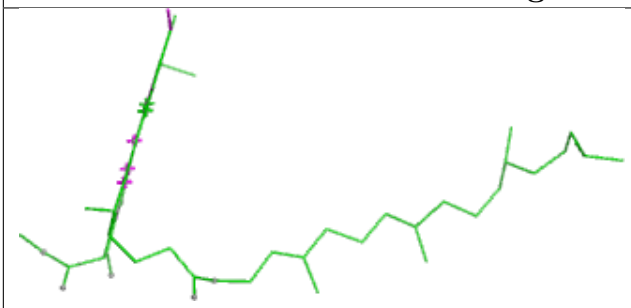
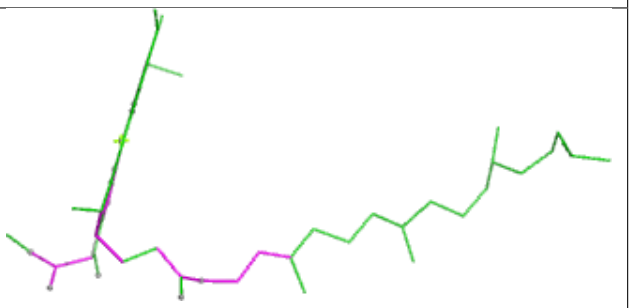
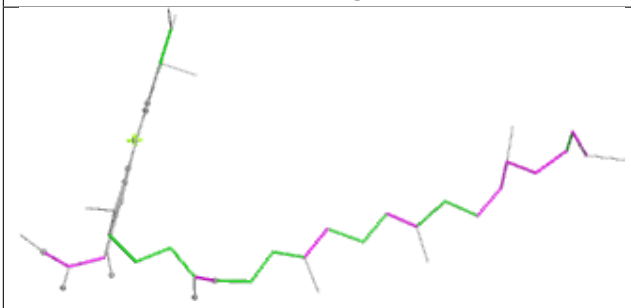
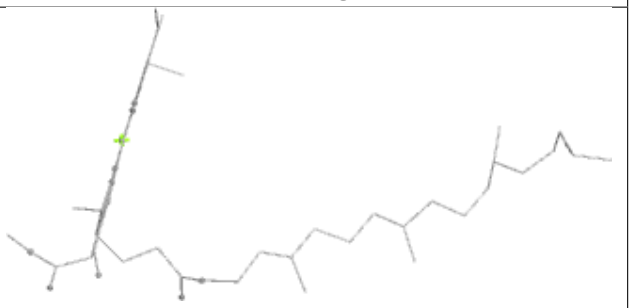


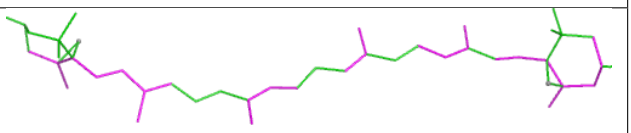
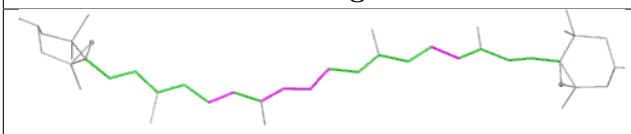
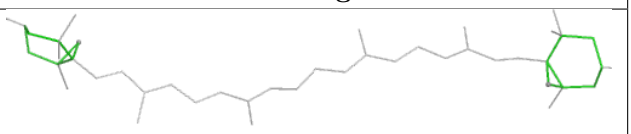
Ligand LMG s 321



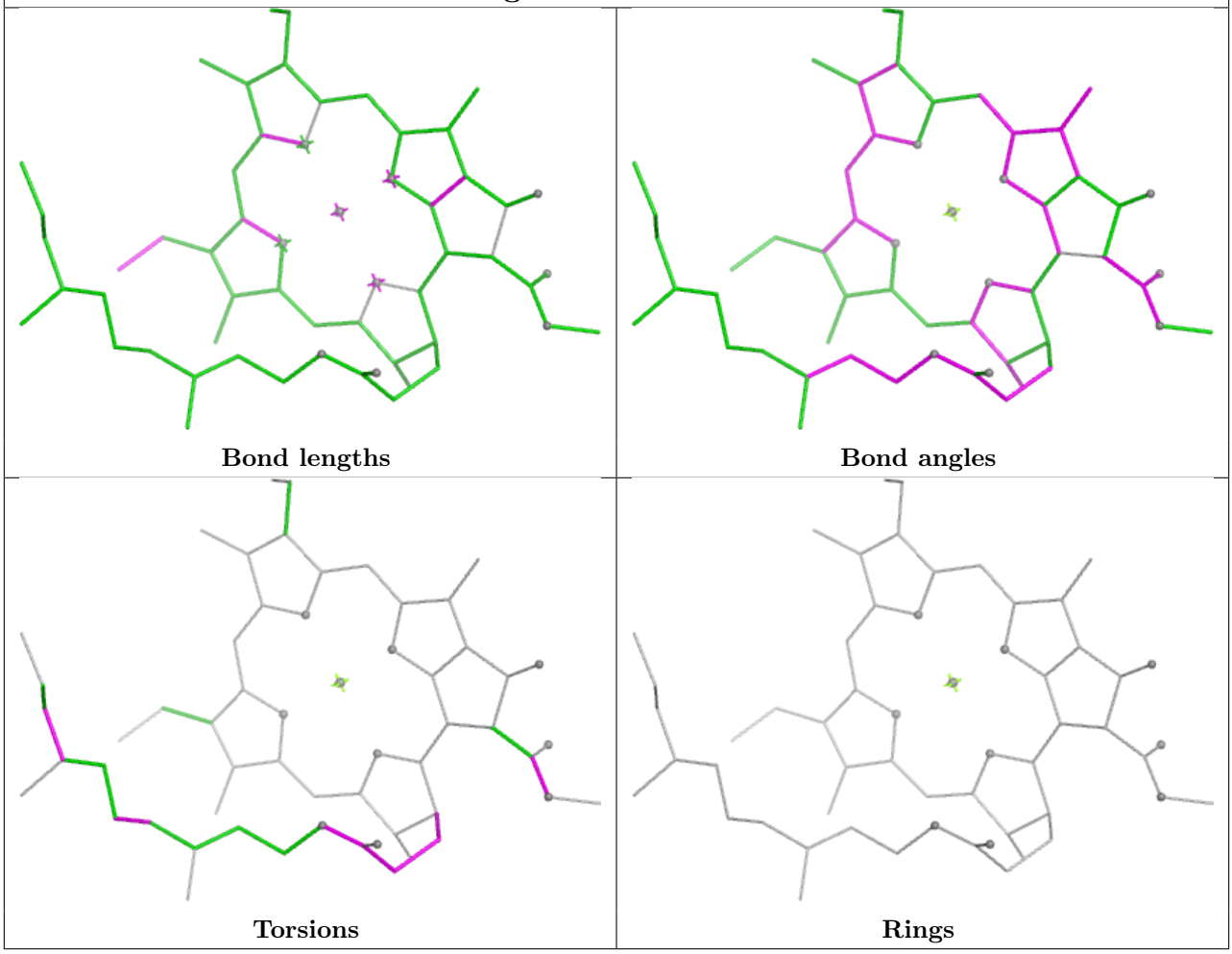
Ligand LUT r 317

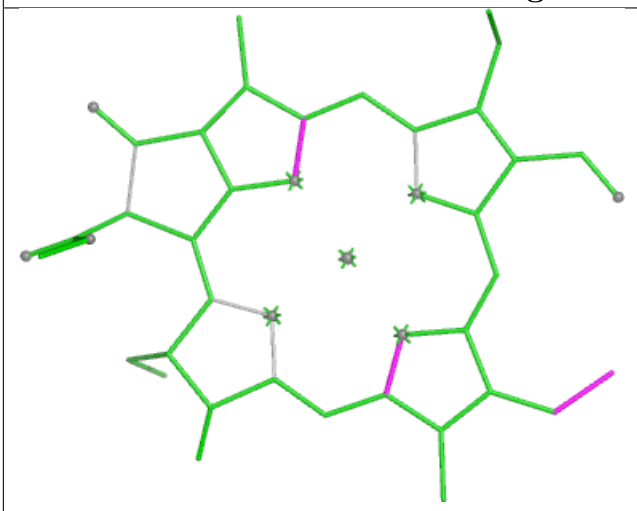
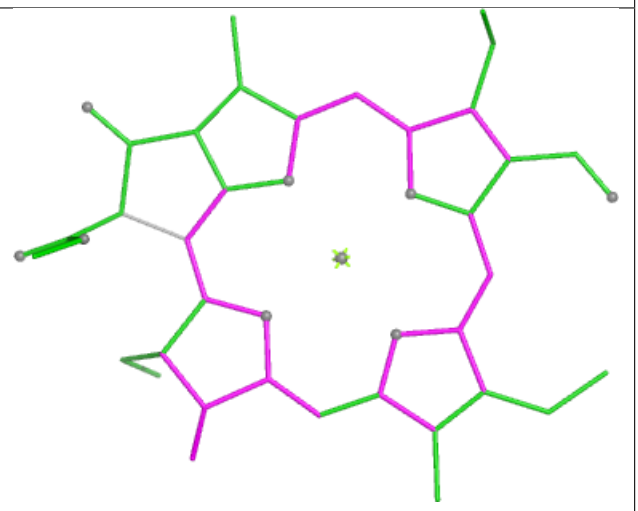
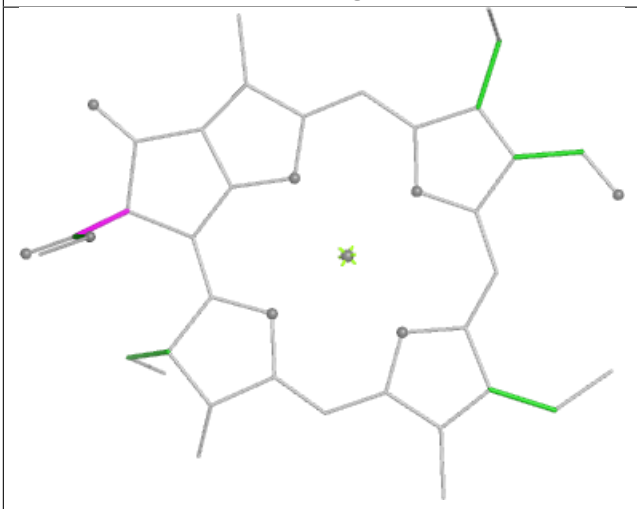
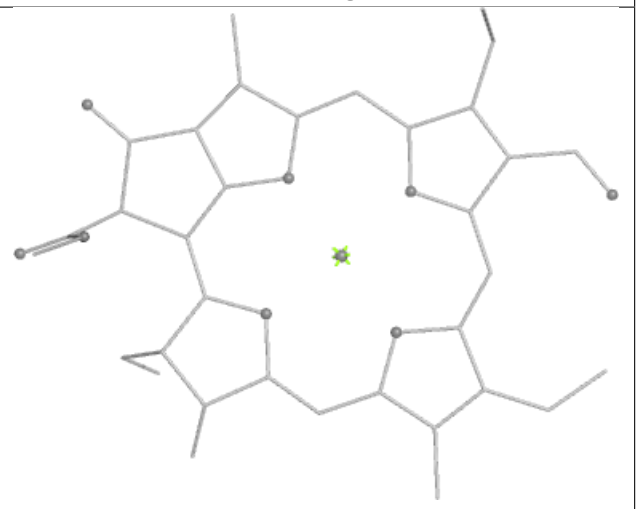


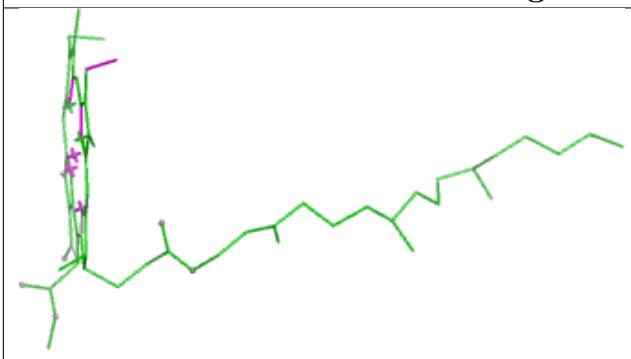
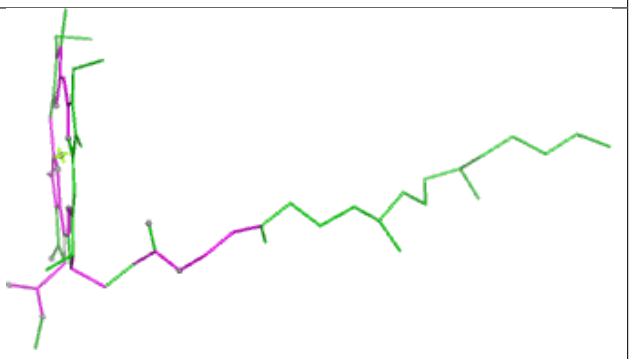
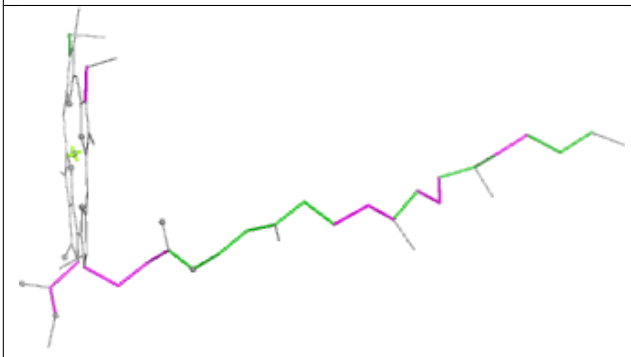
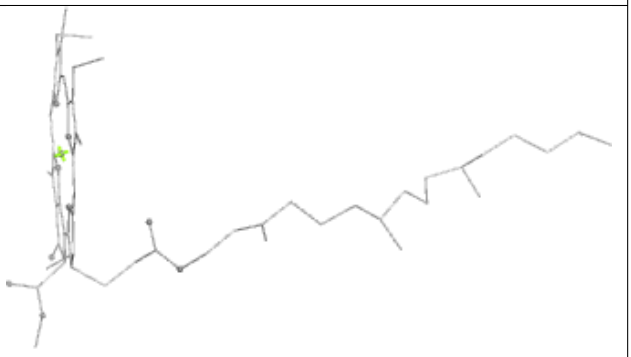
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT R 318	
Bond lengths	 Bond angles
 Torsions	 Rings

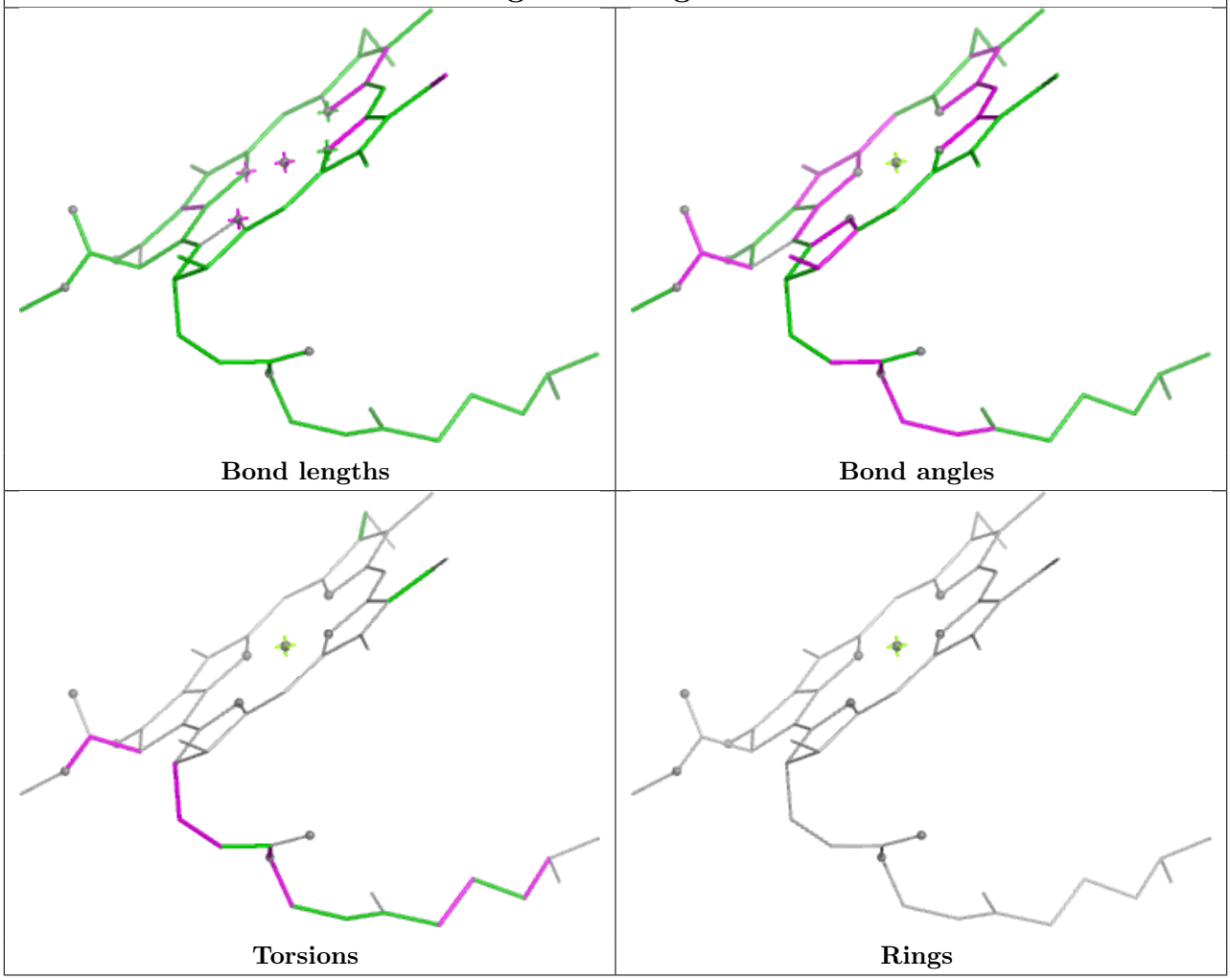
Ligand CLA R 312

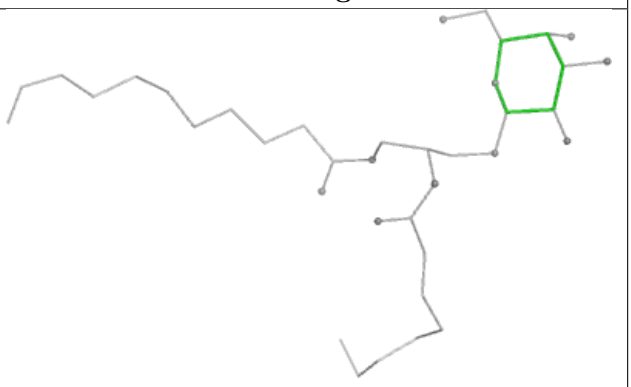


Ligand CHL S 308	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

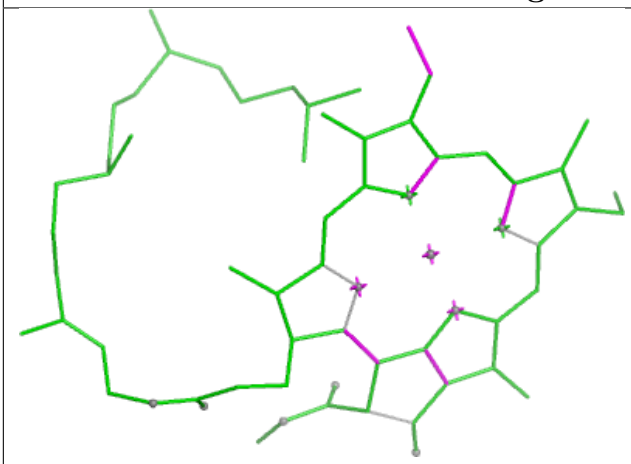
Ligand CLA b 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 305

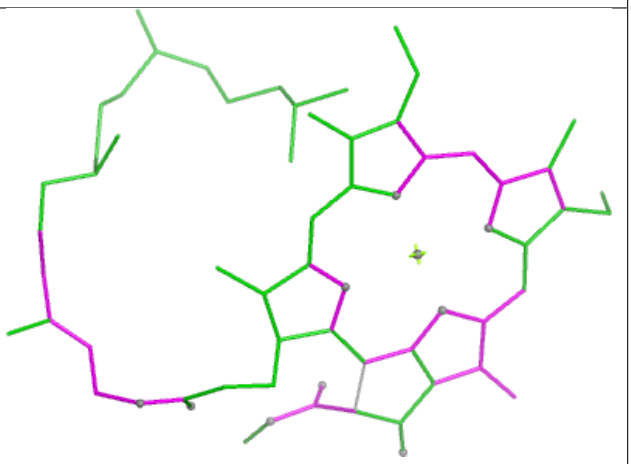


Ligand LMG f 101	
Bond lengths	Bond angles
Torsions	 Rings

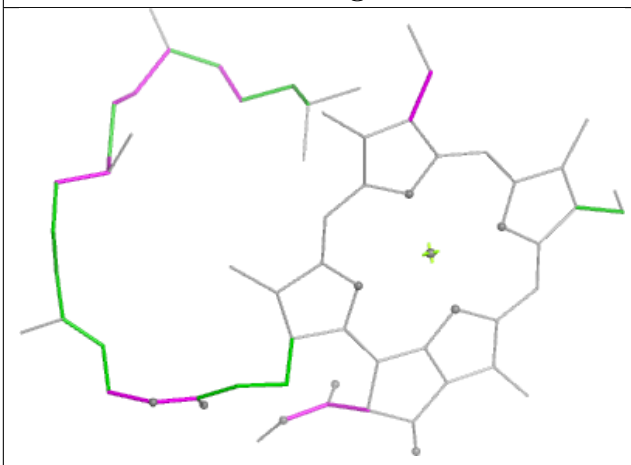
Ligand CLA b 616



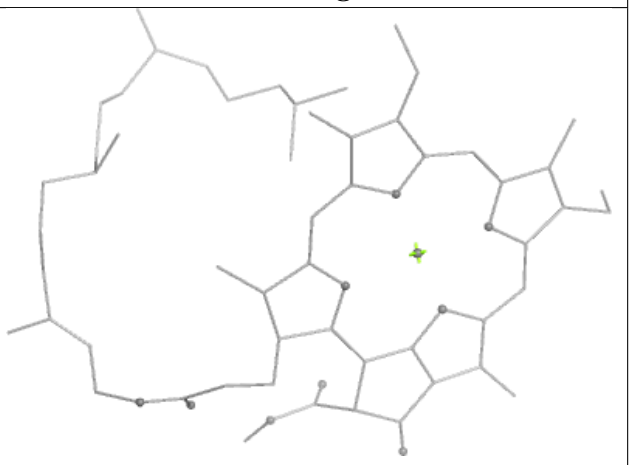
Bond lengths



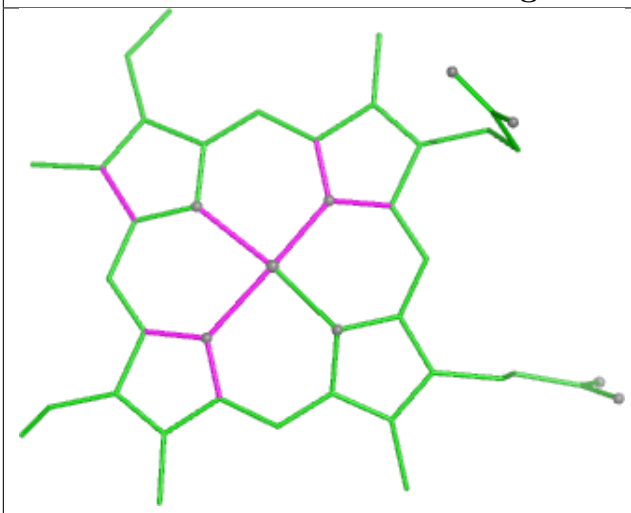
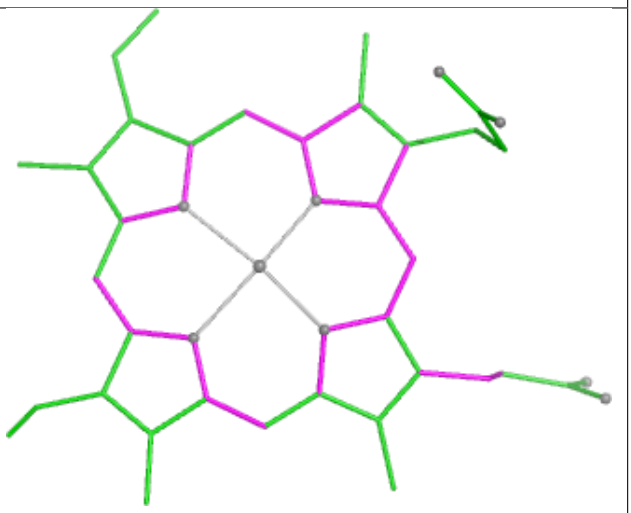
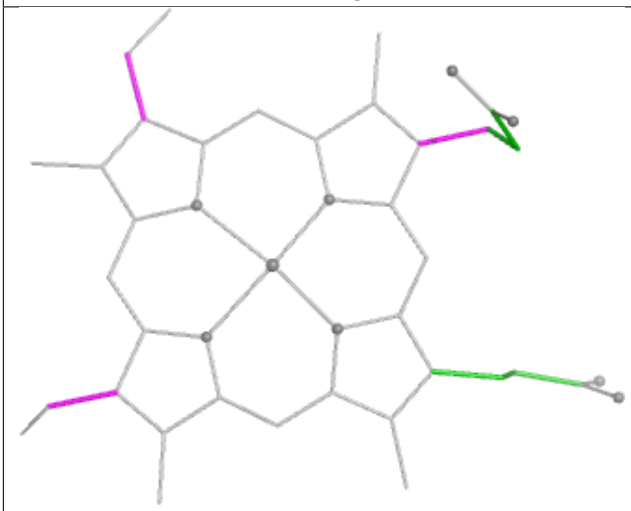
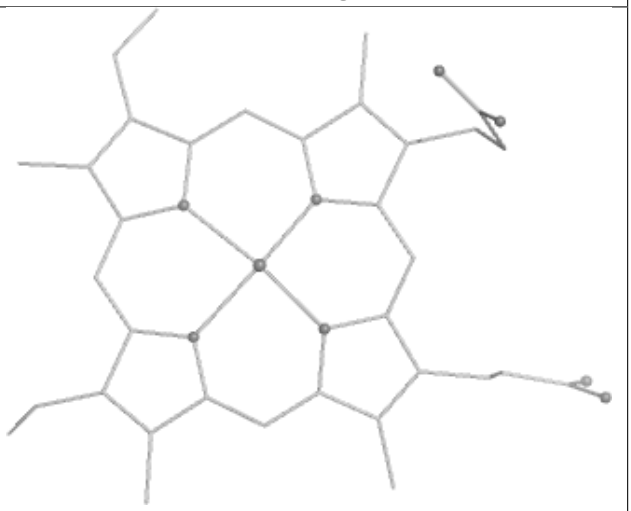
Bond angles



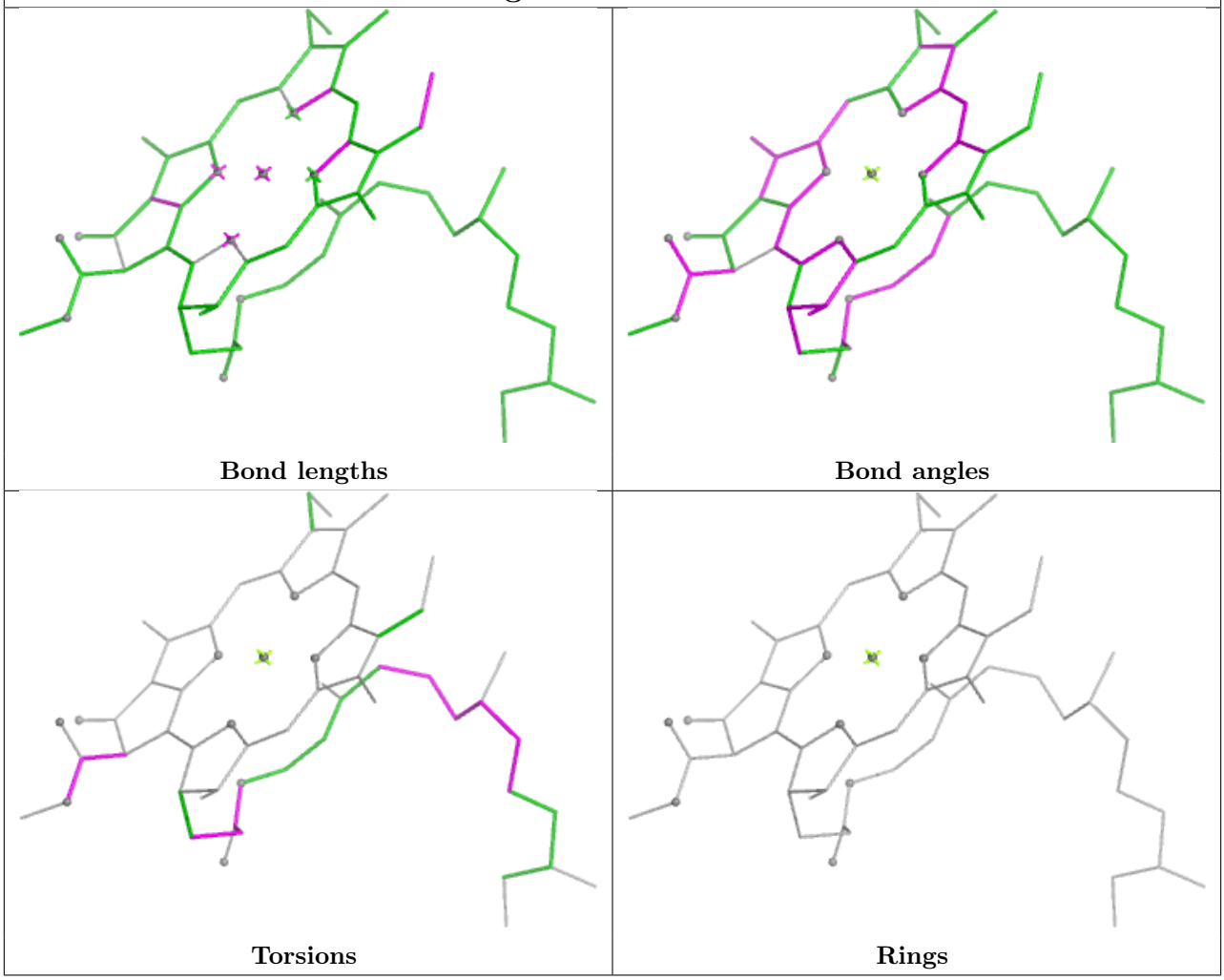
Torsions



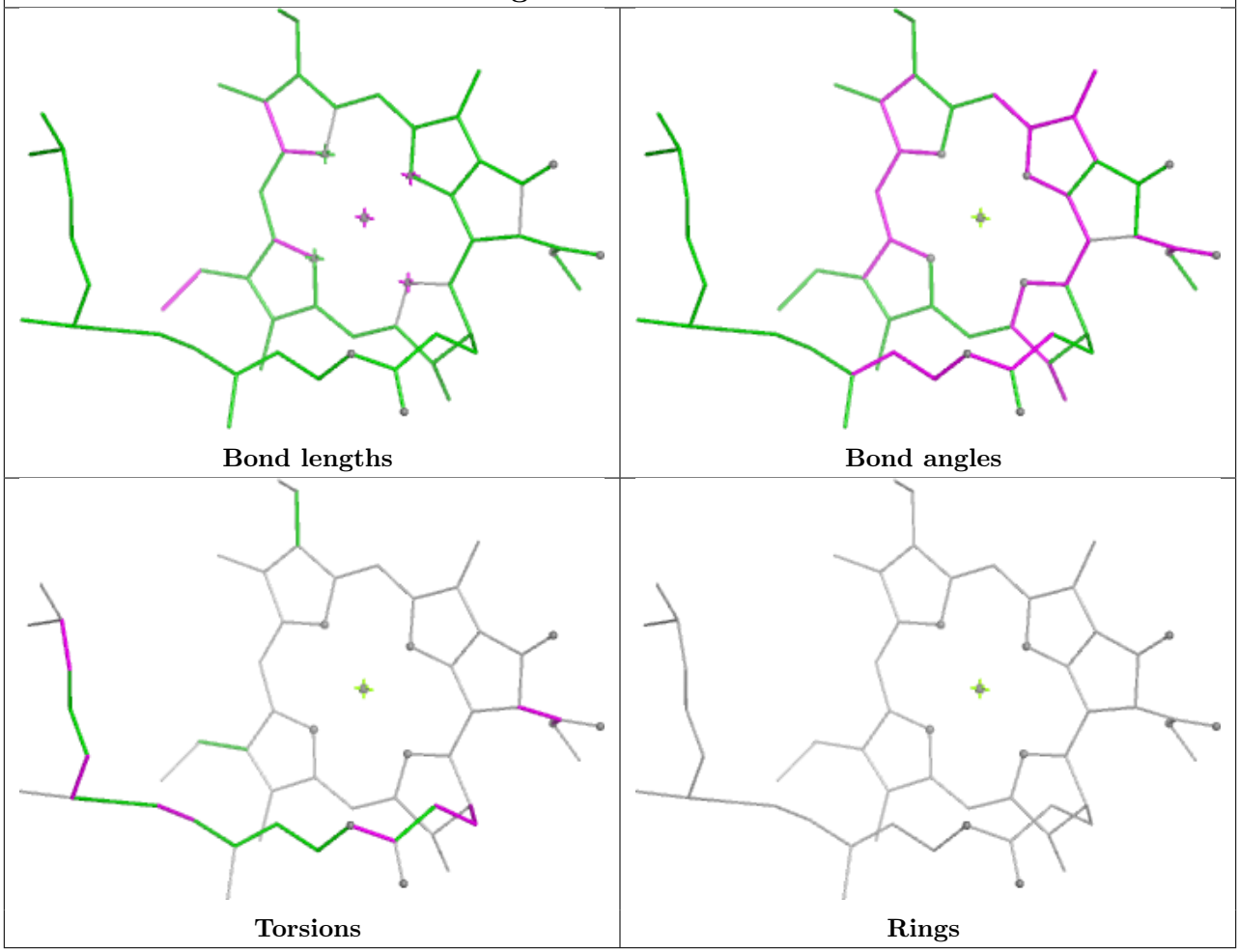
Rings

Ligand HEM E 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

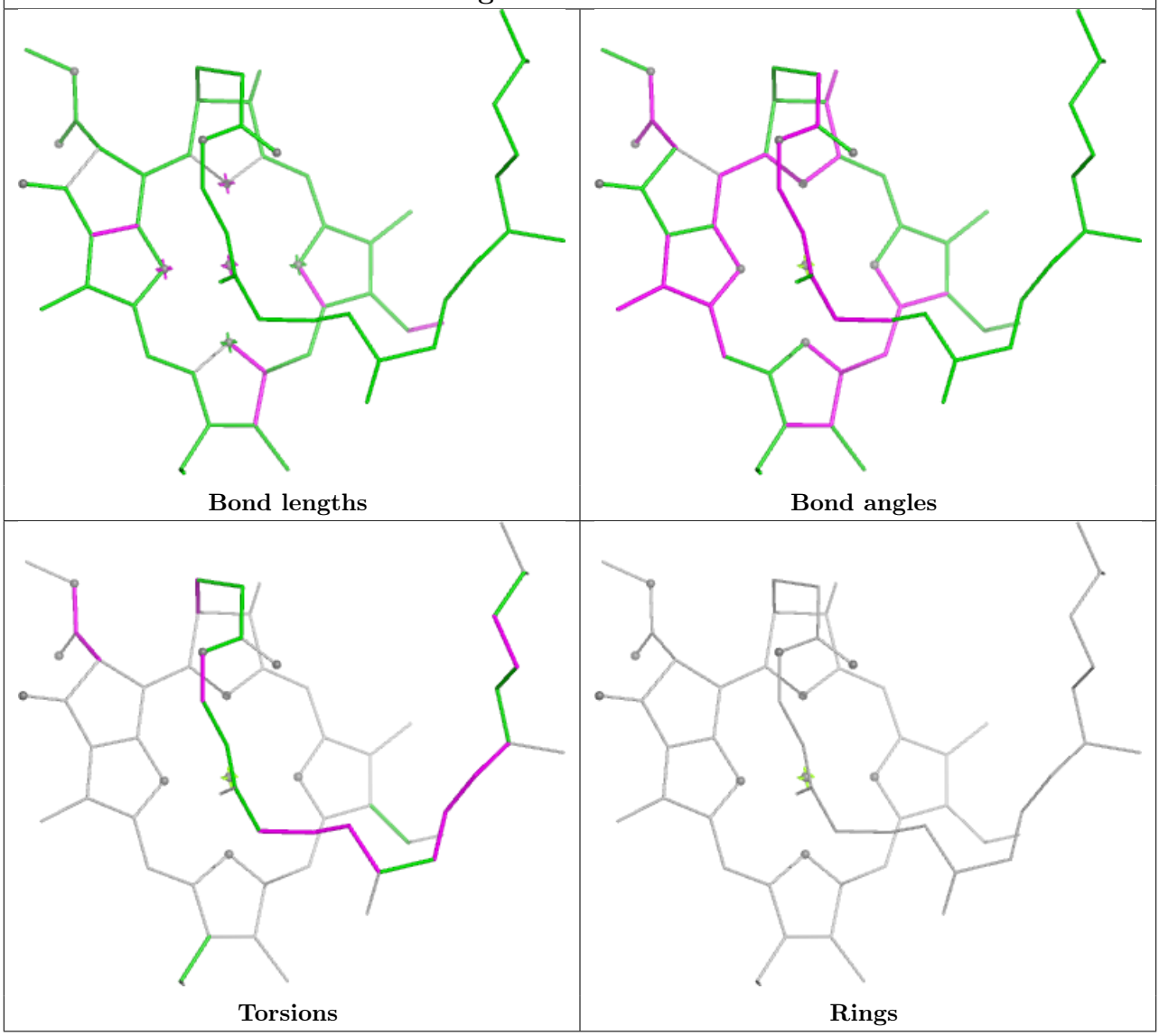
Ligand CLA 4 613



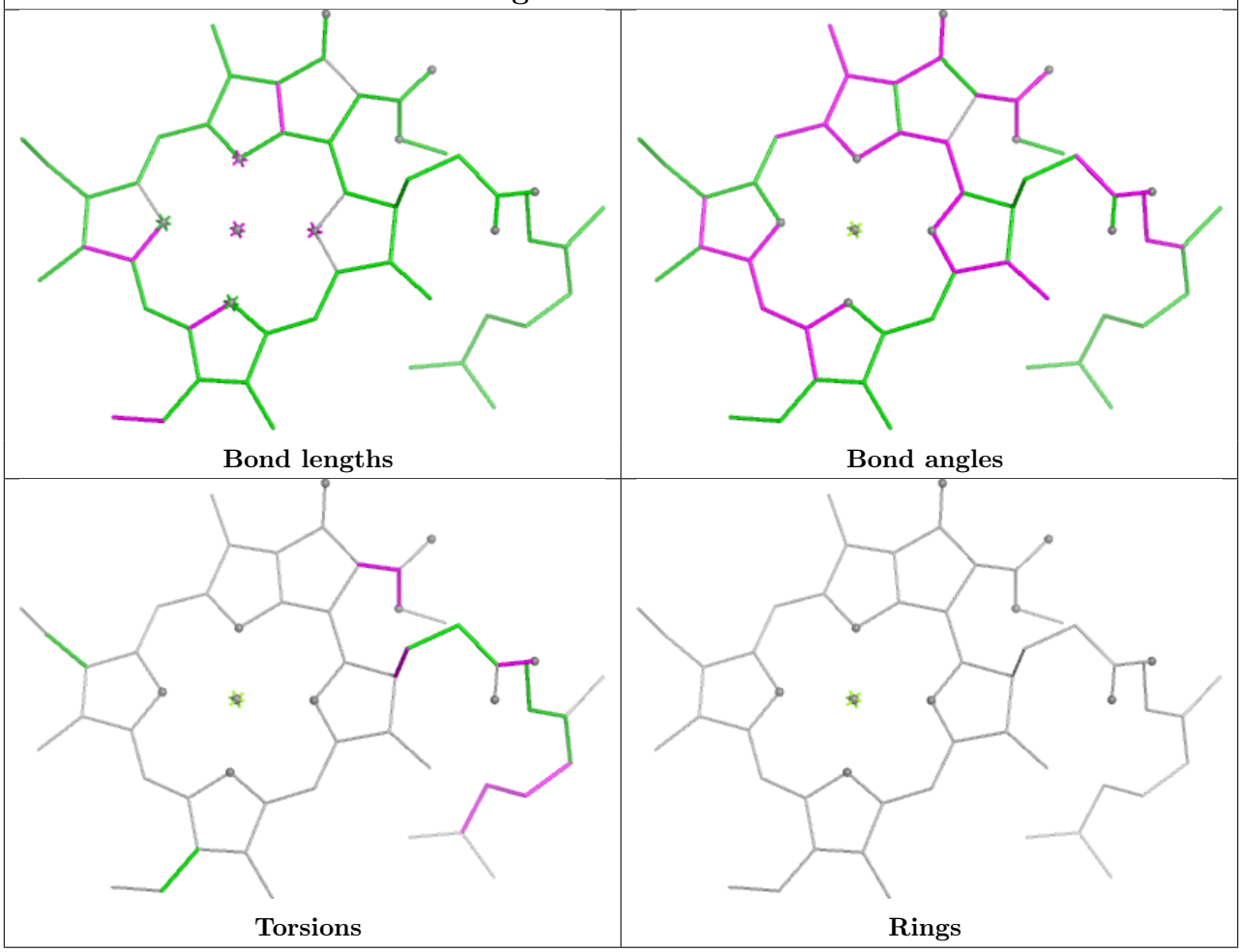
Ligand CLA 7 303



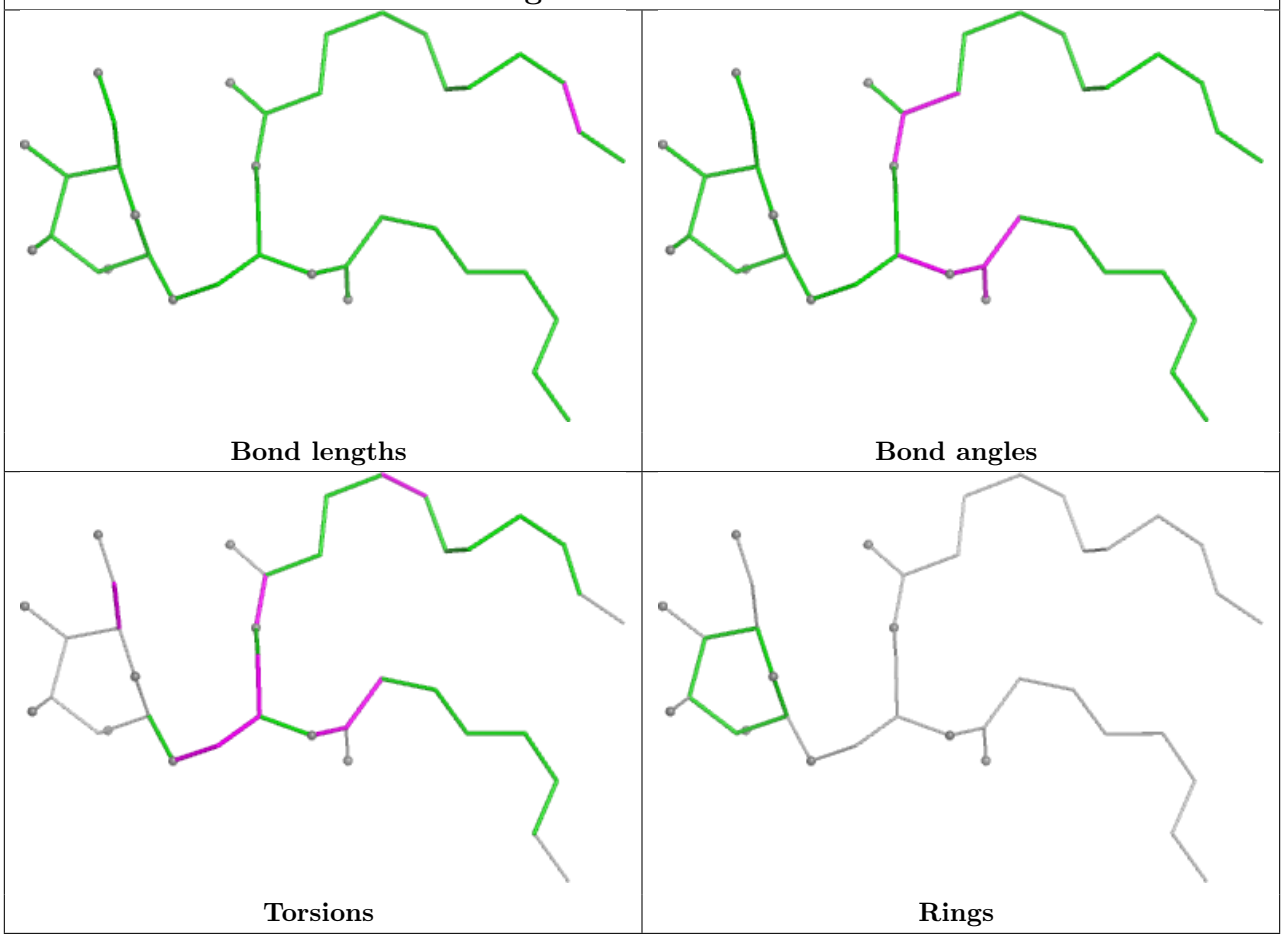
Ligand CLA 8 612



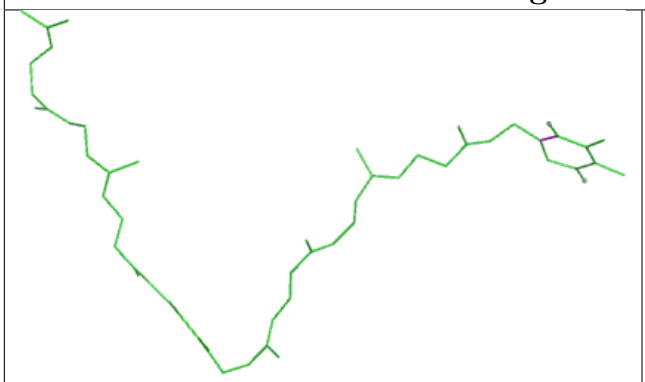
Ligand CLA 9 305



Ligand LMG 7 322



Ligand PL9 D 406



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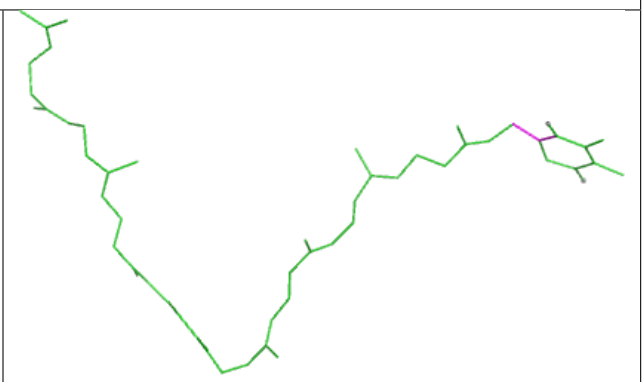
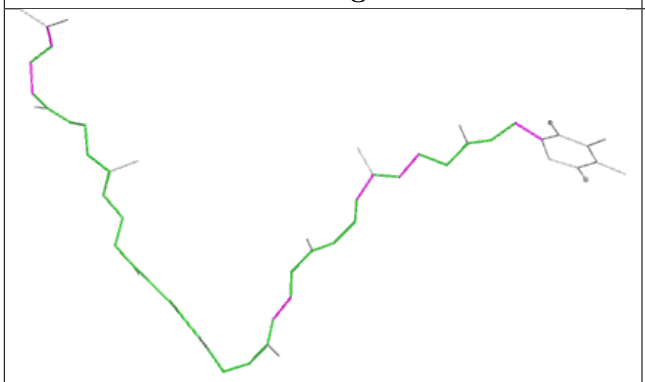


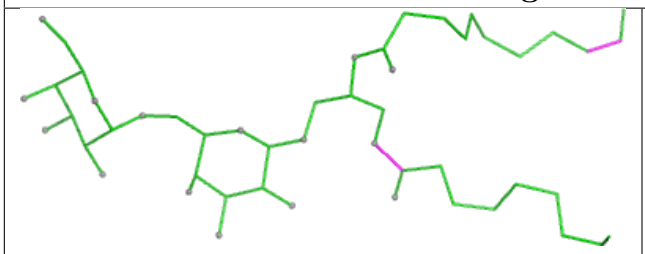
Bond angles



Torsions

Rings

Ligand DGD C 616



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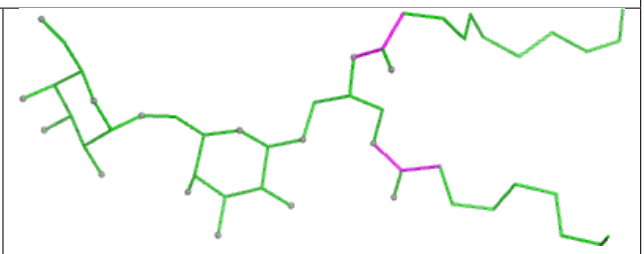
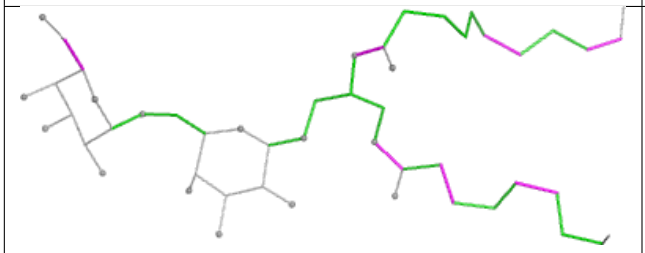


Bond angles



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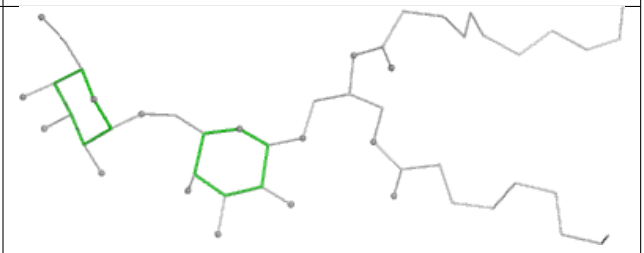
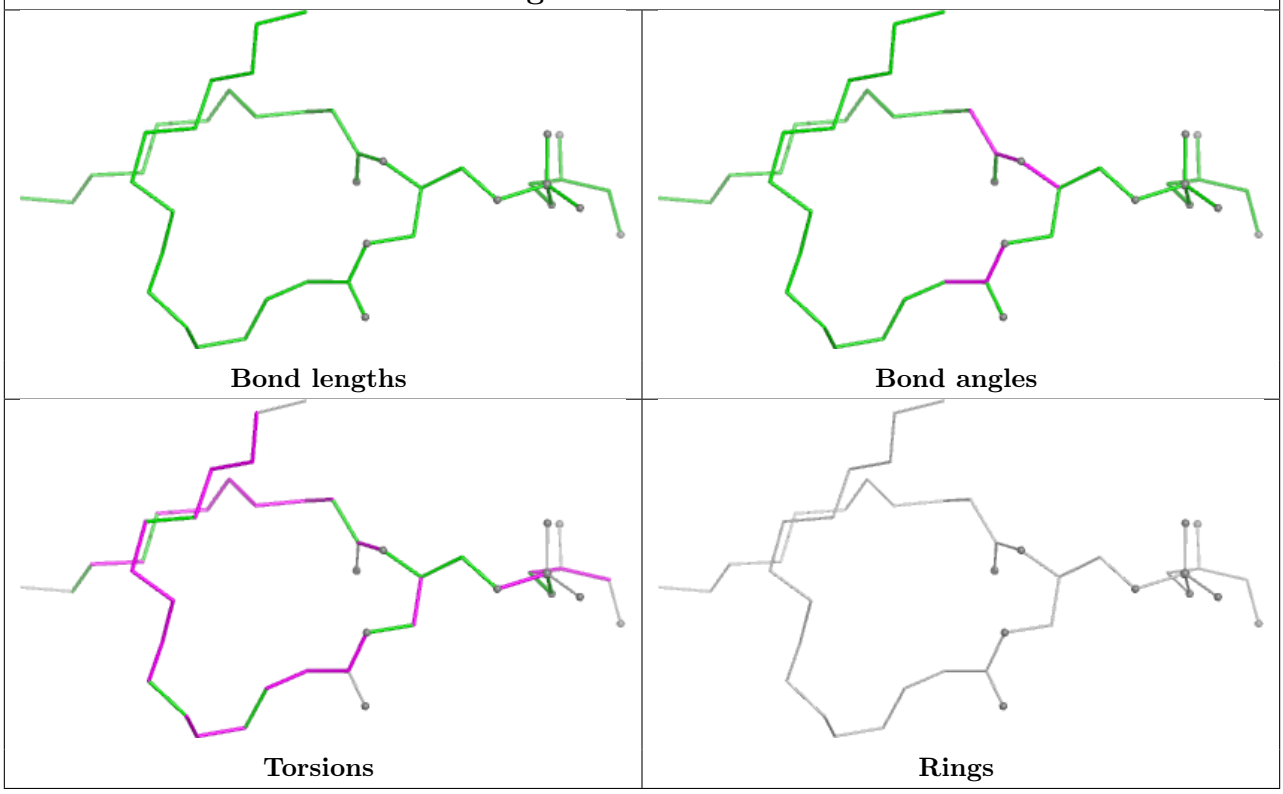
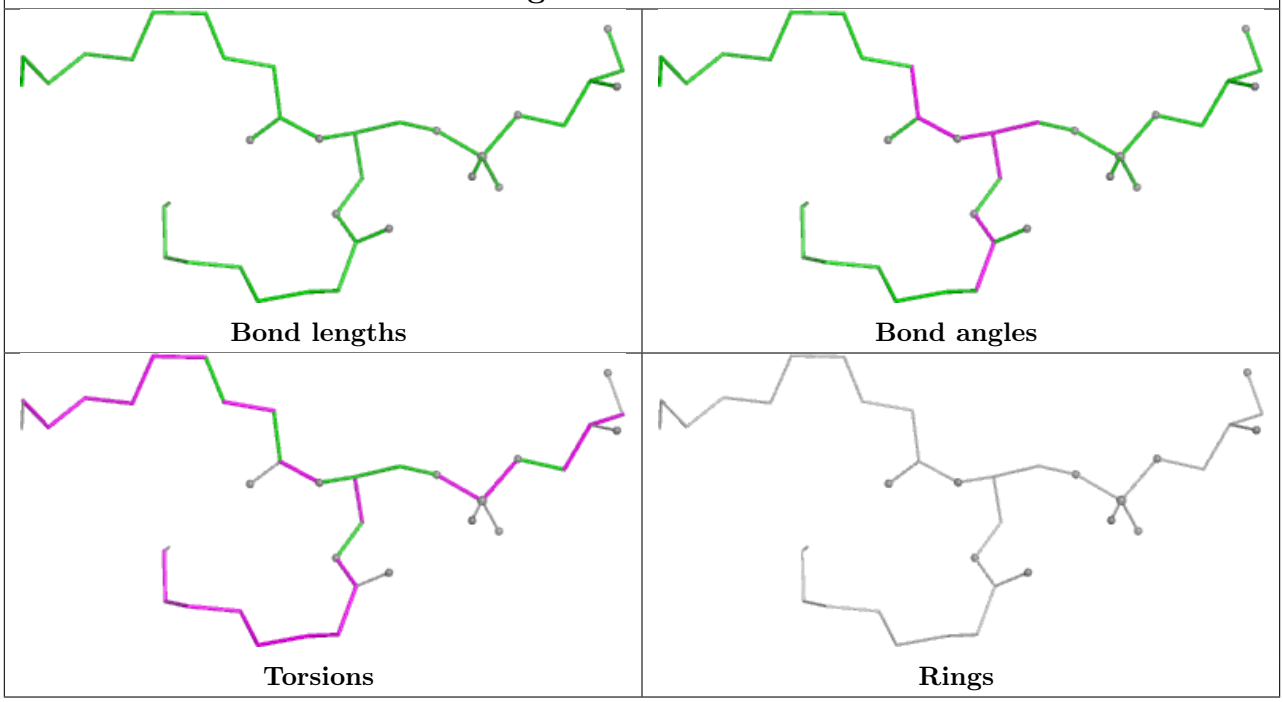


Rings

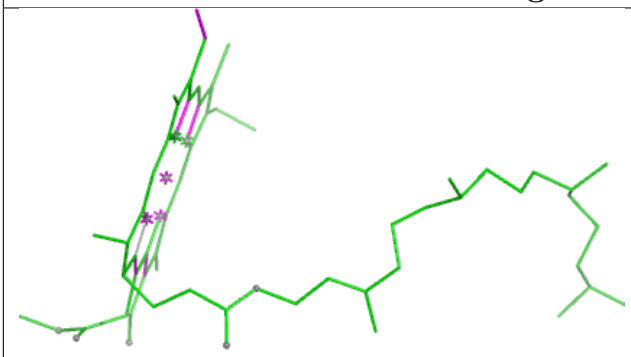
Ligand LHG b 625



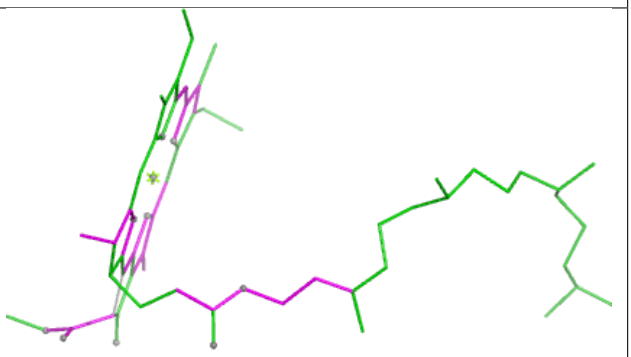
Ligand LHG 0 619



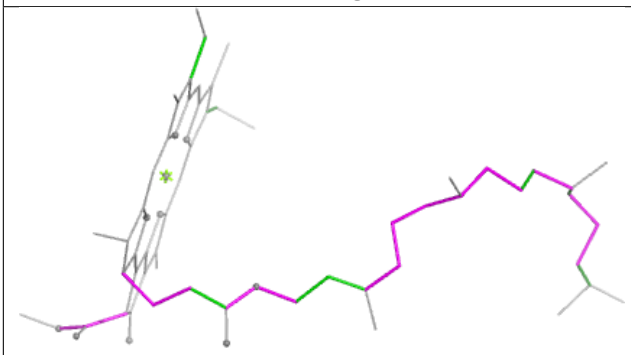
Ligand CLA b 608



Bond lengths



Bond angles



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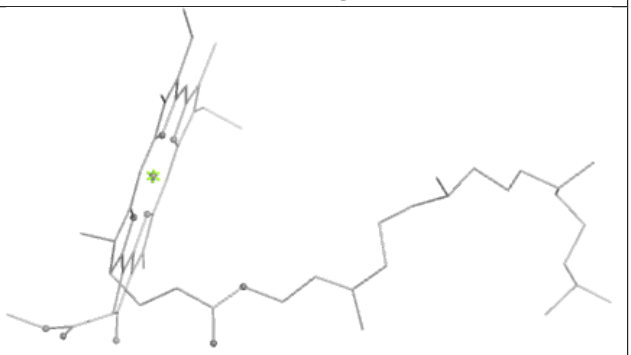
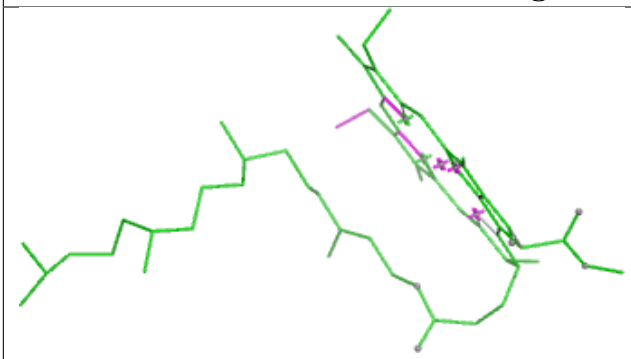


Rings

Ligand CLA r 316



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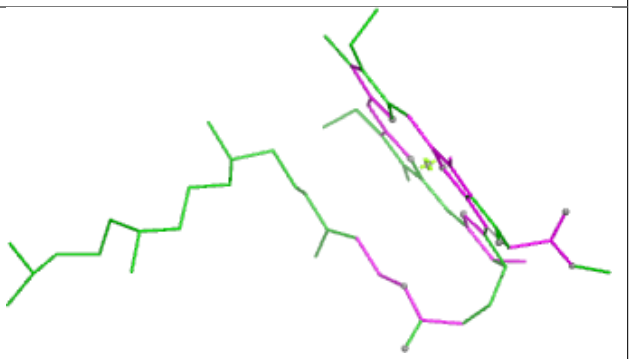
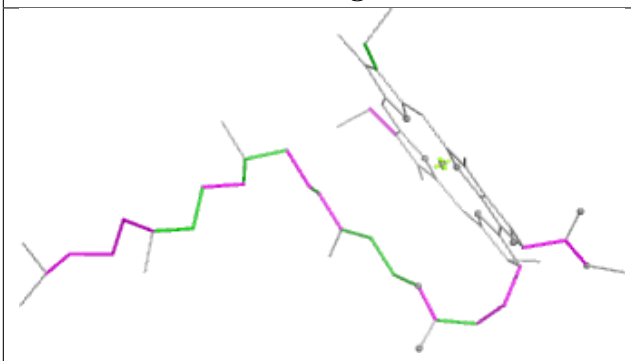


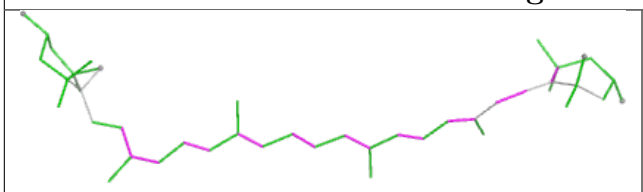
Bond angles



Torsions

Rings

Ligand NEX S 319



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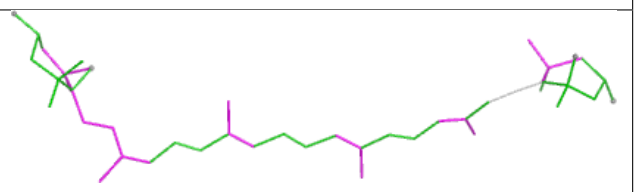
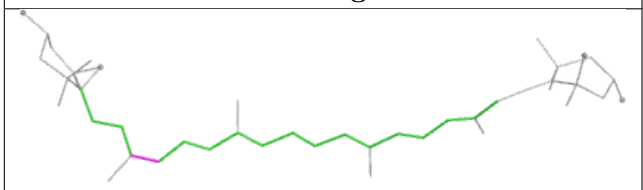


Bond angles



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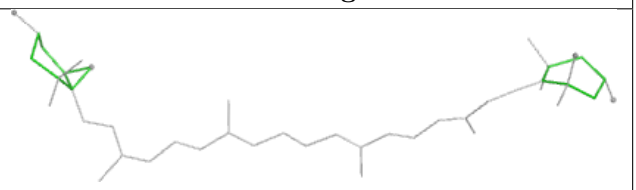
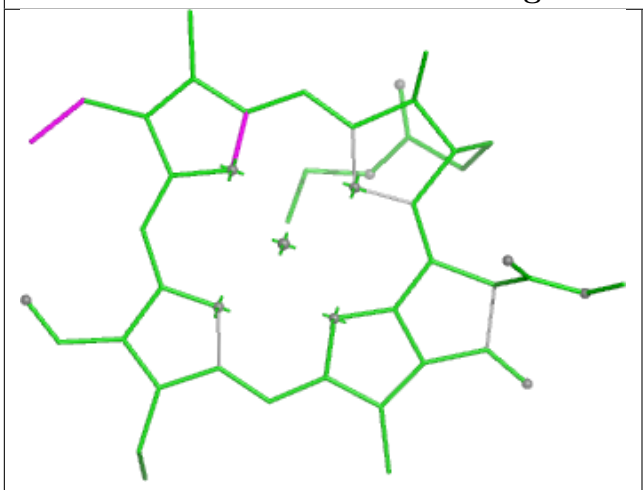


Rings

Ligand CHL G 605



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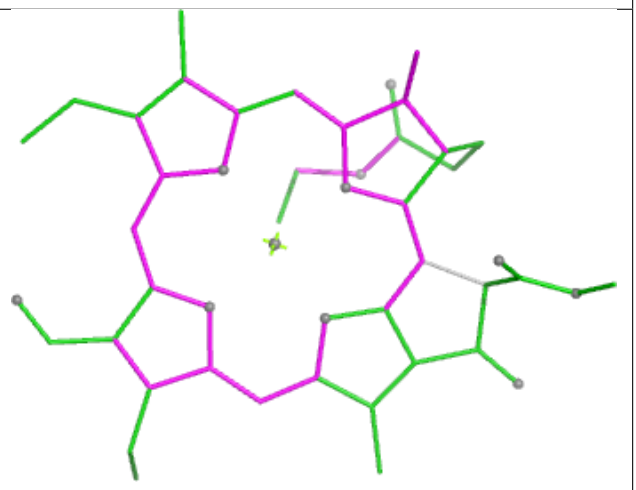
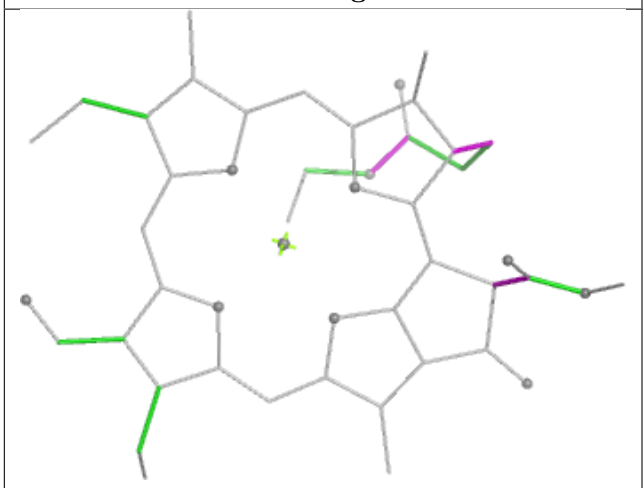


Bond angles



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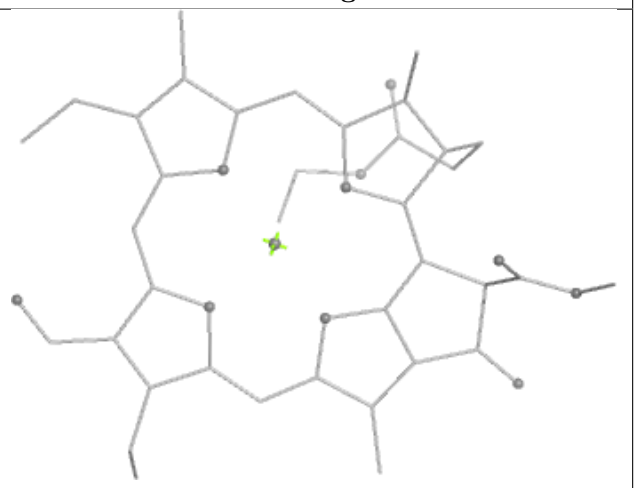
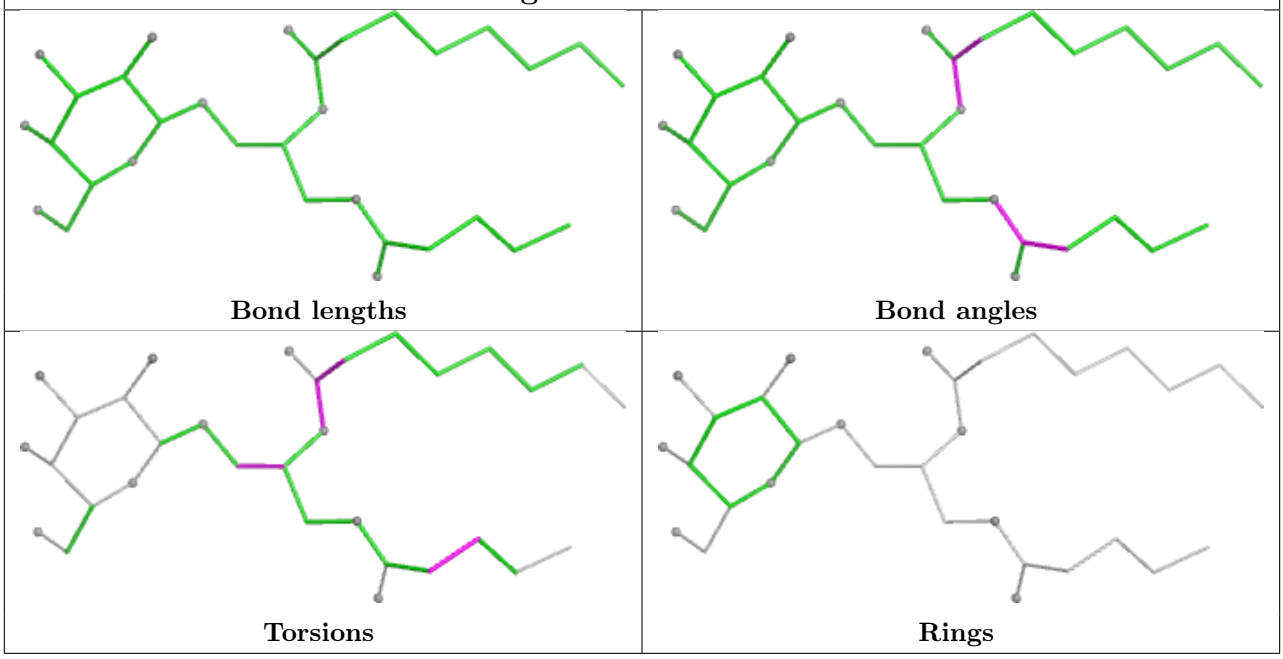
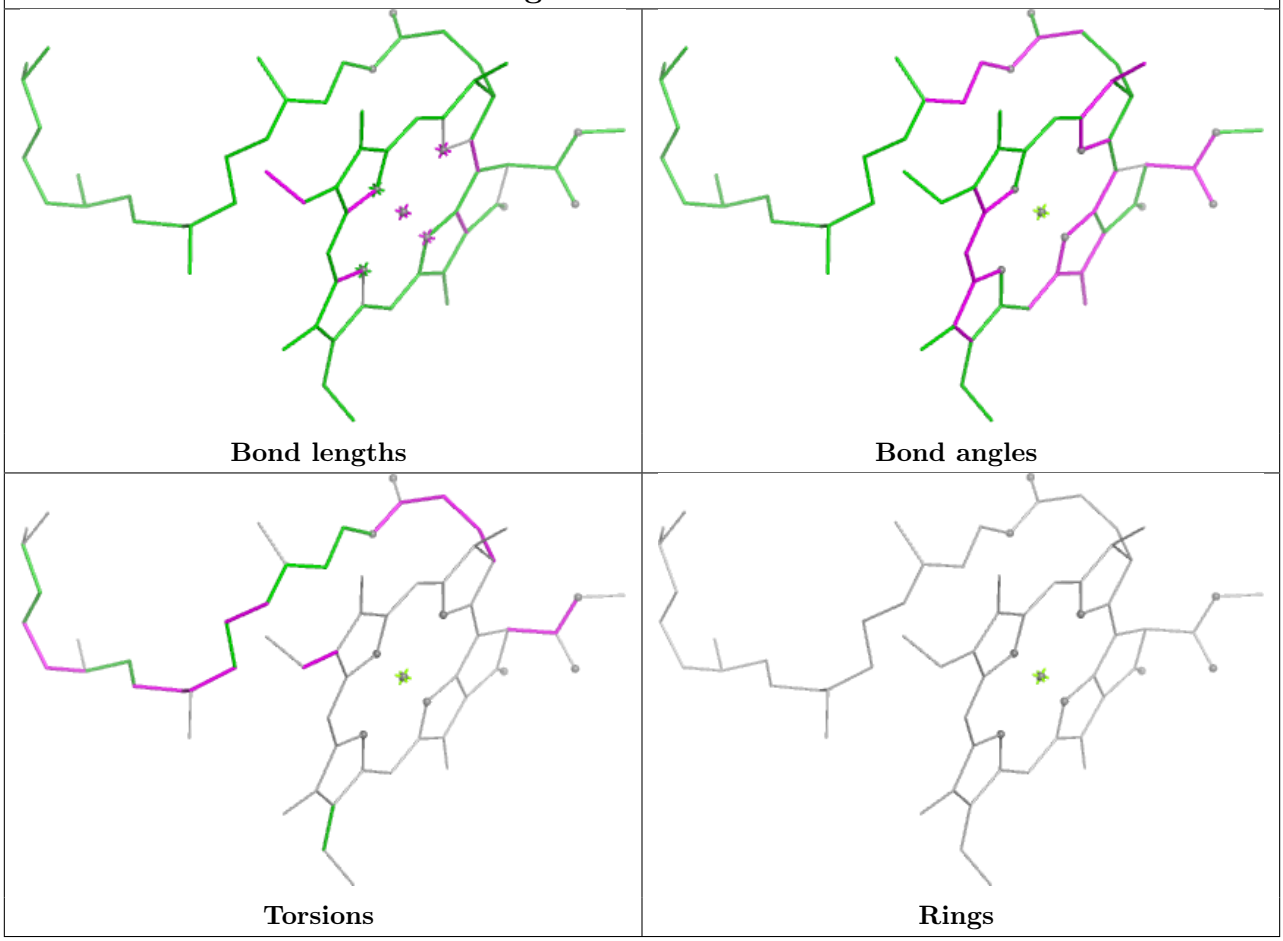


Rings

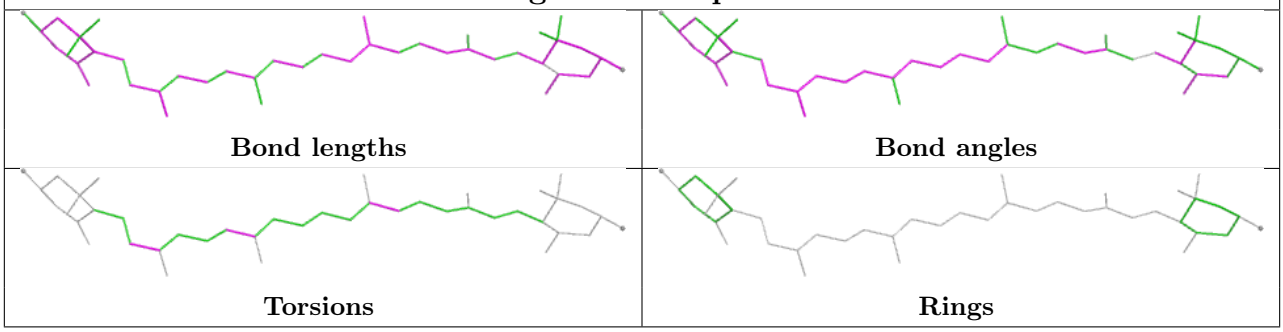
Ligand LMG C 622



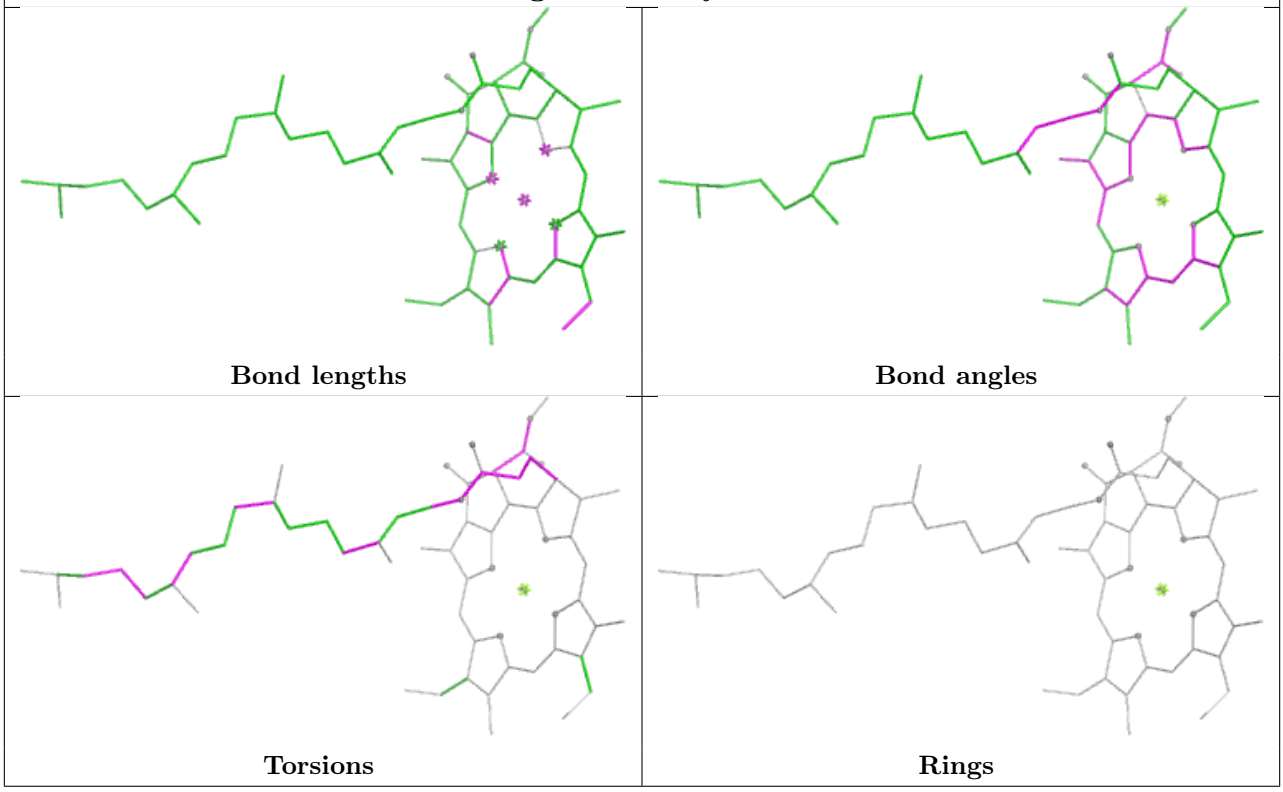
Ligand CLA R 316



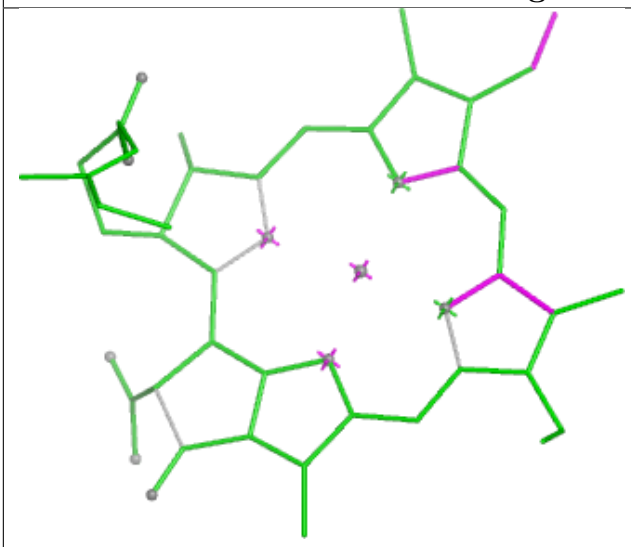
Ligand LUT q 318



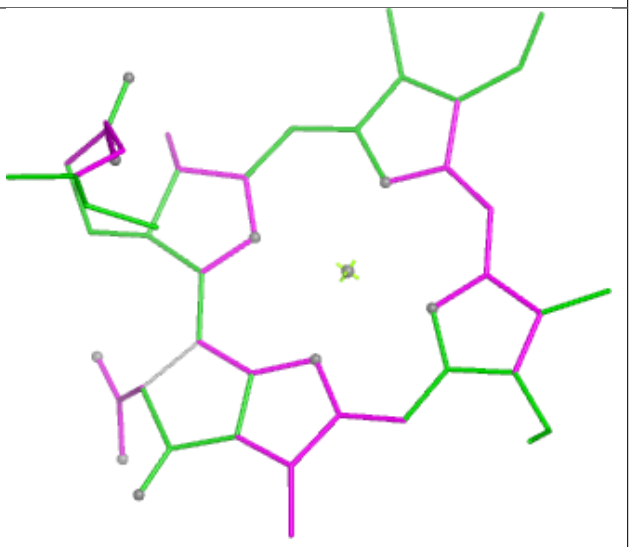
Ligand CLA y 611



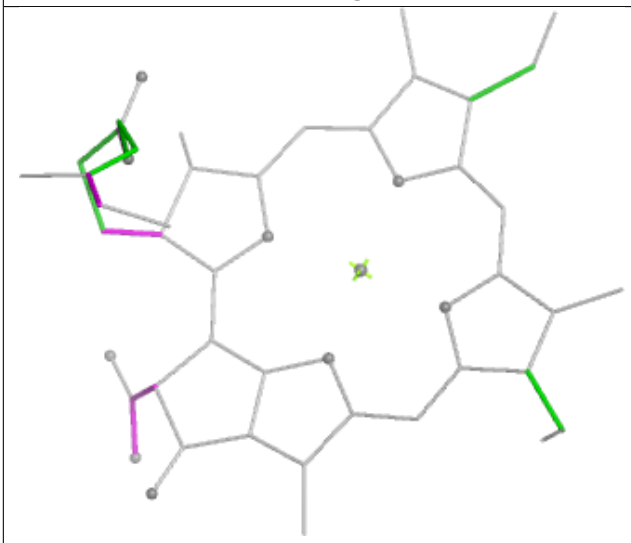
Ligand CLA 4 604



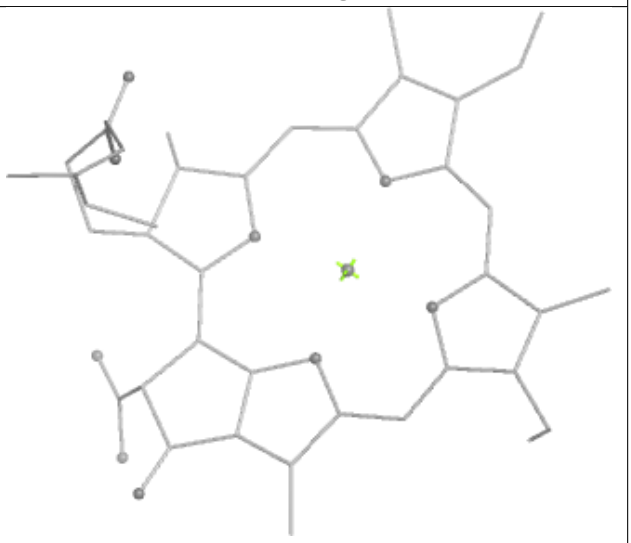
Bond lengths



Bond angles

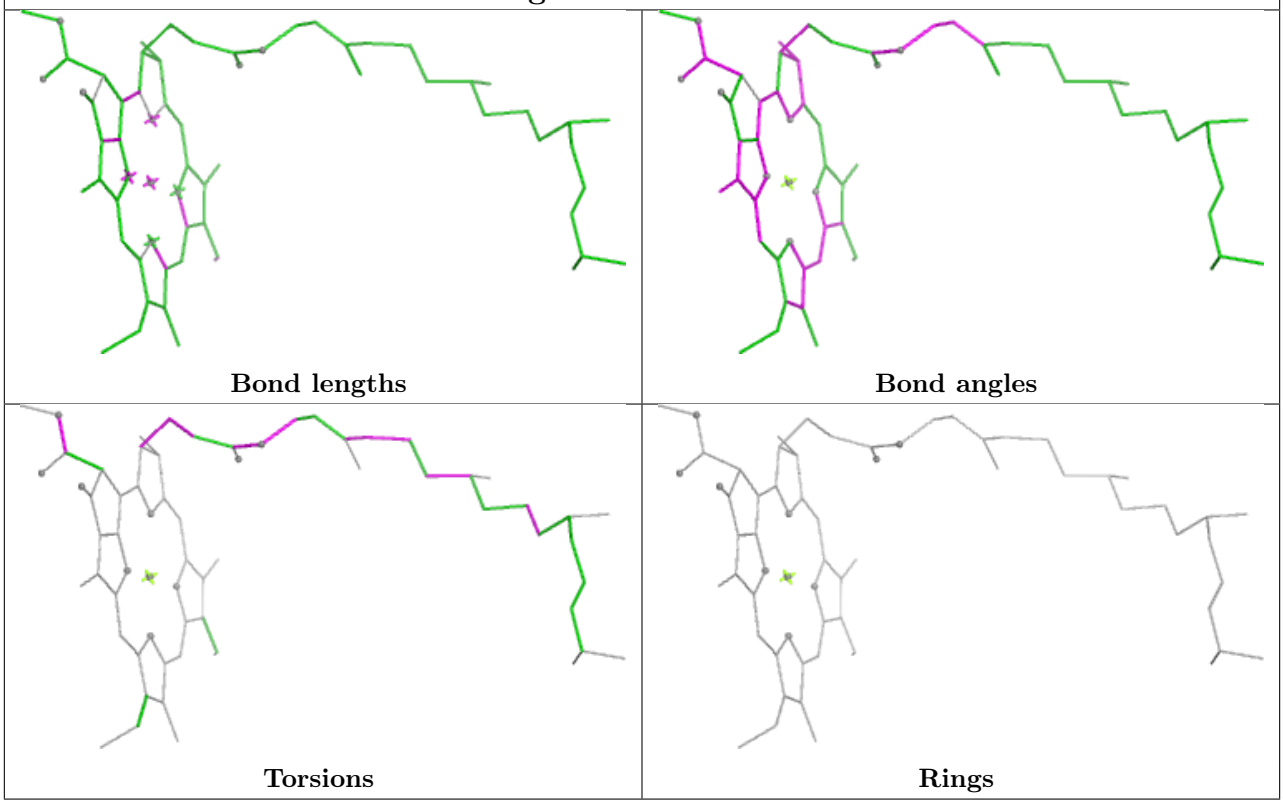


Torsions

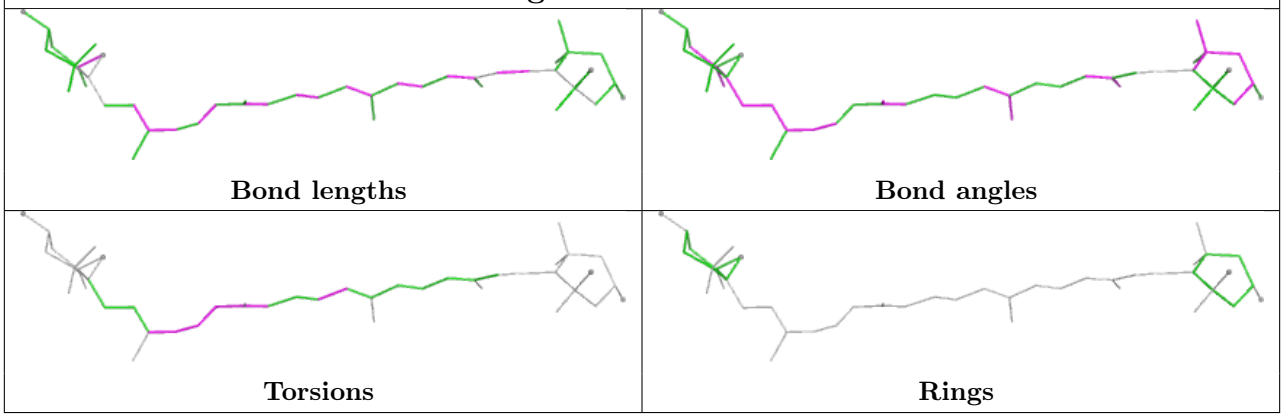


Rings

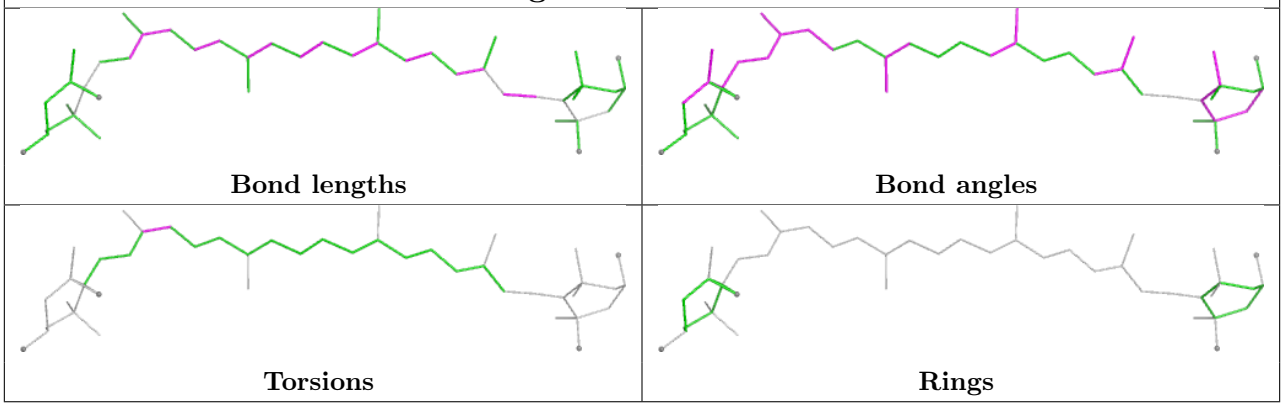
Ligand CLA d 405



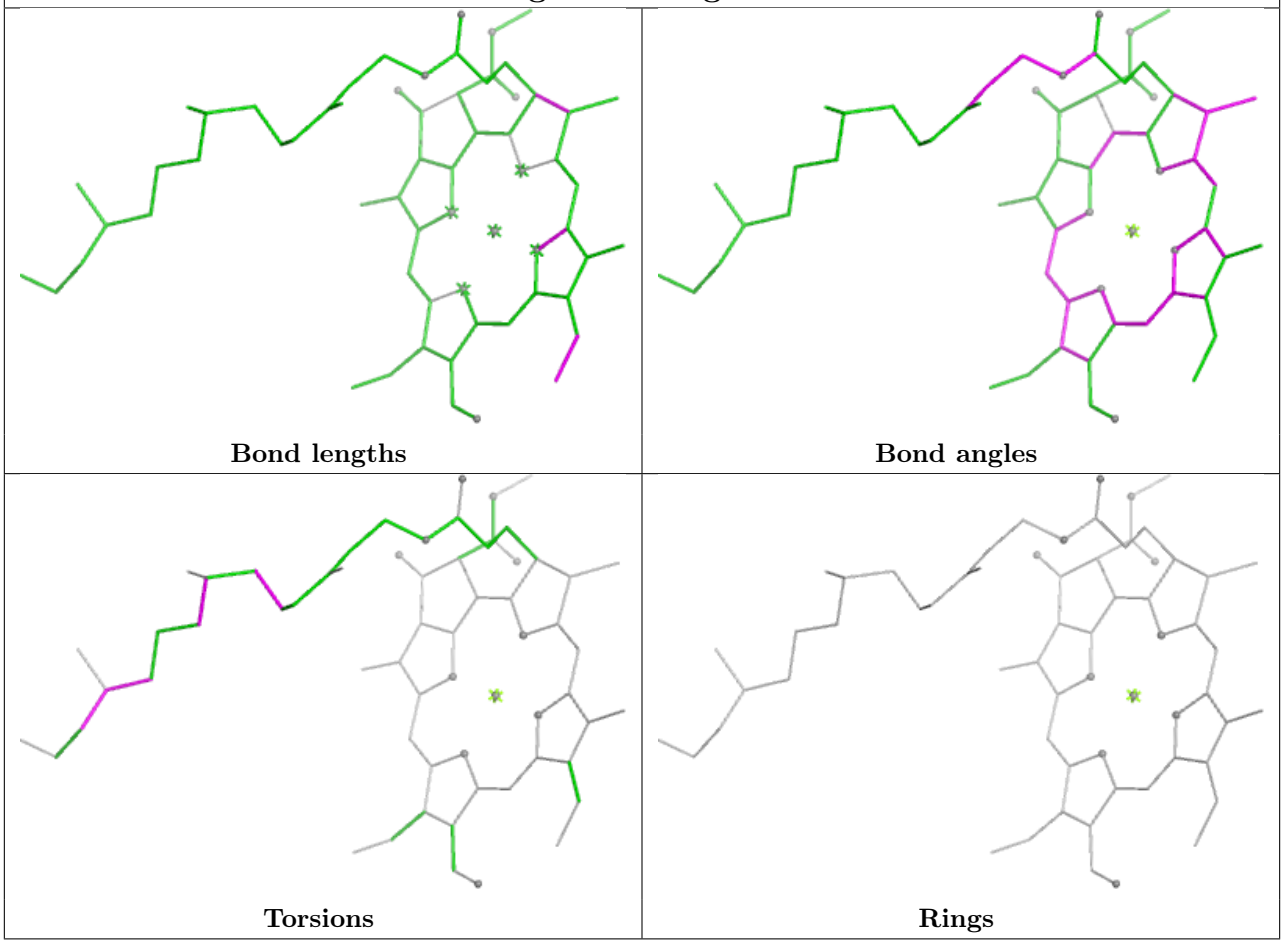
Ligand NEX 0 618



Ligand NEX r 301



Ligand CHL g 309



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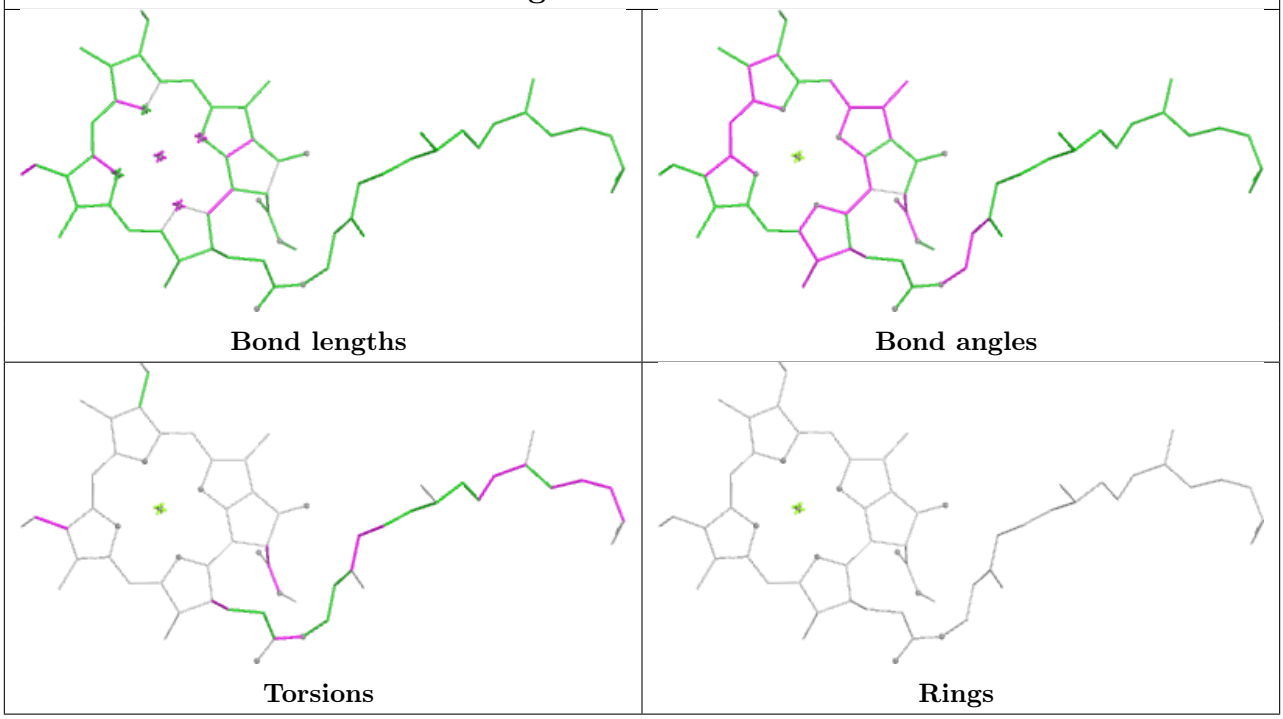
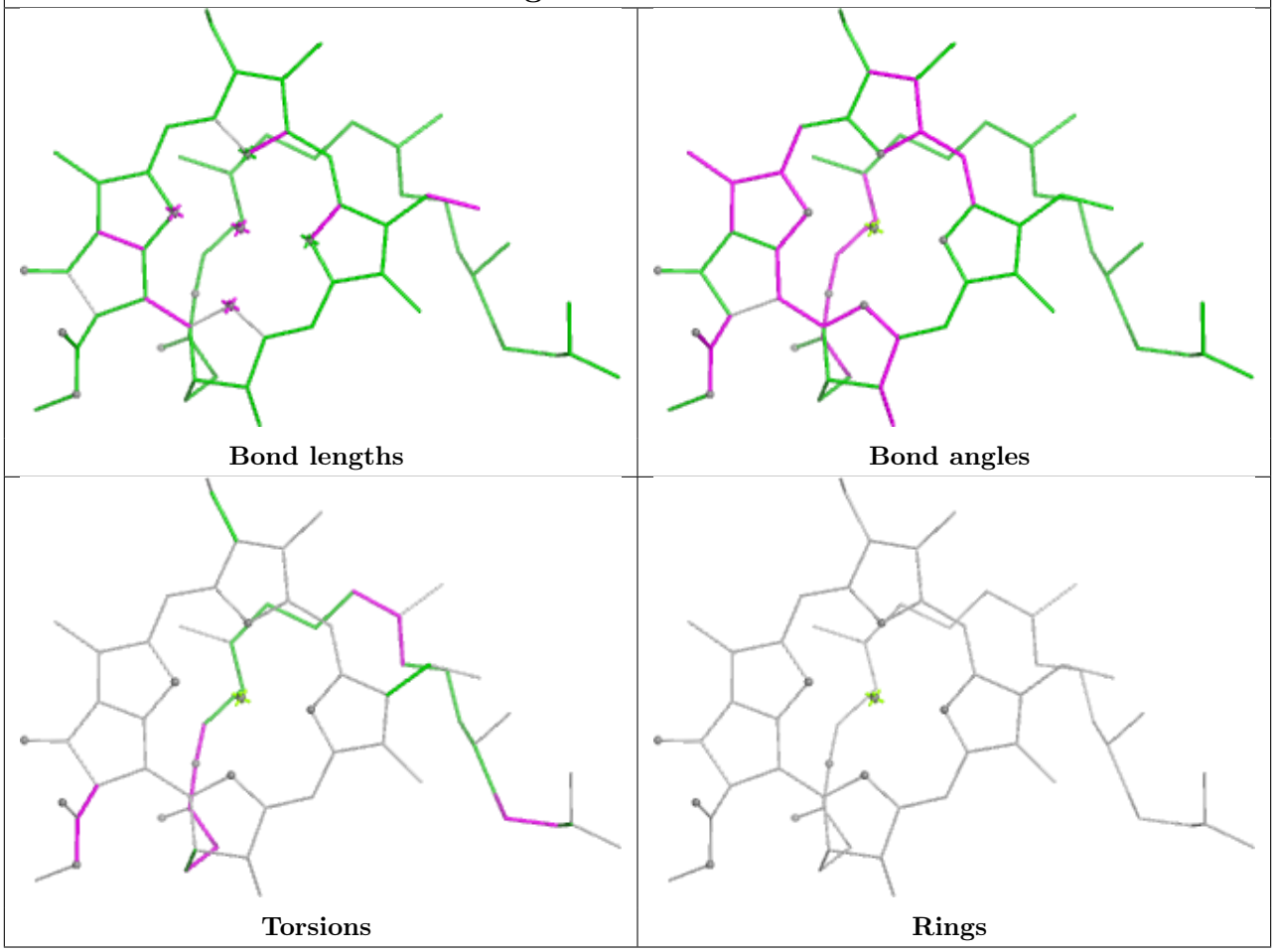
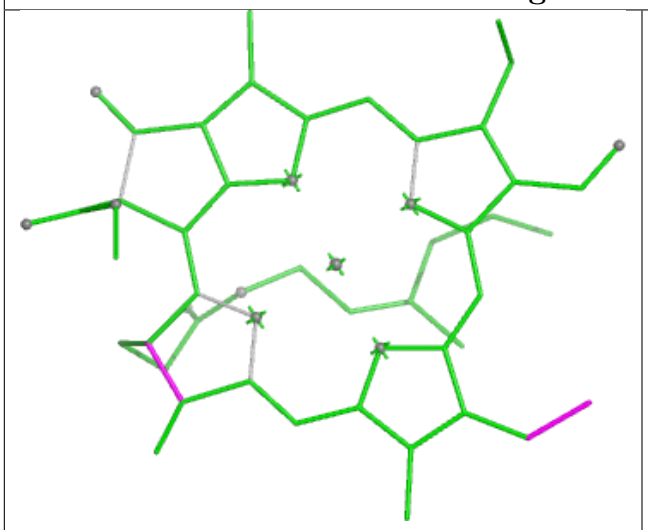


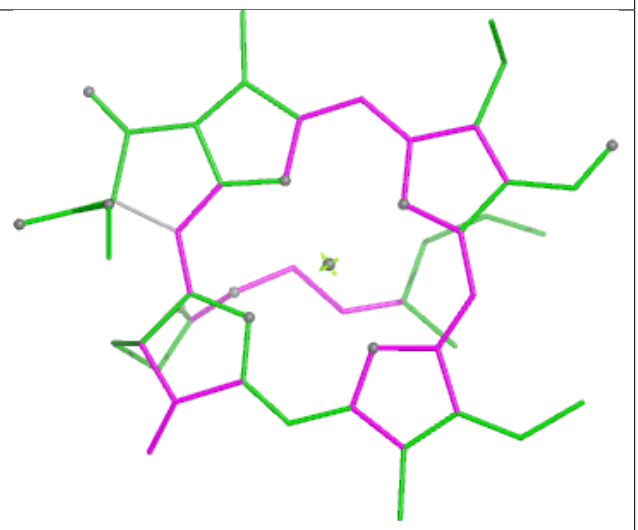
Ligand CLA S 314



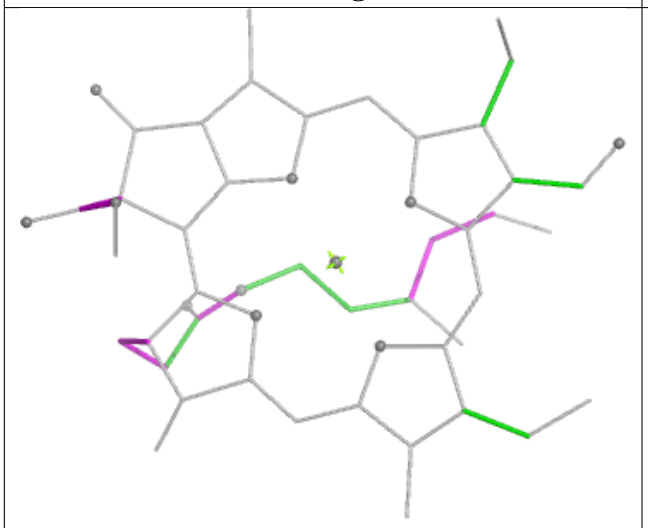
Ligand CHL 9 309



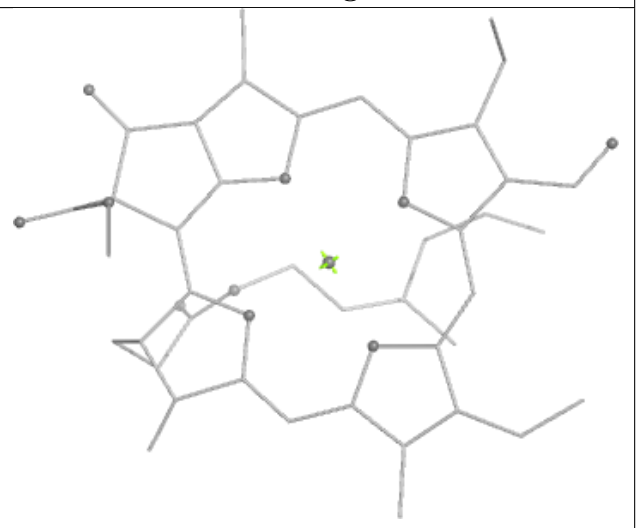
Bond lengths



Bond angles

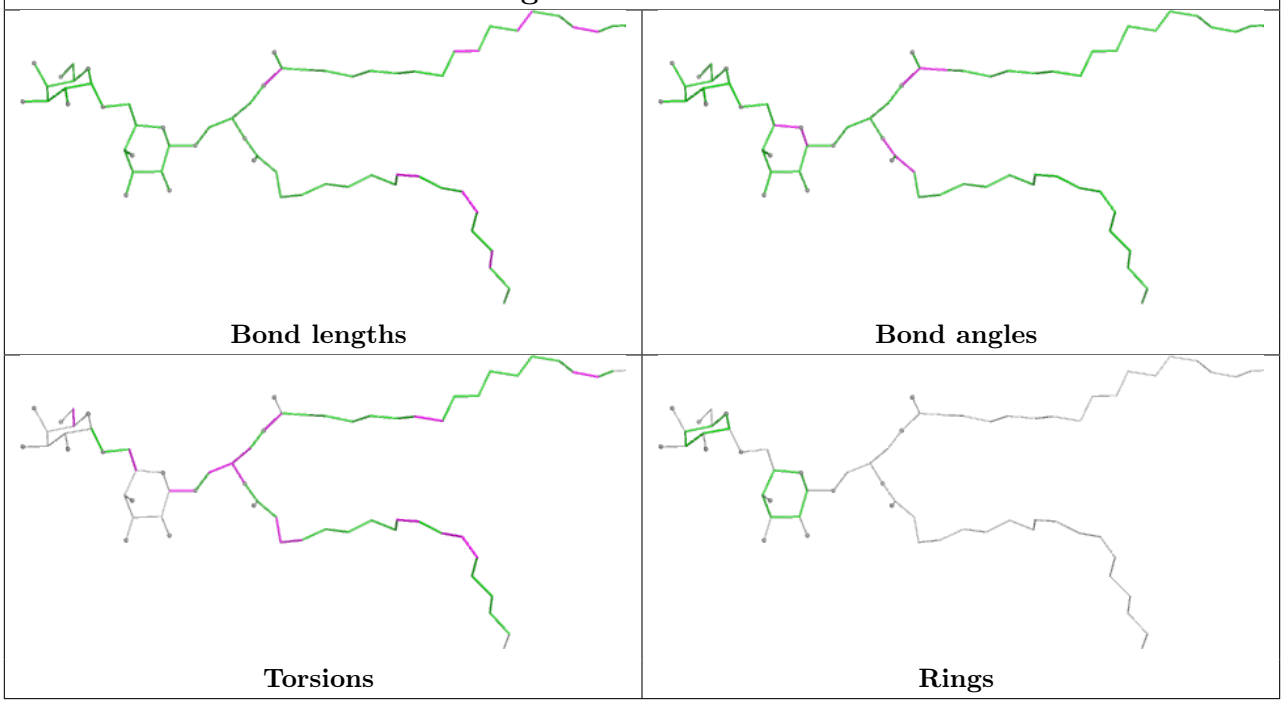


Torsions

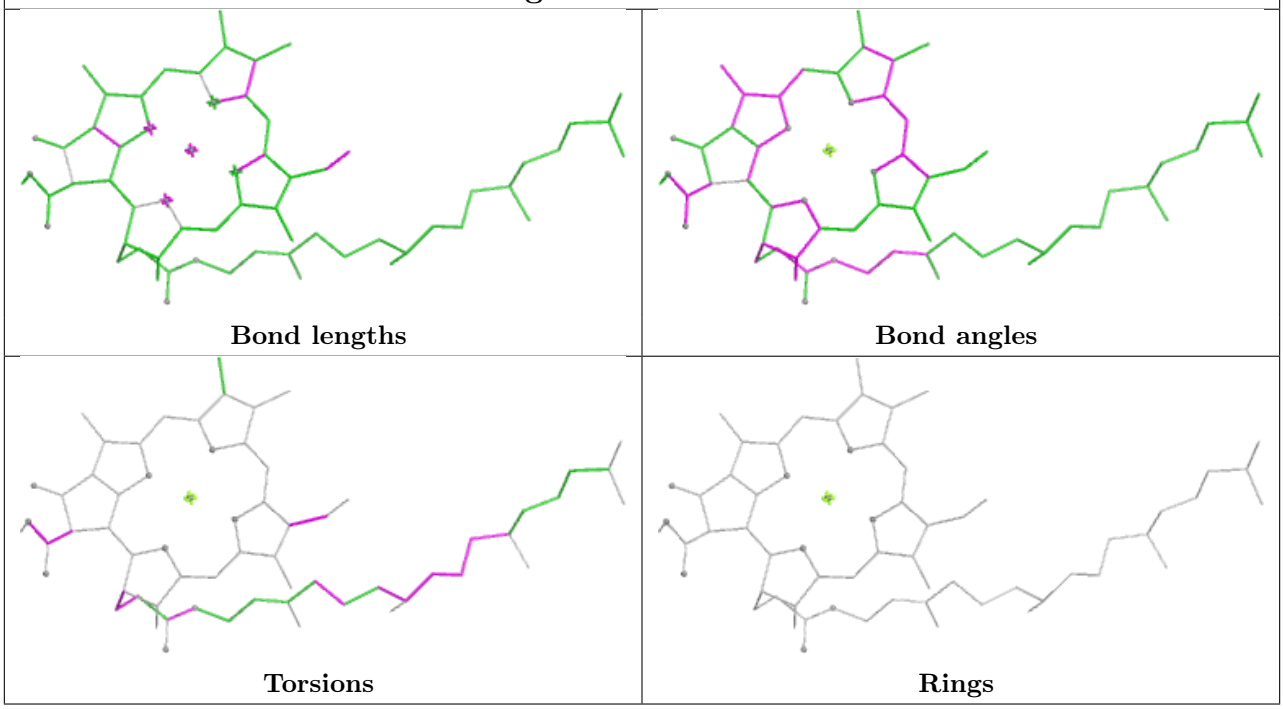


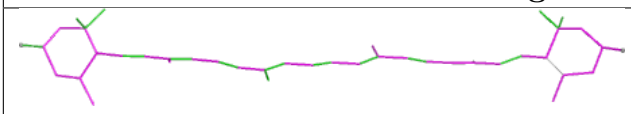
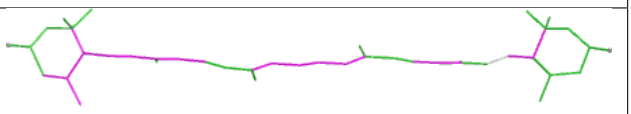
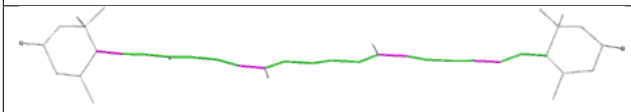
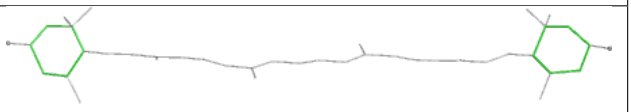
Rings

Ligand DGD C 618



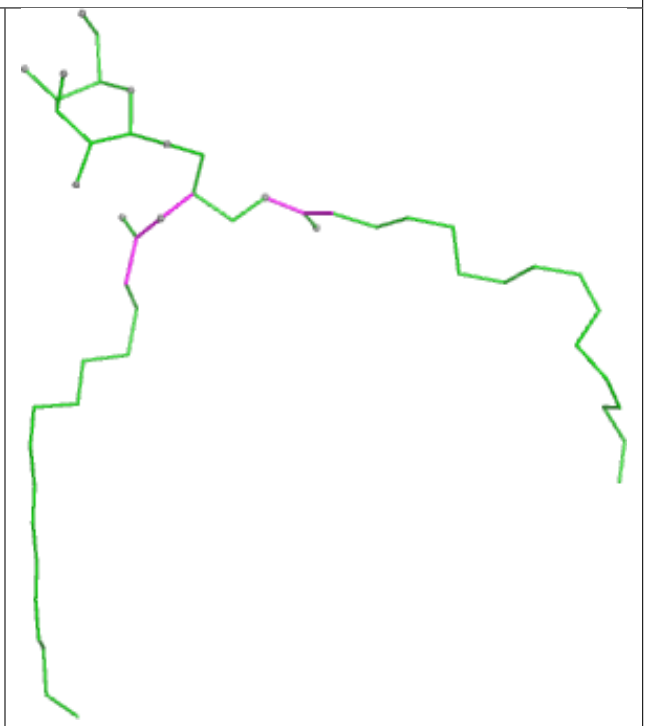
Ligand CLA C 601



Ligand LUT 5 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

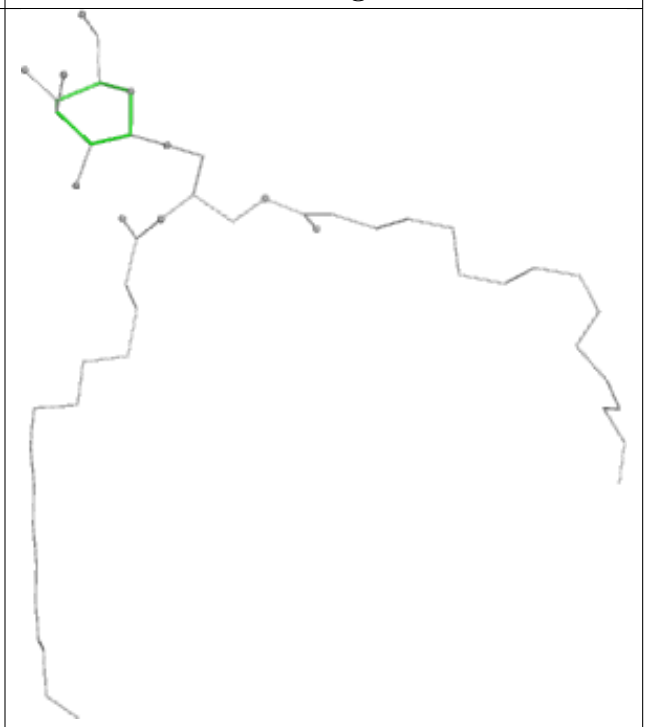
Ligand LMG G 621

Bond lengths



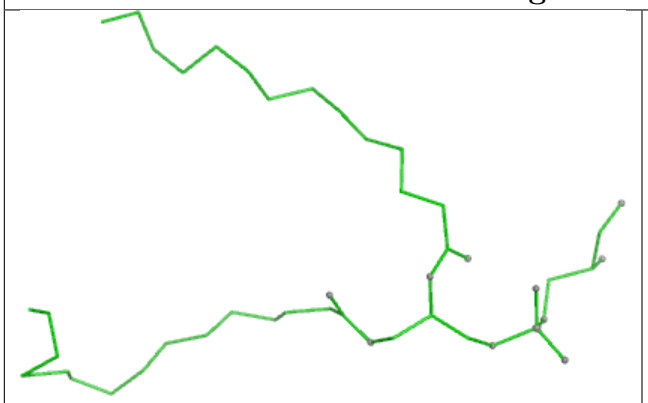
Bond angles

Torsions



Rings

Ligand LHG c 622



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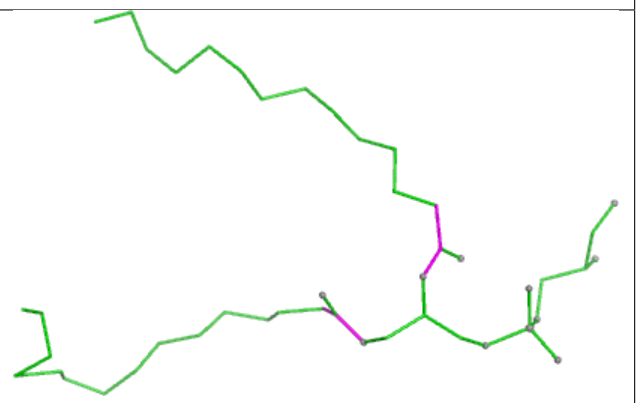
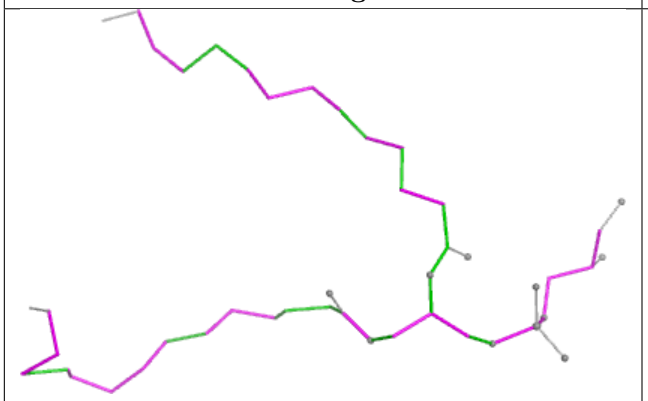


Bond angles



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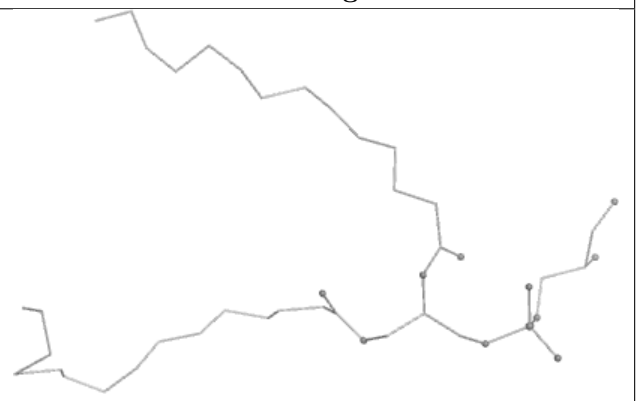
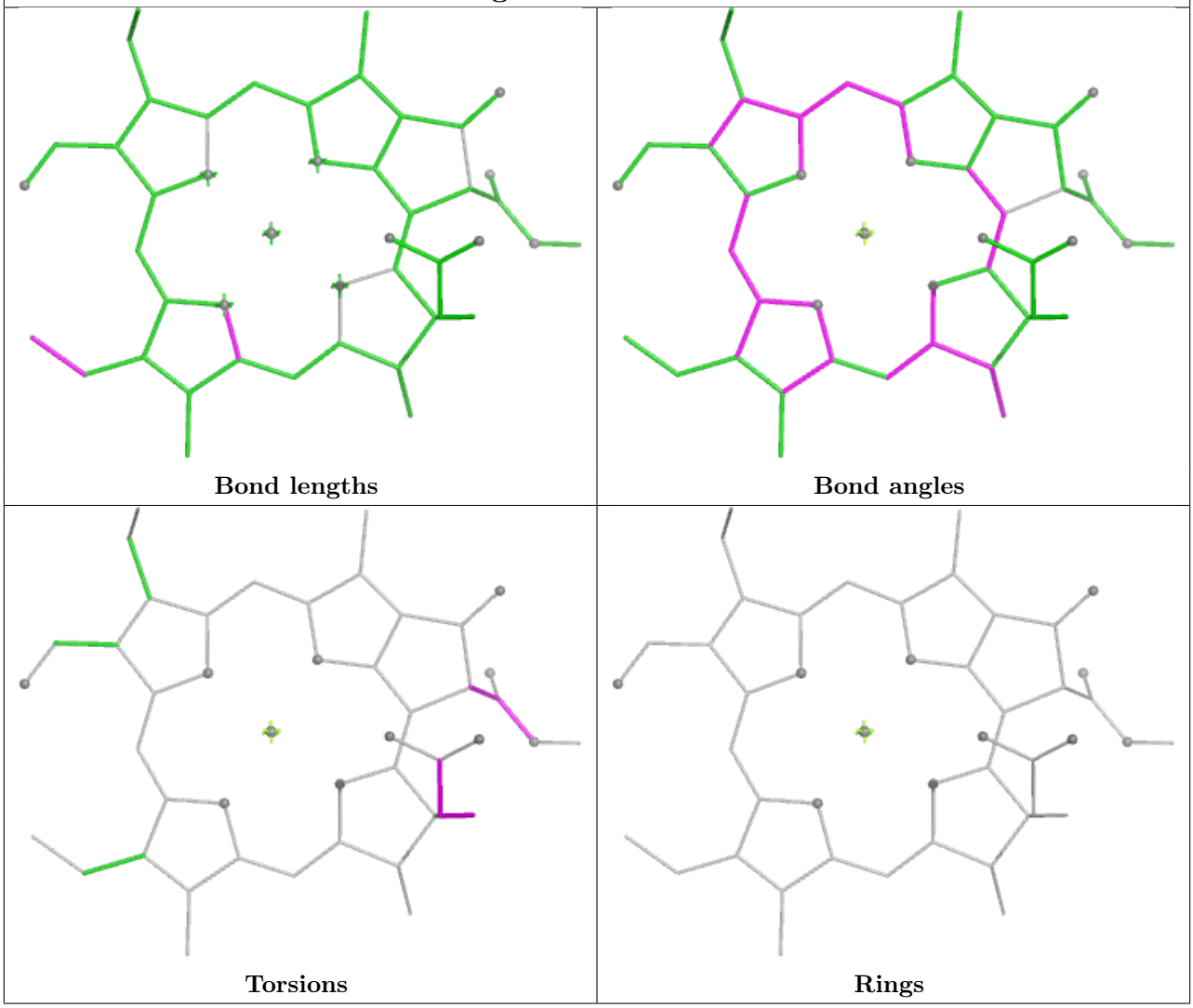
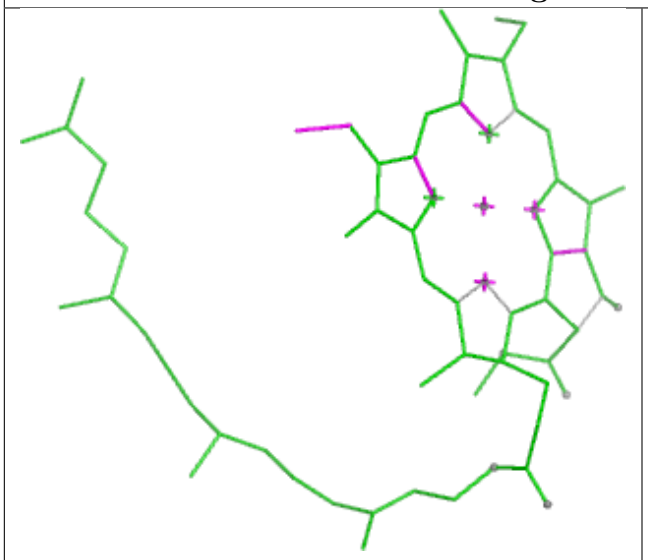


Rings

Ligand CHL 9 307



Ligand CLA c 607



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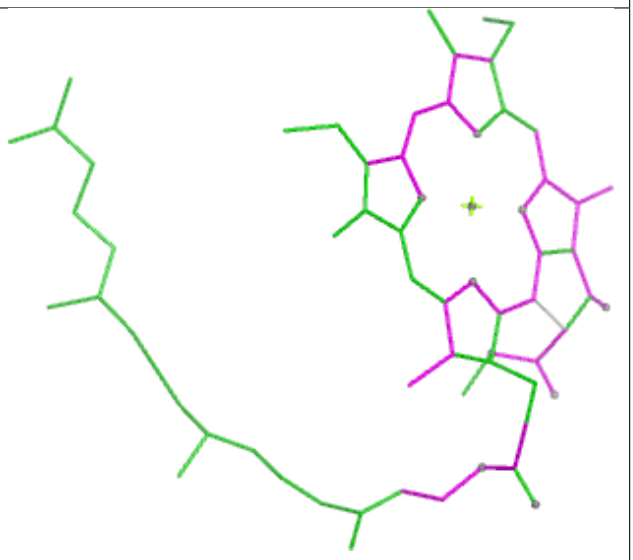
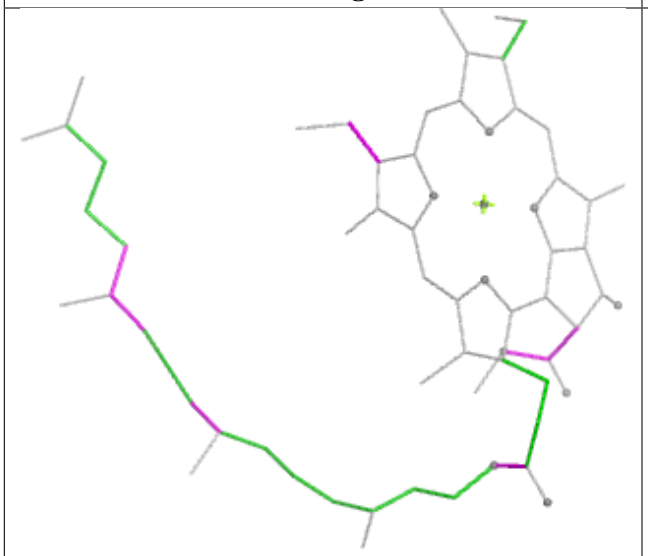
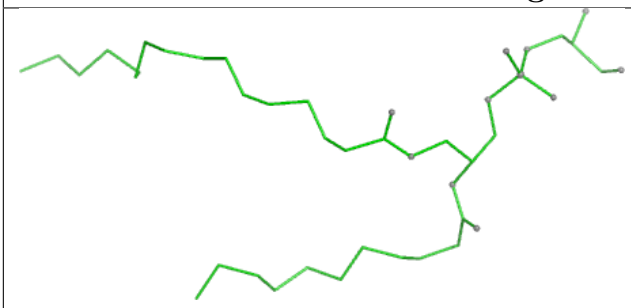
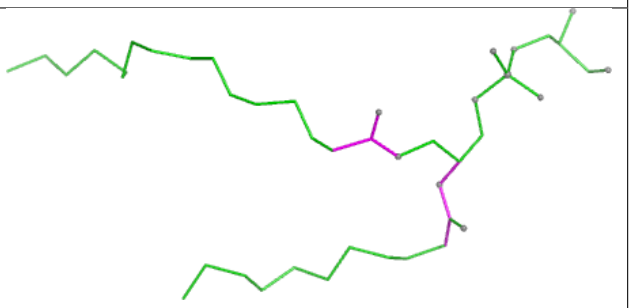
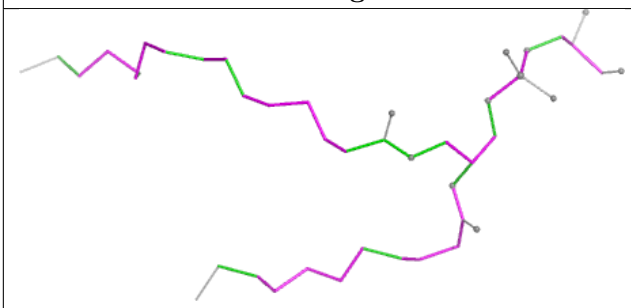


Bond angles

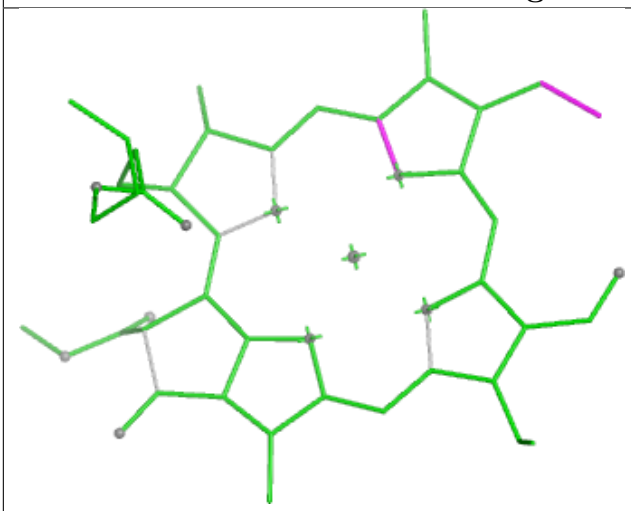


Torsions

Rings

Ligand LHG e 101	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CHL p 608



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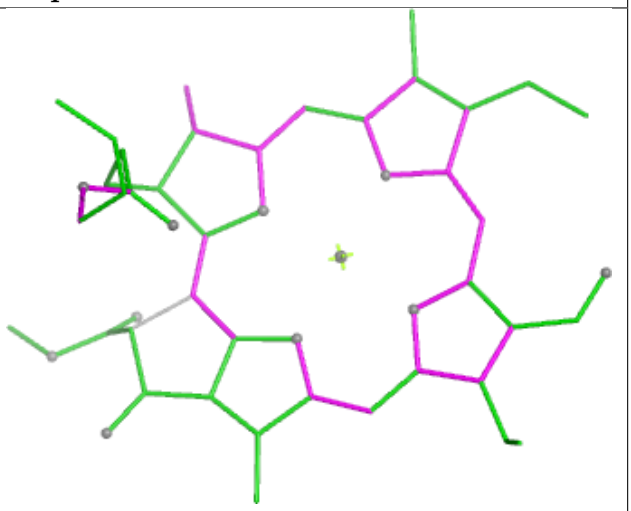
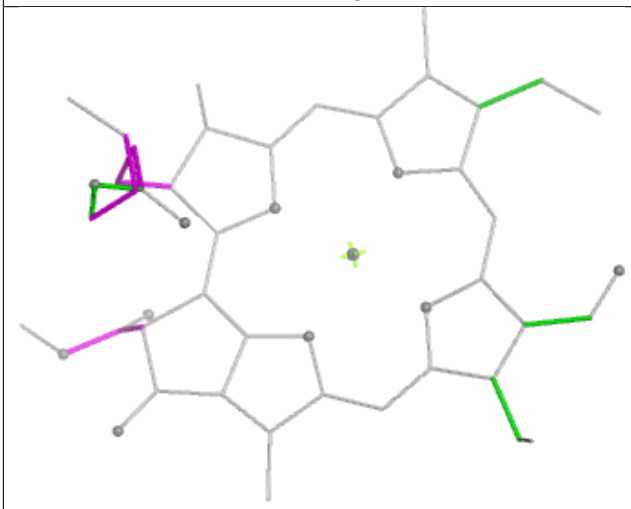


Bond angles



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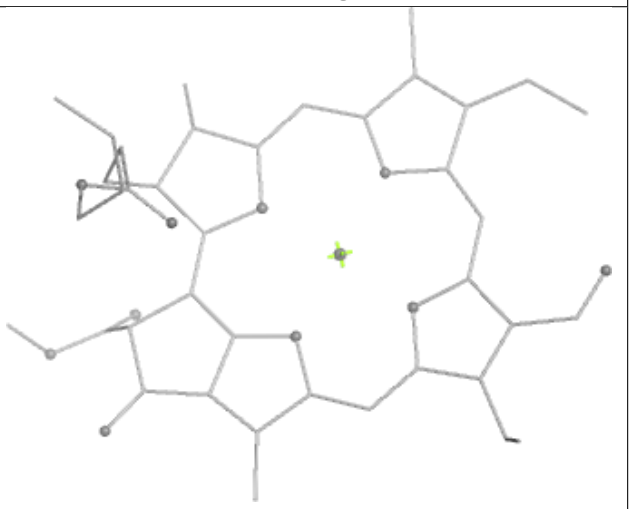
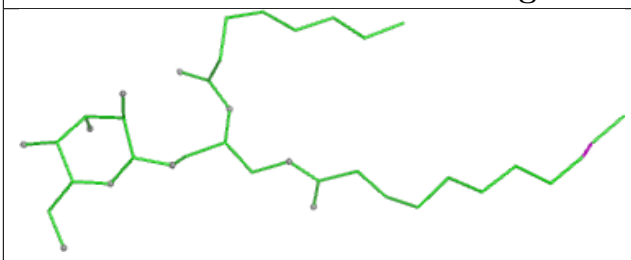


Rings

Ligand LMG A 414



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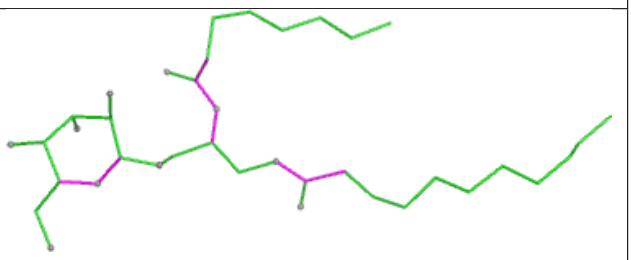

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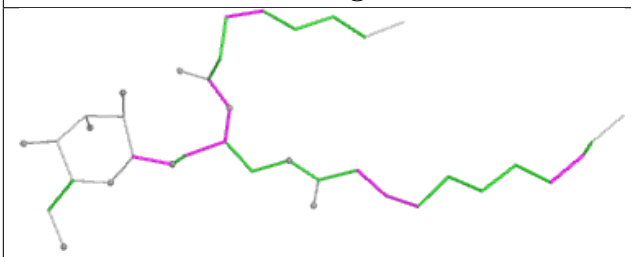

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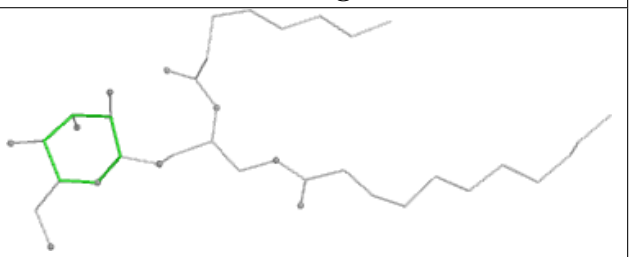
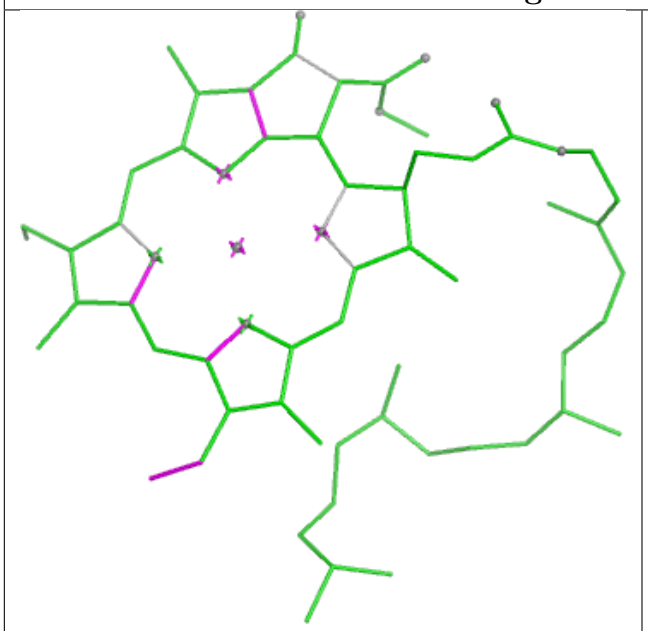


Rings

Ligand CLA Y 312



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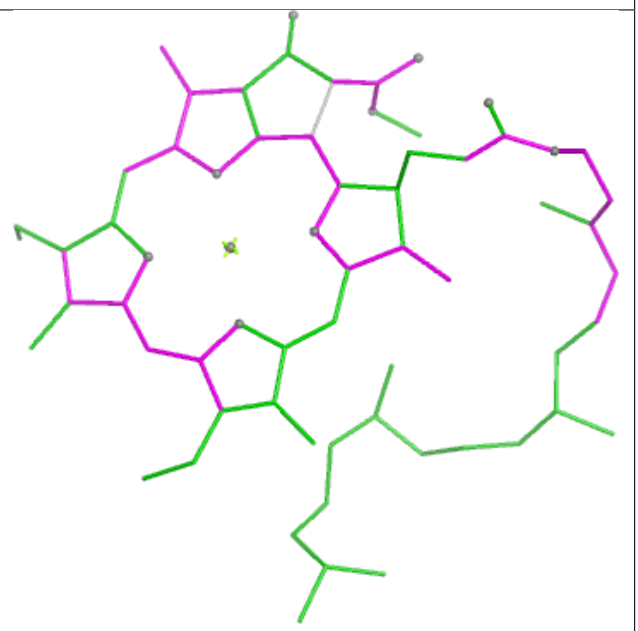
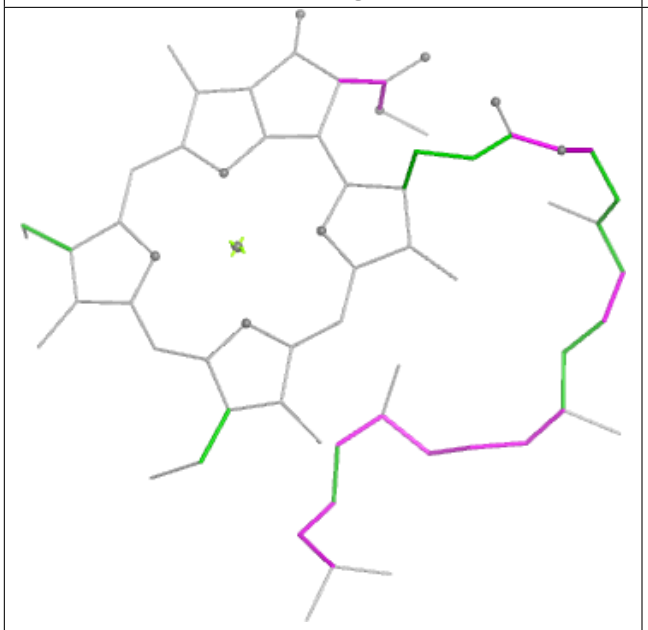


Bond angles



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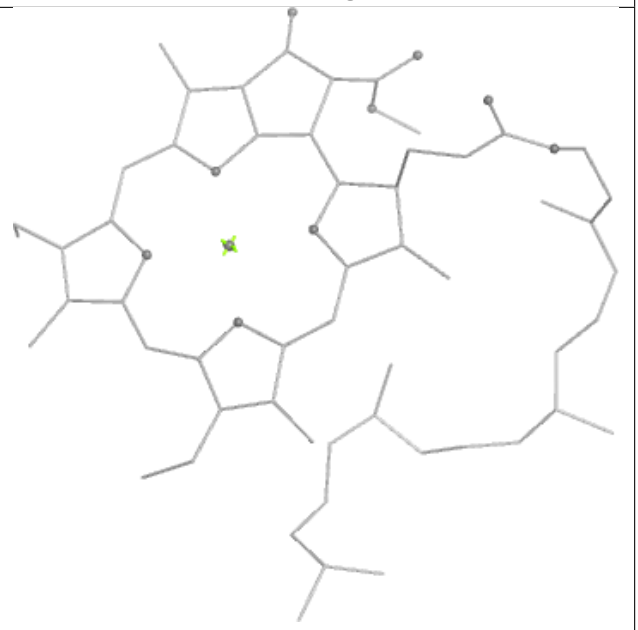
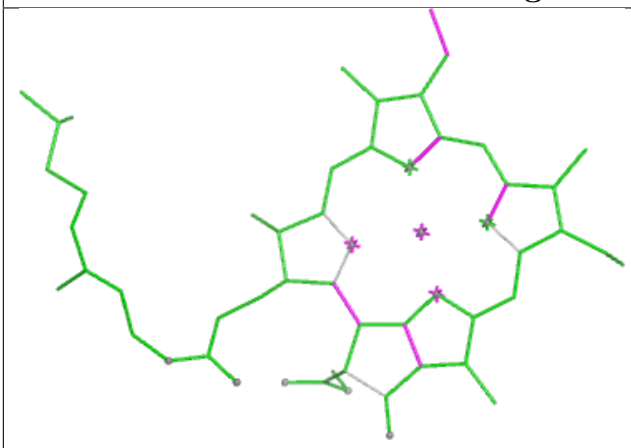
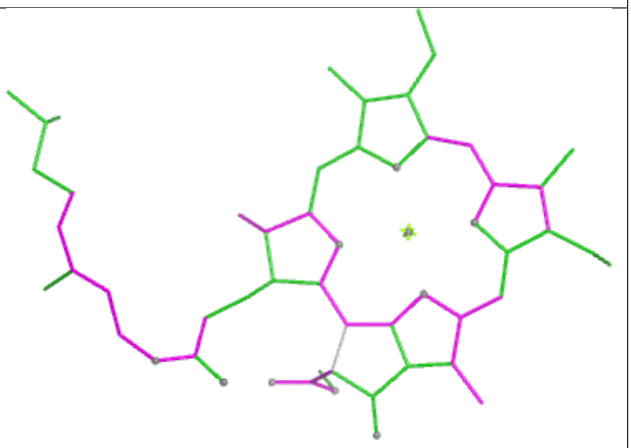
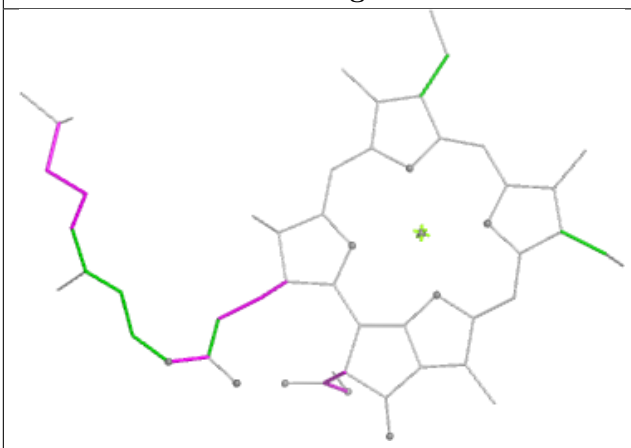
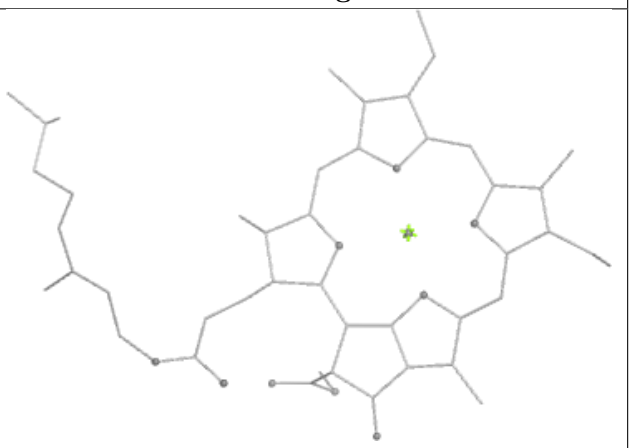
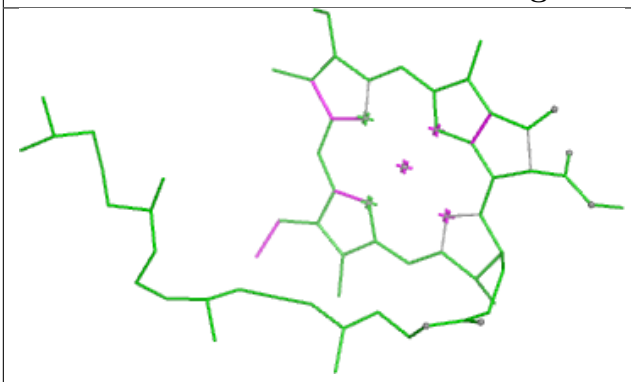


Rings

Ligand CLA C 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 303



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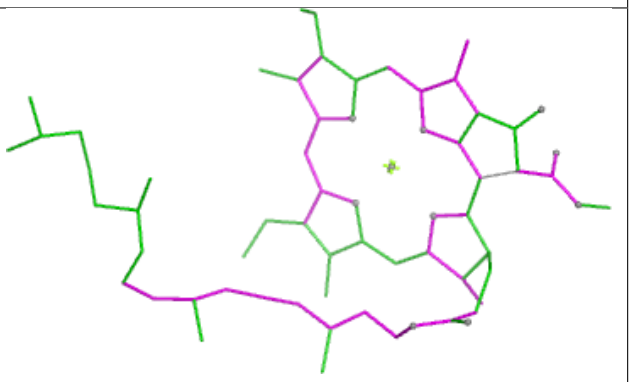
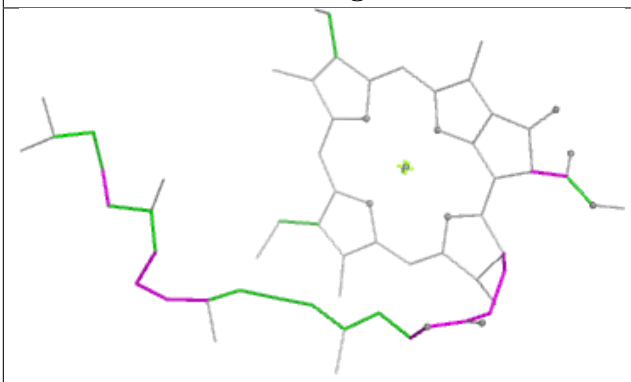


Bond angles



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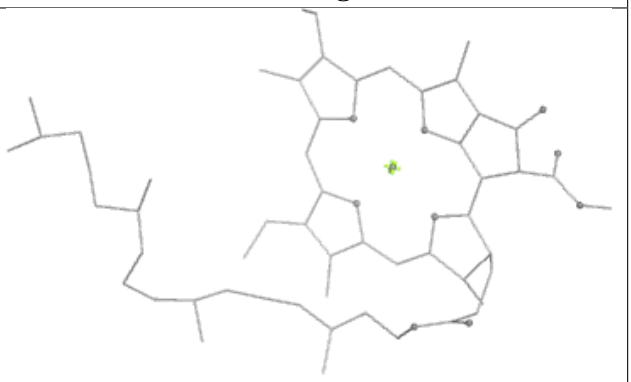
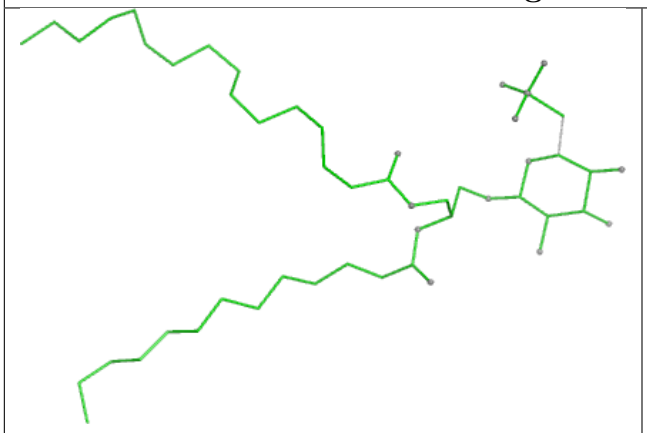


Rings

Ligand SQD A 411



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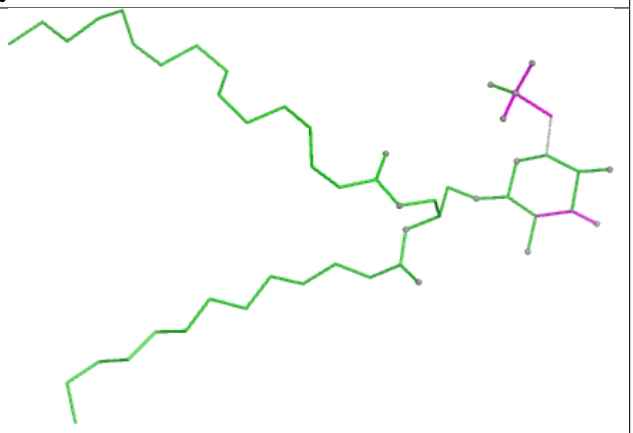
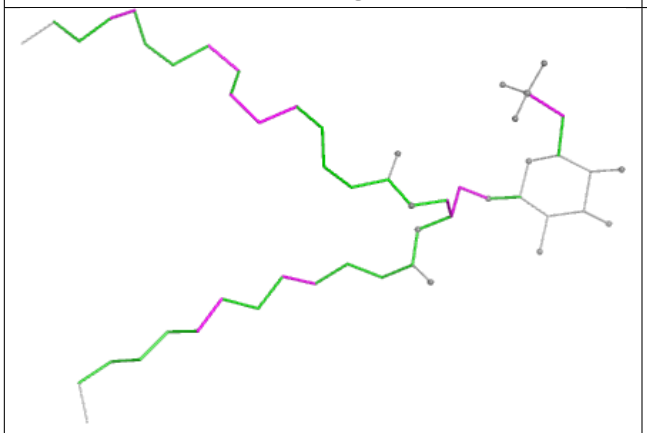


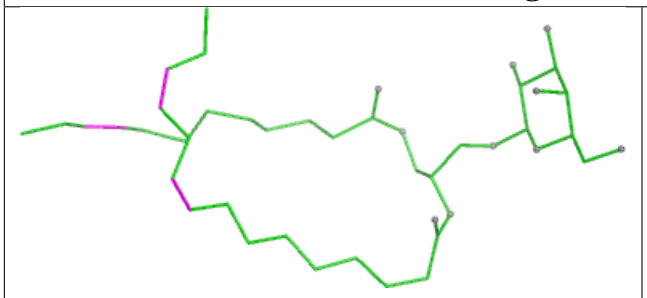
Bond angles



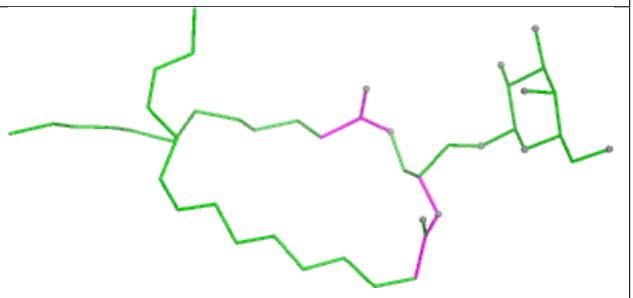
Torsions

Rings

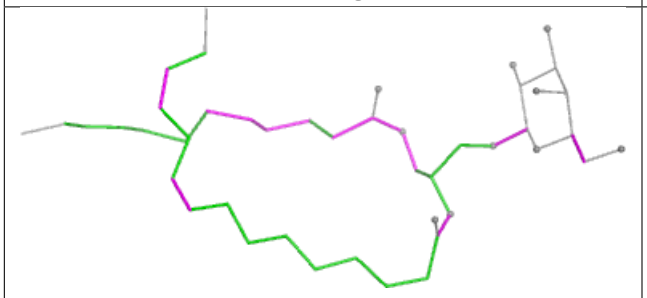
Ligand LMG b 626



Bond lengths

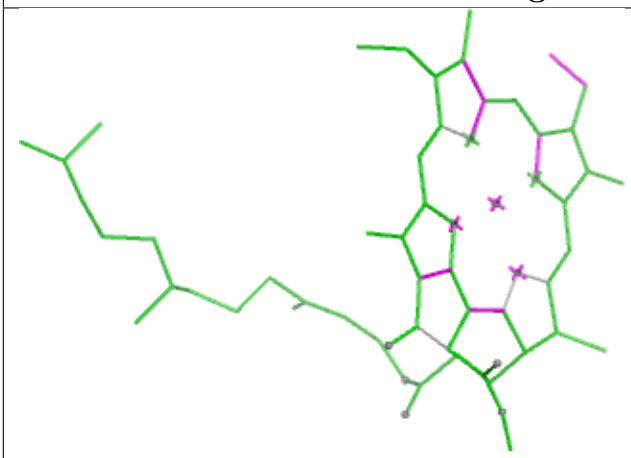
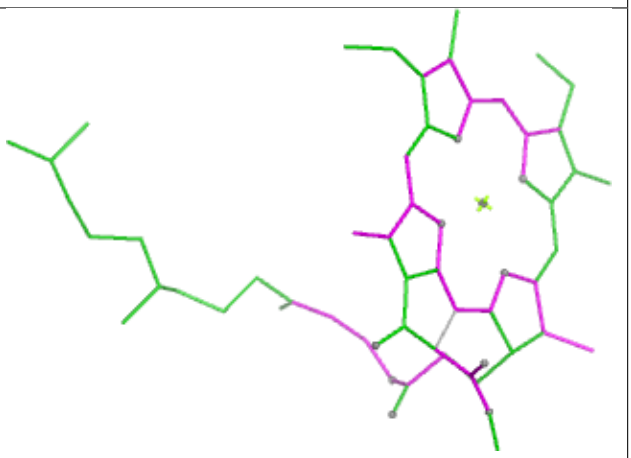
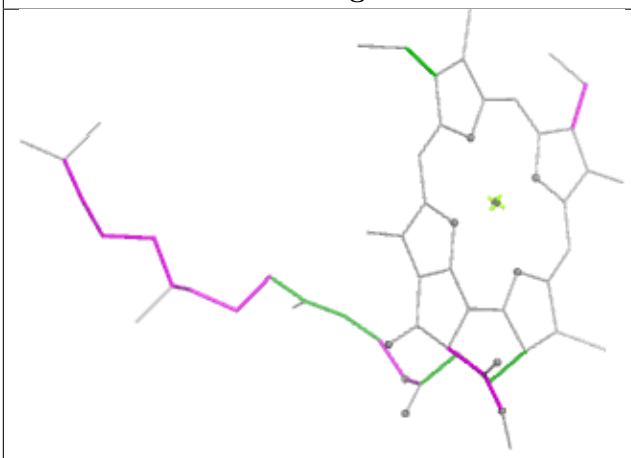


Bond angles



Torsions

Rings

Ligand CLA 6 312	
 Bond lengths	 Bond angles
 Torsions	Rings

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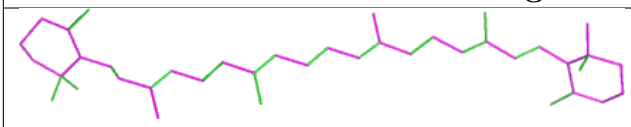
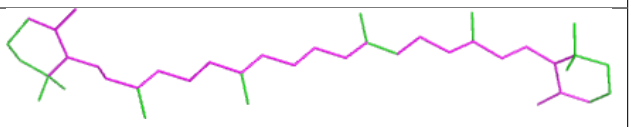
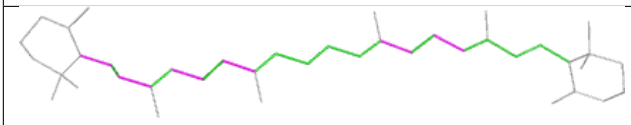
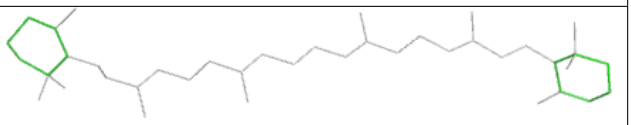
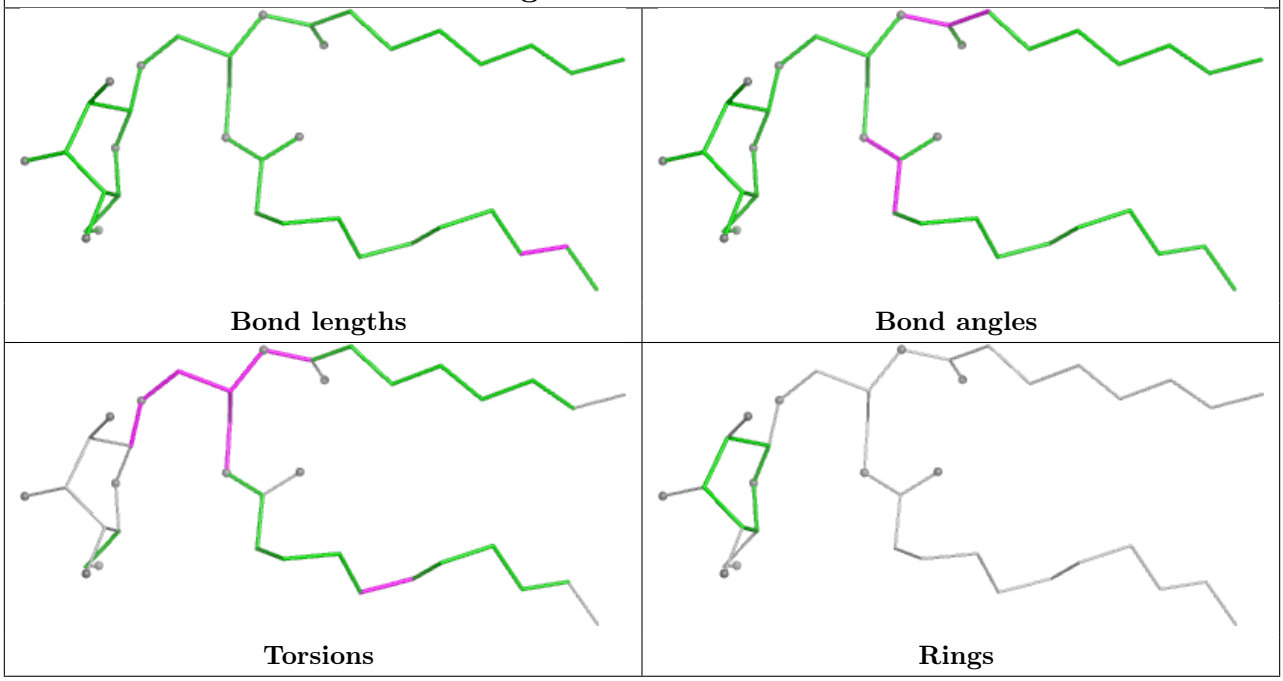
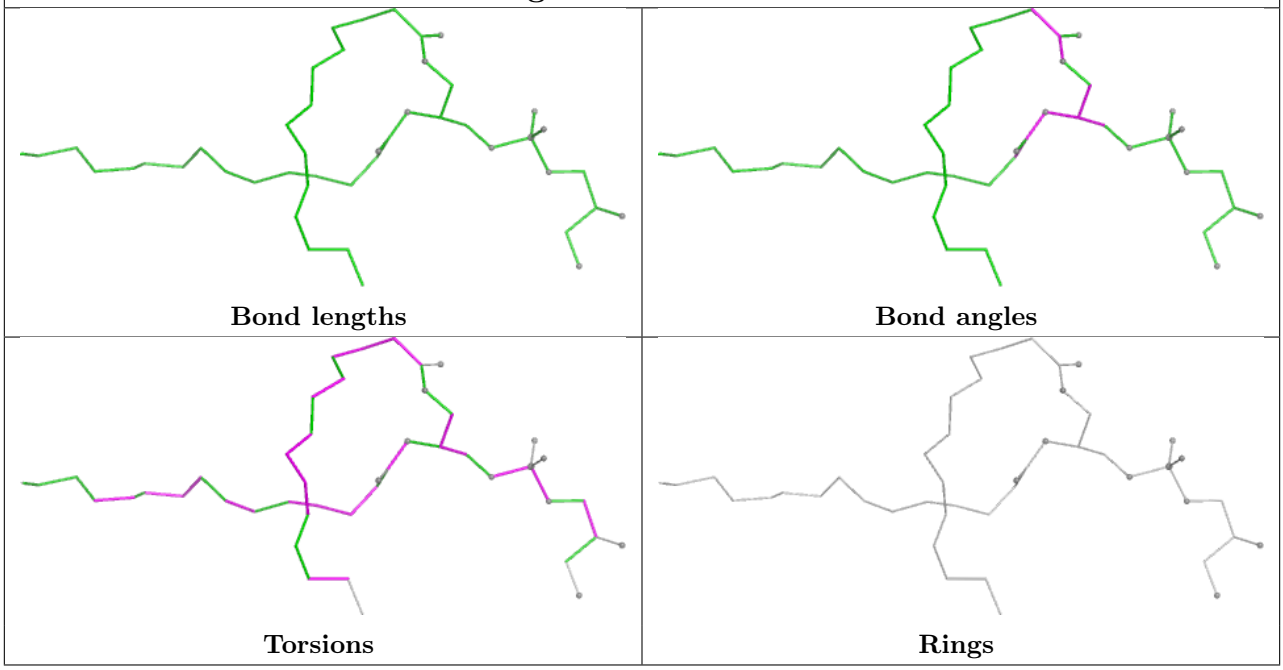
 Bond lengths	 Bond angles
 Torsions	 Rings

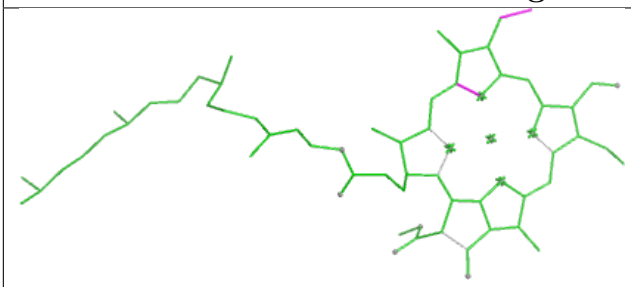
Ligand LMG w 205



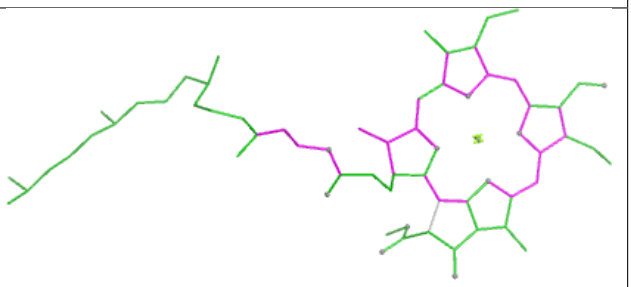
Ligand LHG 4 618



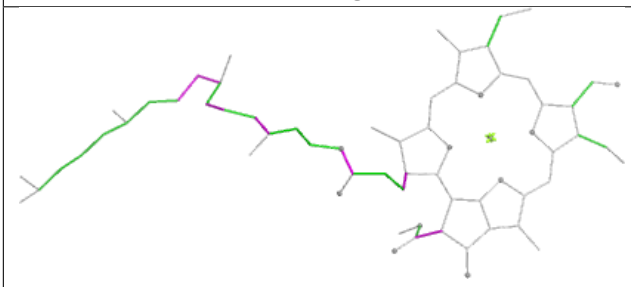
Ligand CHL 2 601



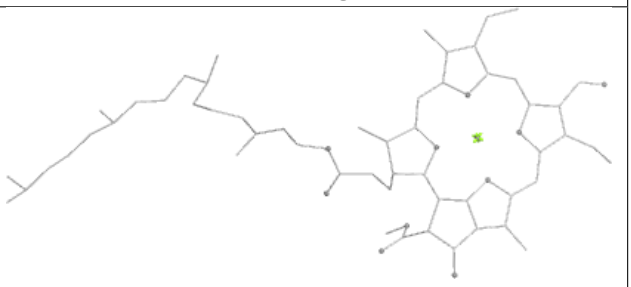
Bond lengths



Bond angles

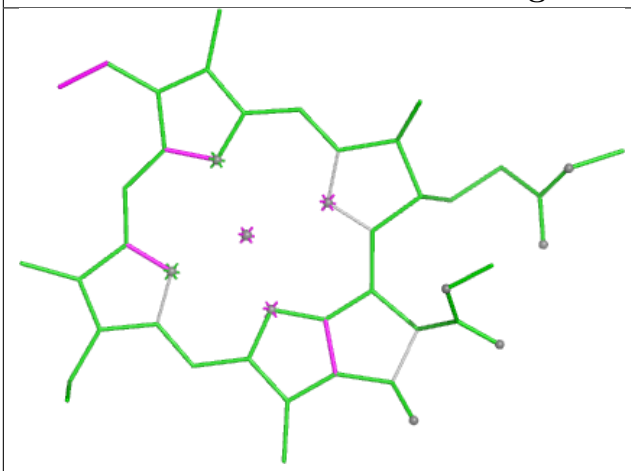


Torsions



Rings

Ligand CLA 4 612



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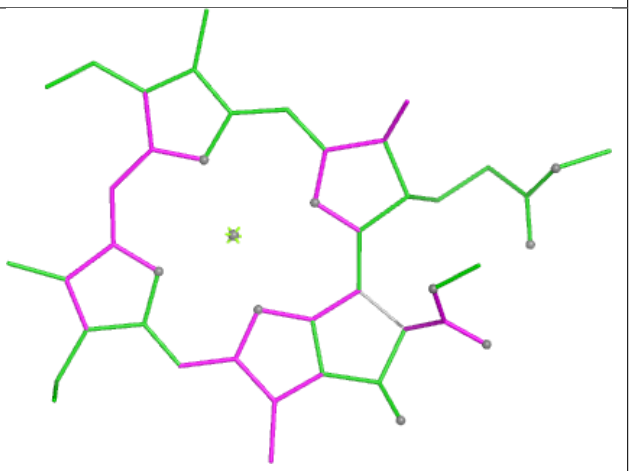
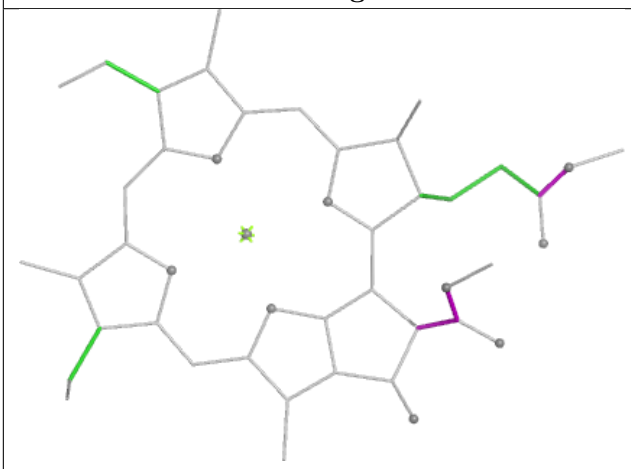


Bond angles



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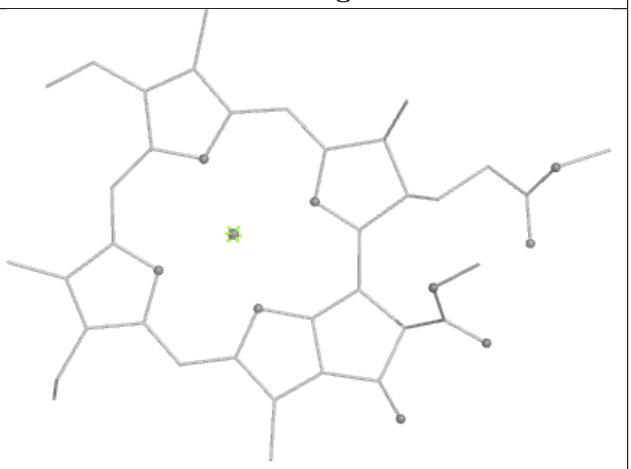
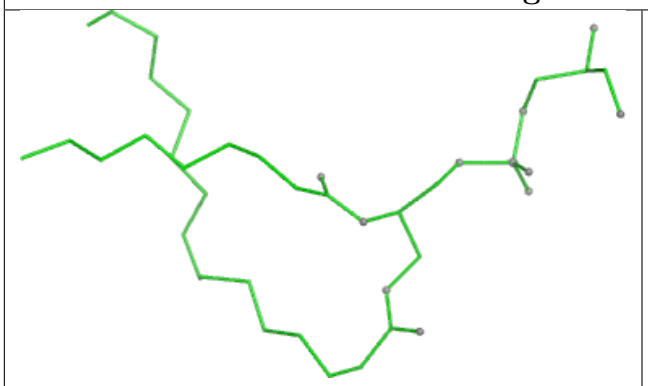


Rings

Ligand LHG Y 318



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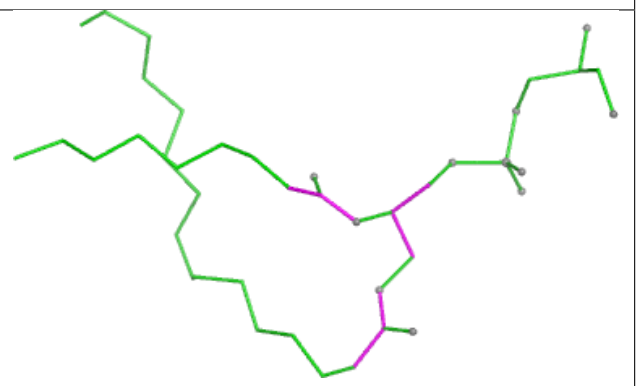
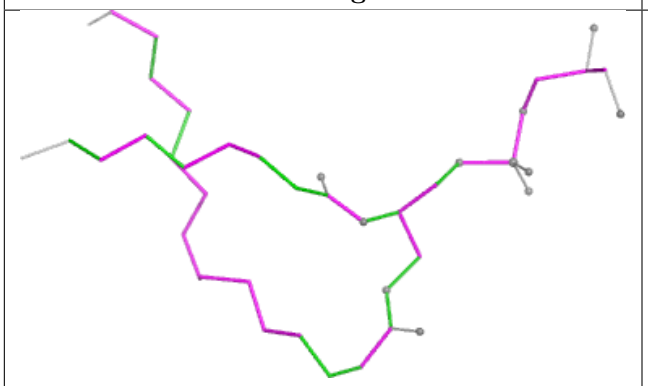


Bond angles



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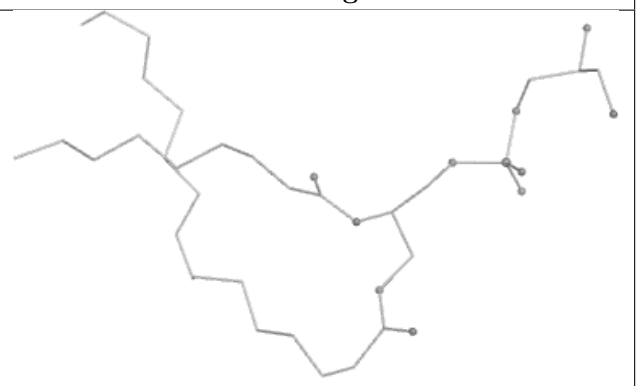
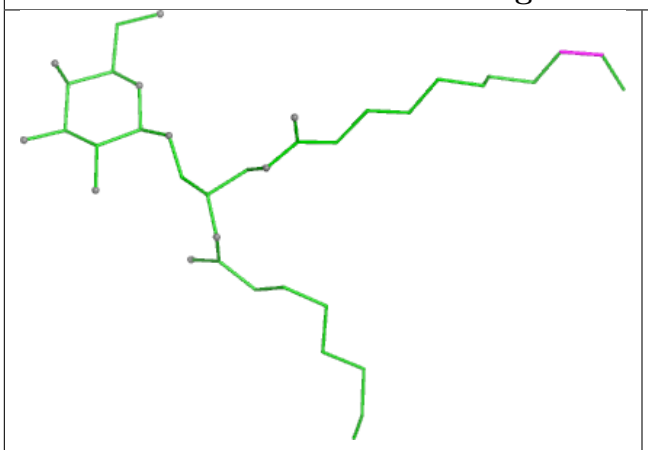


Rings

Ligand LMG W 202



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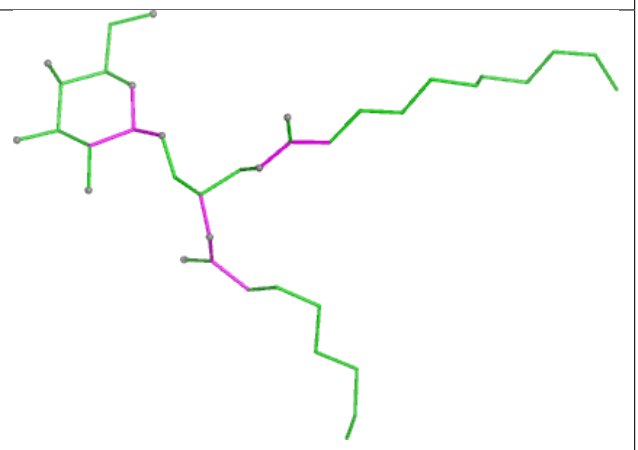
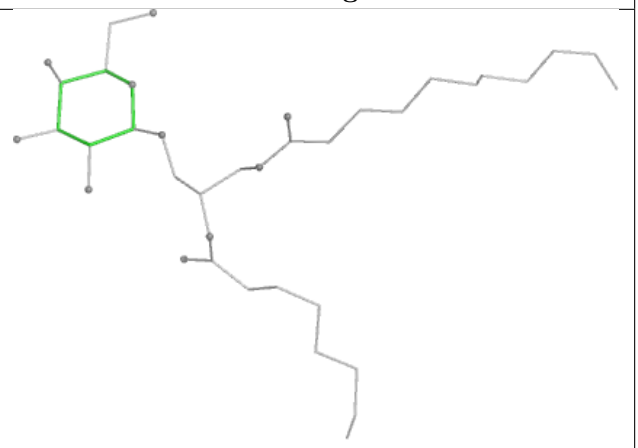


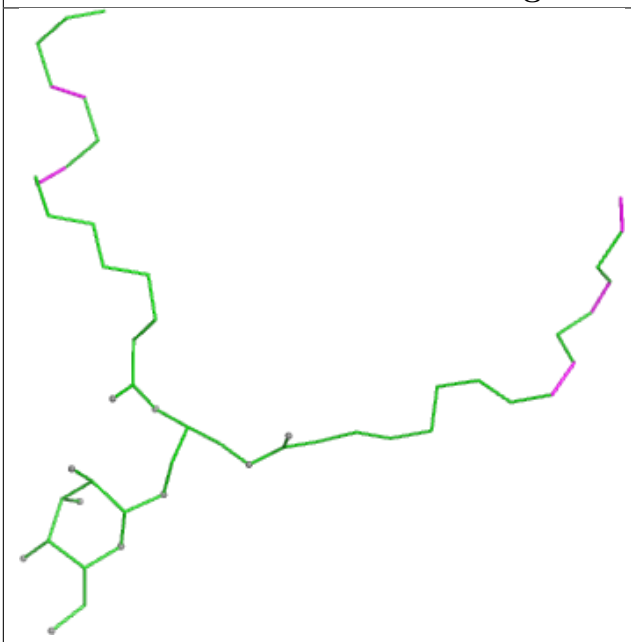
Bond angles

Torsions



Rings

Ligand LMG 4 620



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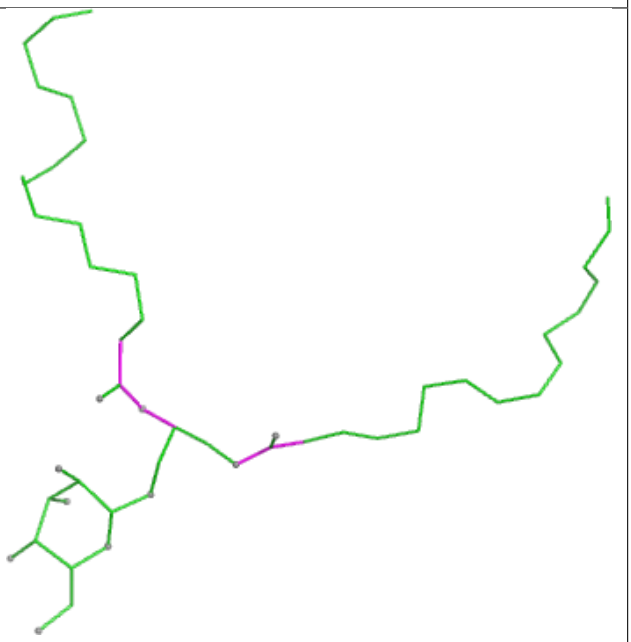
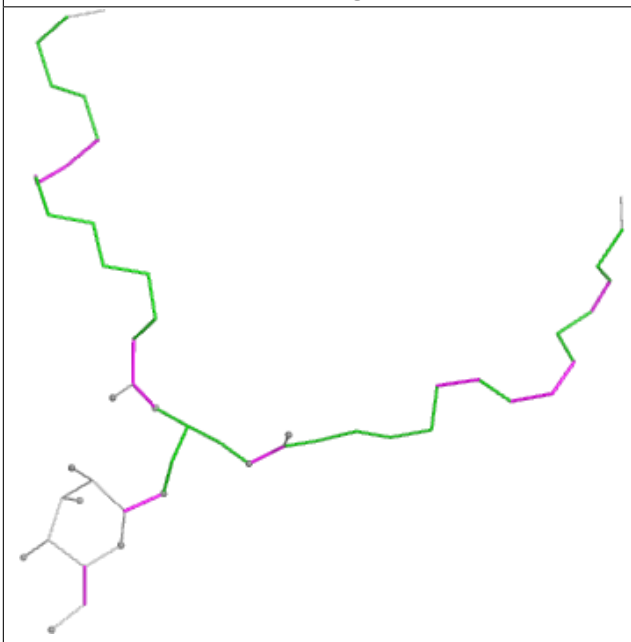


Bond angles



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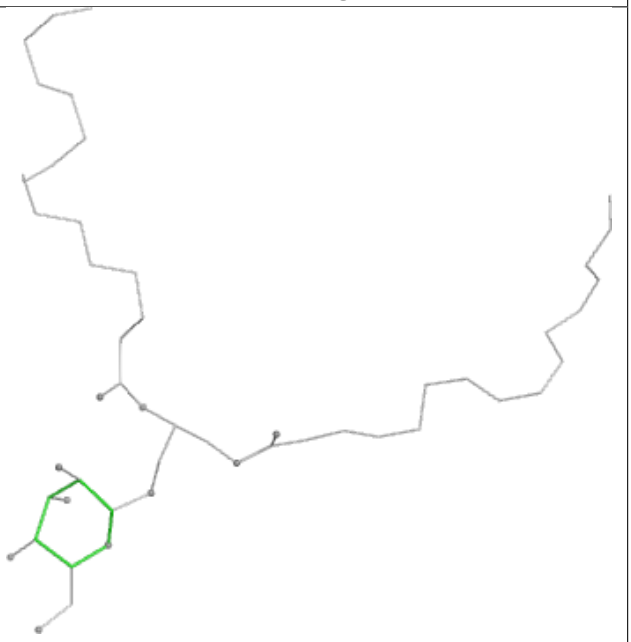
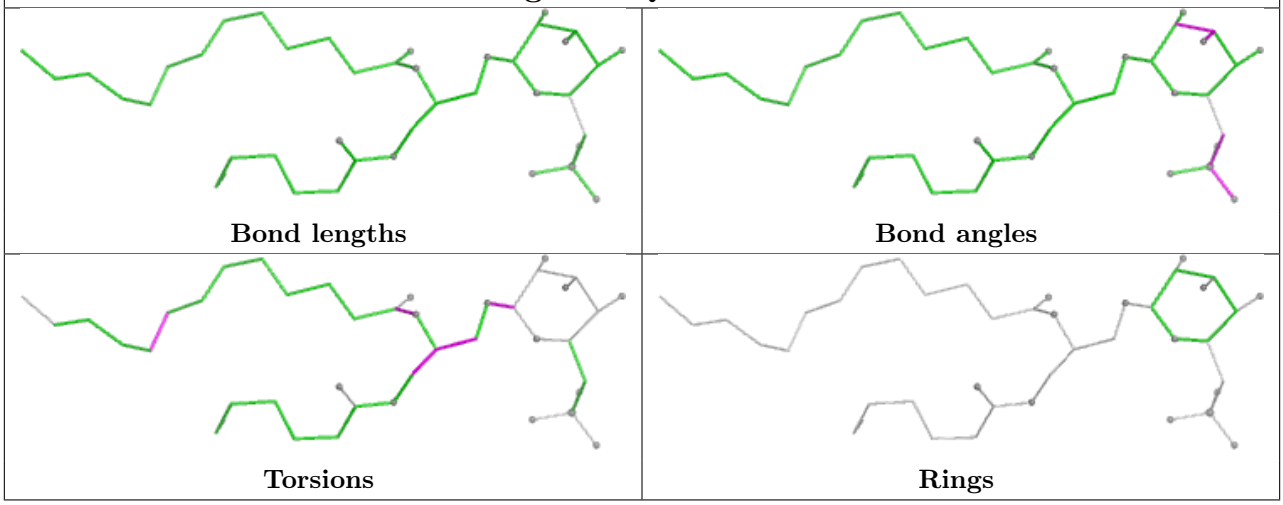
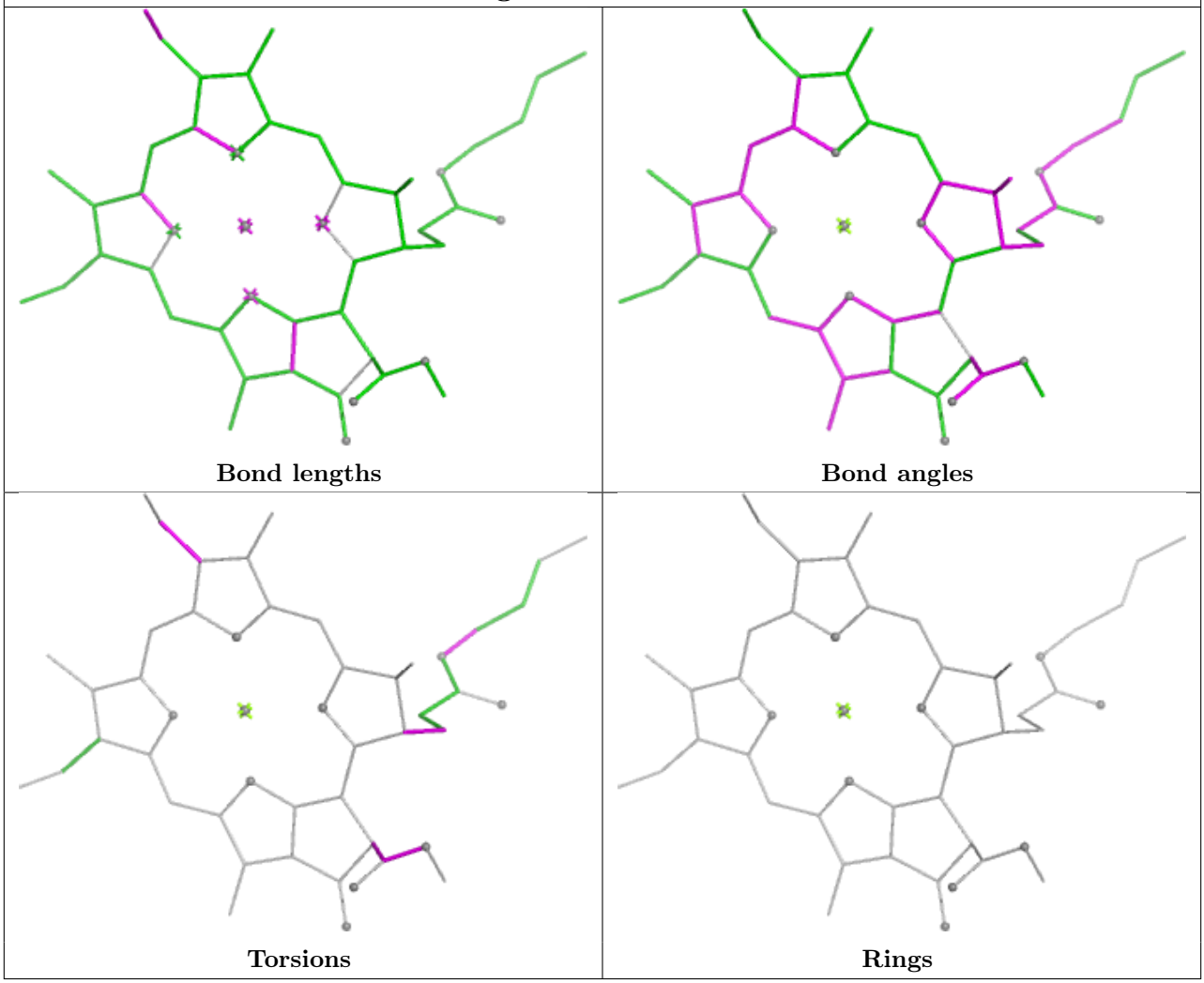


Rings

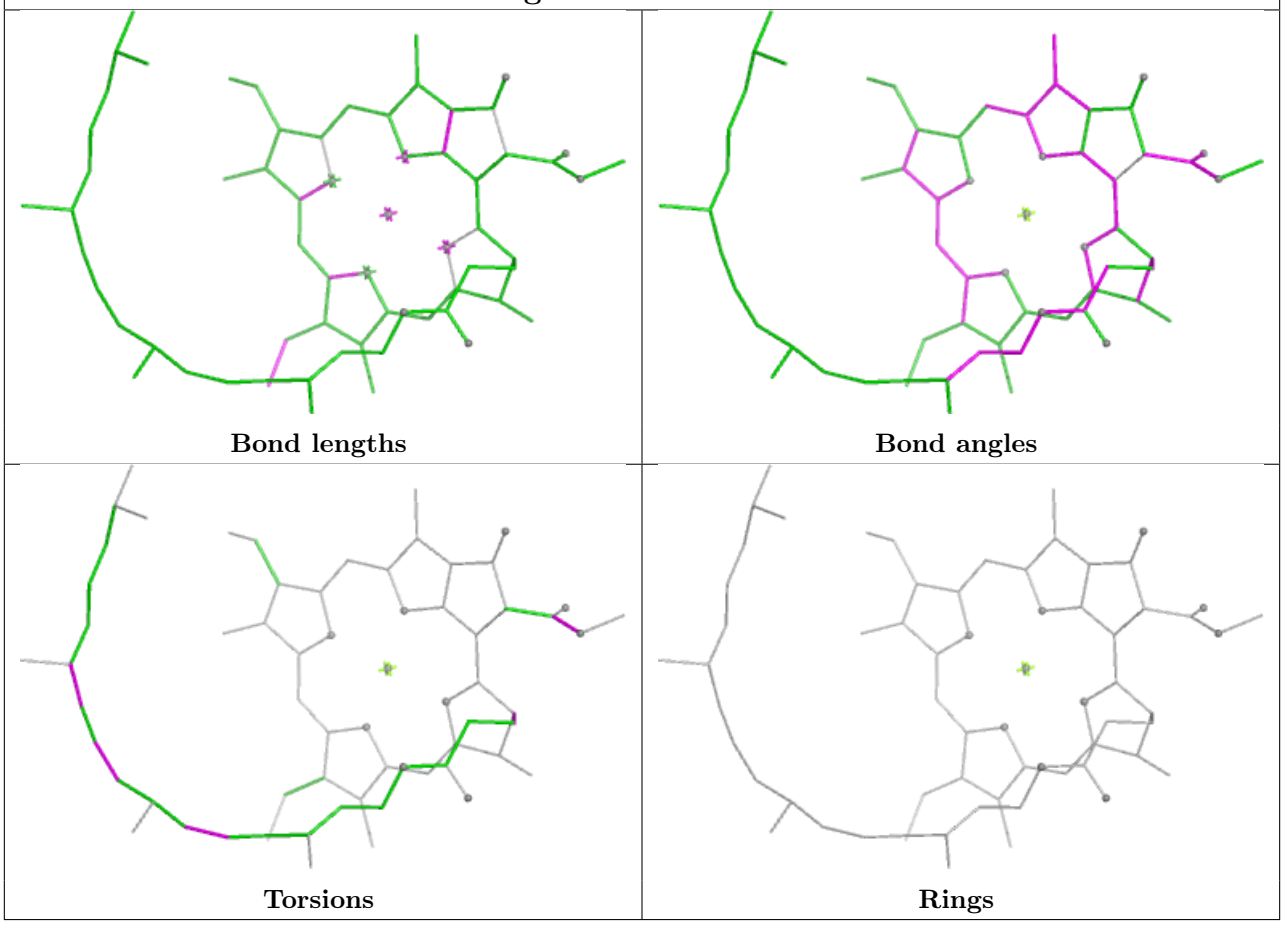
Ligand SQD Y 320



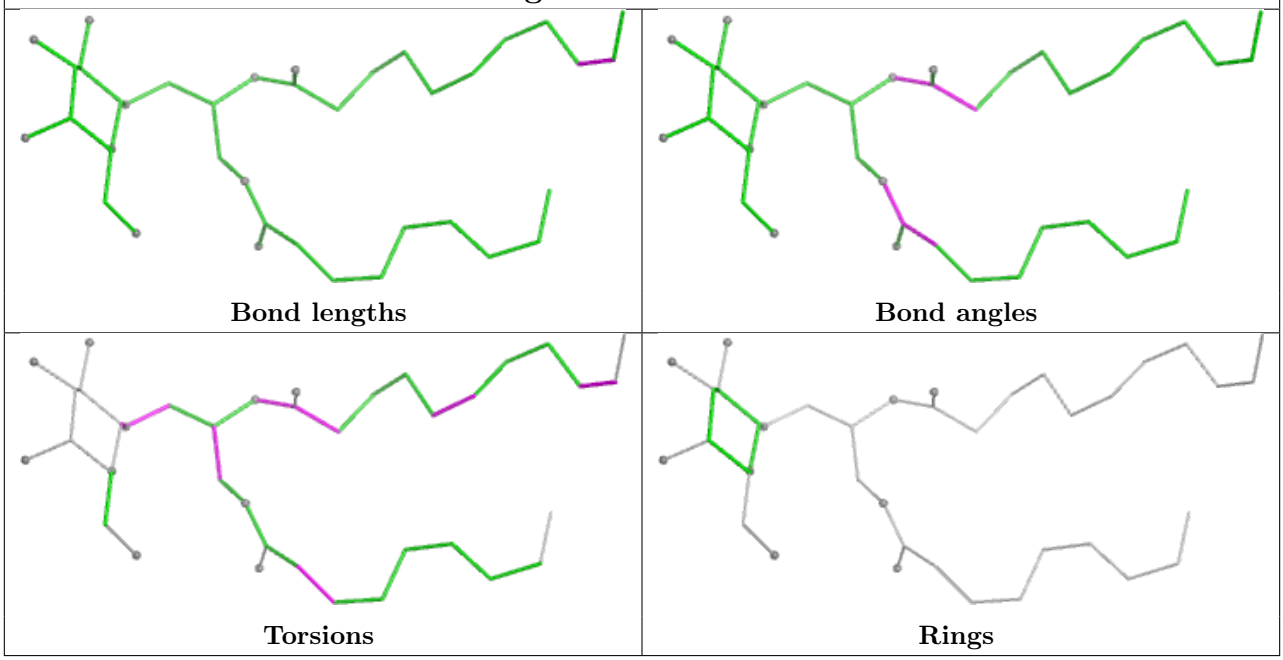
Ligand CLA d 401



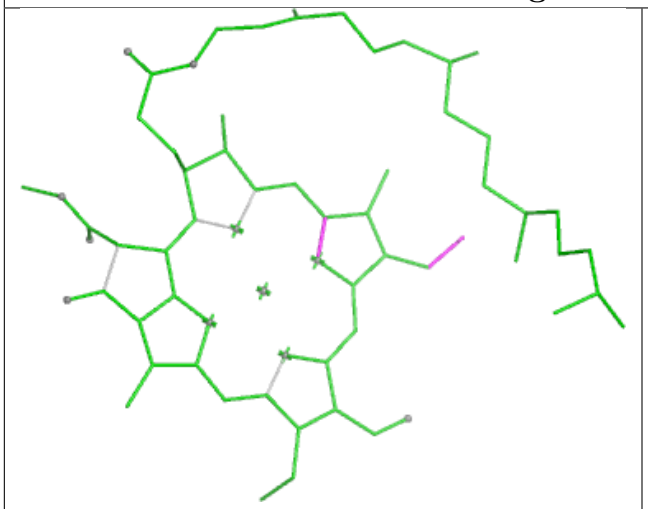
Ligand CLA G 609



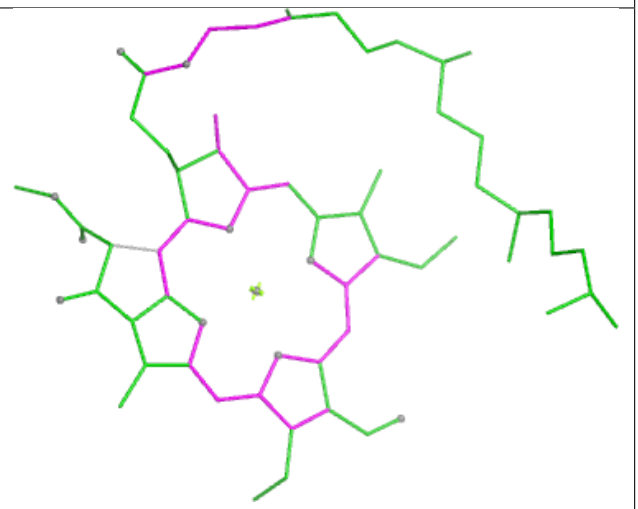
Ligand LMG 7 301



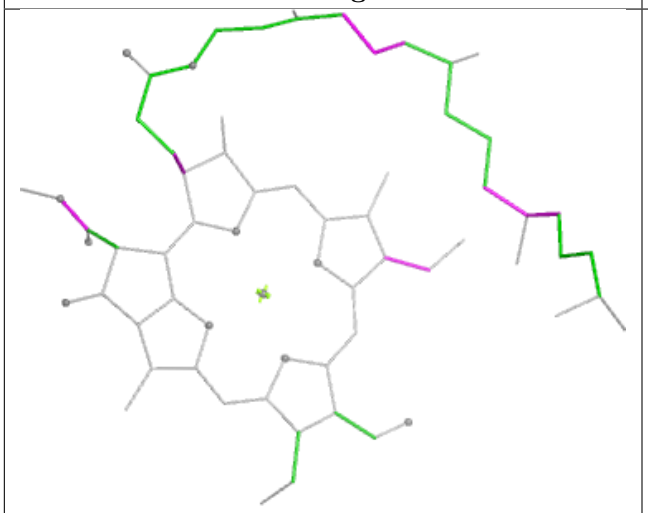
Ligand CHL 7 308



Bond lengths



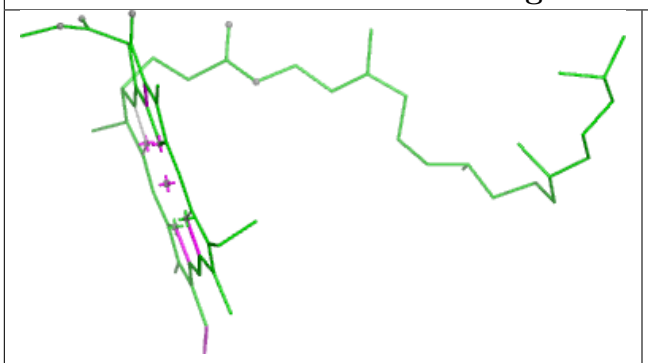
Bond angles



Torsions

Rings

Ligand CLA B 607



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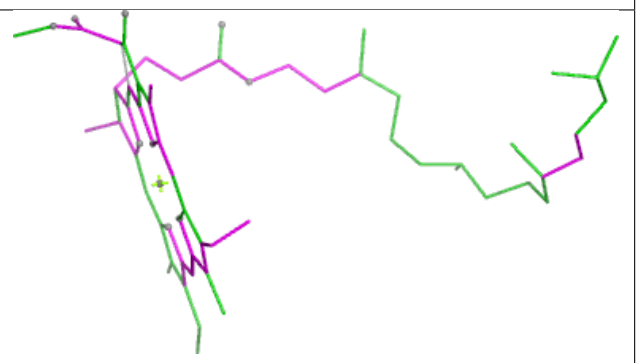
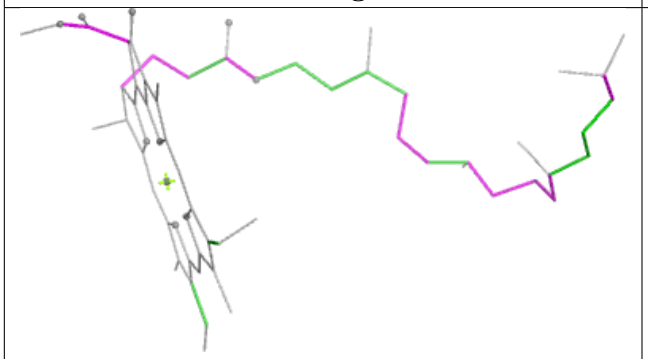


Bond angles



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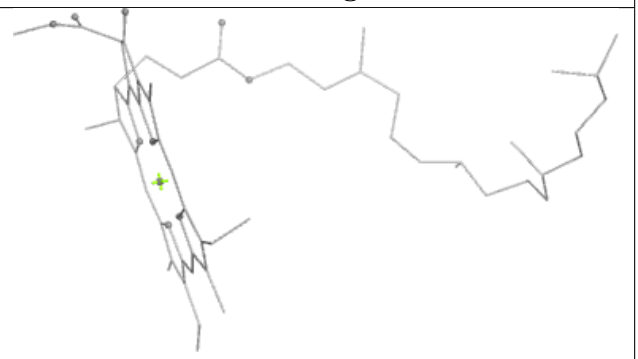
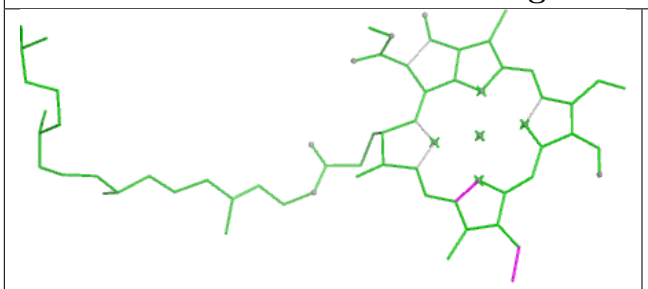
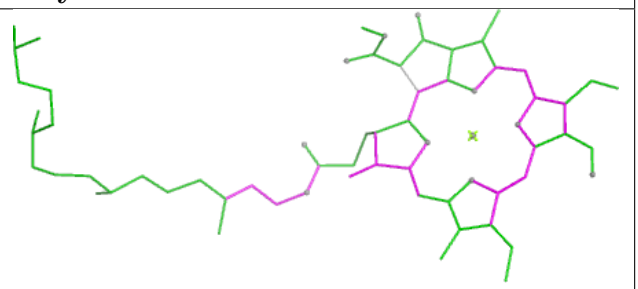


Rings

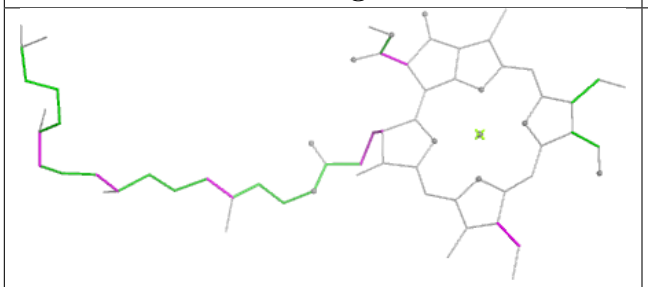
Ligand CHL y 601



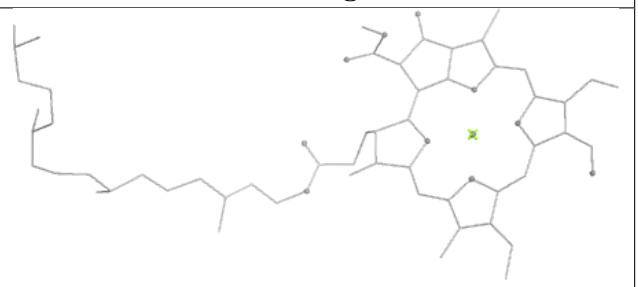
Bond lengths



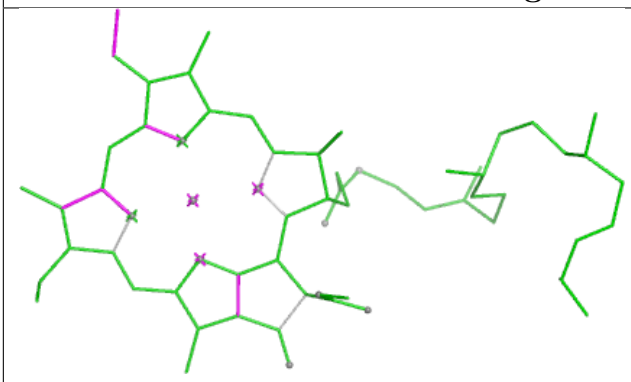
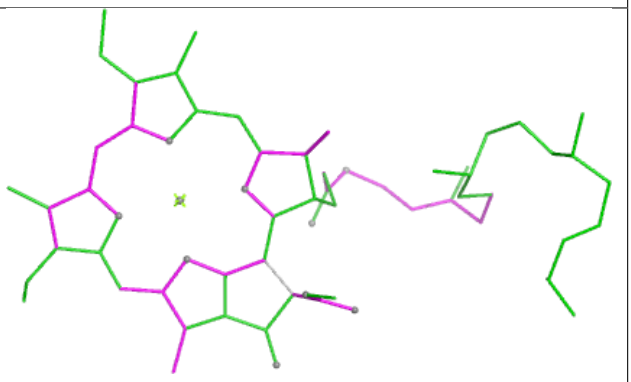
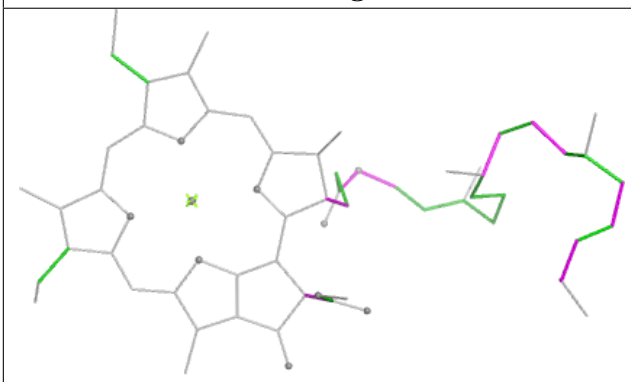
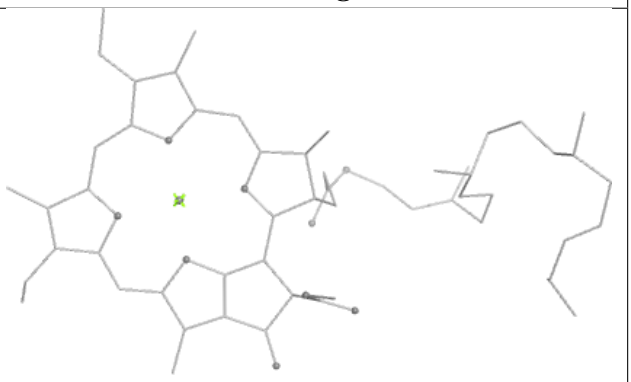
Bond angles



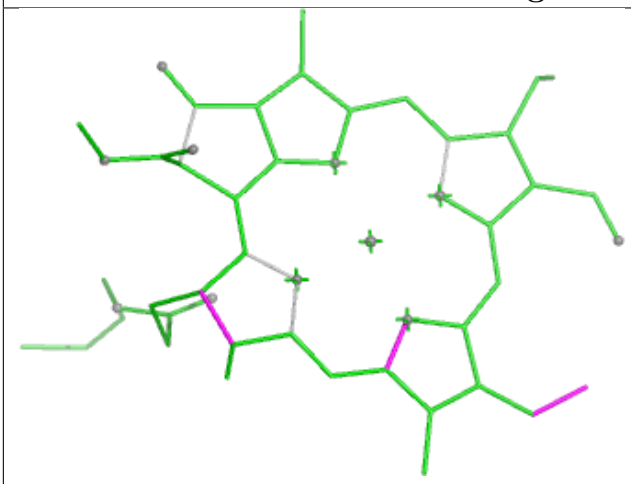
Torsions



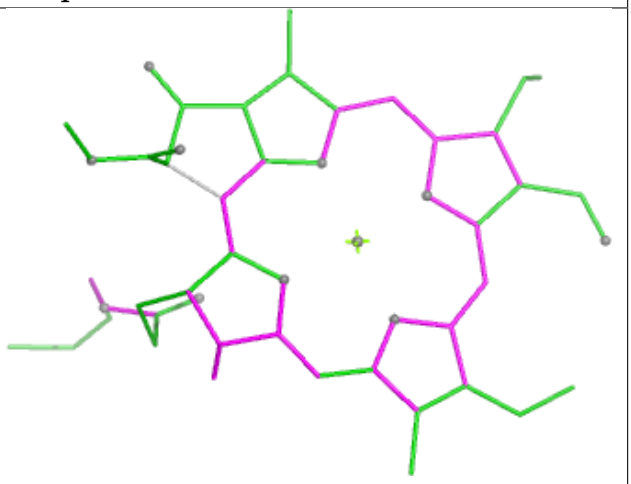
Rings

Ligand CLA B 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

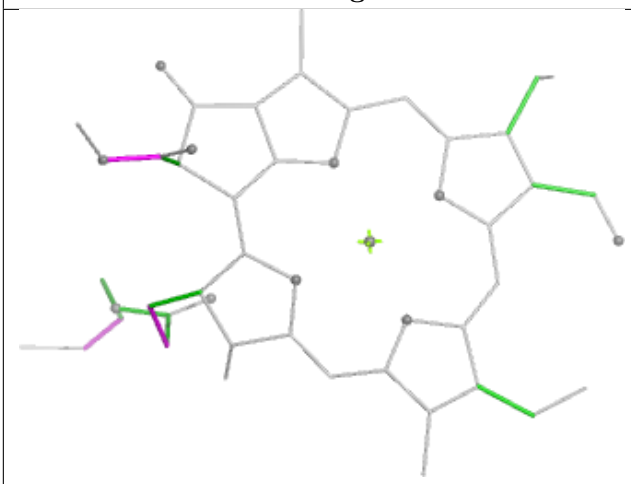
Ligand CHL q 310



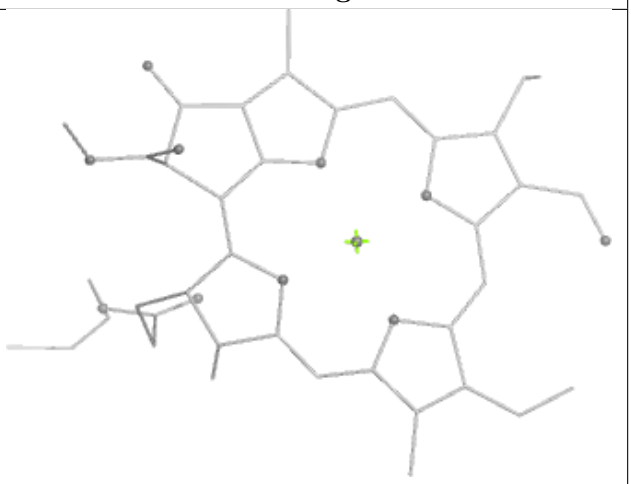
Bond lengths



Bond angles

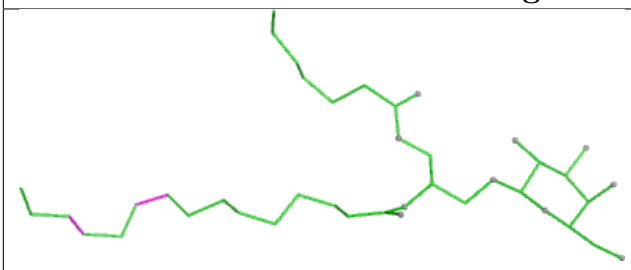


Torsions



Rings

Ligand LMG S 321



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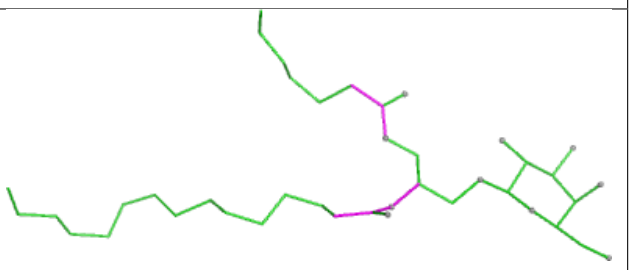
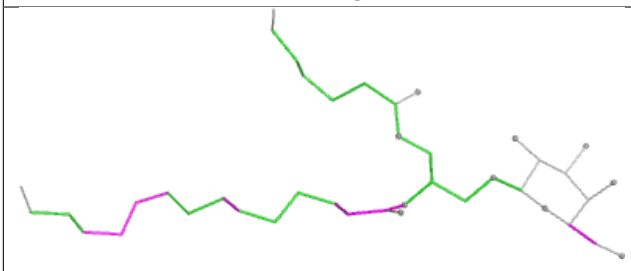


Bond angles



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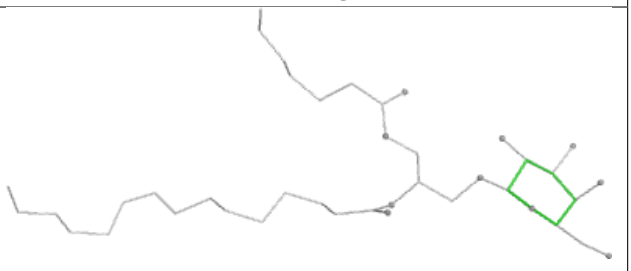
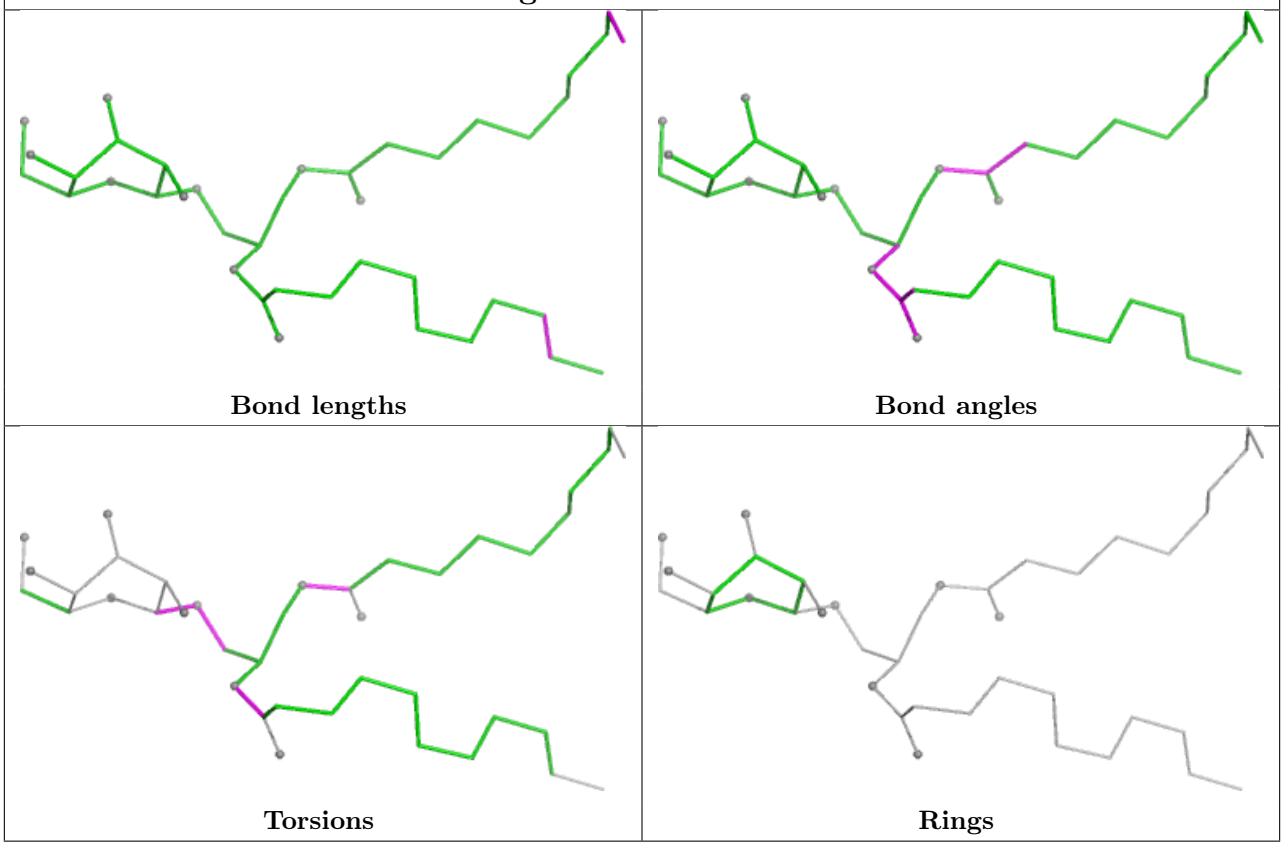
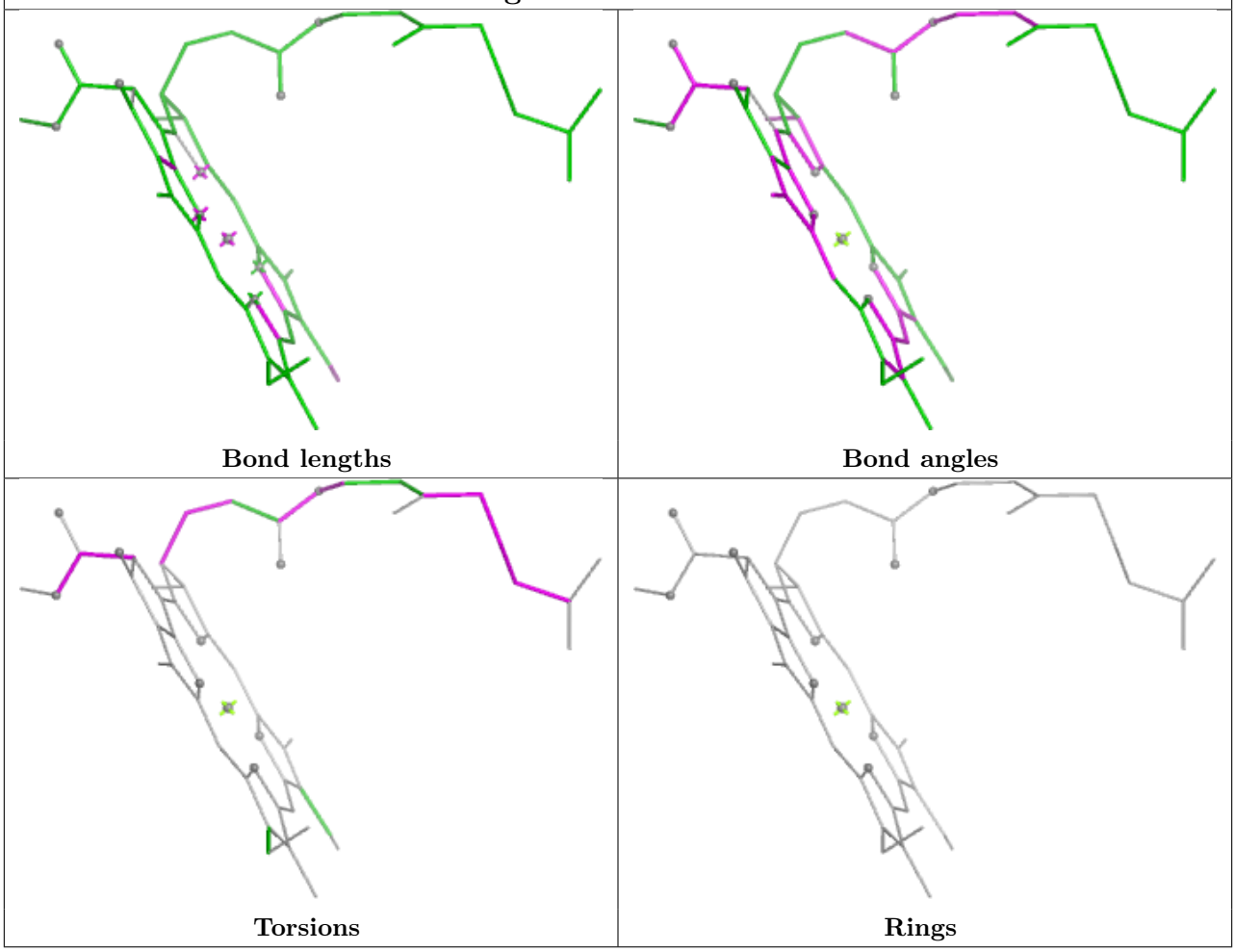


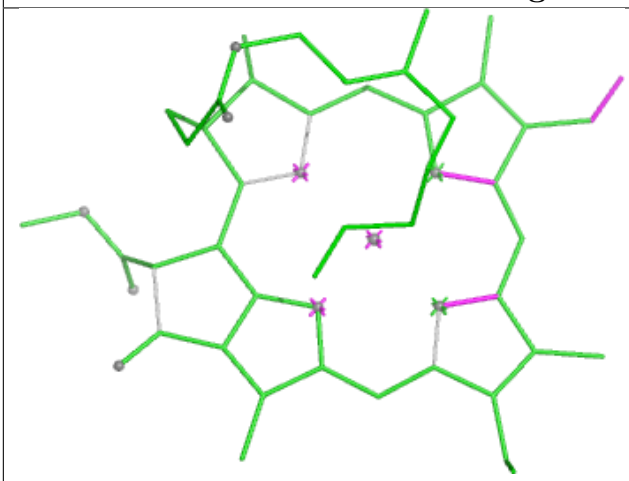
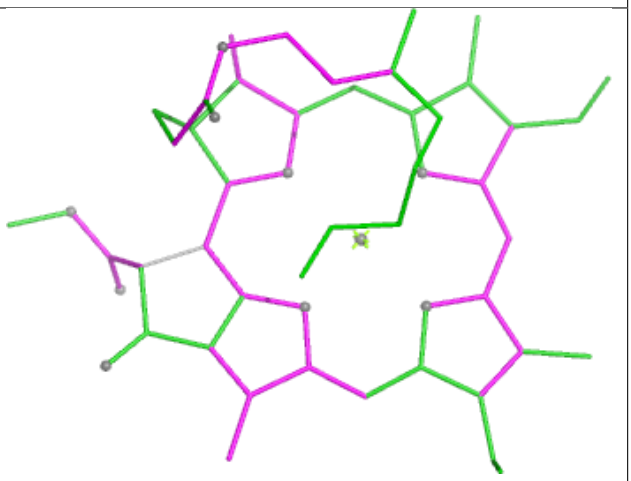
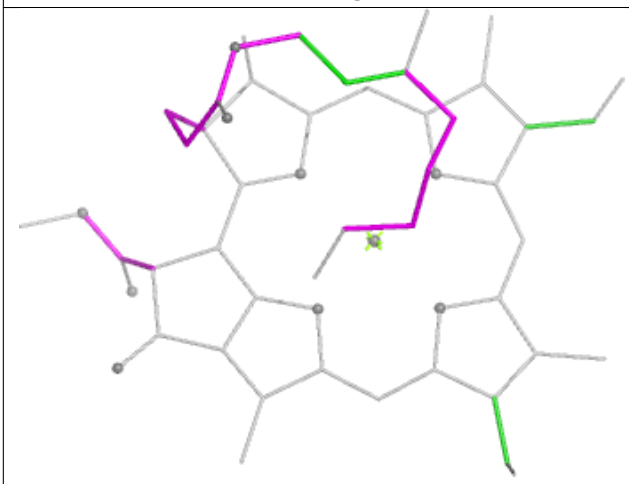
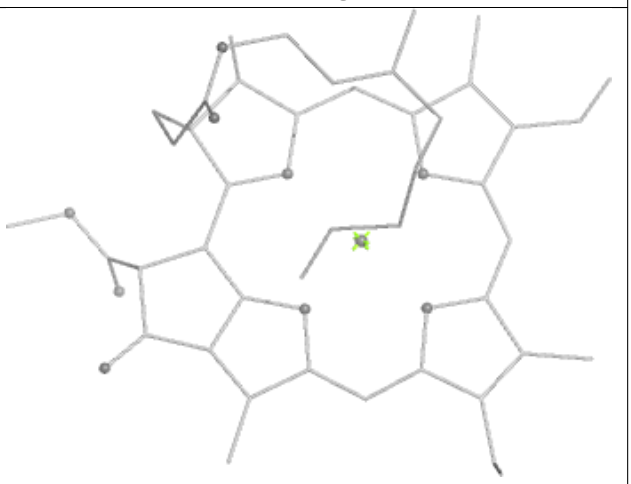
Rings

Ligand LMG G 622

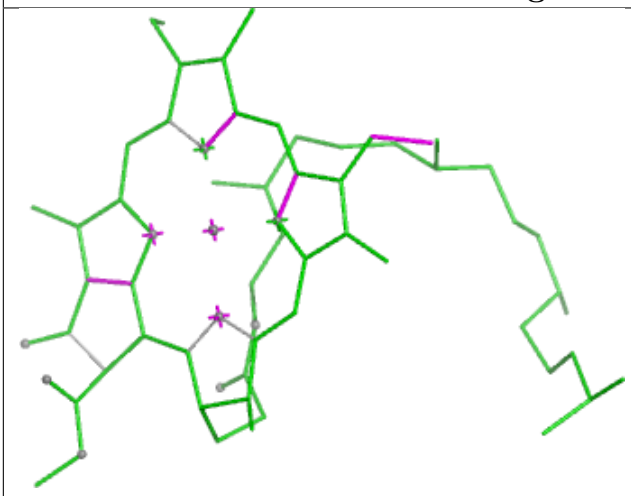


Ligand CLA G 604

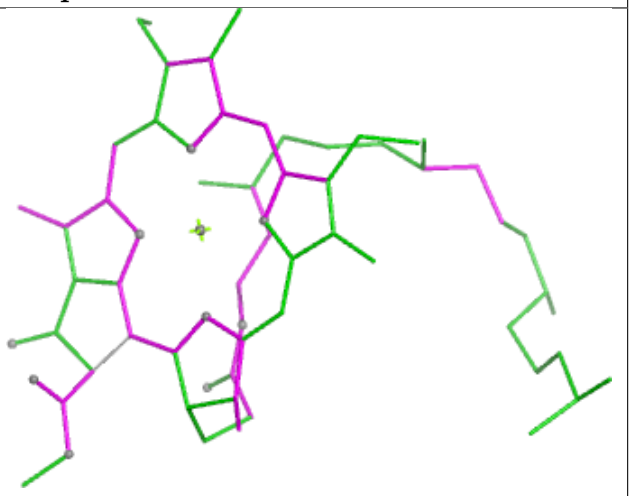


Ligand CLA 7 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

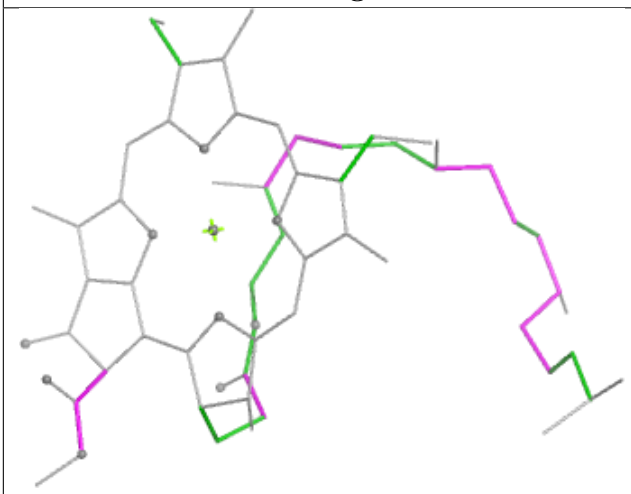
Ligand CLA q 315



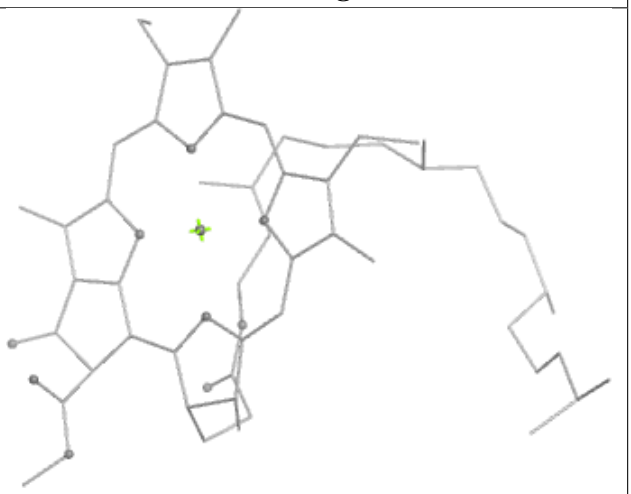
Bond lengths



Bond angles

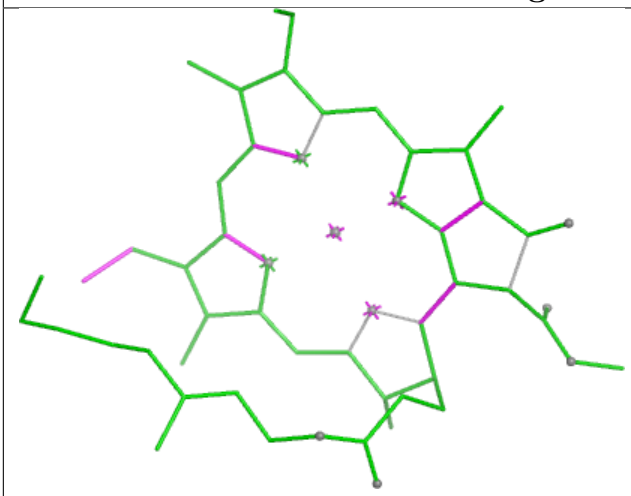


Torsions

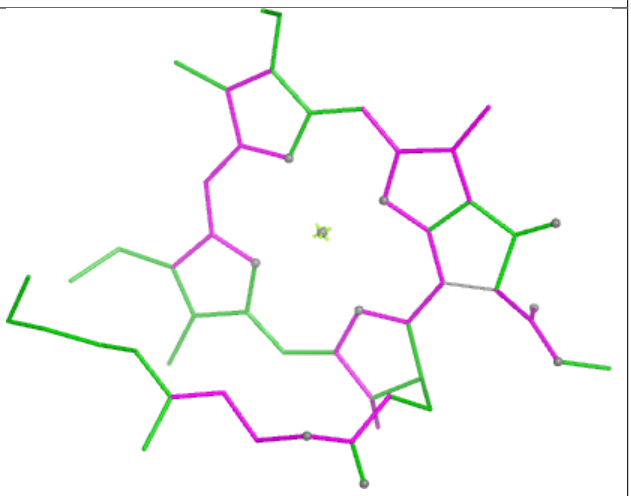


Rings

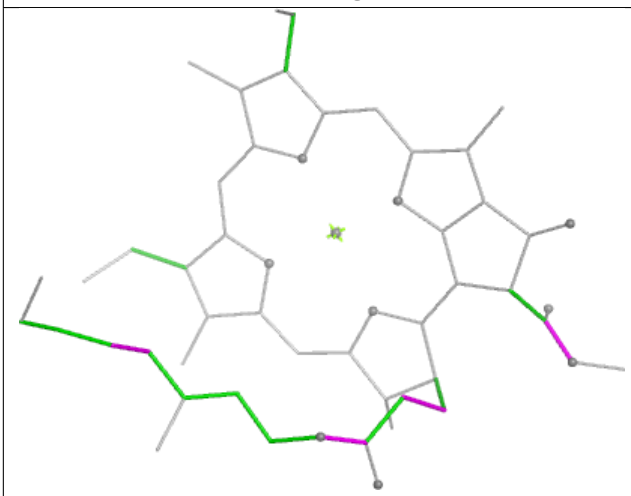
Ligand CLA 3 311



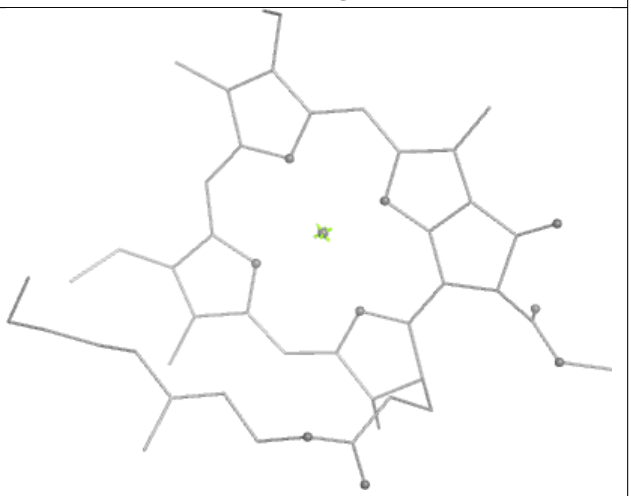
Bond lengths



Bond angles

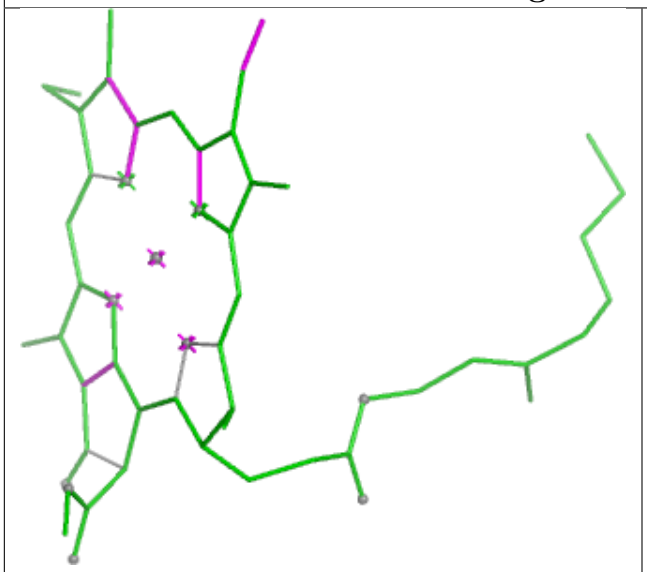


Torsions



Rings

Ligand CLA y 615



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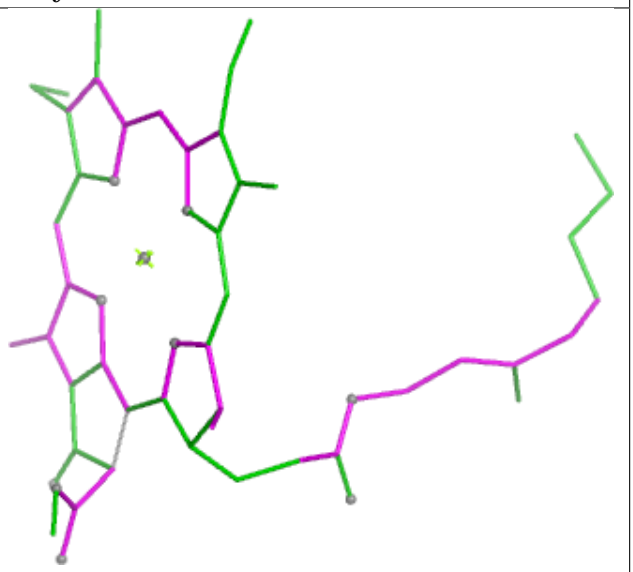

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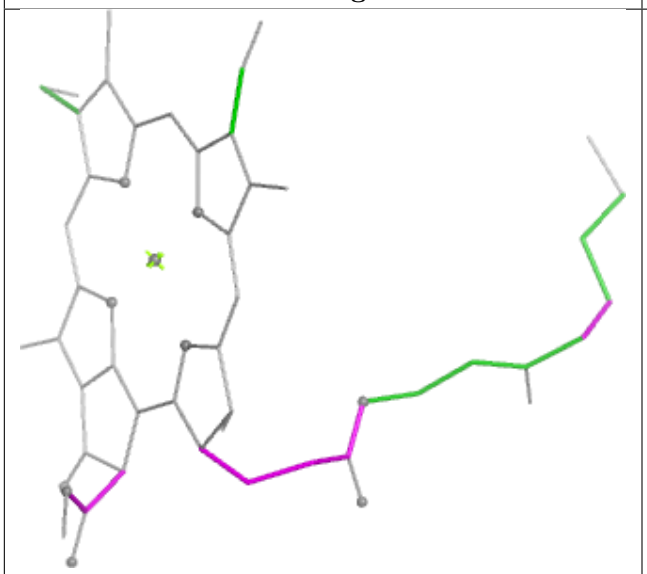

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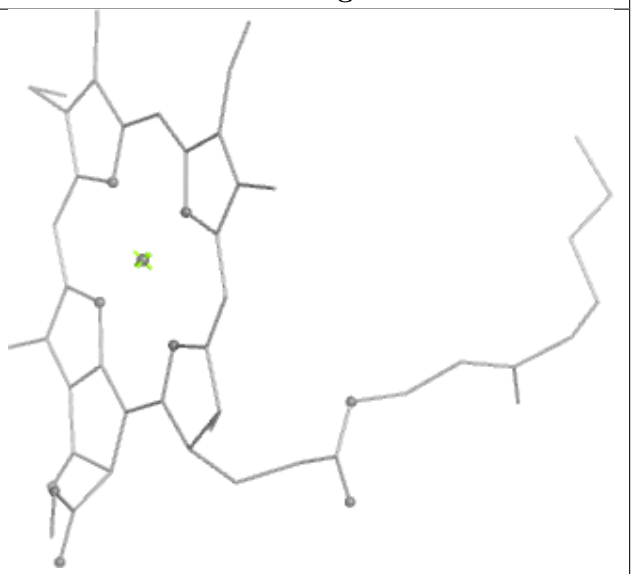
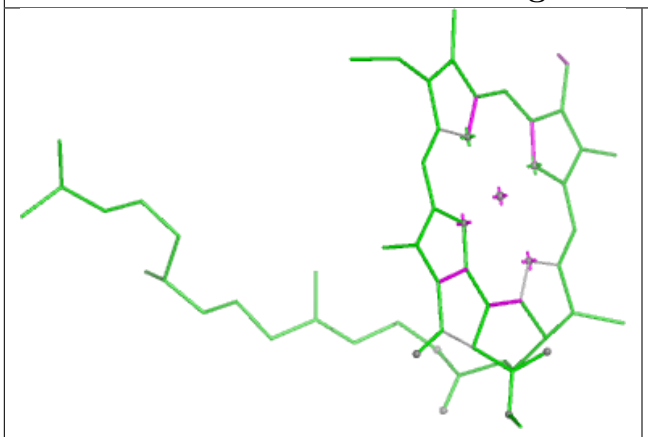


Rings

Ligand CLA S 310



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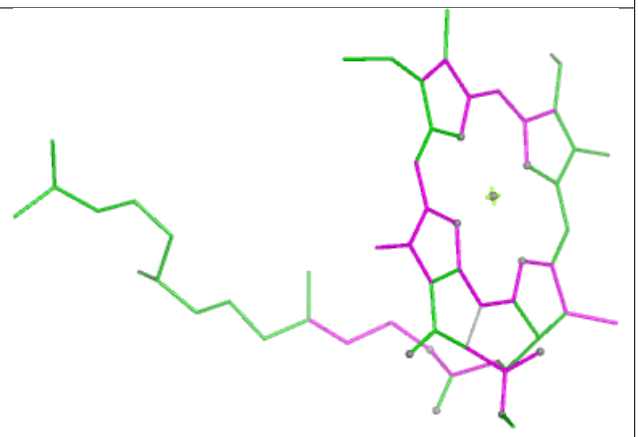
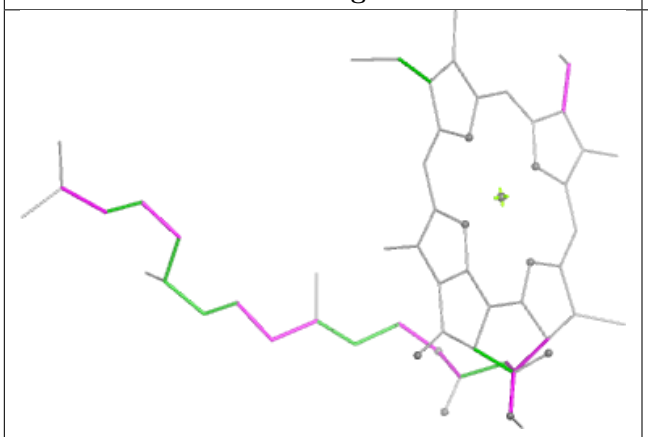


Bond angles



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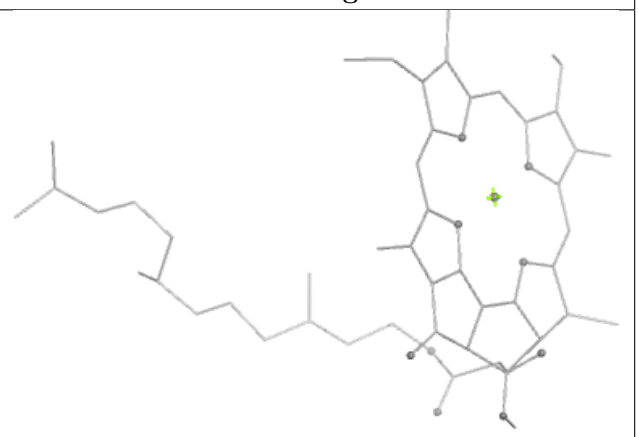
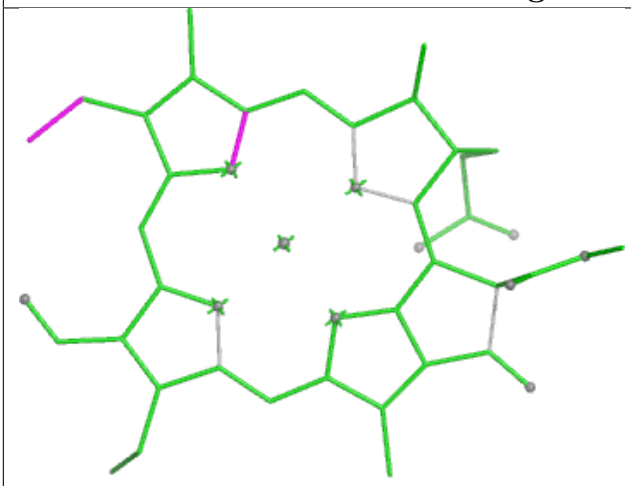


Rings

Ligand CHL 5 605



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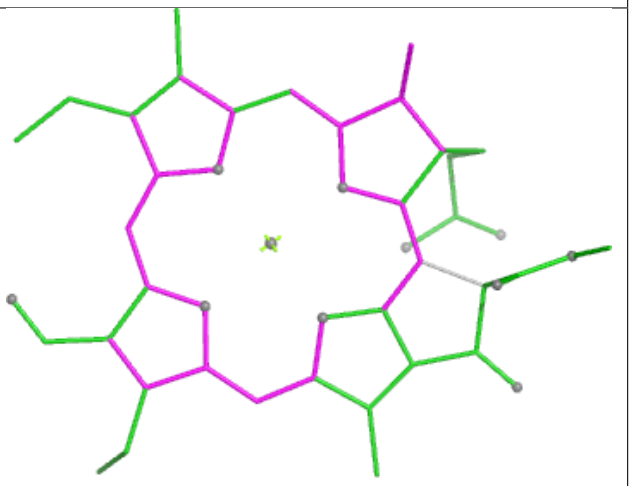

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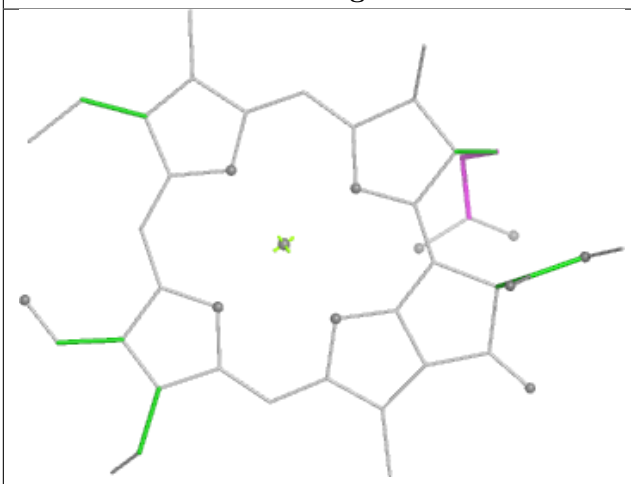

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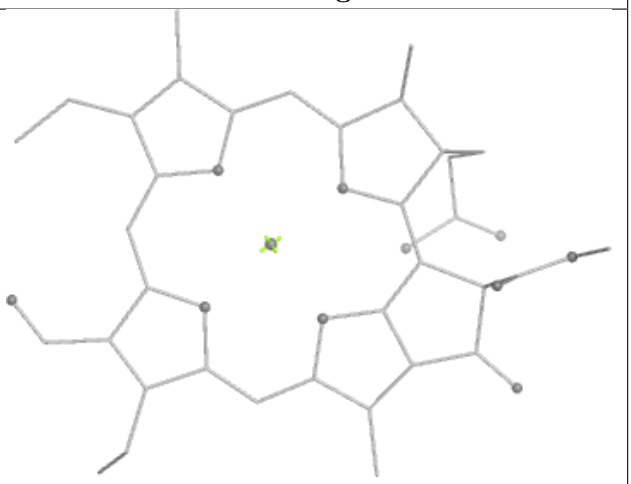
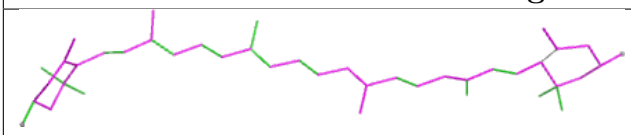


Rings

Ligand LUT n 318



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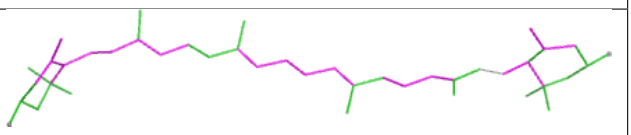

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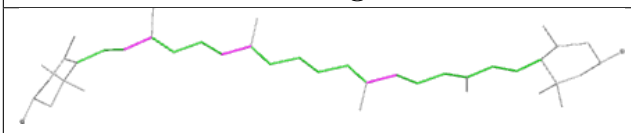

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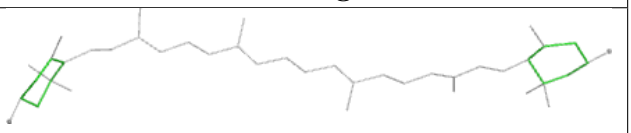
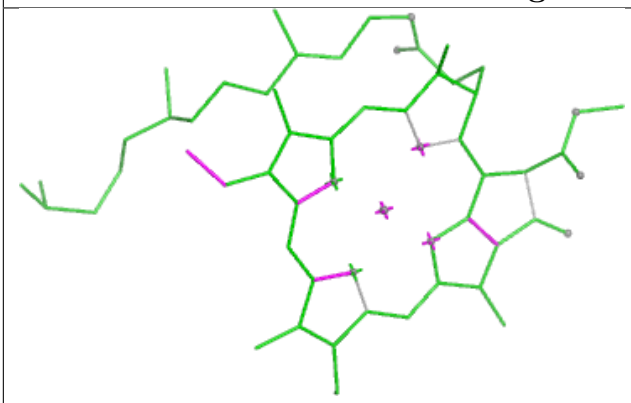


Rings

Ligand CLA 4 610



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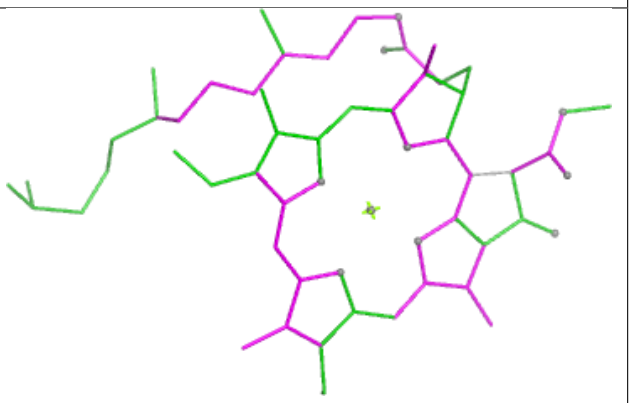

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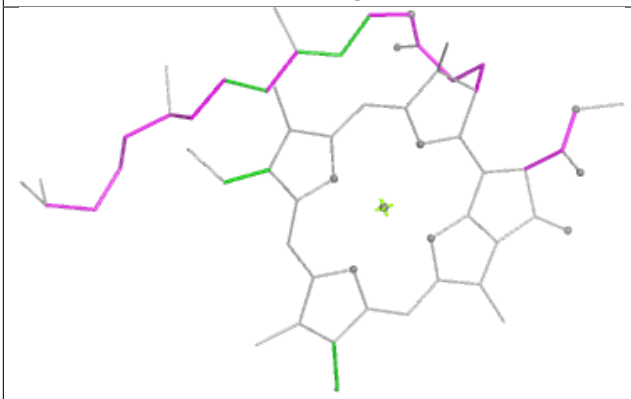

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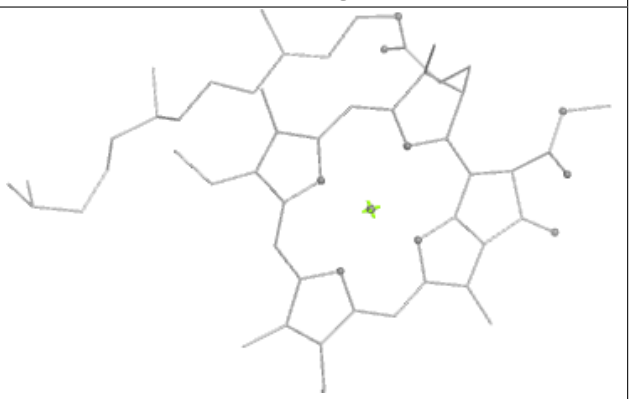
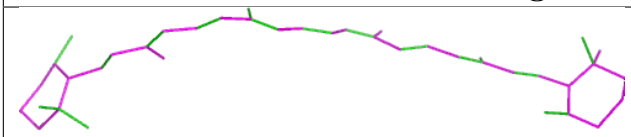


Rings

Ligand BCR t 101



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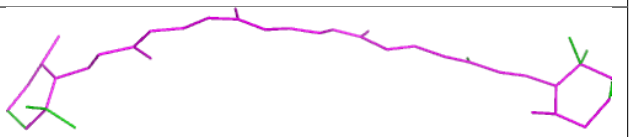

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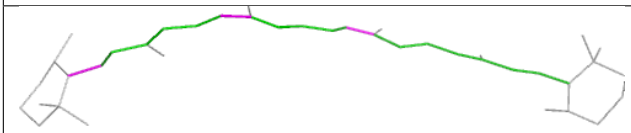

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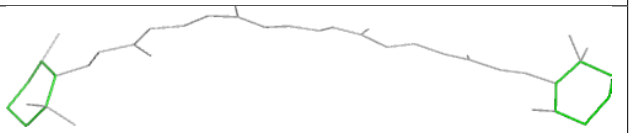

Rings

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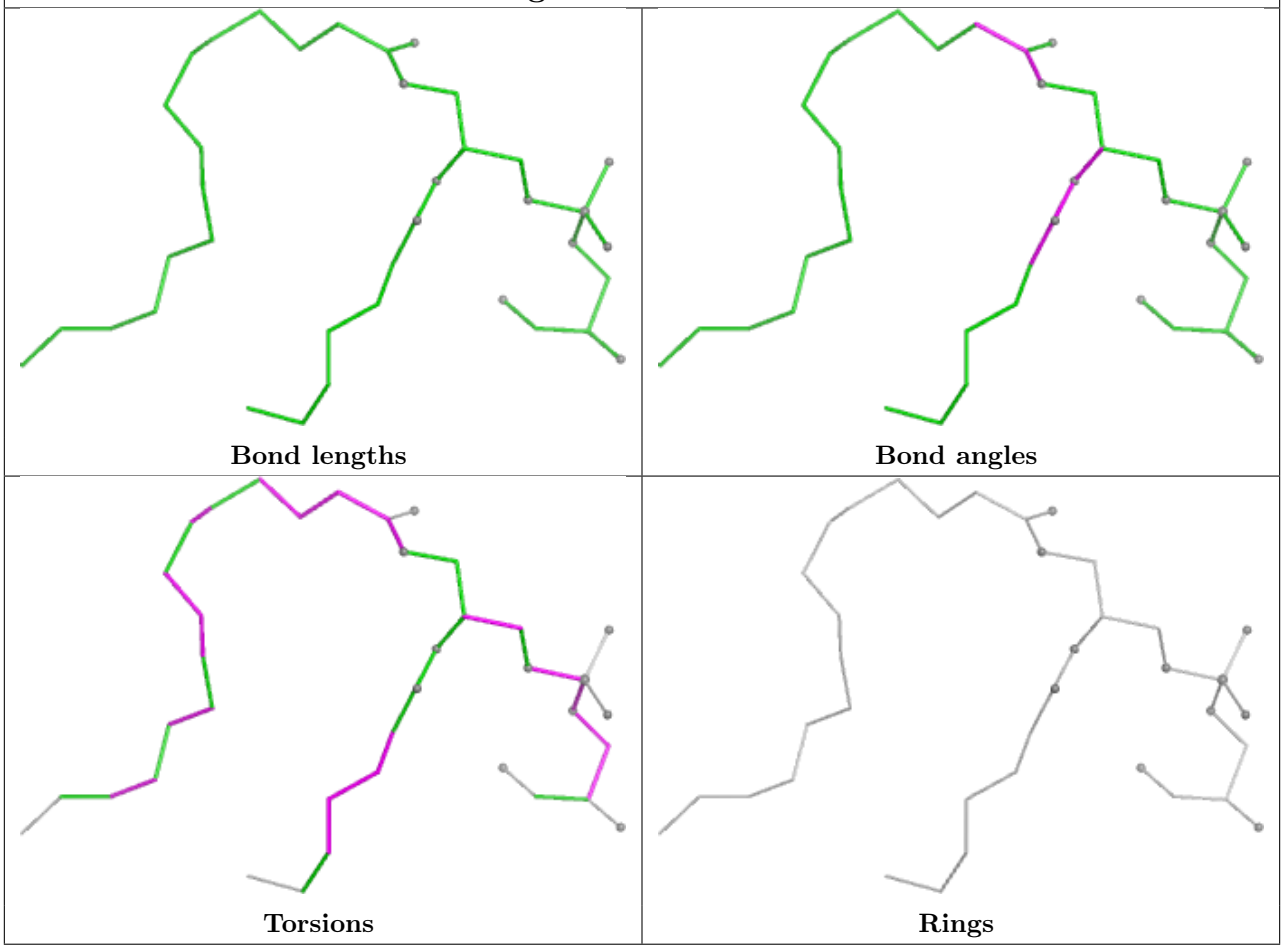
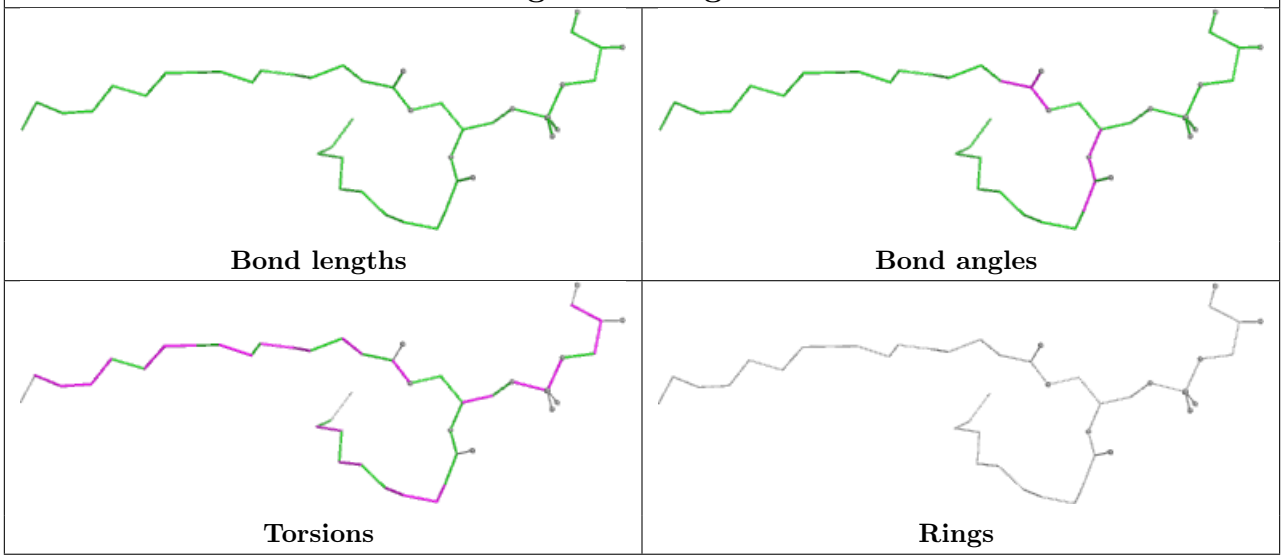


Ligand LHG g 319



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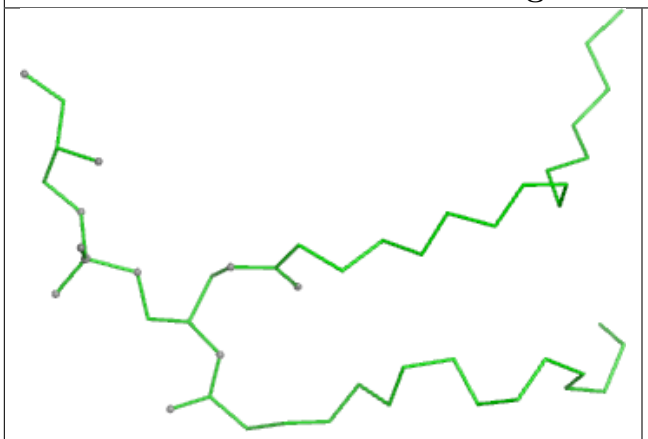

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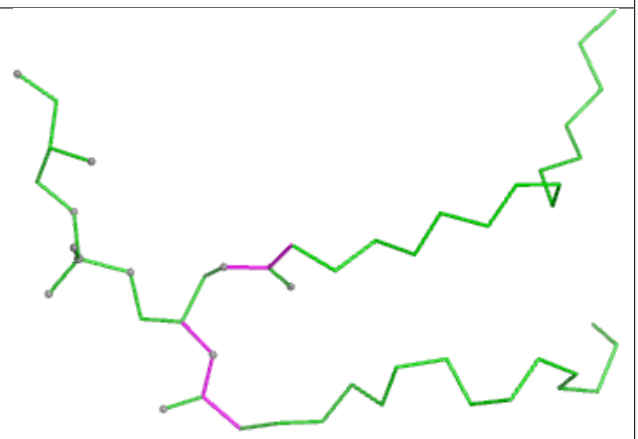

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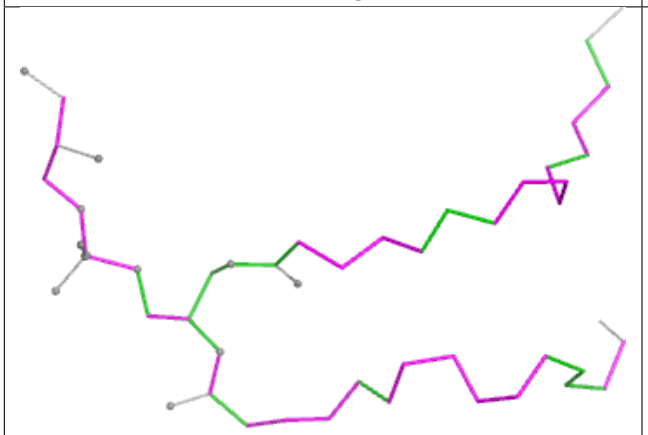
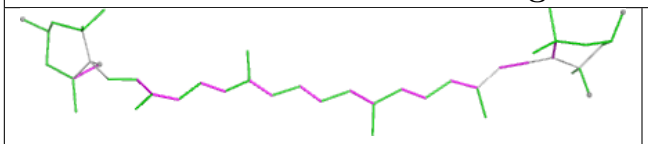


Torsions

Rings

Ligand NEX r 319



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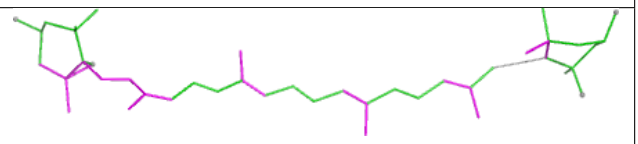
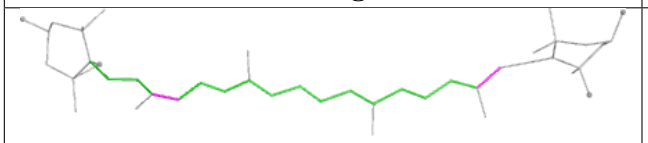


Bond angles



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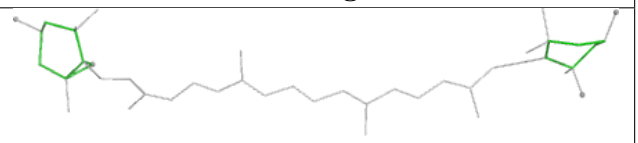
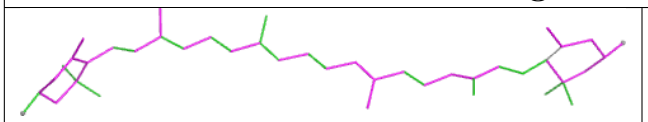


Rings

Ligand LUT 1 616



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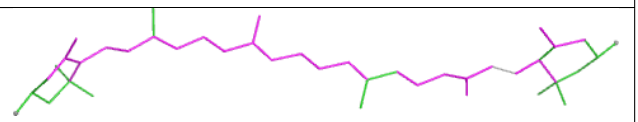
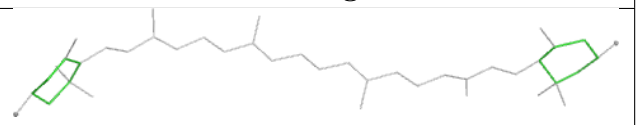


Bond angles

Torsions



Rings

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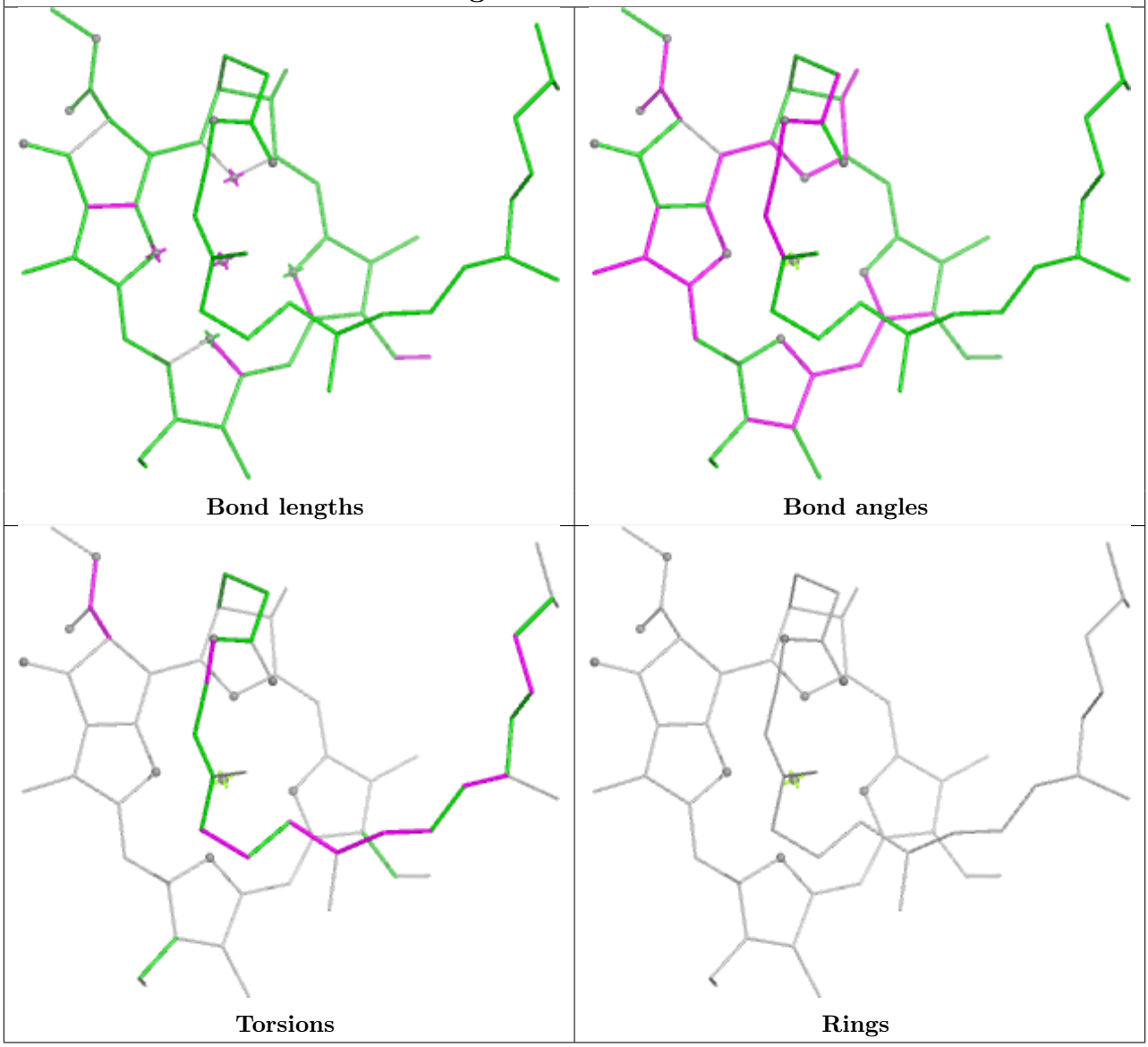

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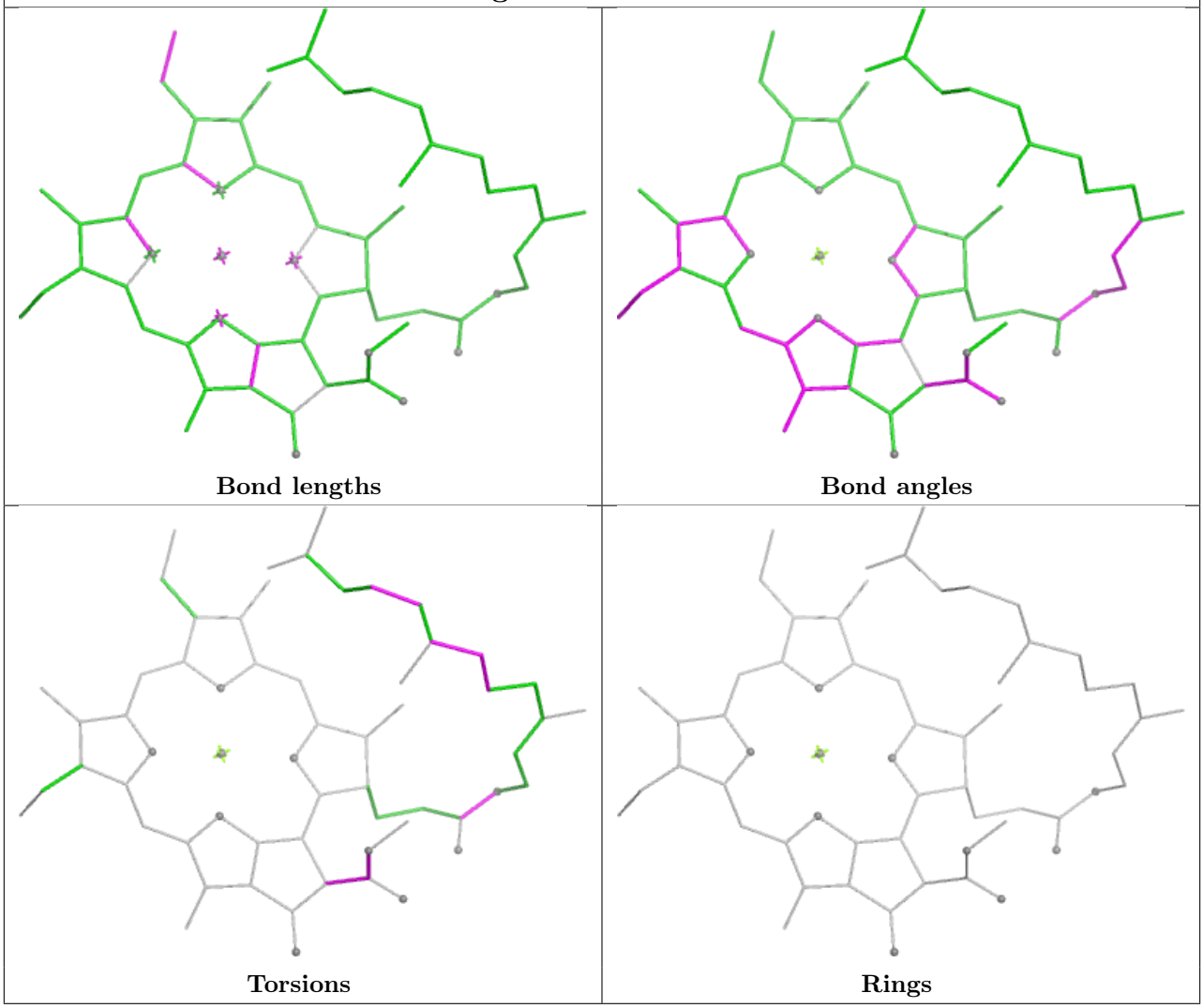

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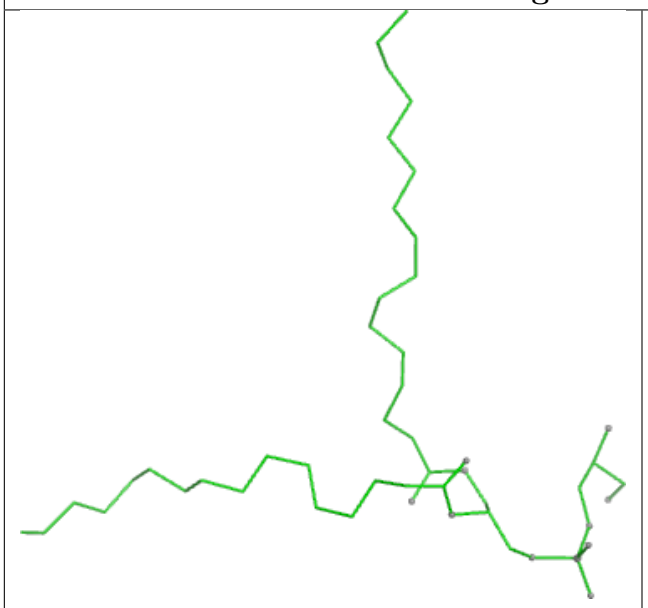

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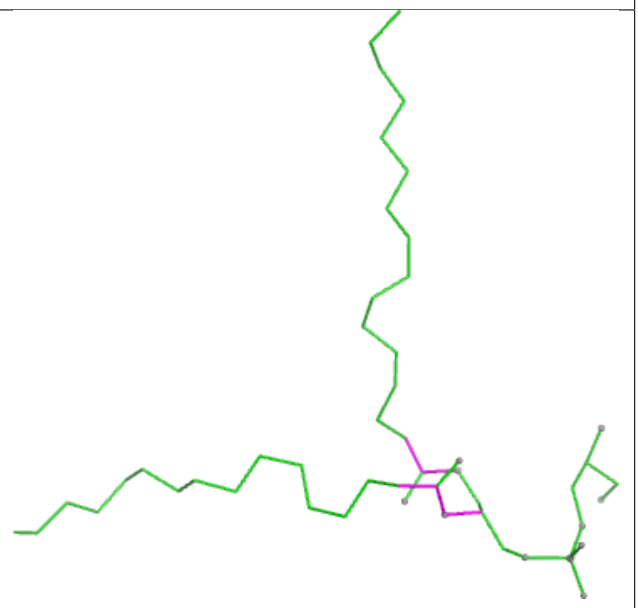

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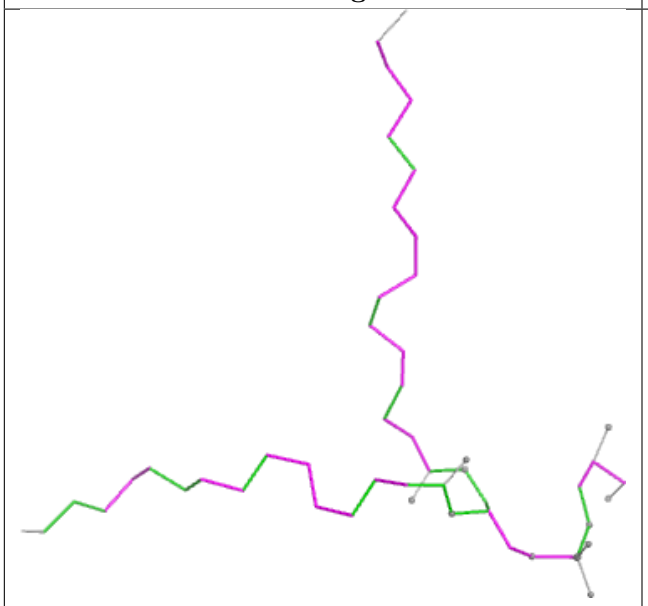
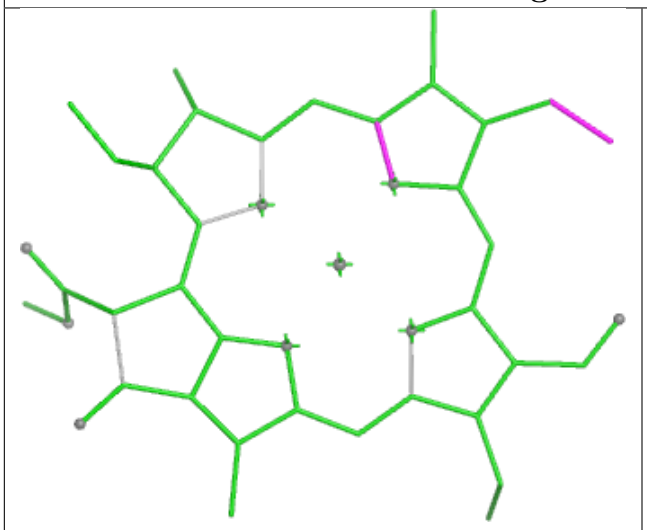


Torsions

Rings

Ligand CHL s 308



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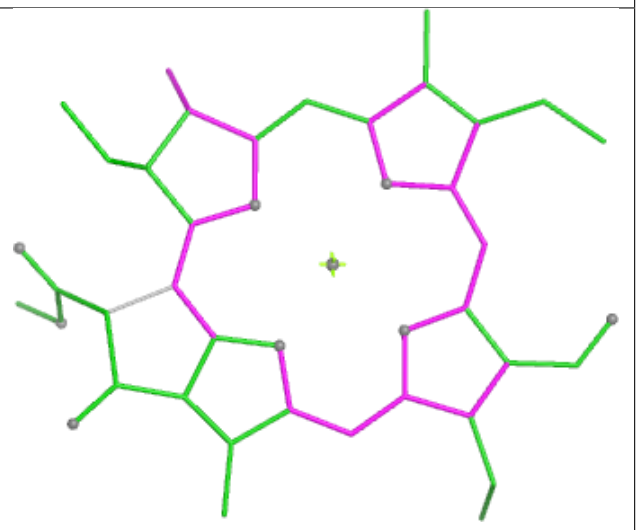

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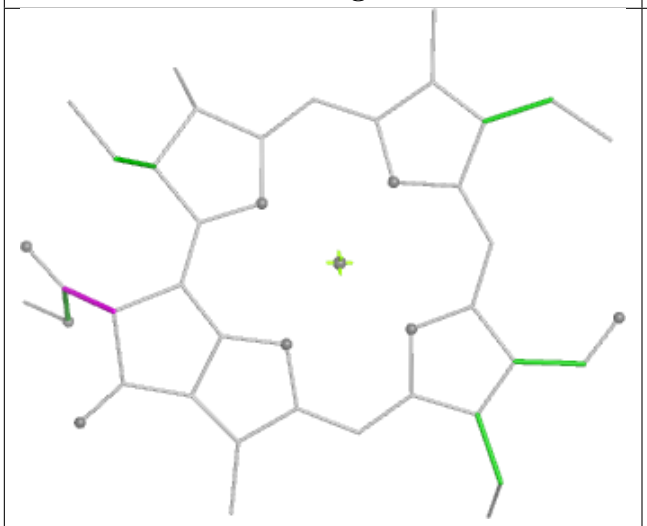

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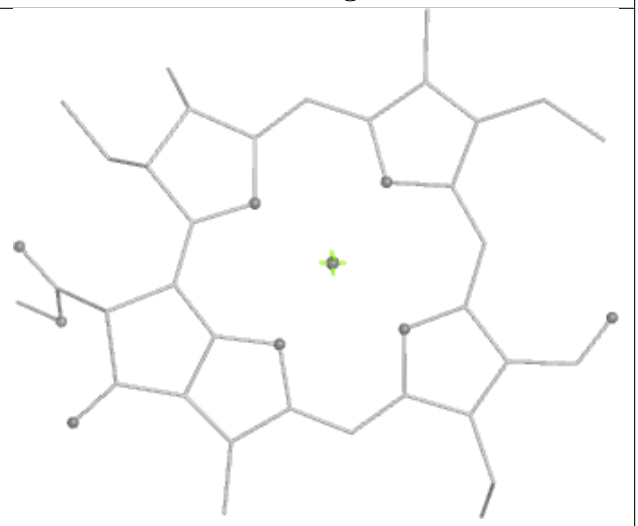
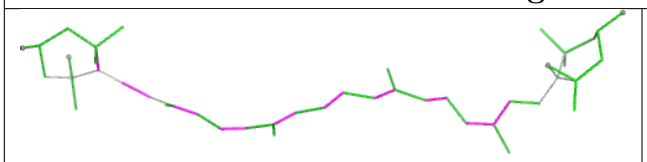


Rings

Ligand NEX 5 618



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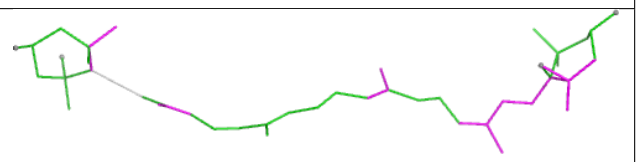

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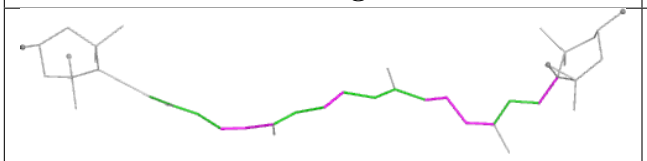

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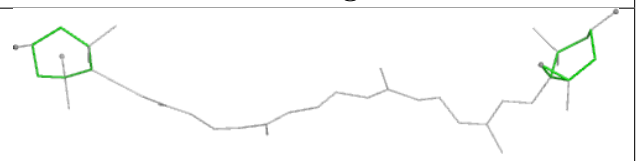
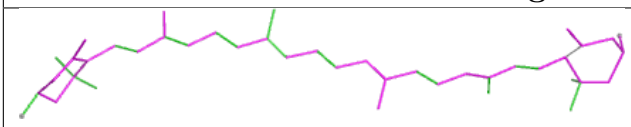
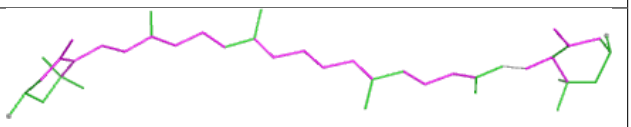
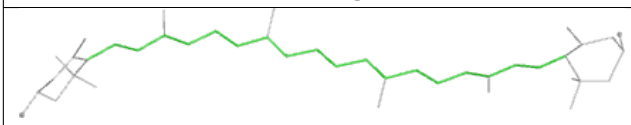
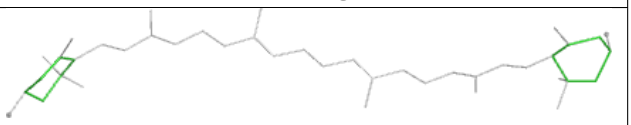
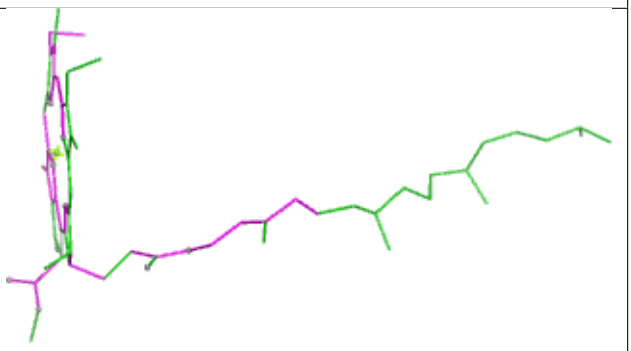
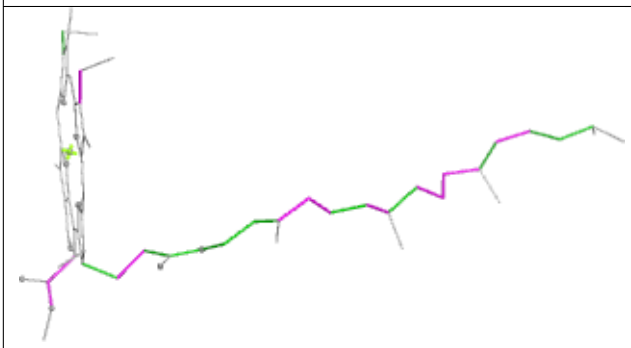
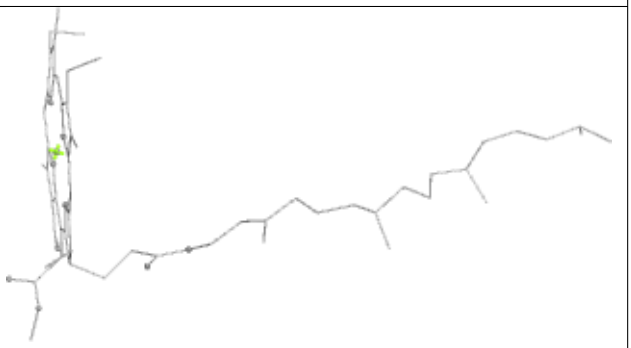
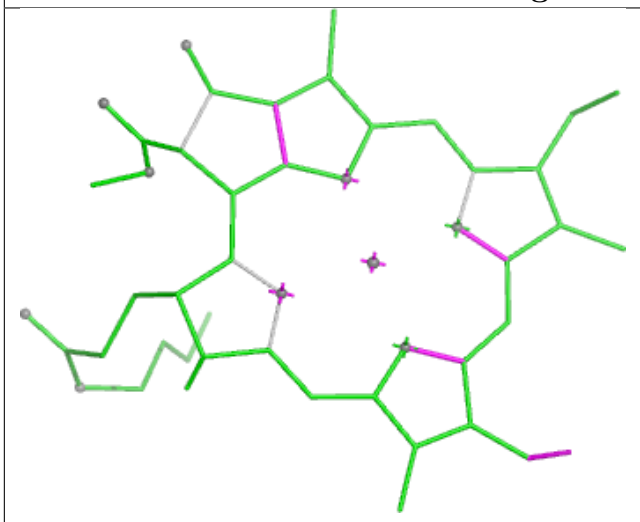
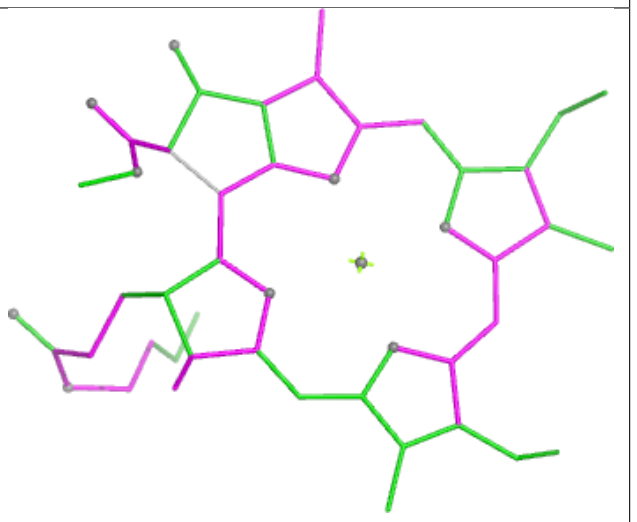
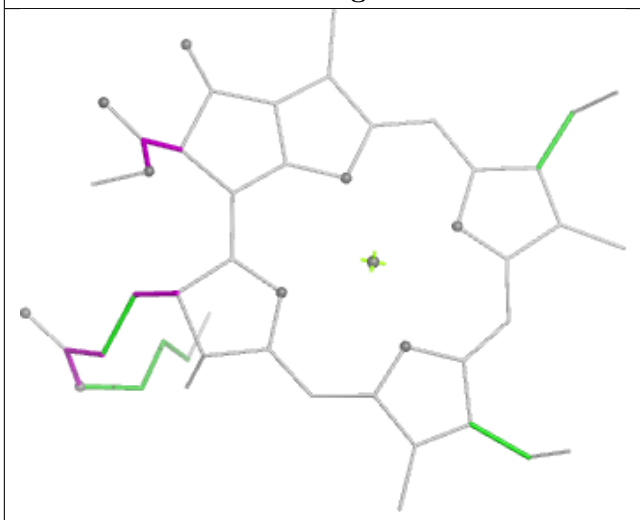
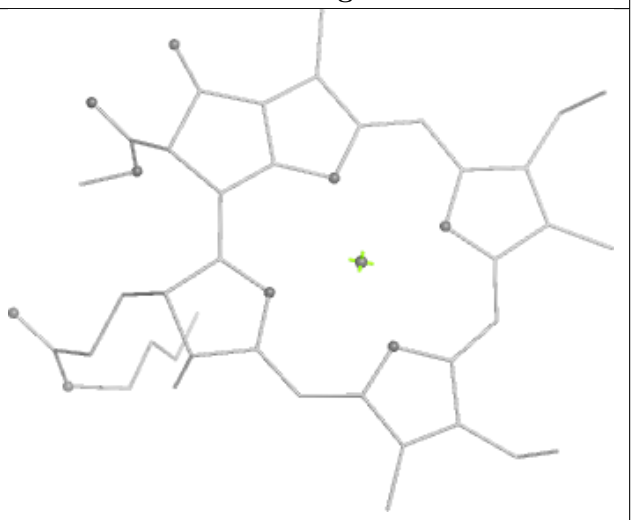


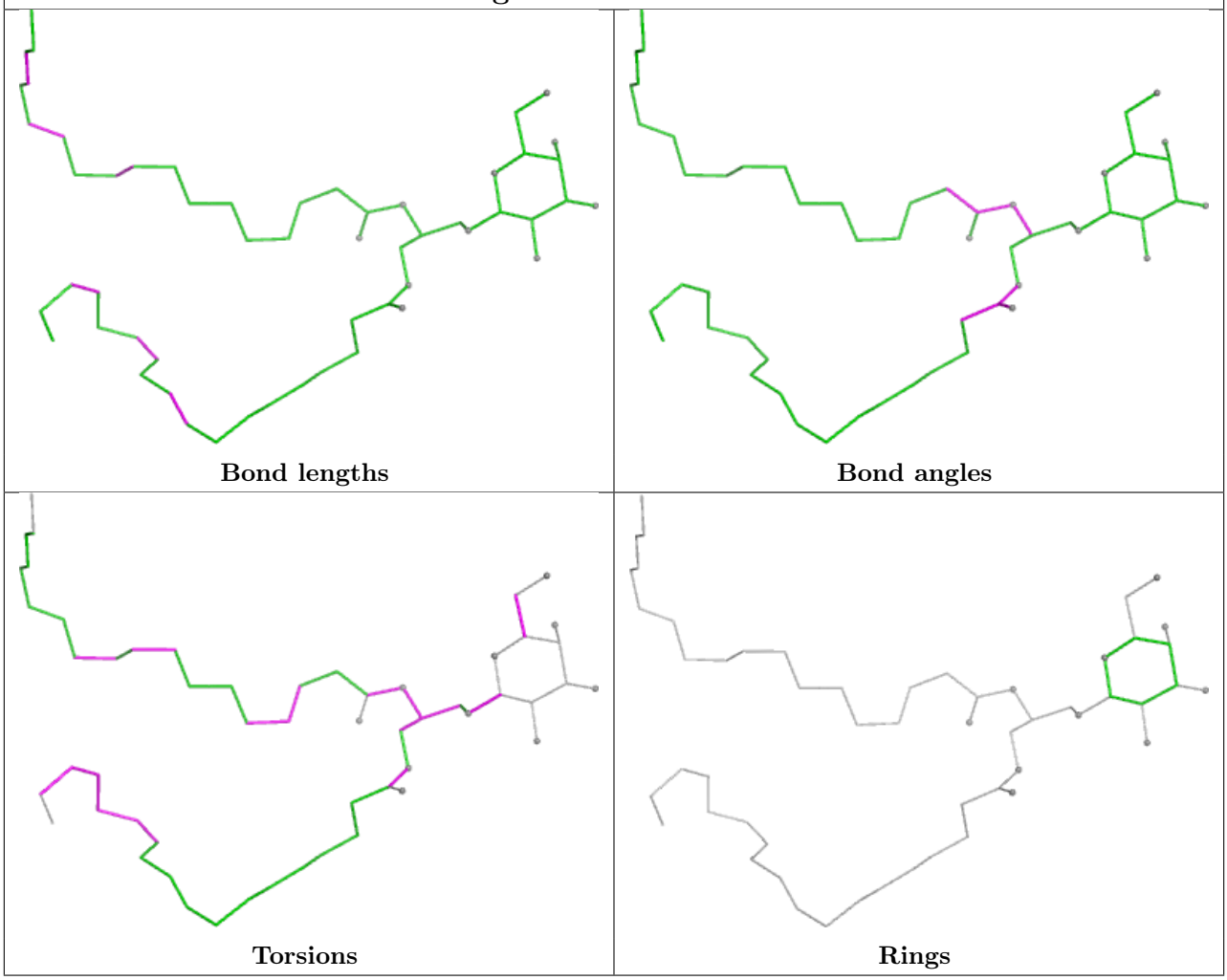
Rings

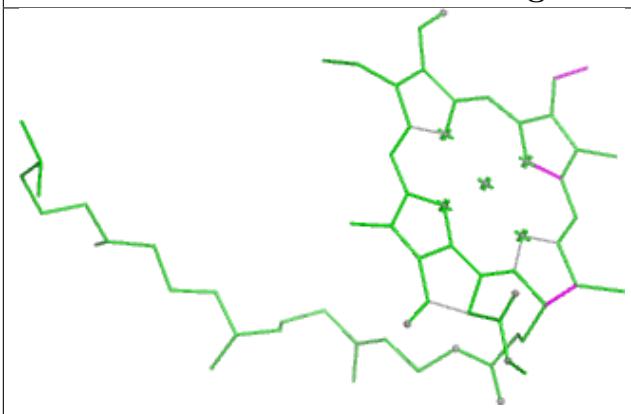
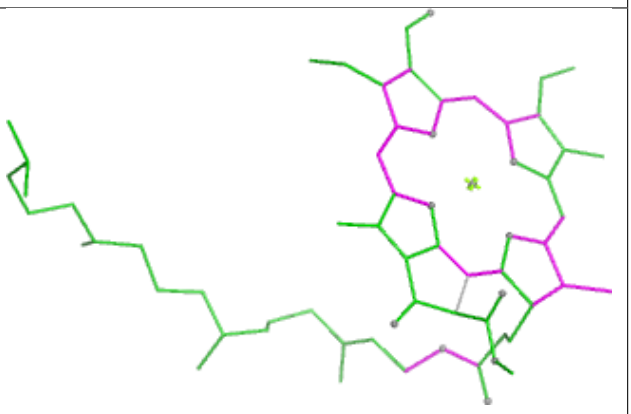
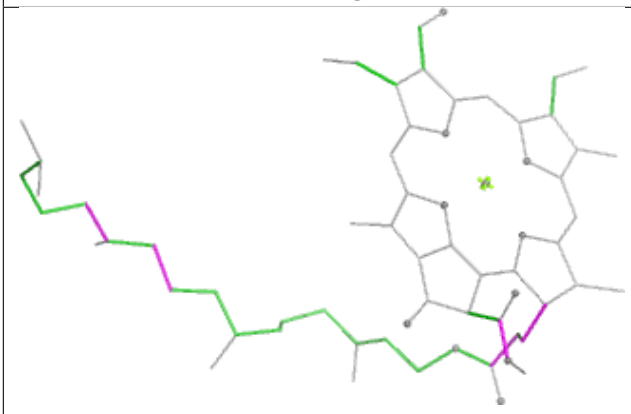
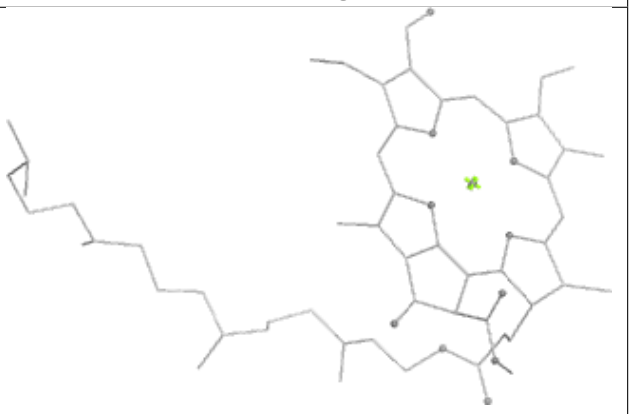
Ligand LUT 0 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 606	
Bond lengths	 Bond angles
 Torsions	 Rings

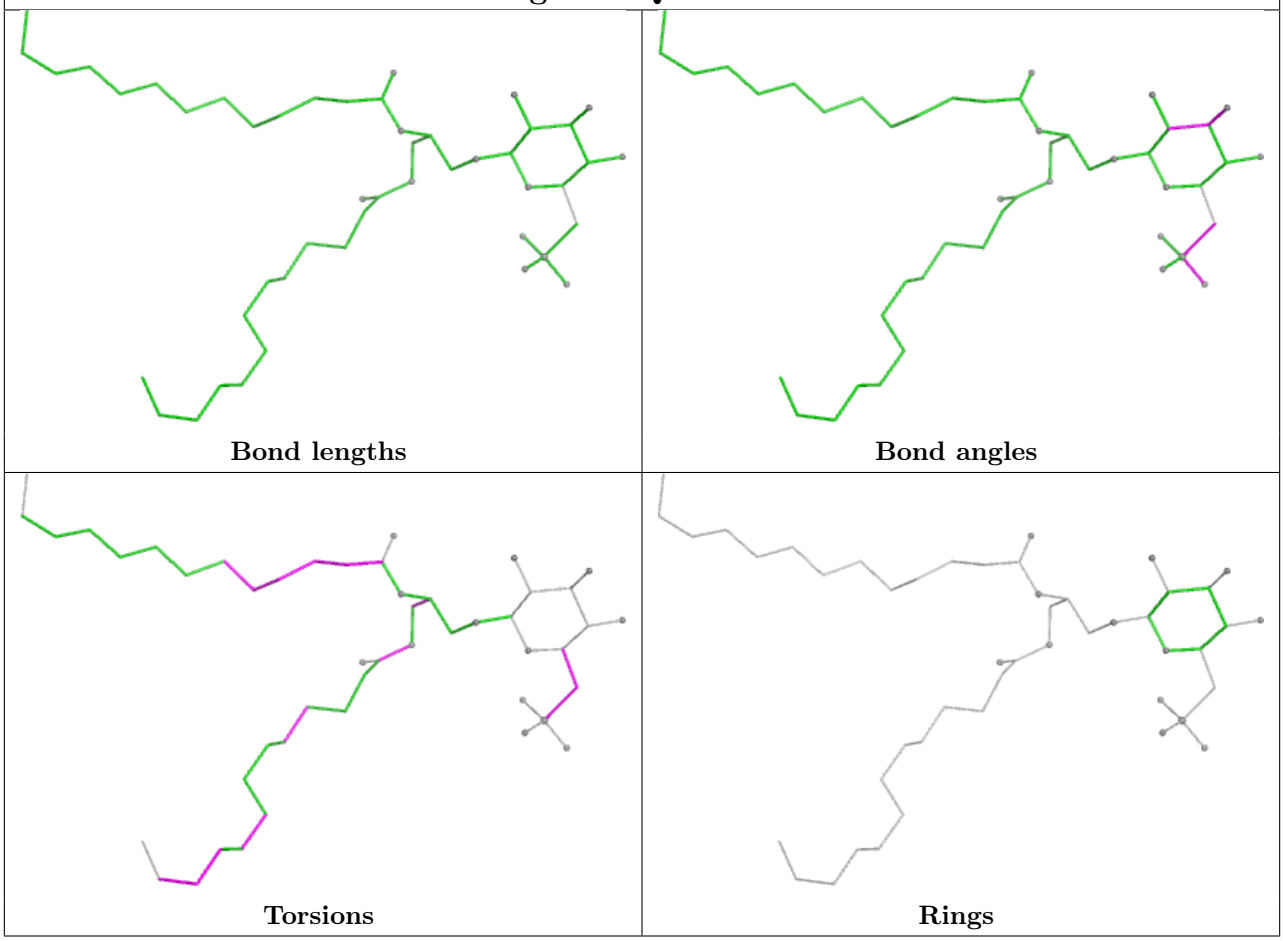
Ligand CLA r 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG W 201

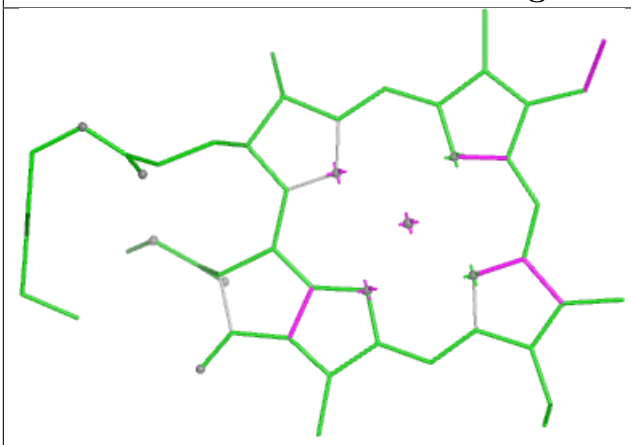


Ligand CHL 8 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

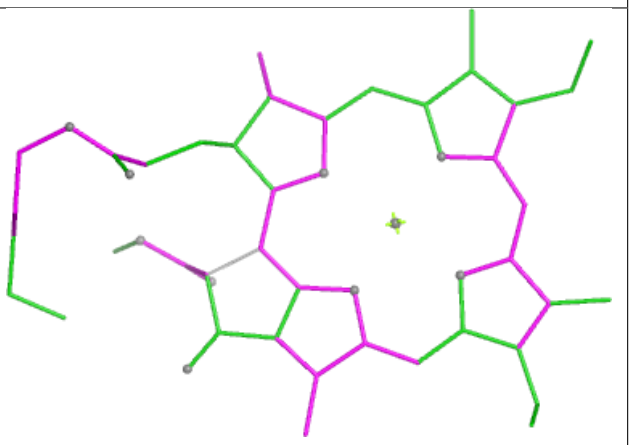
Ligand SQD a 411



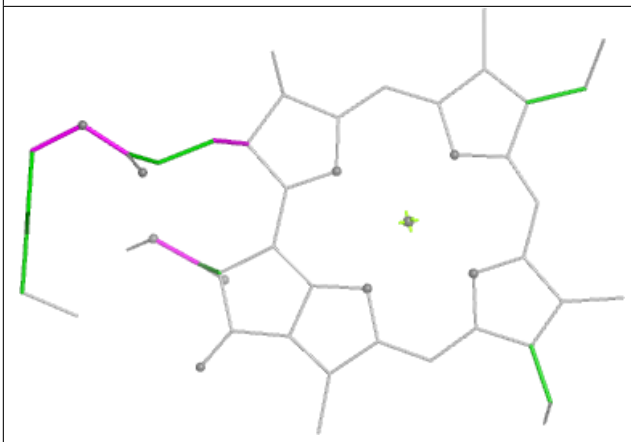
Ligand CLA 7 316



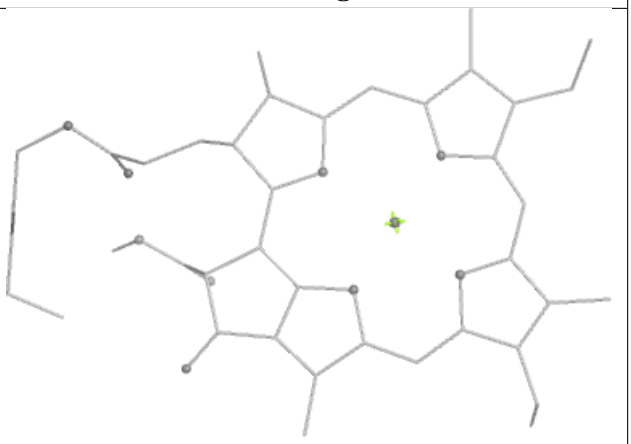
Bond lengths



Bond angles

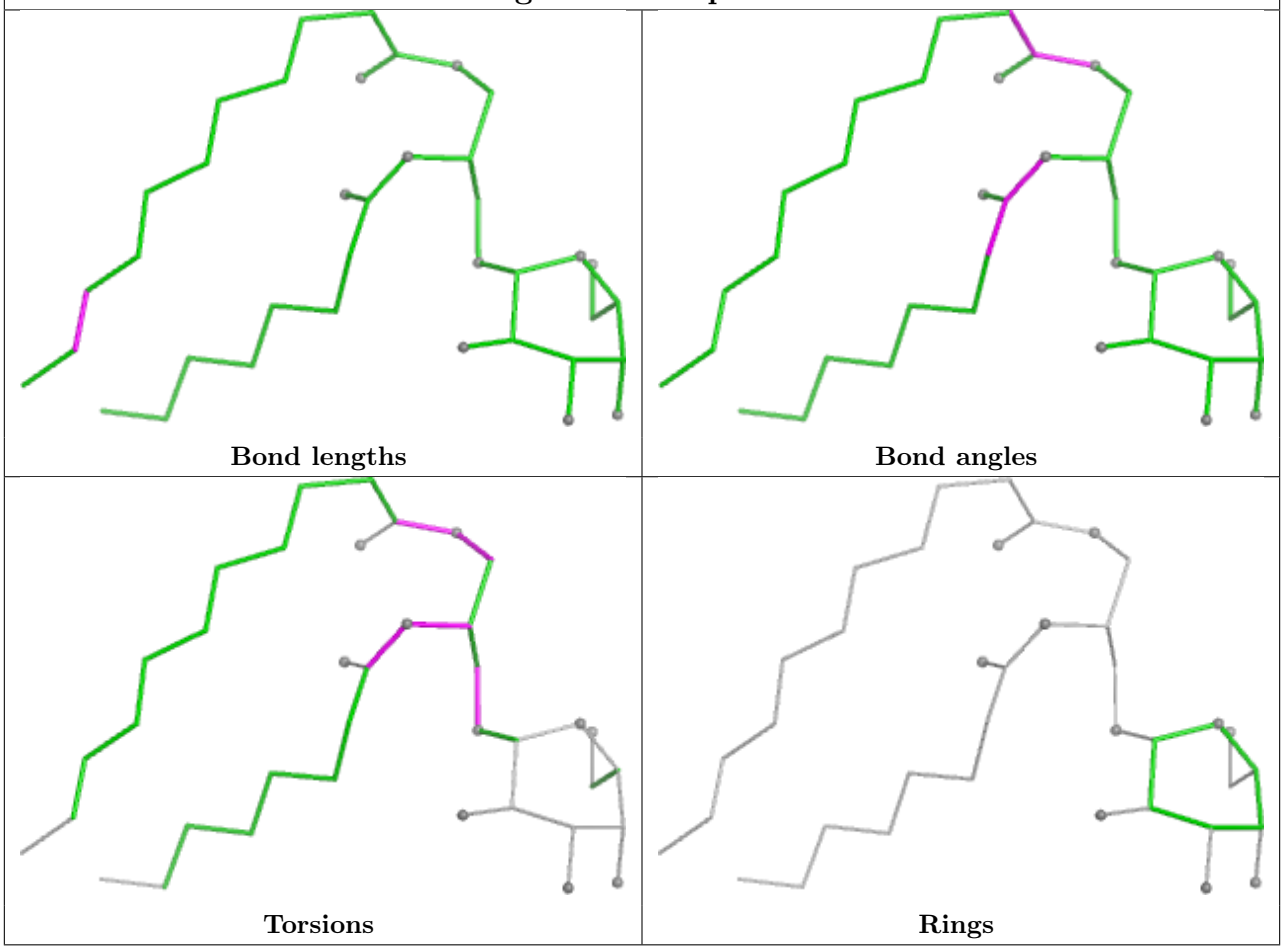


Torsions

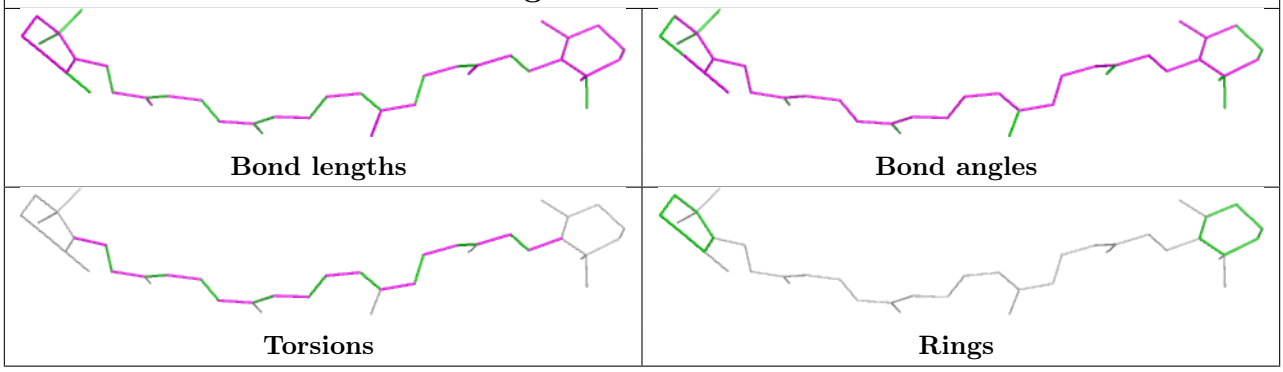


Rings

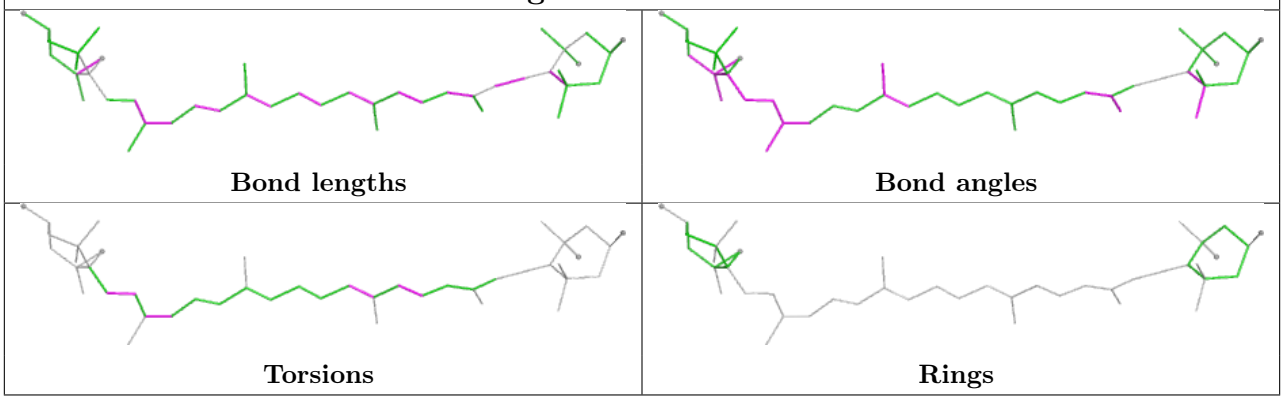
Ligand LMG q1 101



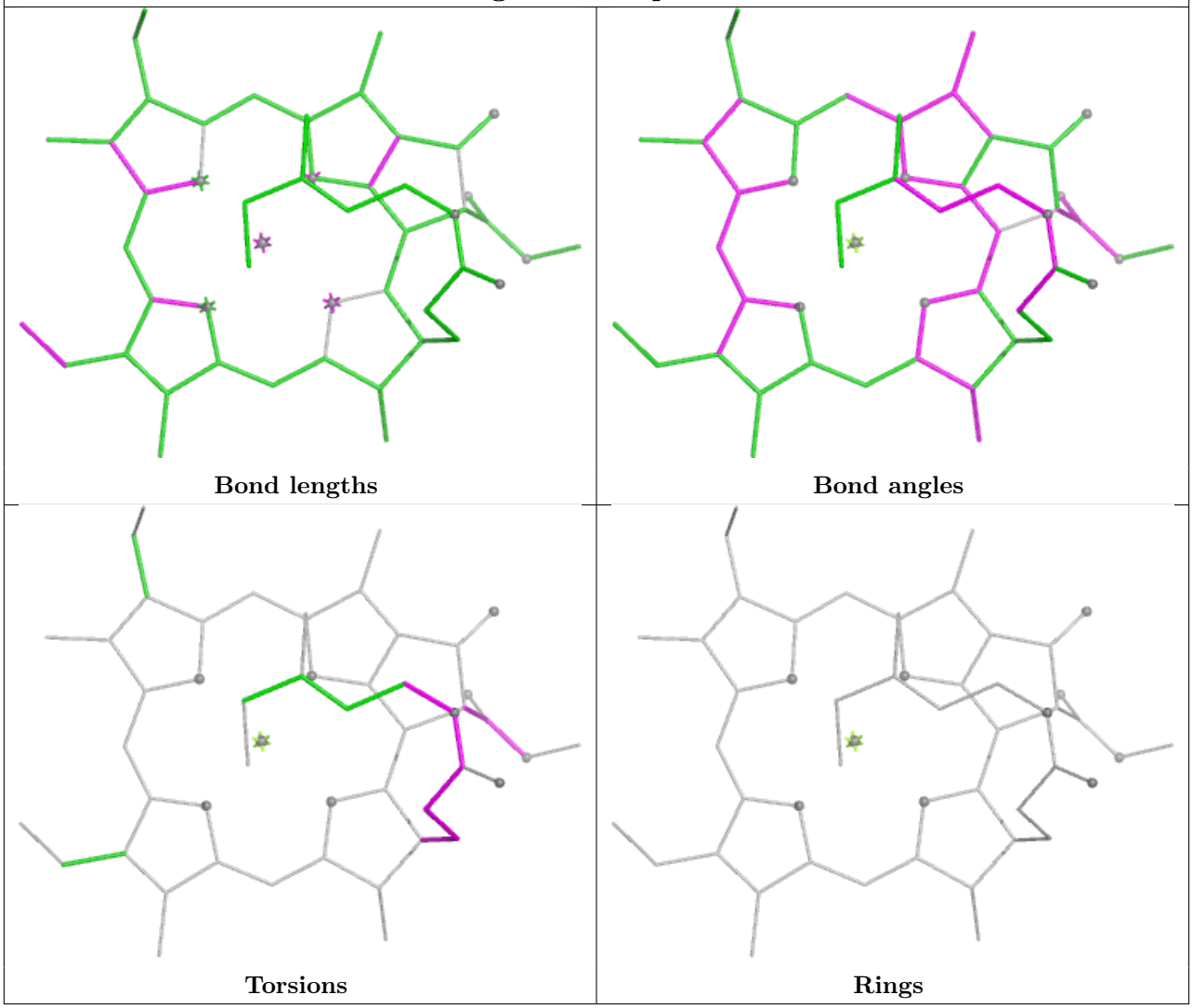
Ligand BCR T 101



Ligand NEX 4 617



Ligand CLA p 614



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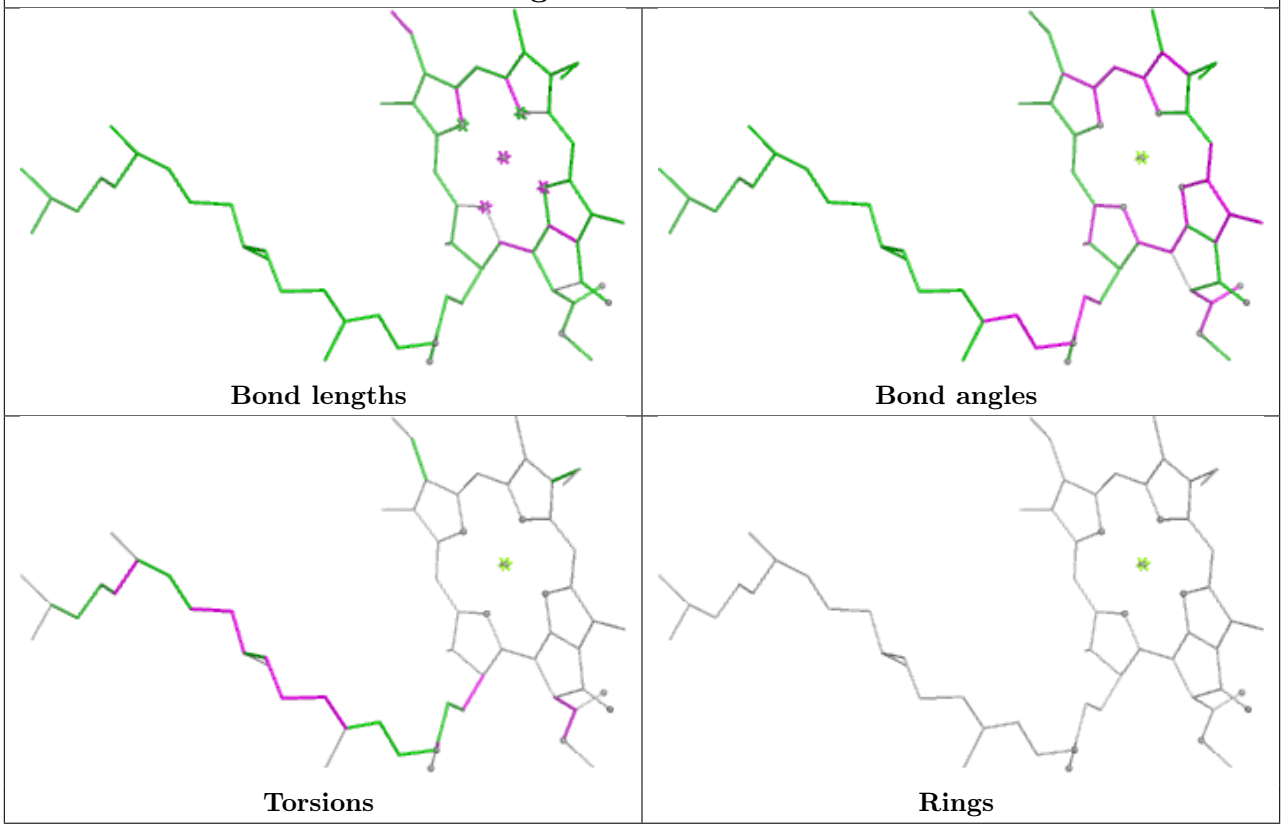

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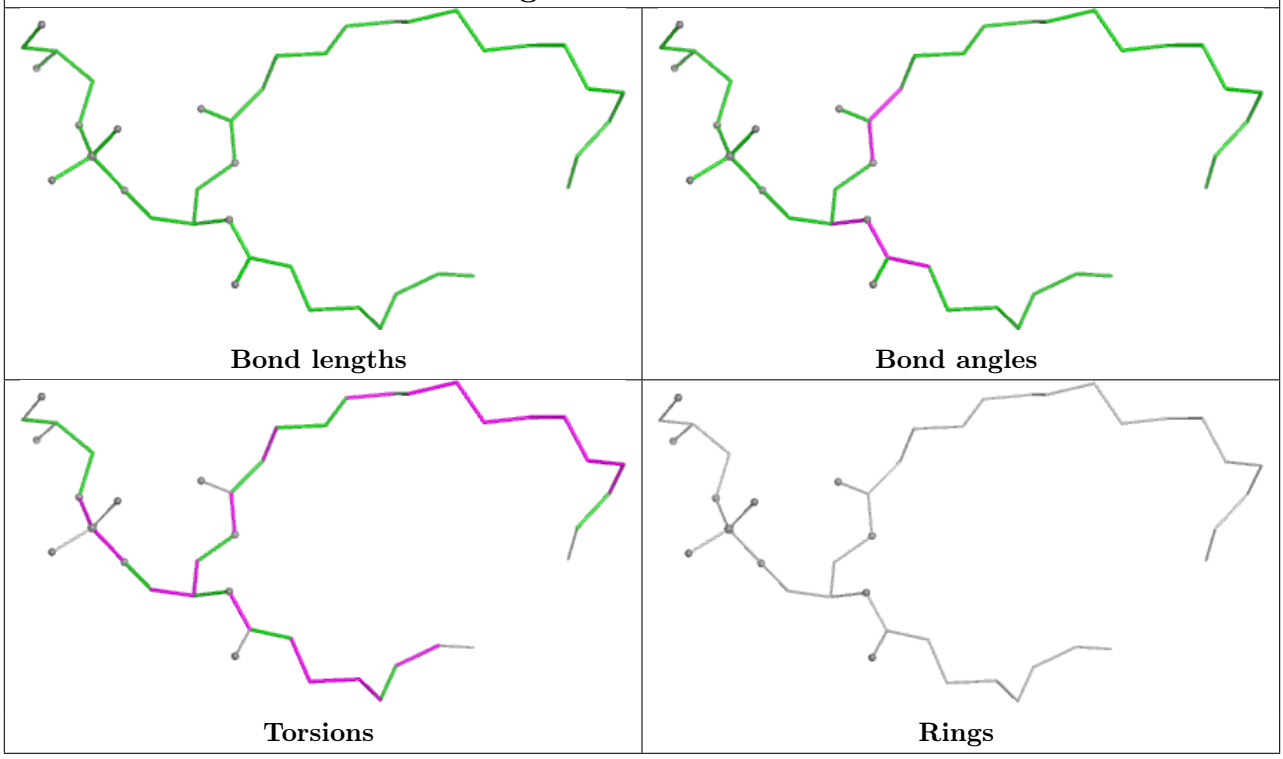

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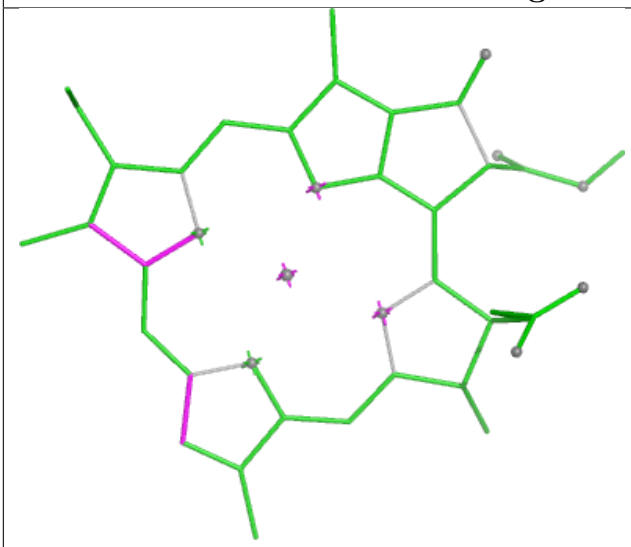
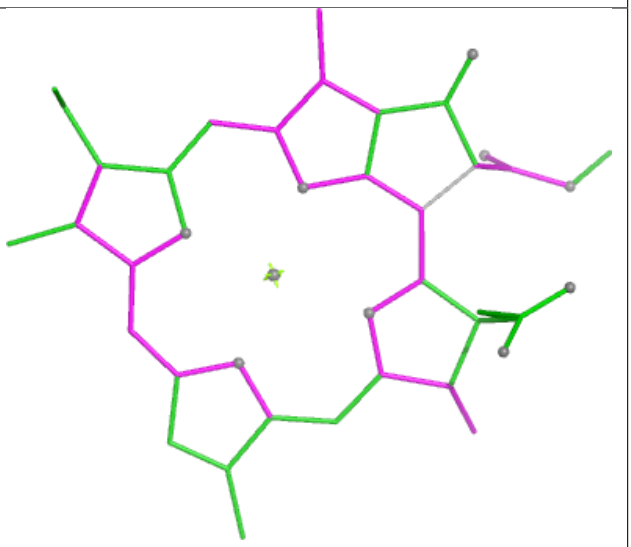
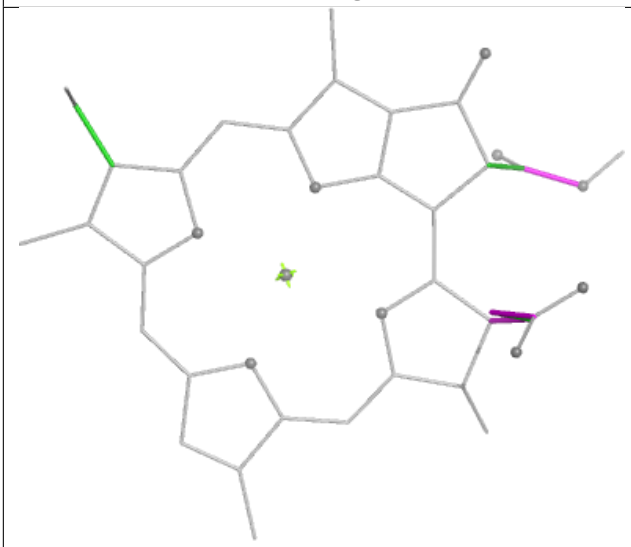


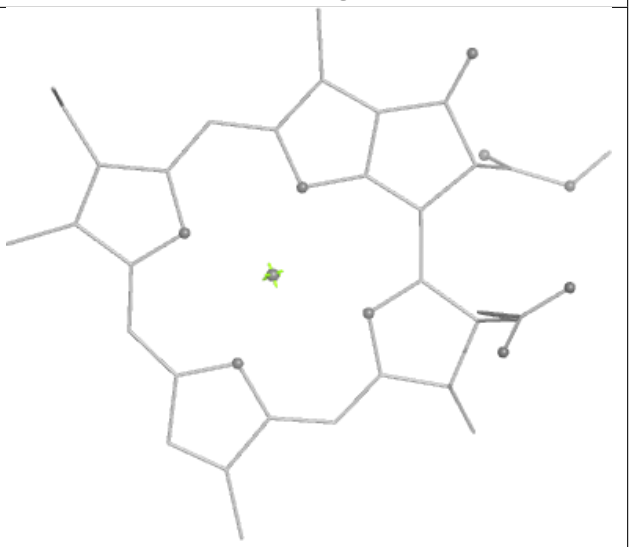
Bond lengths



Bond angles

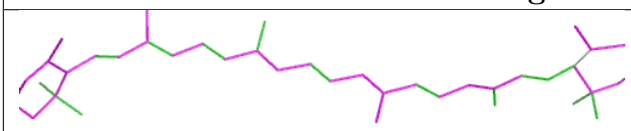


Torsions



Rings

Ligand LUT y 617



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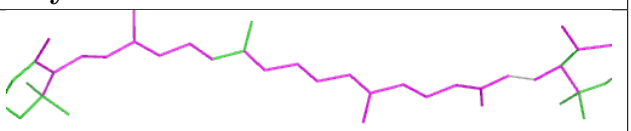
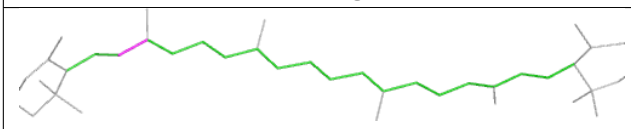


Bond angles



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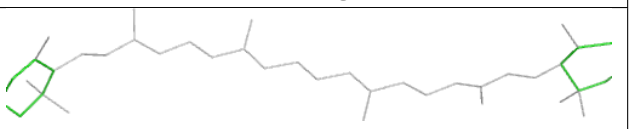
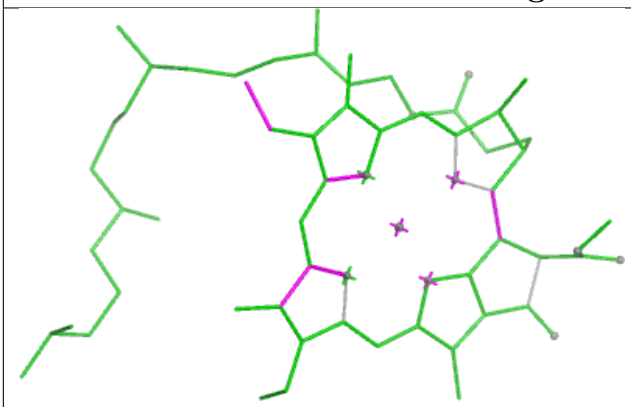
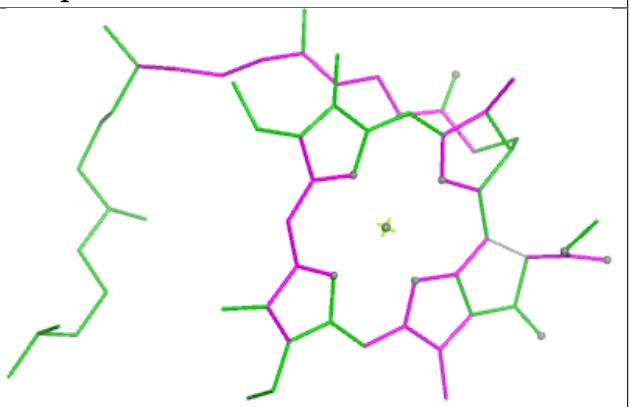


Rings

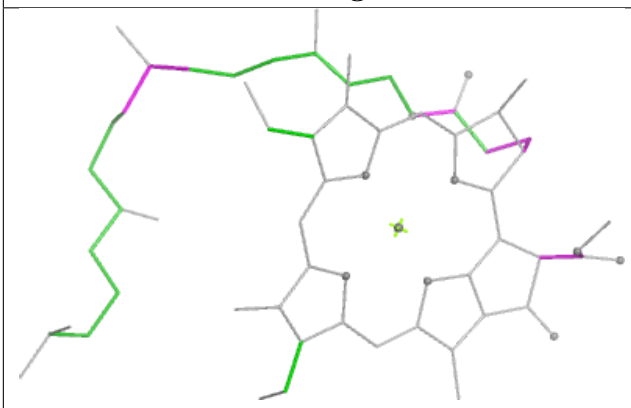
Ligand CLA q 304



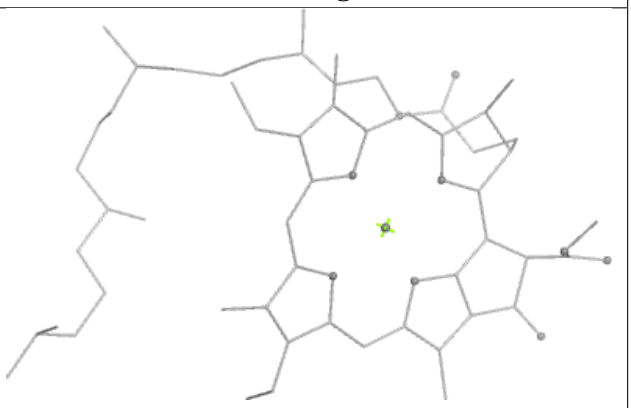
Bond lengths



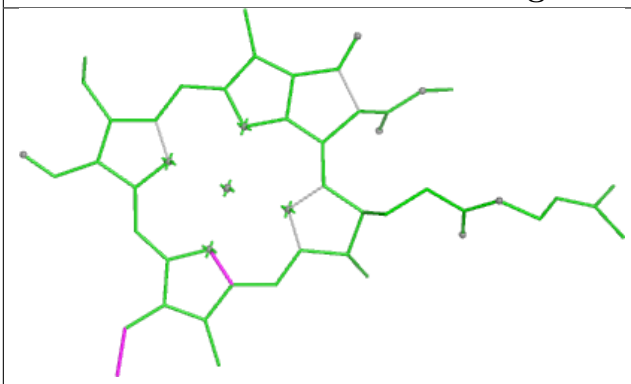
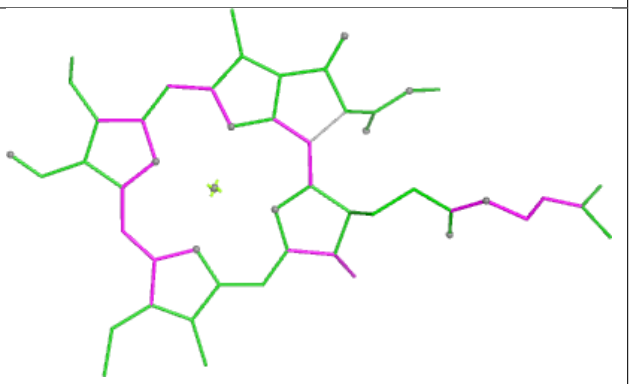
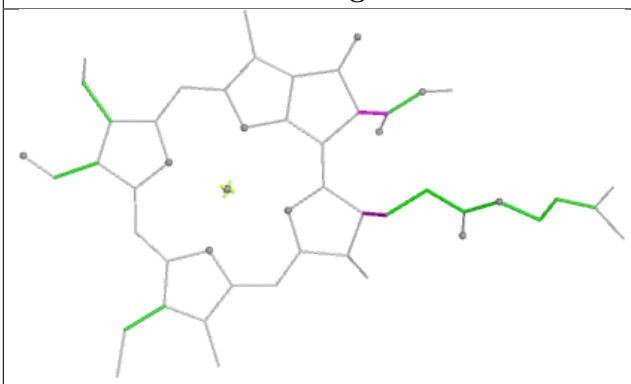
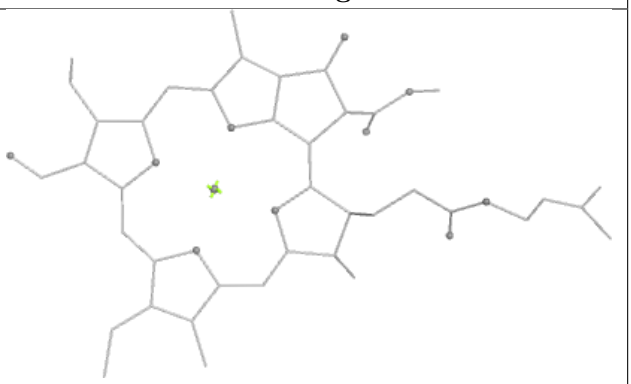
Bond angles



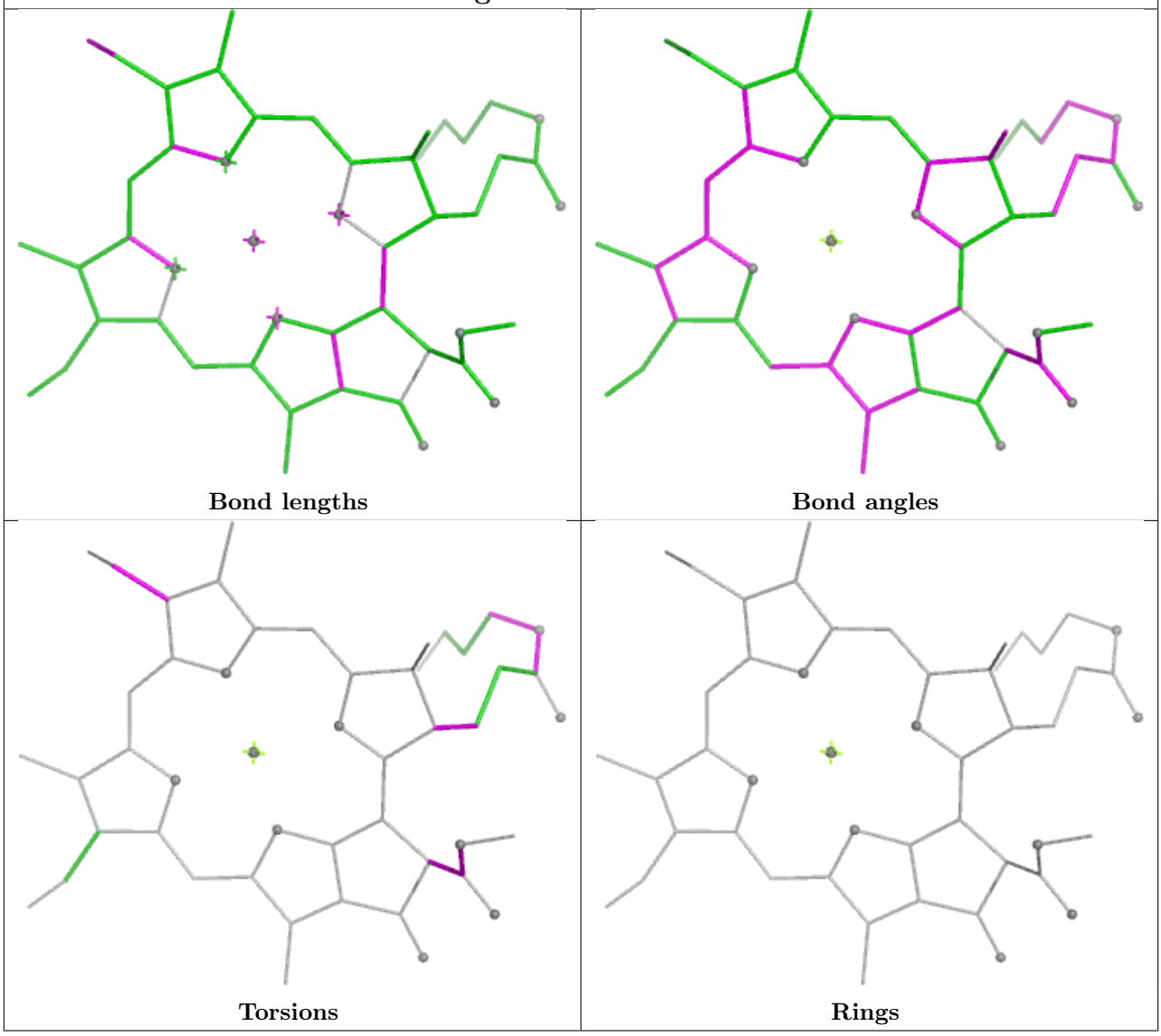
Torsions



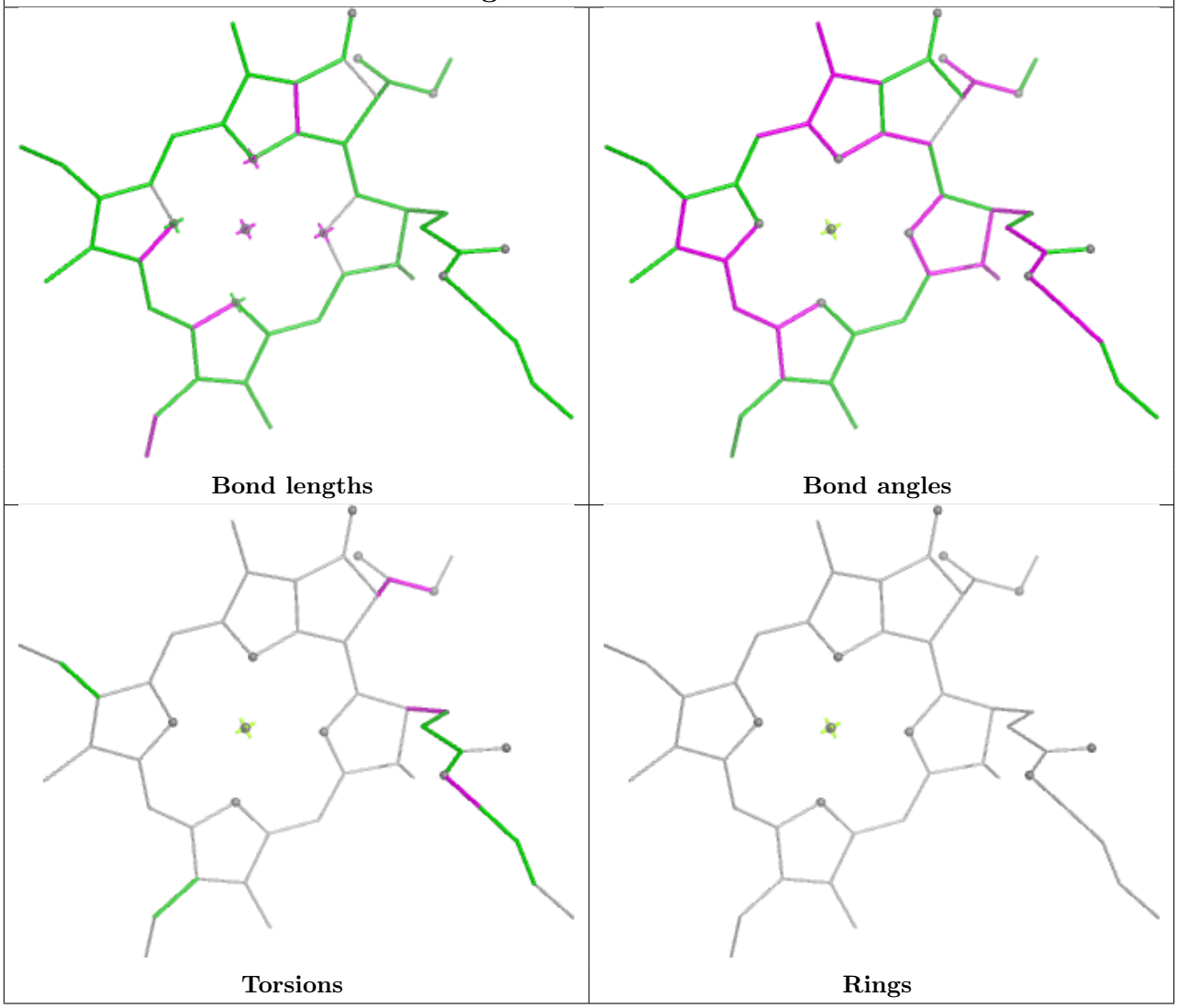
Rings

Ligand CHL 0 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

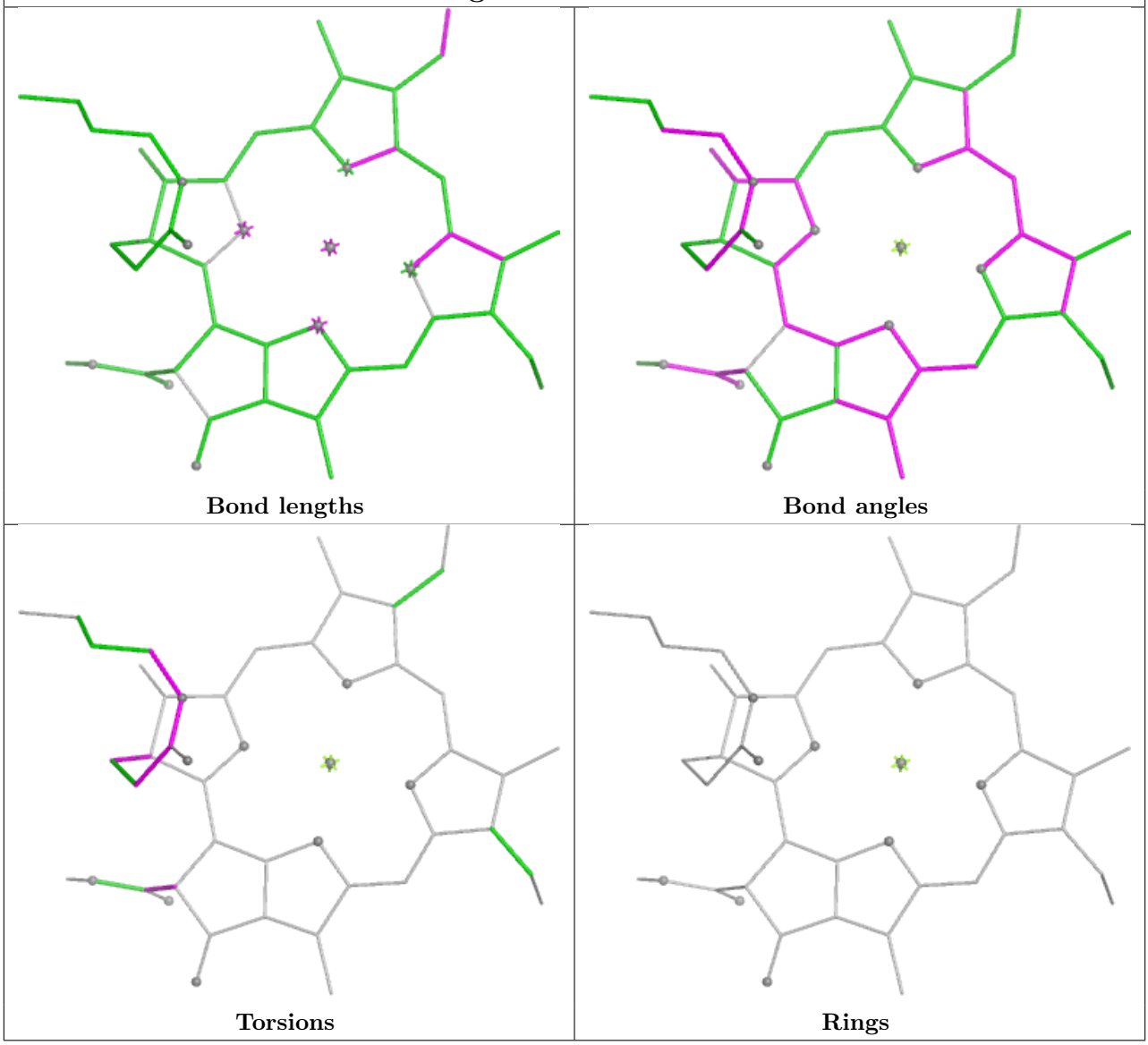
Ligand CLA R 303



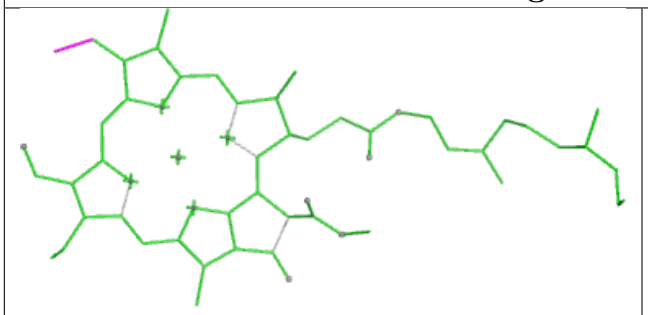
Ligand CLA A 407



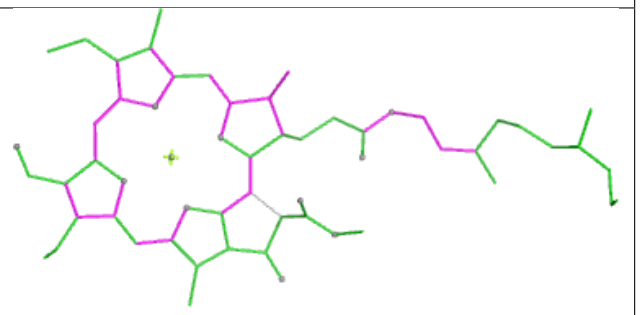
Ligand CLA N 314



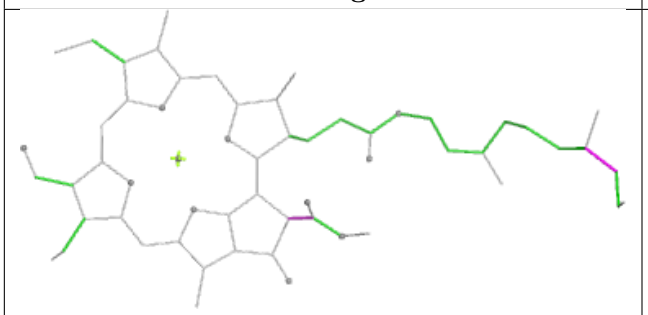
Ligand CHL n 307



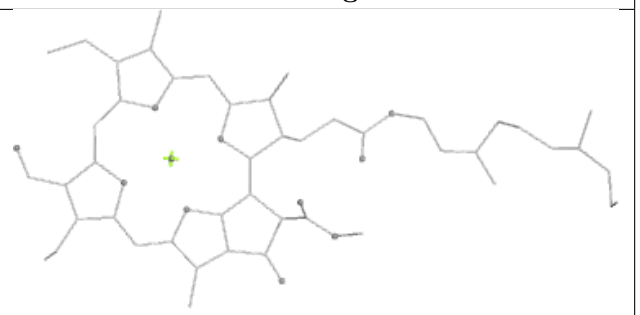
Bond lengths



Bond angles

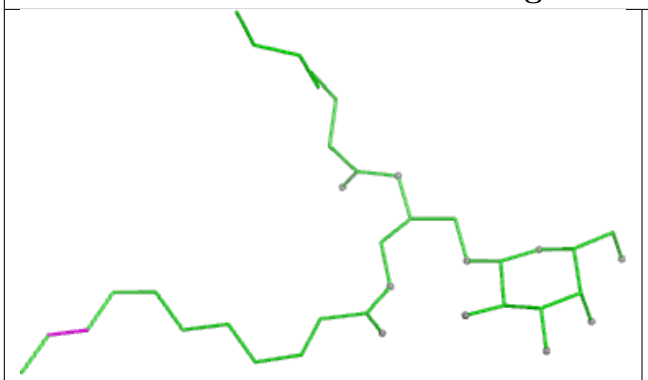


Torsions

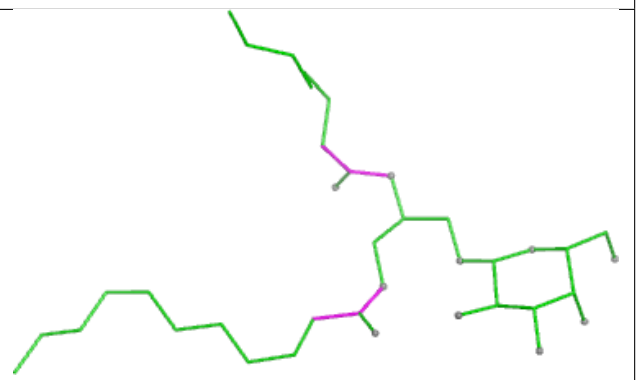


Rings

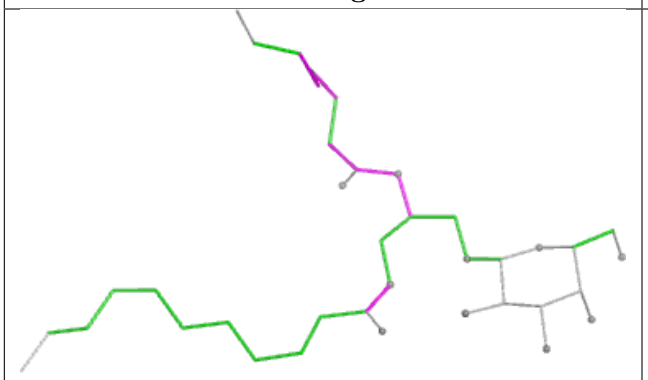
Ligand LMG 1 618



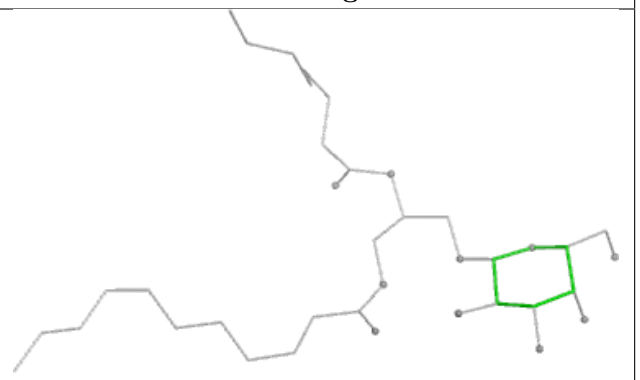
Bond lengths



Bond angles

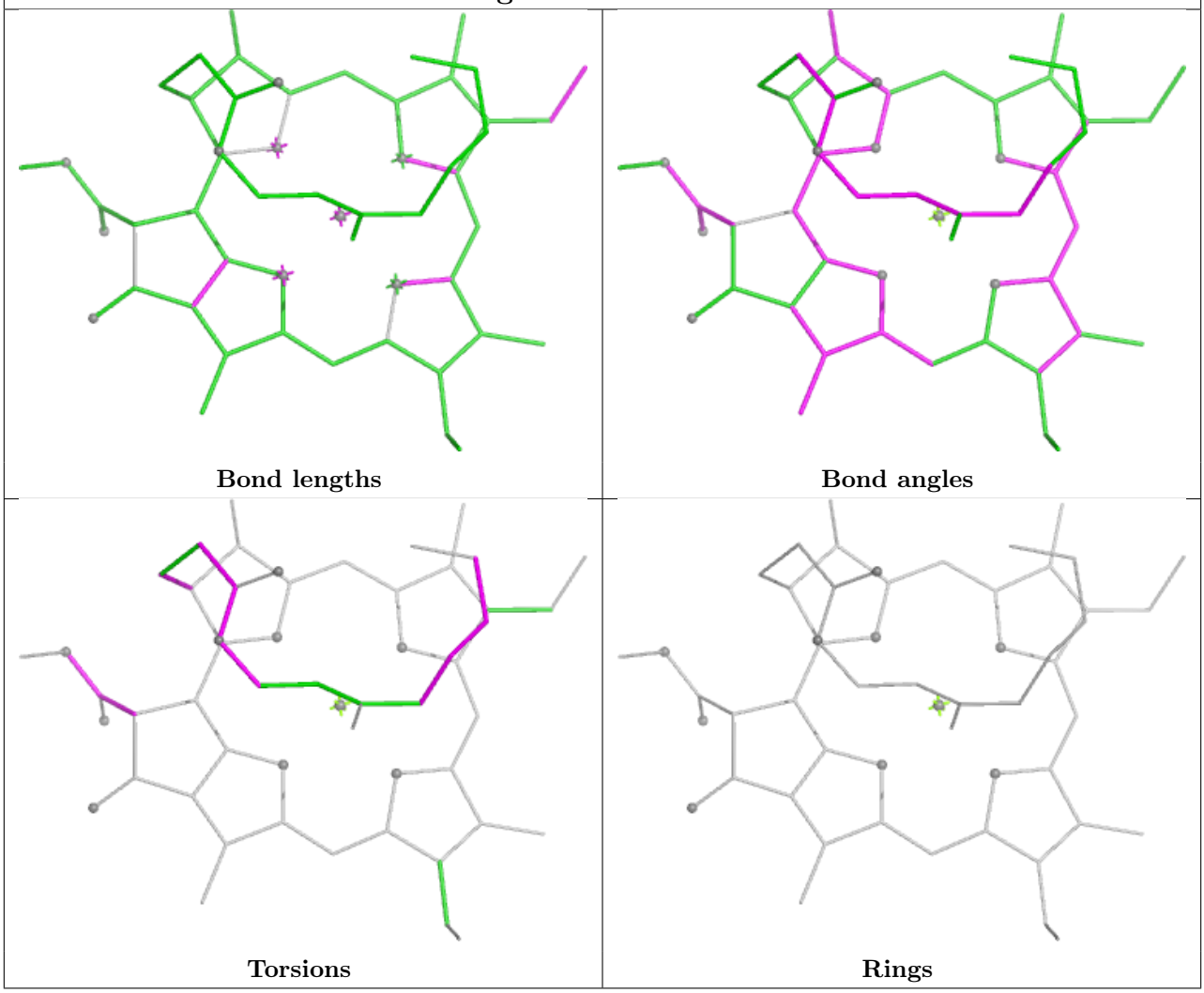


Torsions

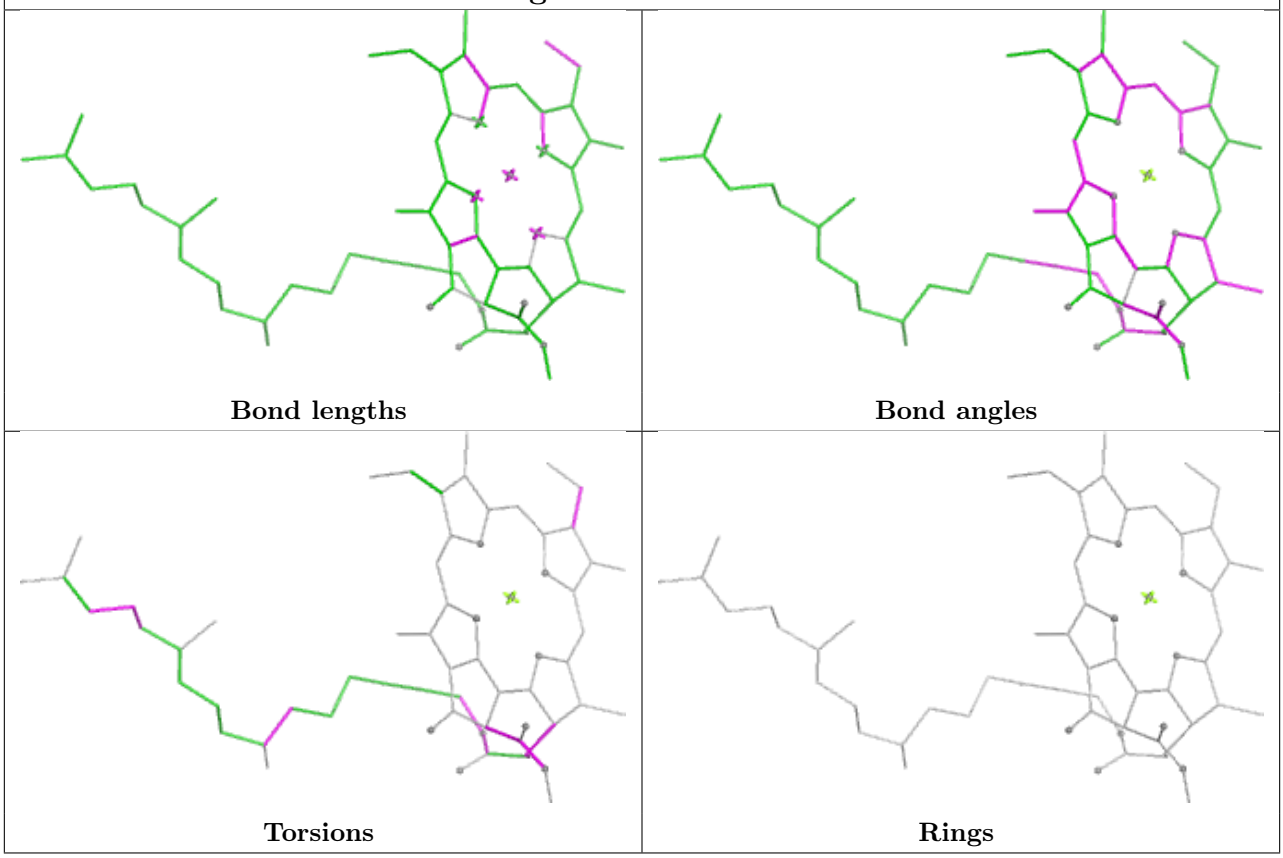


Rings

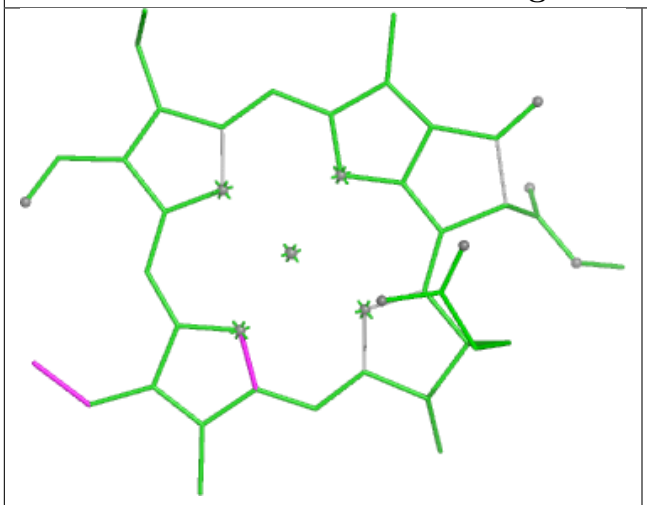
Ligand CLA 0 614



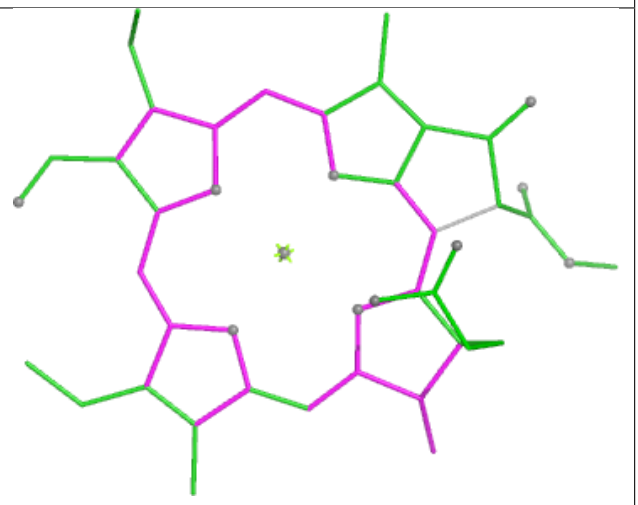
Ligand CLA 3 312



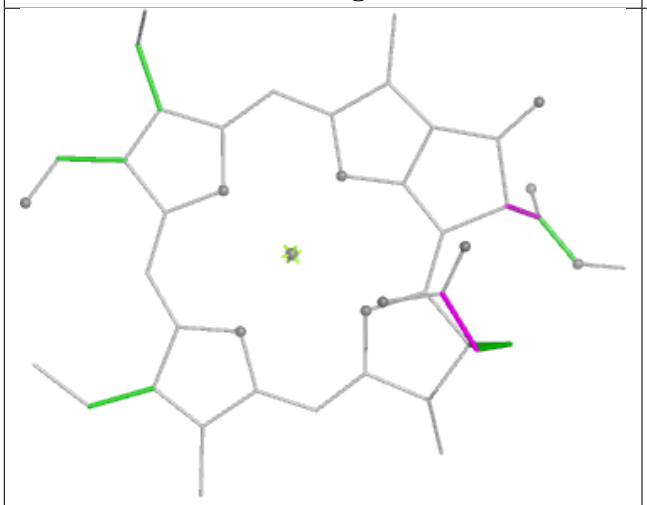
Ligand CHL 2 605



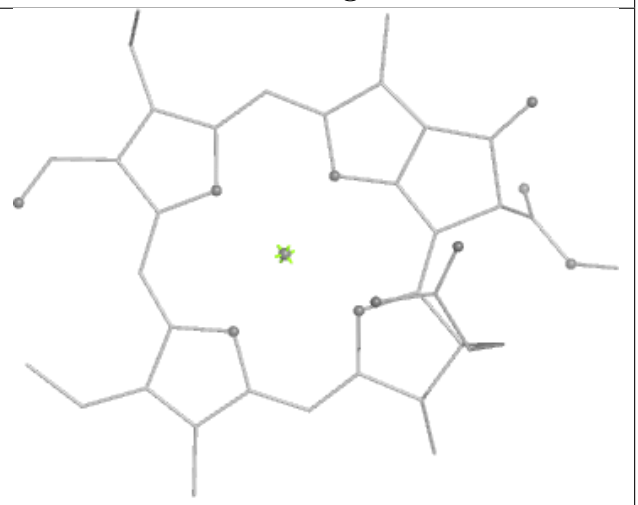
Bond lengths



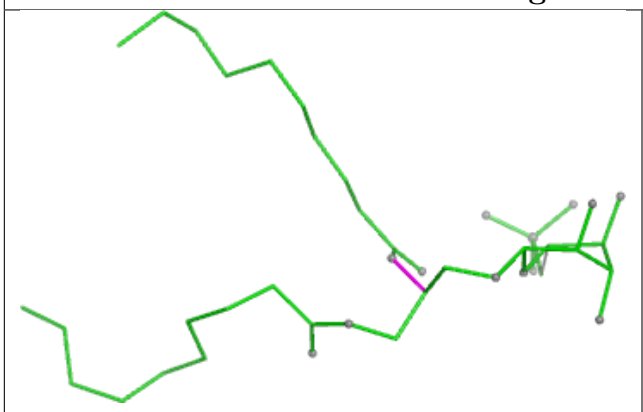
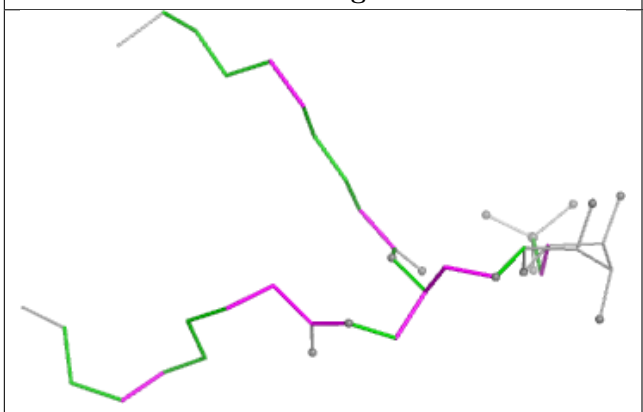
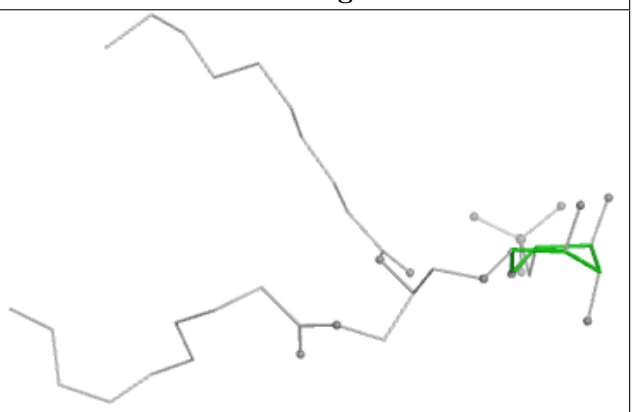
Bond angles

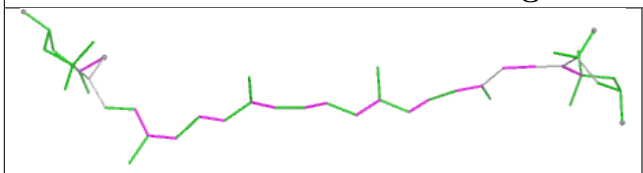
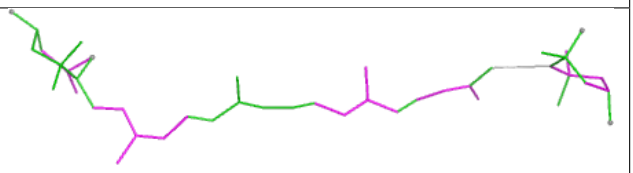
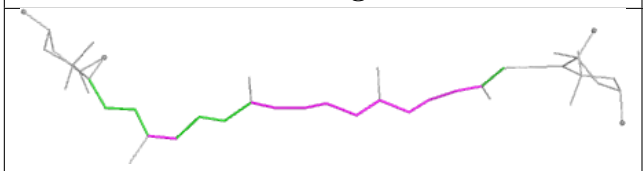
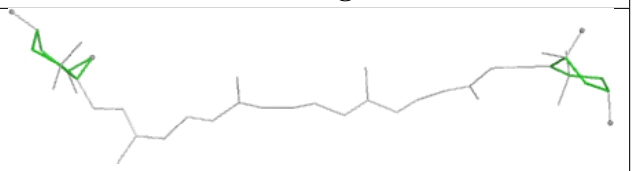


Torsions

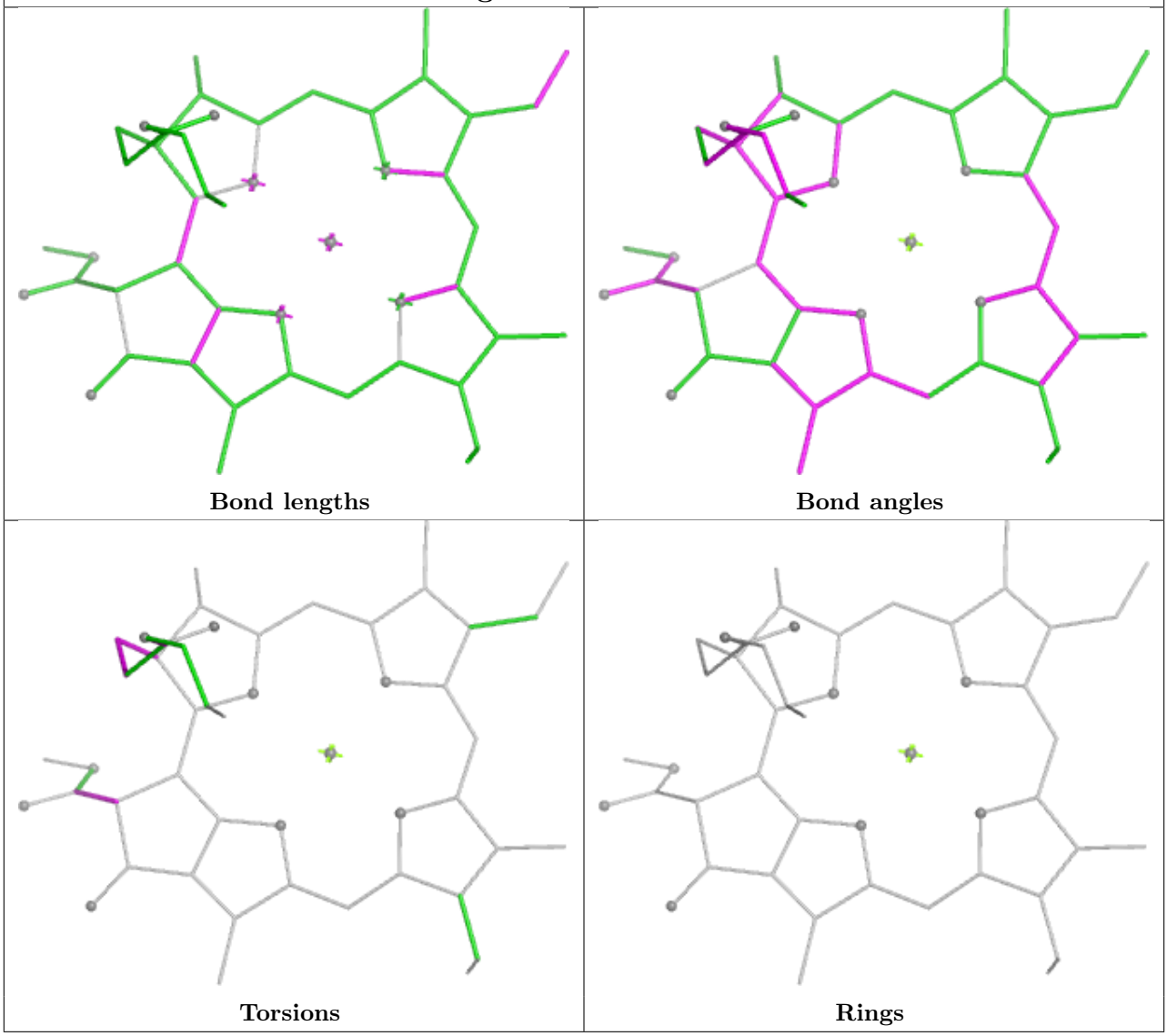


Rings

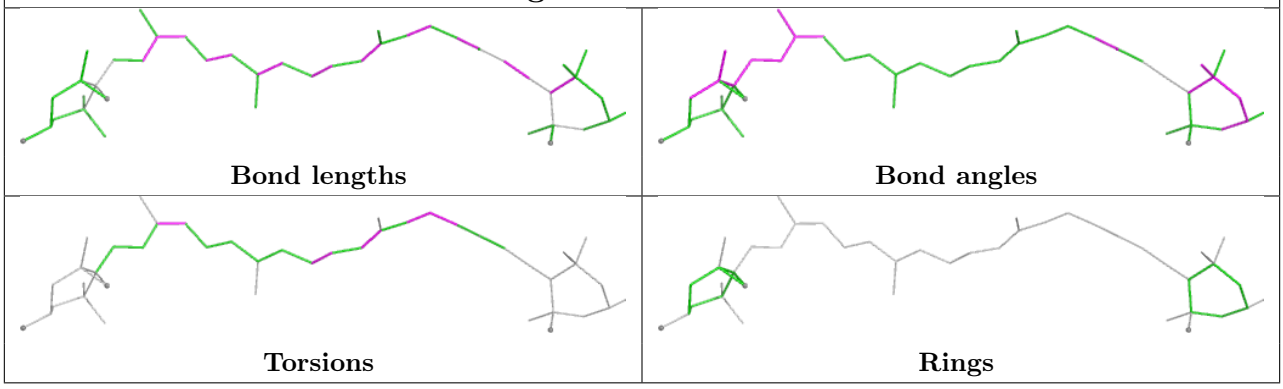
Ligand SQD x 201	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand NEX N 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

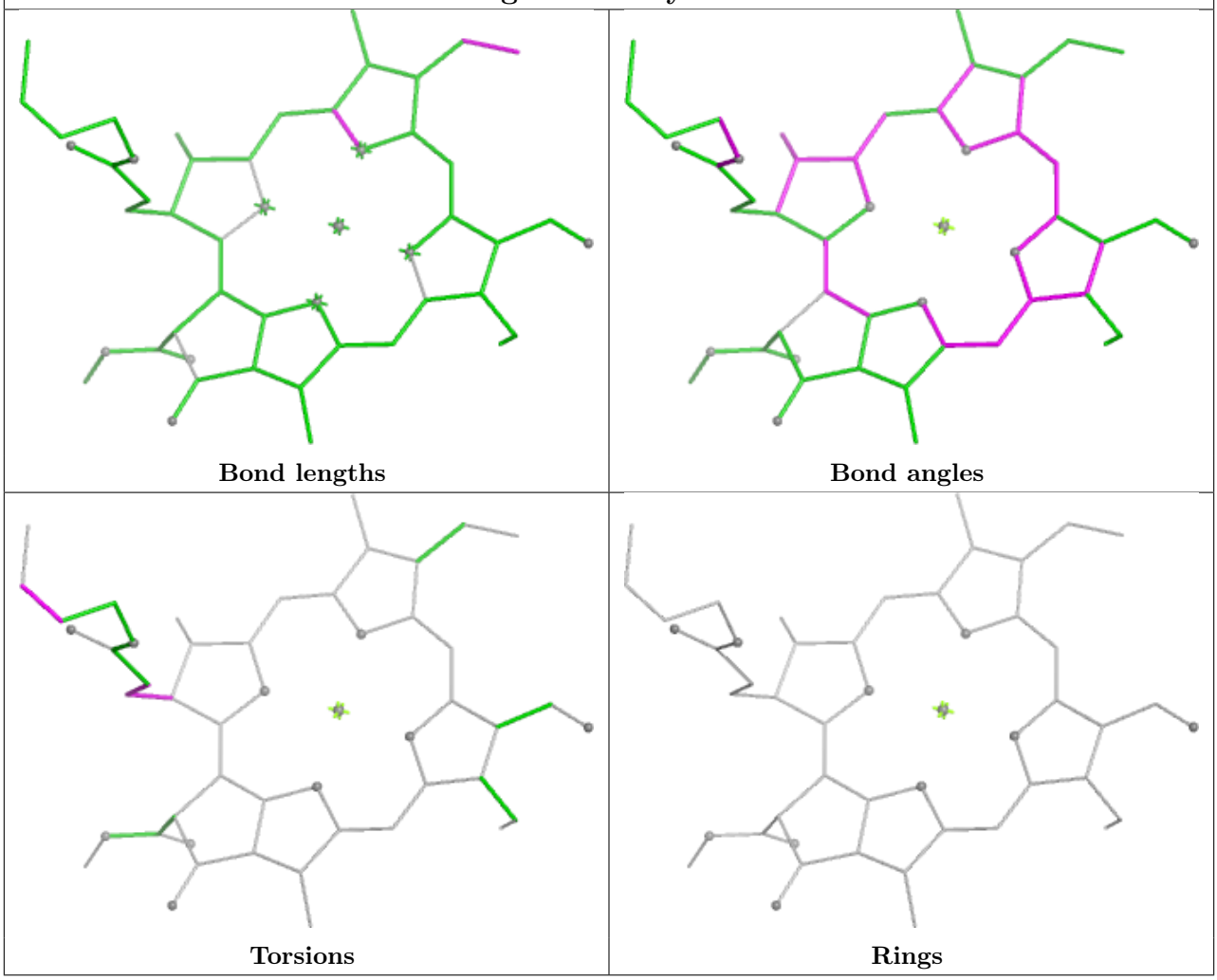
Ligand CLA R 306



Ligand NEX 9 319



Ligand CHL y 608



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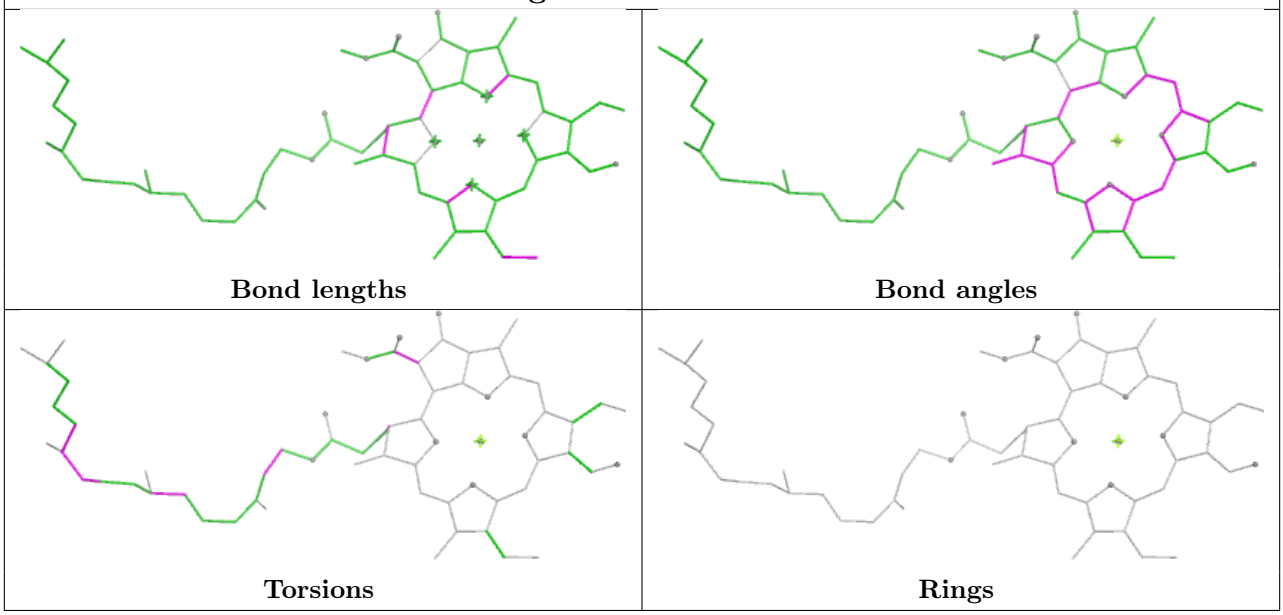

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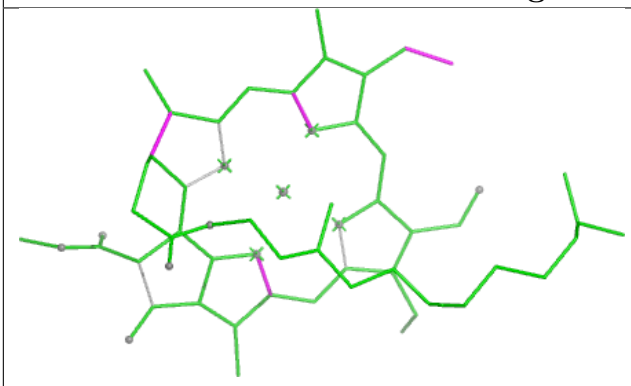
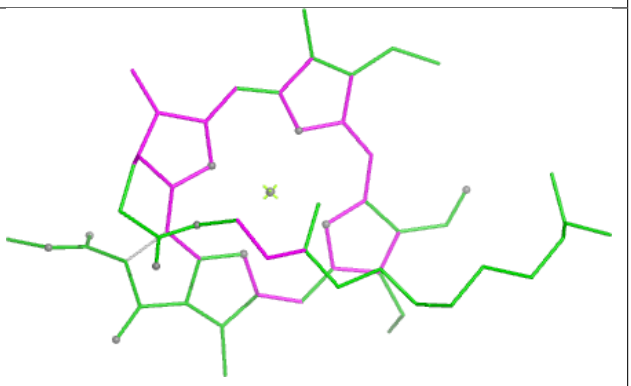
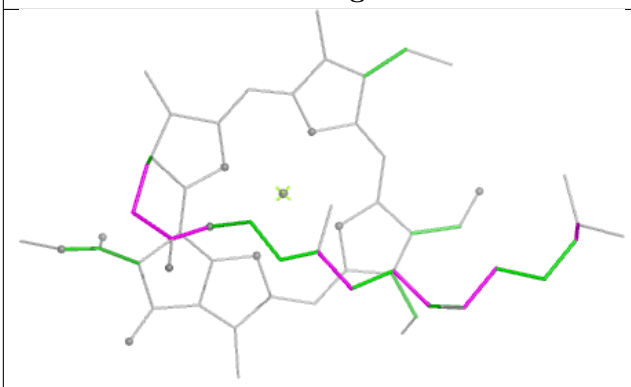


Bond lengths



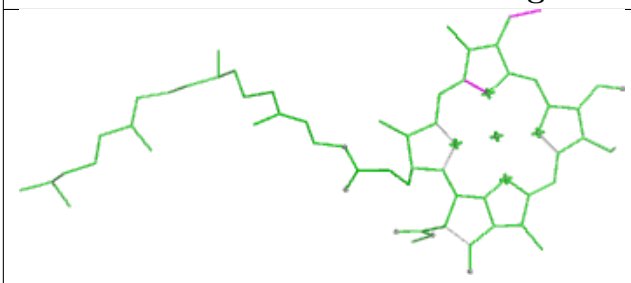
Bond angles



Torsions

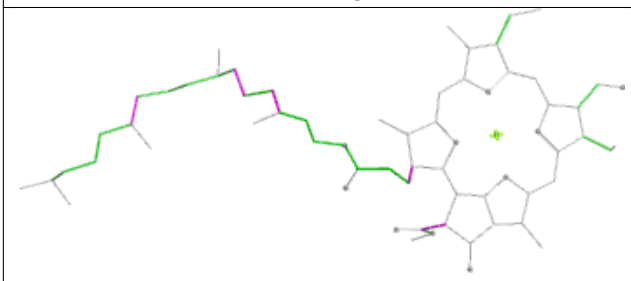
Rings

Ligand CHL q 303

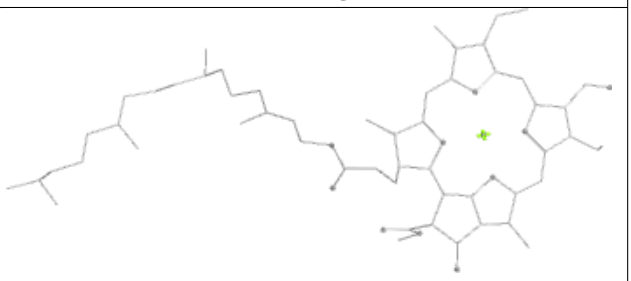


Bond lengths

Bond angles

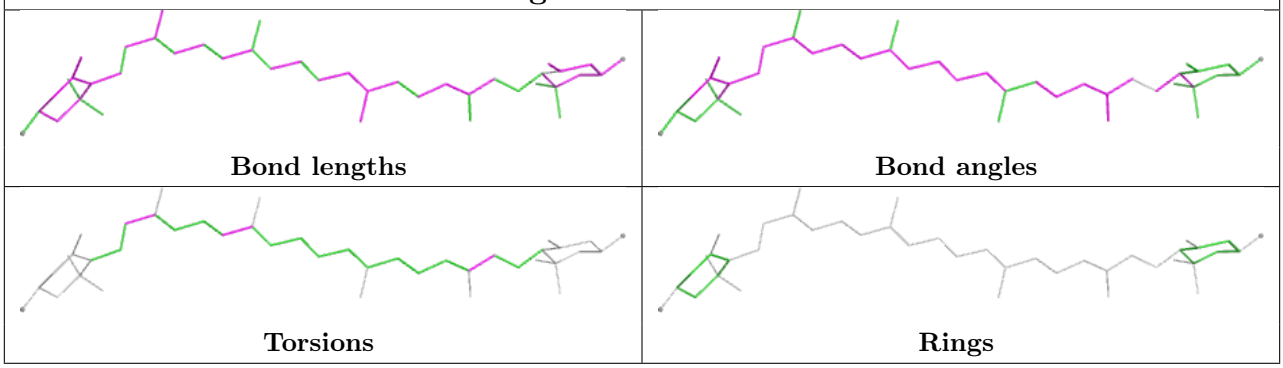


Torsions

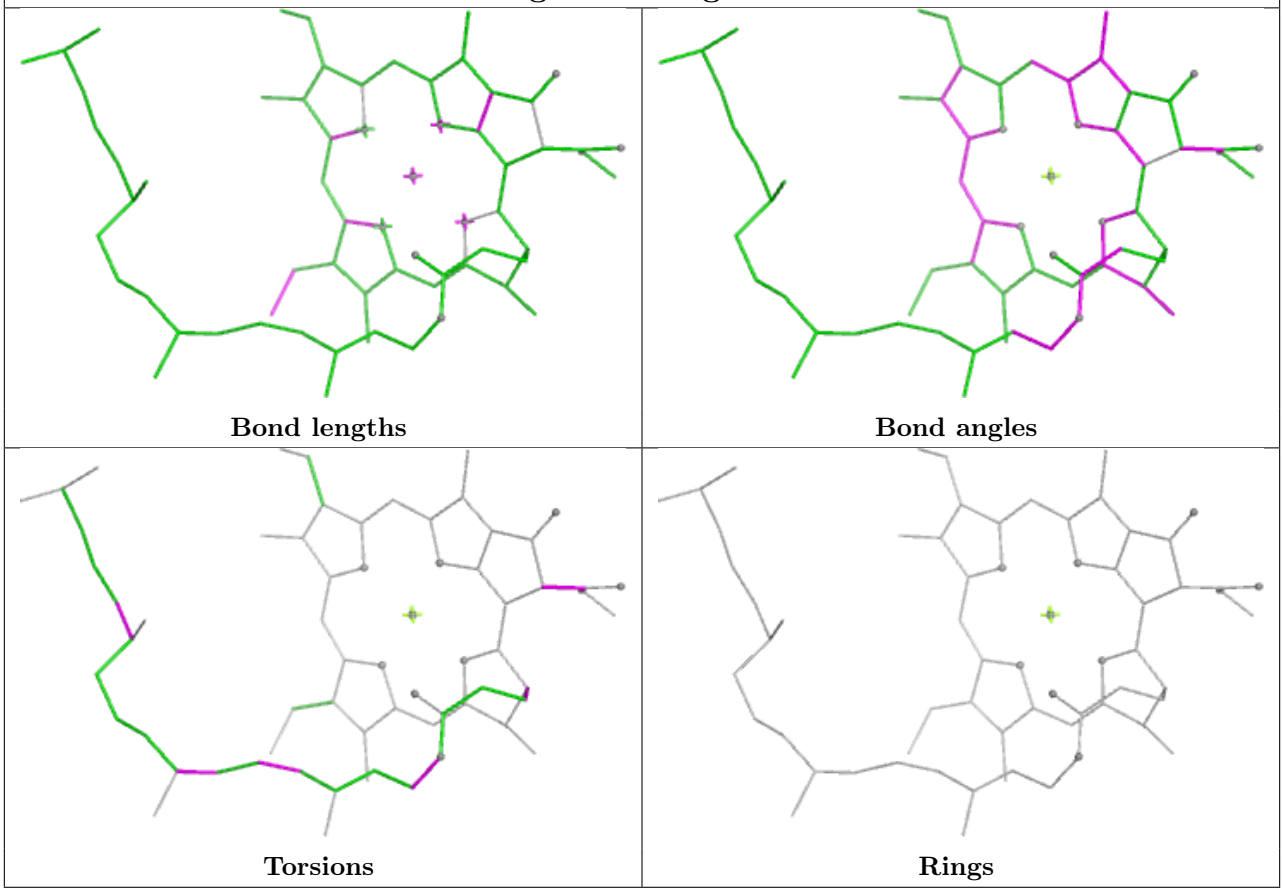


Rings

Ligand LUT 7 317

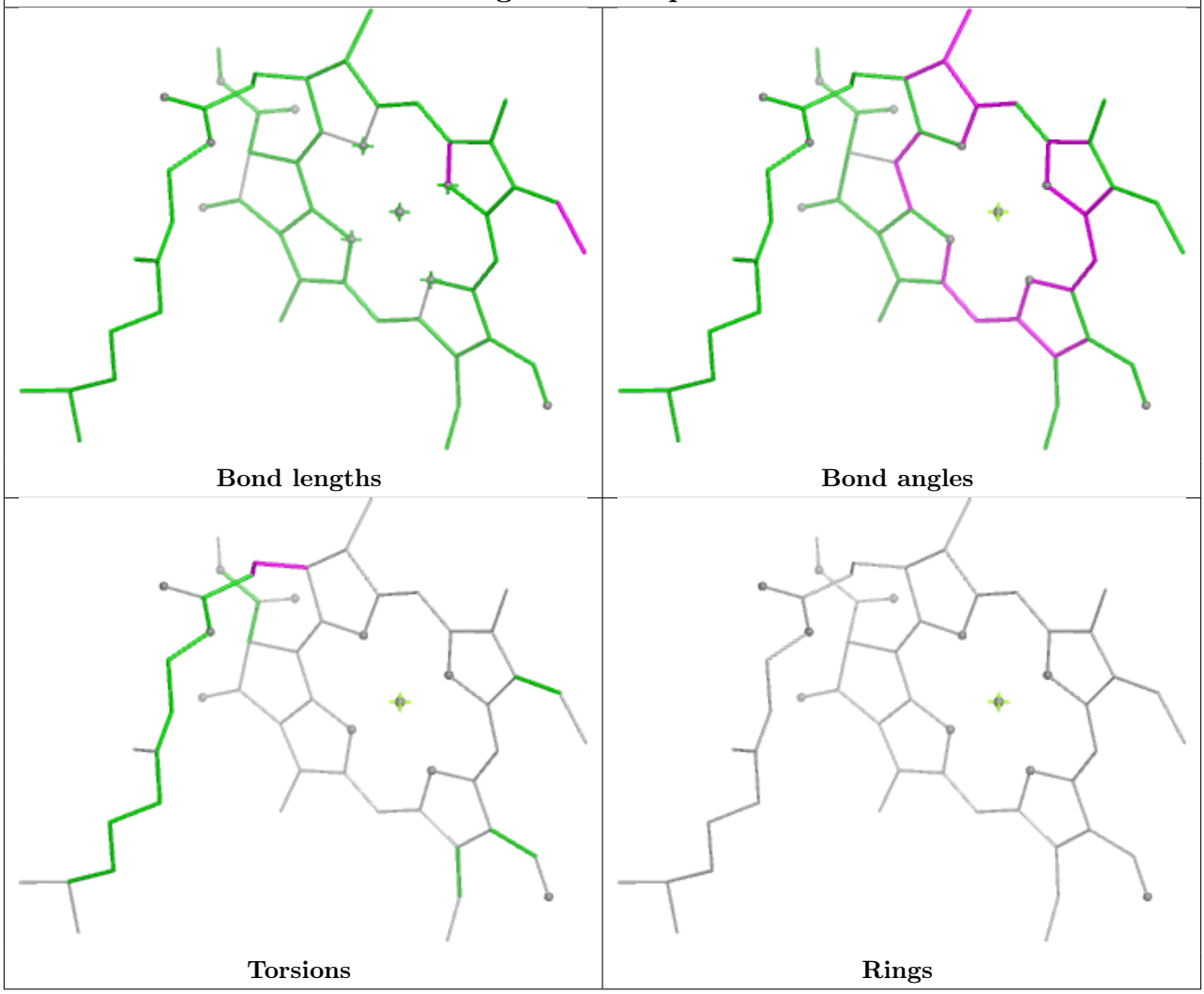


Ligand CLA g 303



Ligand RRX 2 614

Ligand CHL q 311



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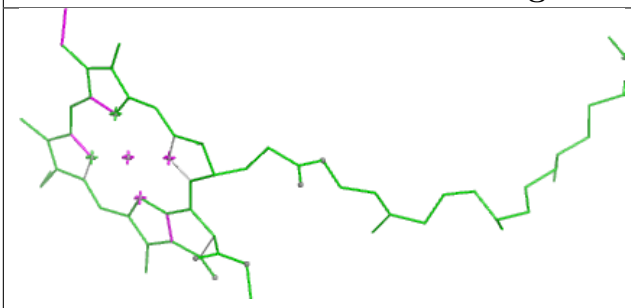
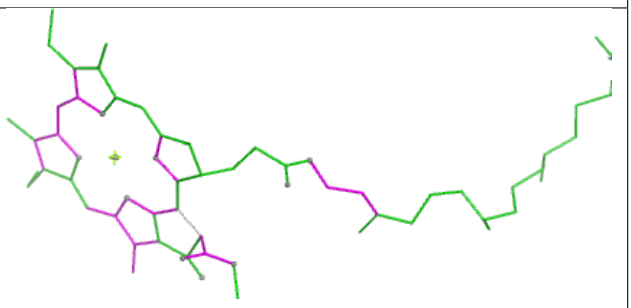
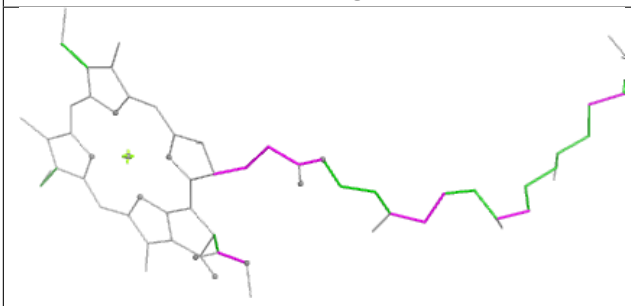
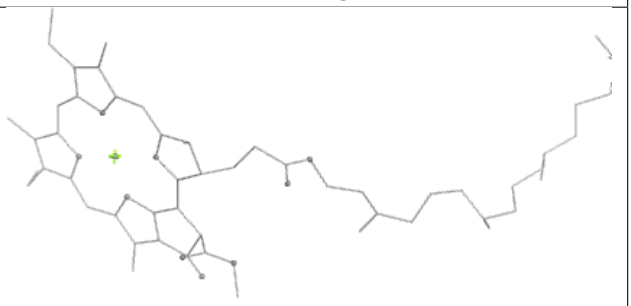
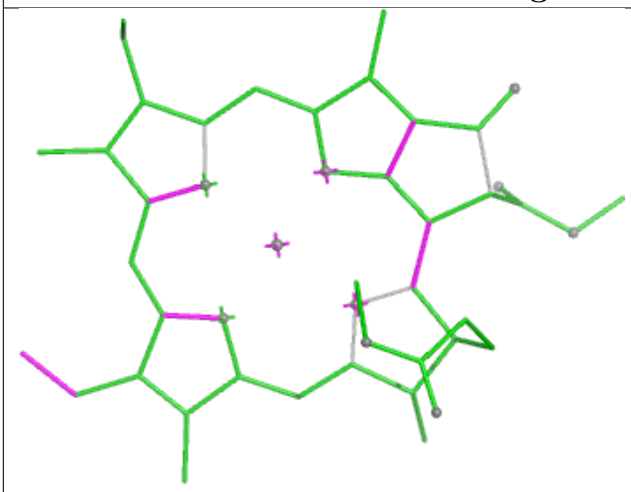
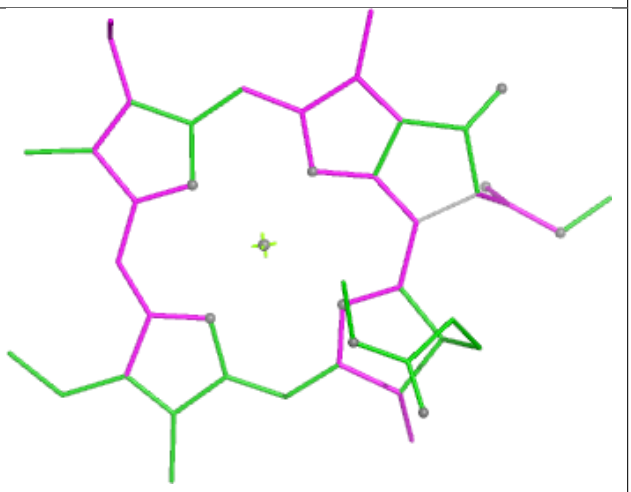
 Bond lengths	 Bond angles
 Torsions	 Rings

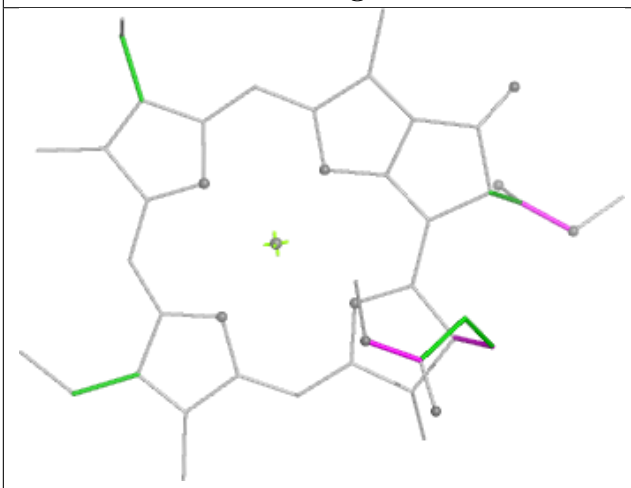
Ligand CLA s 316



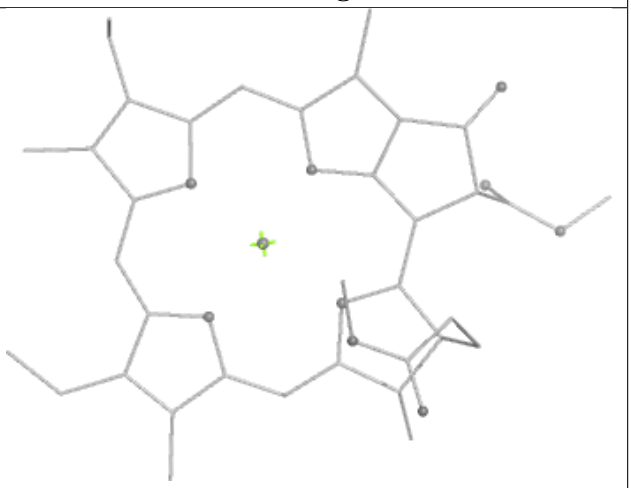
Bond lengths



Bond angles

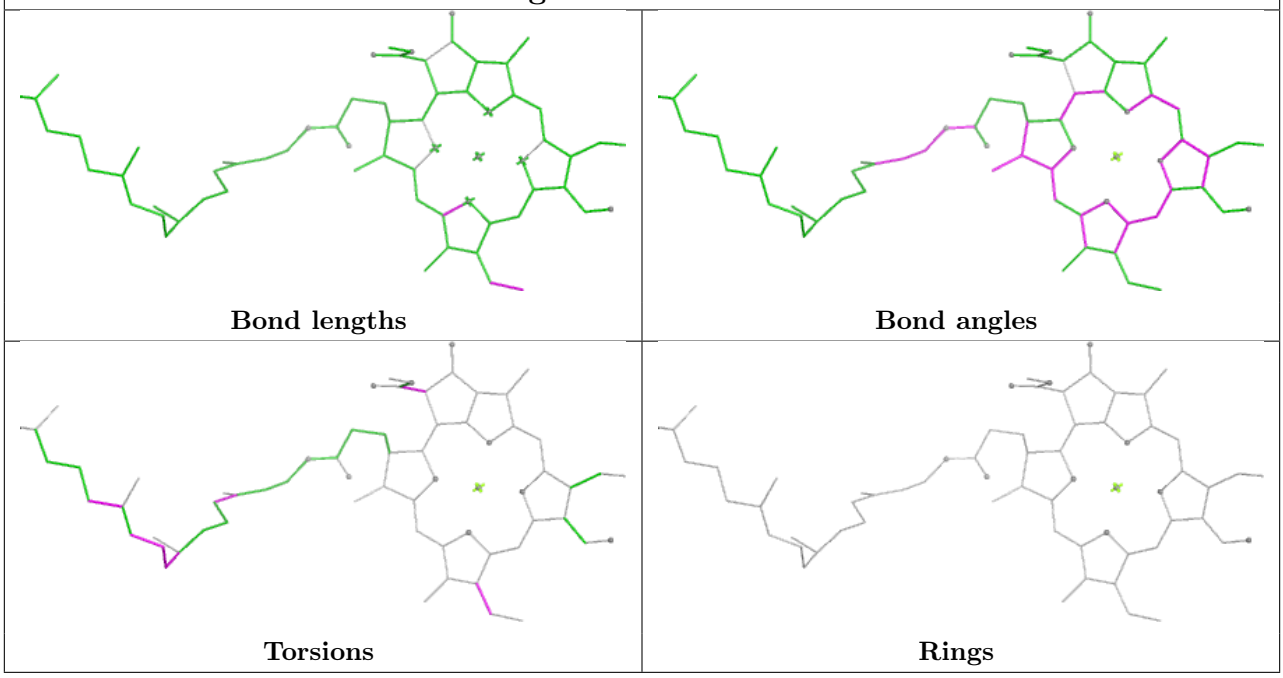


Torsions

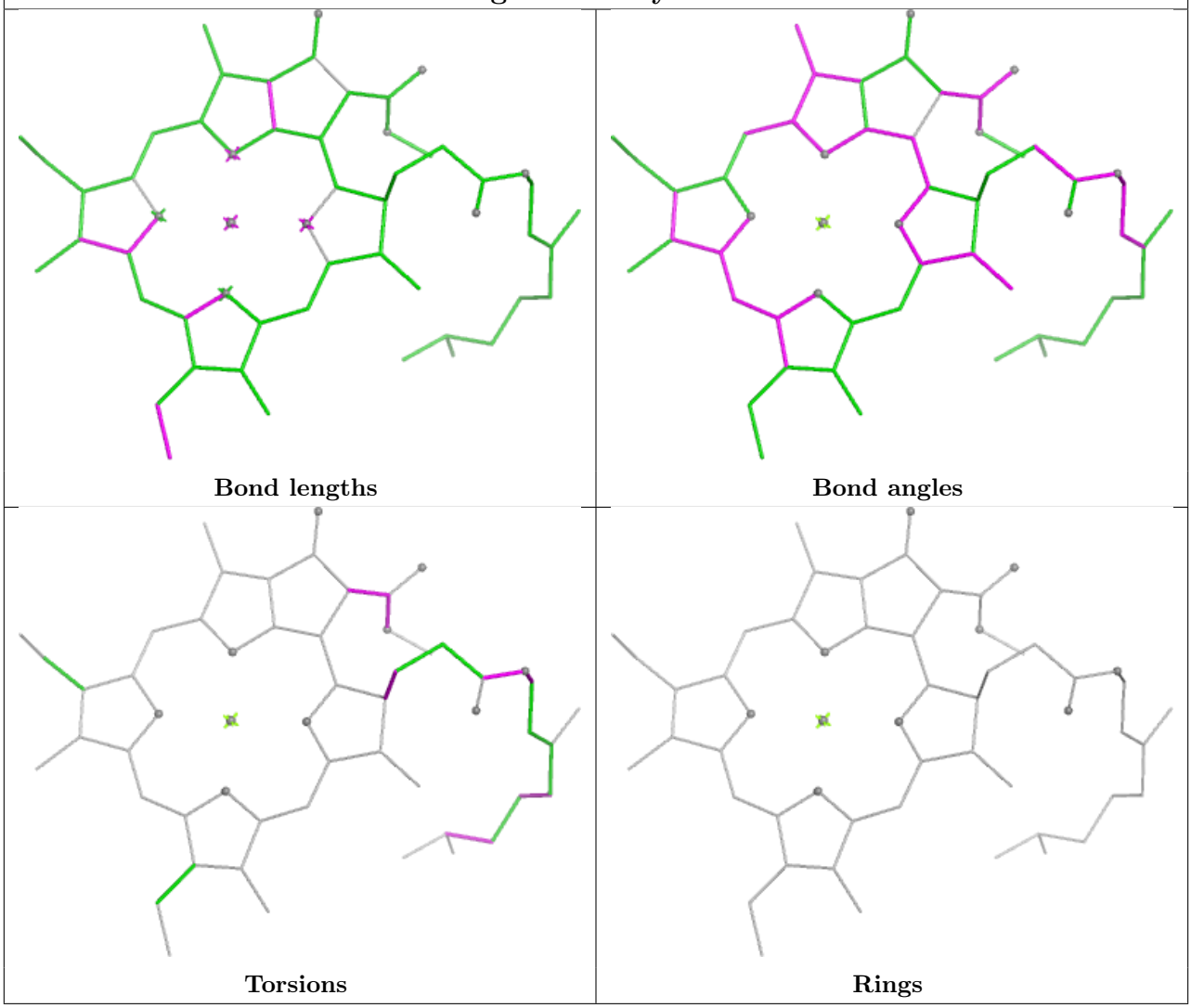


Rings

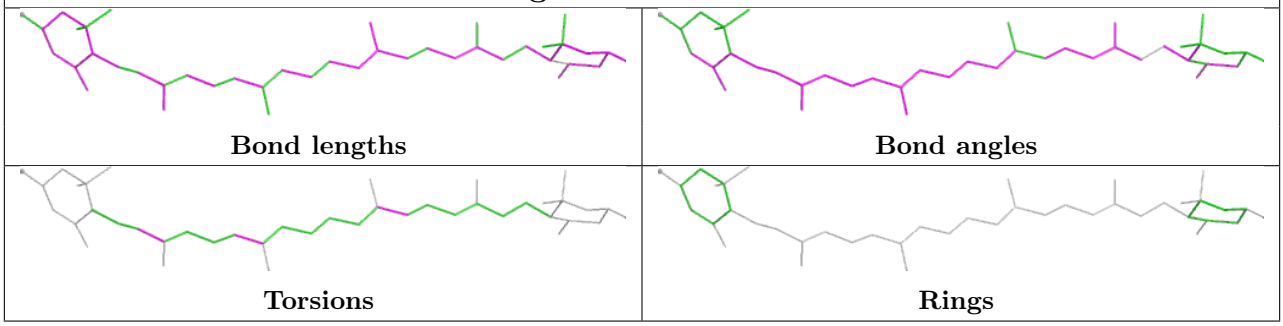
Ligand CHL 9 303



Ligand CLA y 603



Ligand LUT 8 615



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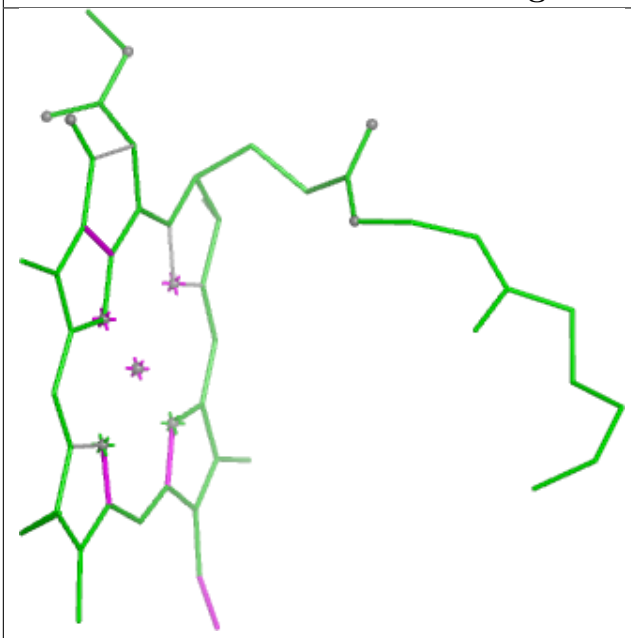
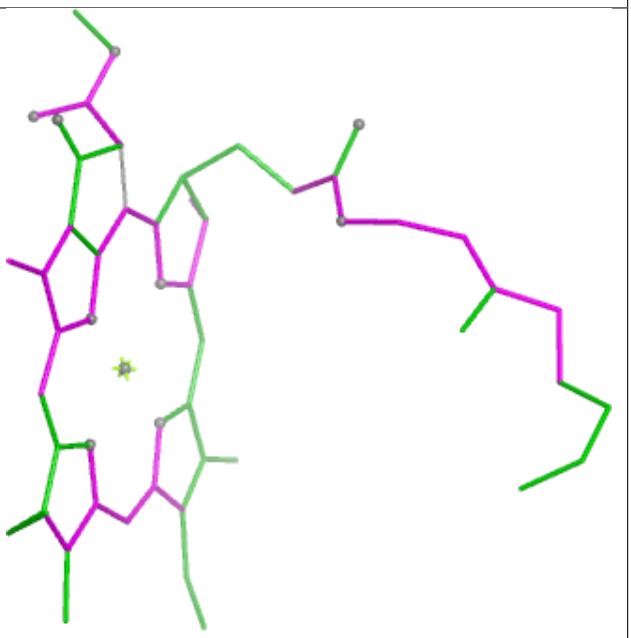
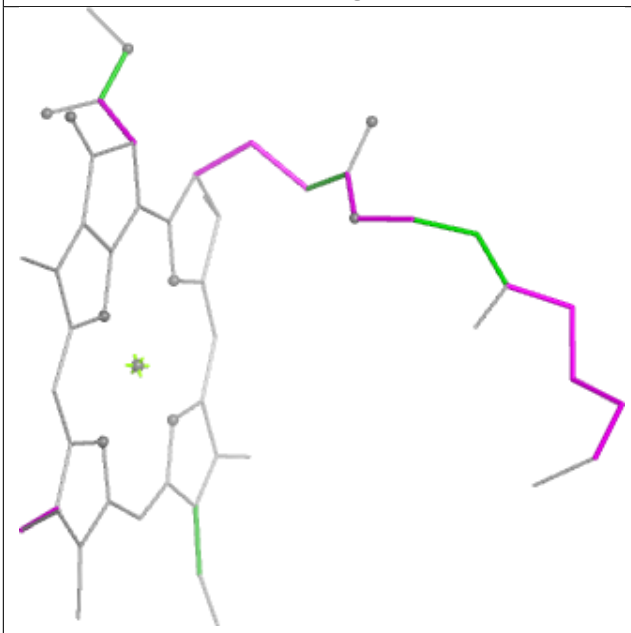


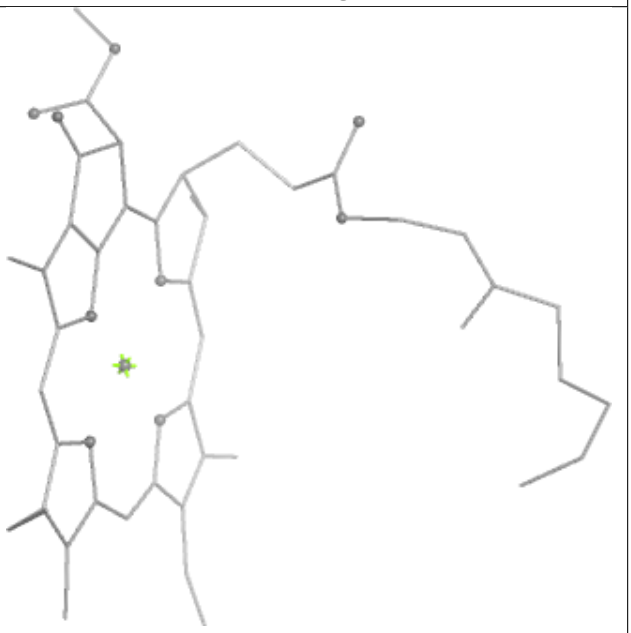
Bond lengths



Bond angles

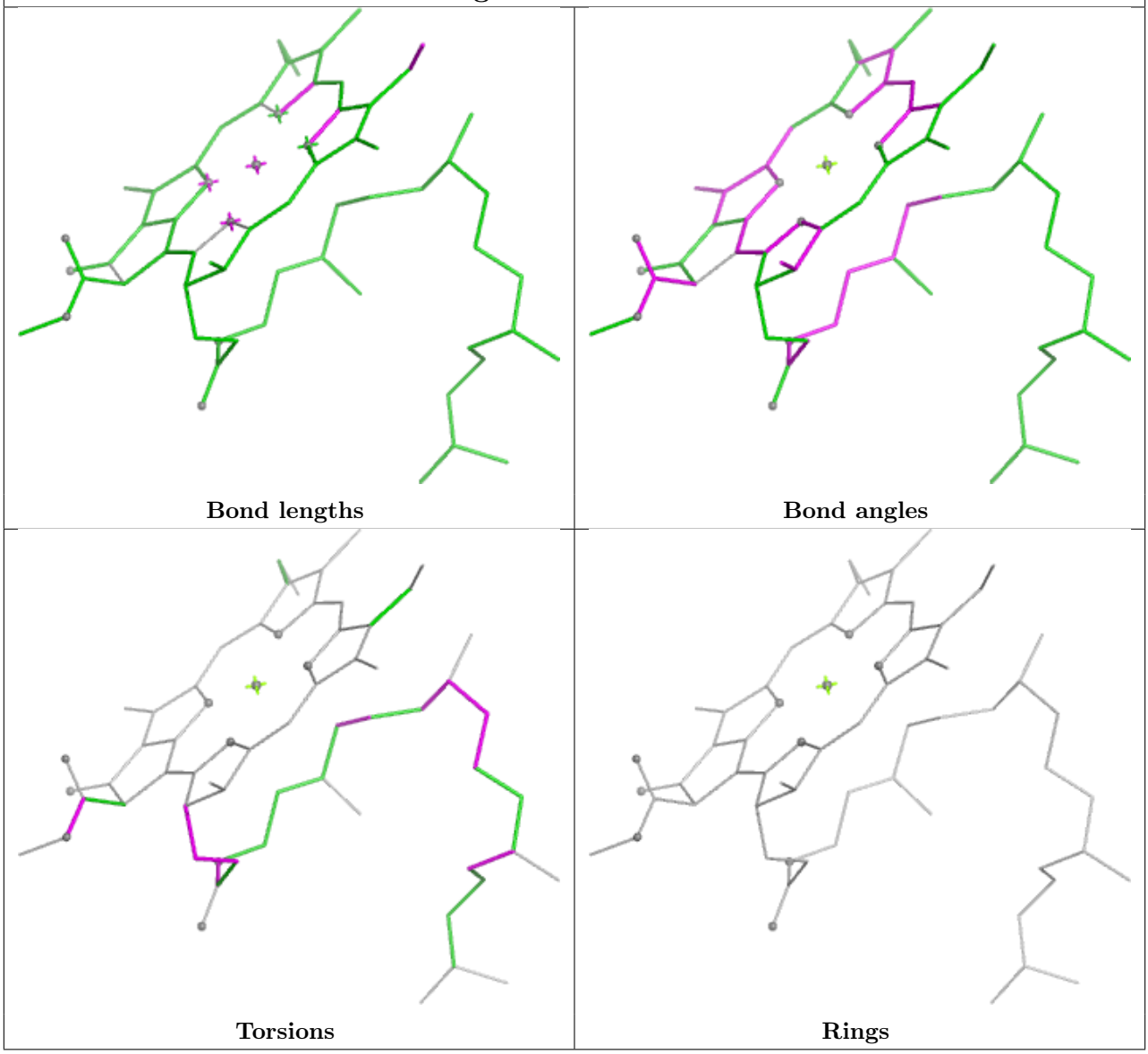


Torsions



Rings

Ligand CLA 6 314



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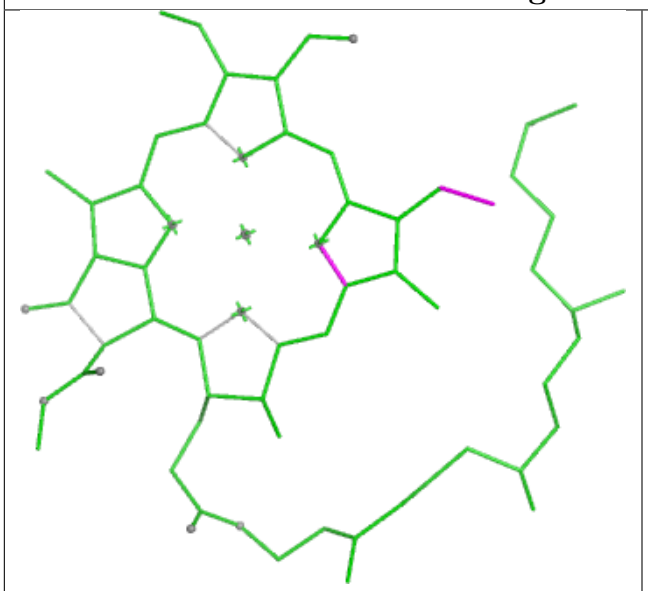

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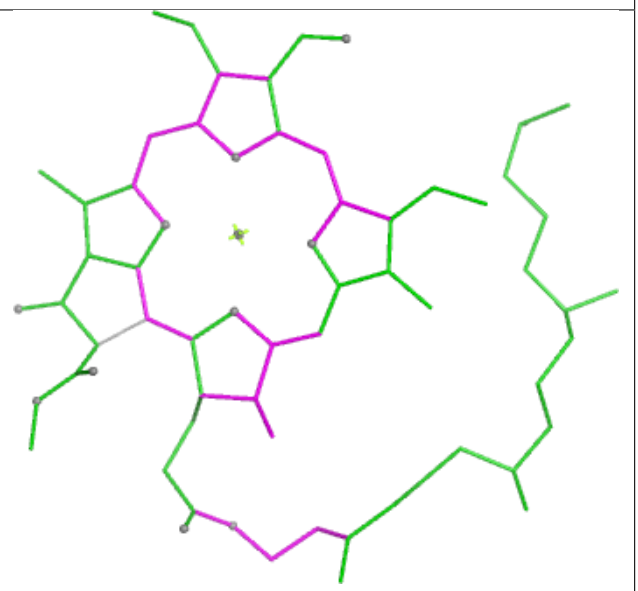
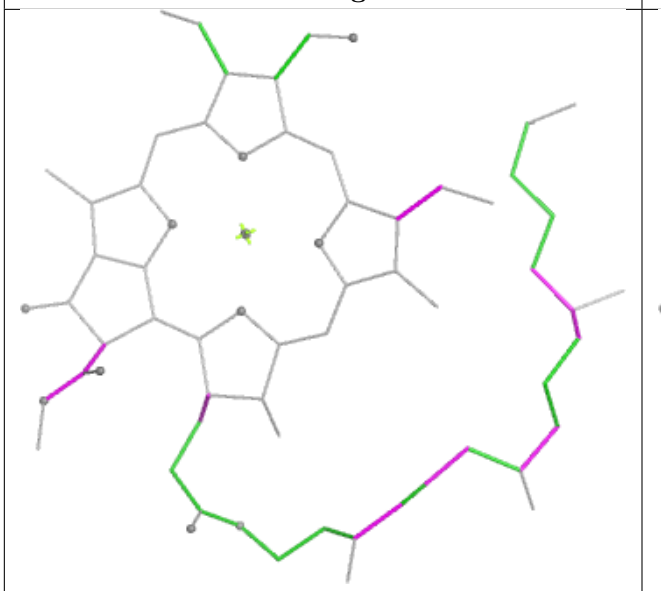


Bond angles



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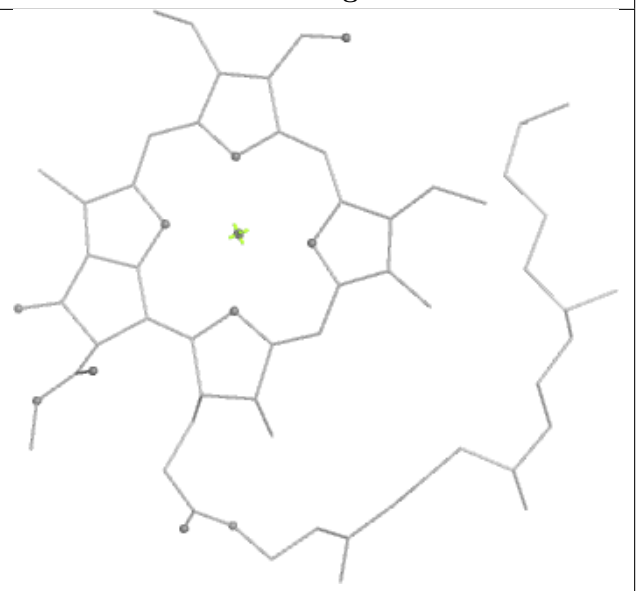
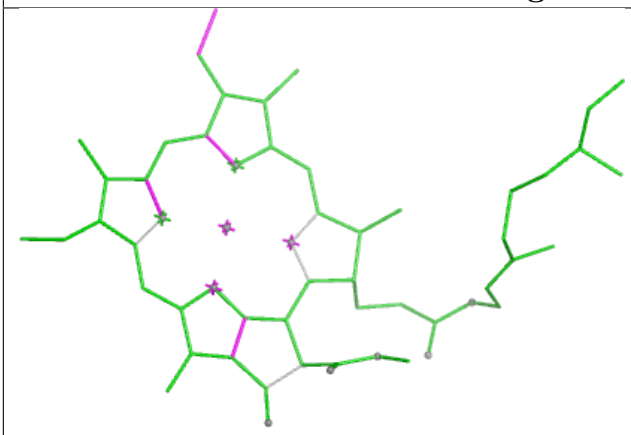
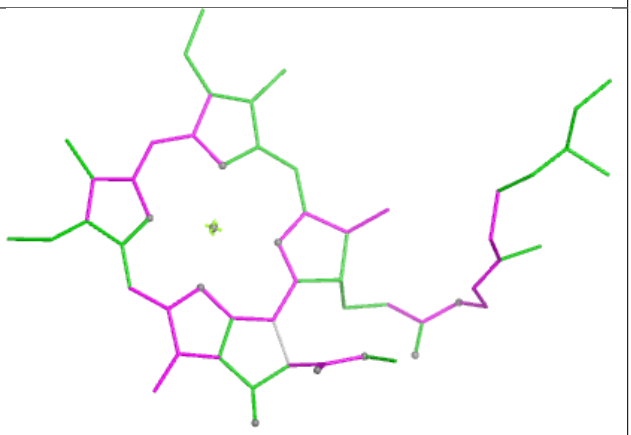
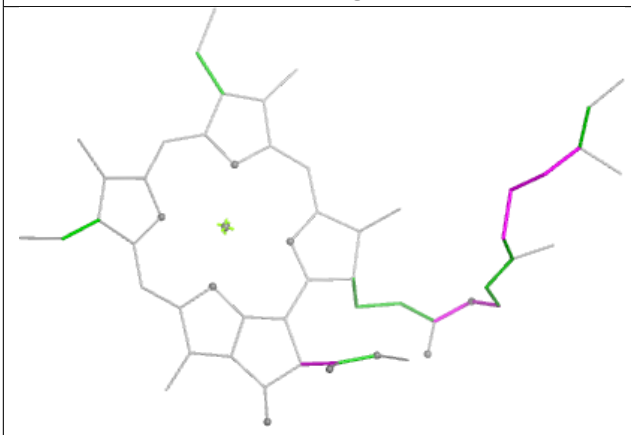
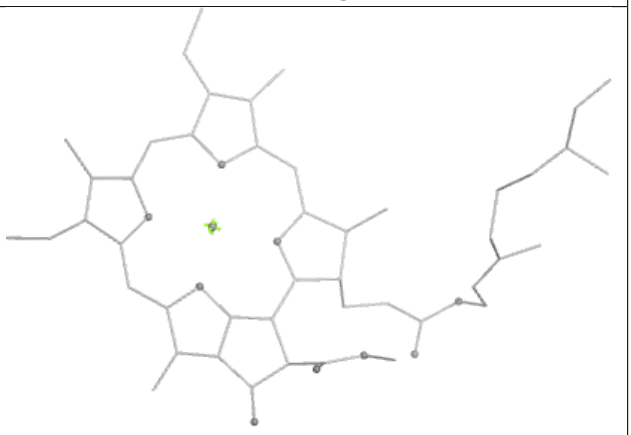
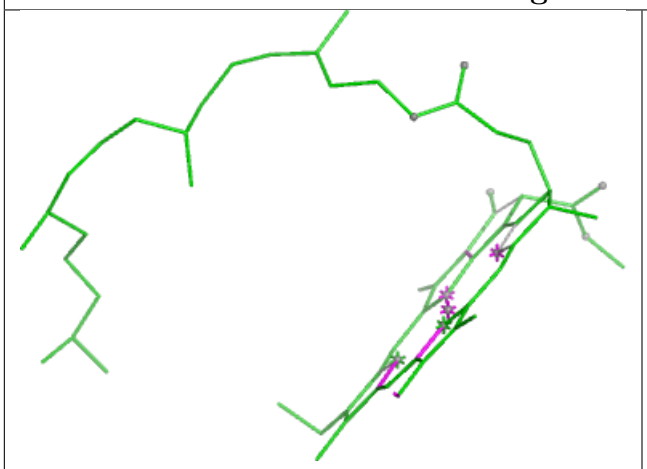


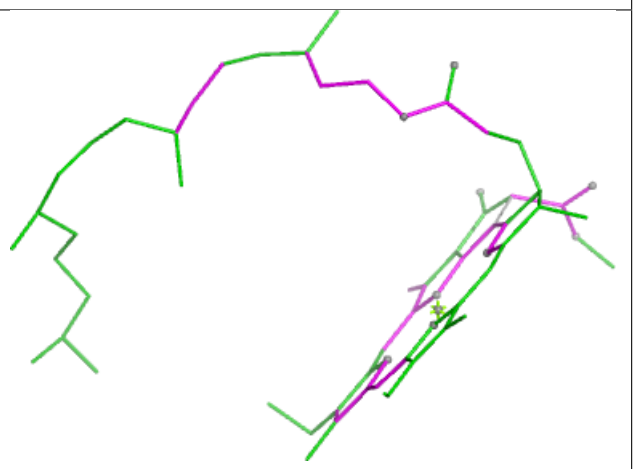
Rings

Ligand CLA S 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

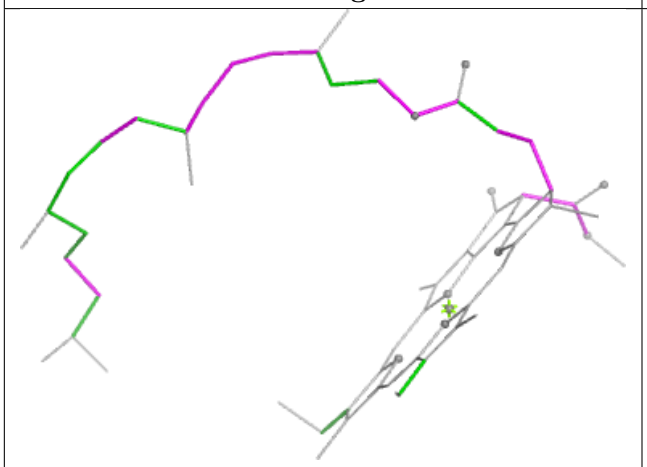
Ligand CLA c 606



Bond lengths

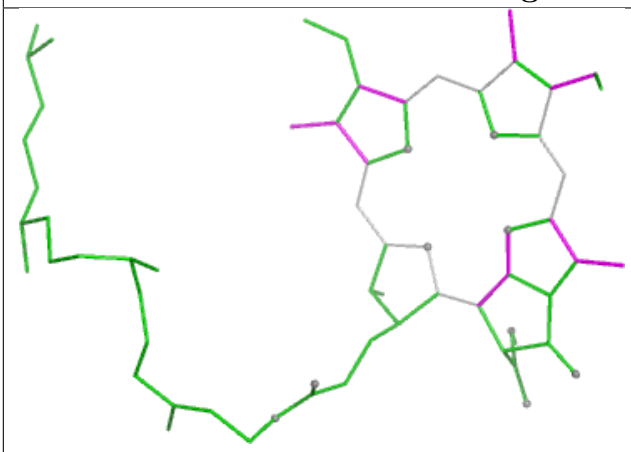
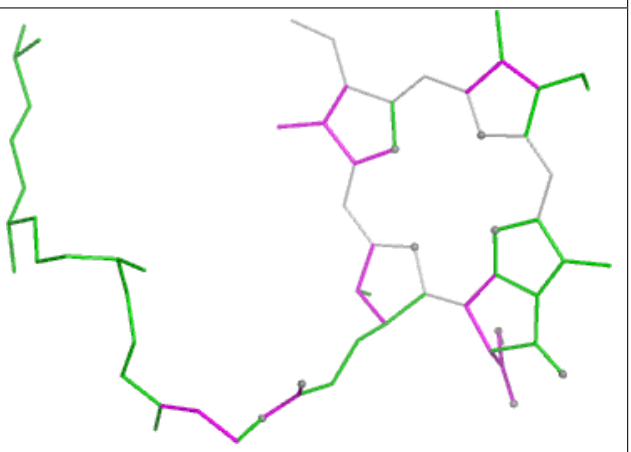
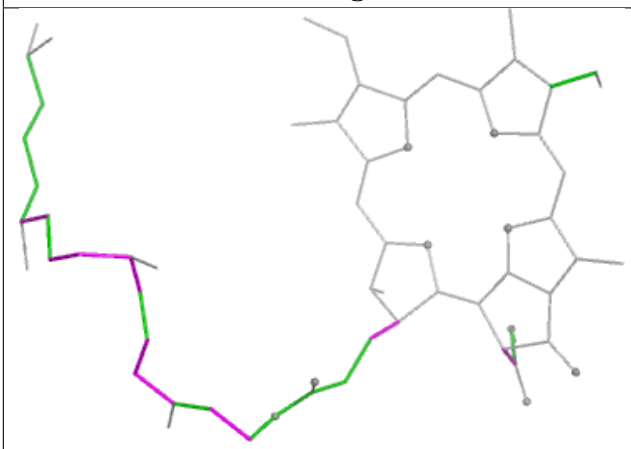
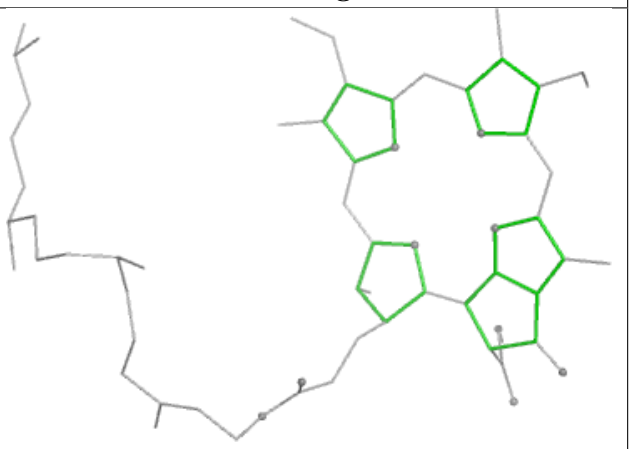


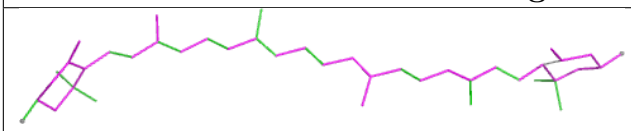
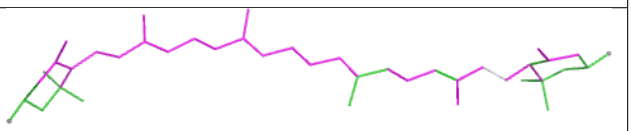
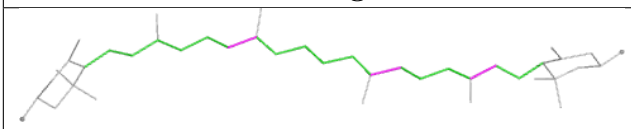
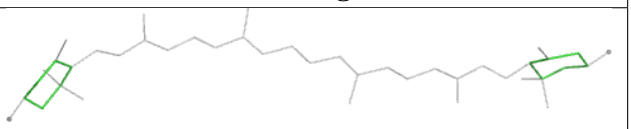
Bond angles



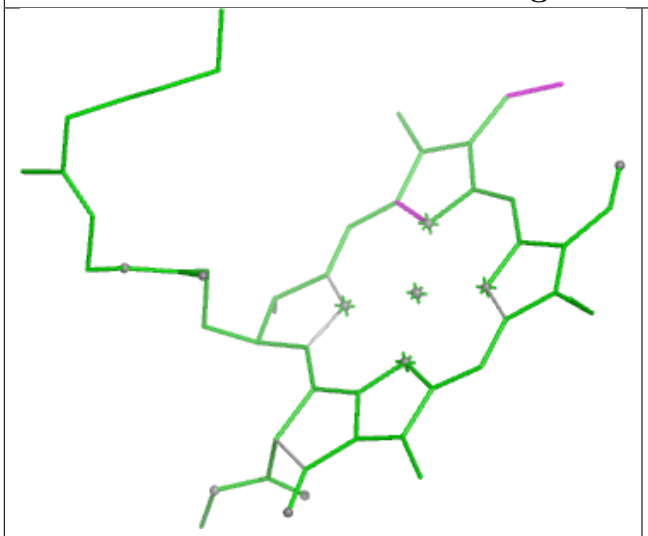
Torsions

Rings

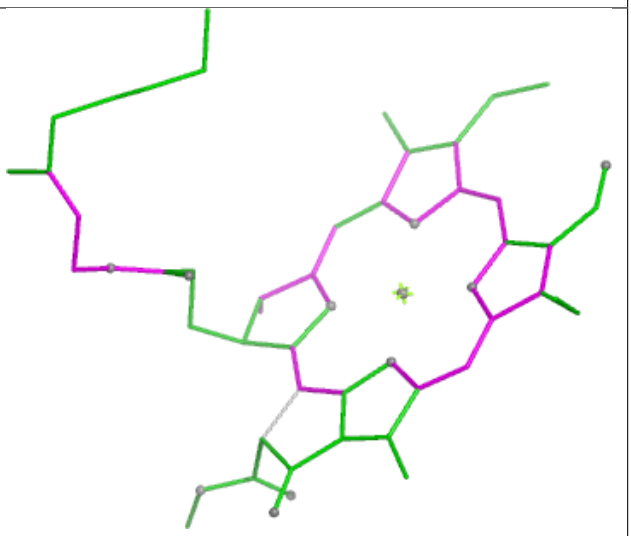
Ligand PHO D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 6 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

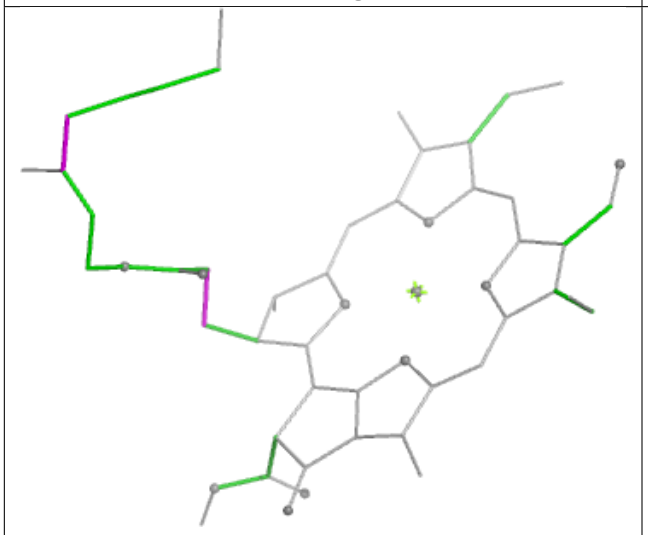
Ligand CHL r 310



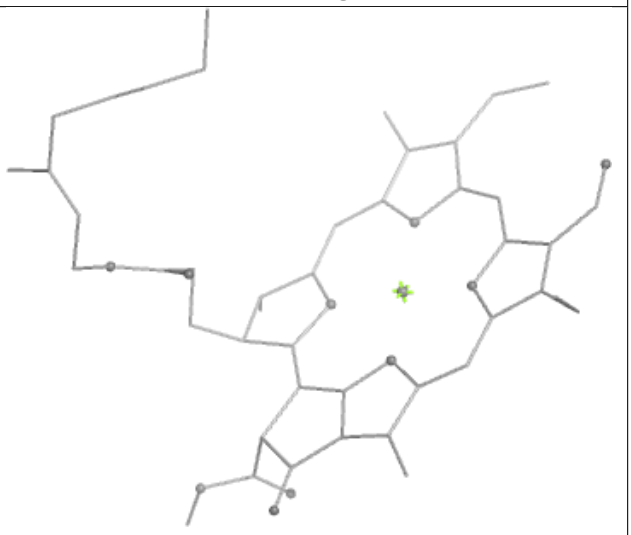
Bond lengths



Bond angles

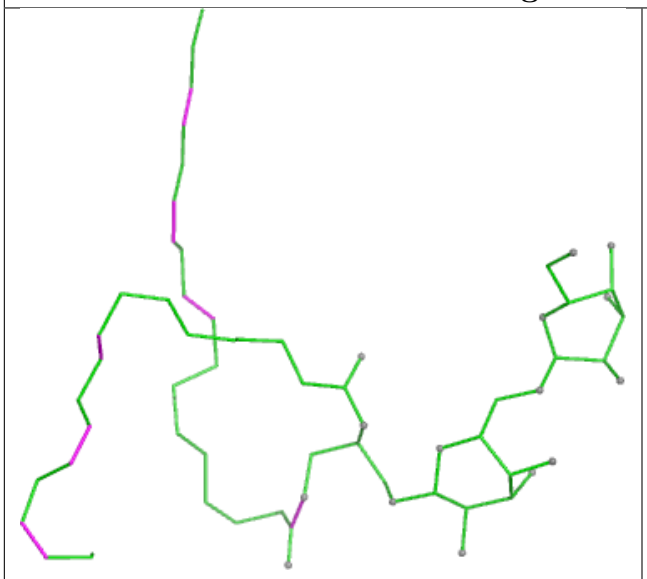


Torsions

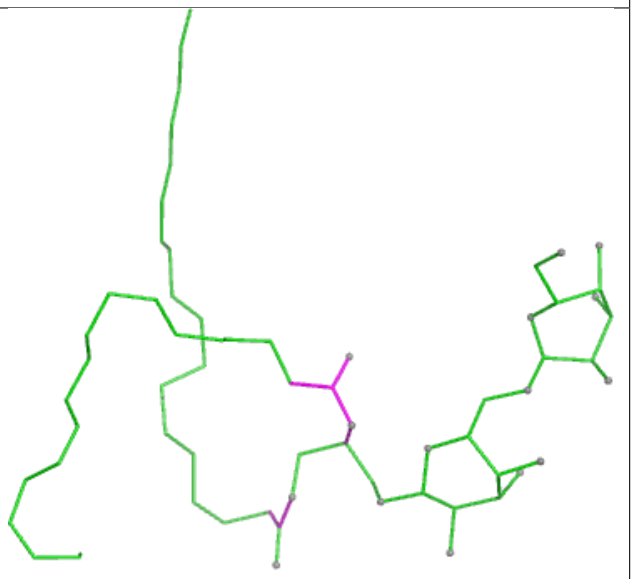


Rings

Ligand DGD C 620

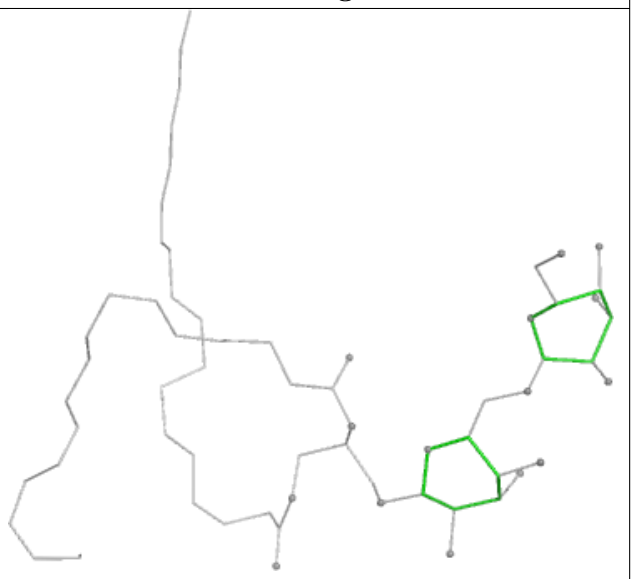


Bond lengths



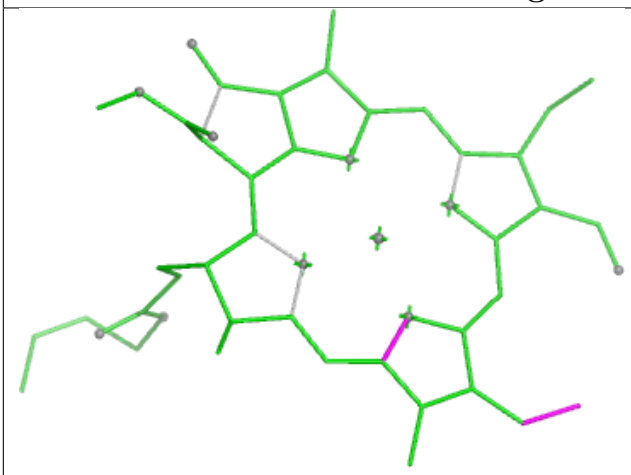
Bond angles

Torsions



Rings

Ligand CHL 2 607



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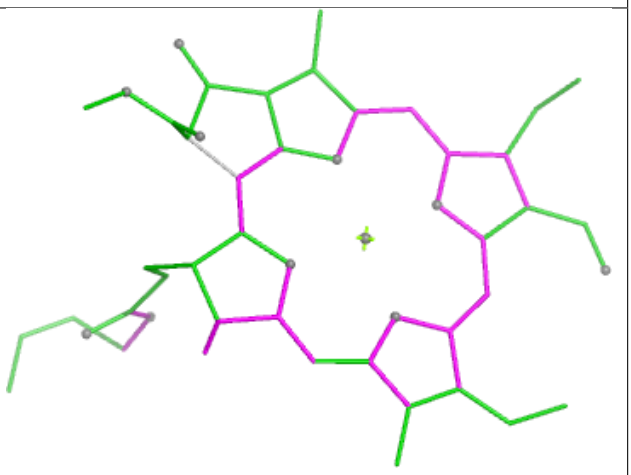
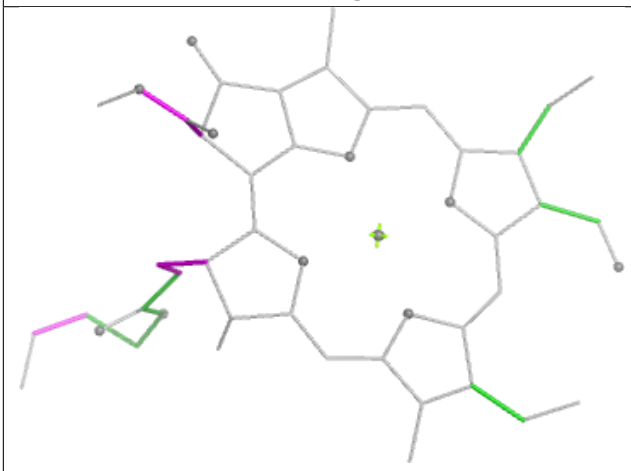
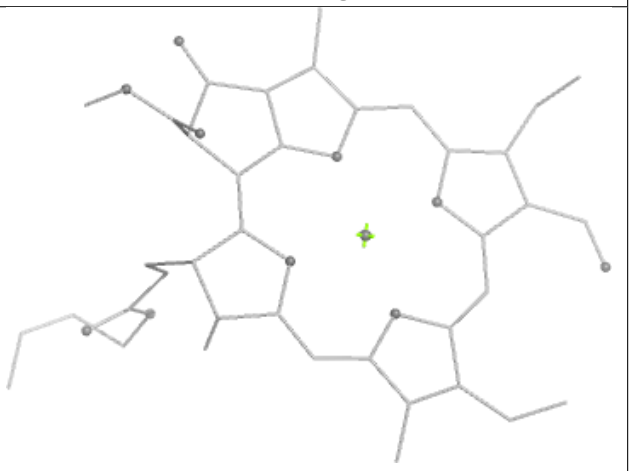


Bond angles

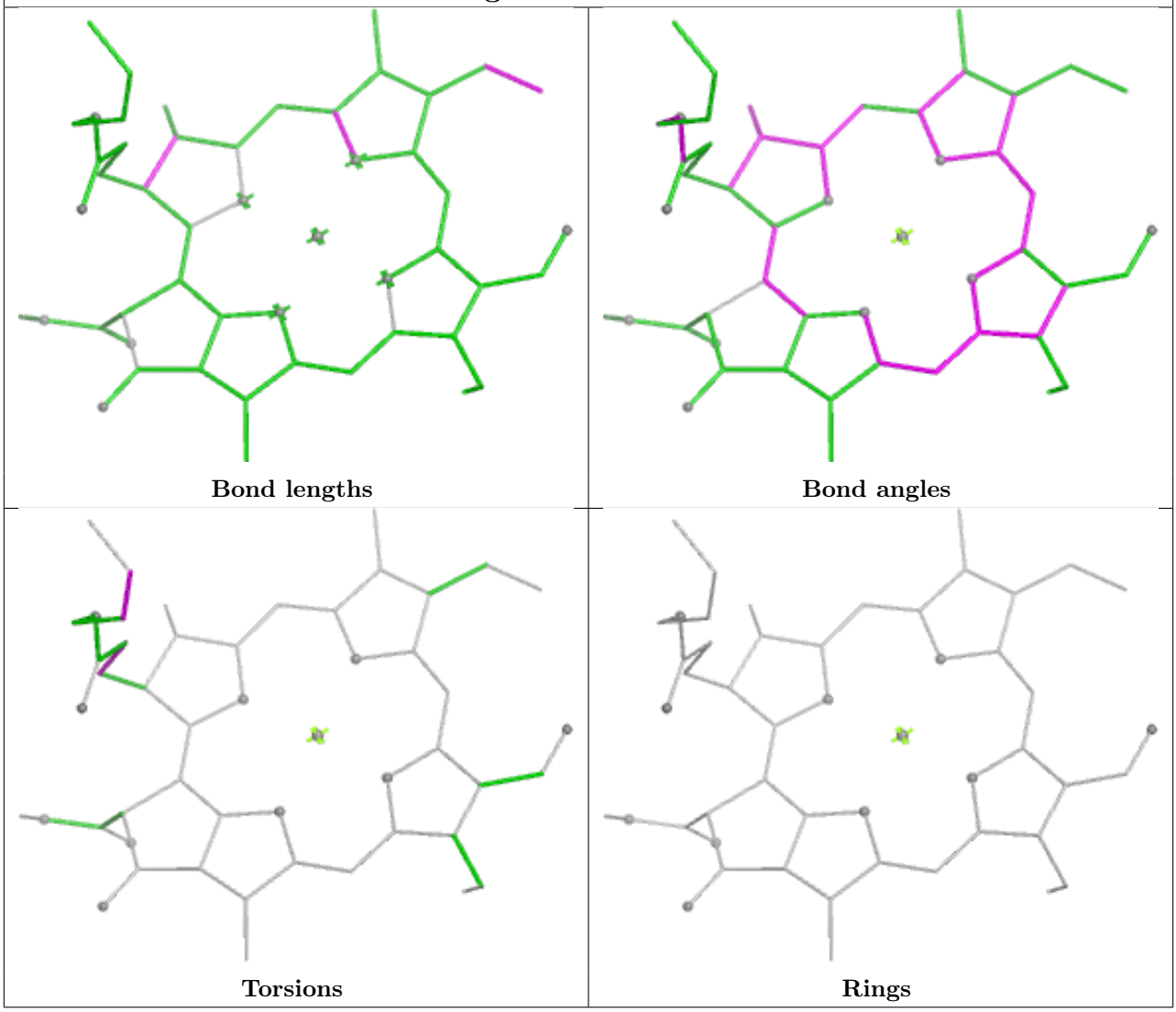


Torsions

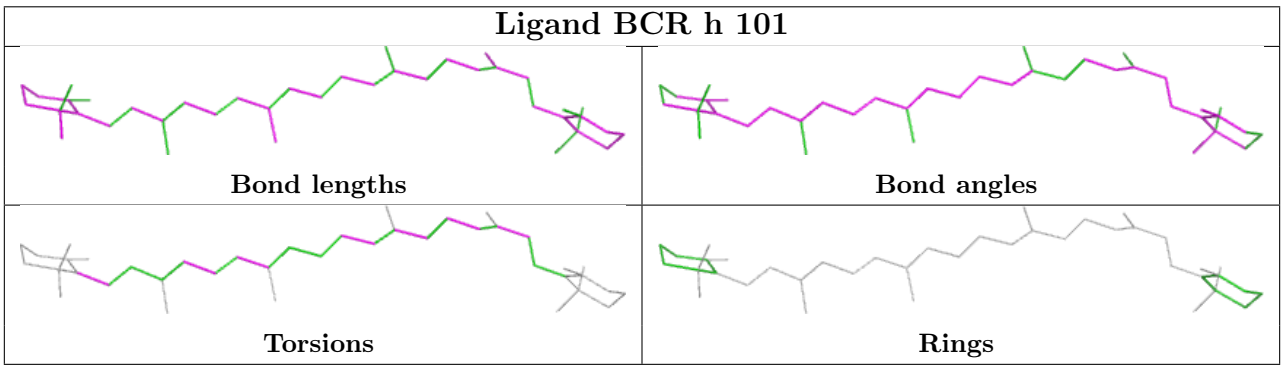


Rings

Ligand CHL 6 309



Ligand BCR h 101



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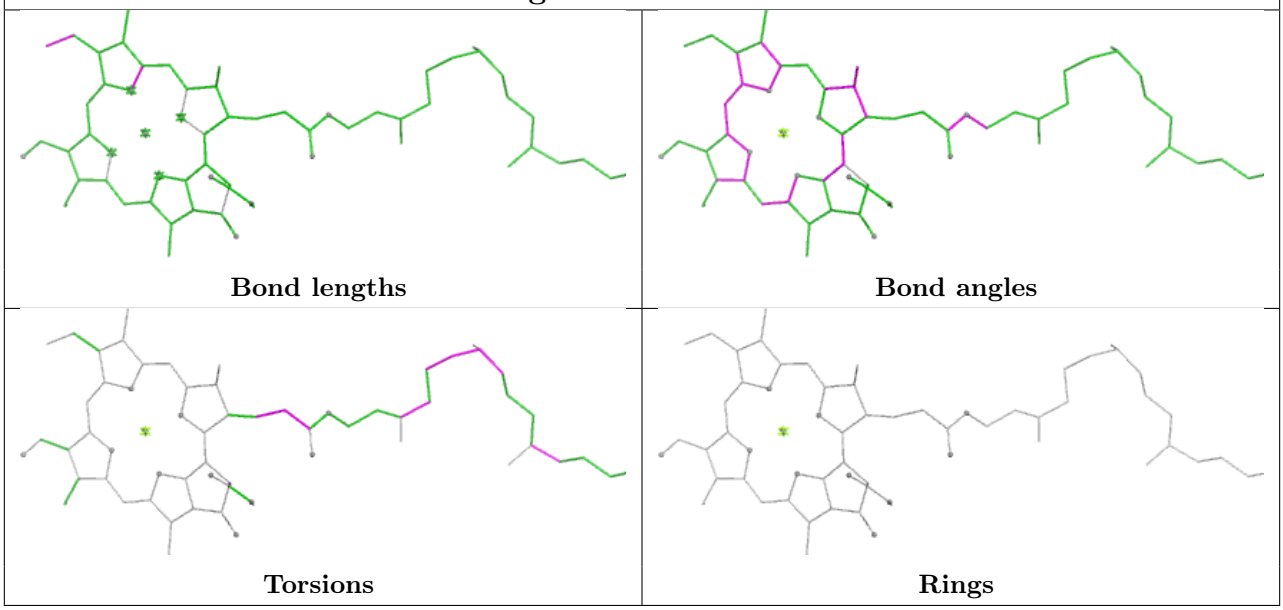
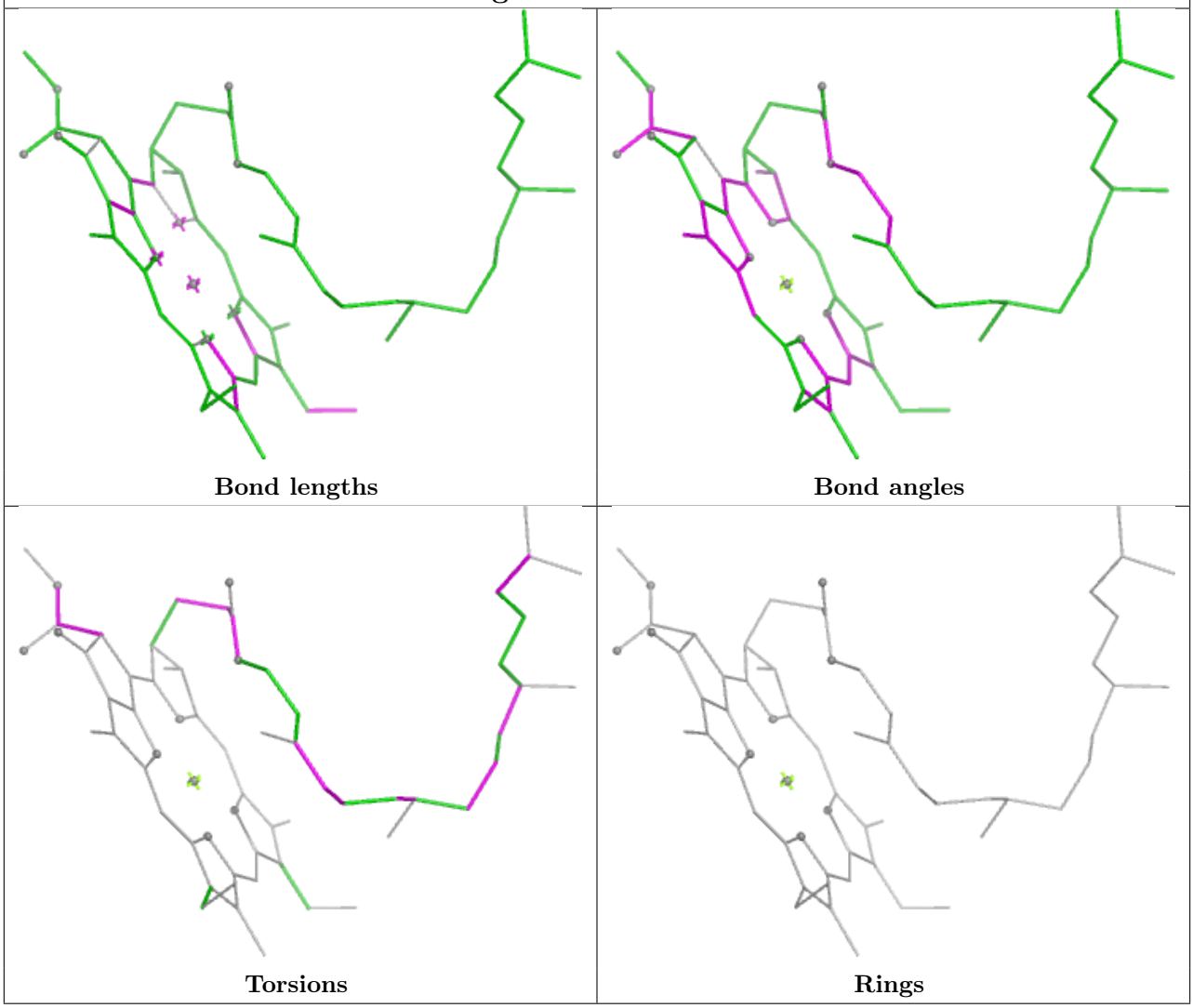
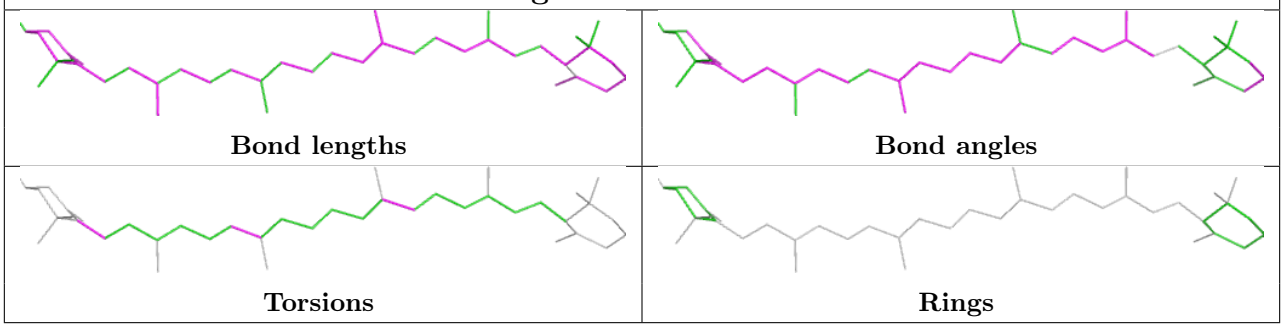


Ligand CLA 2 612



Ligand LUT s 318



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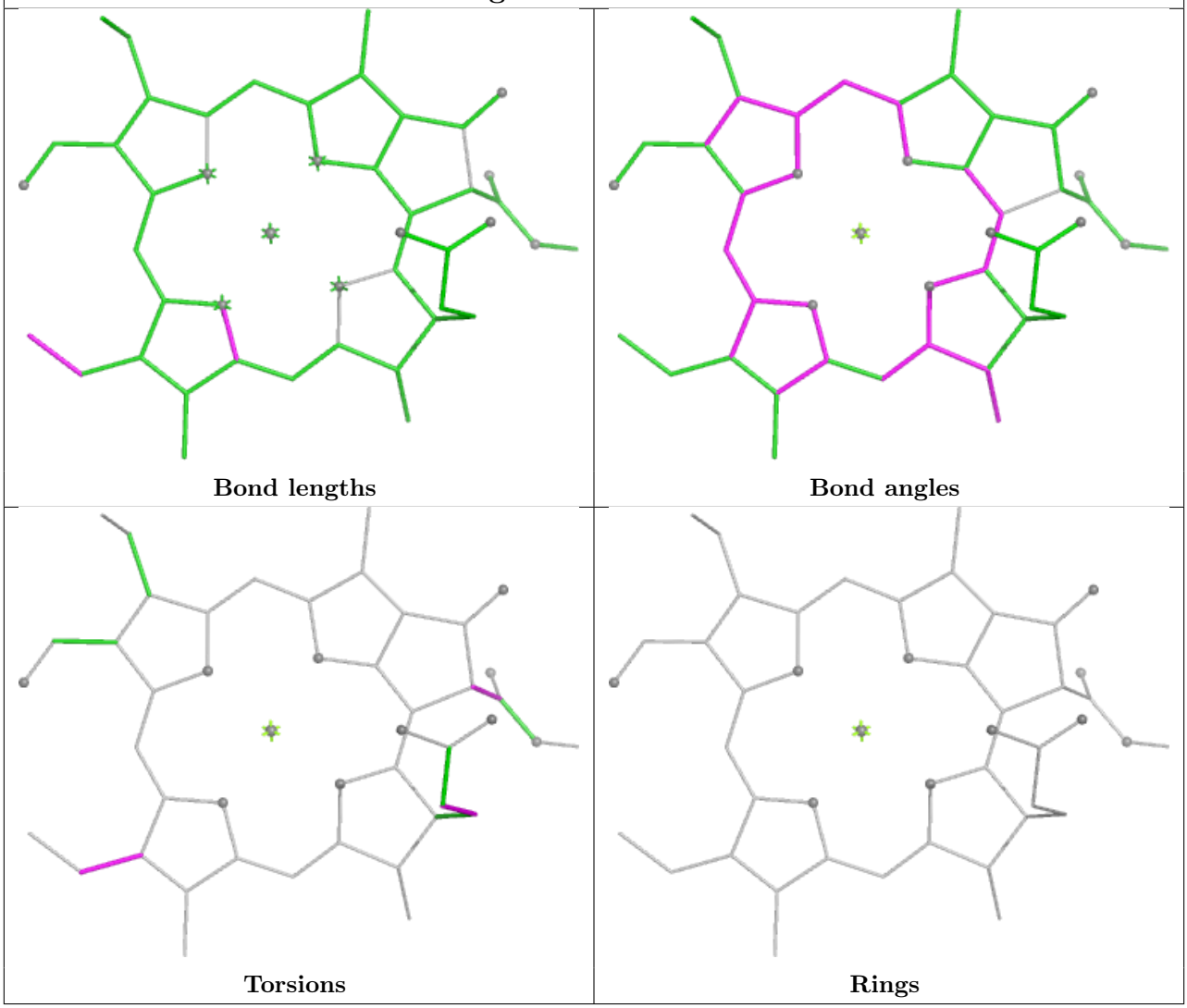
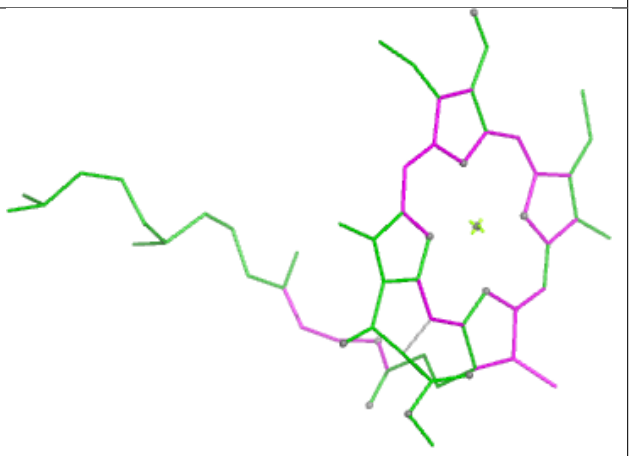
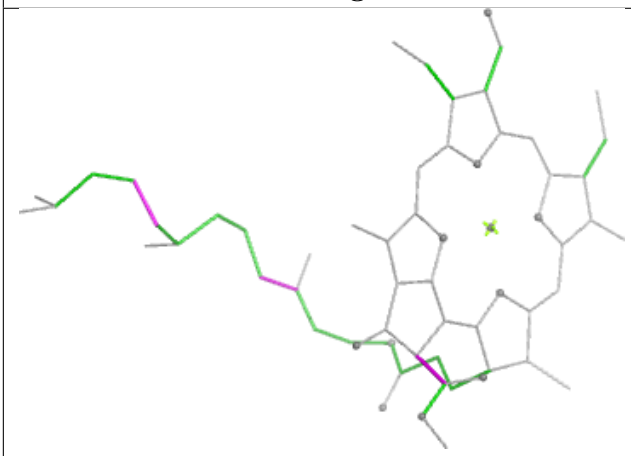


Ligand CHL 0 609

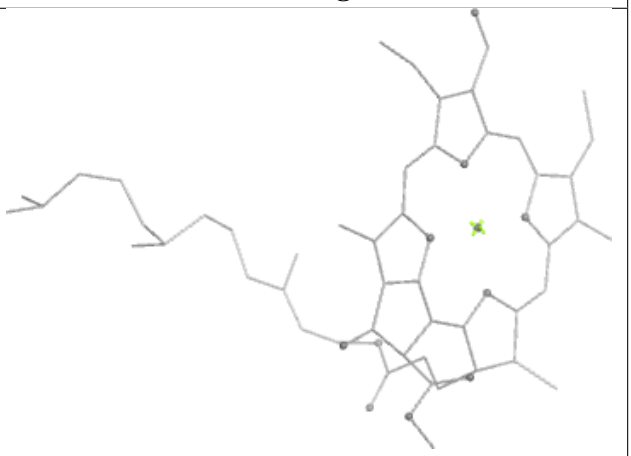
Bond lengths



Bond angles

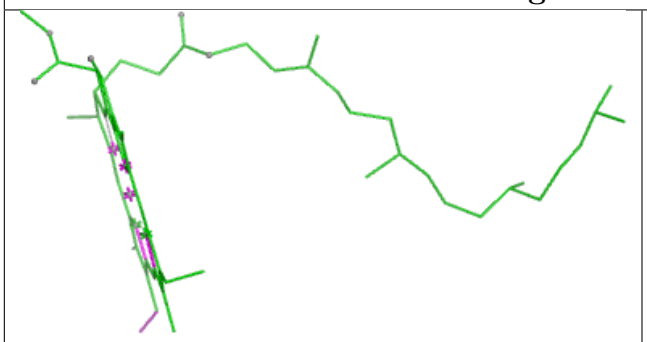


Torsions



Rings

Ligand CLA S 305



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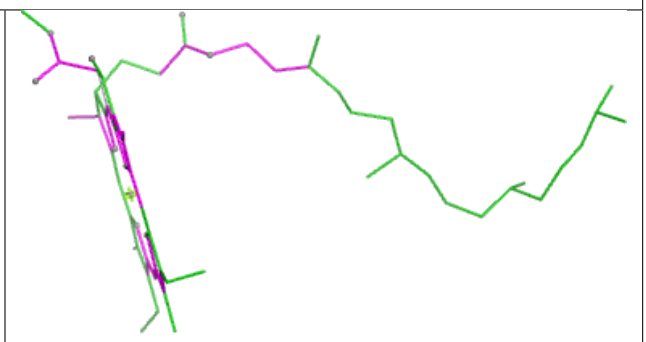
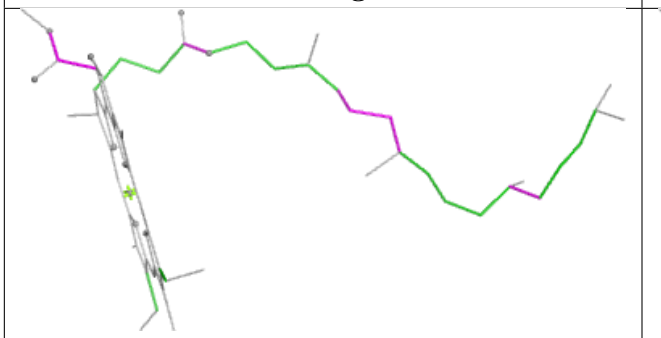


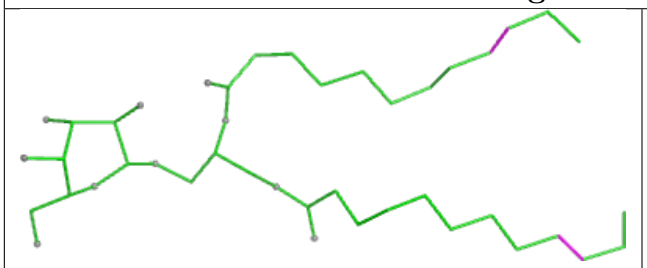
Bond angles



Torsions

Rings

Ligand LMG j 101



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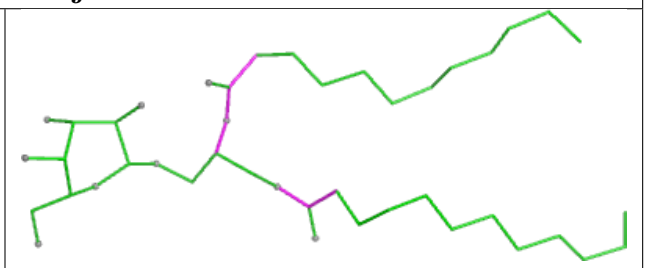
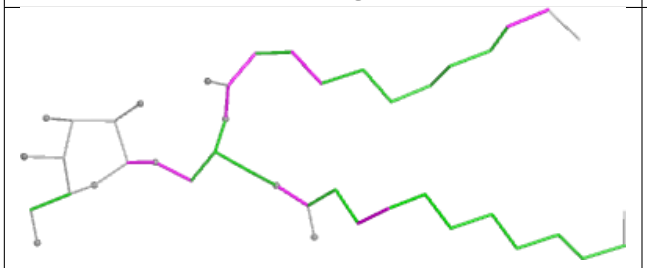


Bond angles



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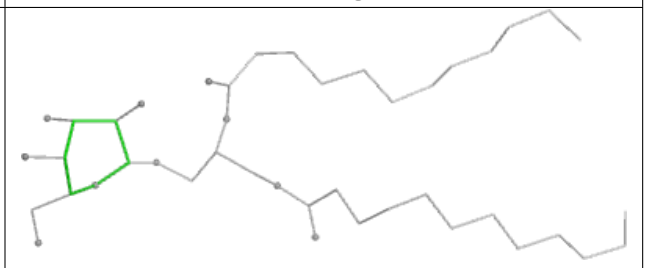
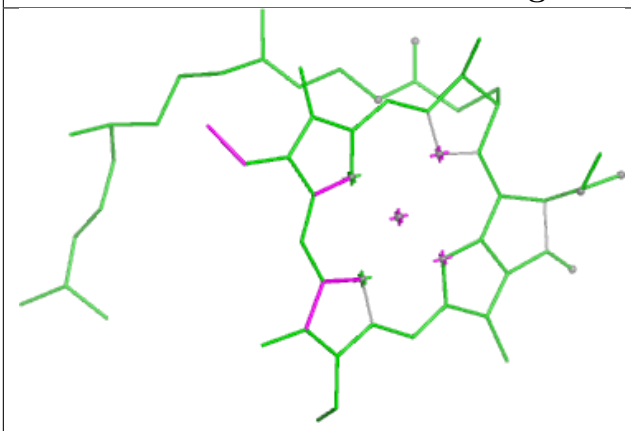


Rings

Ligand CLA 3 304



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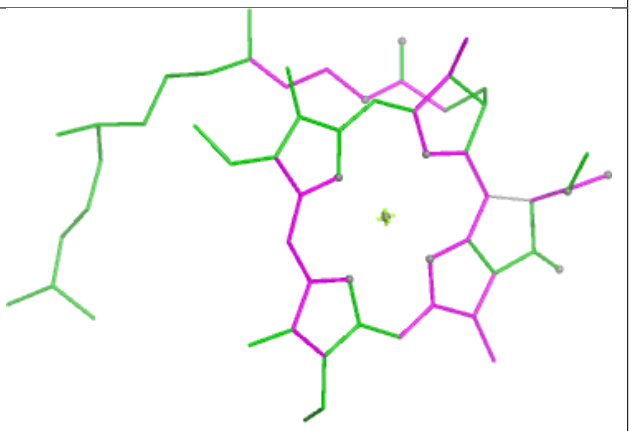
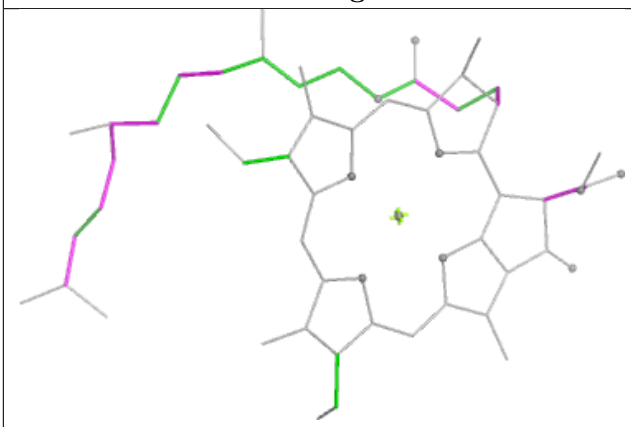


Bond angles



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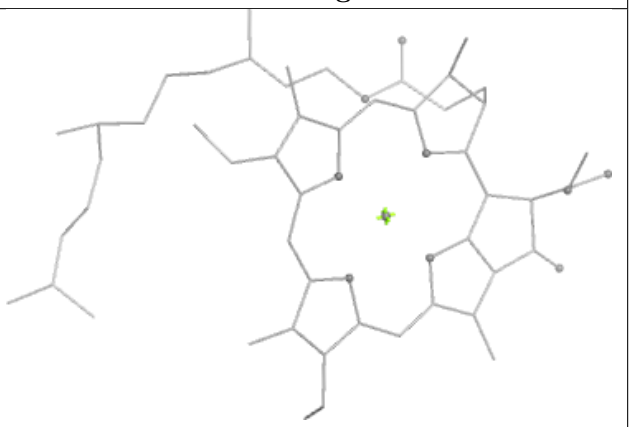
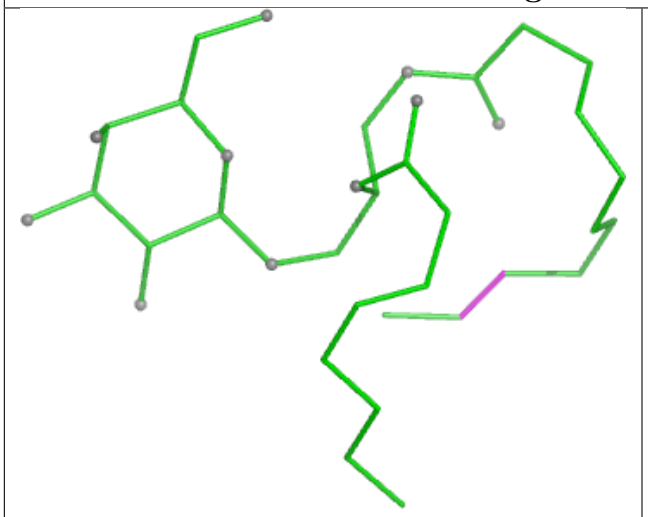


Rings

Ligand LMG 5 620



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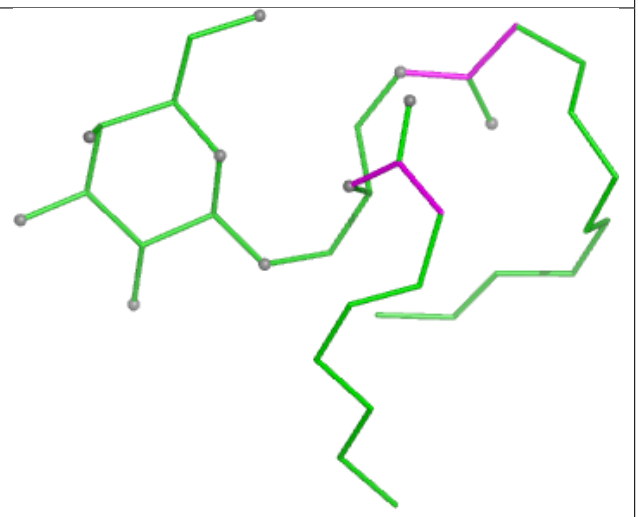
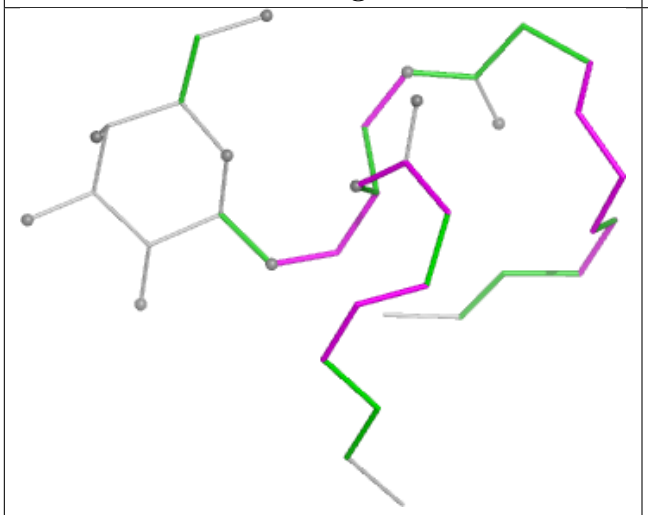


Bond angles



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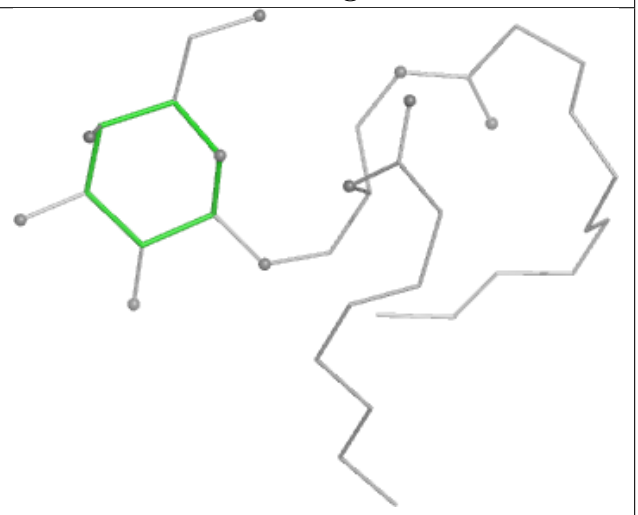
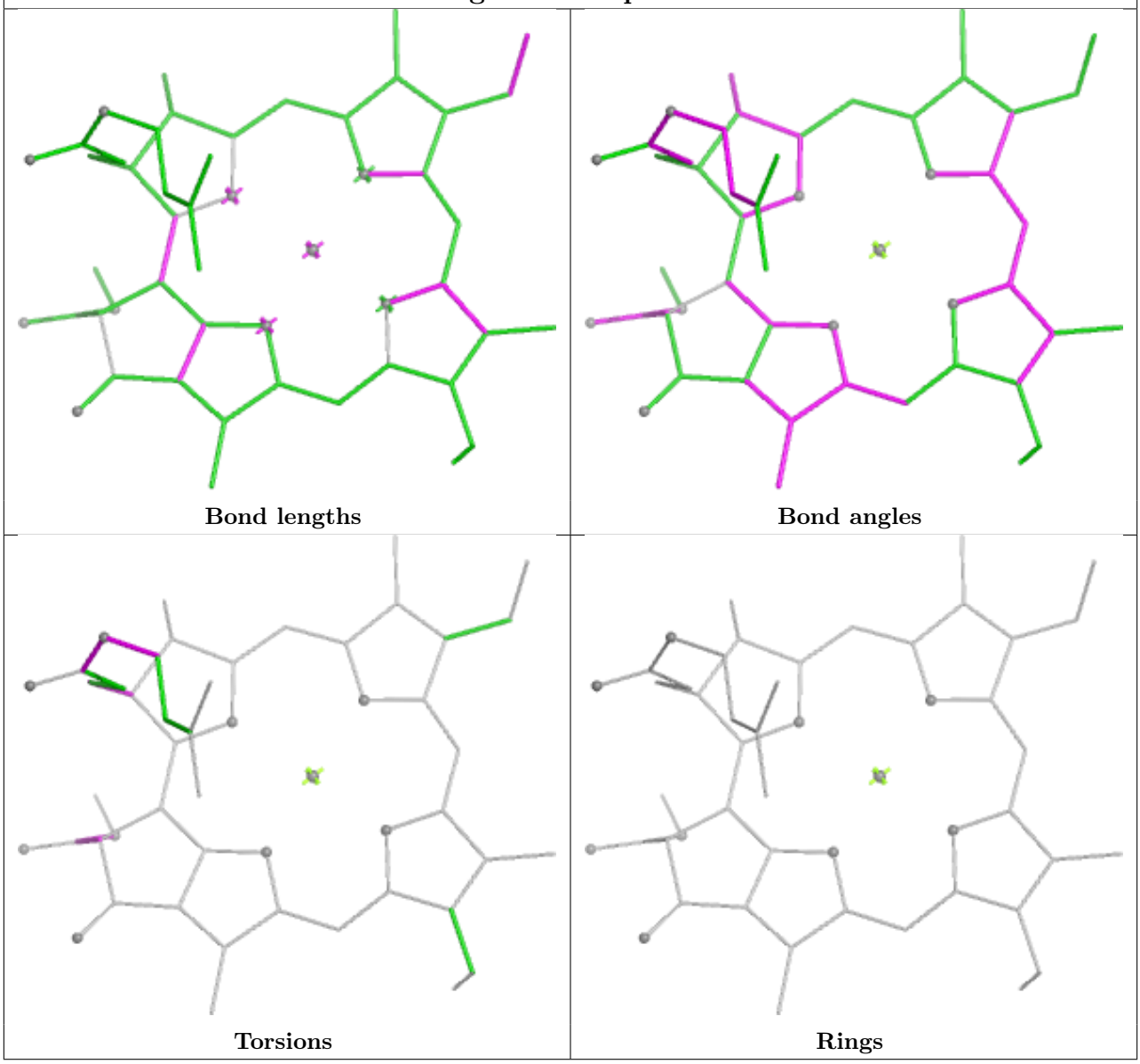
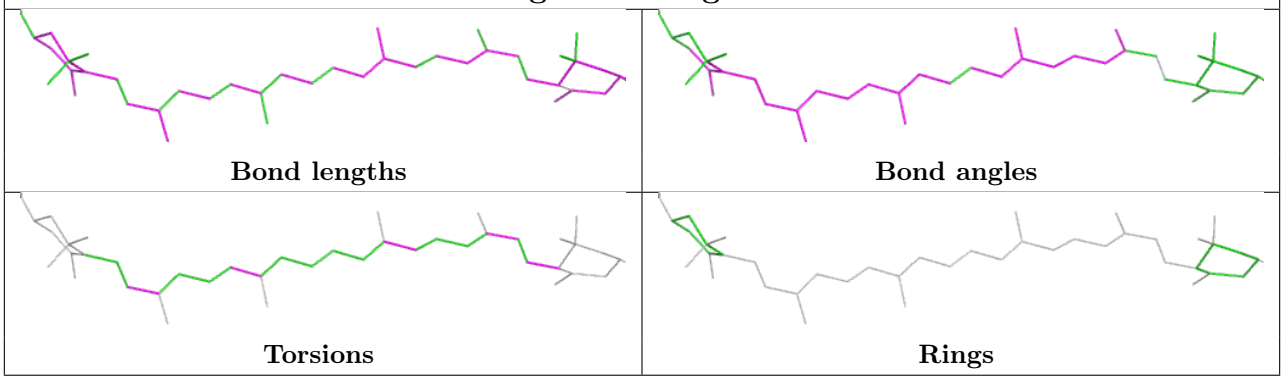


Rings

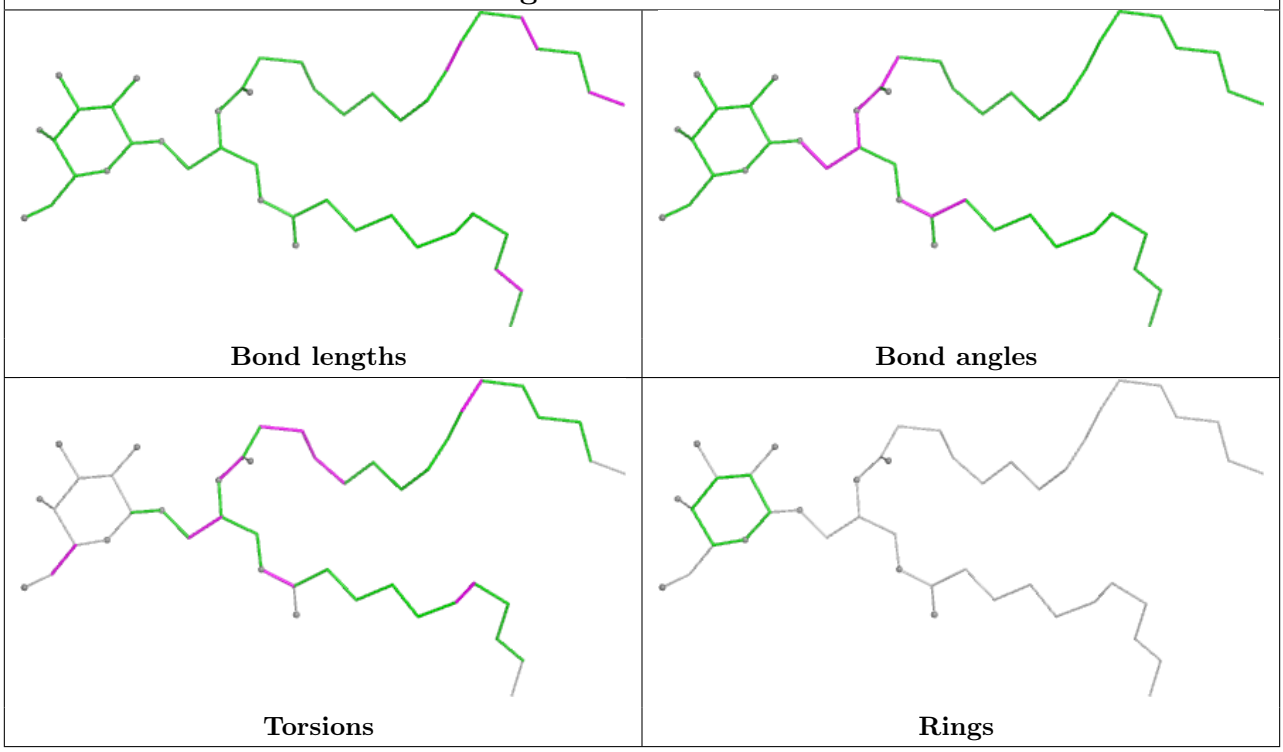
Ligand CLA p 604



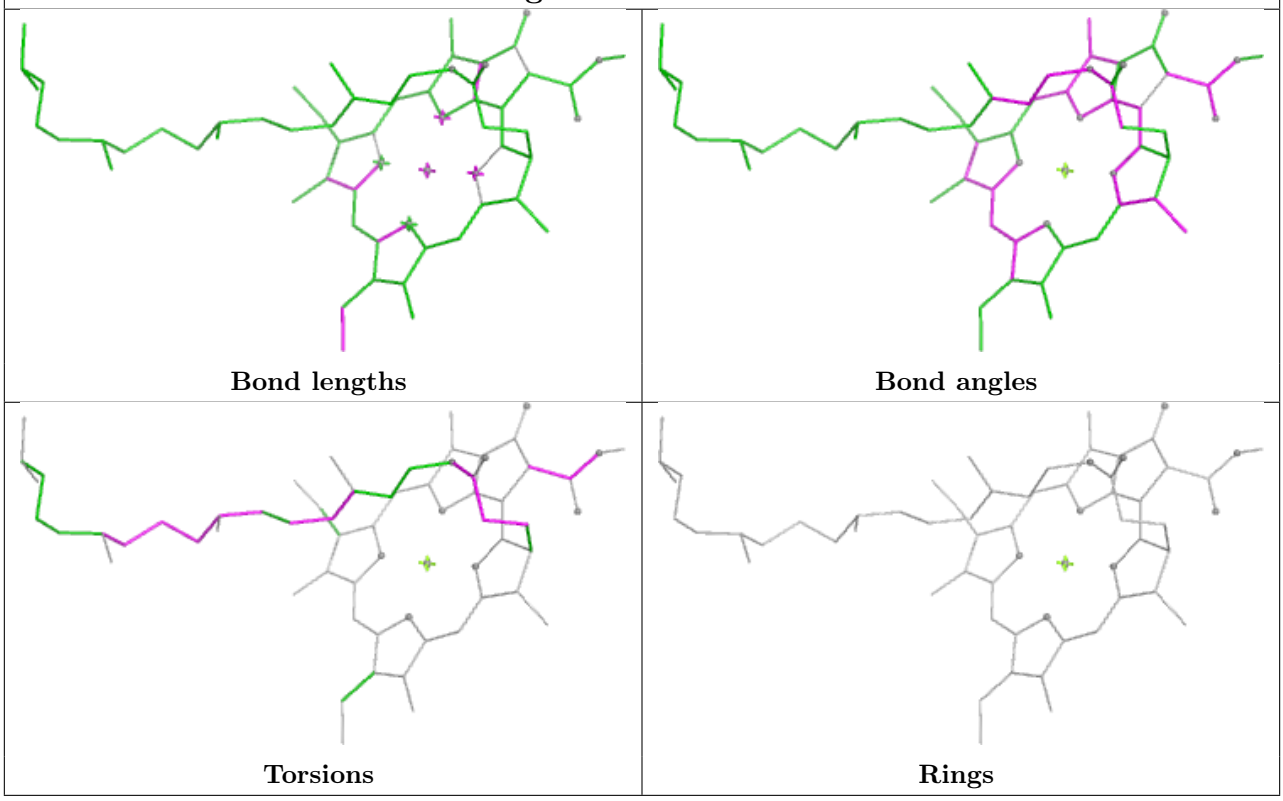
Ligand LUT g 316



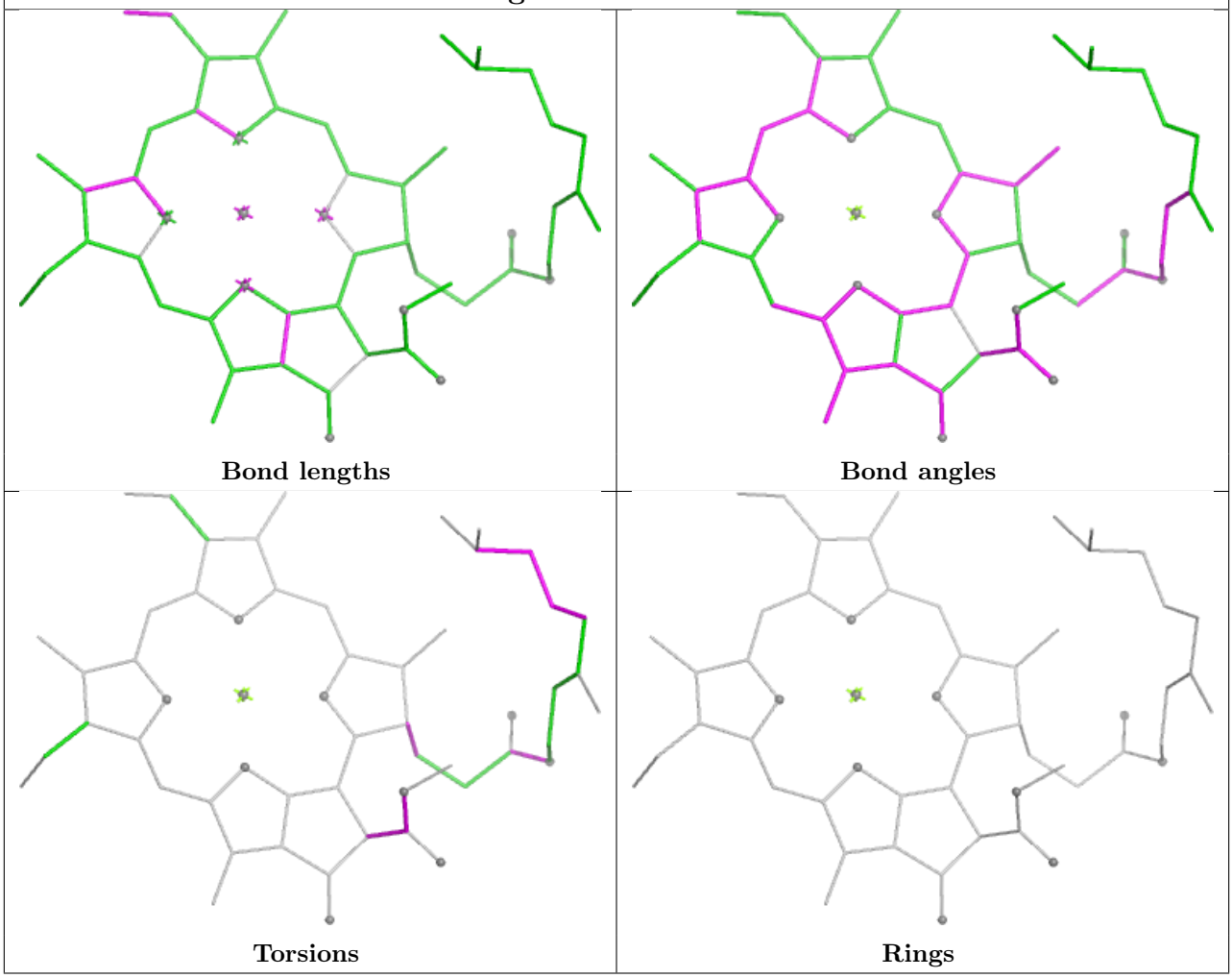
Ligand LMG D 409



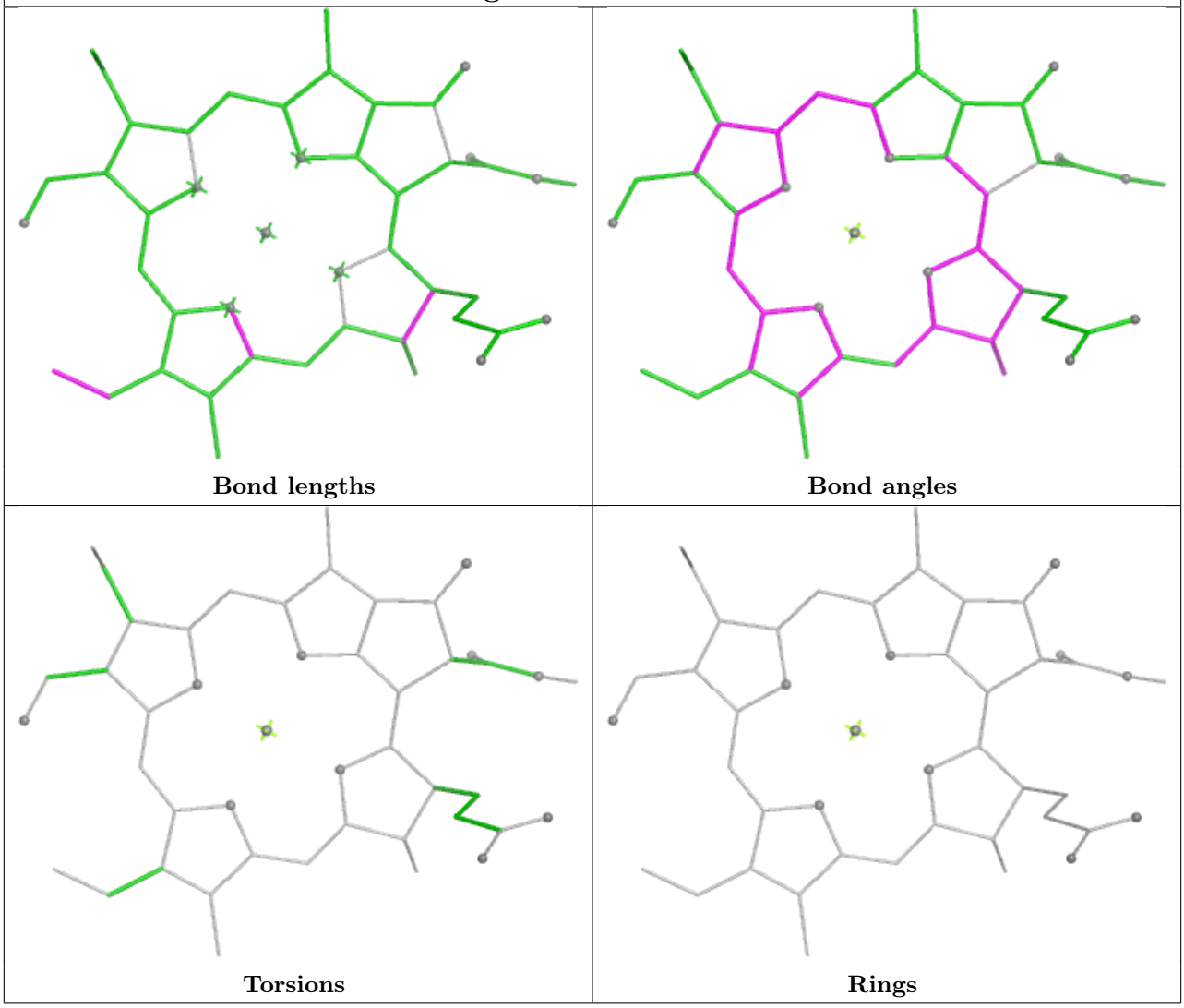
Ligand CLA B 614



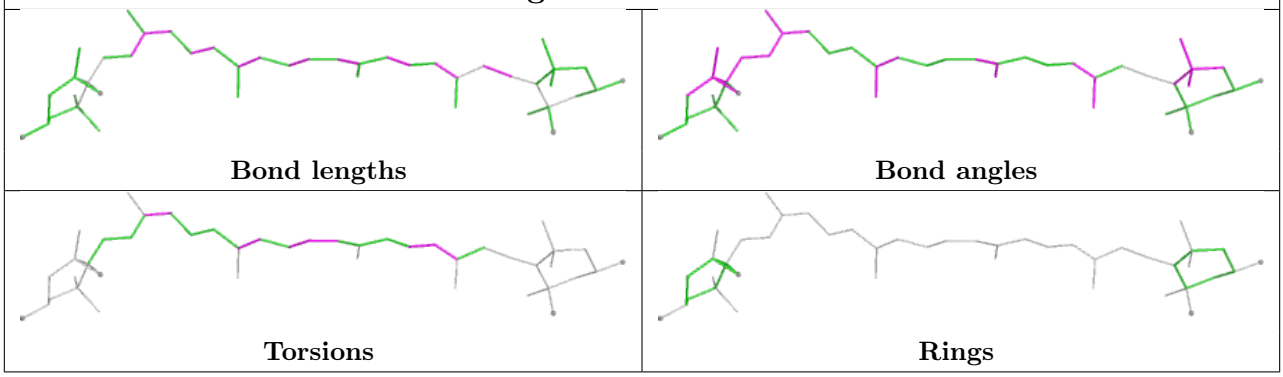
Ligand CLA 7 304

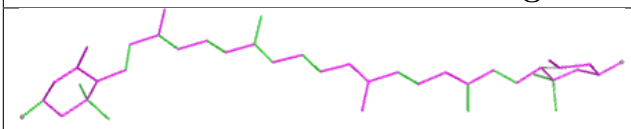
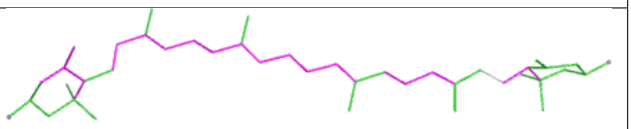
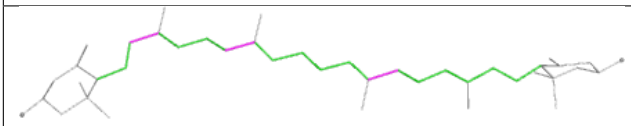
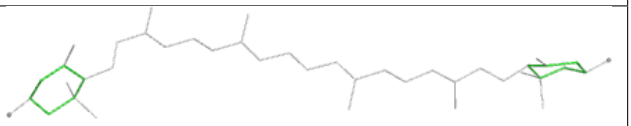


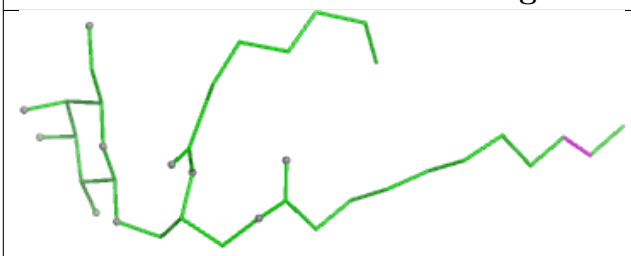
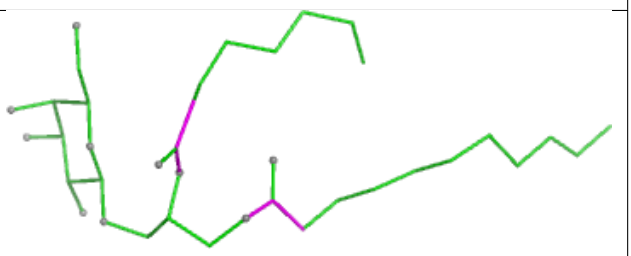
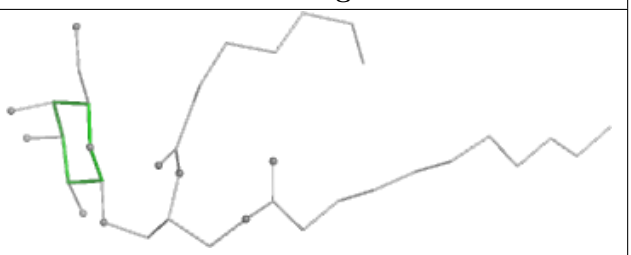
Ligand CHL Y 306



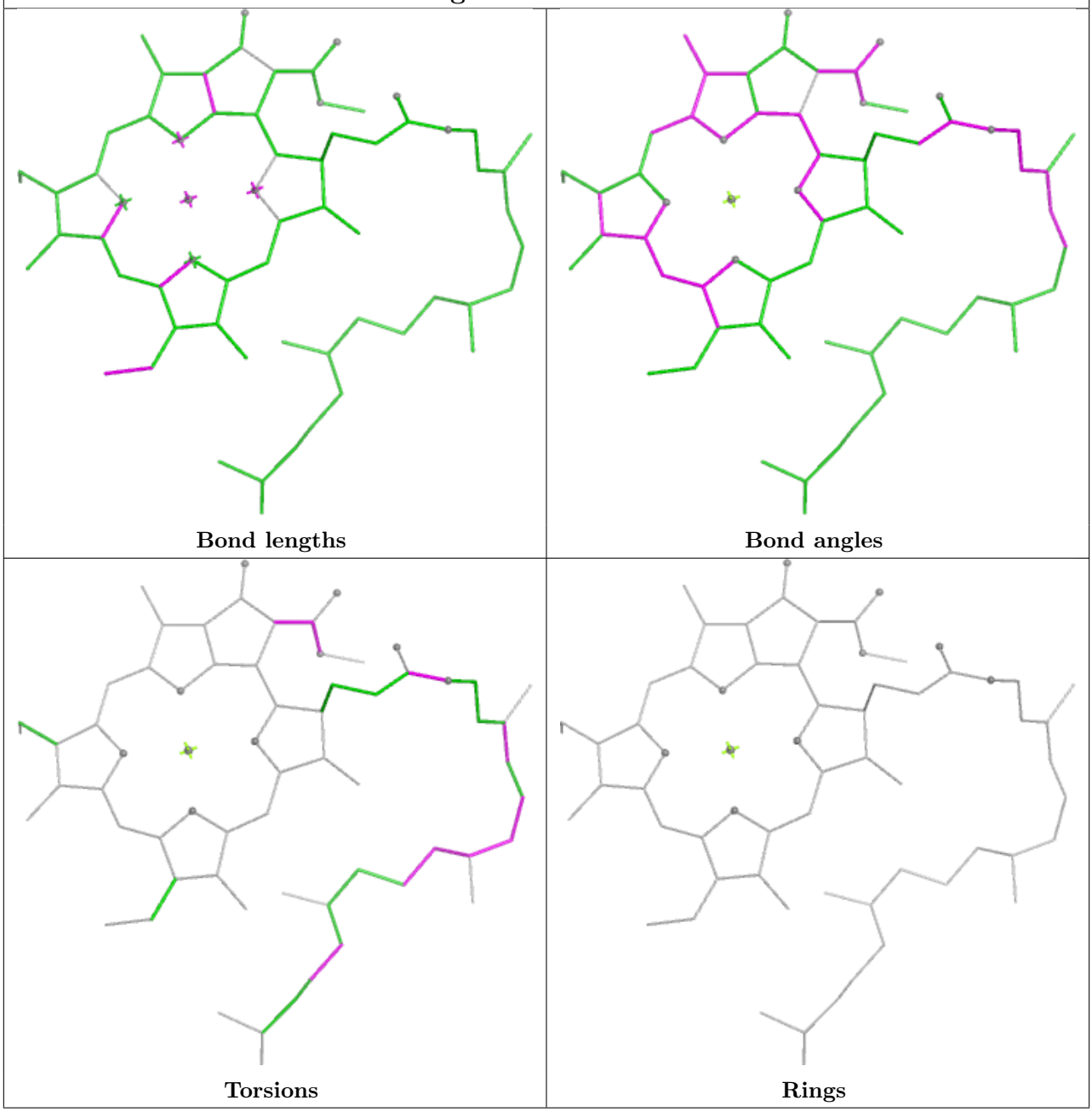
Ligand NEX 3 319



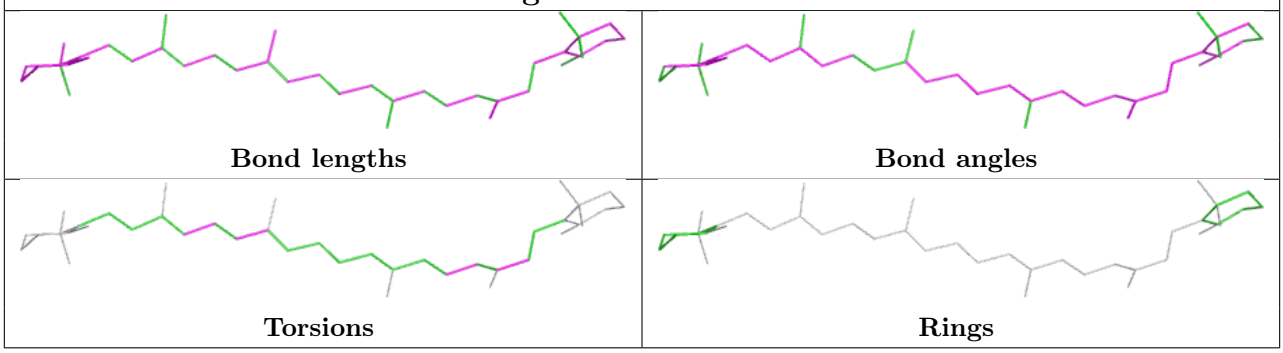
Ligand LUT N 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

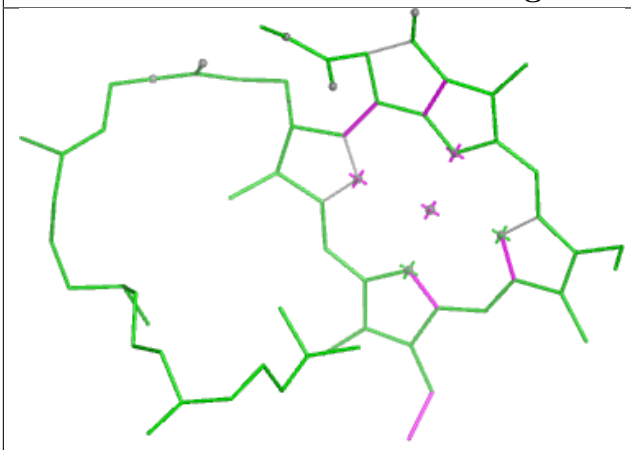
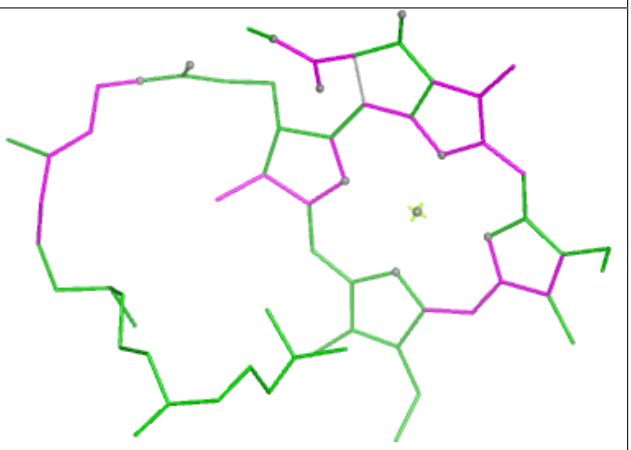
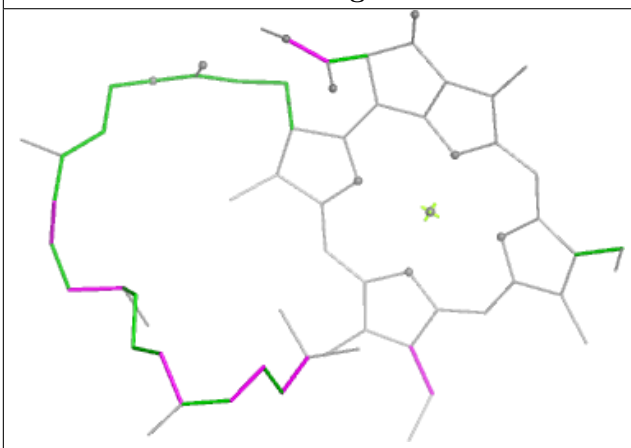
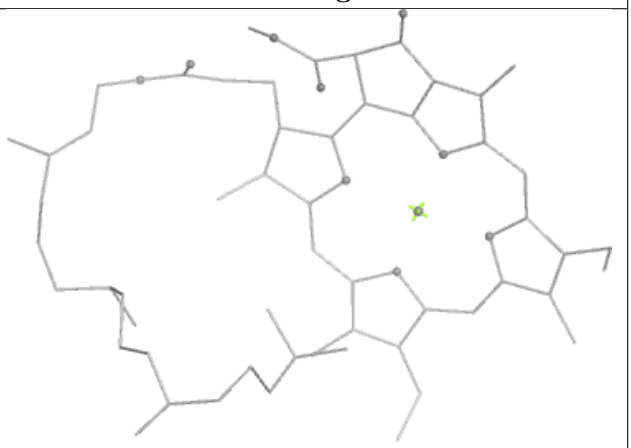
Ligand LMG R 321	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA 7 313

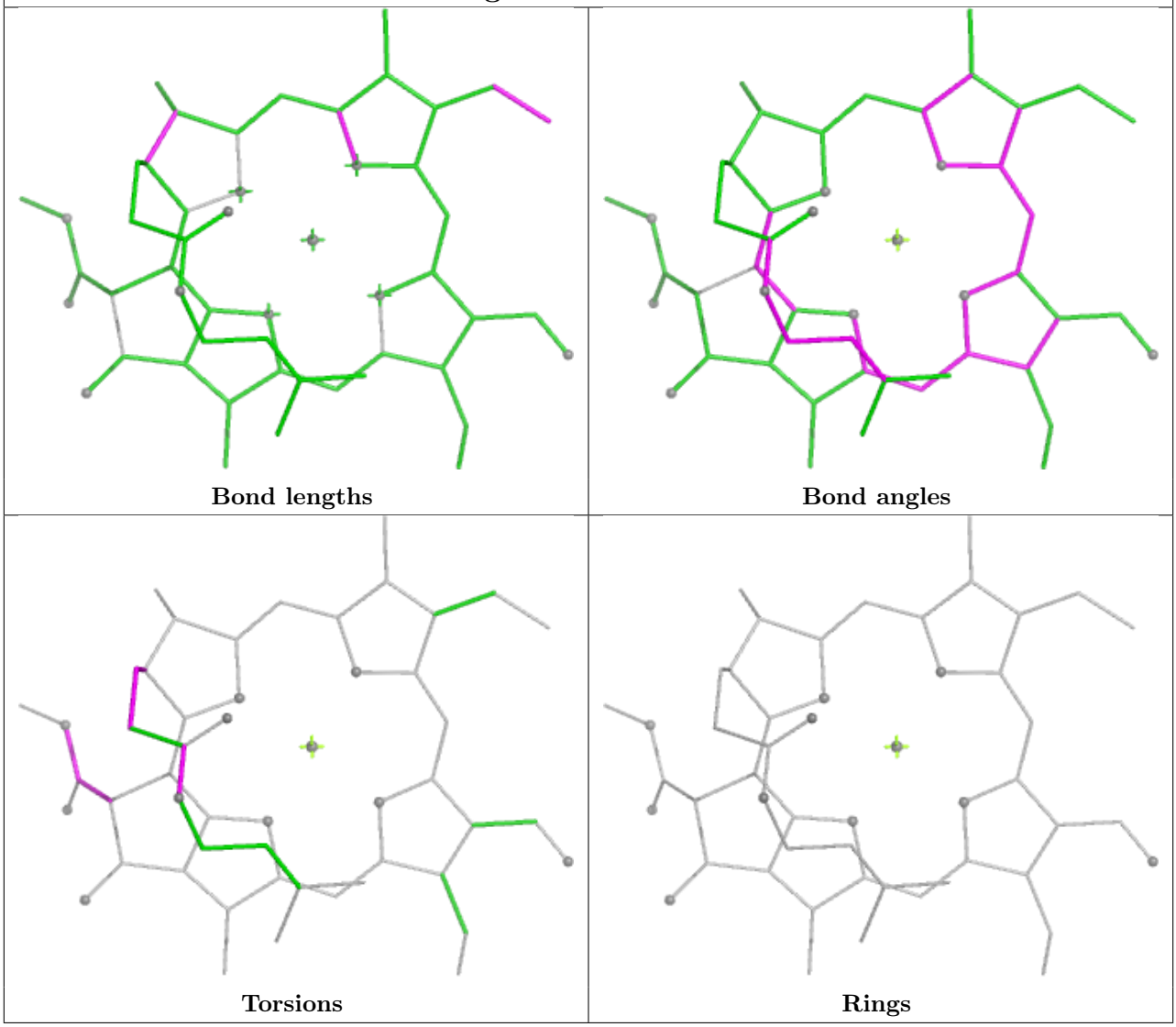


Ligand BCR H 101

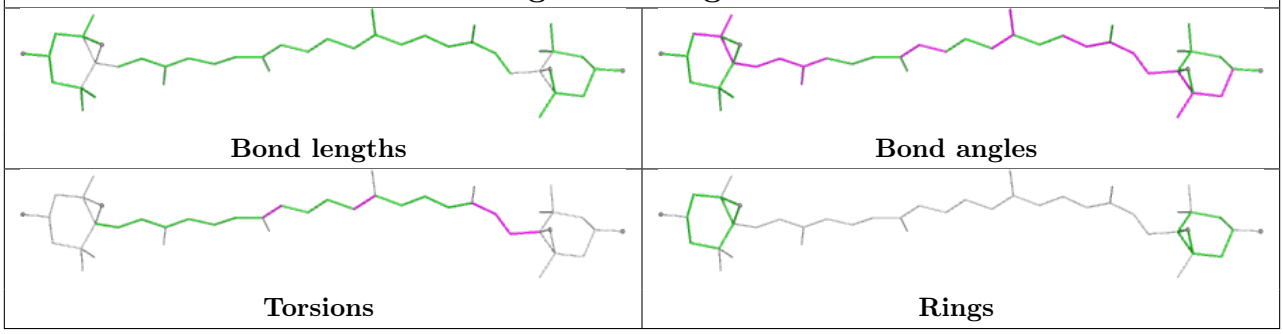


Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

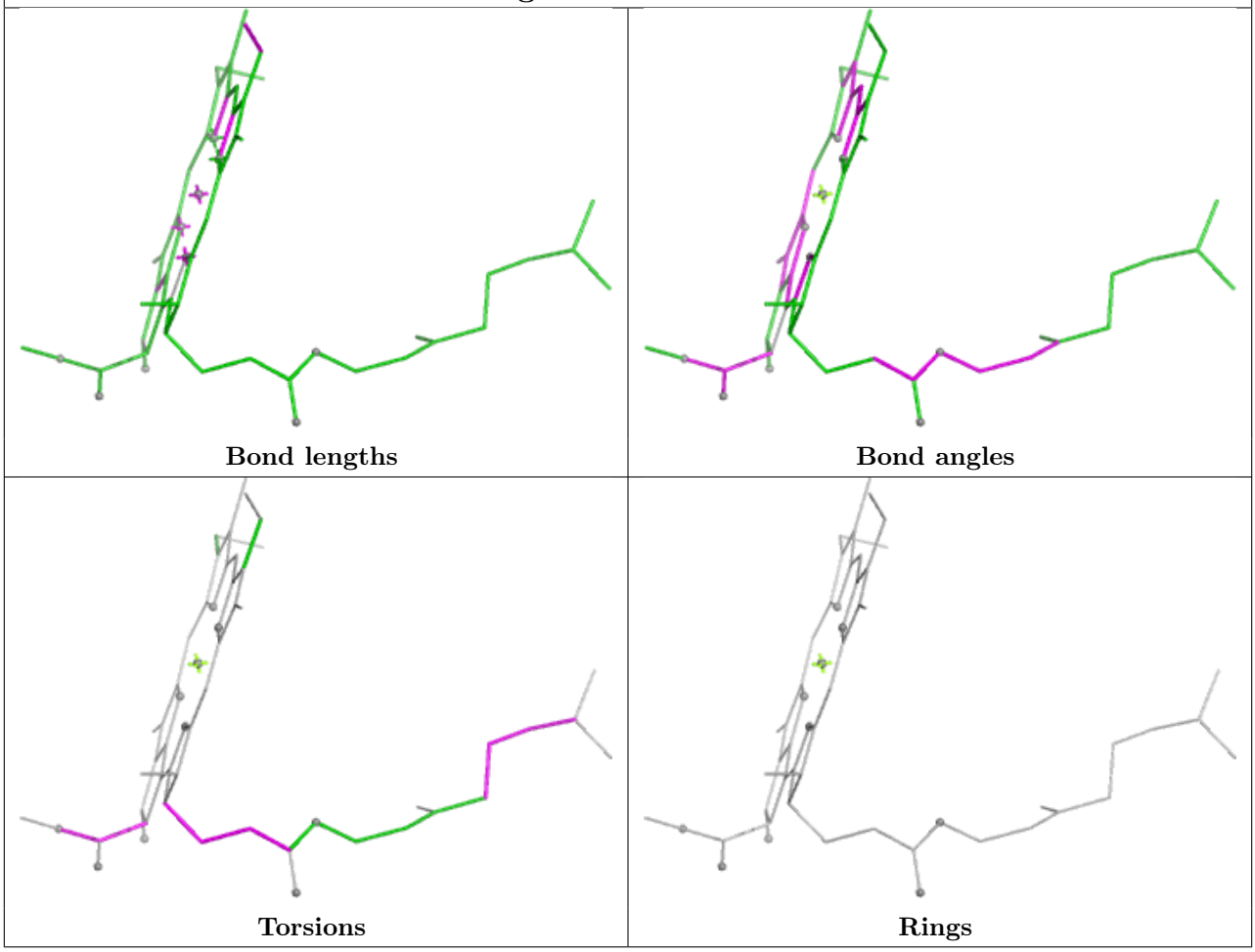
Ligand CHL 5 607



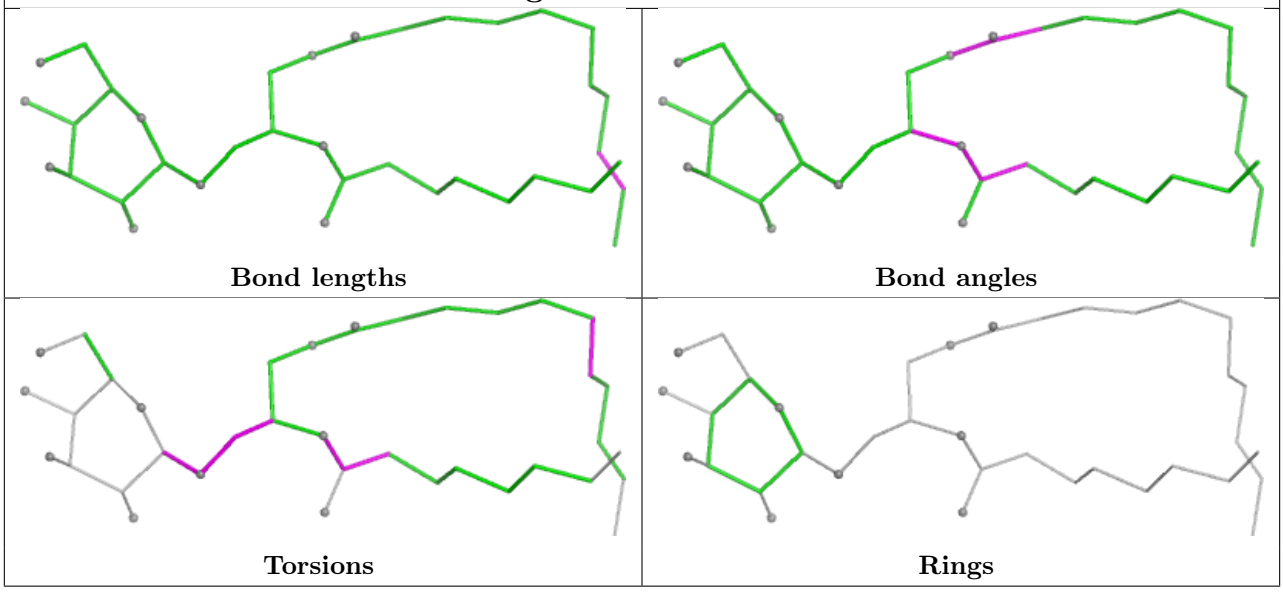
Ligand XAT g 321



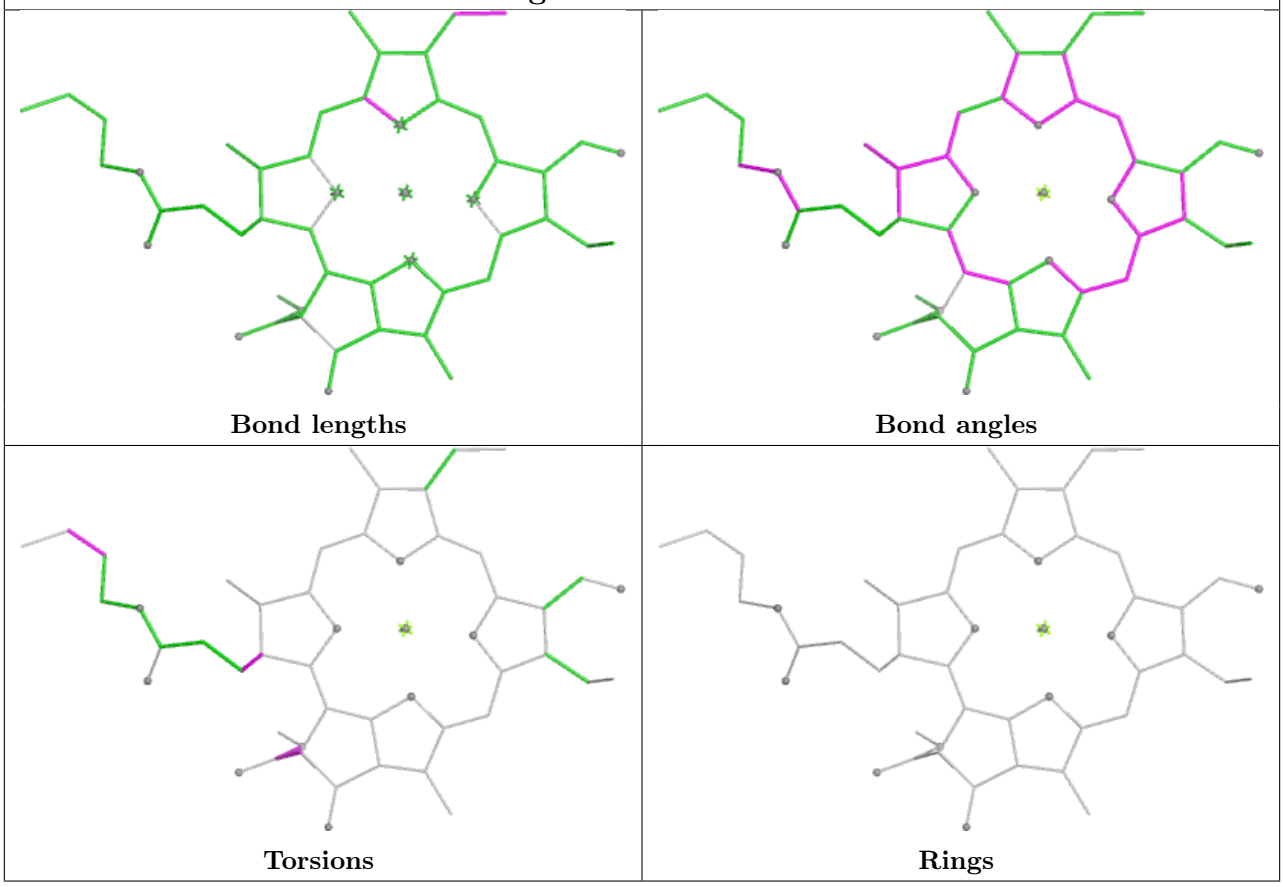
Ligand CLA 0 604



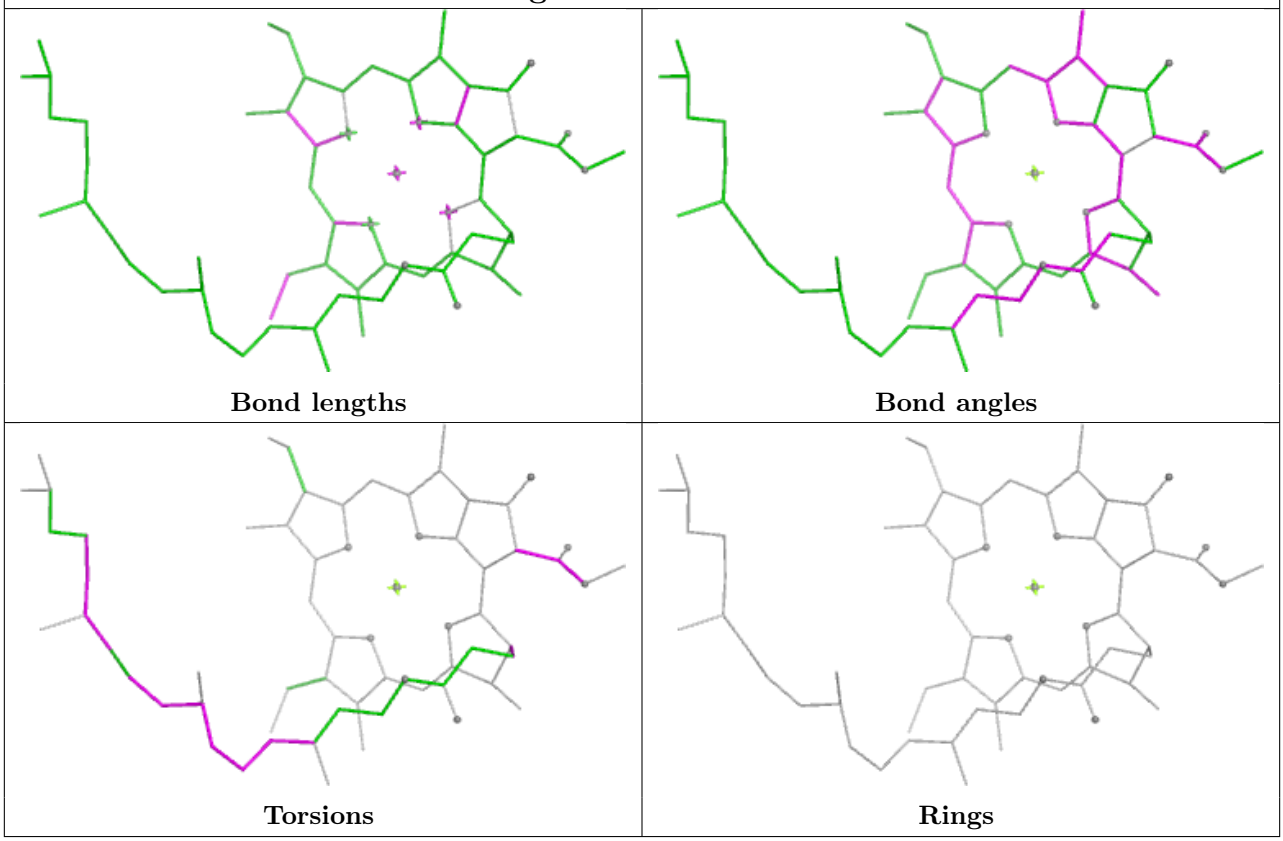
Ligand LMG c 621



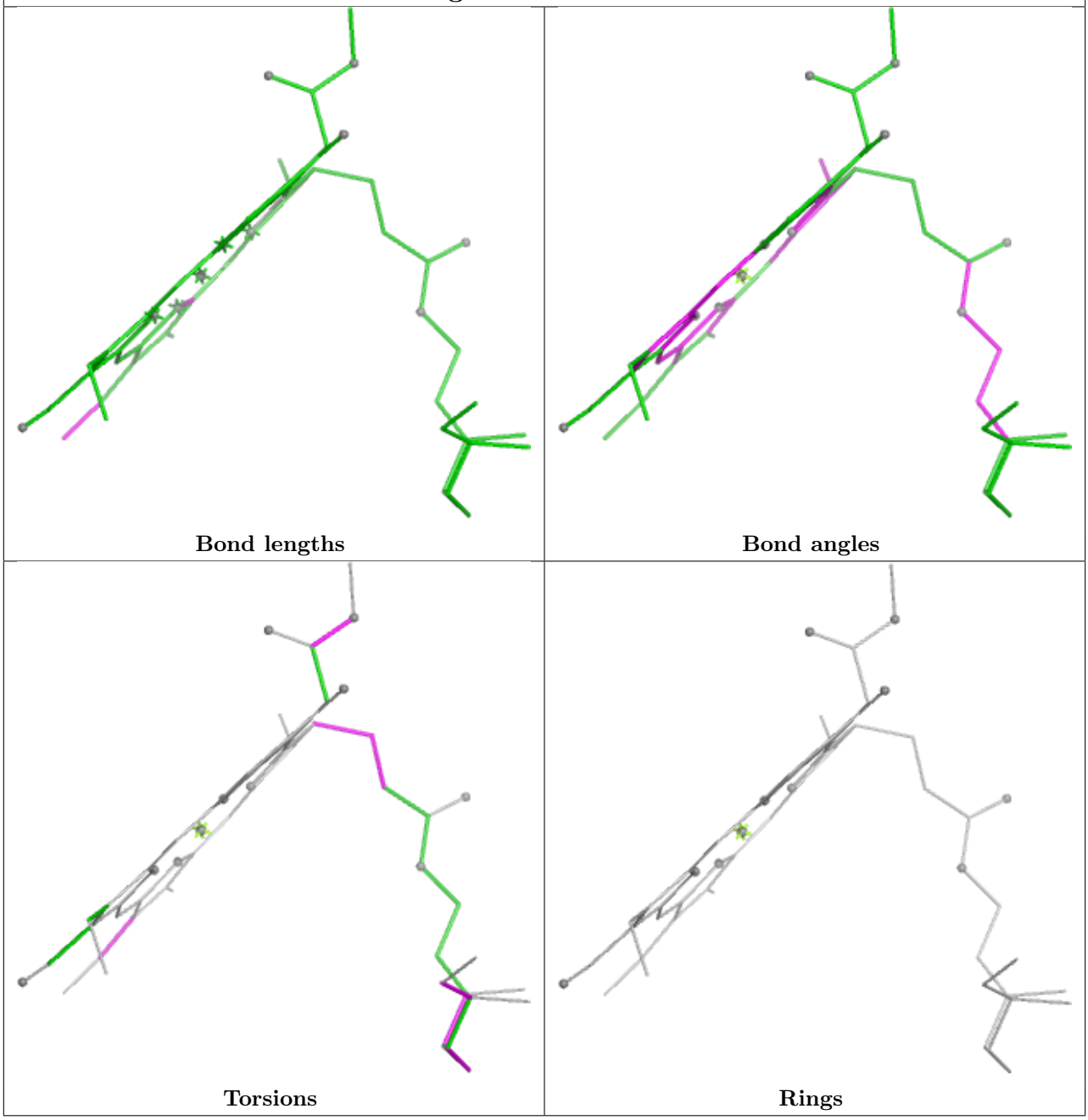
Ligand CHL 3 303



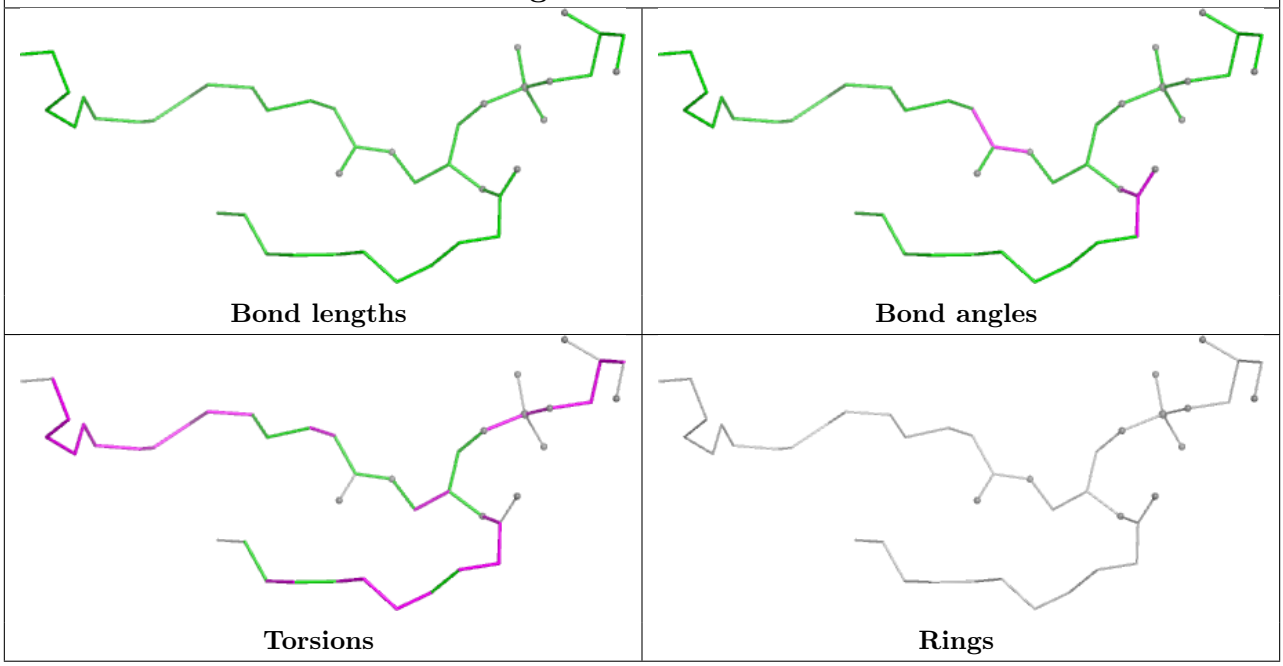
Ligand CLA 1 610



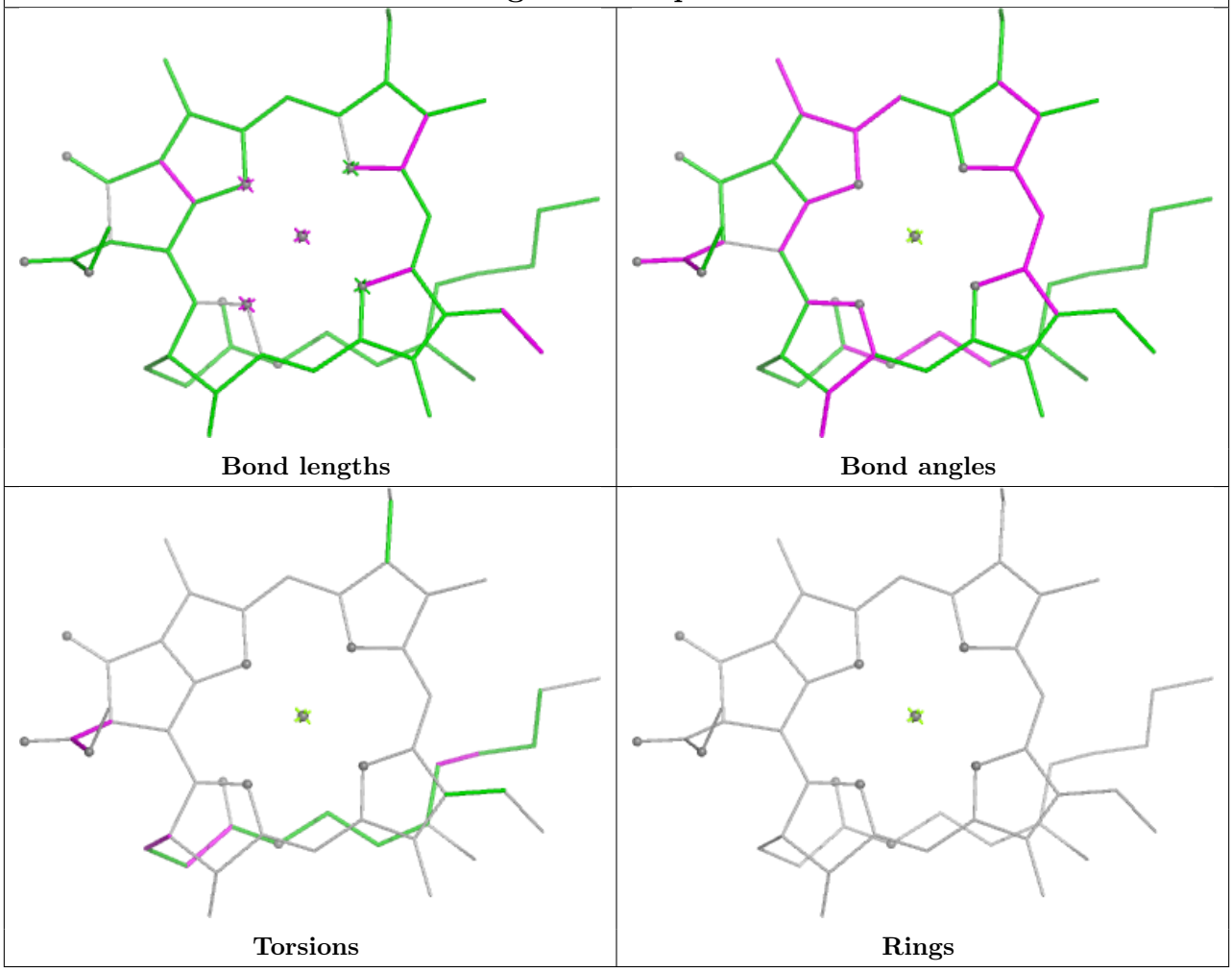
Ligand CHL 4 609



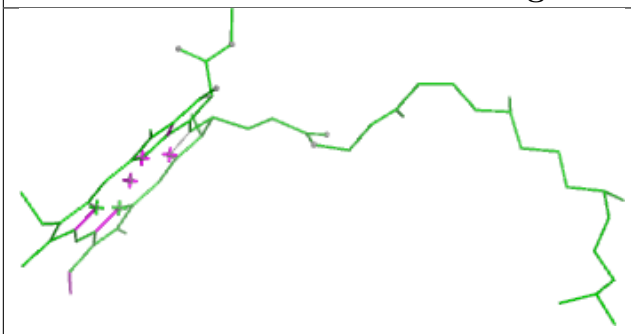
Ligand LHG s 322



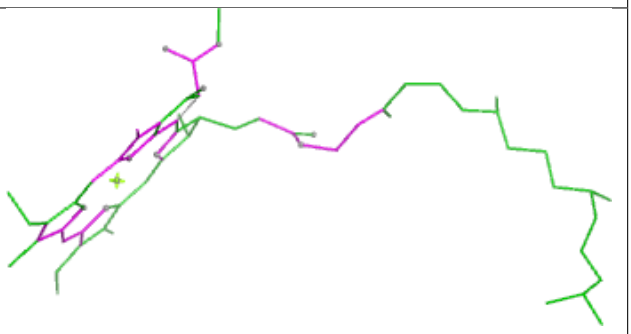
Ligand CLA p 613



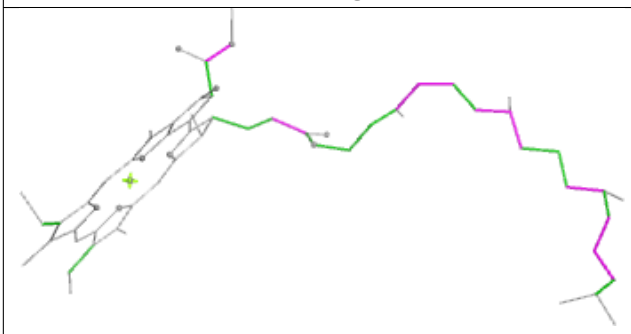
Ligand CLA d 404



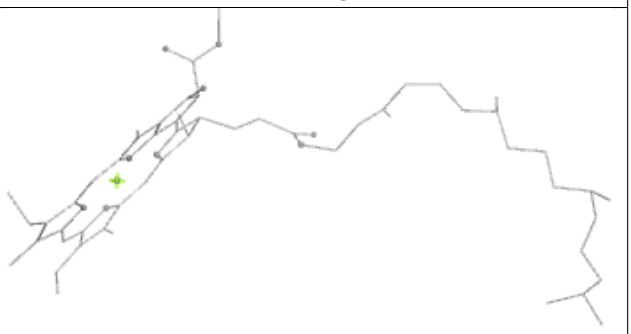
Bond lengths



Bond angles

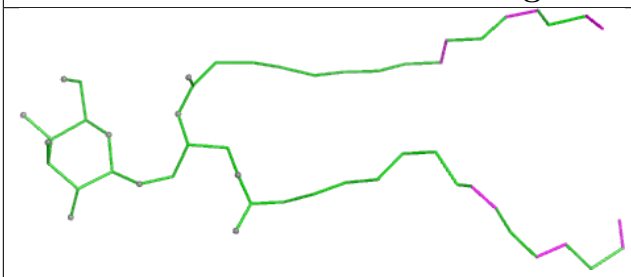


Torsions



Rings

Ligand LMG J 101



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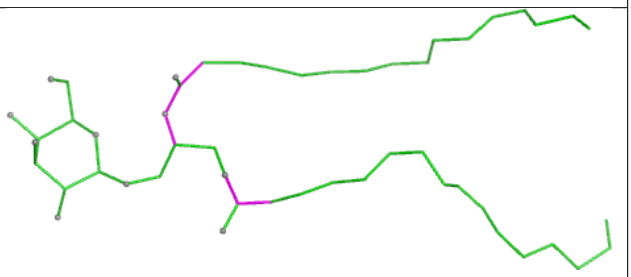
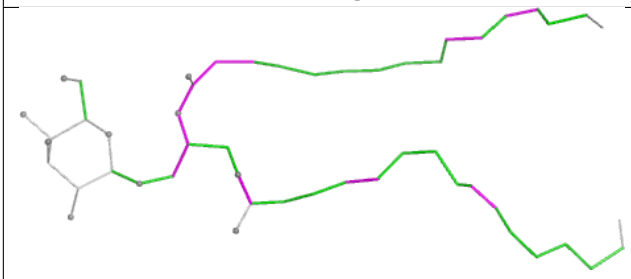


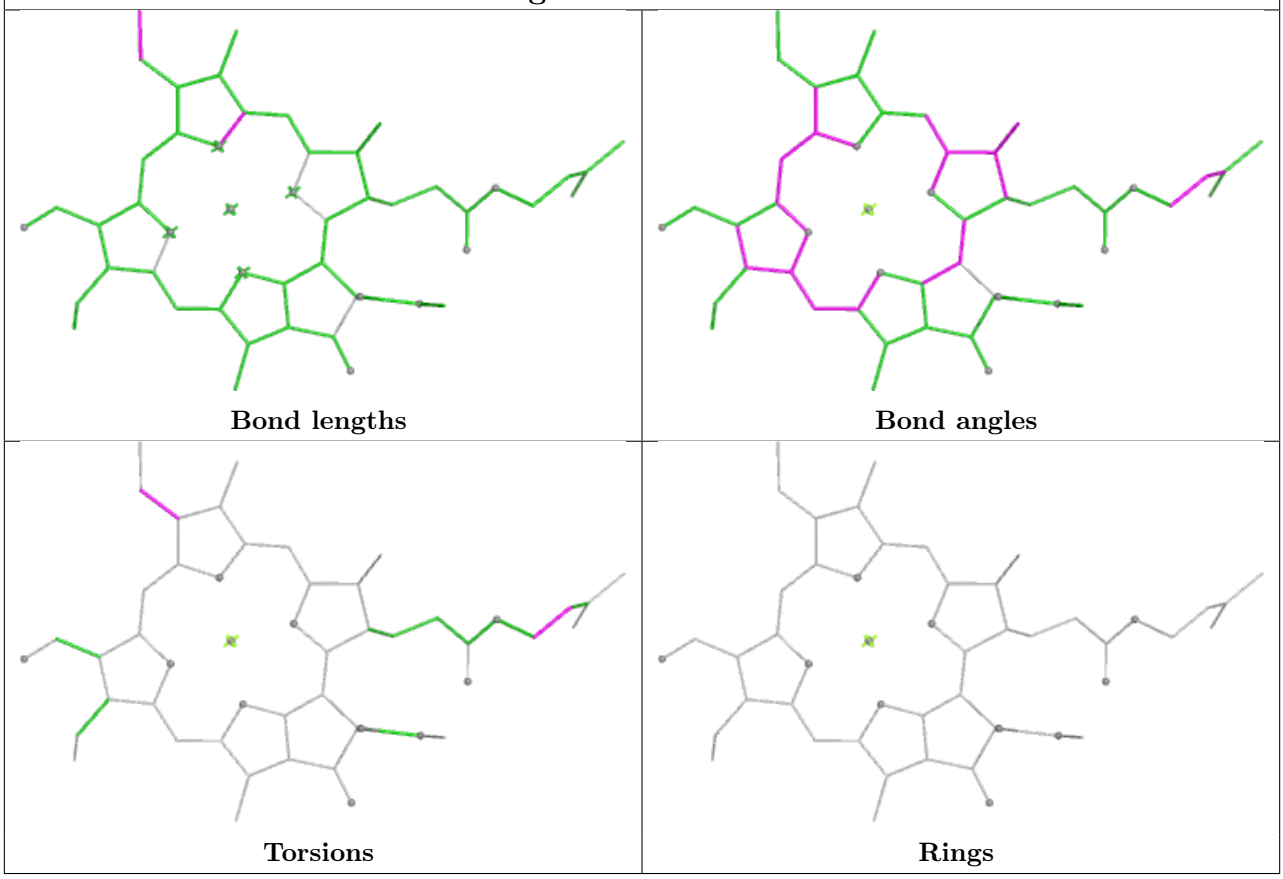
Bond angles



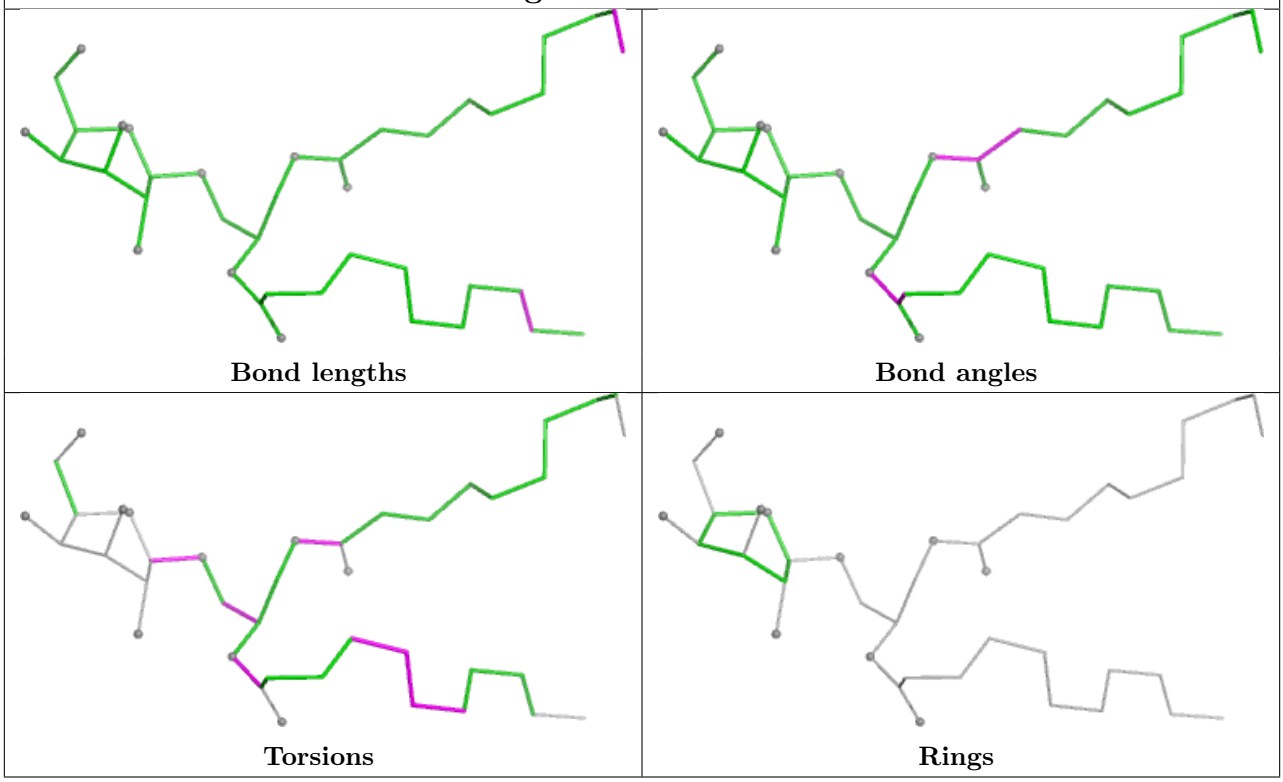
Torsions

Rings

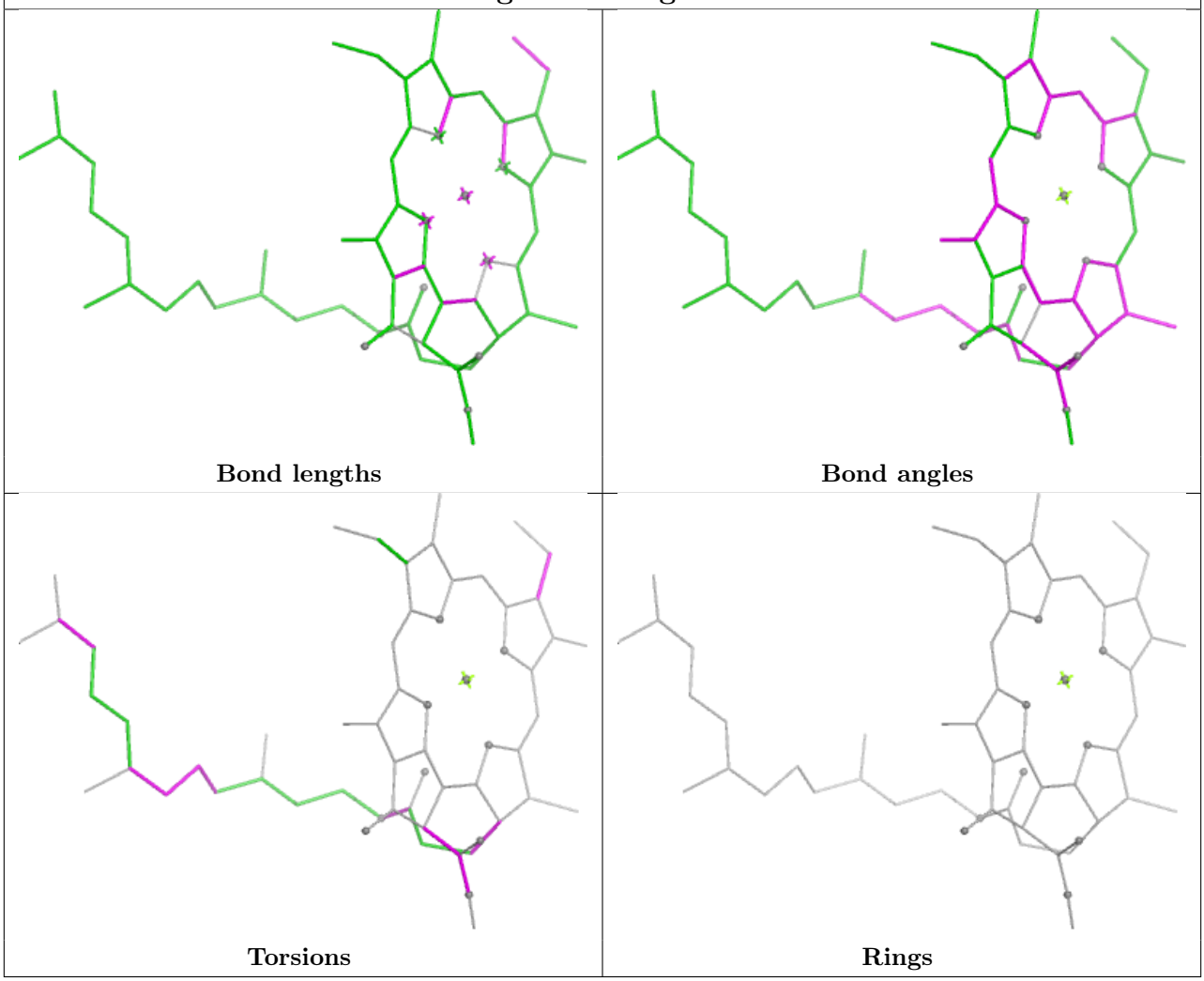
Ligand CHL 5 606



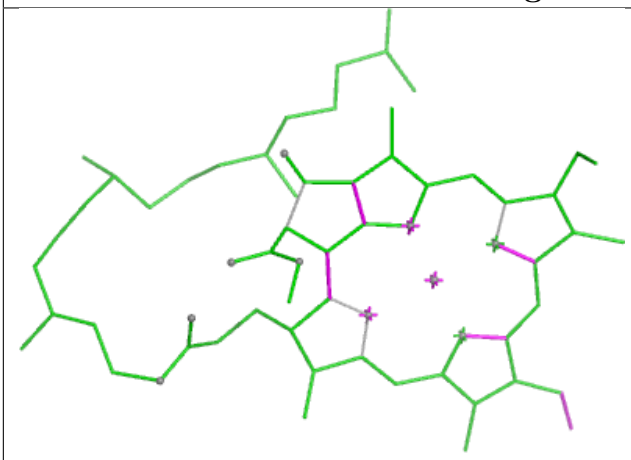
Ligand LMG 4 621



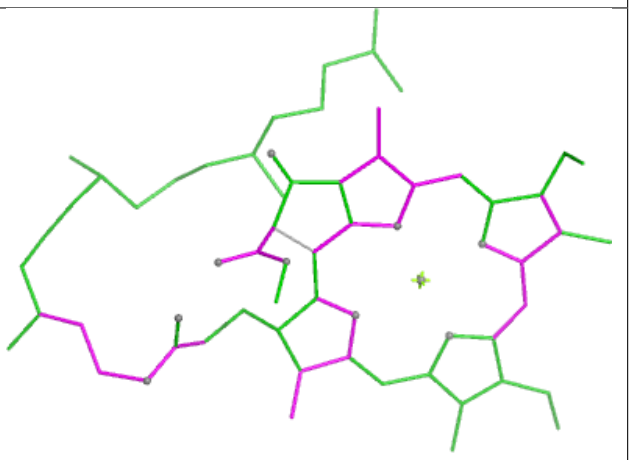
Ligand CLA g 311



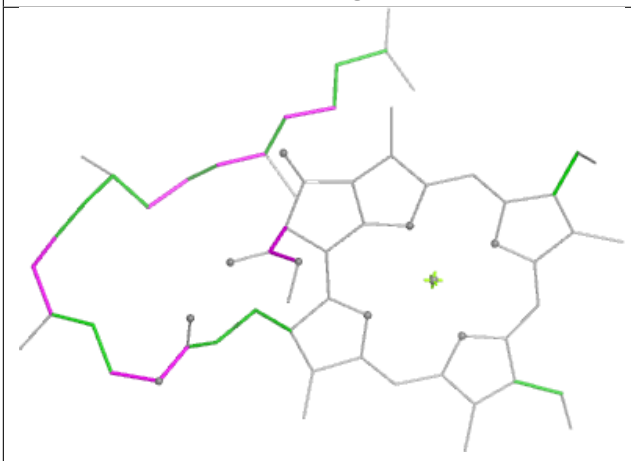
Ligand CLA C 609



Bond lengths



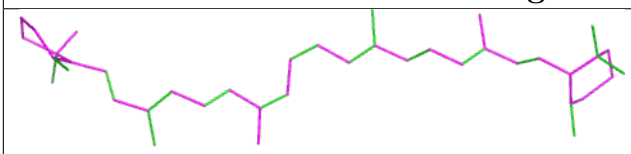
Bond angles



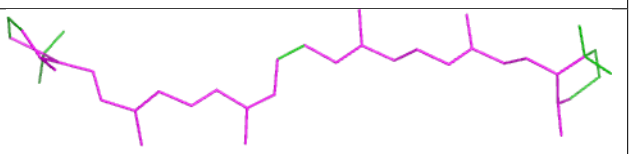
Torsions

Rings

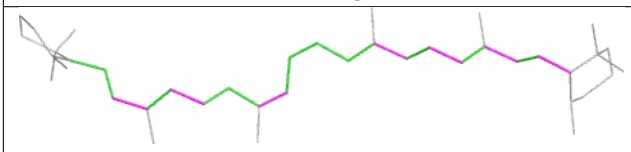
Ligand BCR c 615



Bond lengths



Bond angles



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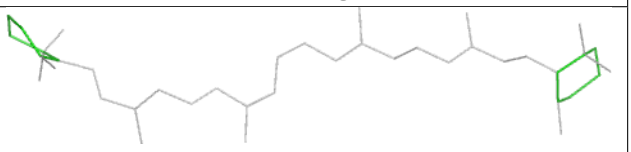
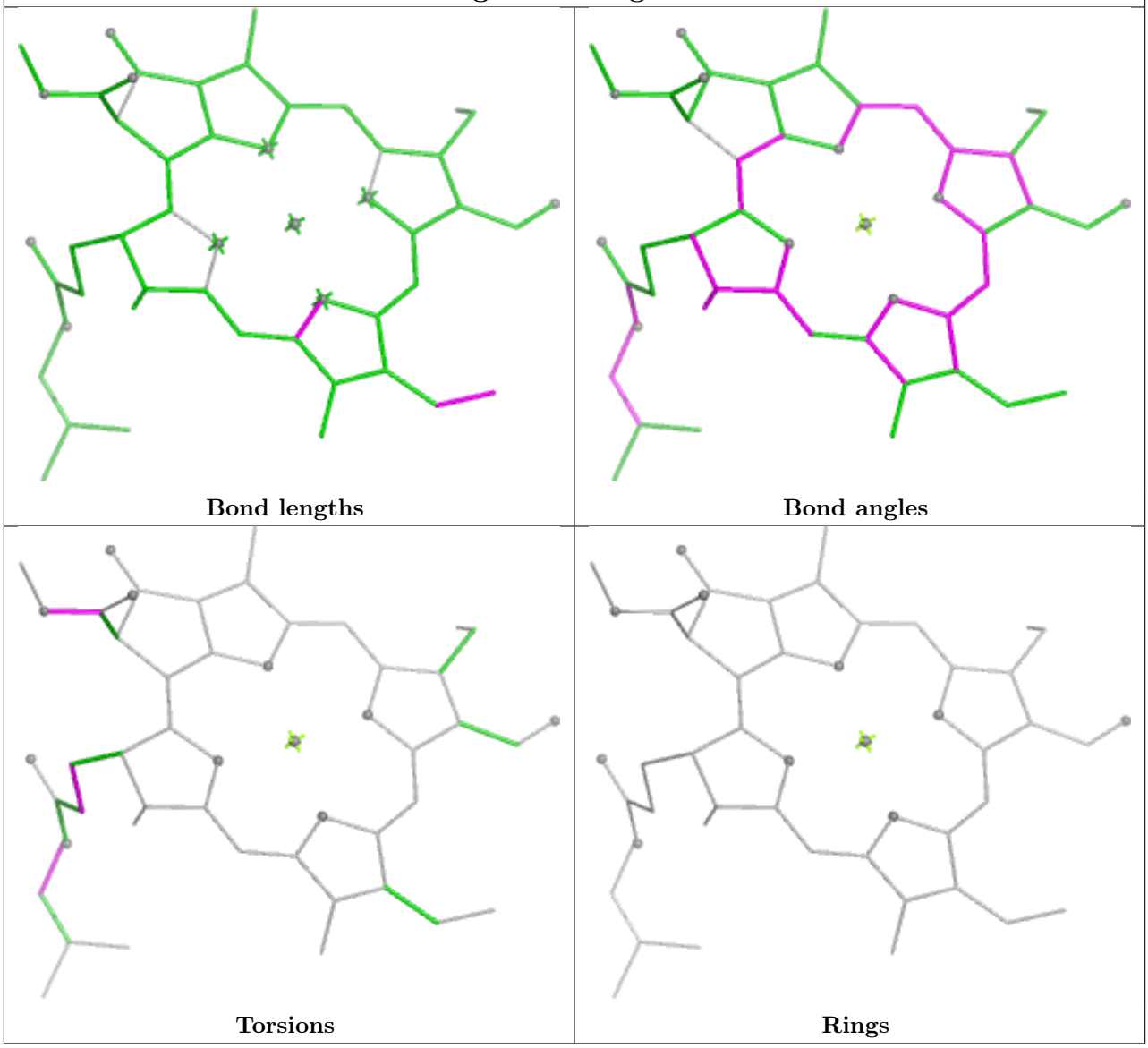
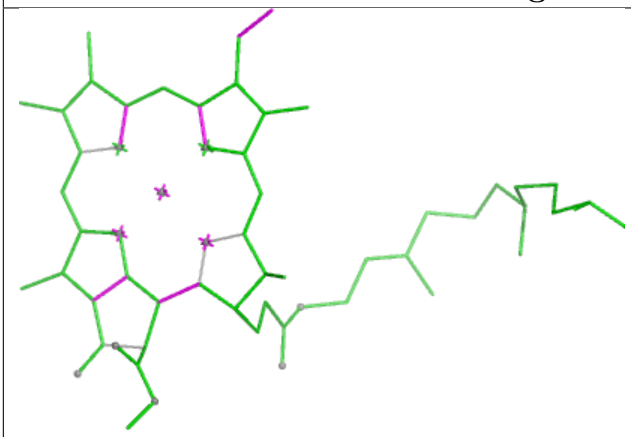


Rings

Ligand CHL g 308



Ligand CLA a 409



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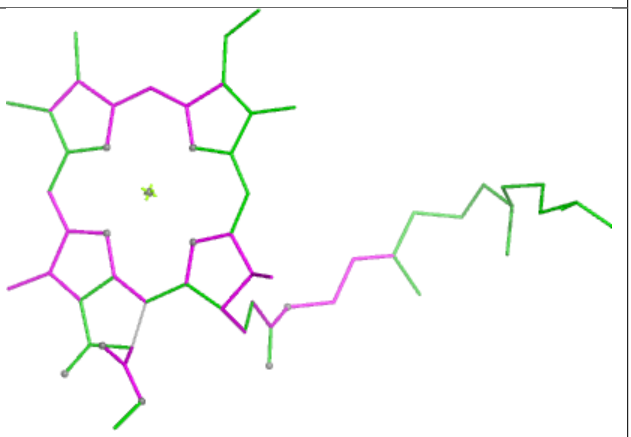
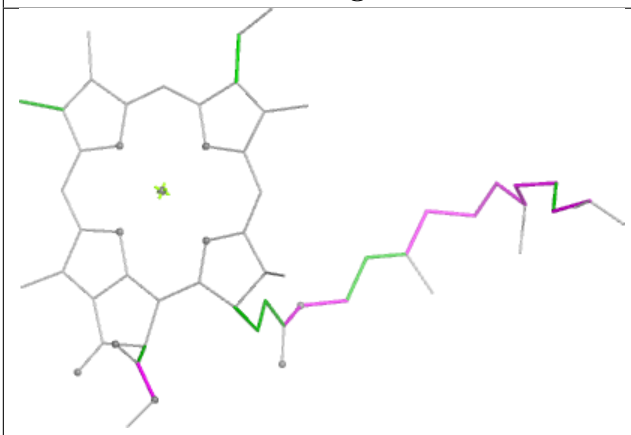


Bond angles



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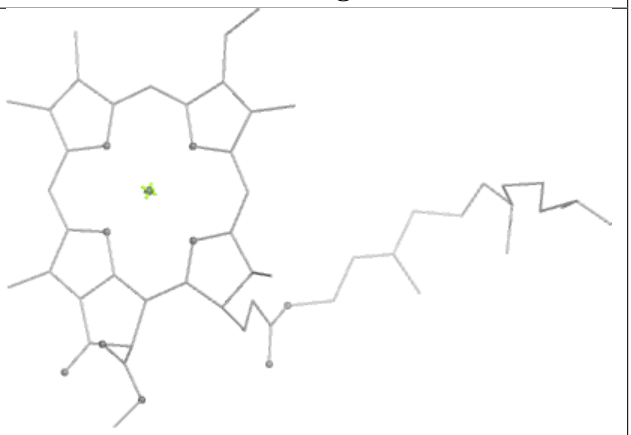
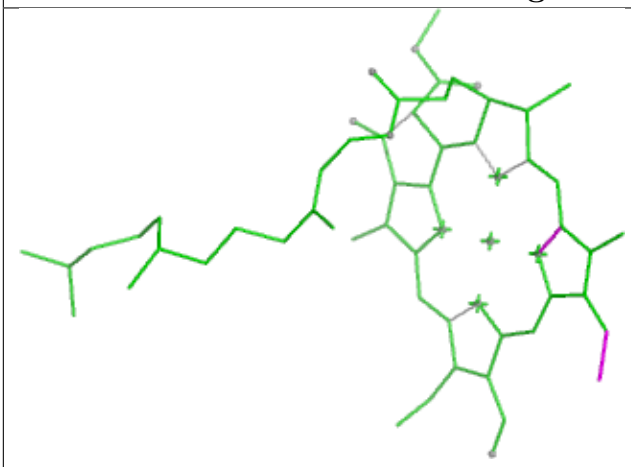
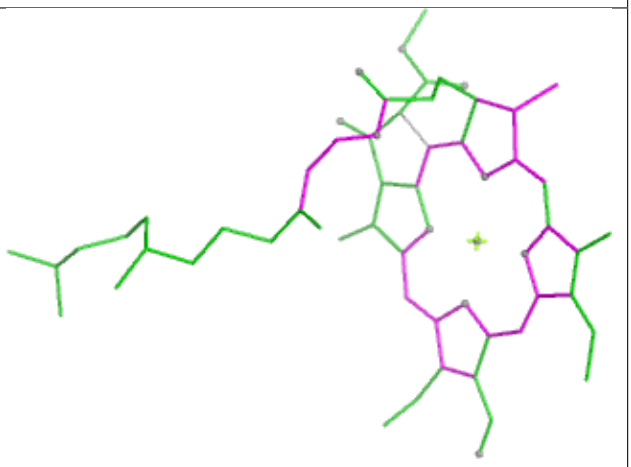


Rings

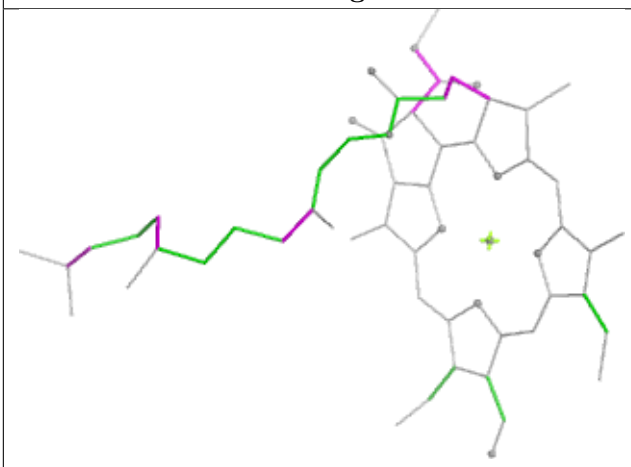
Ligand CHL 6 310



Bond lengths



Bond angles



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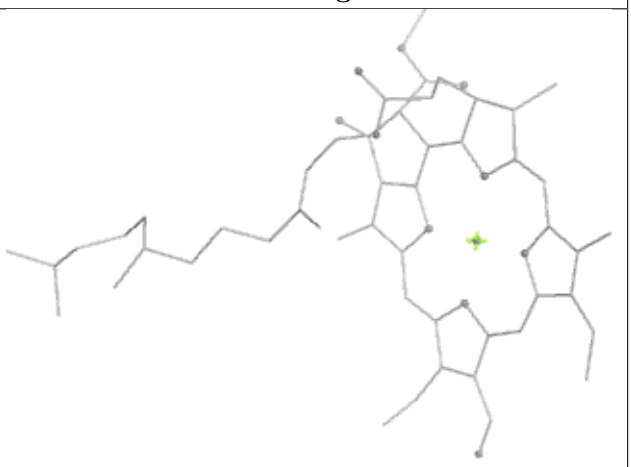
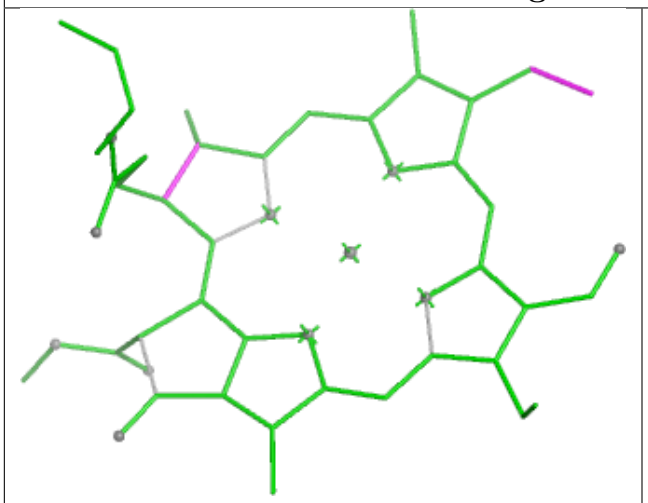
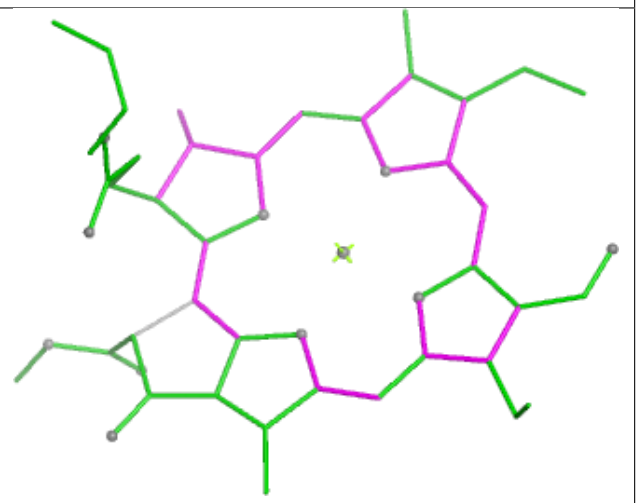


Rings

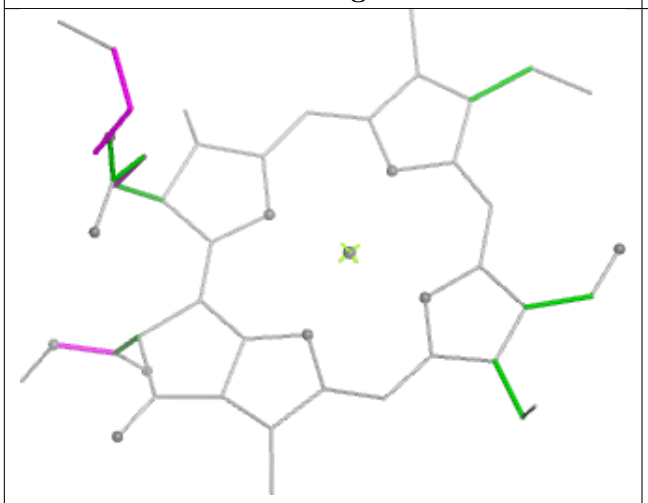
Ligand CHL 1 608



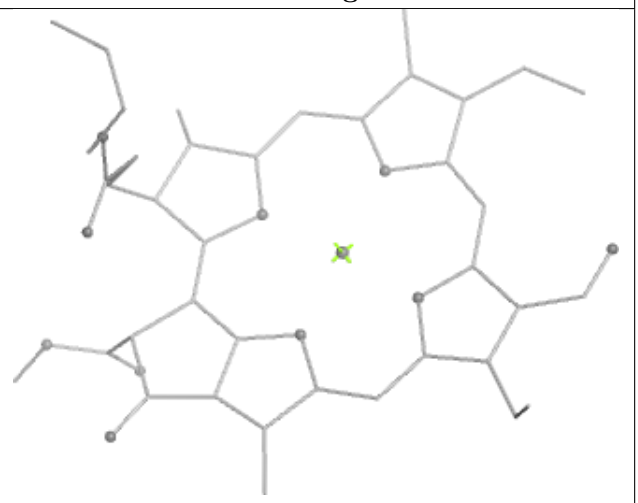
Bond lengths



Bond angles

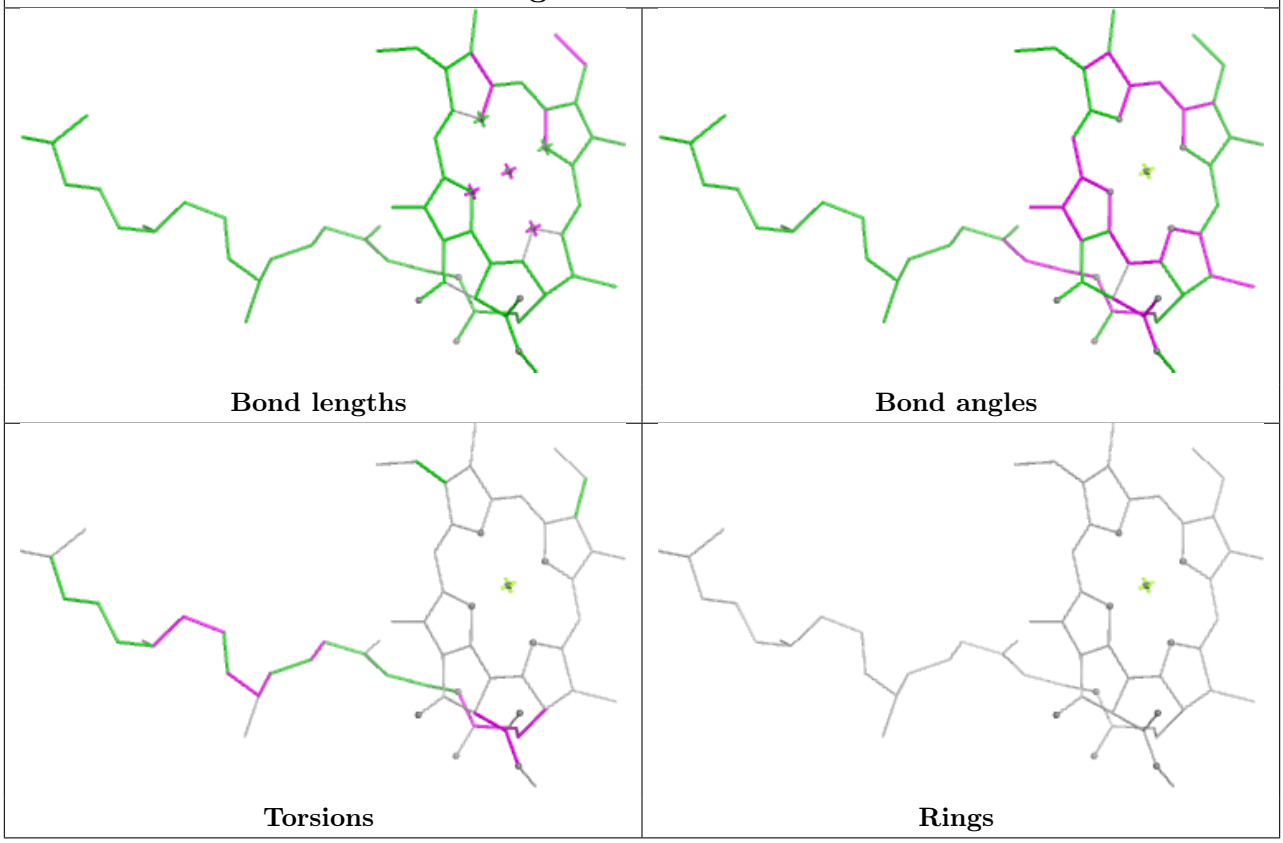


Torsions

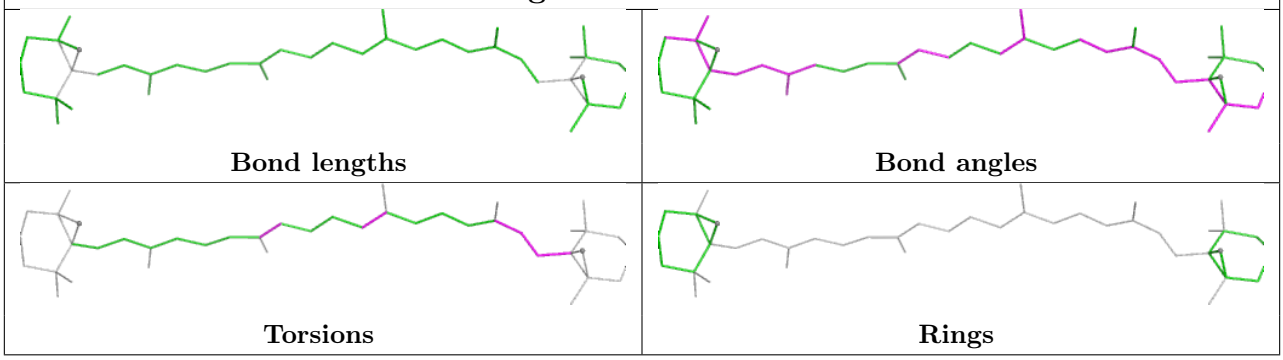


Rings

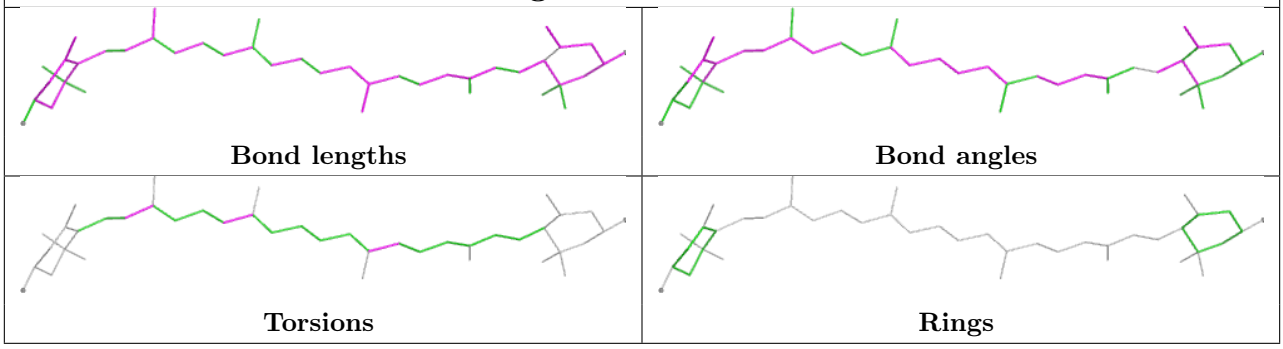
Ligand CLA 7 312

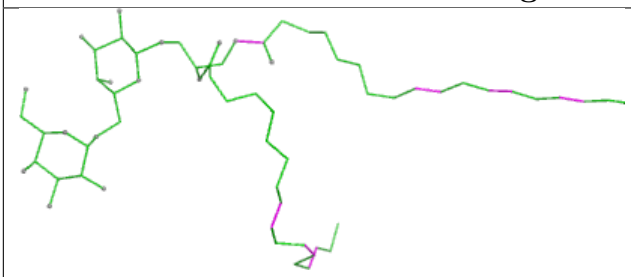
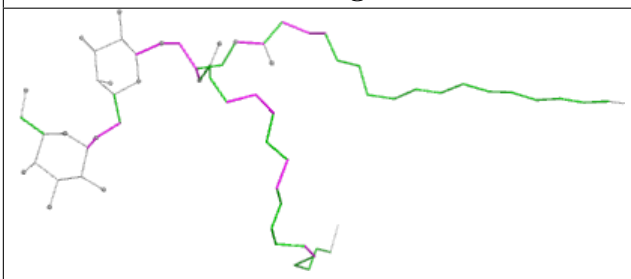


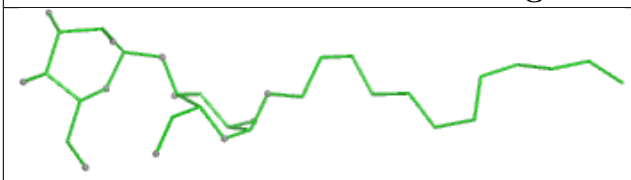
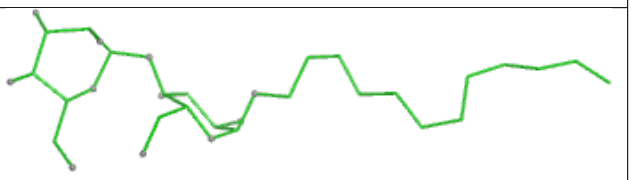
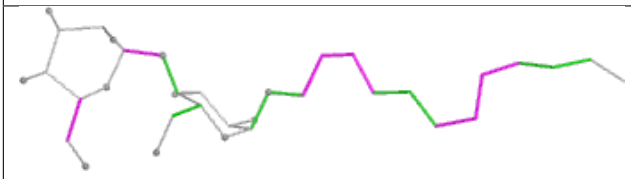
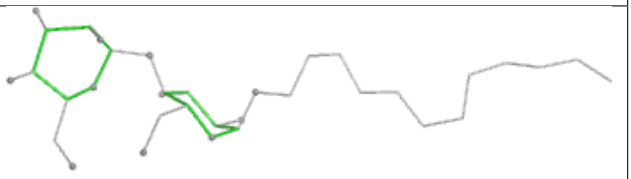
Ligand XAT 9 322



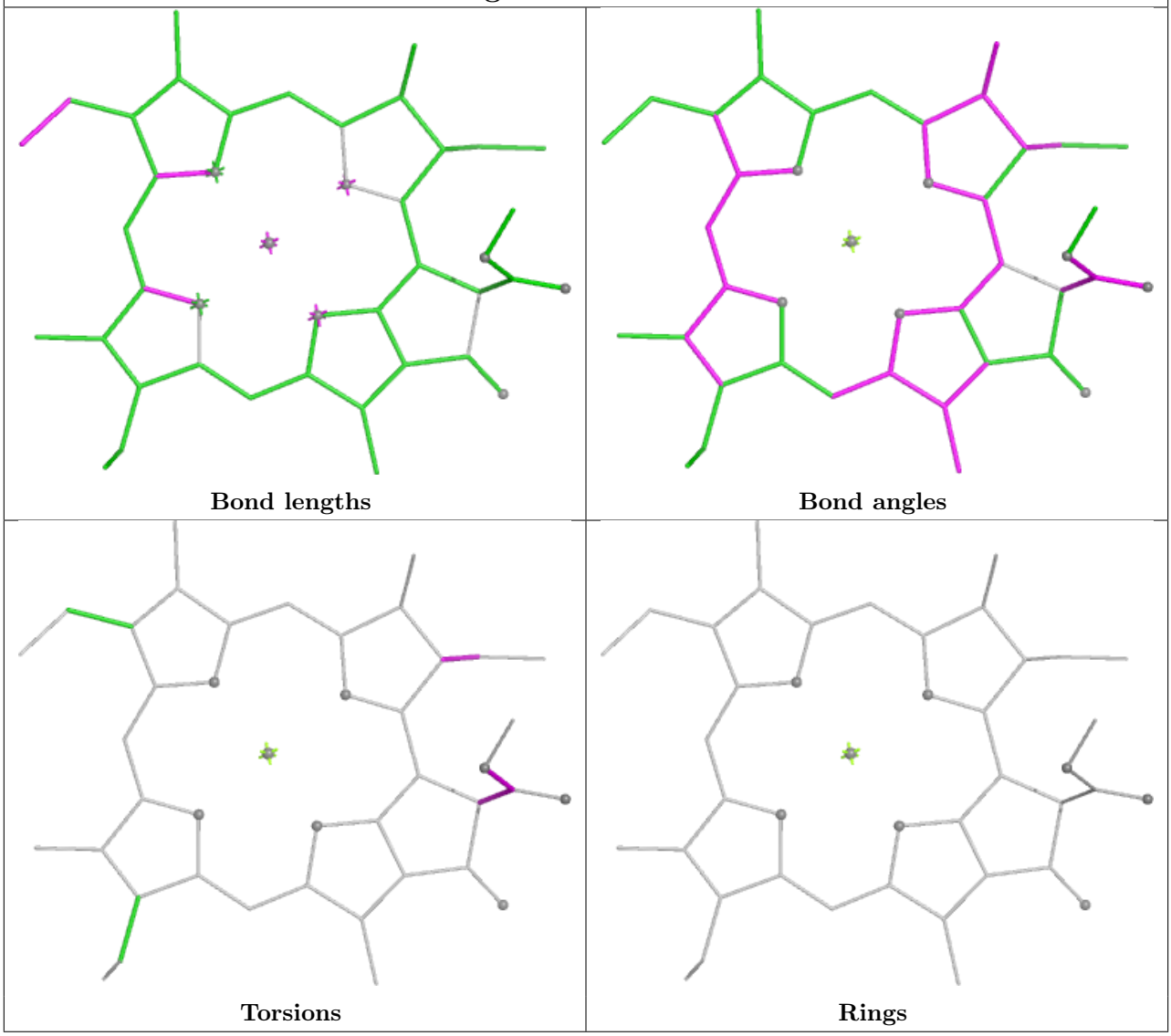
Ligand LUT 8 616



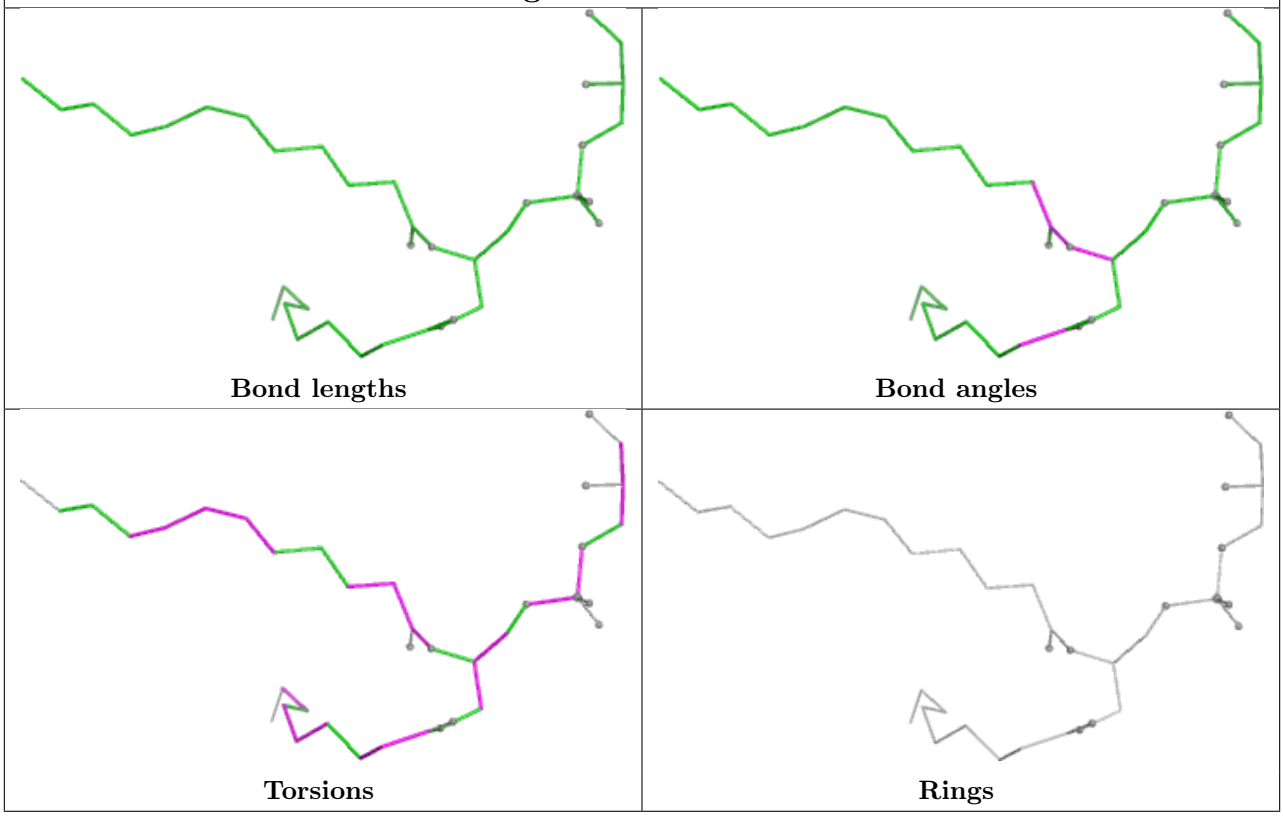
Ligand DGD C 617	
 Bond lengths	Bond angles
 Torsions	Rings

Ligand LMU r 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

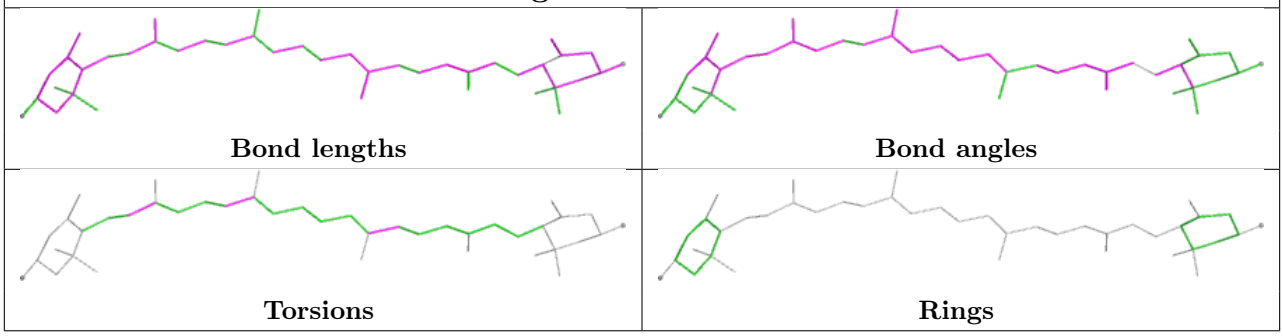
Ligand CLA s 304



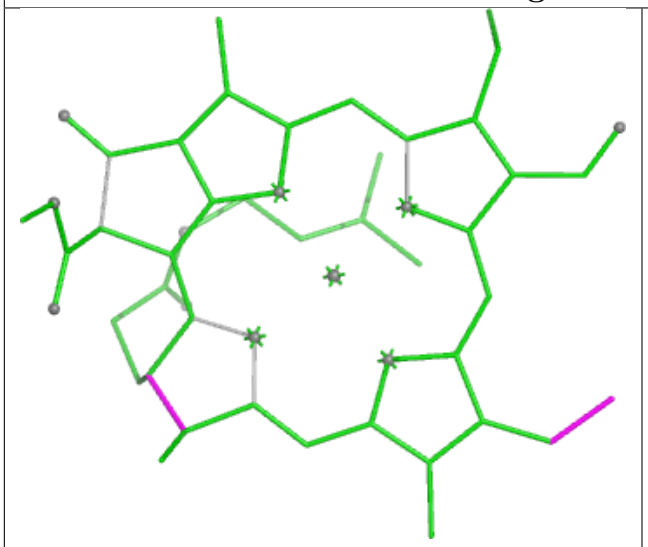
Ligand LHG R 320



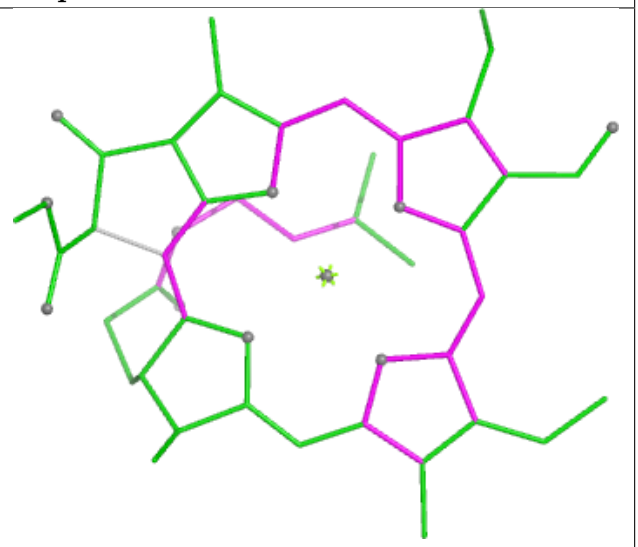
Ligand LUT s 317



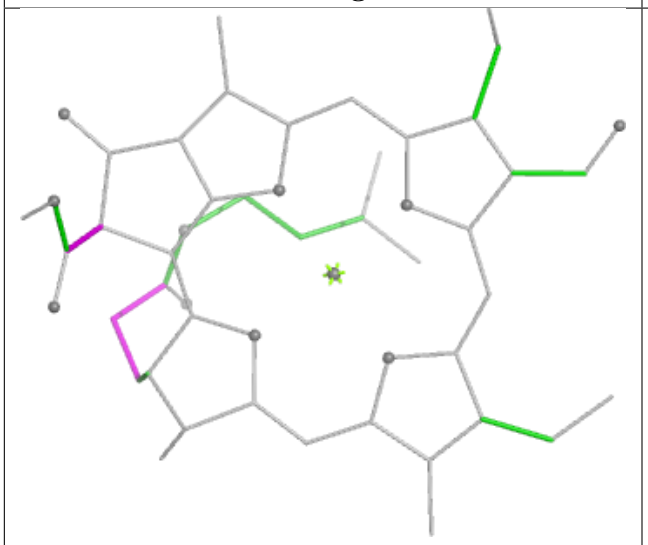
Ligand CHL p 607



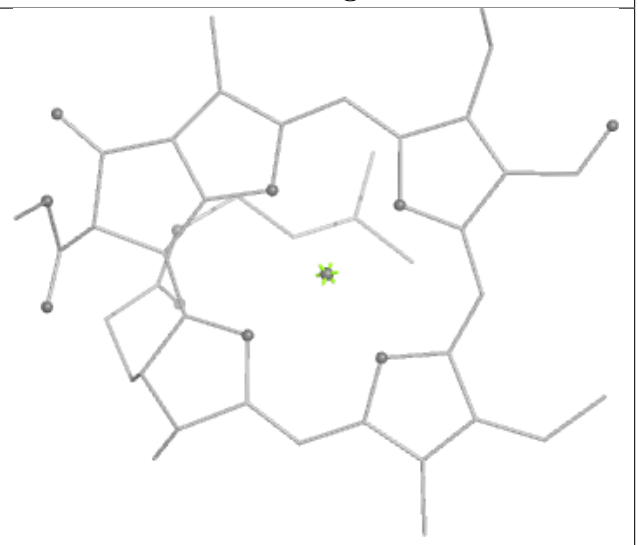
Bond lengths



Bond angles

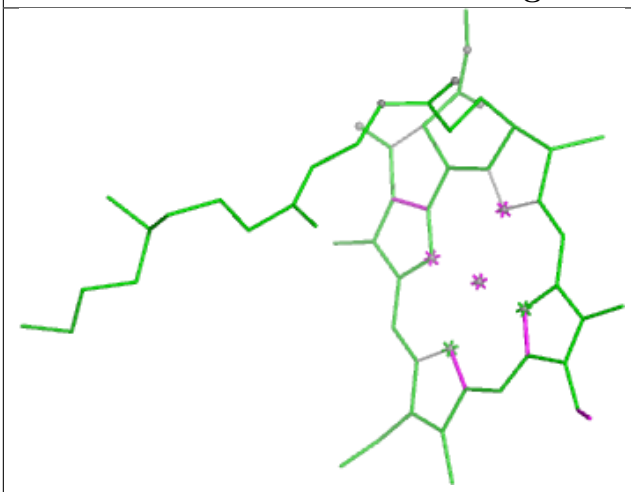


Torsions



Rings

Ligand CLA R 311



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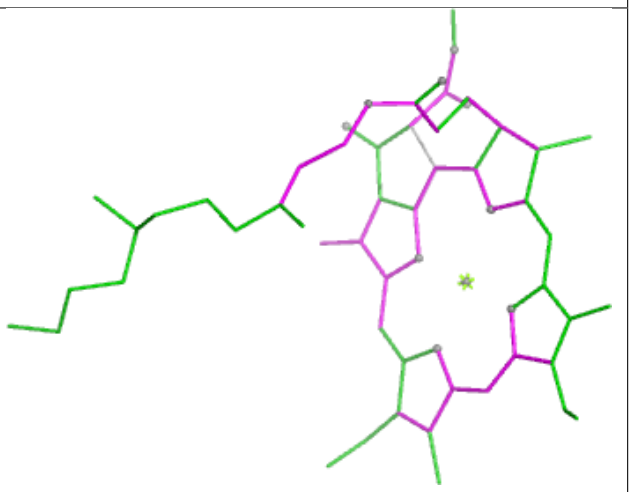
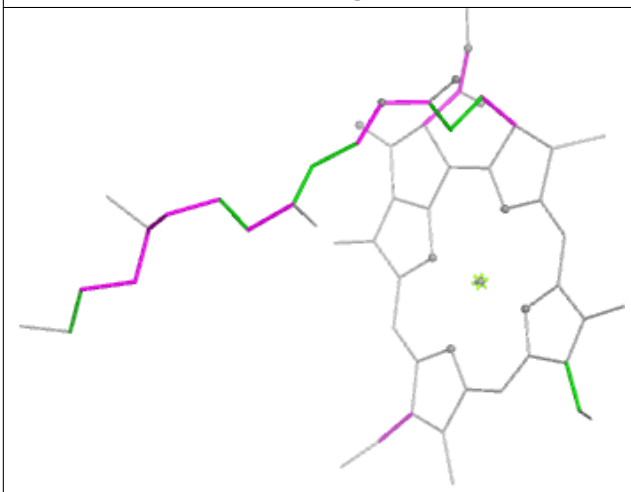
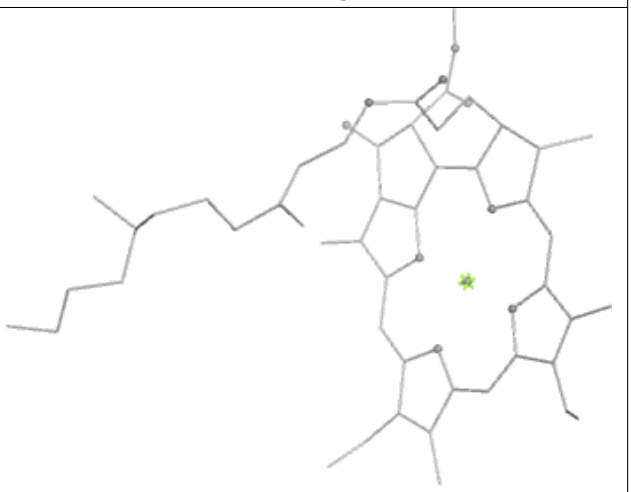


Bond angles

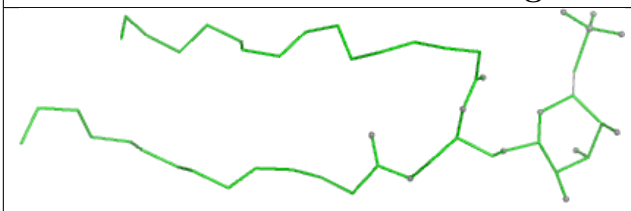


Torsions

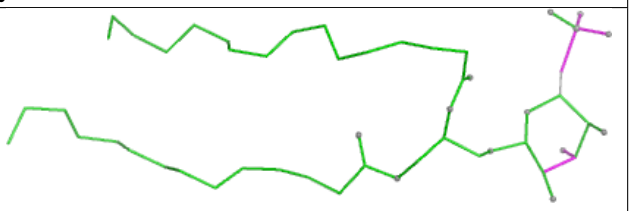


Rings

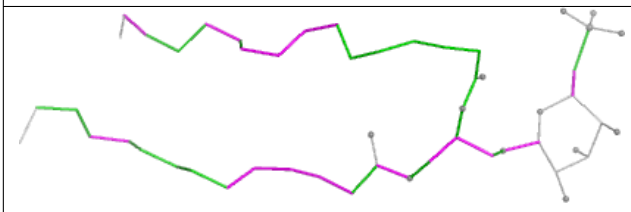
Ligand SQD B 623



Bond lengths



Bond angles



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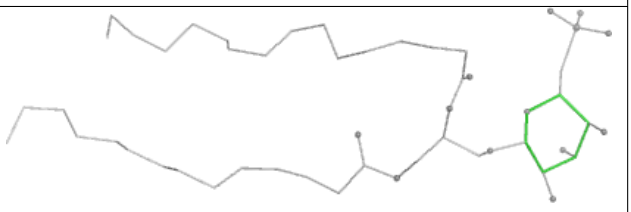
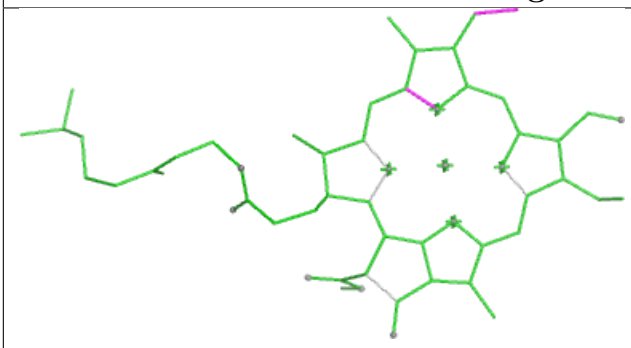


Rings

Ligand CHL 0 601



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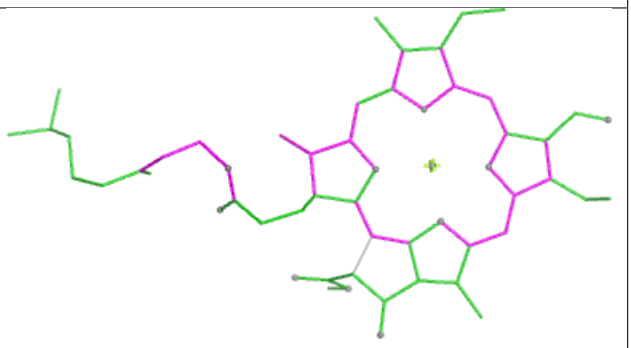

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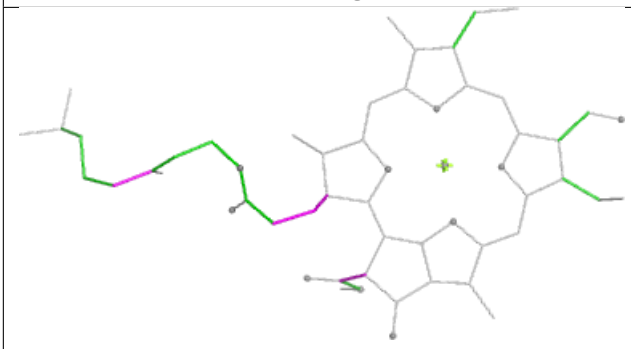

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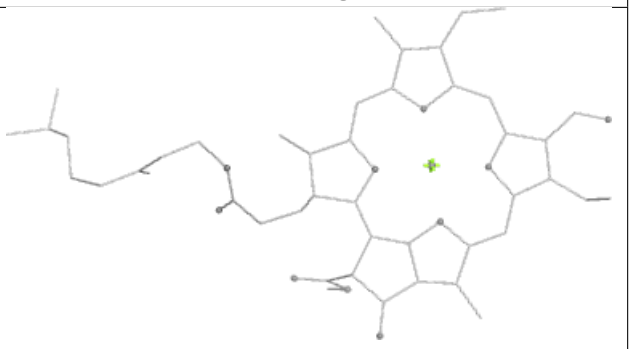

Rings

Ligand LMG A 412

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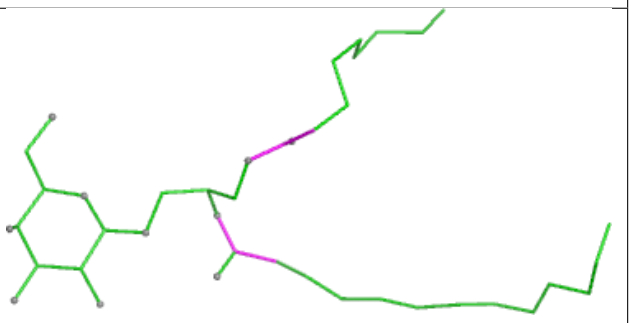

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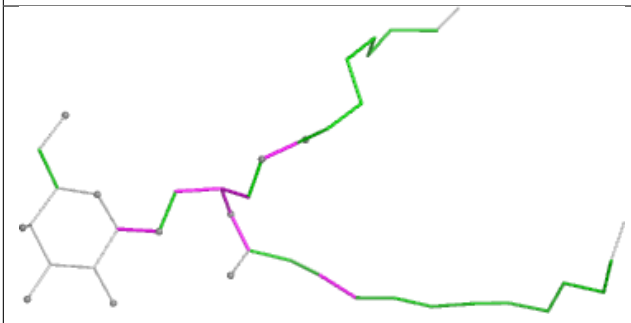
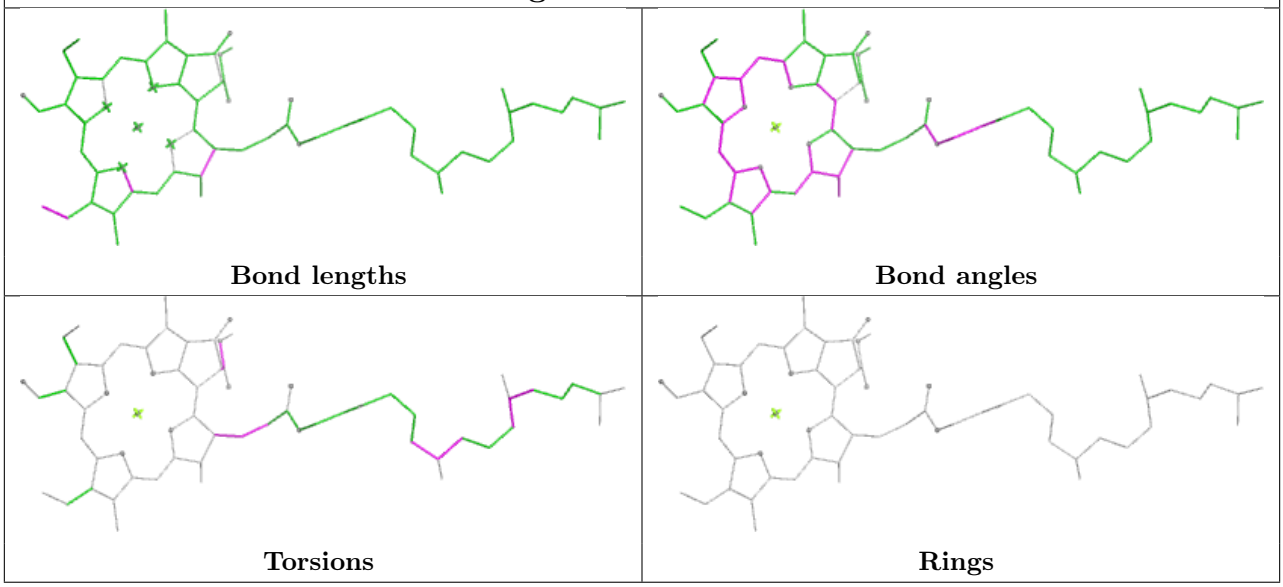


Torsions

Rings

Ligand CHL 7 306



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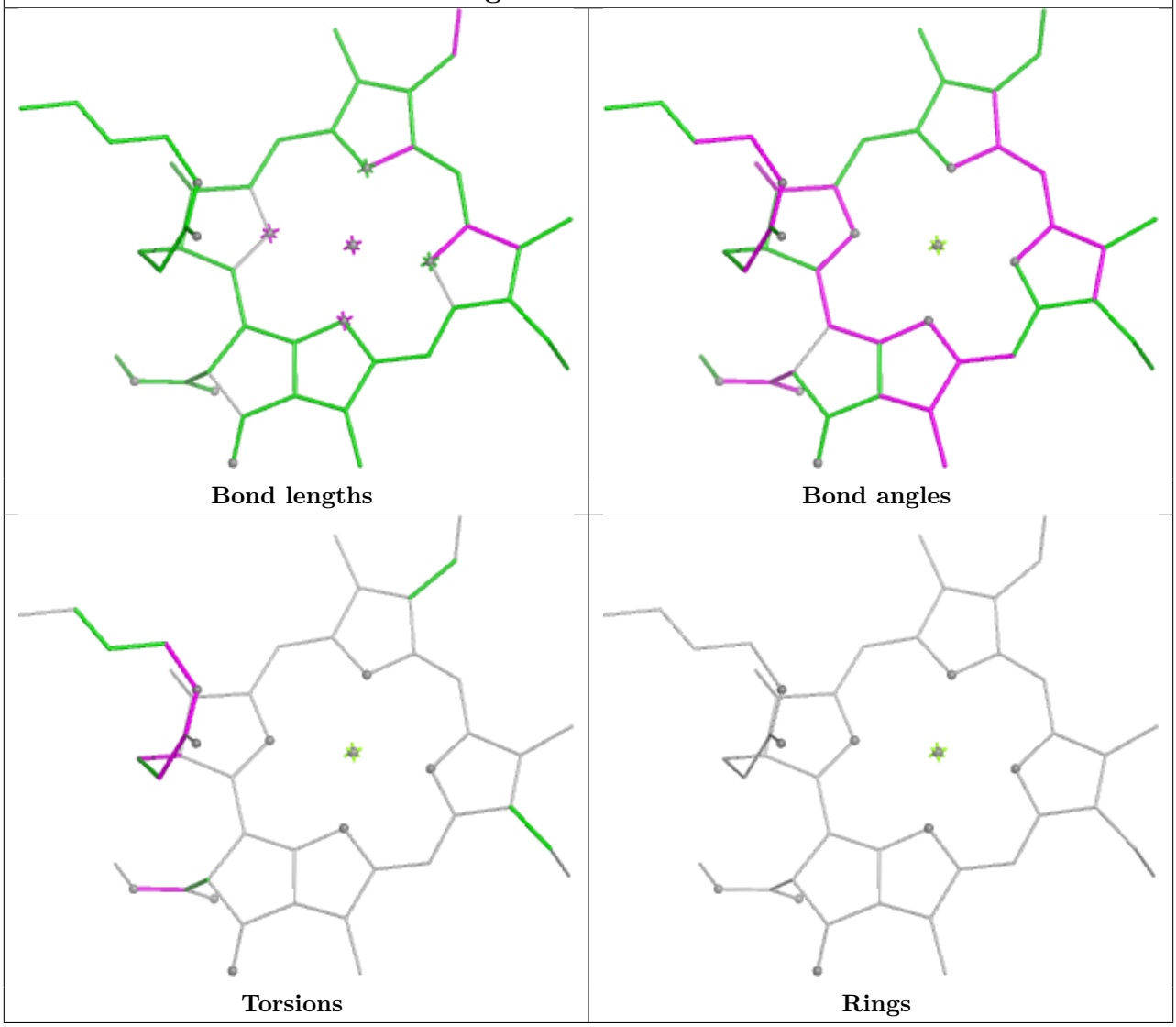

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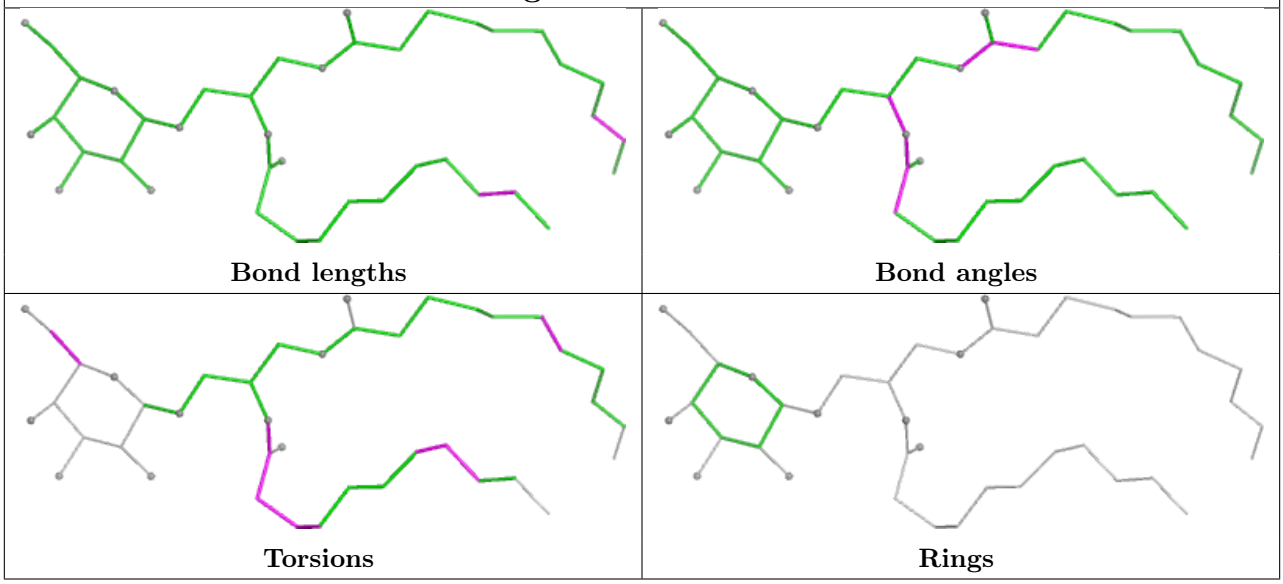

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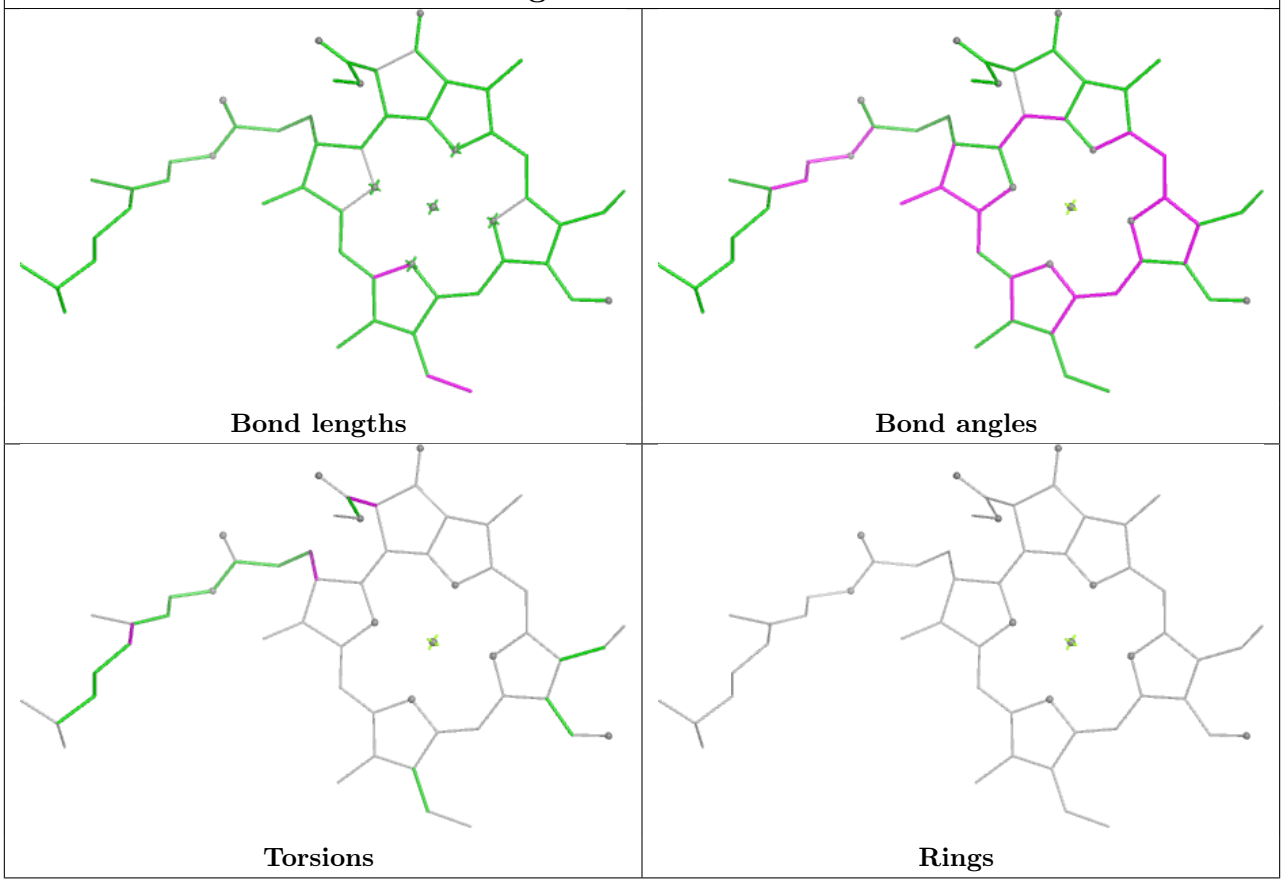
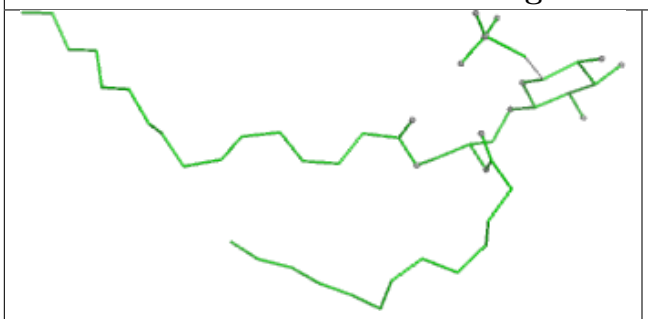
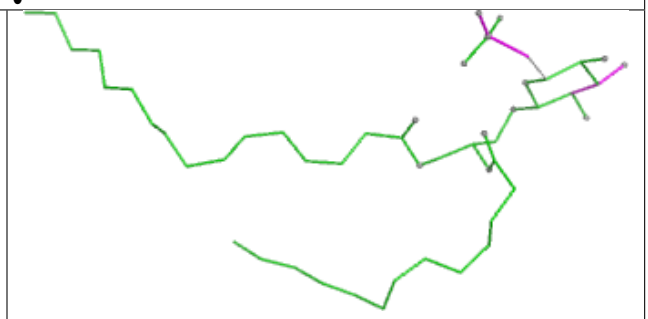


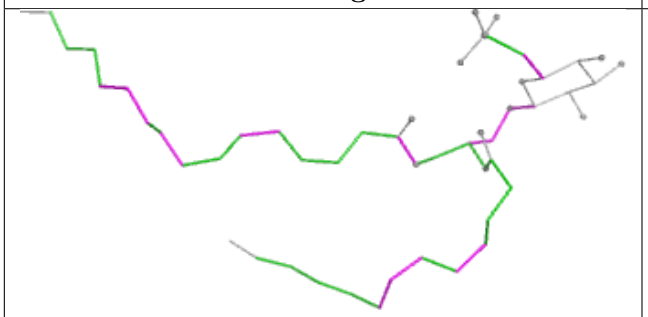
Ligand SQD R 322



Bond lengths



Bond angles



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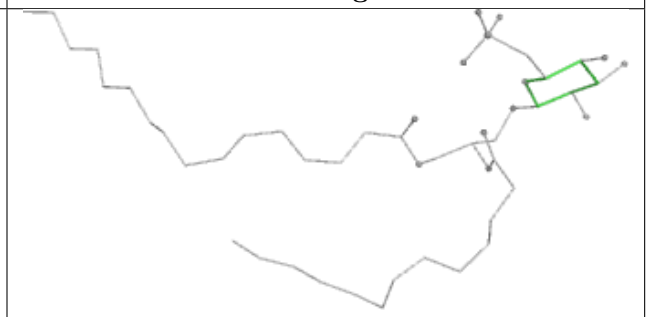
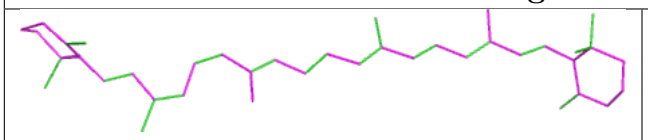


Rings

Ligand BCR a 410



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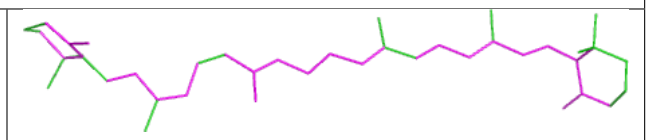

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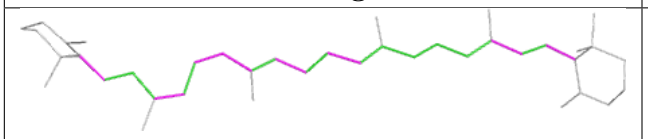

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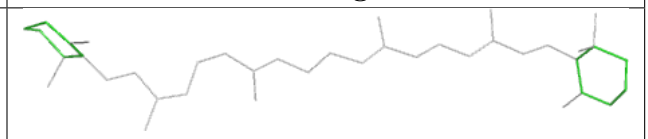
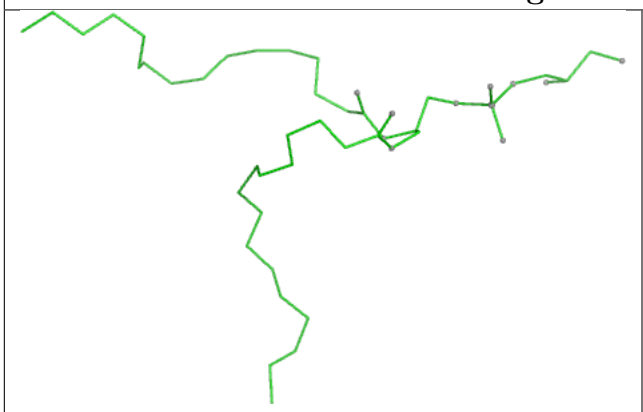
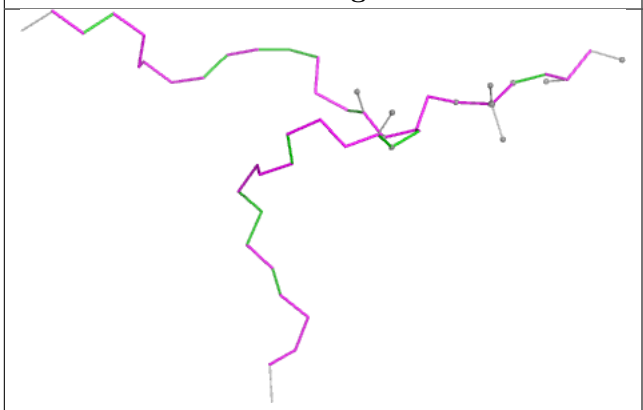
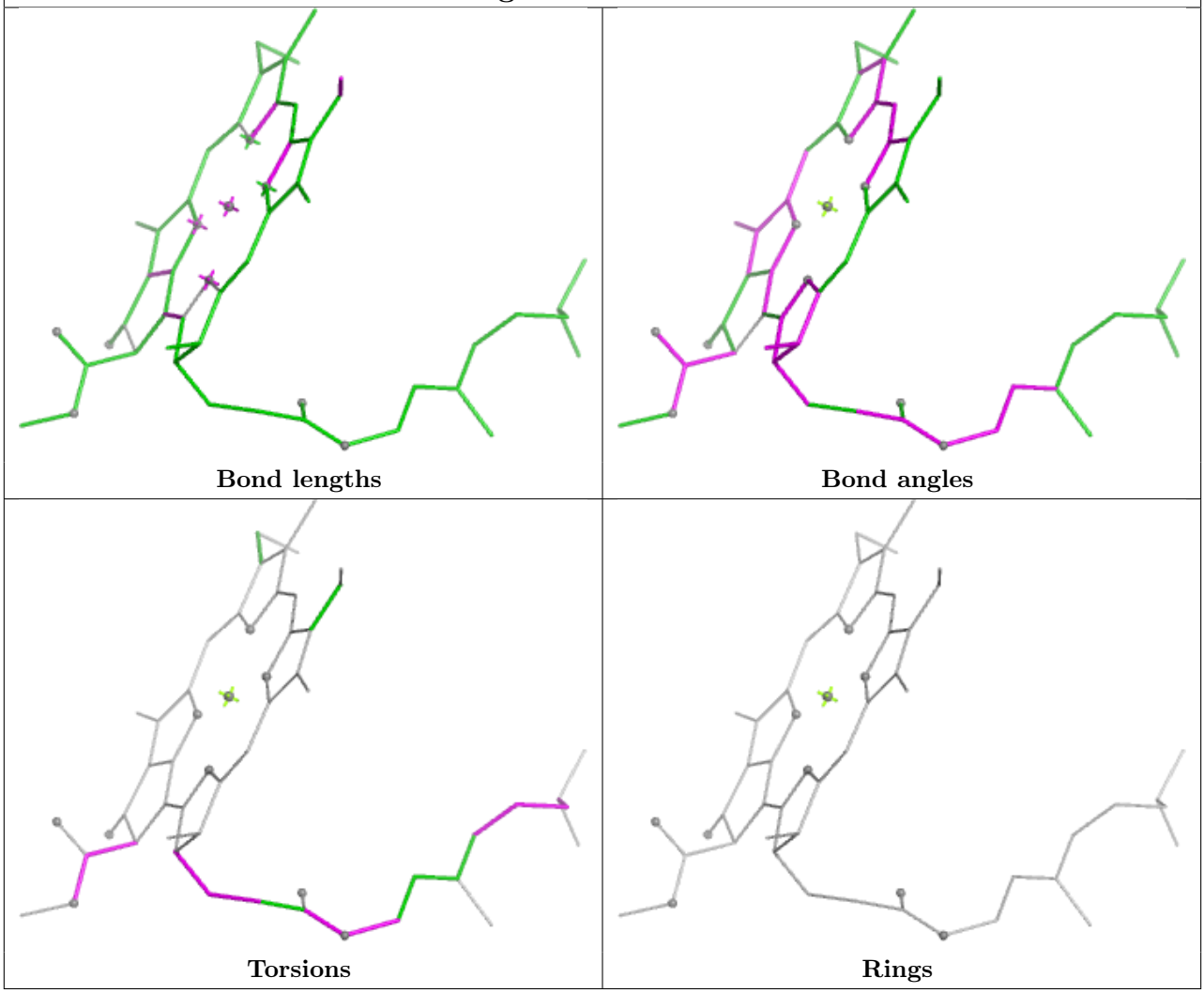


Rings

Ligand LHG n 320	
 Bond lengths	Bond angles
 Torsions	Rings

Ligand CLA r 315



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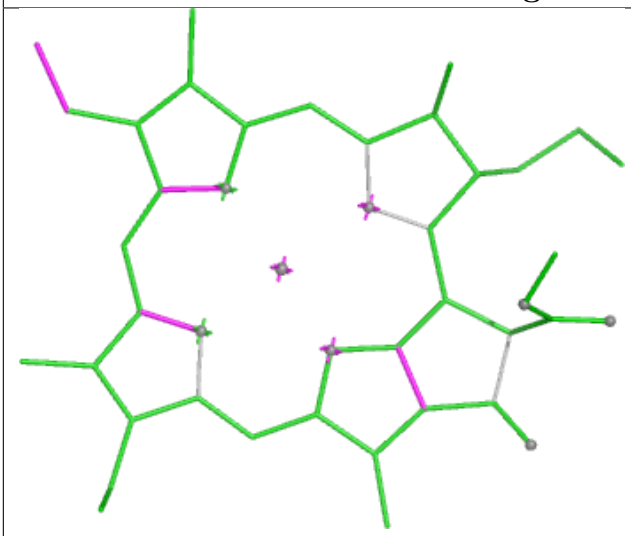

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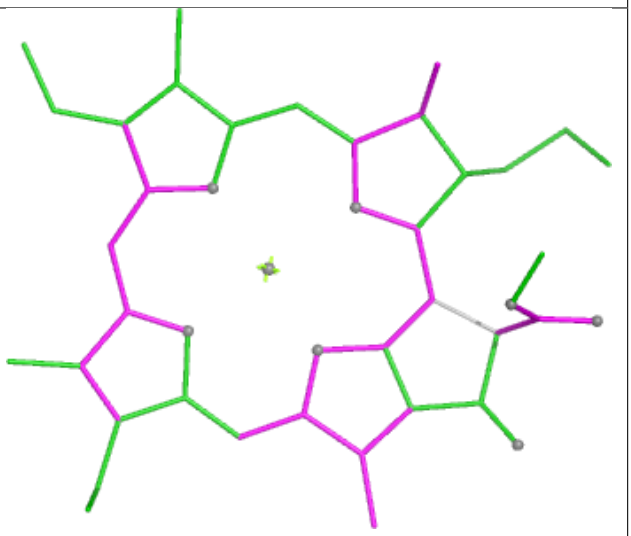

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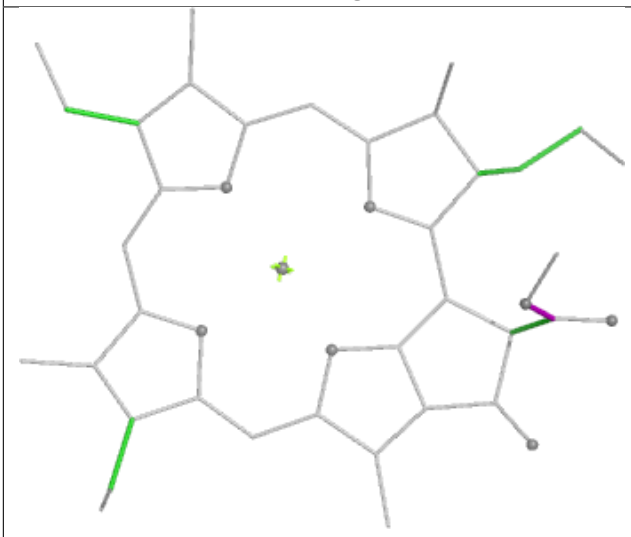

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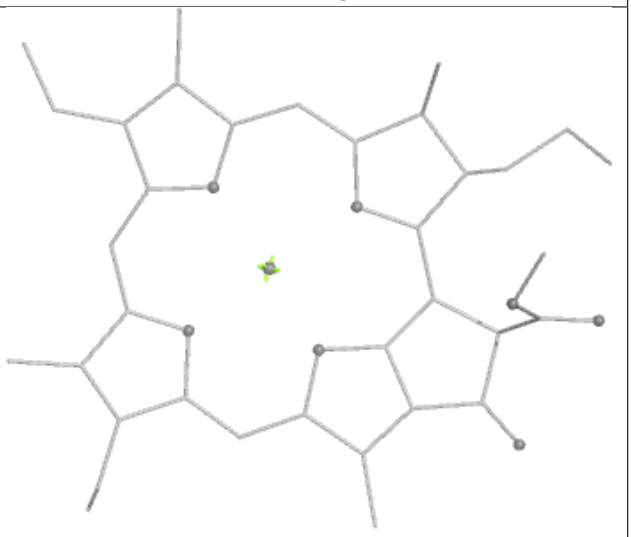
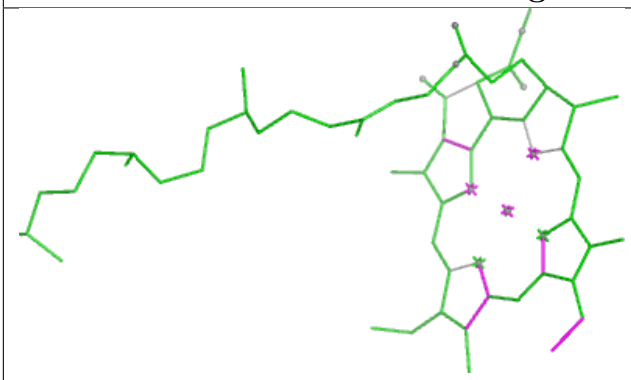


Rings

Ligand CLA 1 611



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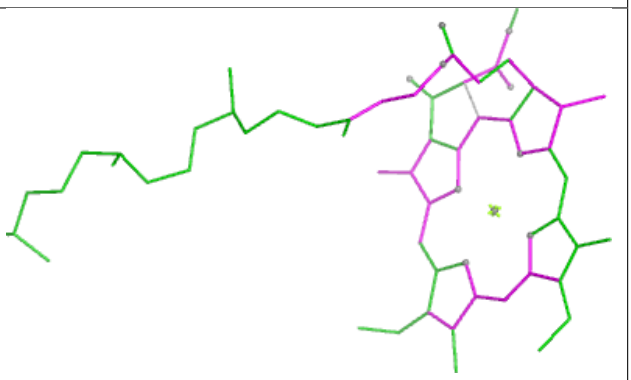

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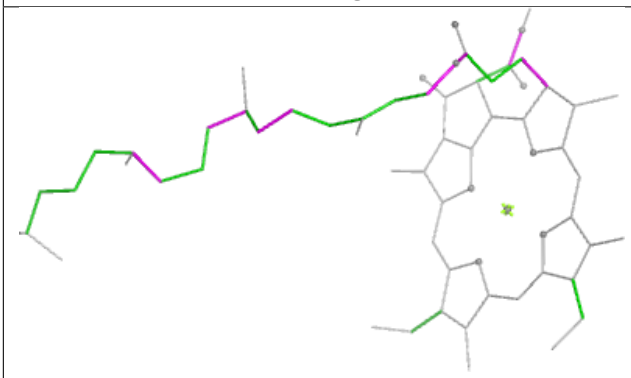
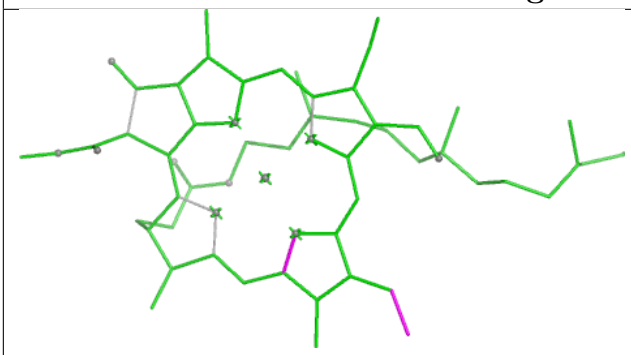


Torsions

Rings

Ligand CHL n 308



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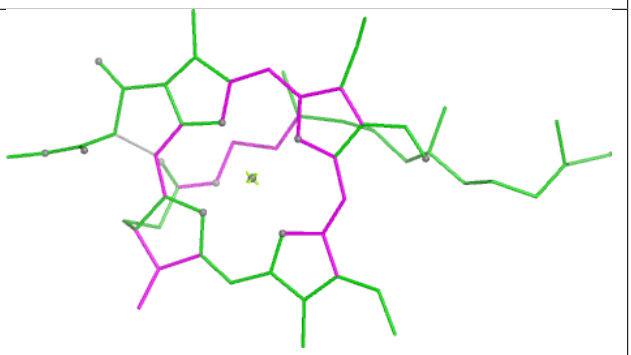
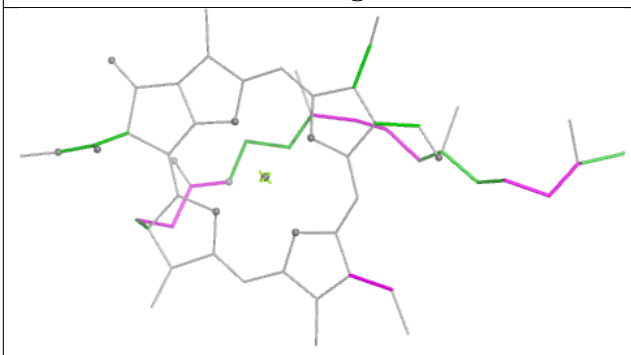


Bond angles



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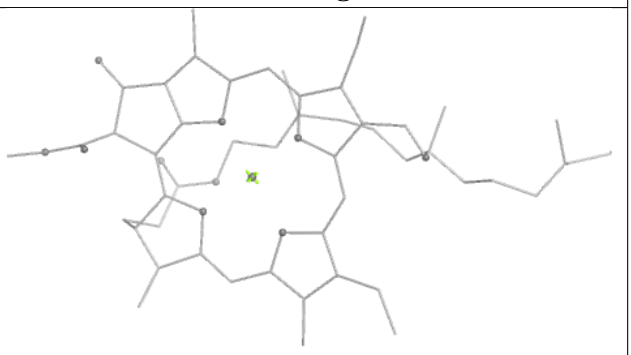
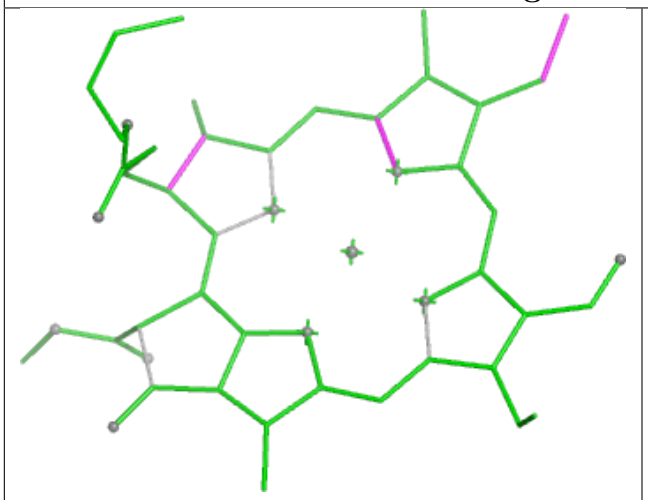


Rings

Ligand CHL N 308



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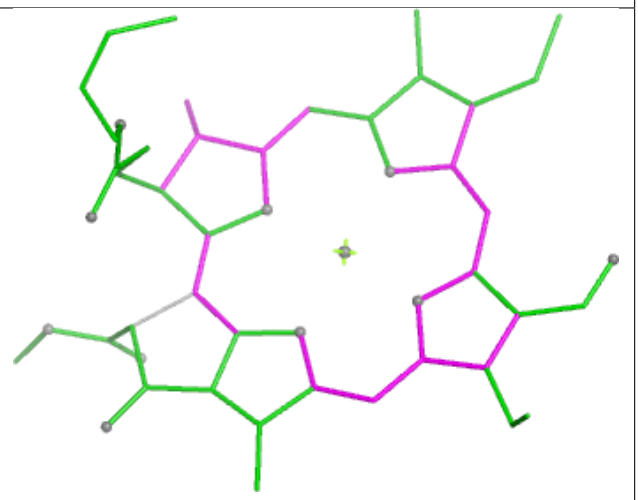

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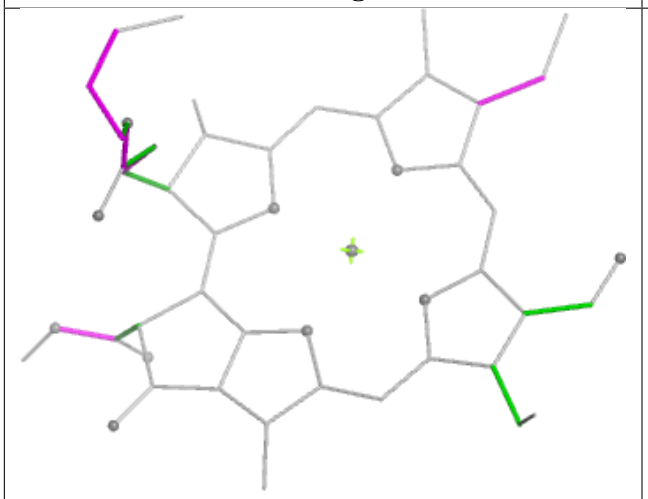

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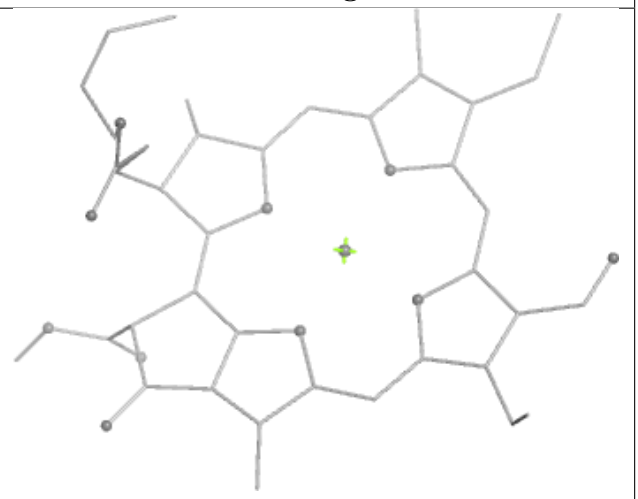
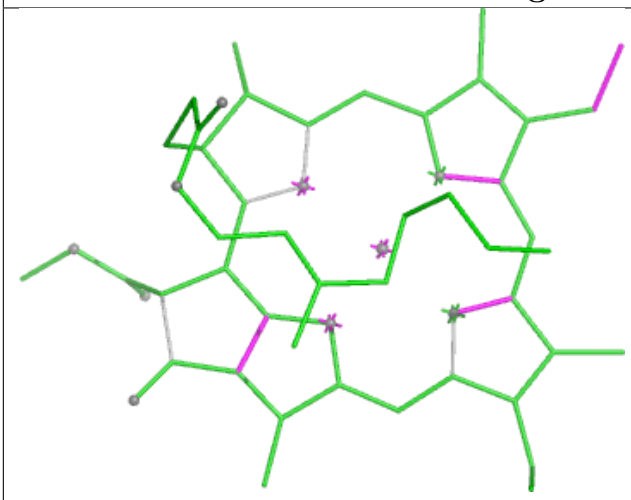


Rings

Ligand CLA 2 613



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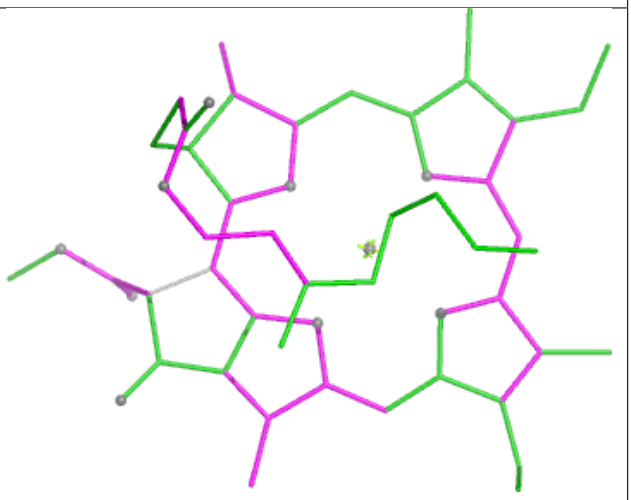
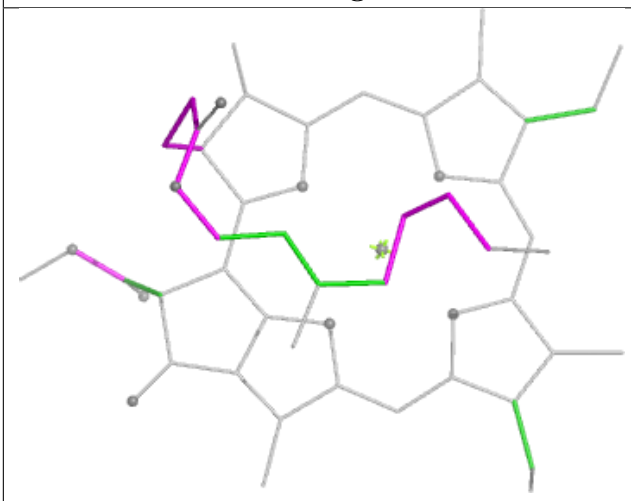


Bond angles



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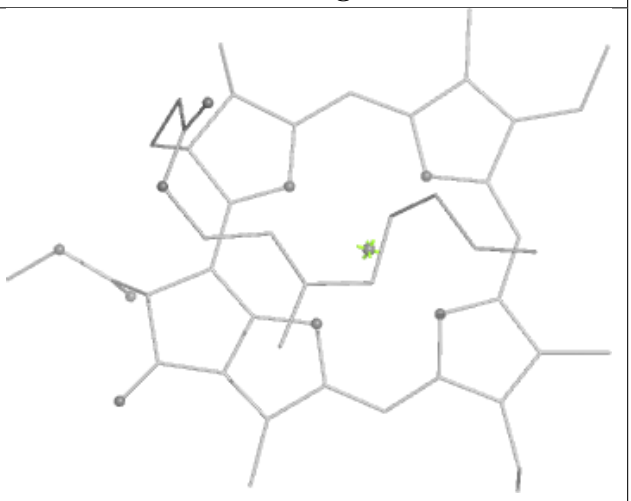
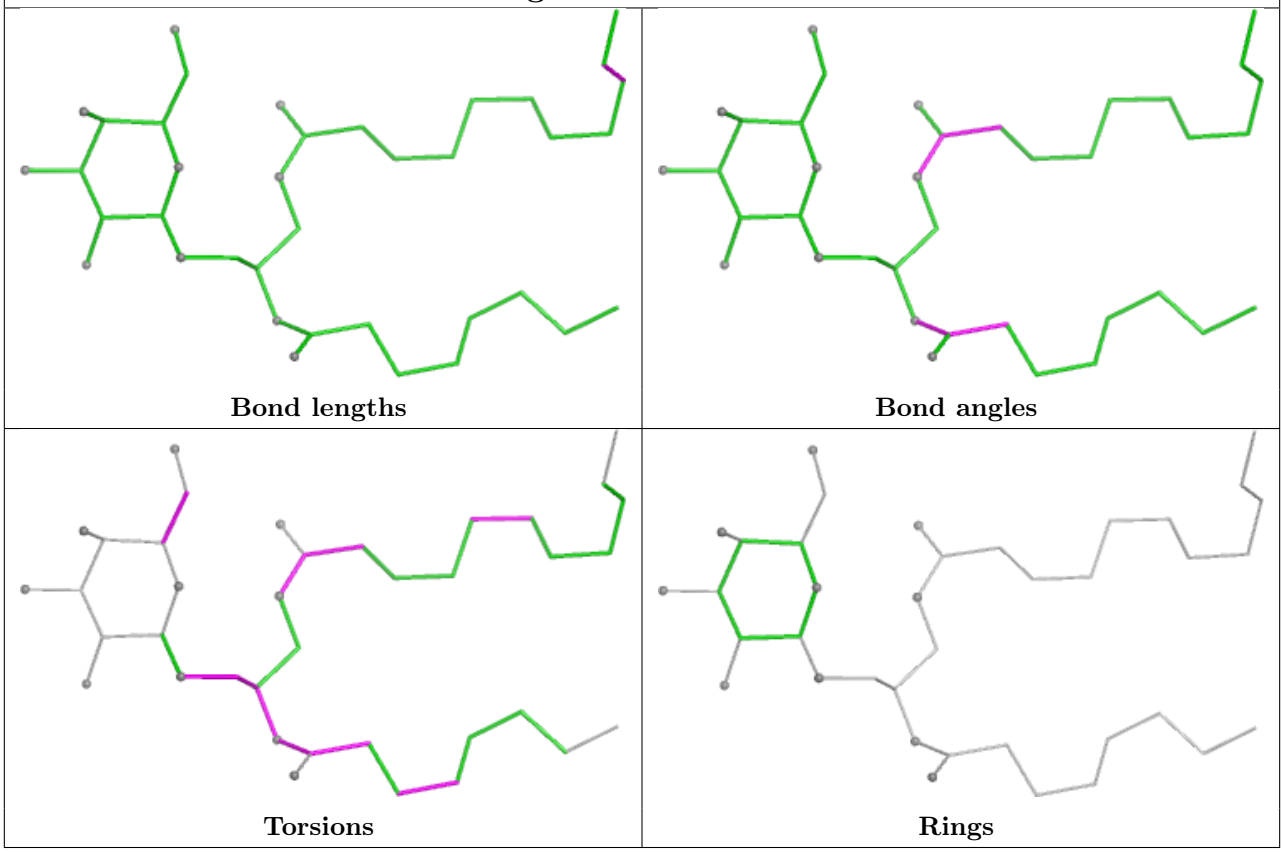


Rings

Ligand LMG I 101



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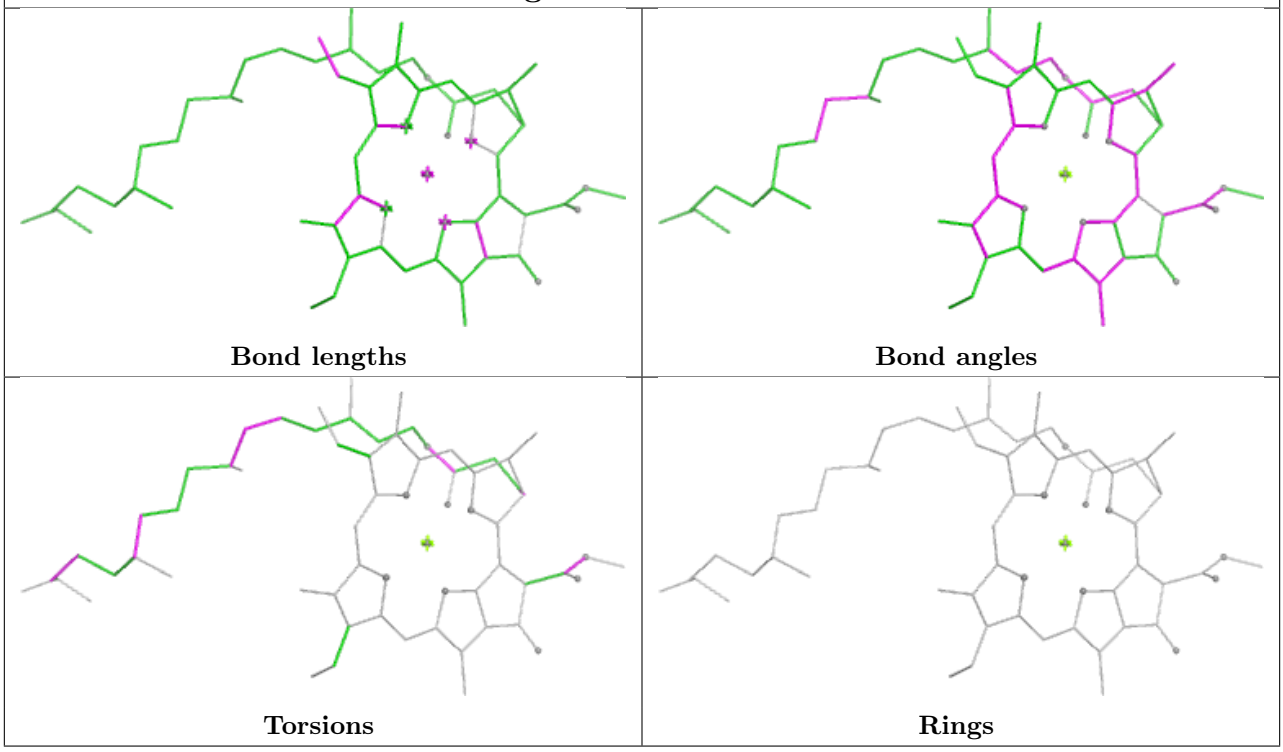

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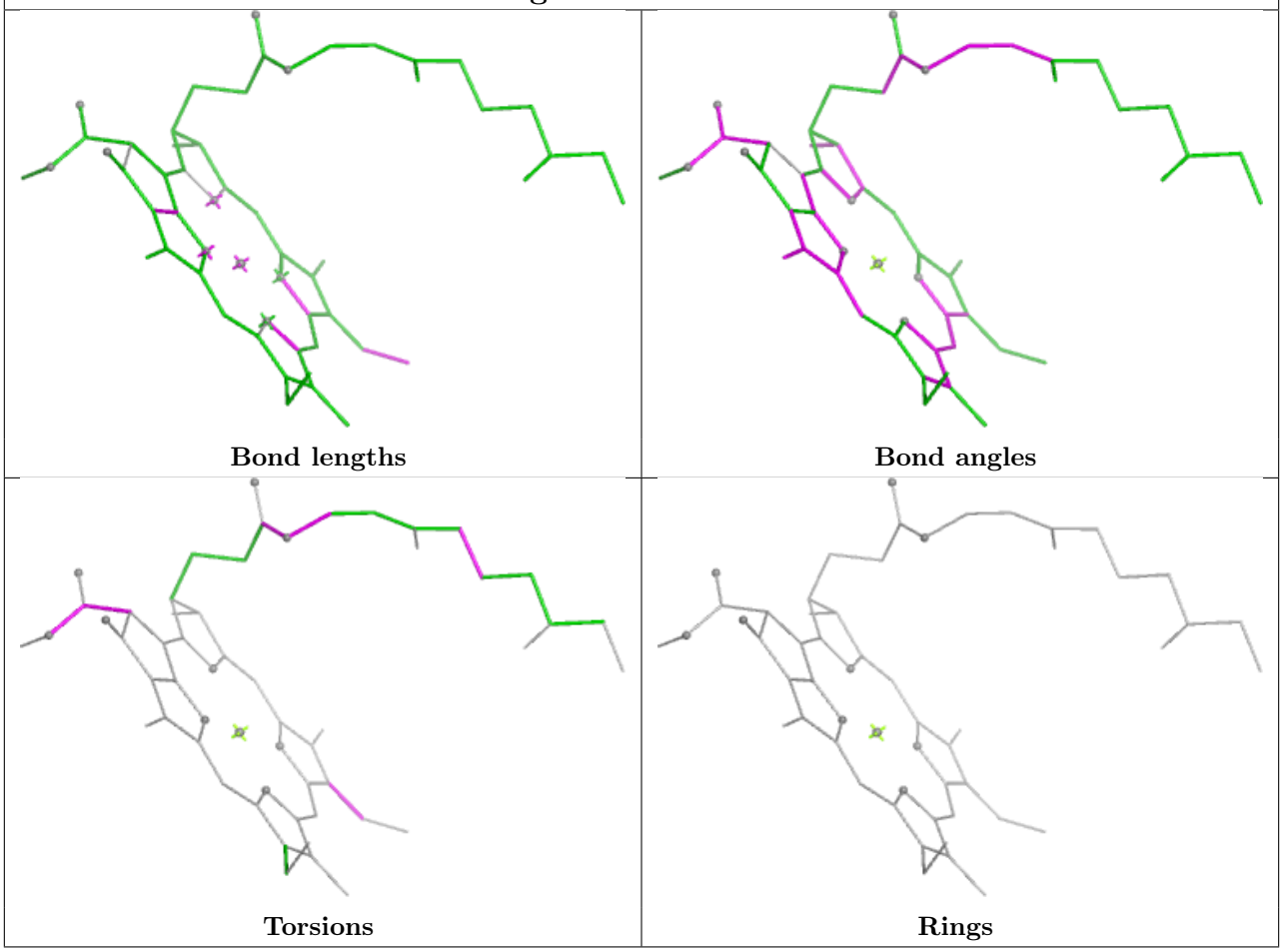

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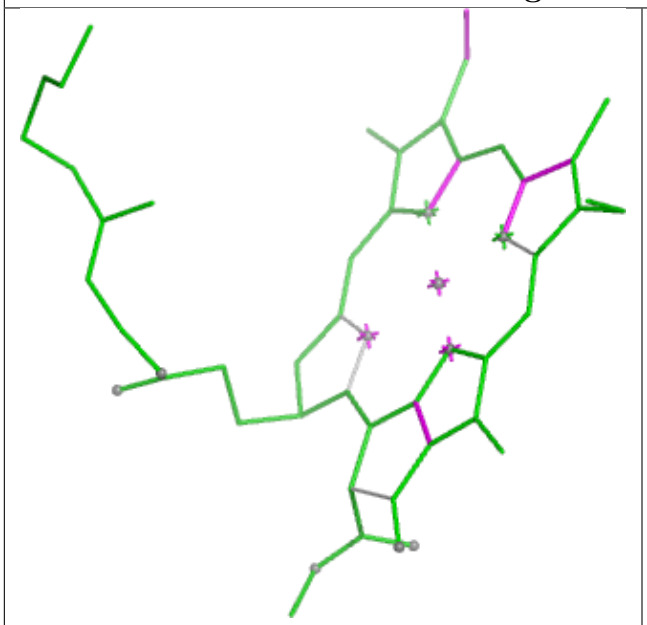
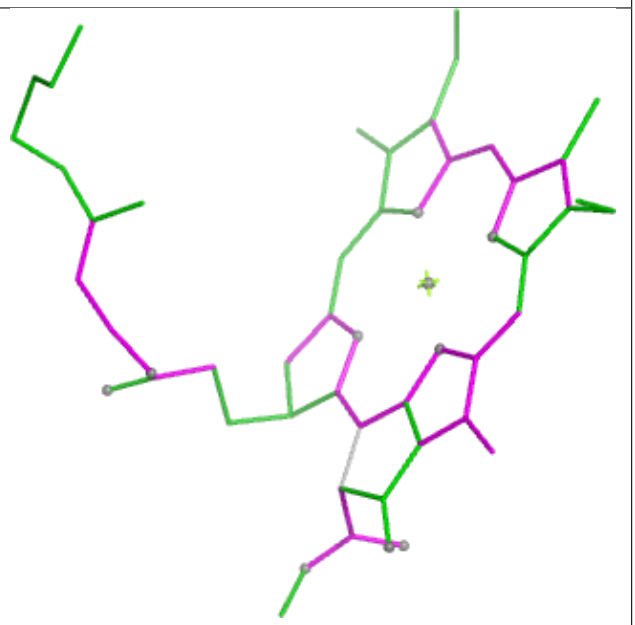
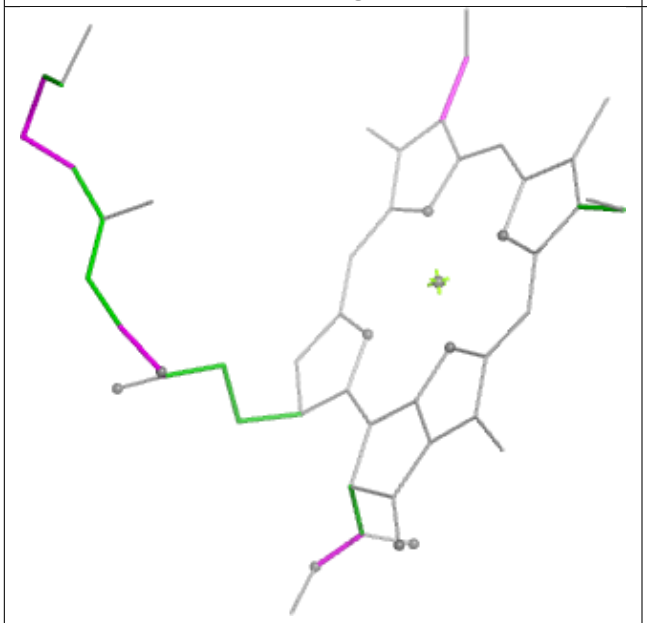


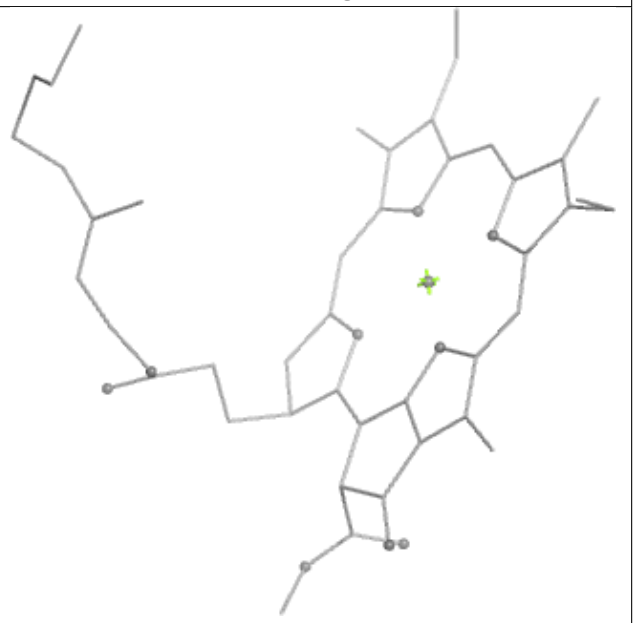
Bond lengths



Bond angles

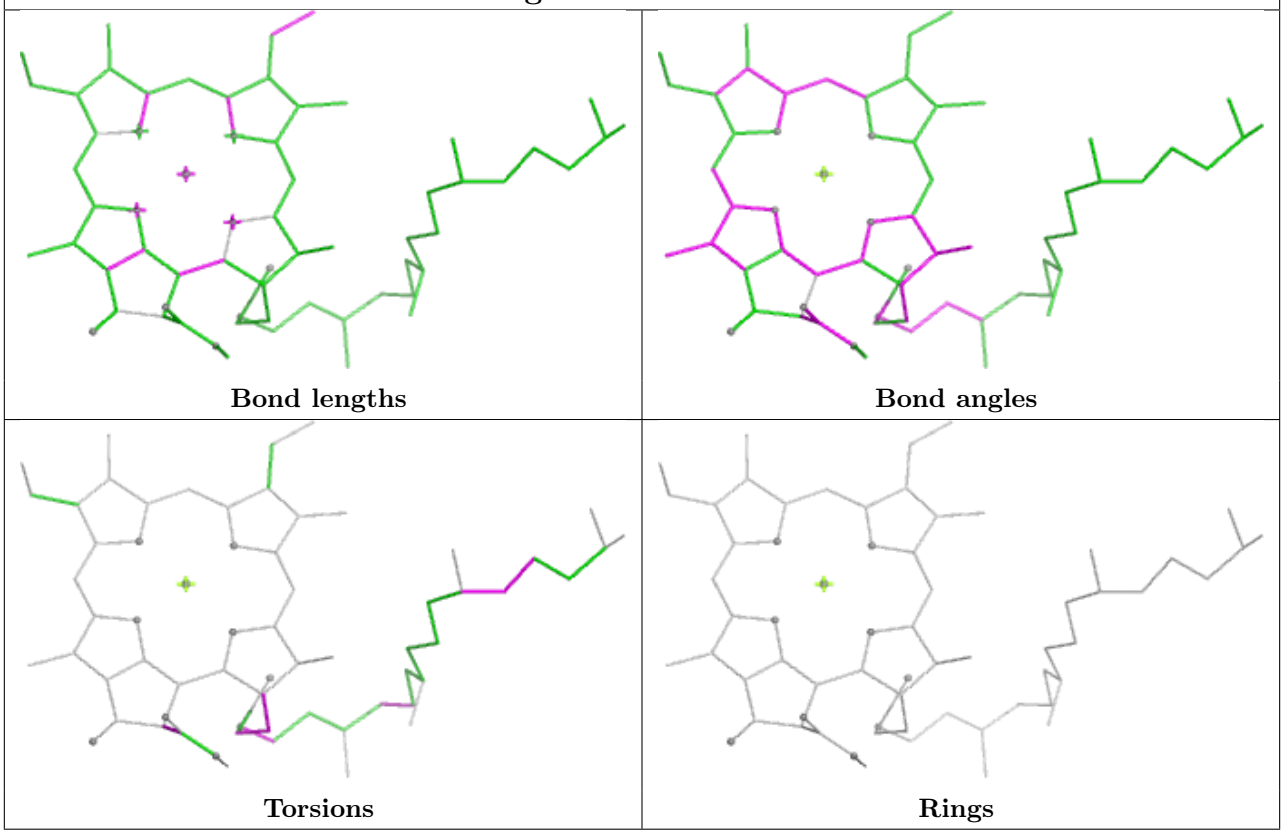


Torsions

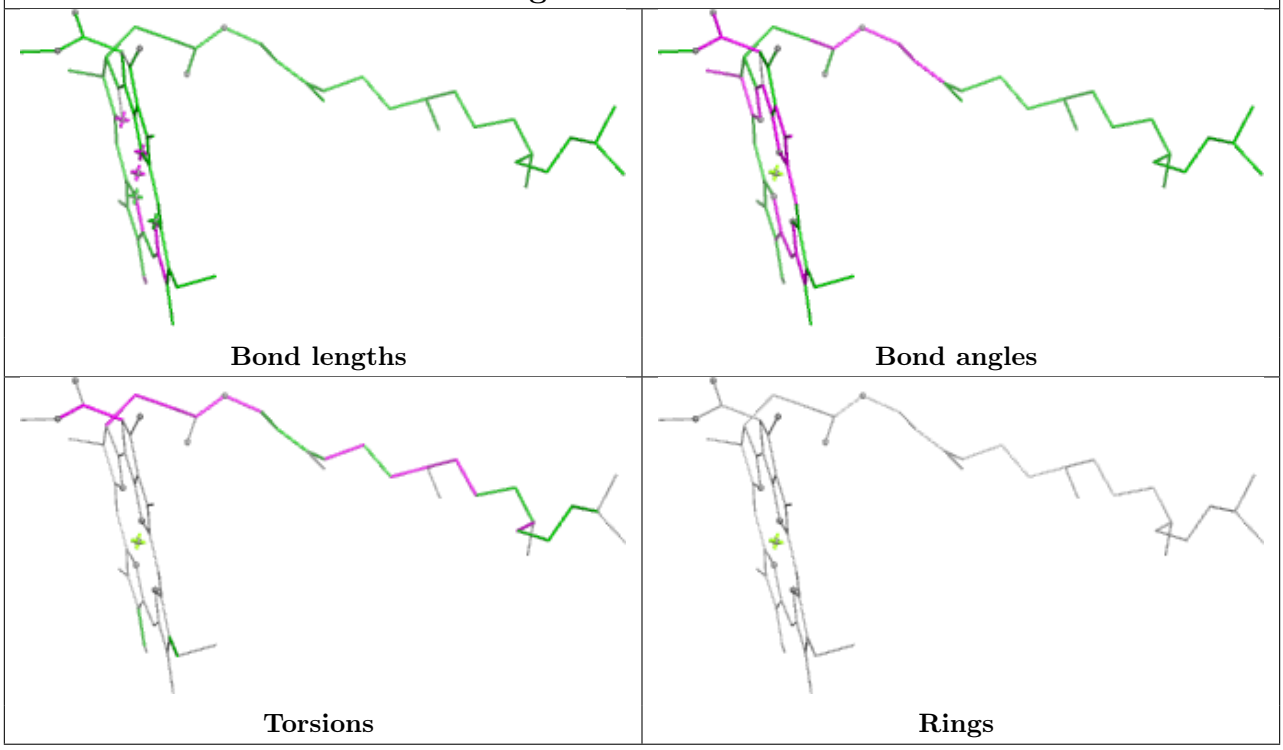


Rings

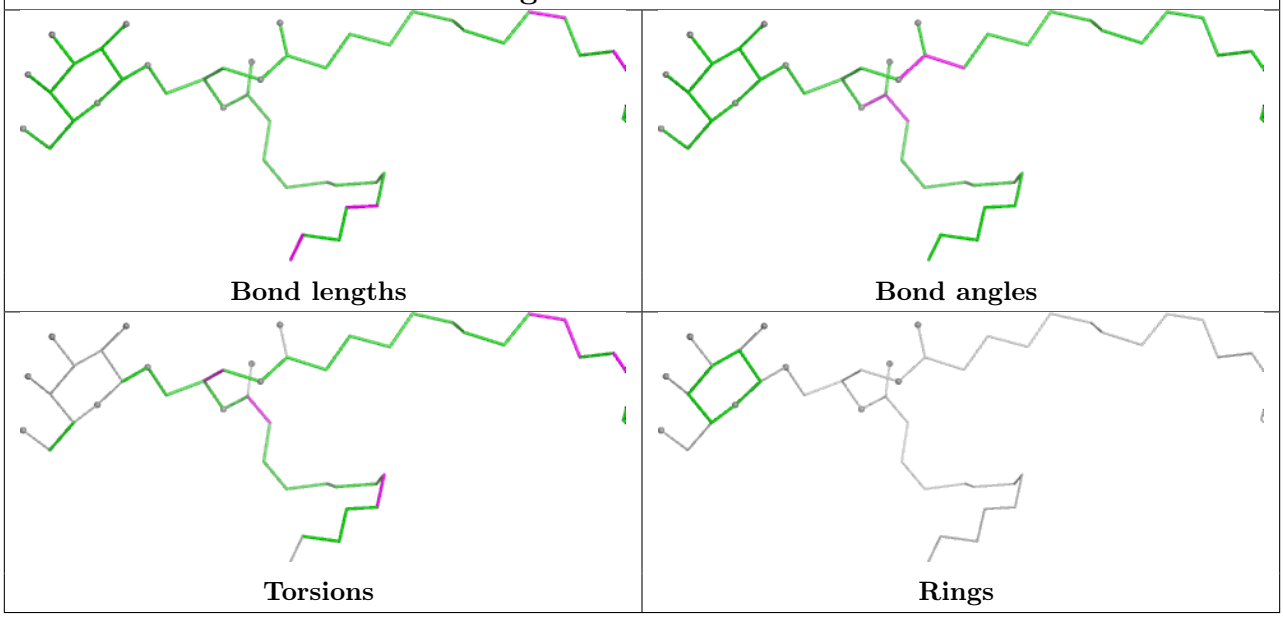
Ligand CLA A 406



Ligand CLA 8 604



Ligand LMG D 412



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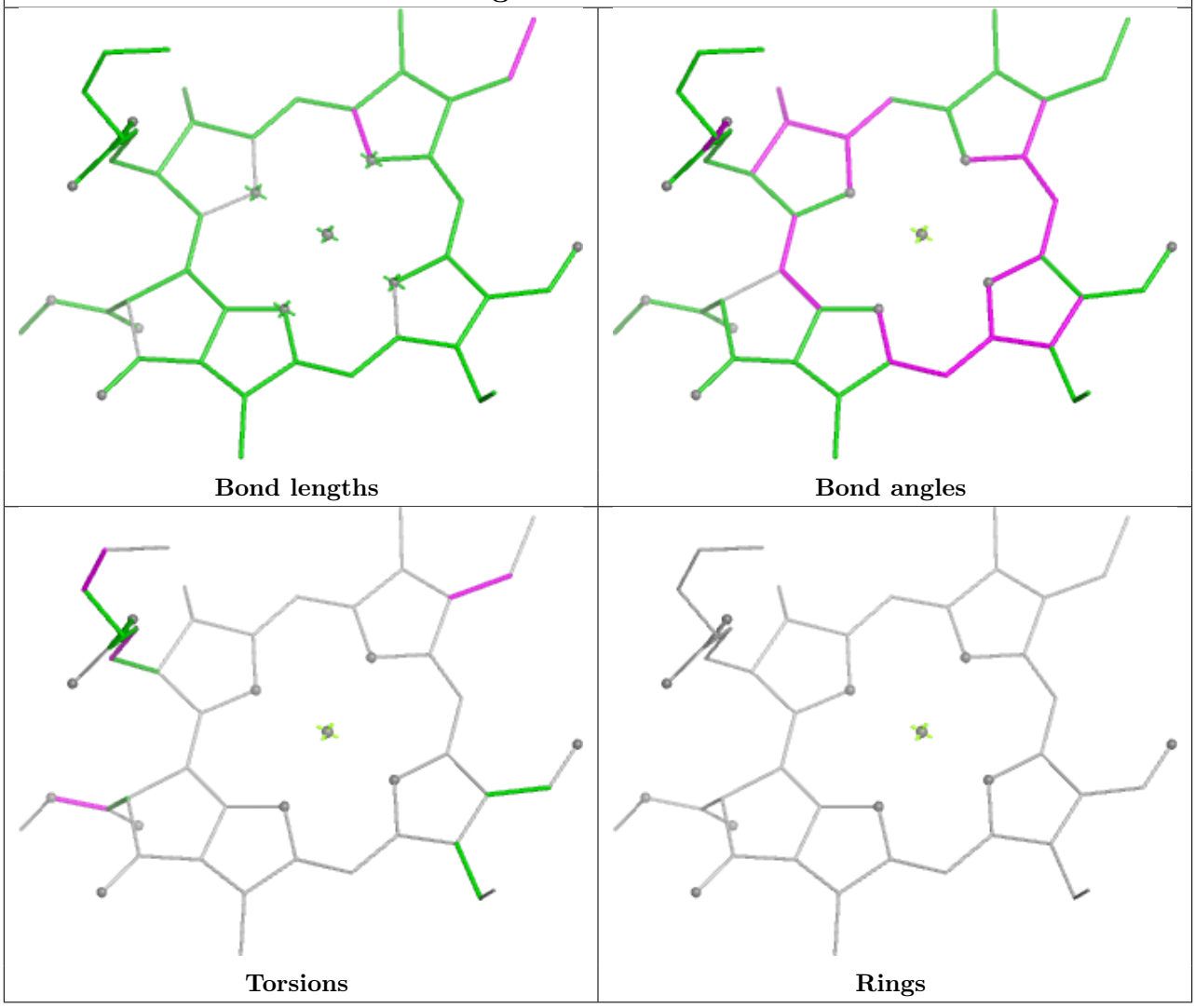

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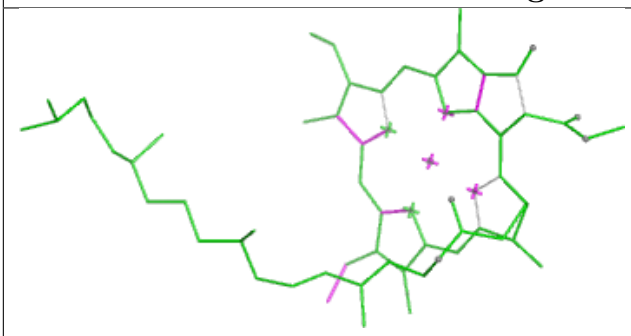
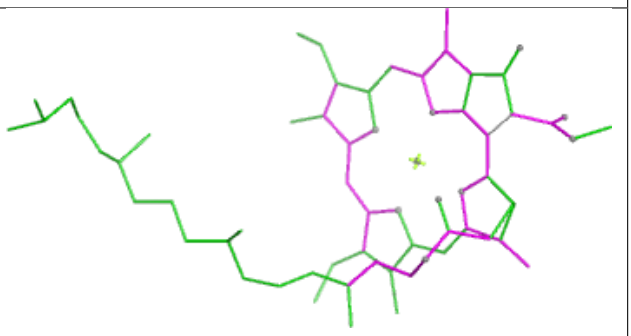
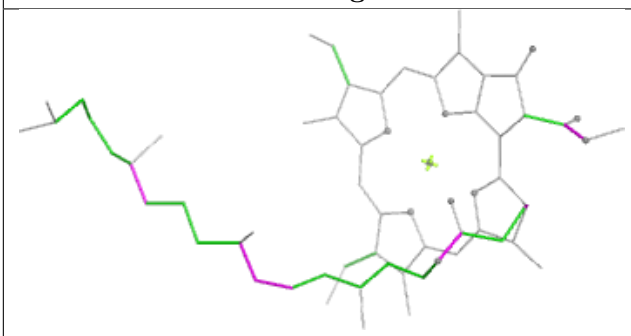
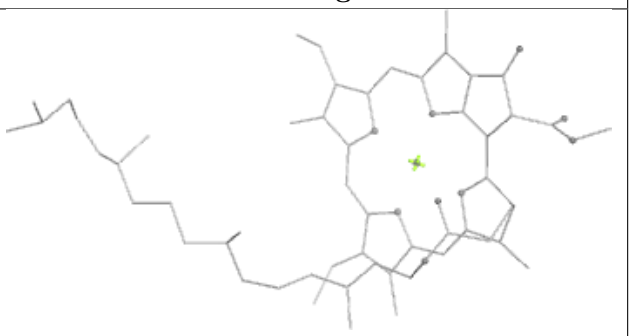
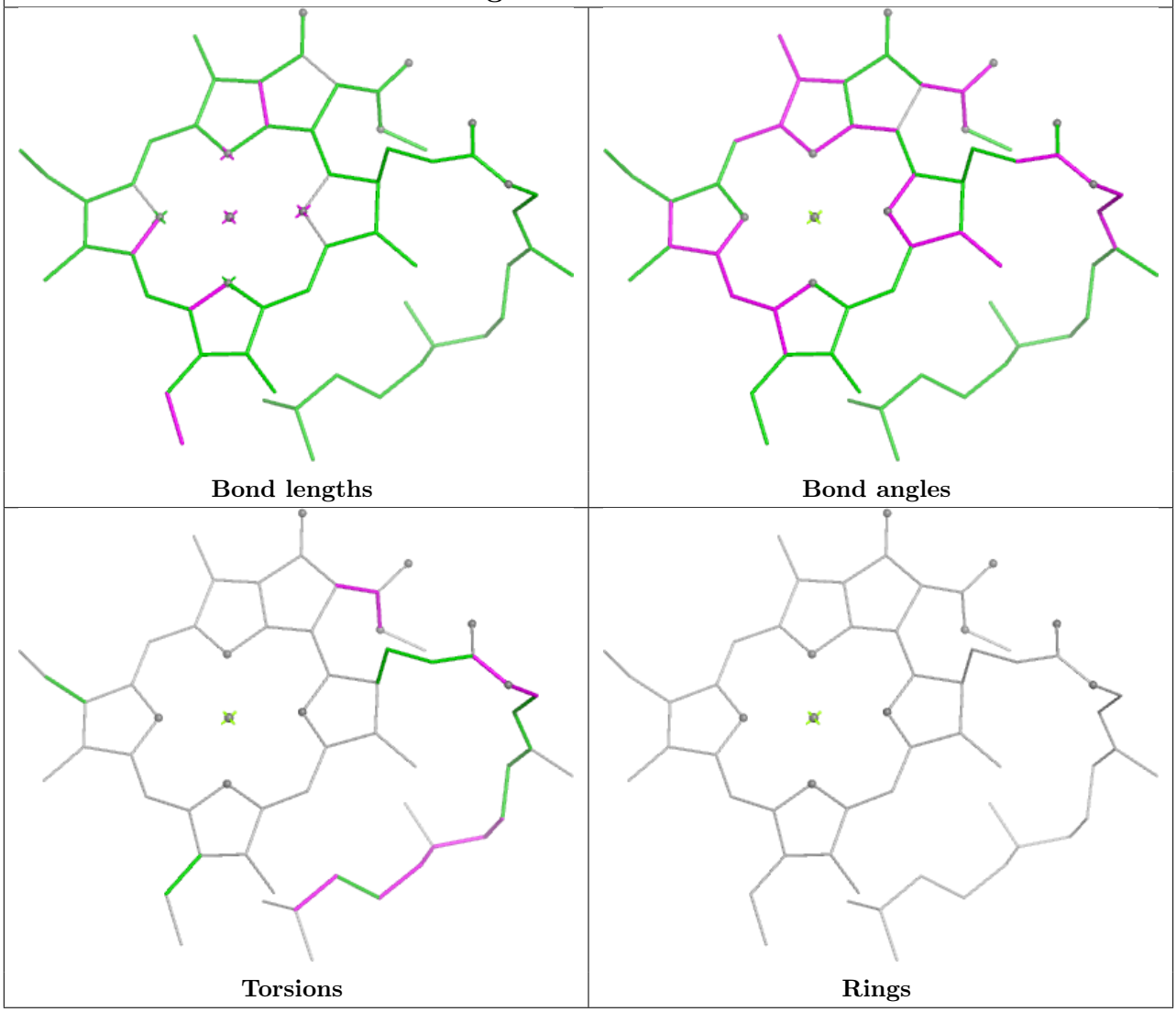
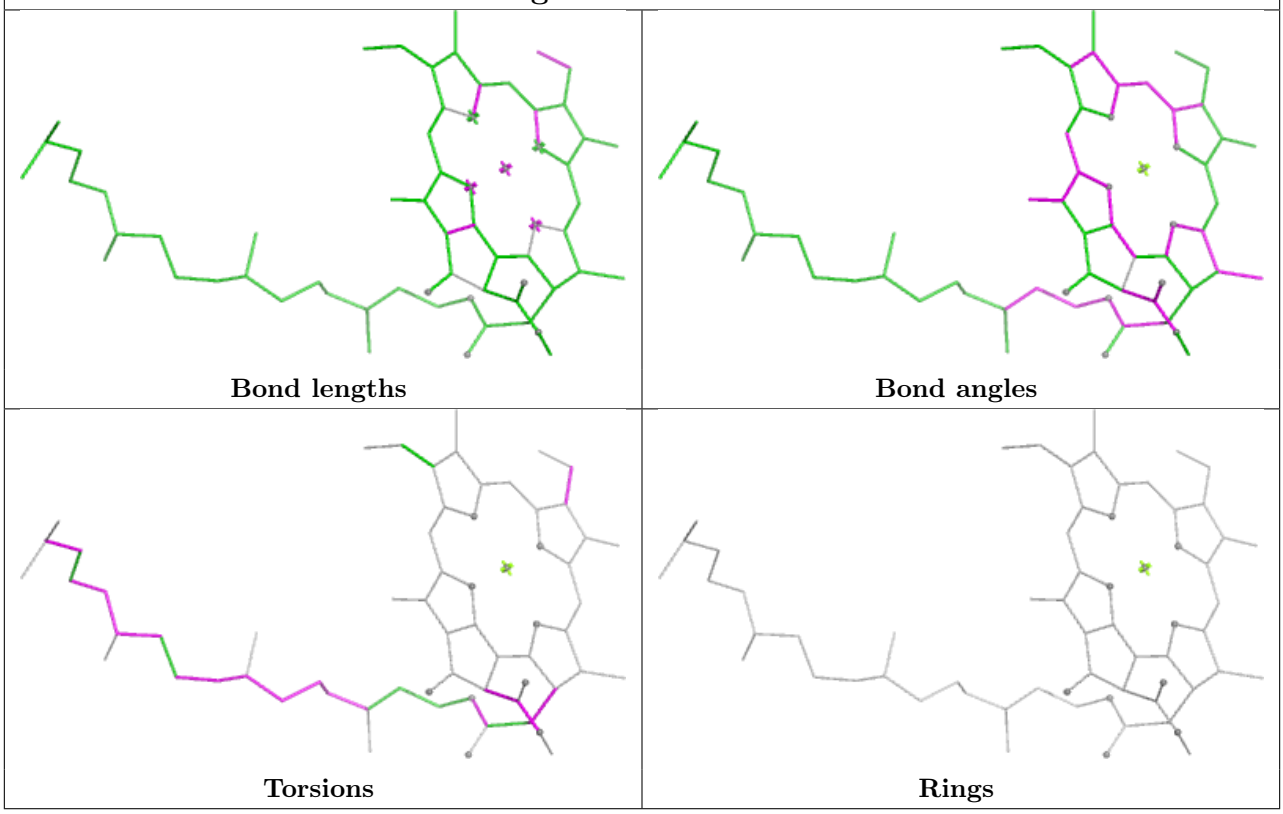
 Bond lengths	 Bond angles
 Torsions	 Rings

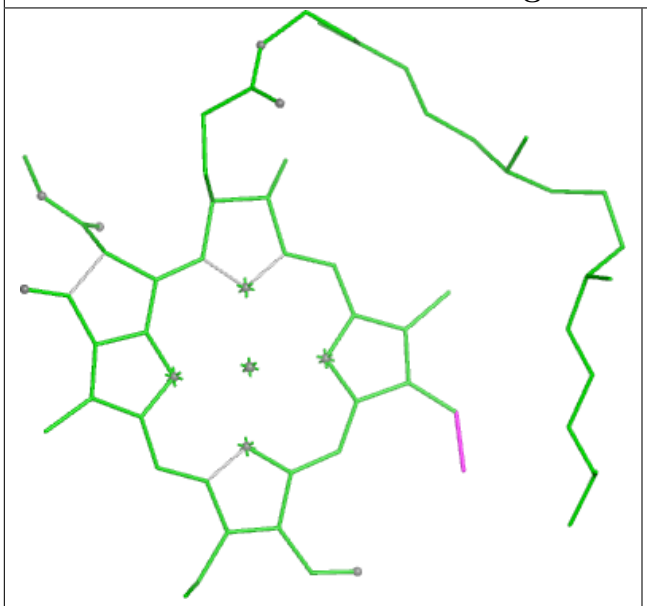
Ligand CLA r 305



Ligand CLA s 312



Ligand CHL G 623



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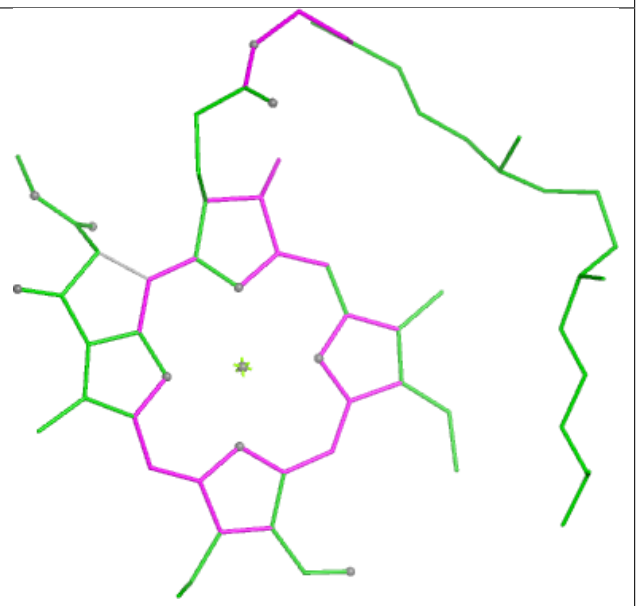

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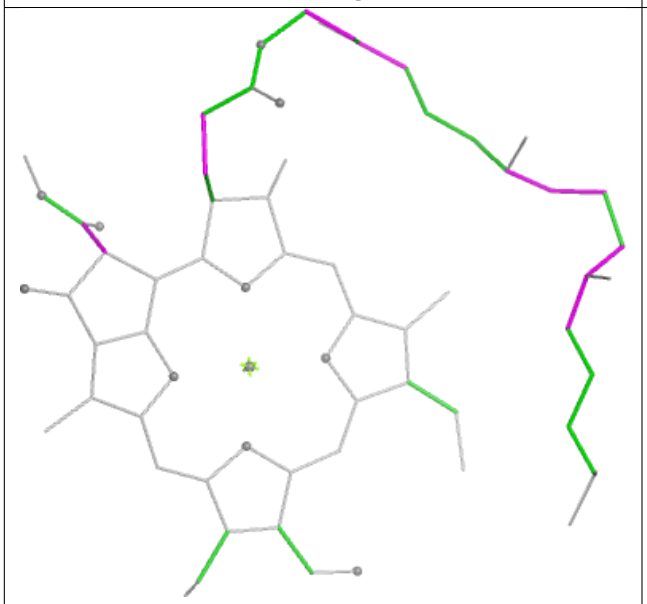

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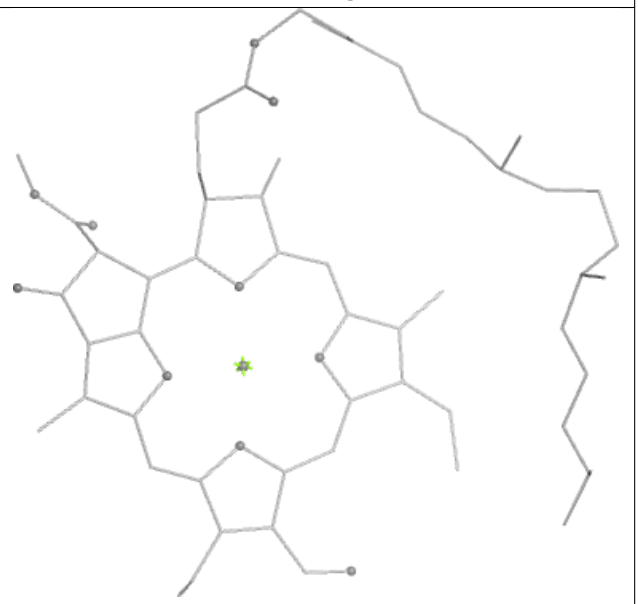
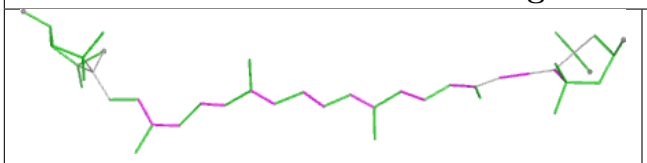


Rings

Ligand NEX 2 616



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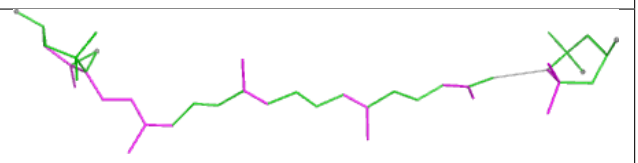
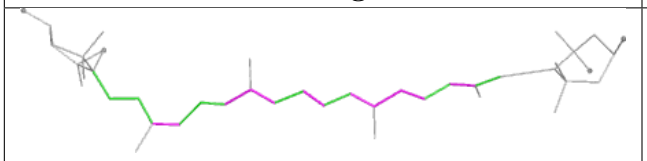


Bond angles



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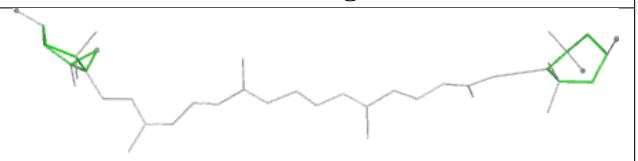
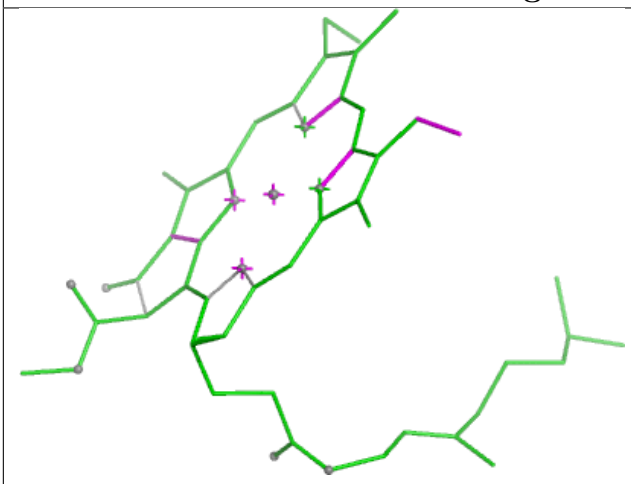


Rings

Ligand CLA R 315



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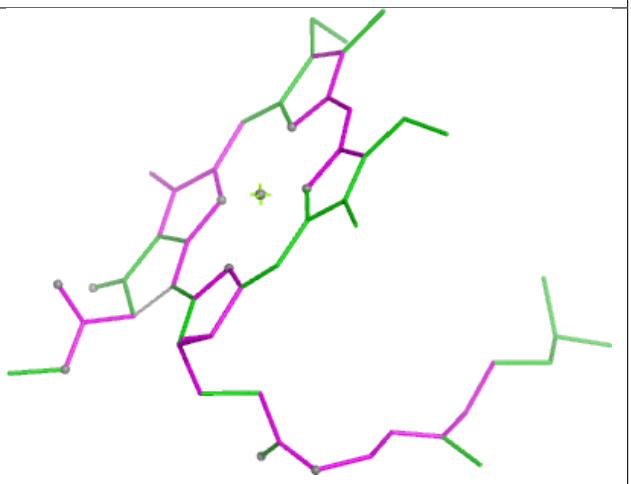

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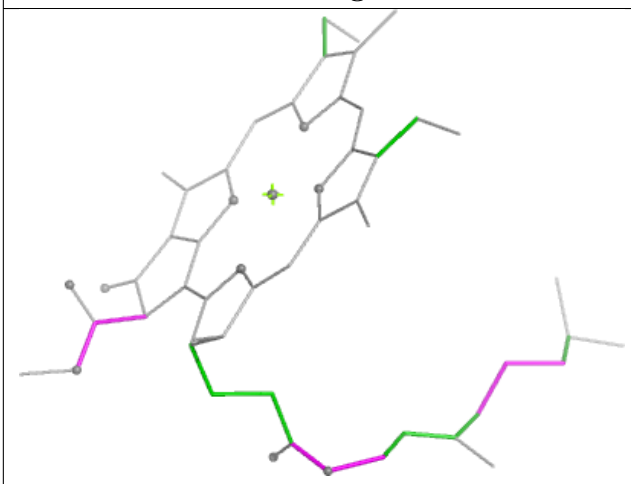
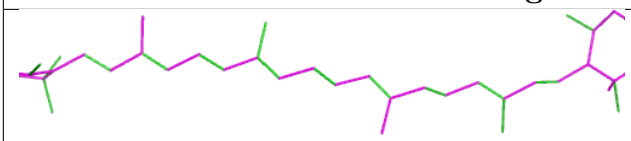


Torsions

Rings

Ligand BCR b 618



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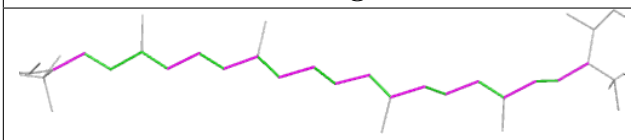
Bond angles



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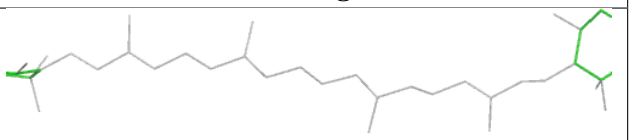
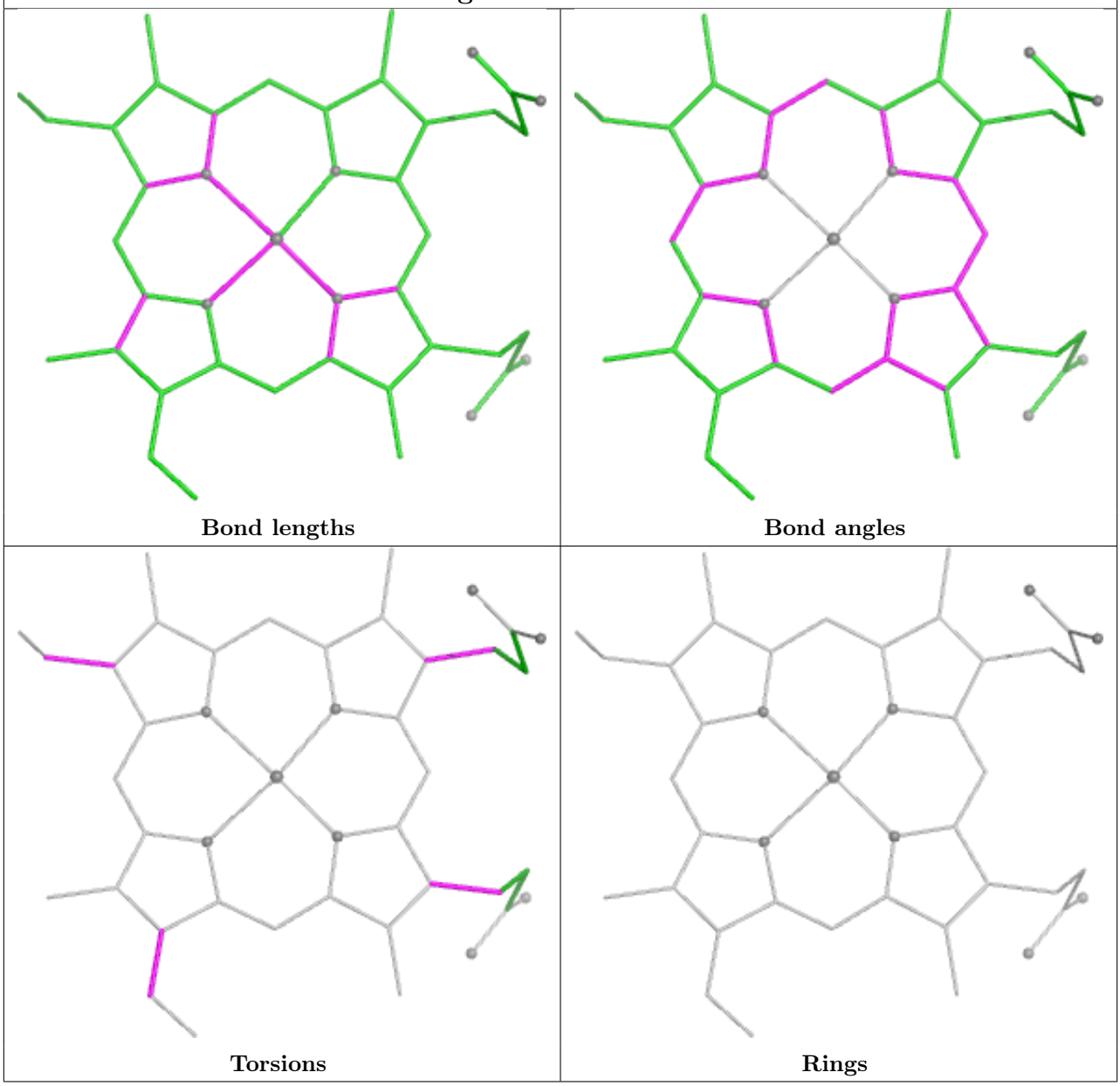
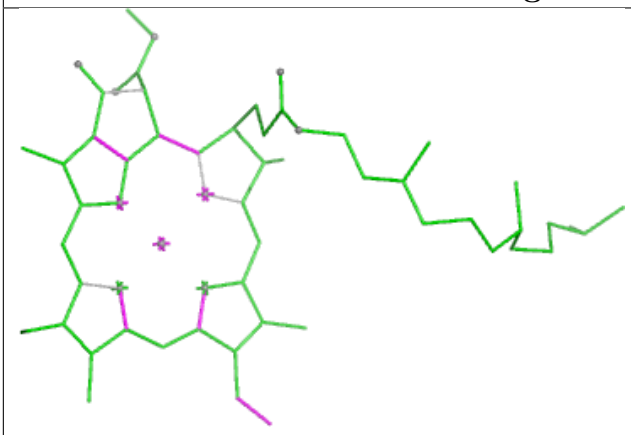


Rings

Ligand HEM e 102



Ligand CLA A 409



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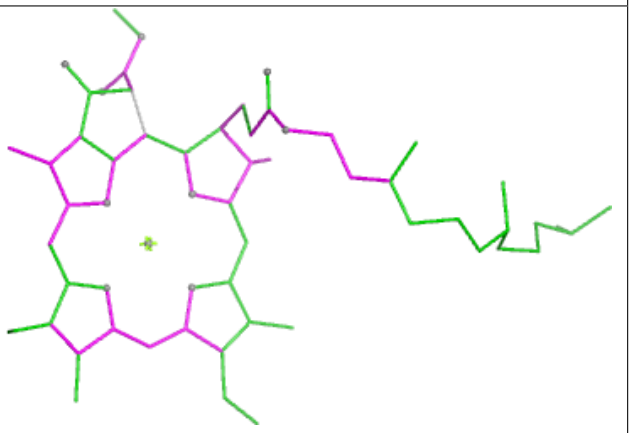
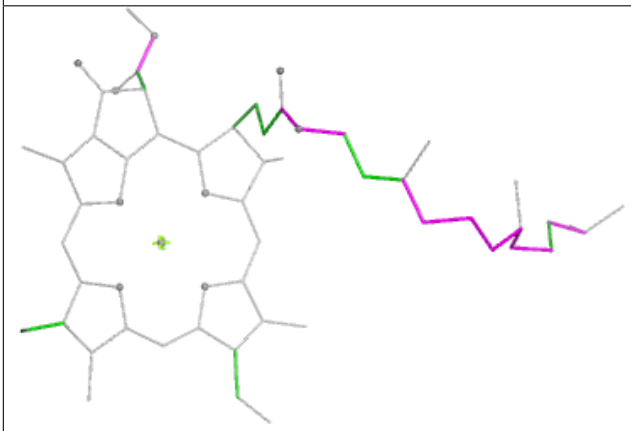


Bond angles



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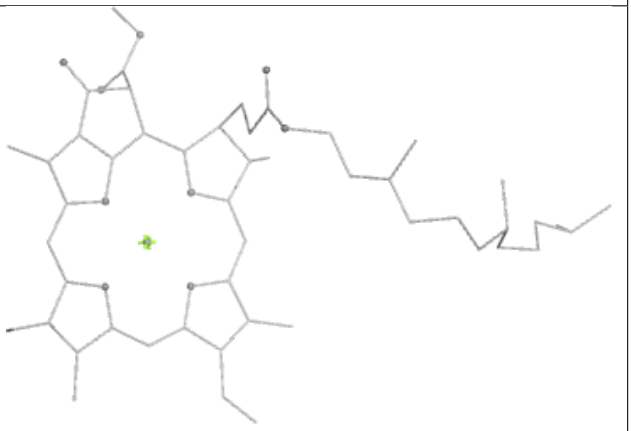
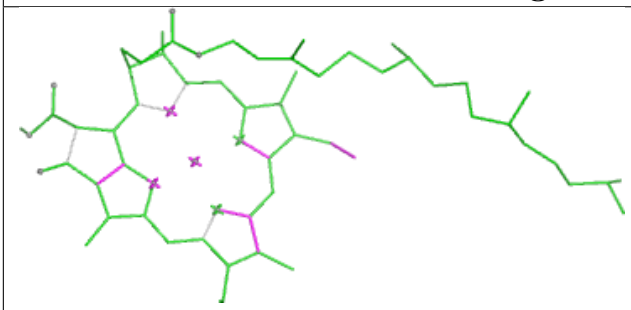


Rings

Ligand CLA c 601



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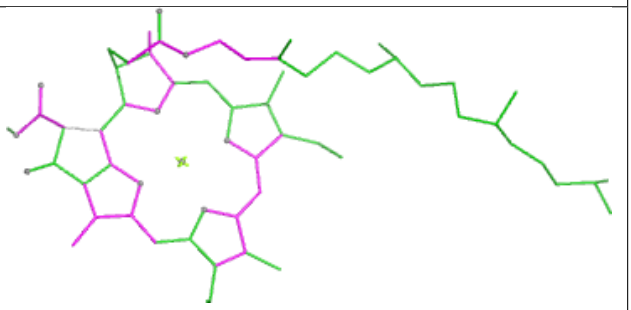

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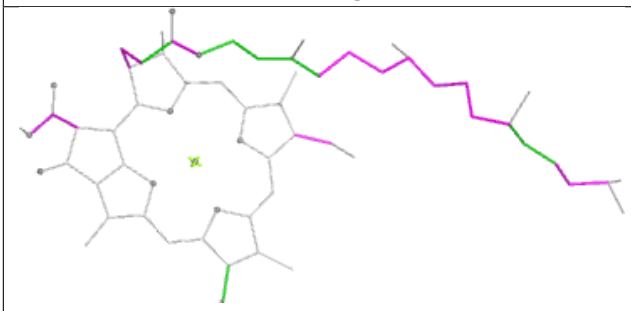

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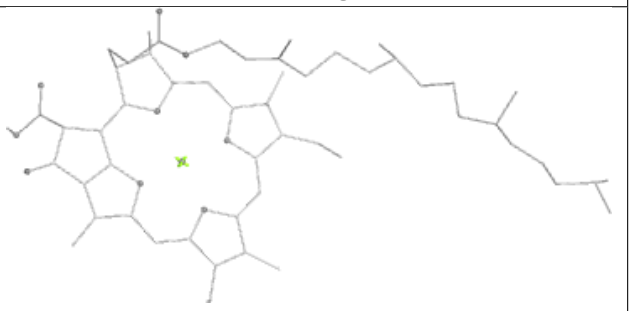
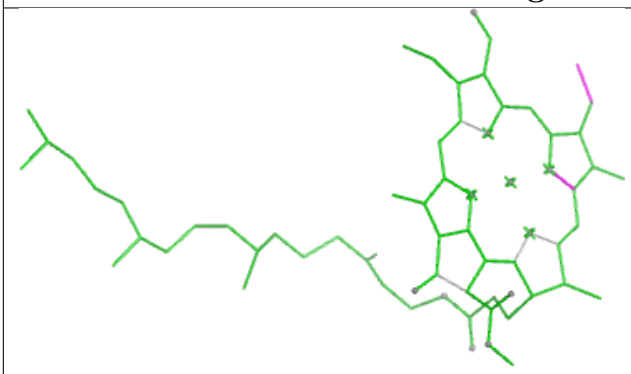
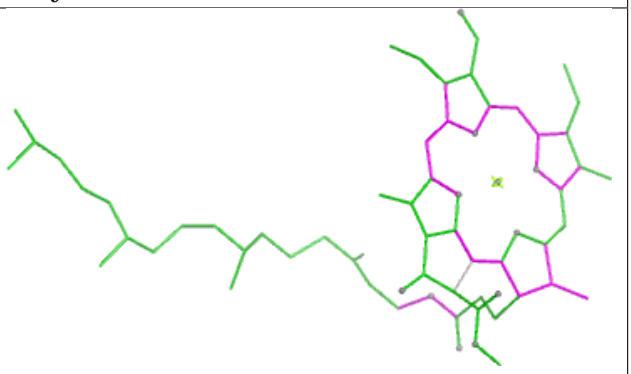
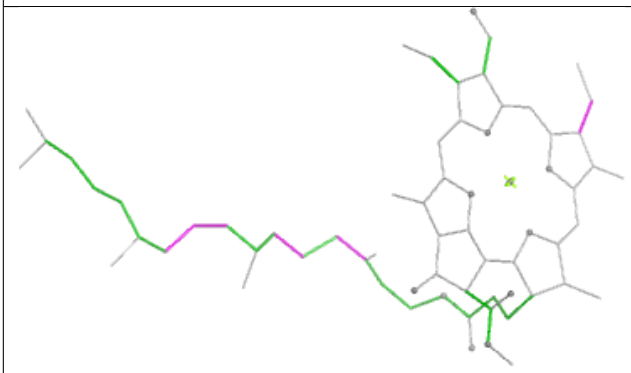
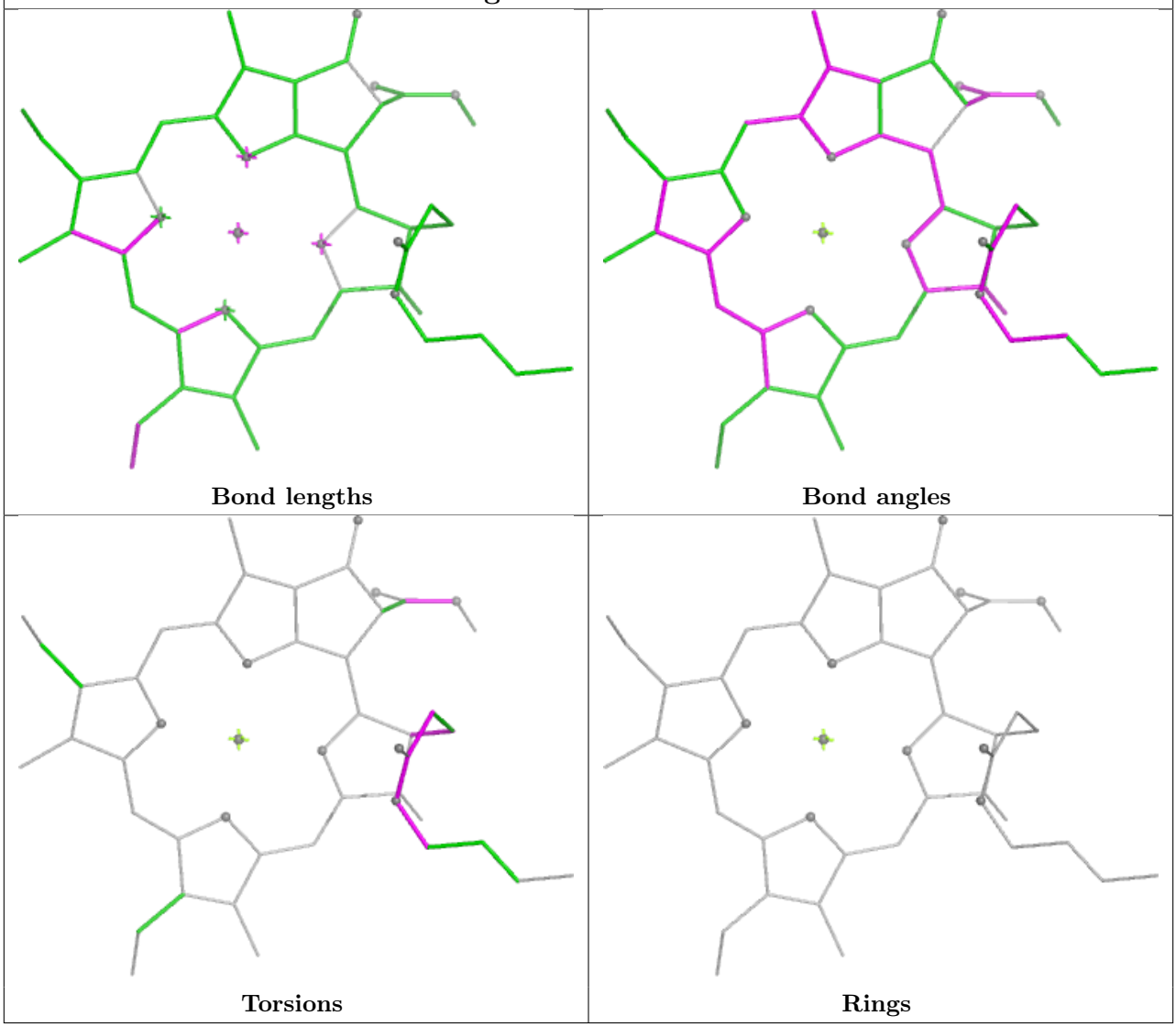


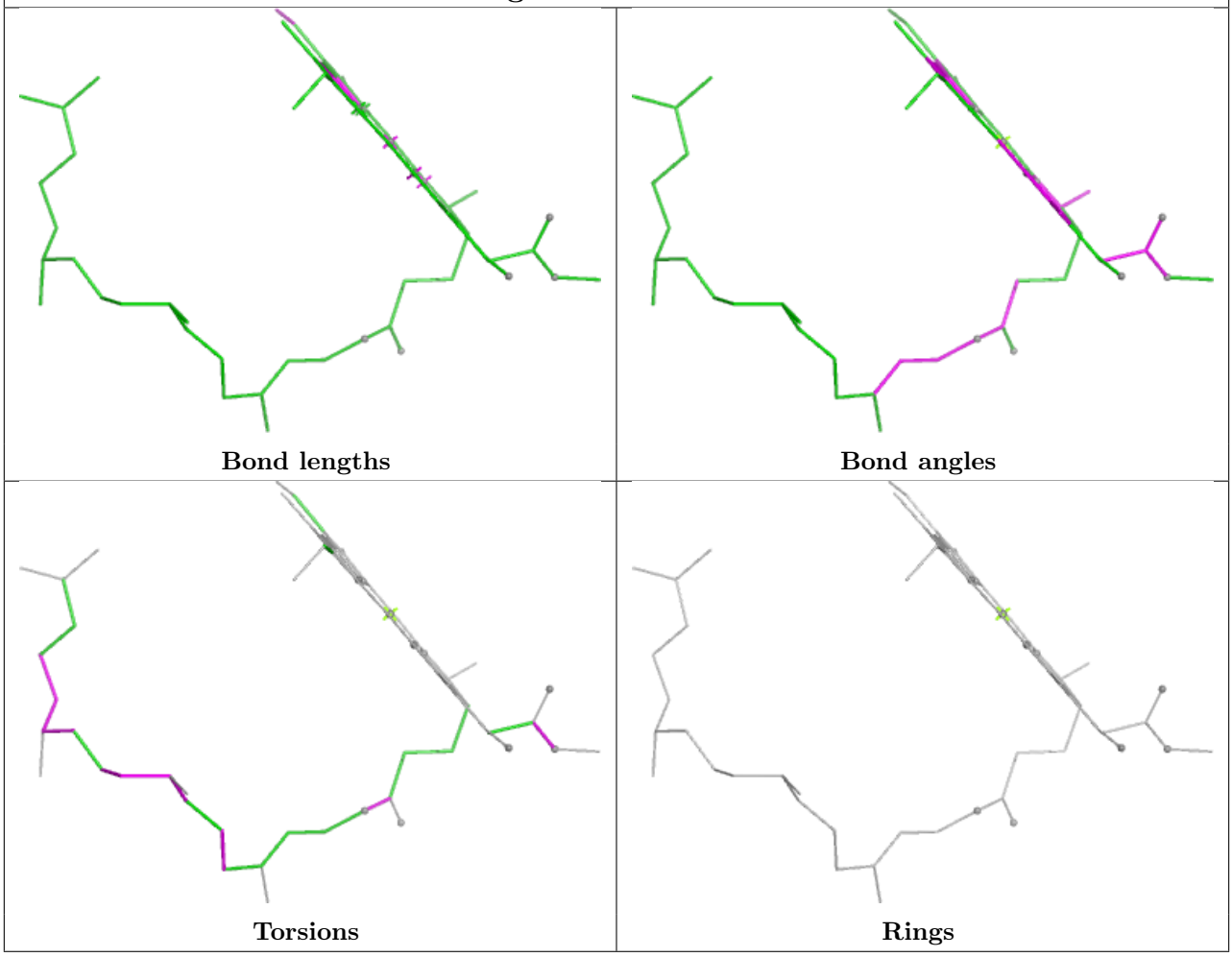
Rings

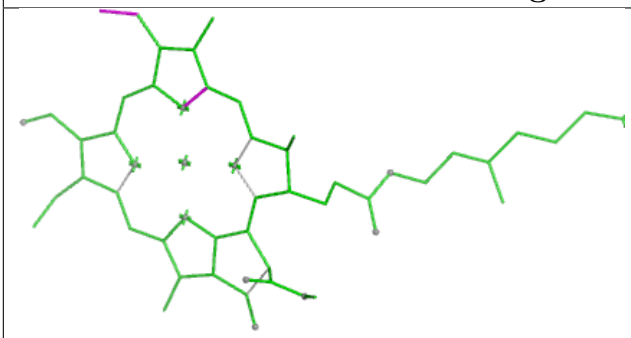
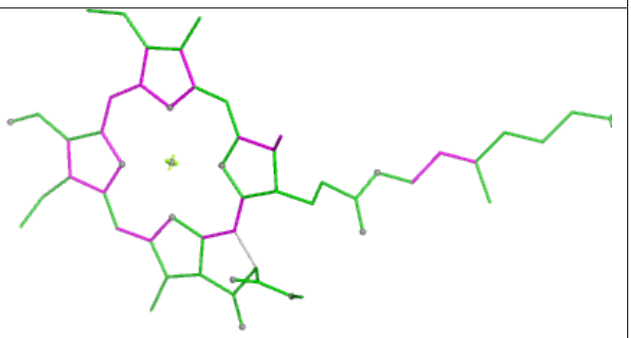
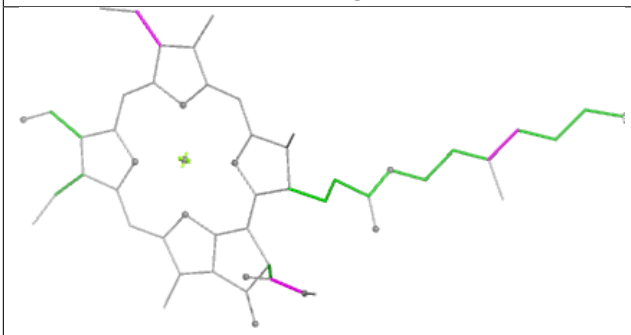
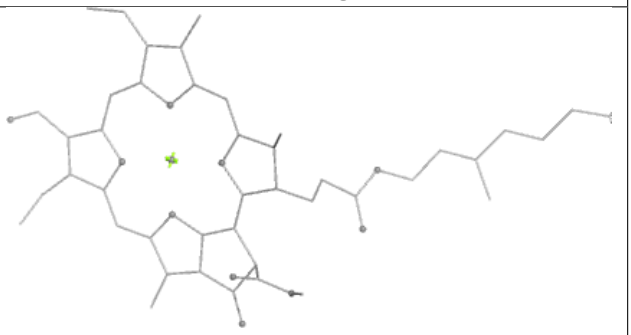
Ligand CHL y 609	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA n 315

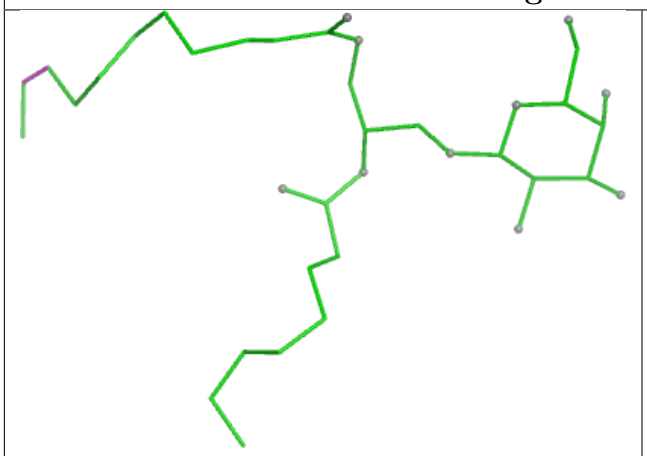


Ligand CLA b 612



Ligand CHL r 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG a 416



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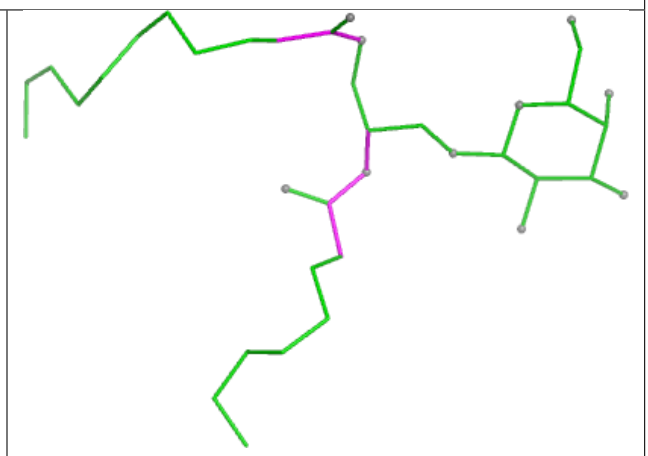
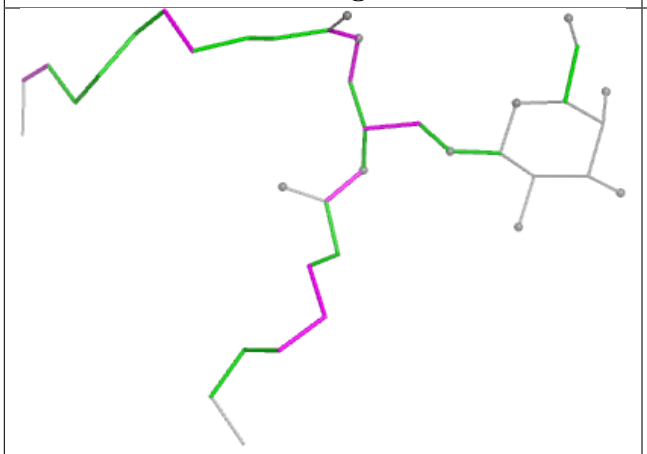


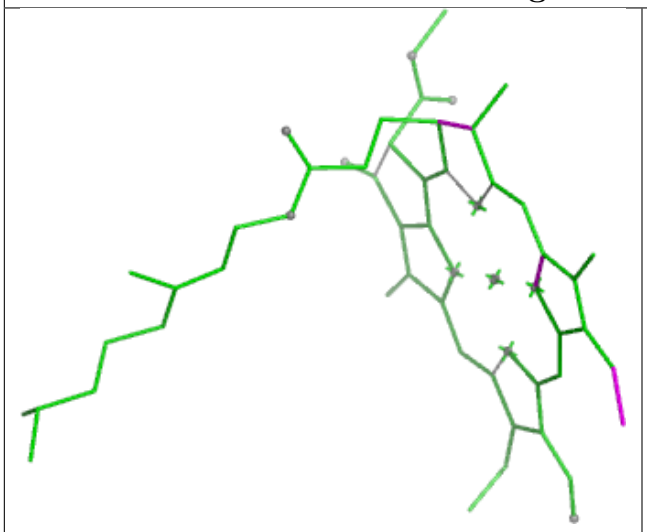
Bond angles



Torsions

Rings

Ligand CHL 5 609



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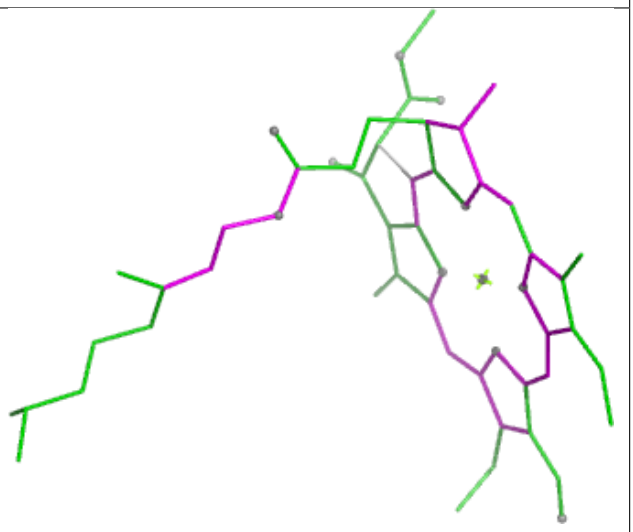

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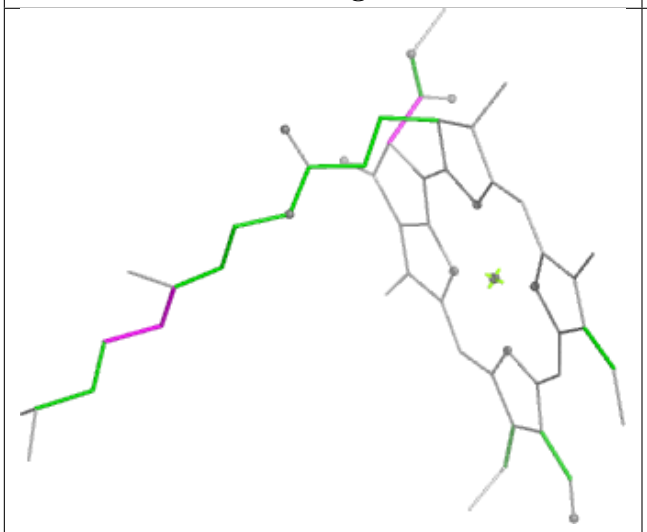

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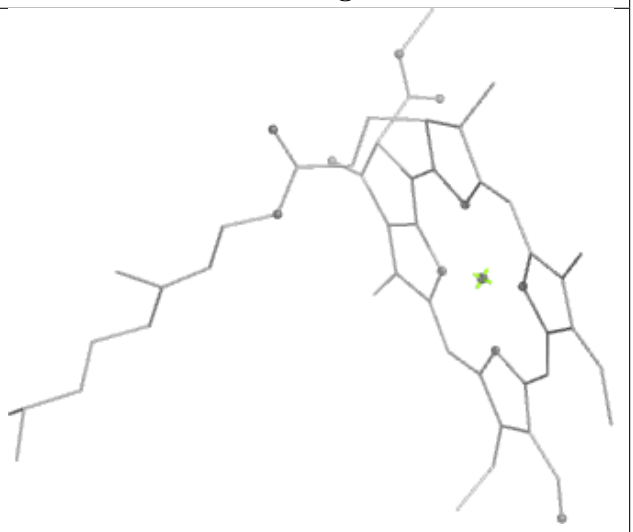
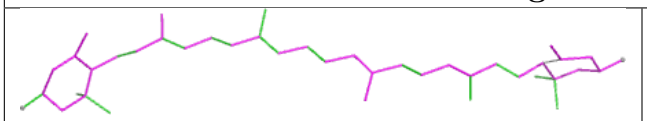


Rings

Ligand LUT n 317



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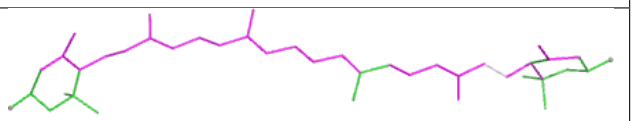

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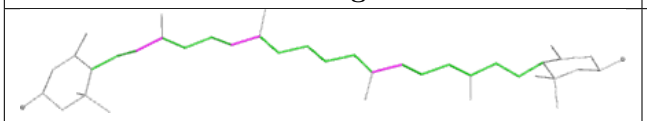

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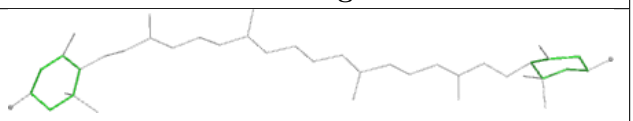
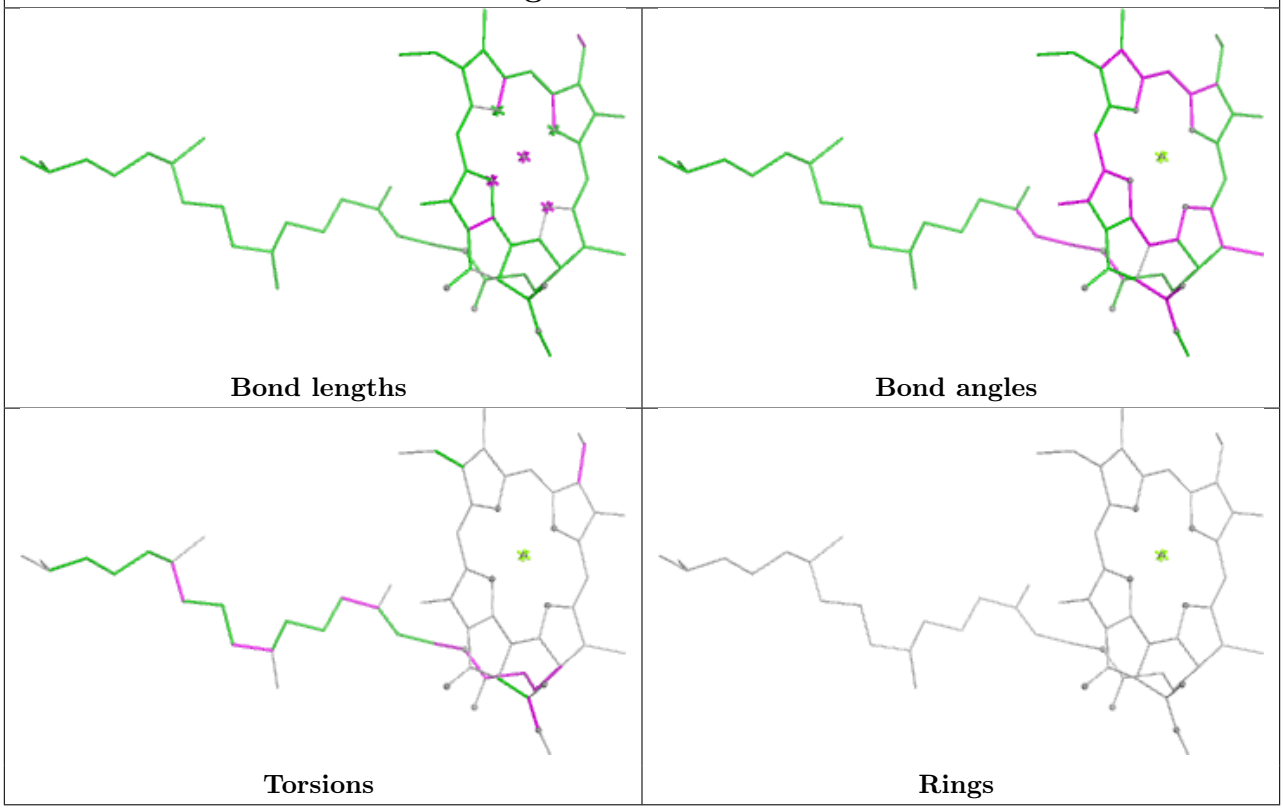
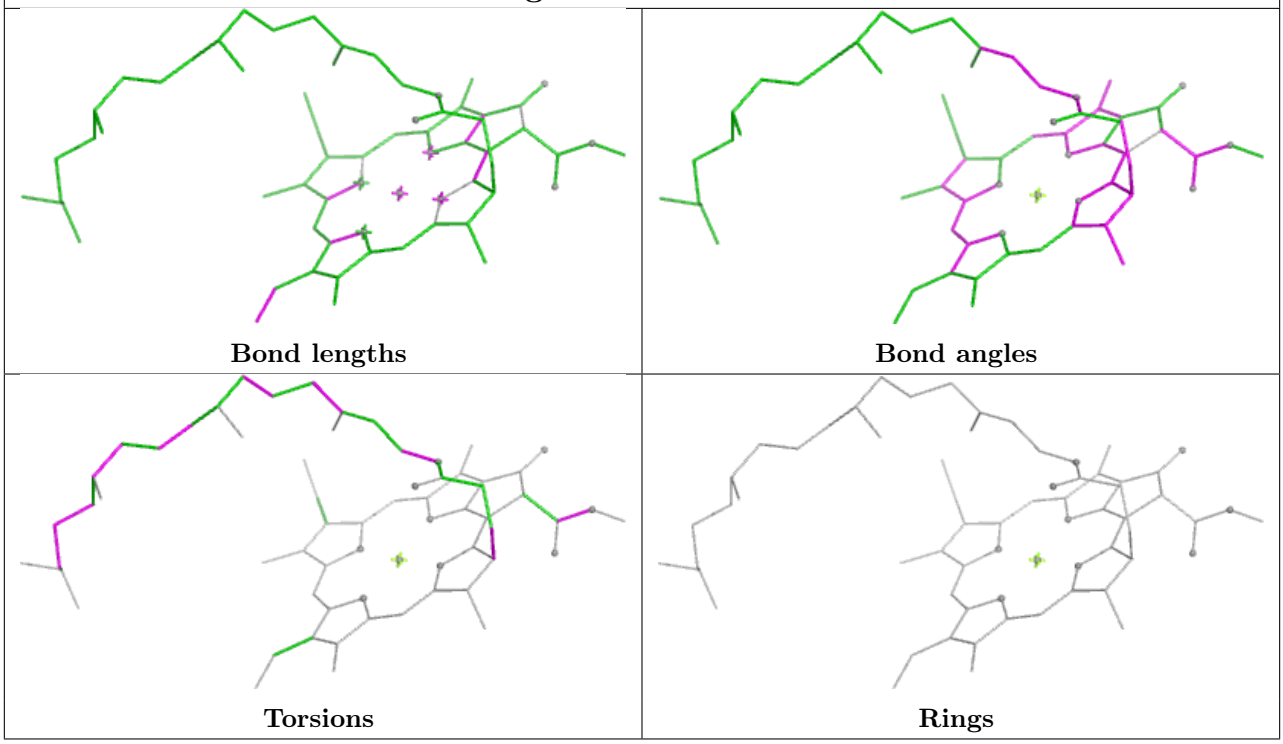


Rings

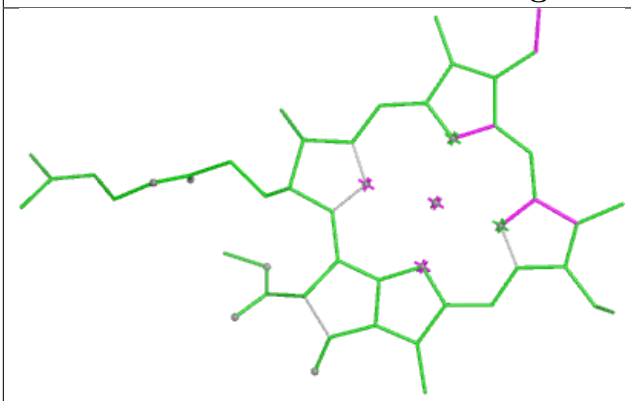
Ligand CLA Y 311



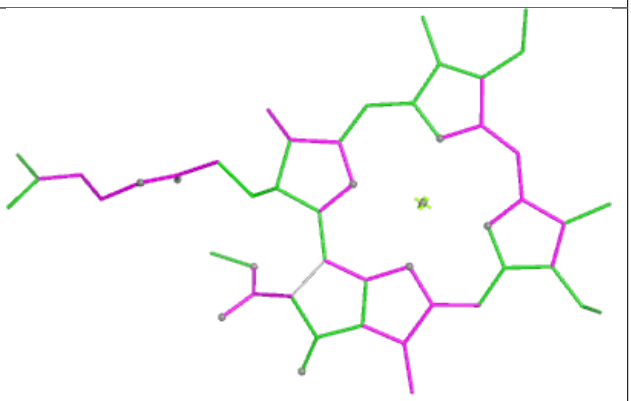
Ligand CLA C 613



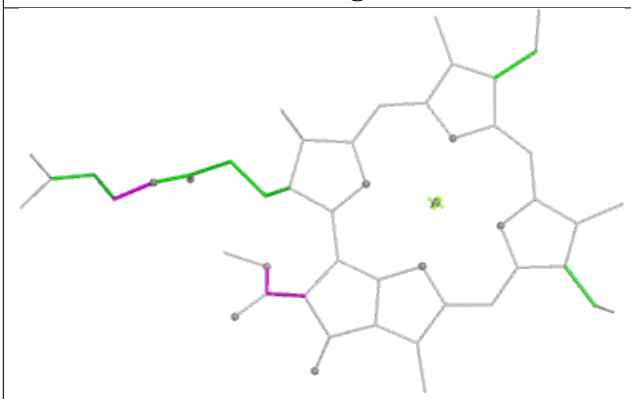
Ligand CLA s 306



Bond lengths



Bond angles



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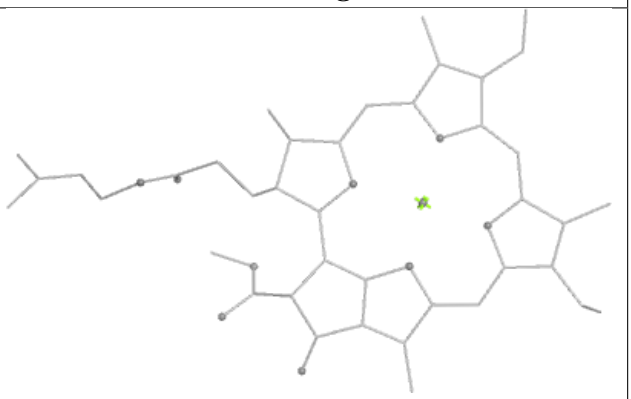
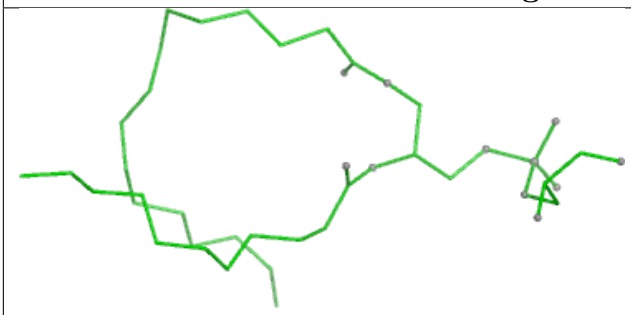
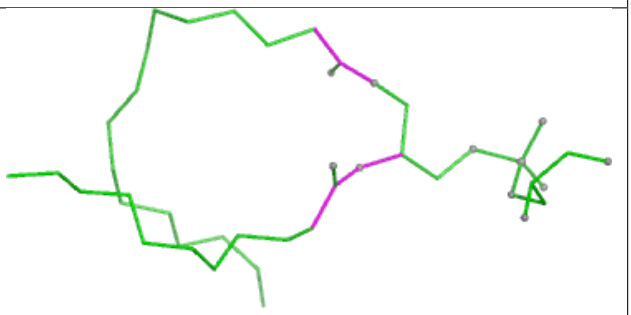


Rings

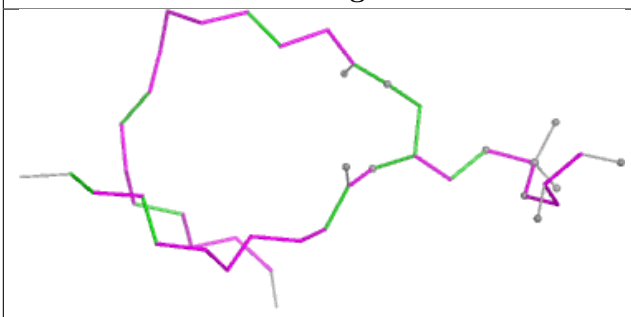
Ligand LHG D 407



Bond lengths



Bond angles



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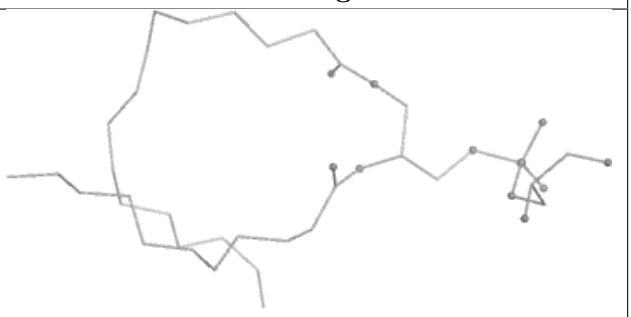
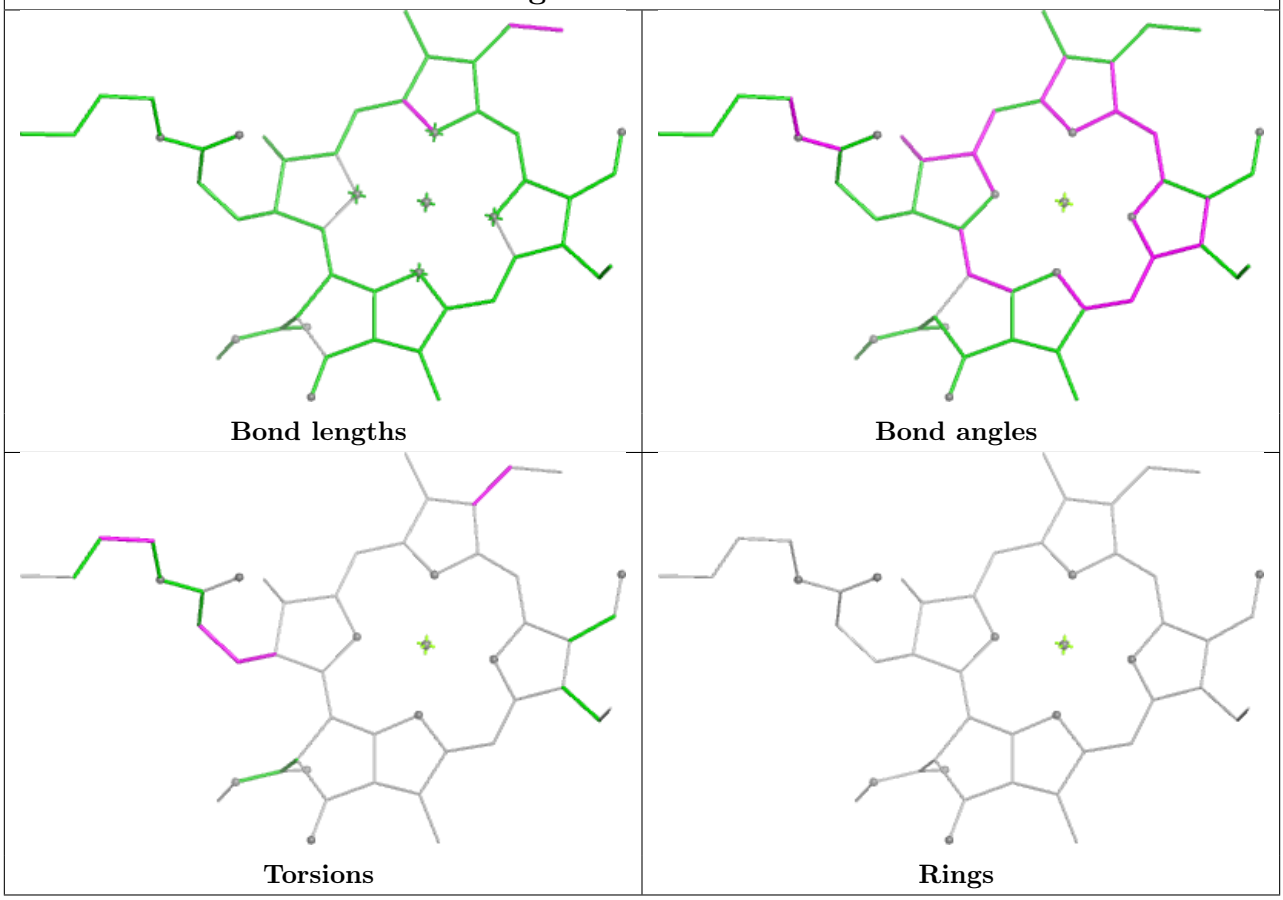
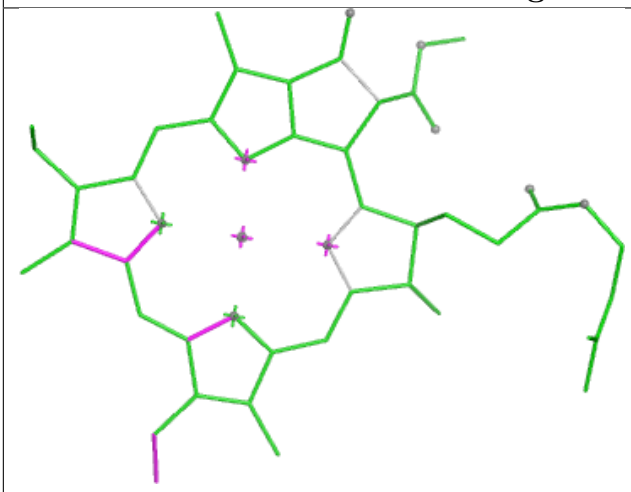


Rings

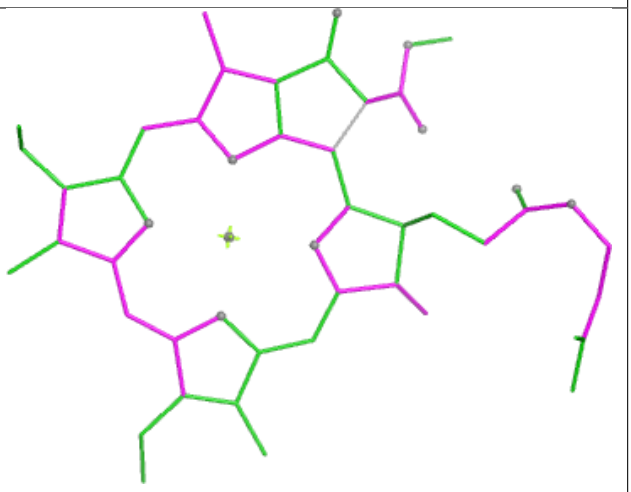
Ligand CHL 4 608



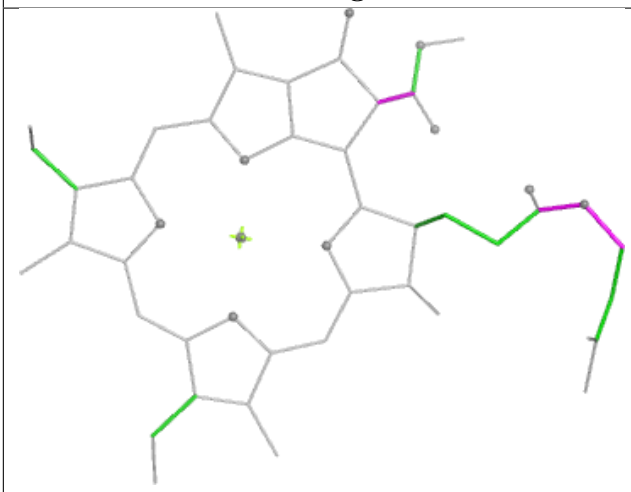
Ligand CLA S 306



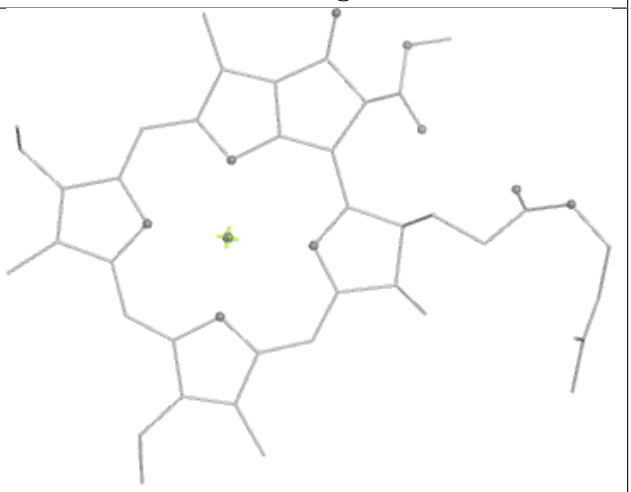
Bond lengths



Bond angles

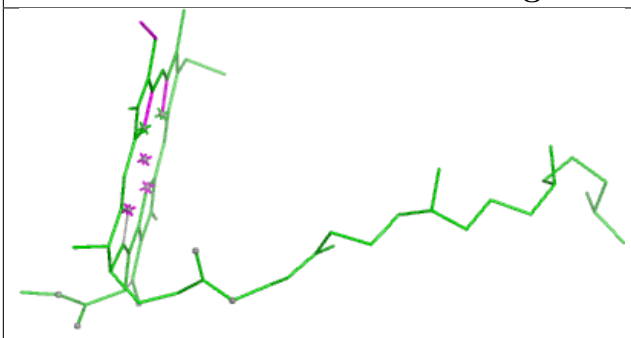


Torsions



Rings

Ligand CLA N 305



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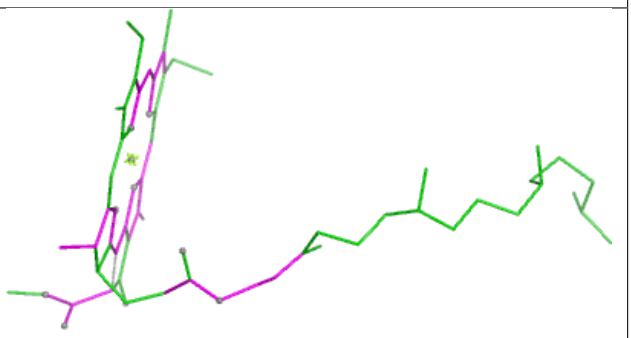
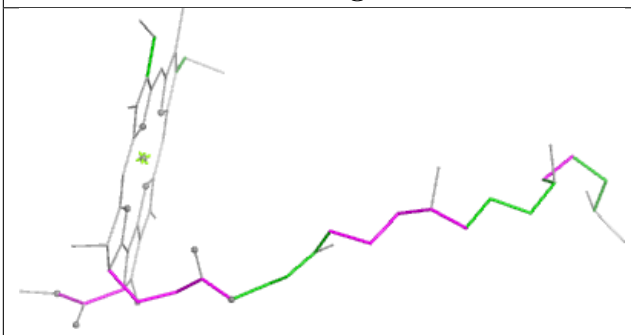
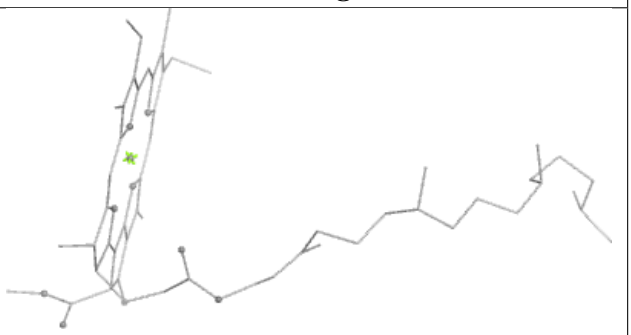


Bond angles

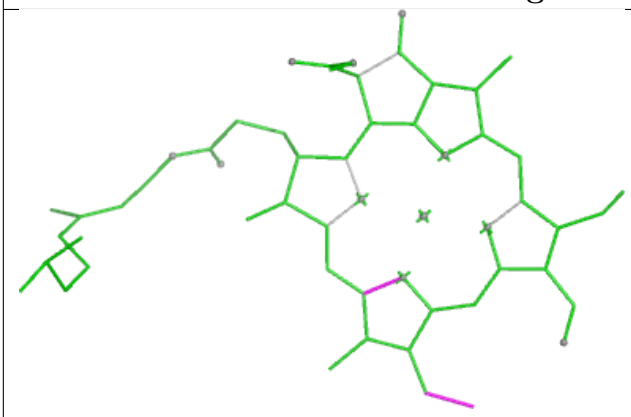


Torsions

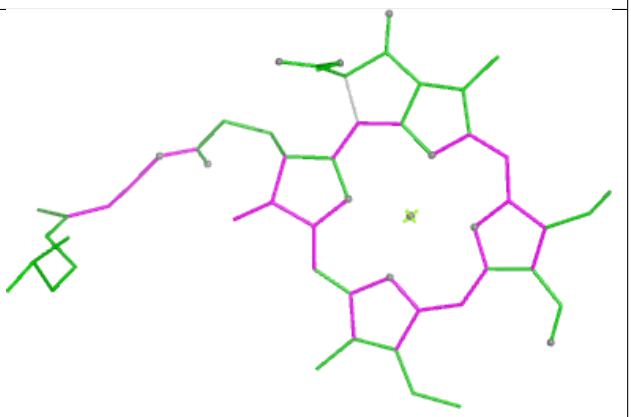


Rings

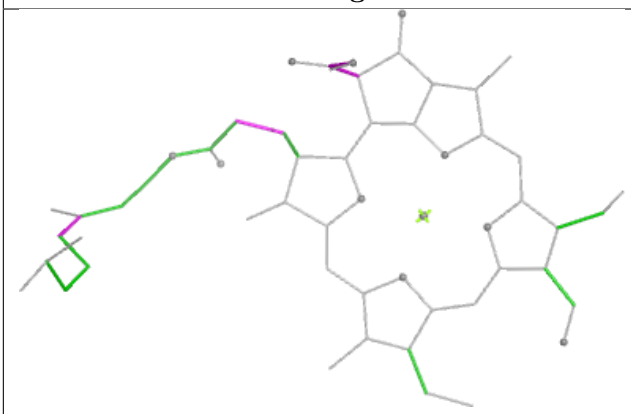
Ligand CHL n 302



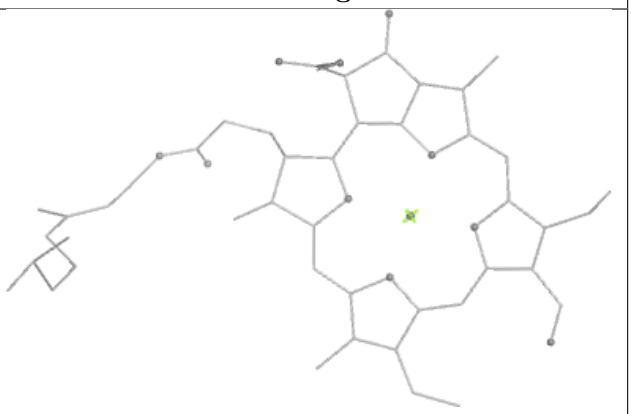
Bond lengths



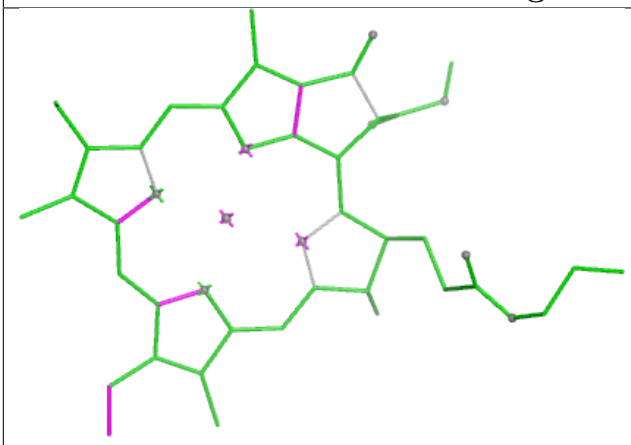
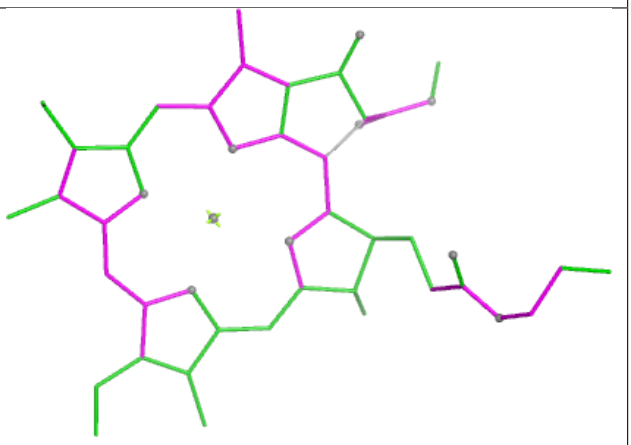
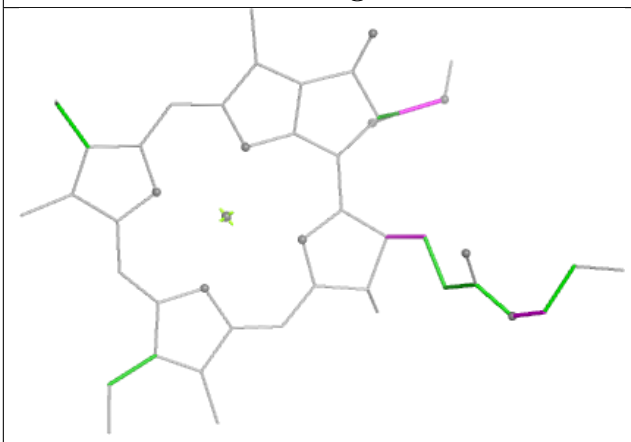
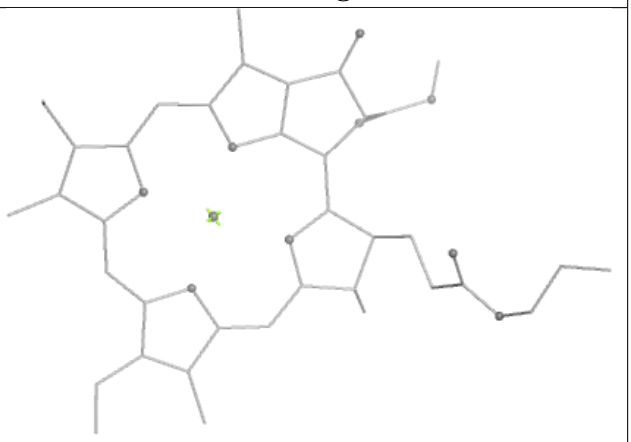
Bond angles



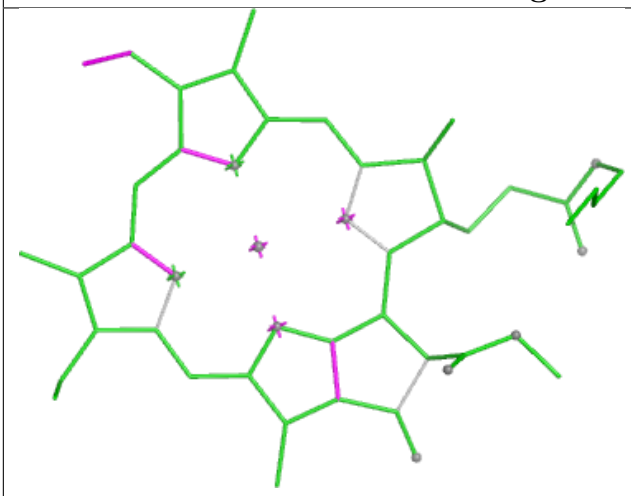
Torsions



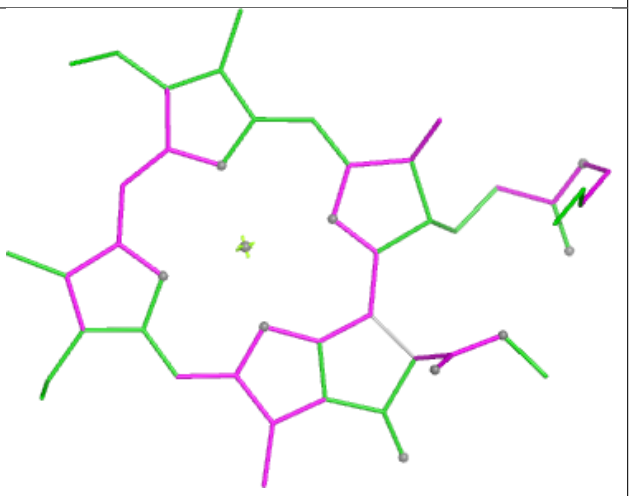
Rings

Ligand CLA S 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

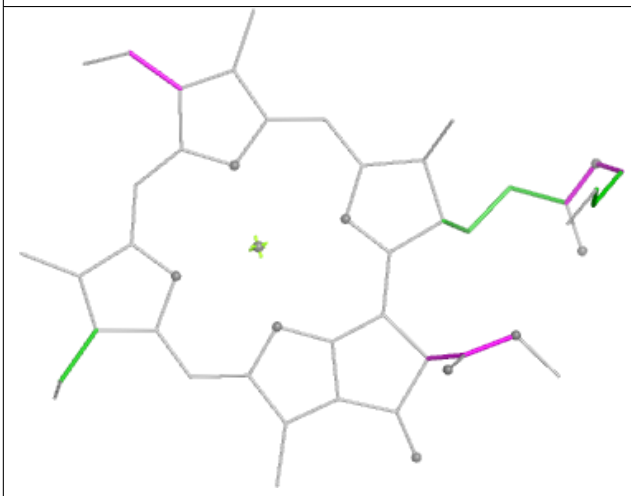
Ligand CLA r 314



Bond lengths



Bond angles



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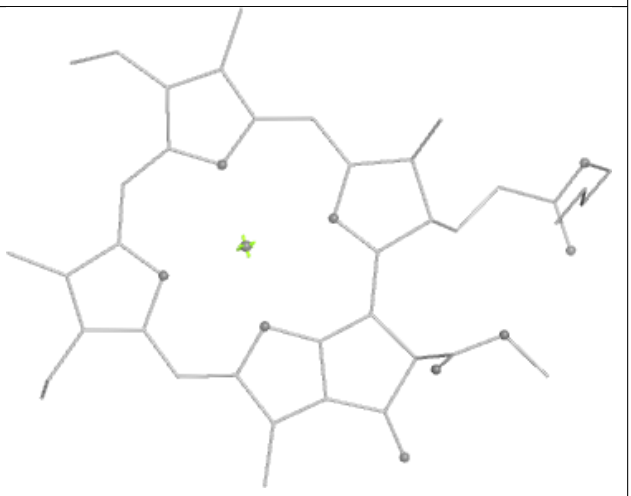
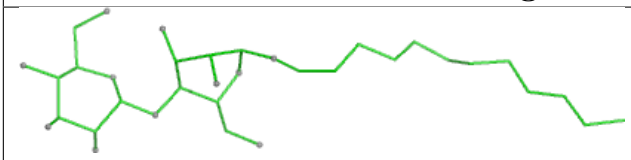


Rings

Ligand LMU R 302



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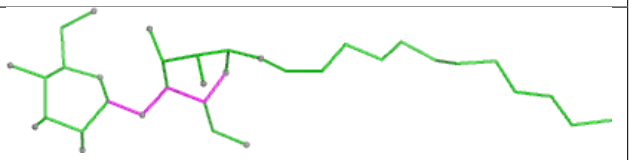
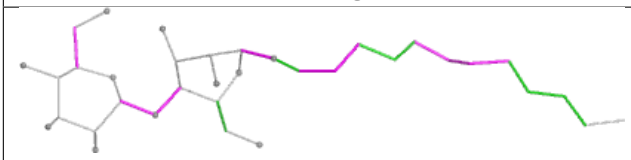


Bond angles



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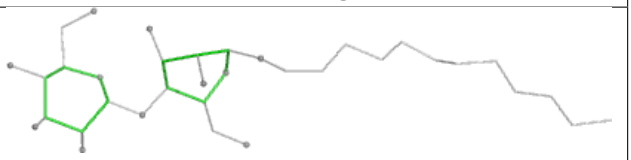
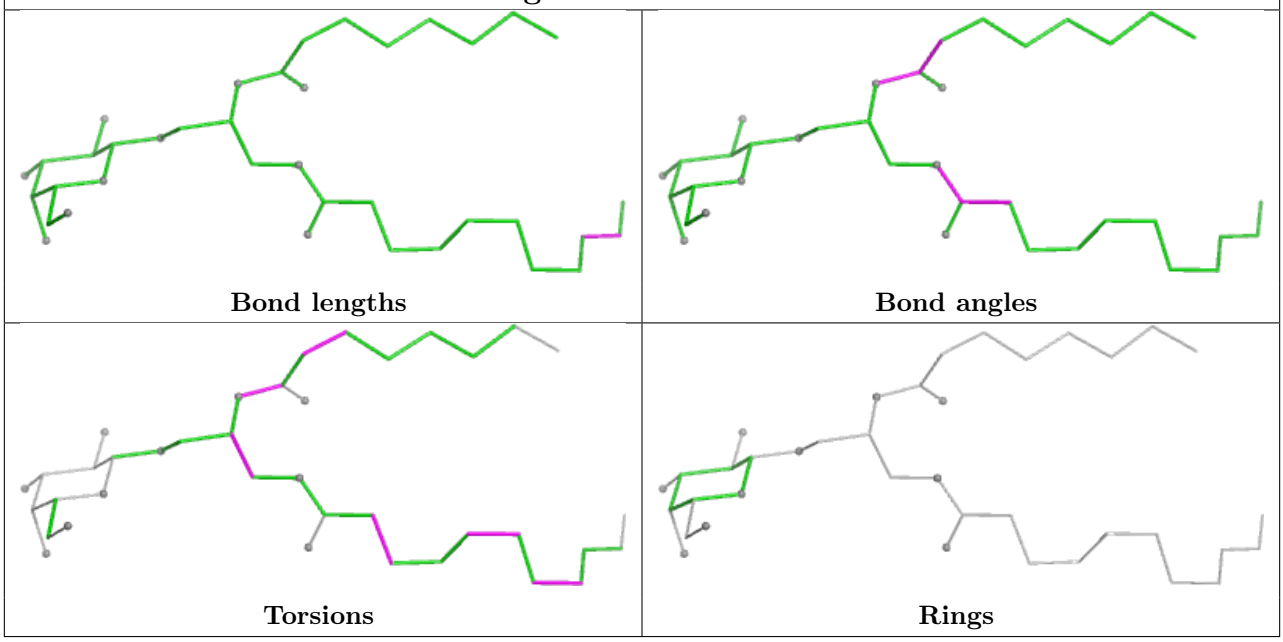
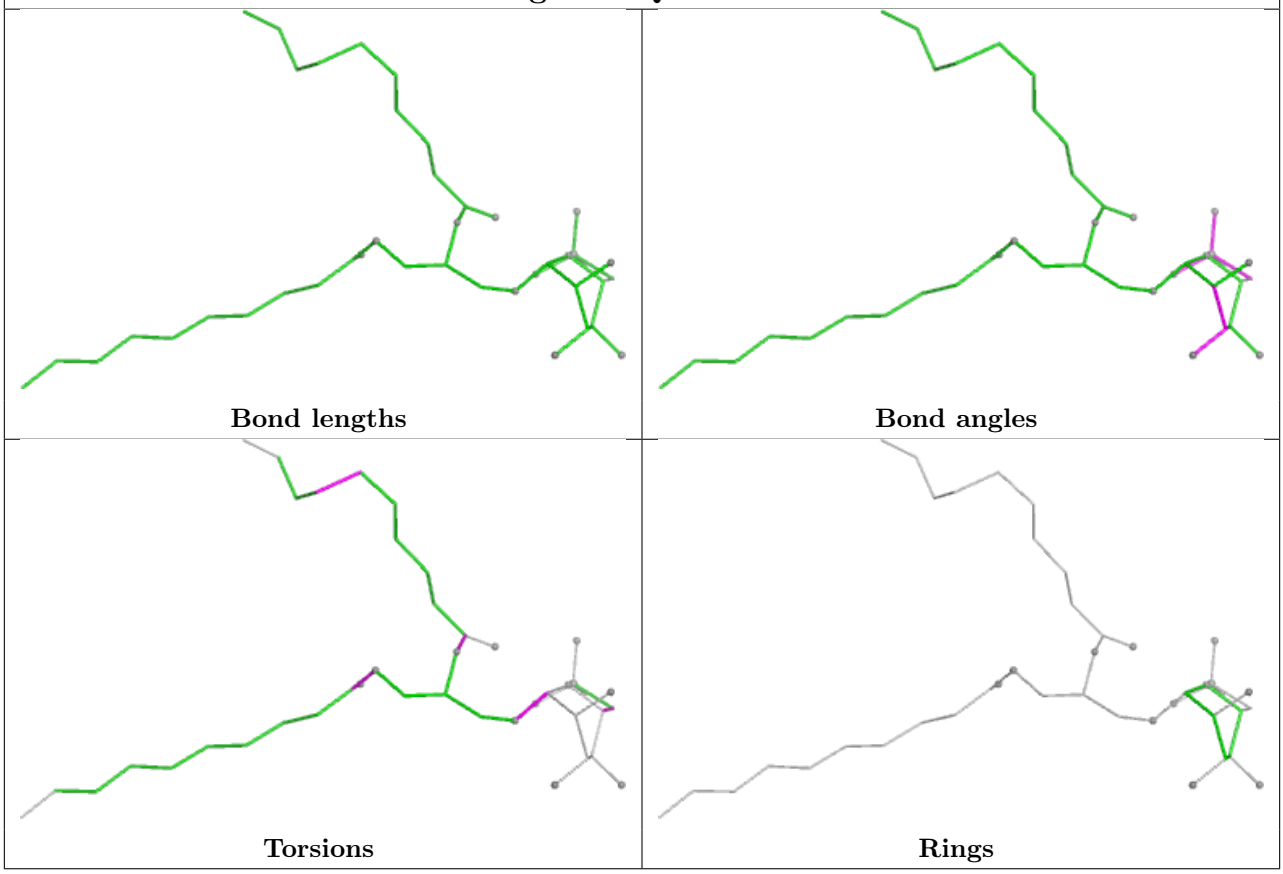


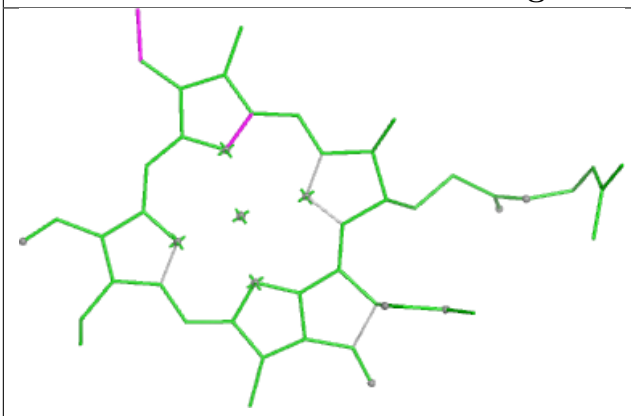
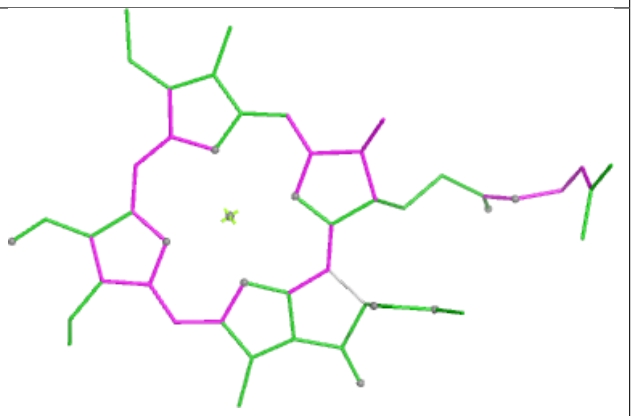
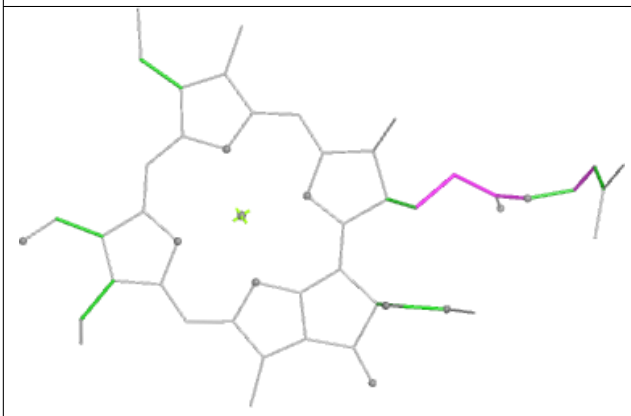
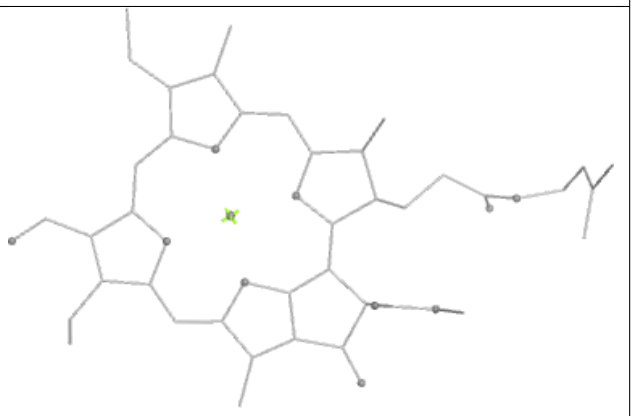
Rings

Ligand LMG b 623

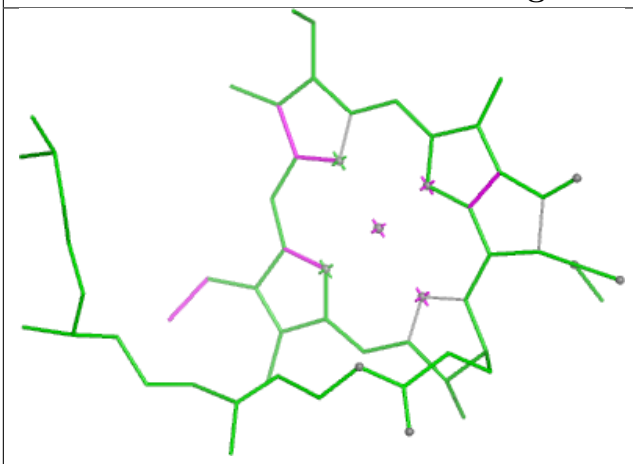


Ligand SQD 0 621

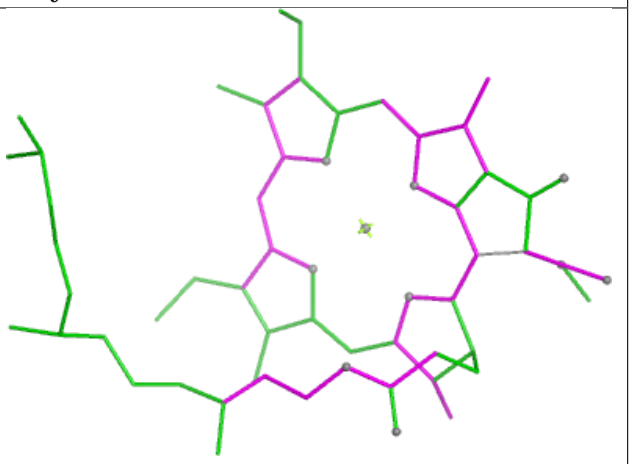


Ligand CHL 2 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

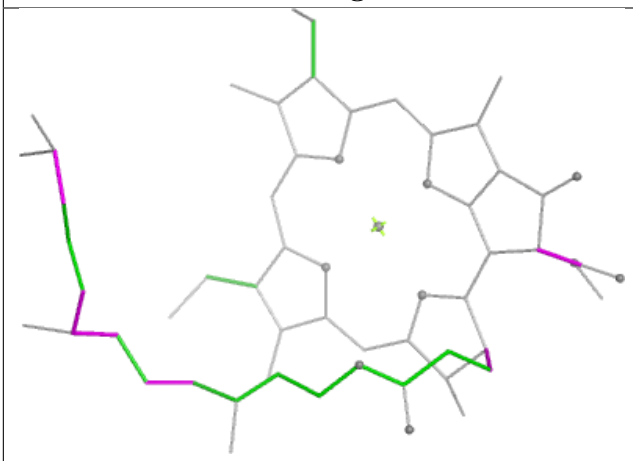
Ligand CLA y 602



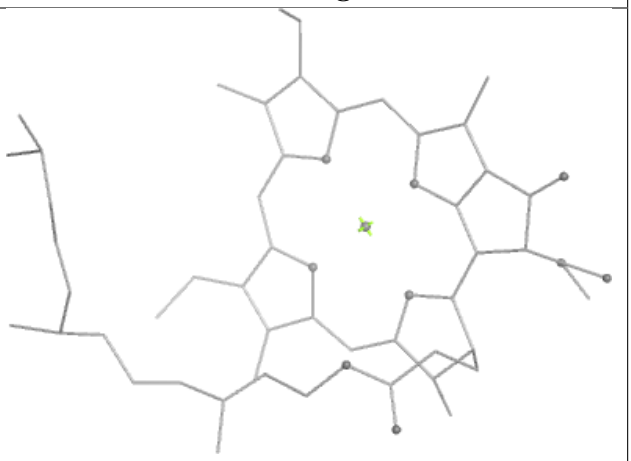
Bond lengths



Bond angles

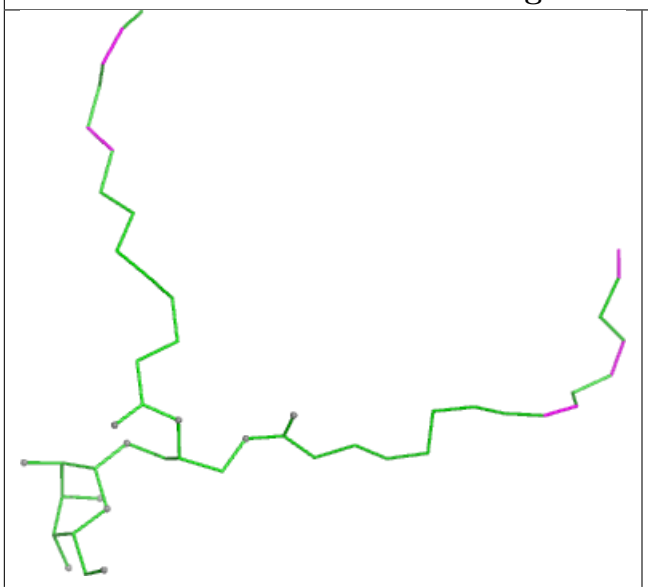


Torsions

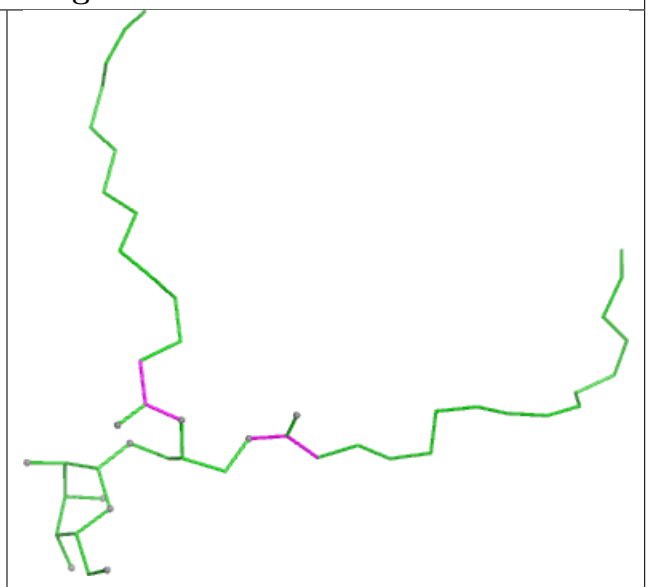


Rings

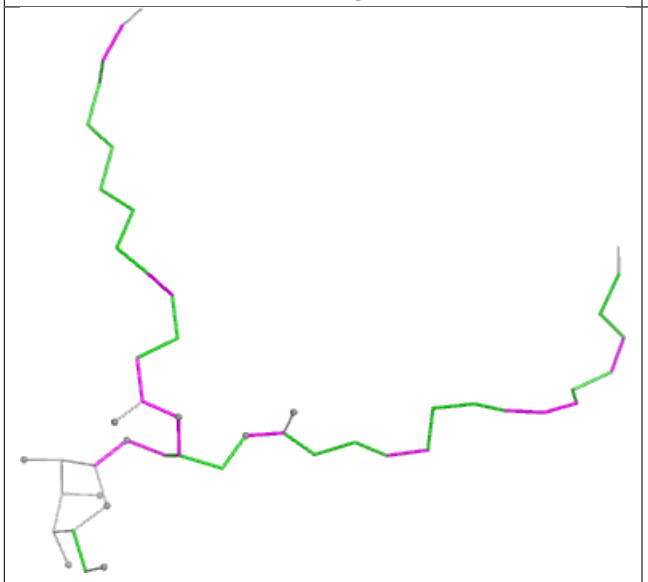
Ligand LMG g 322



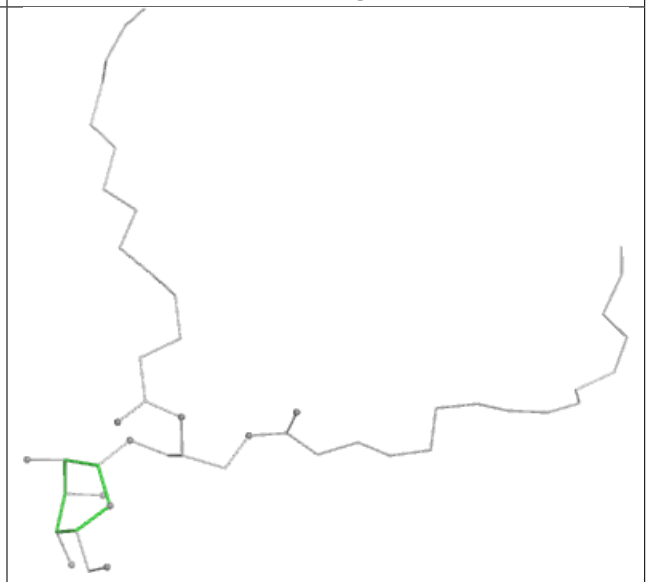
Bond lengths



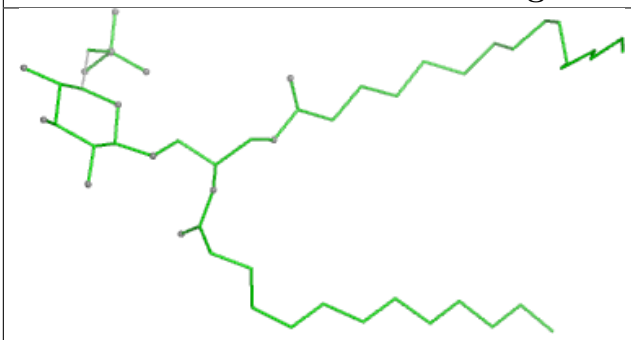
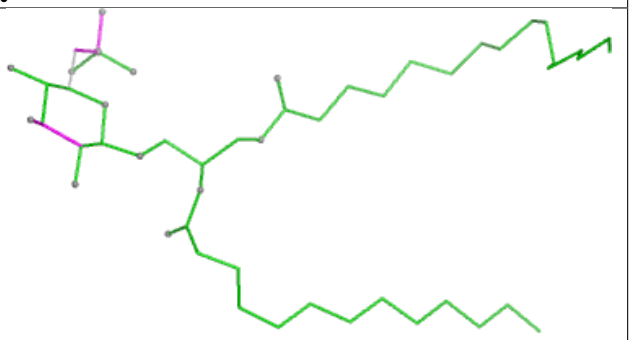
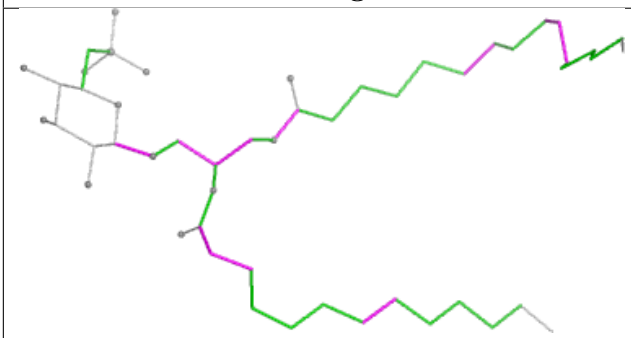
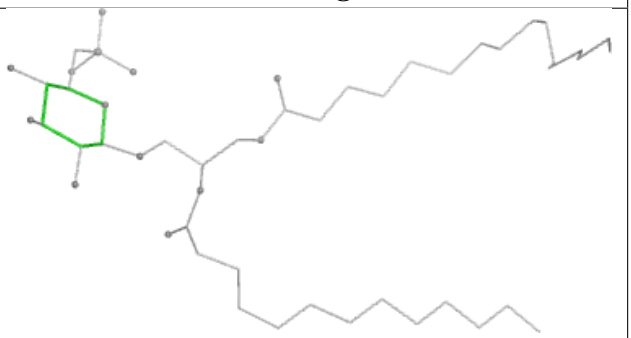
Bond angles



Torsions

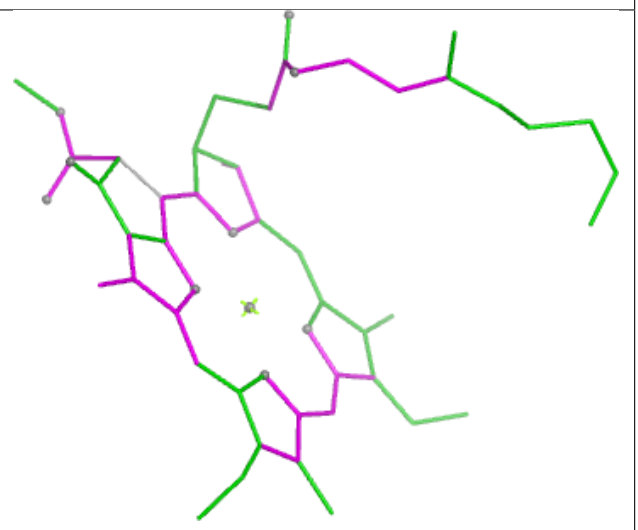


Rings

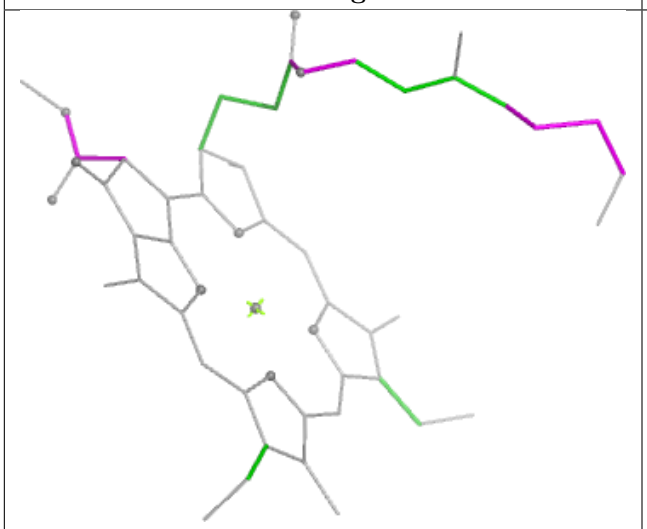
Ligand SQD S 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 316

Bond lengths



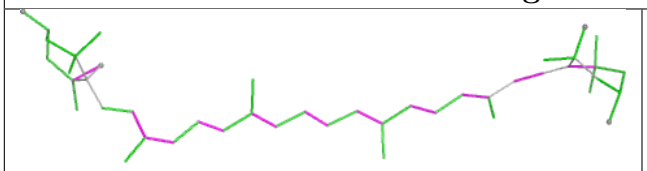
Bond angles



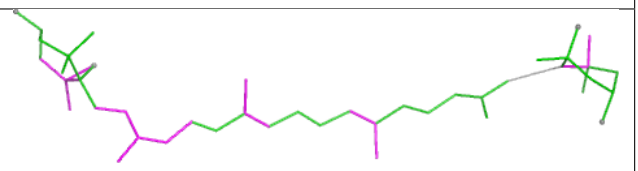
Torsions

Rings

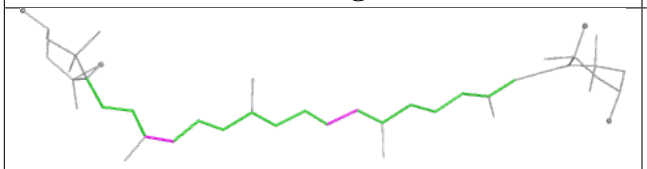
Ligand NEX R 301



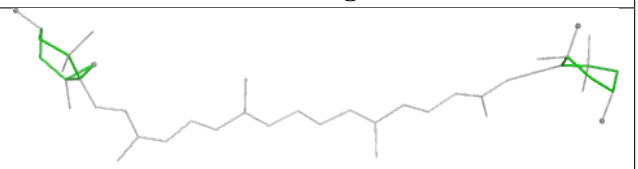
Bond lengths



Bond angles

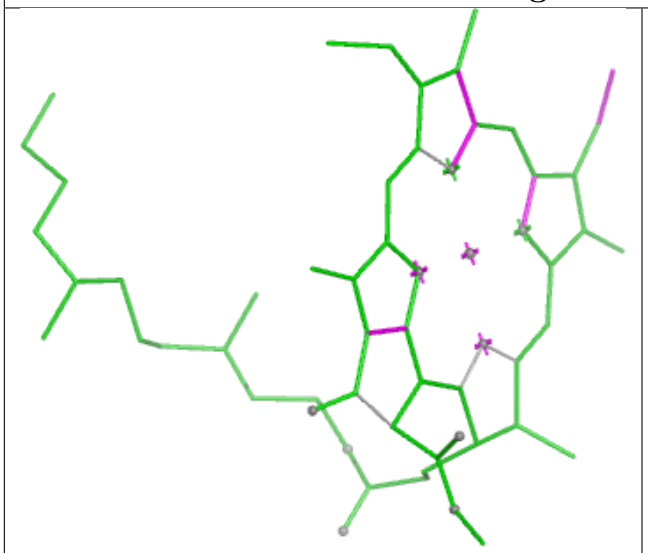


Torsions

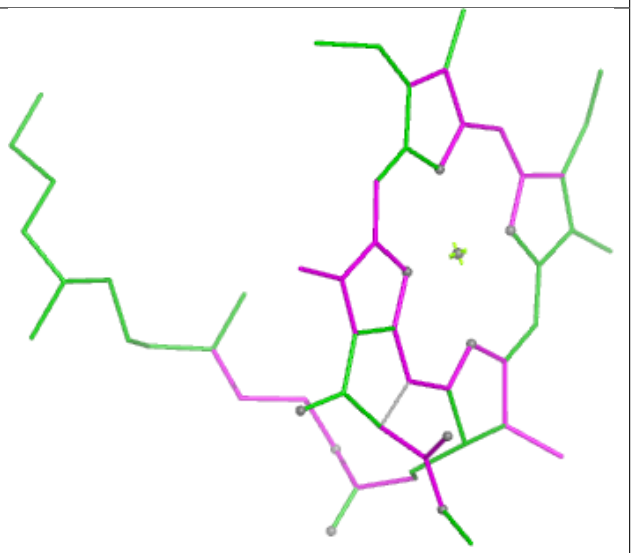


Rings

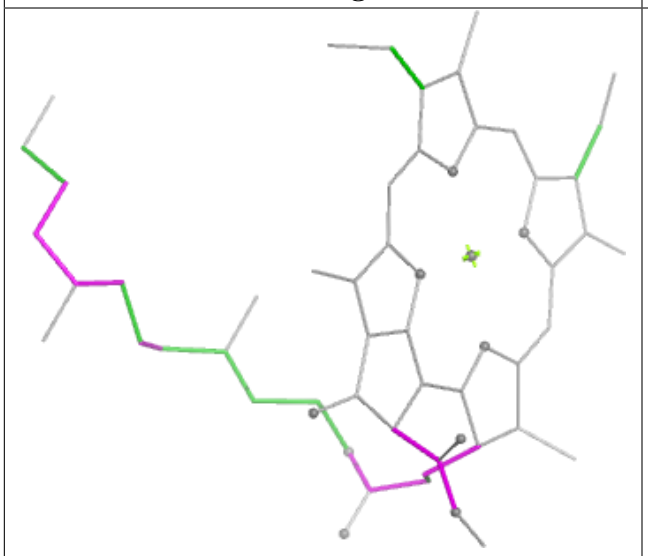
Ligand CLA 5 611



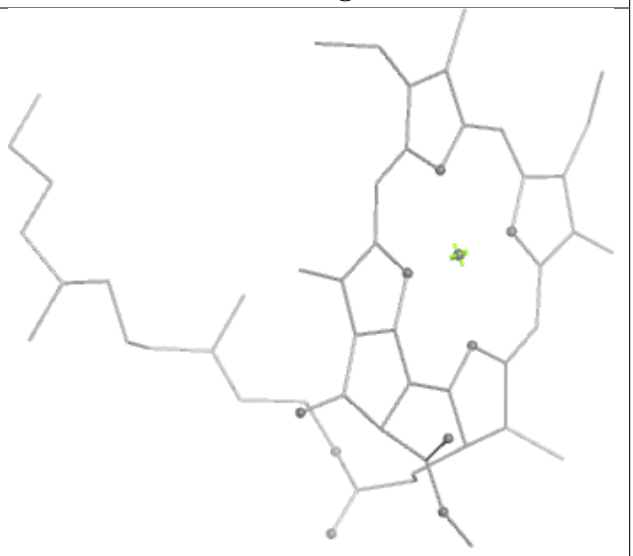
Bond lengths



Bond angles

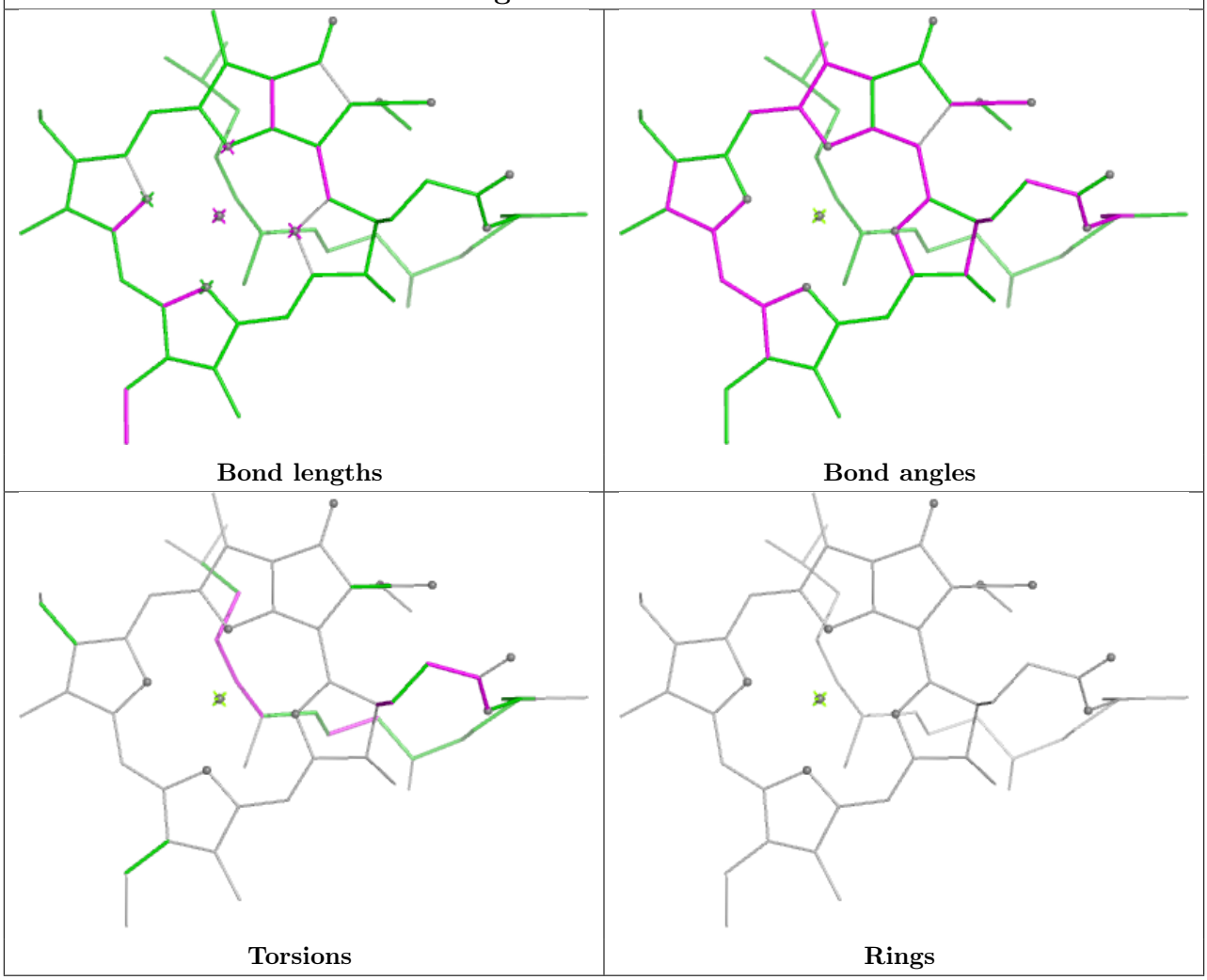


Torsions

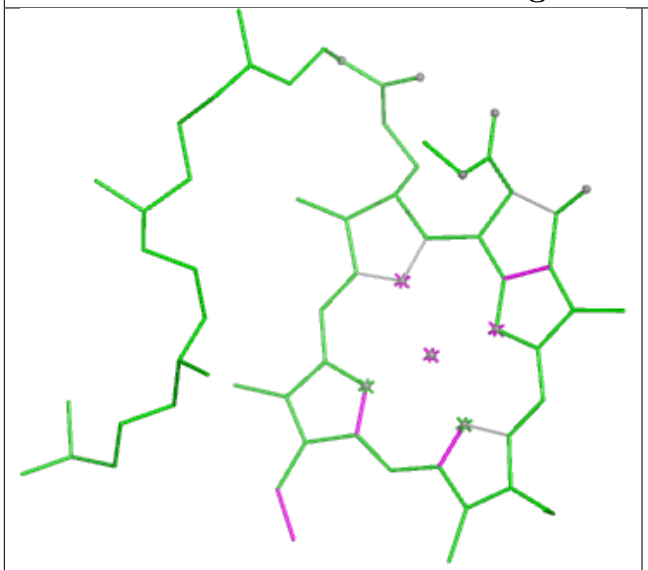


Rings

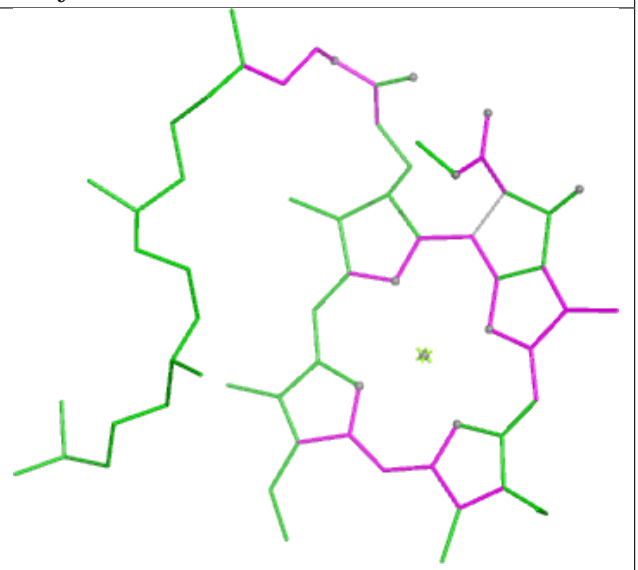
Ligand CLA C 610



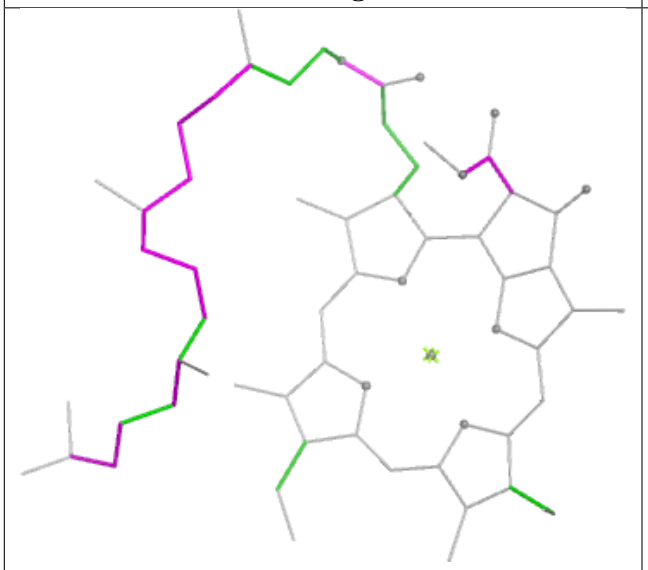
Ligand CLA y 612



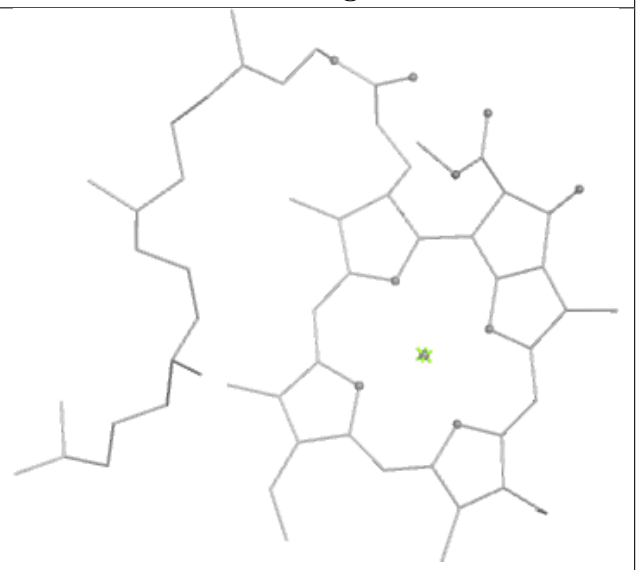
Bond lengths



Bond angles

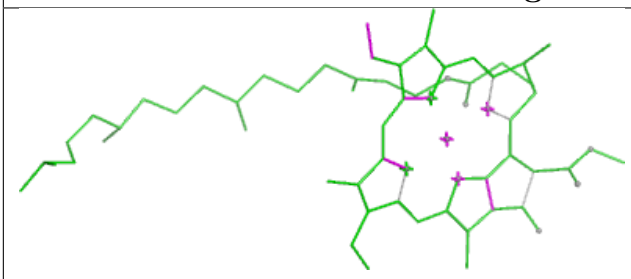


Torsions

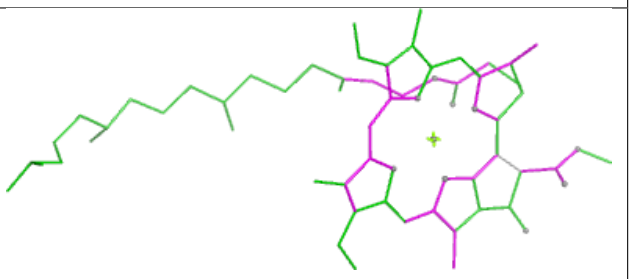


Rings

Ligand CLA B 608



Bond lengths



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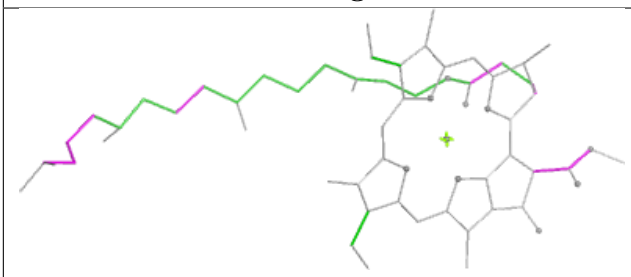
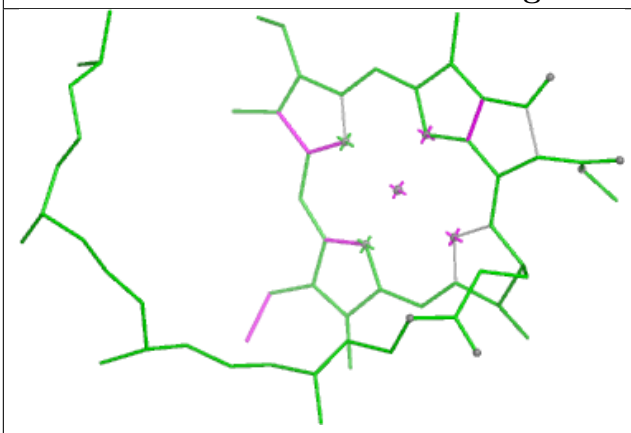


Torsions

Rings

Ligand CLA N 303



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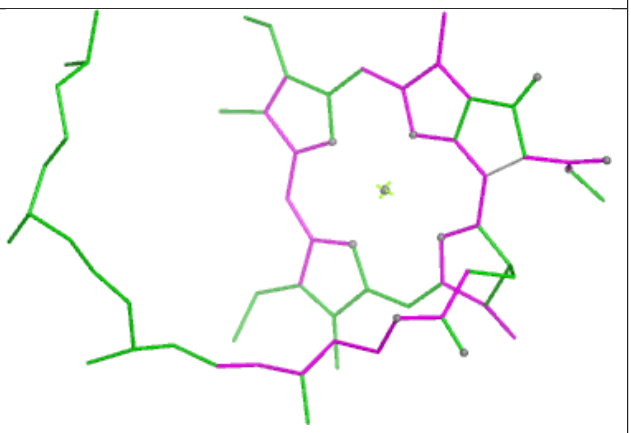

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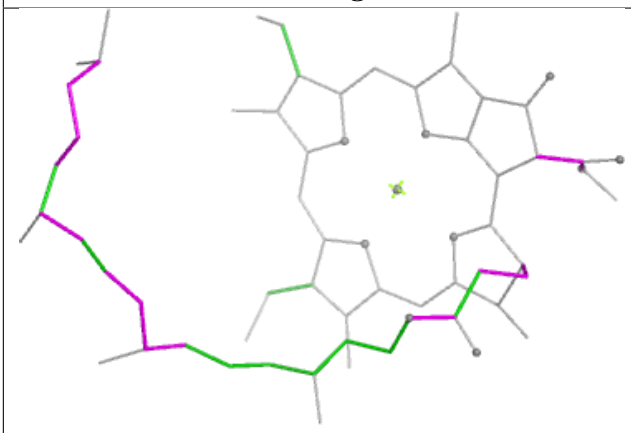

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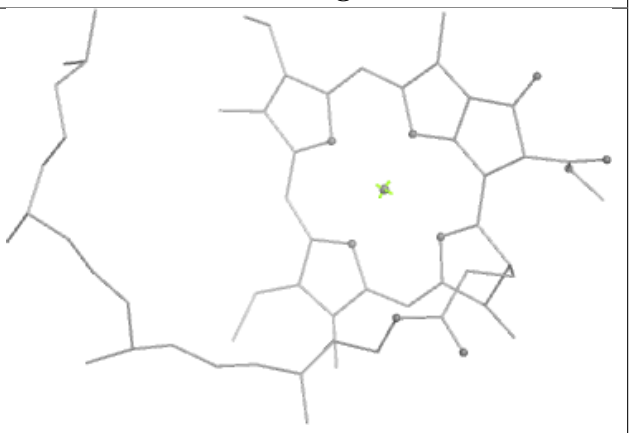
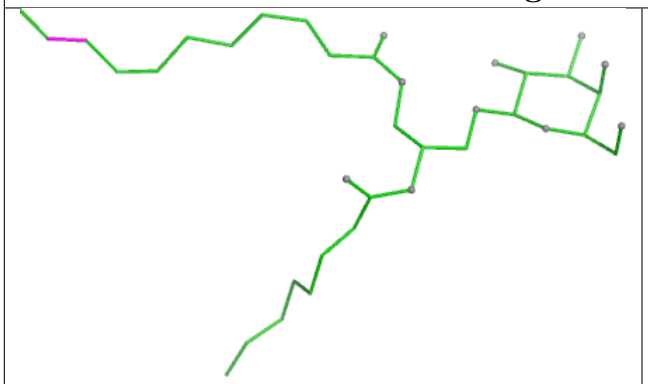


Rings

Ligand LMG 7 320



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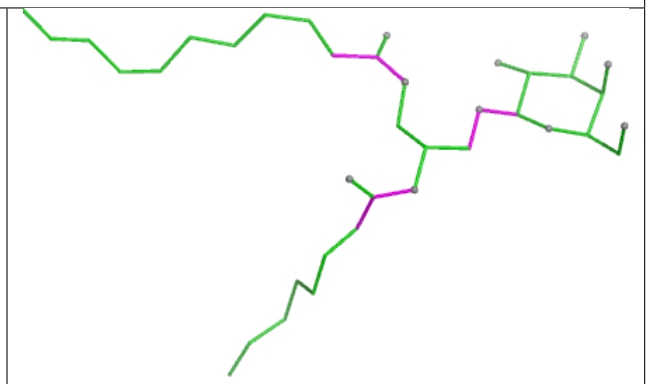
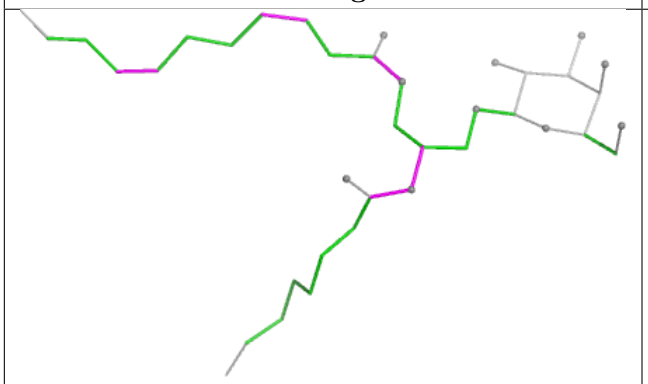


Bond angles



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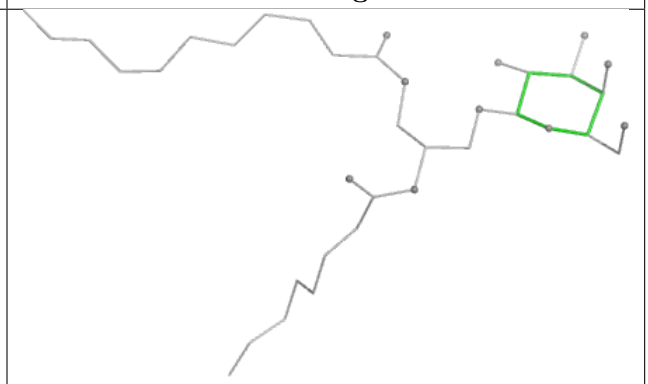
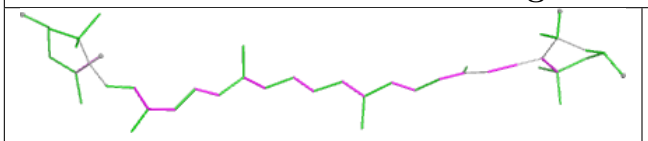


Rings

Ligand NEX 8 617



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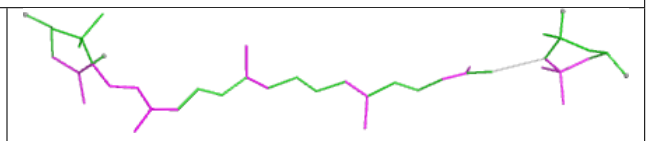

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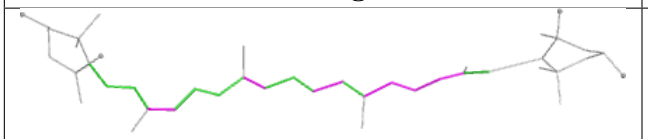

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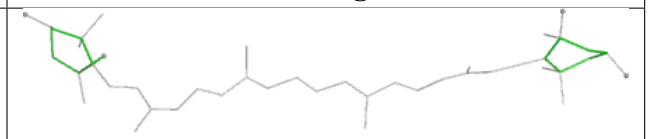
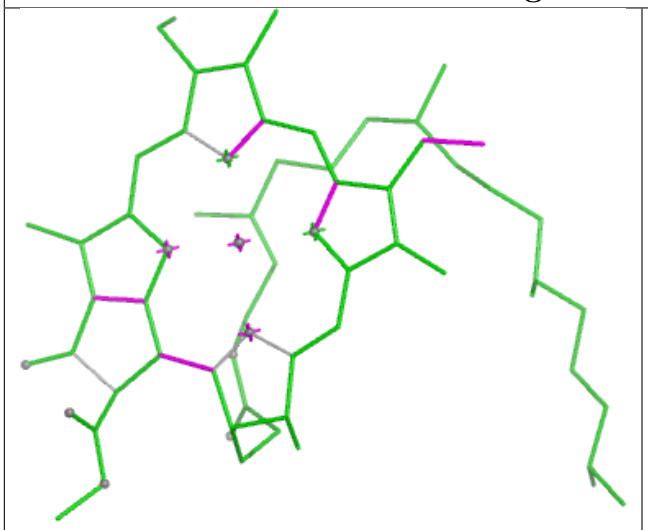


Rings

Ligand CLA Y 313



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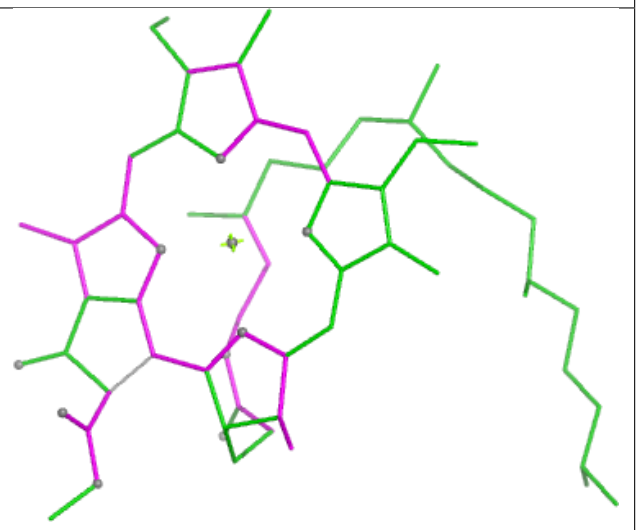

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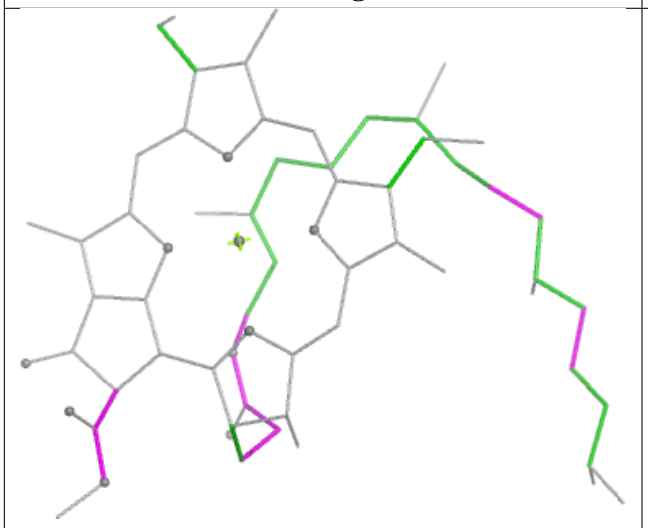
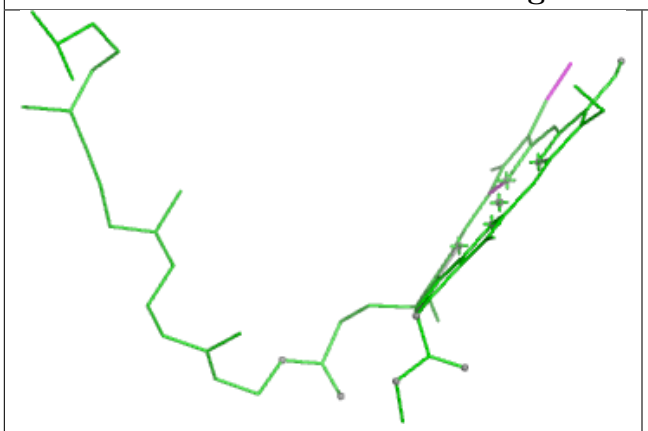


Torsions

Rings

Ligand CHL n 306



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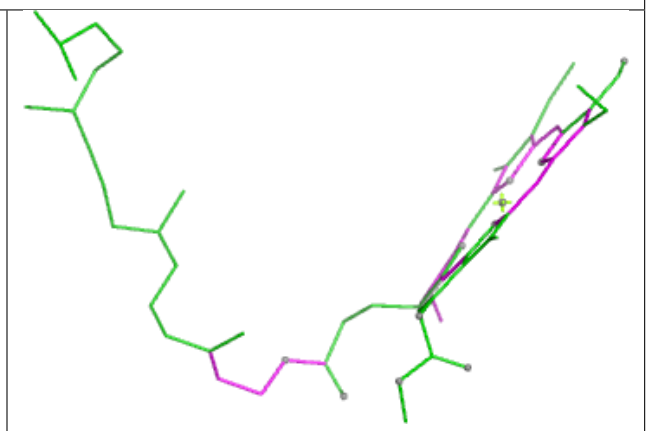

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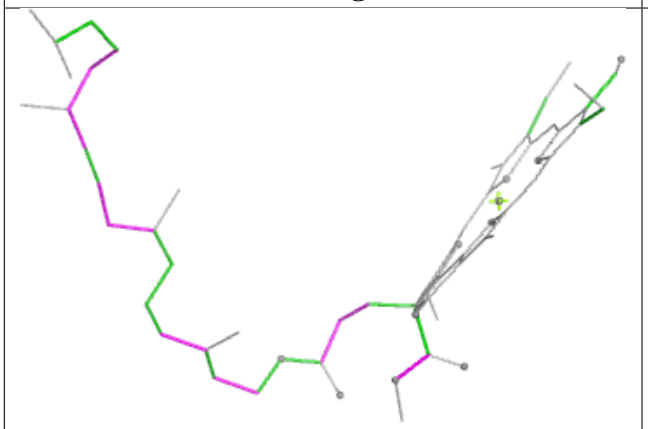

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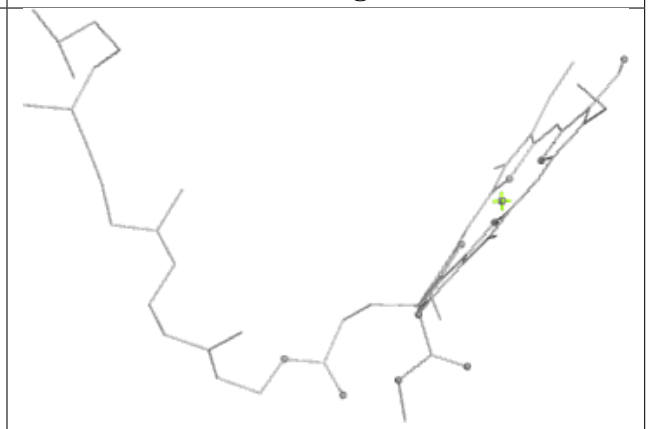
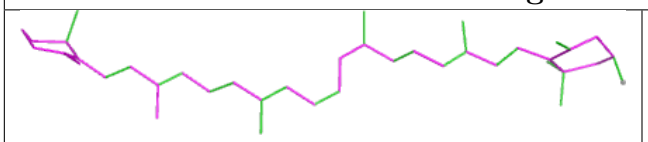


Rings

Ligand RRX 9 317



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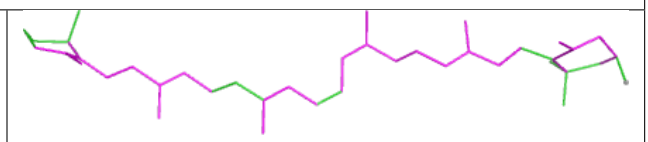

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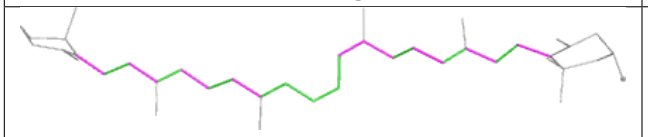

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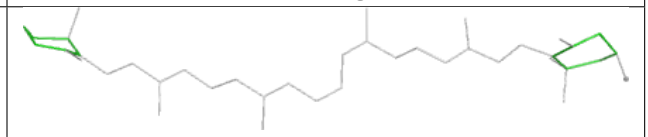
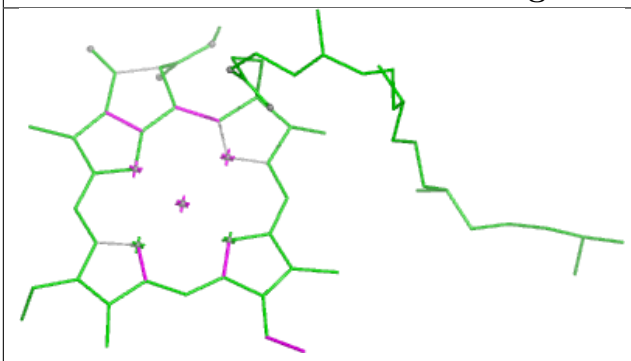


Rings

Ligand CLA a 407



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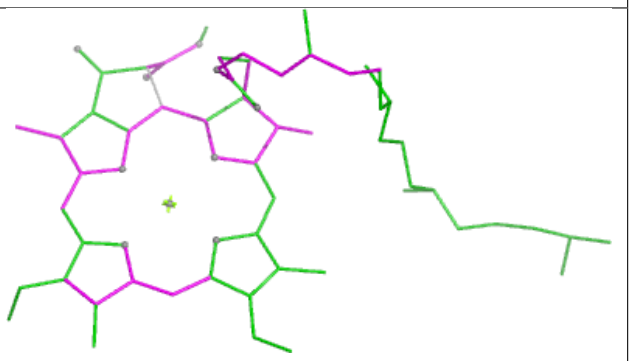

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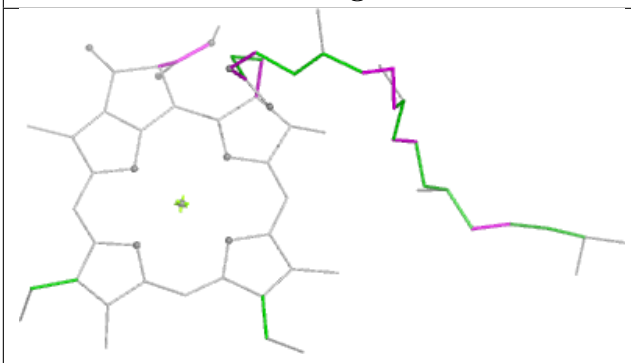

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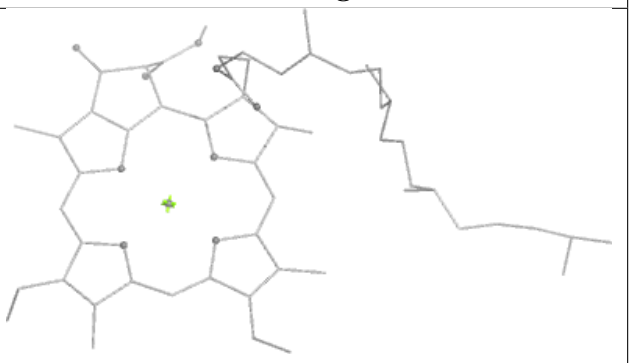
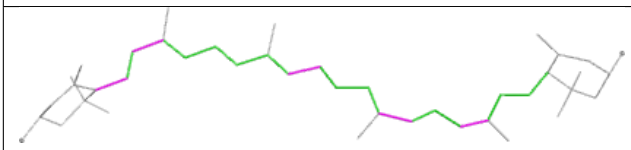


Rings

Ligand LUT p 617

Bond lengths

Bond angles



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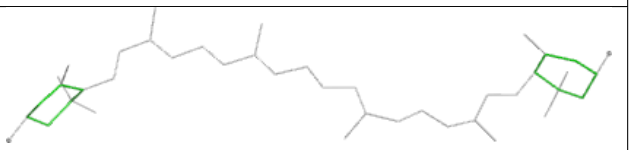
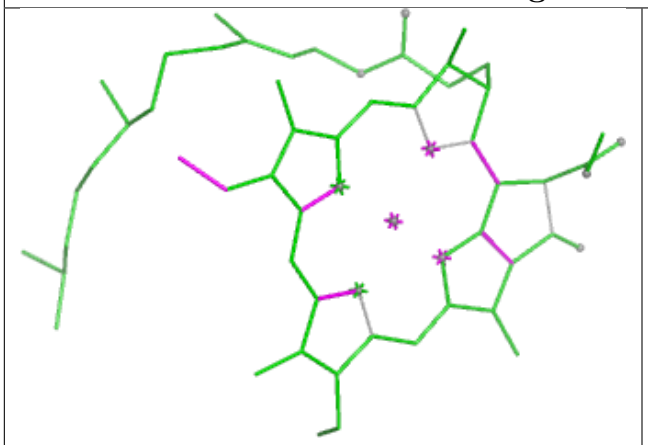
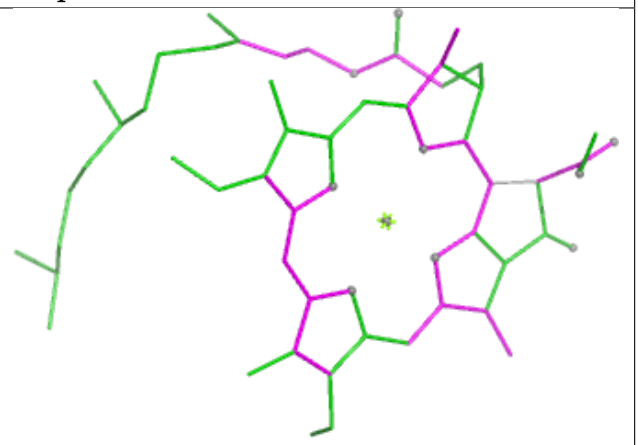


Rings

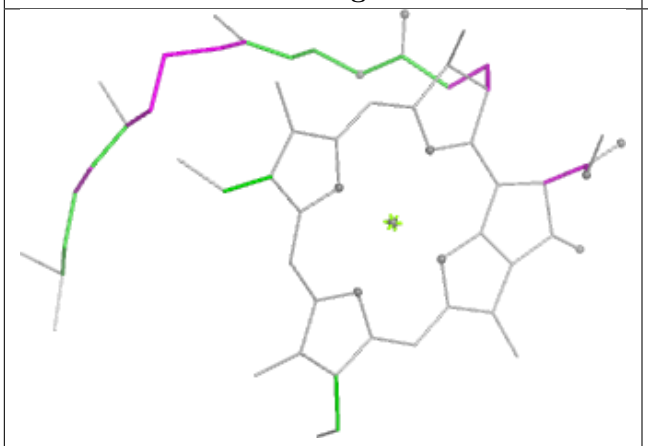
Ligand CLA p 602



Bond lengths



Bond angles



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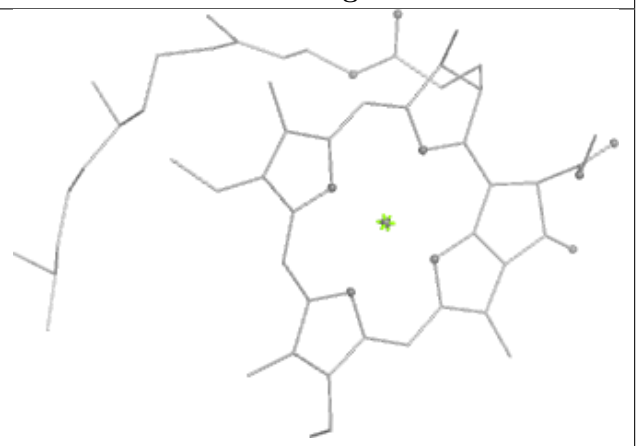
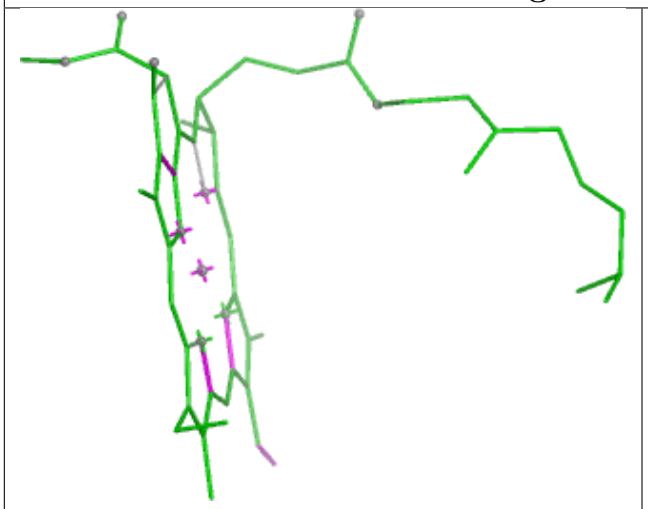


Rings

Ligand CLA 6 305



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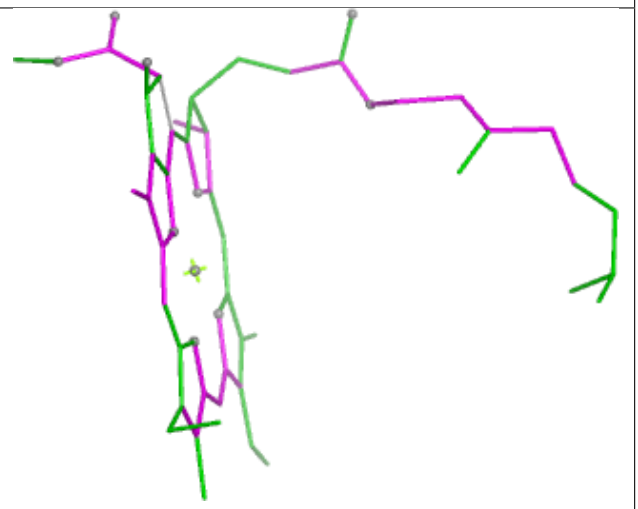
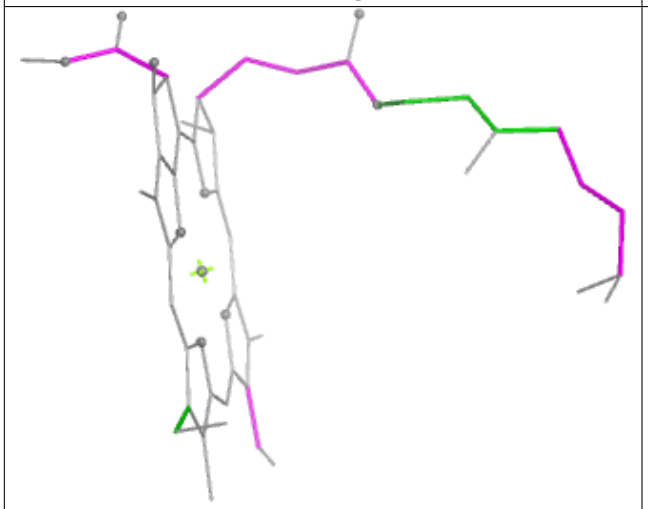


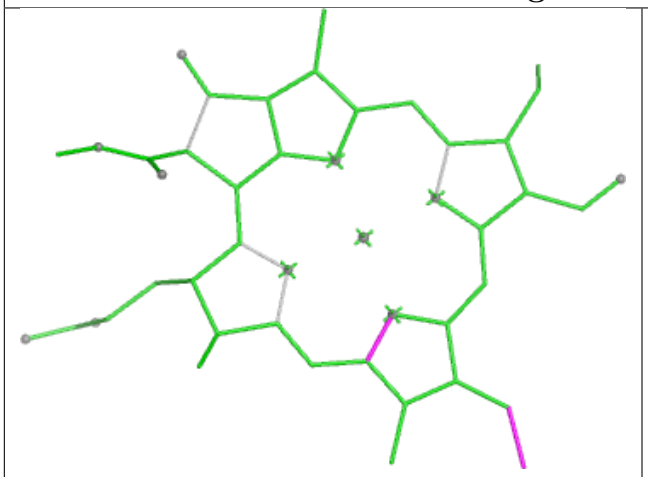
Bond angles



Torsions

Rings

Ligand CHL S 302



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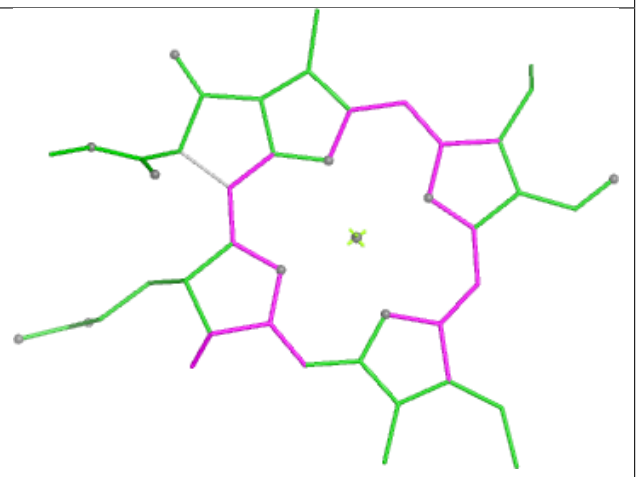

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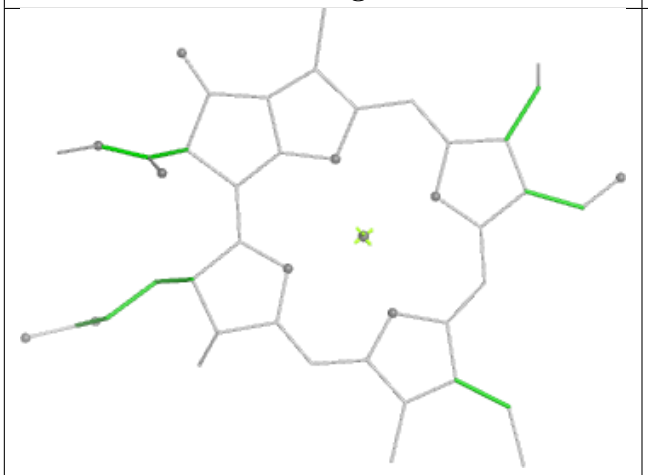

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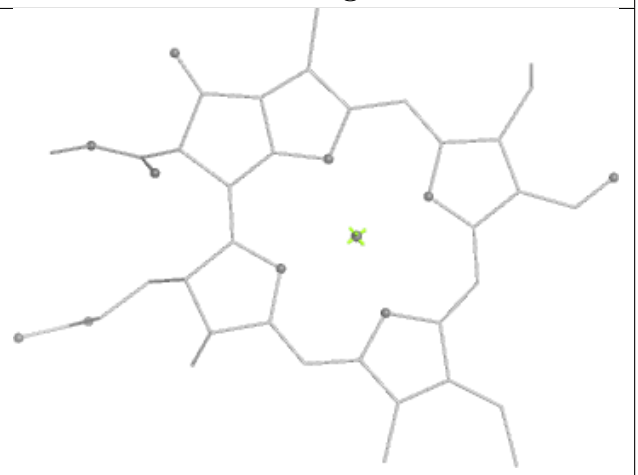
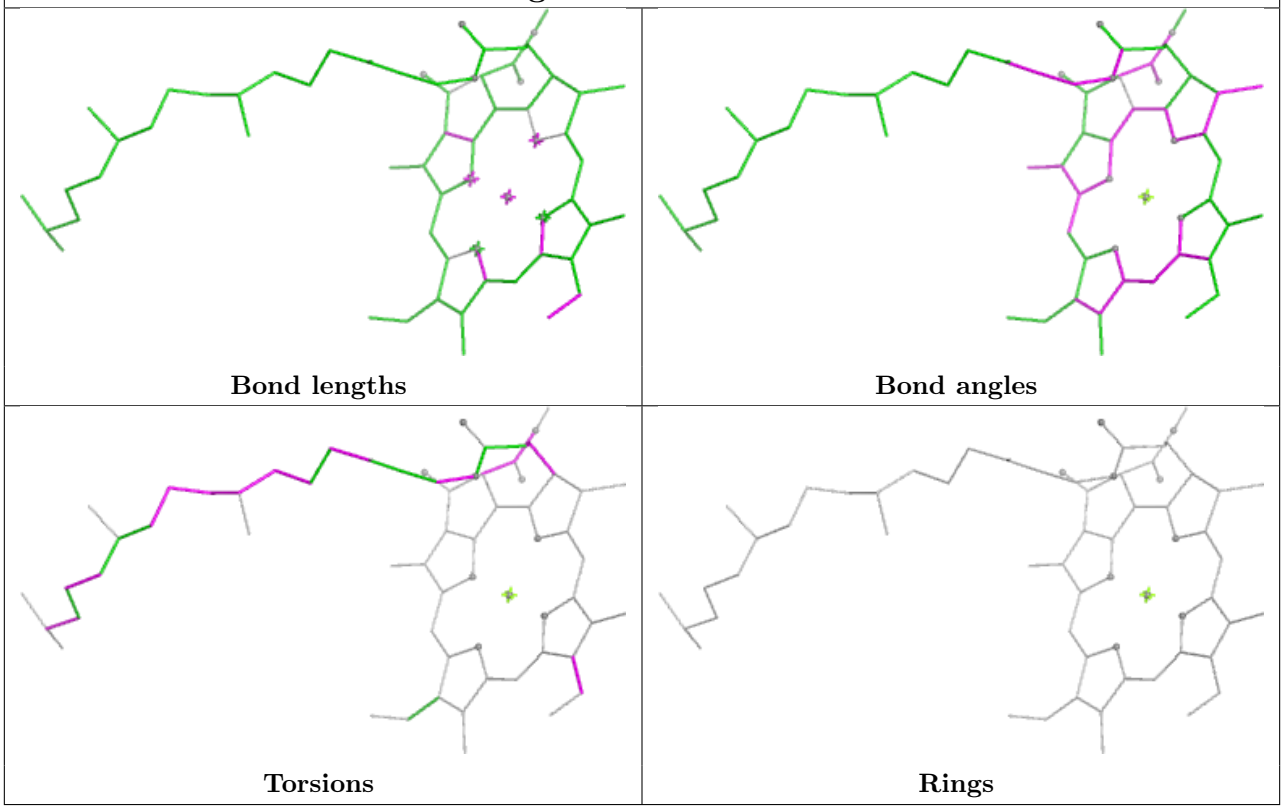
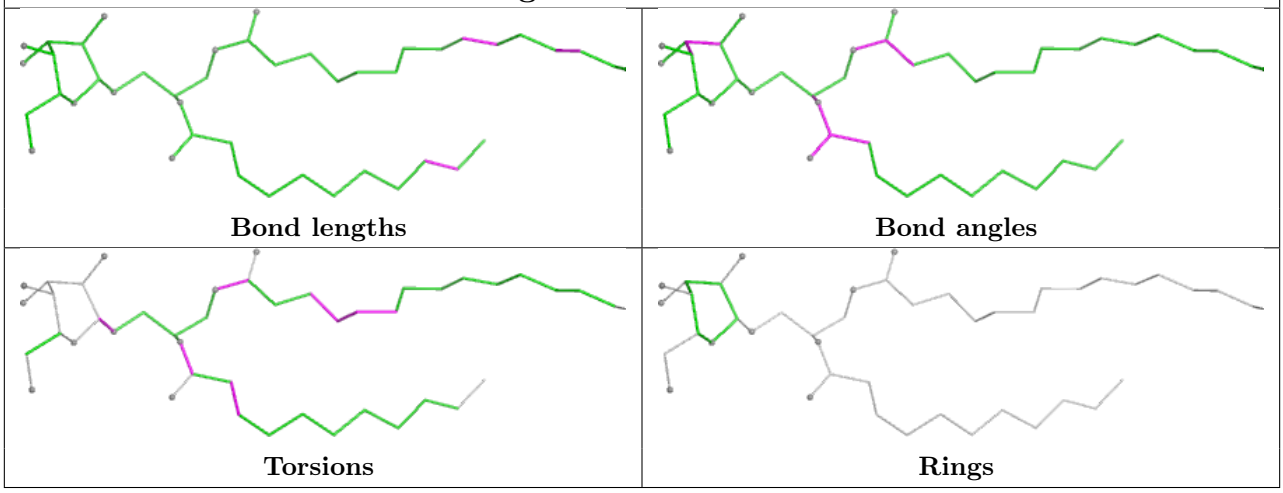


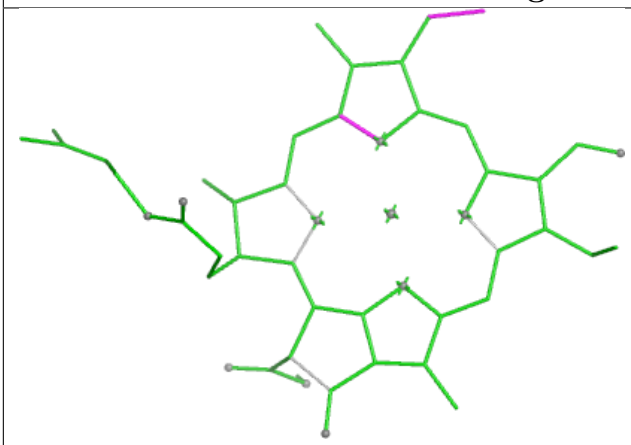
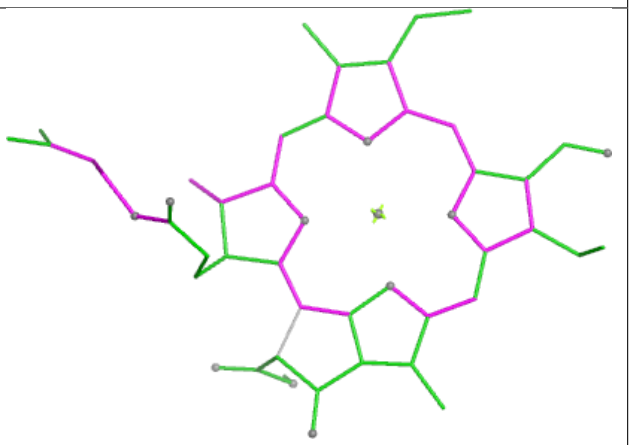
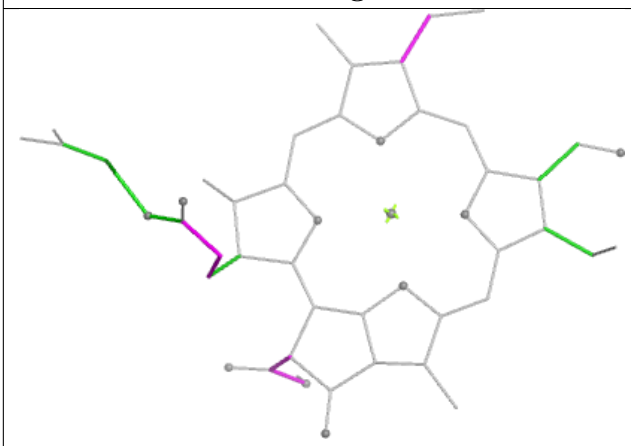
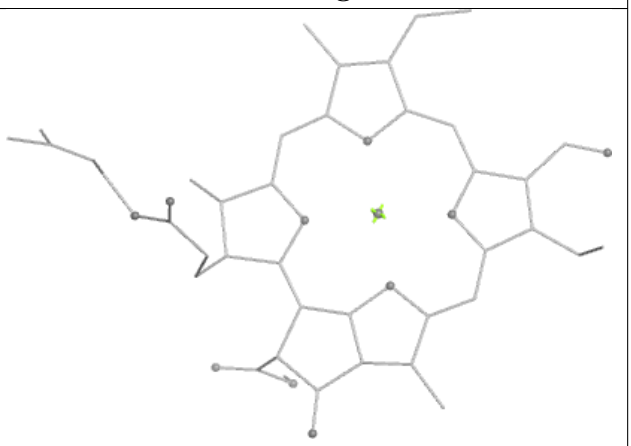
Rings

Ligand CLA S 312

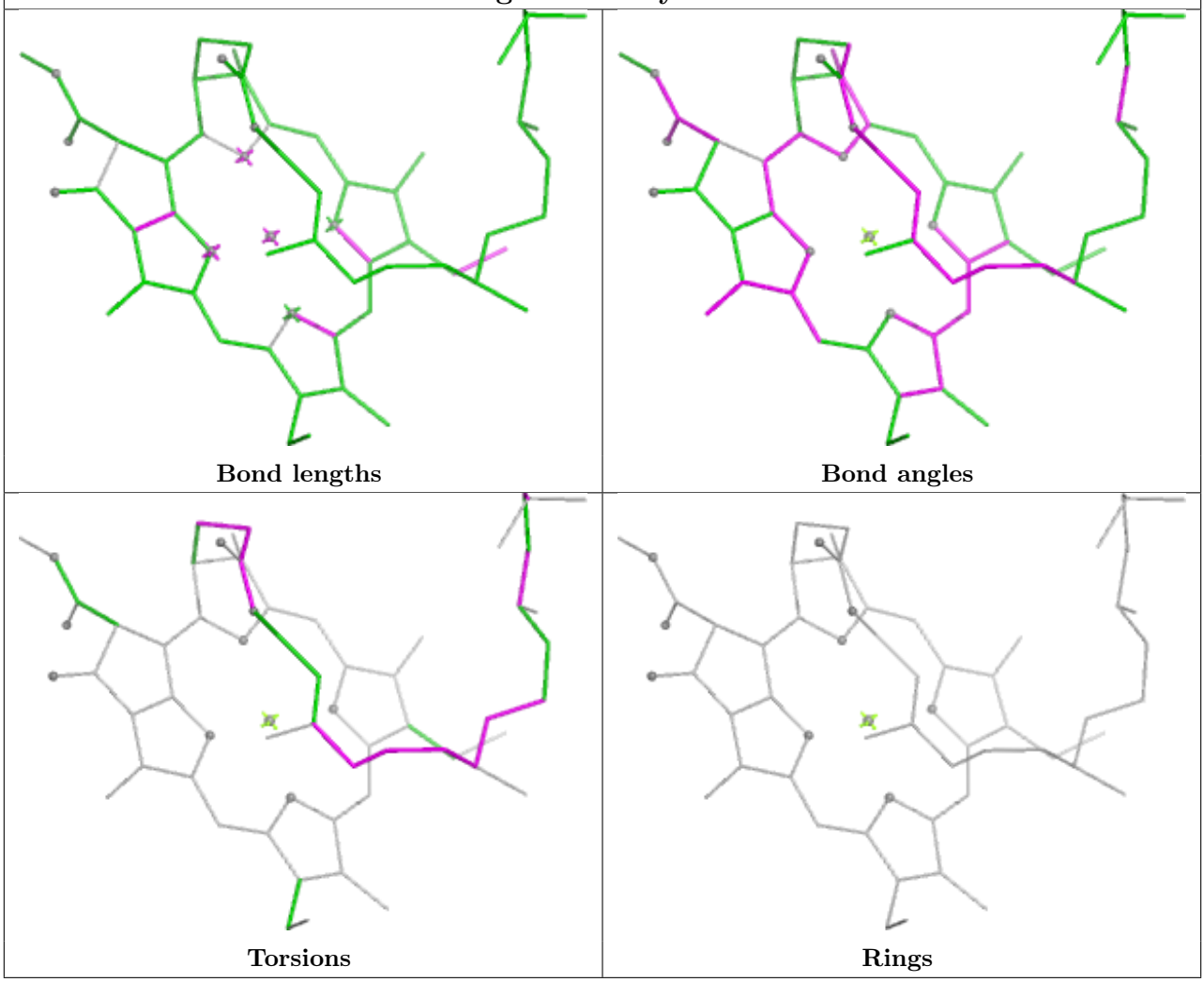


Ligand LMG m 102

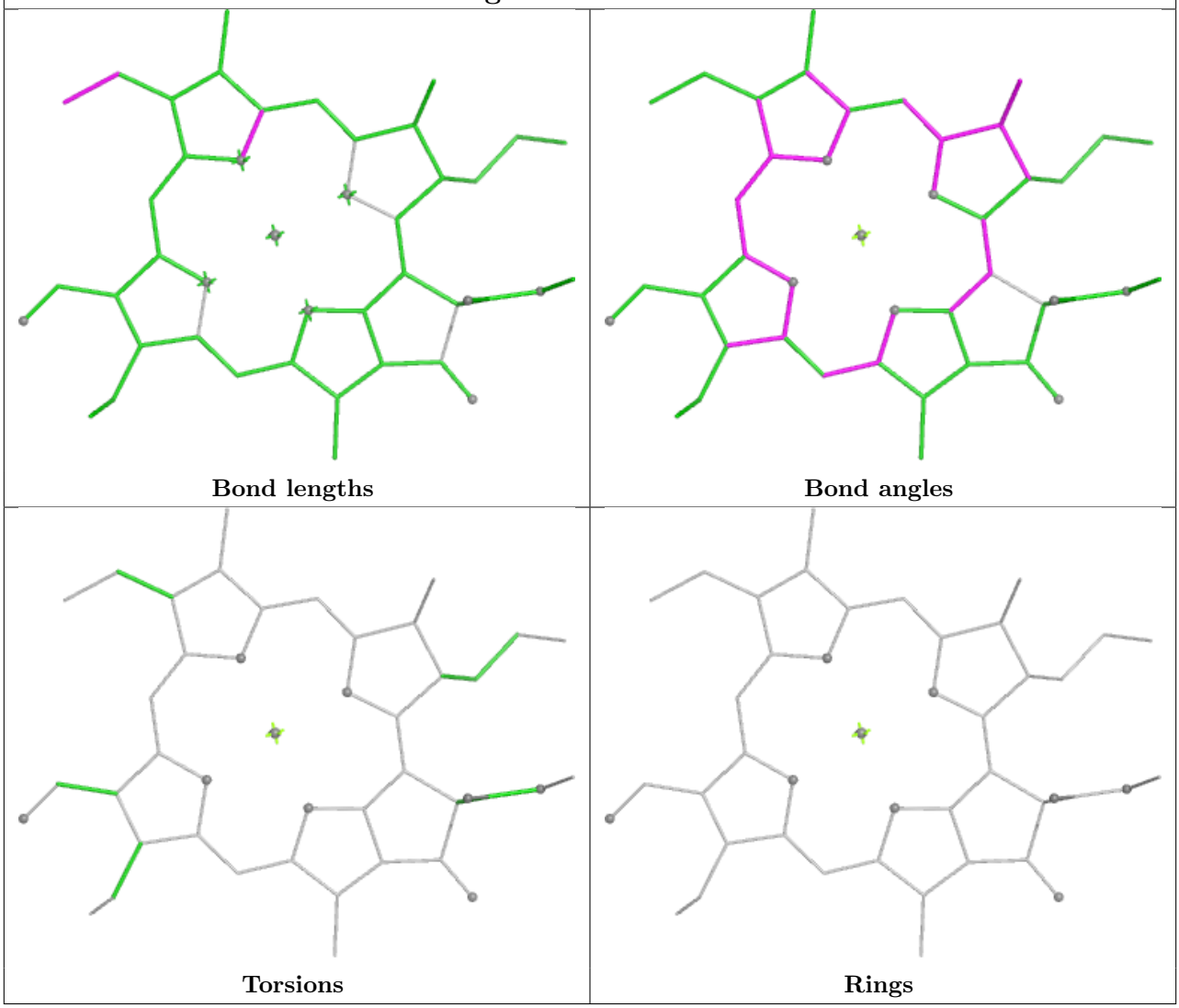


Ligand CHL 5 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

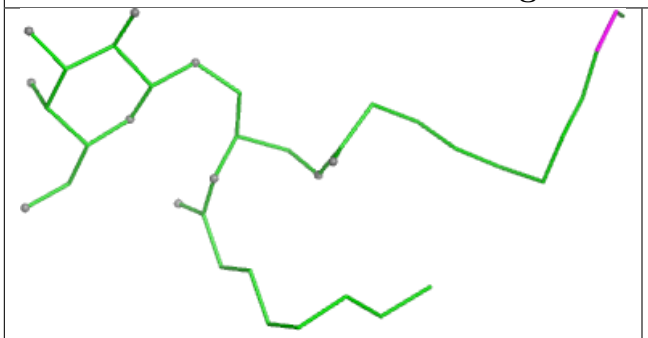
Ligand CLA y 613



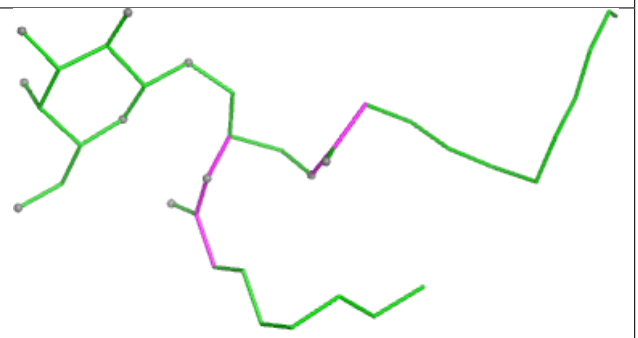
Ligand CHL S 307



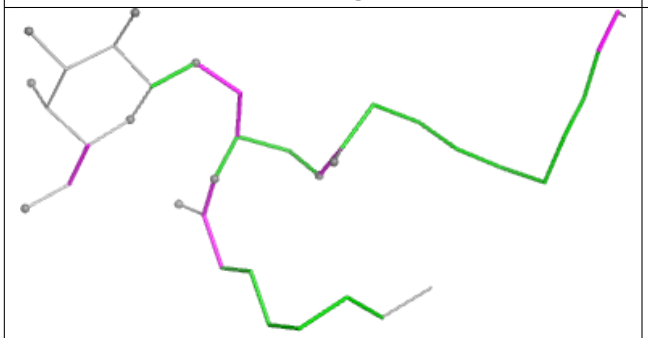
Ligand LMG G 619



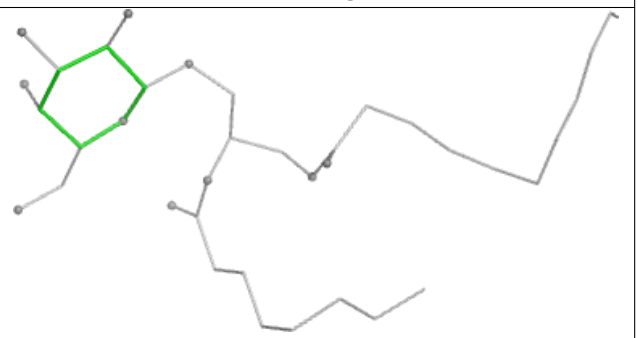
Bond lengths



Bond angles

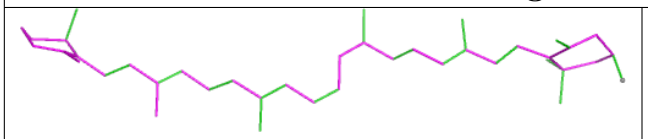


Torsions



Rings

Ligand RRX 4 615



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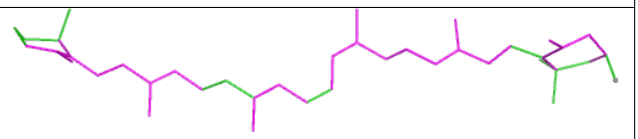
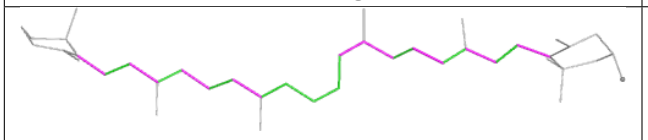


Bond angles



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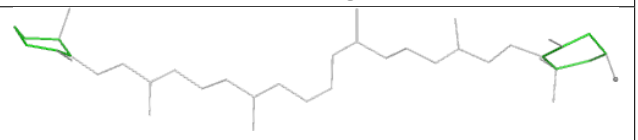
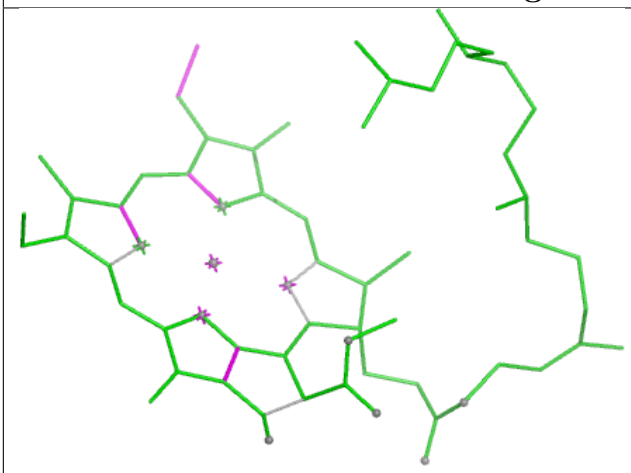


Rings

Ligand CLA B 616



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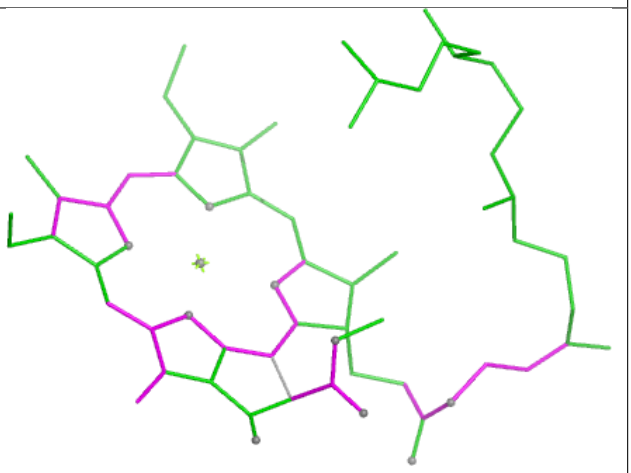

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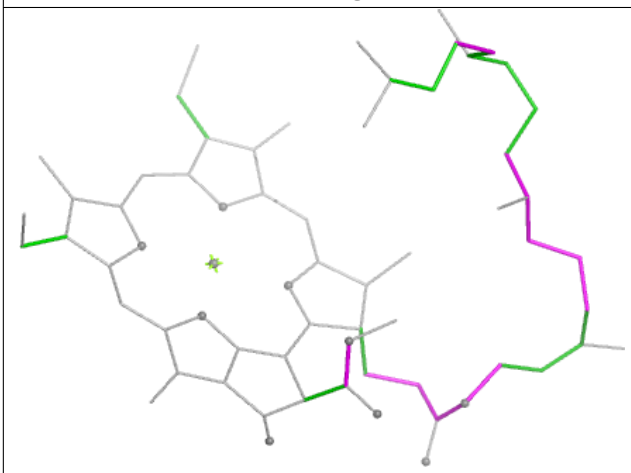

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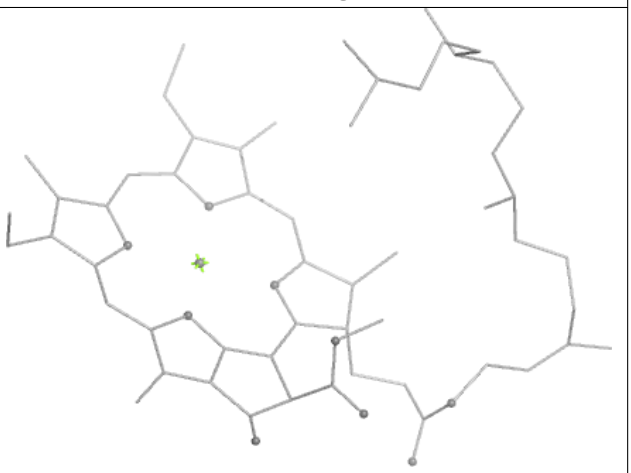

Rings

Ligand LUT 1 615

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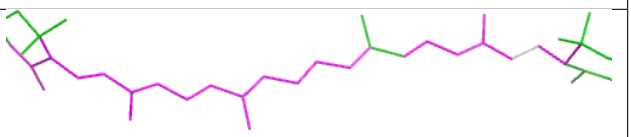

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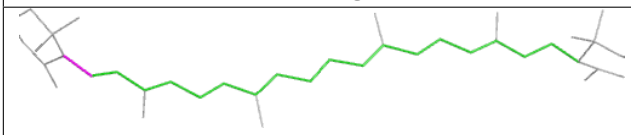

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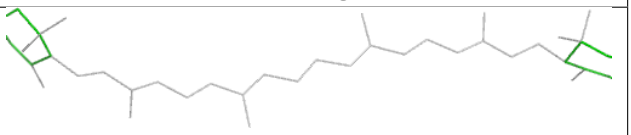
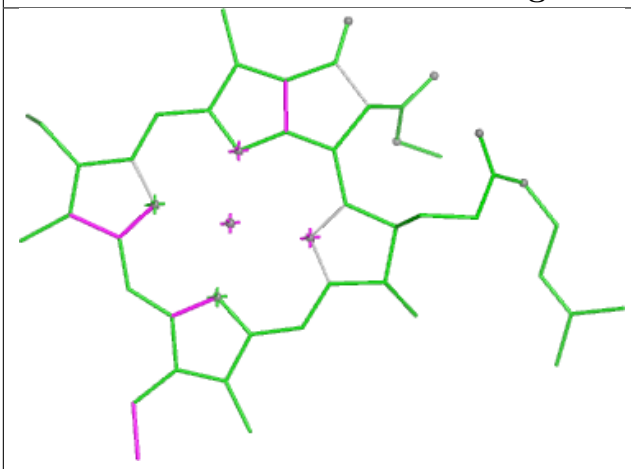


Rings

Ligand CLA 5 612



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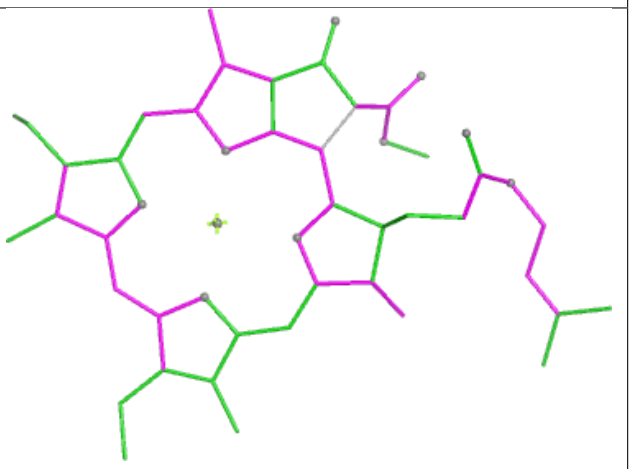

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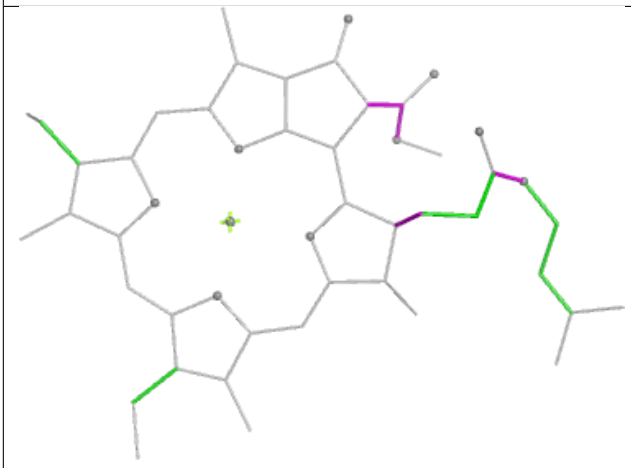

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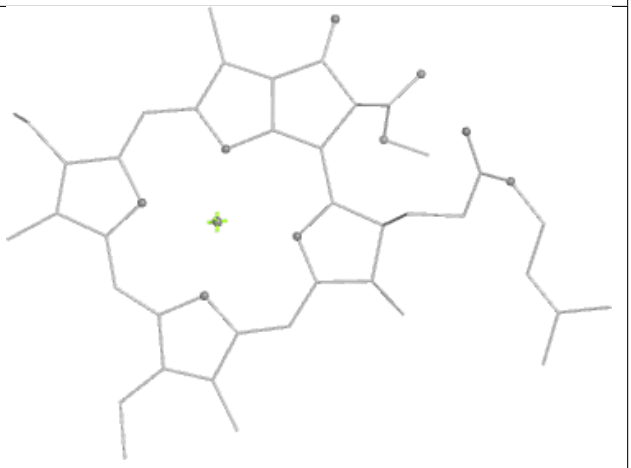
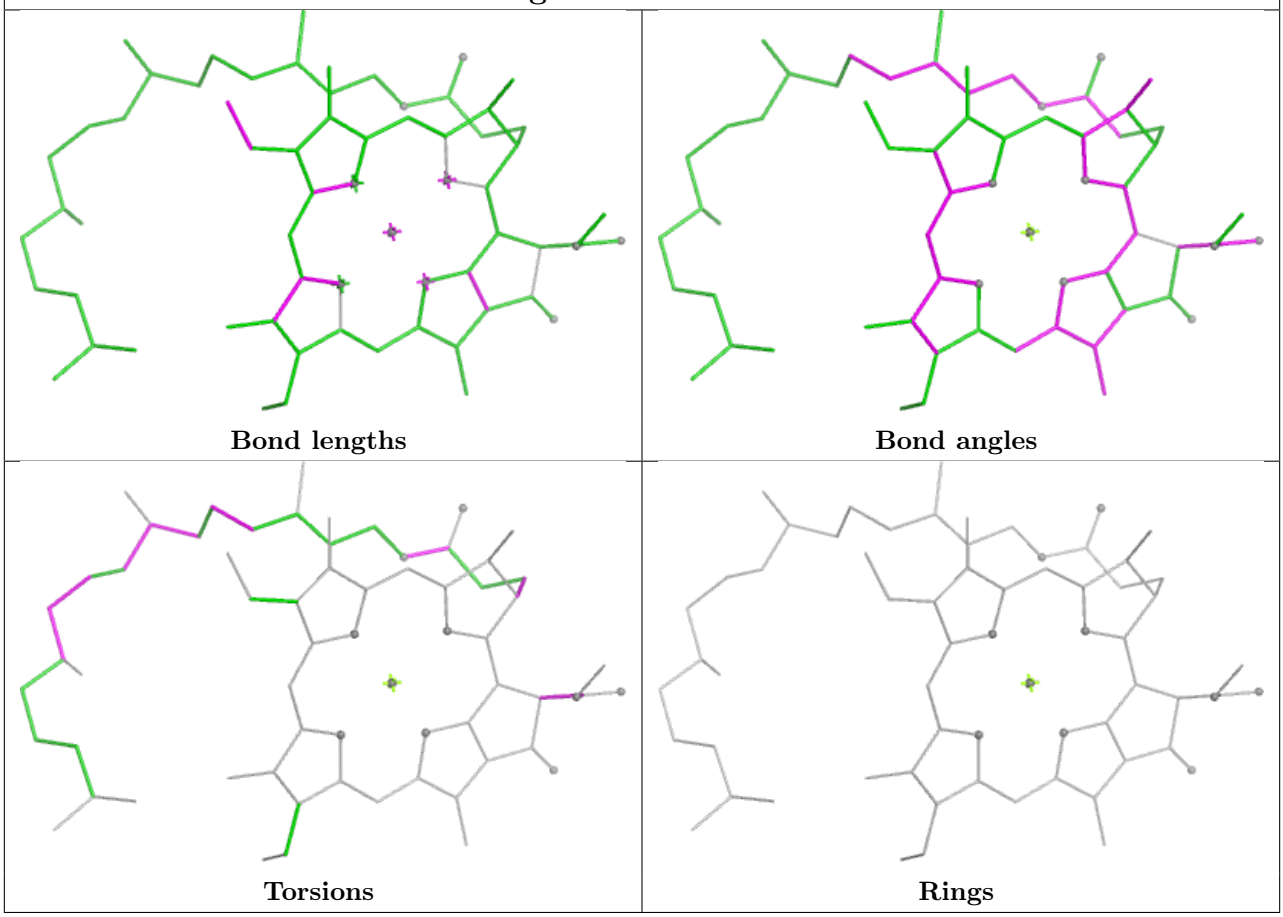


Rings

Ligand CLA 6 303



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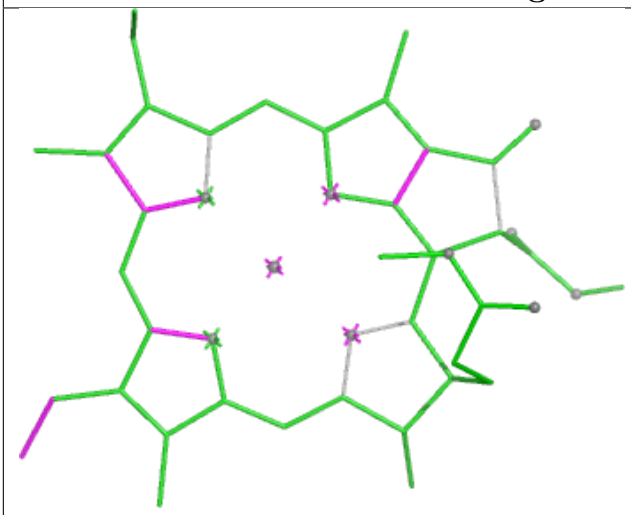
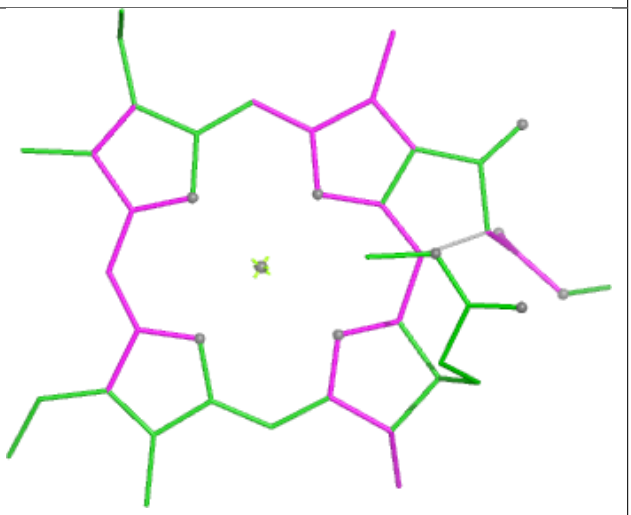
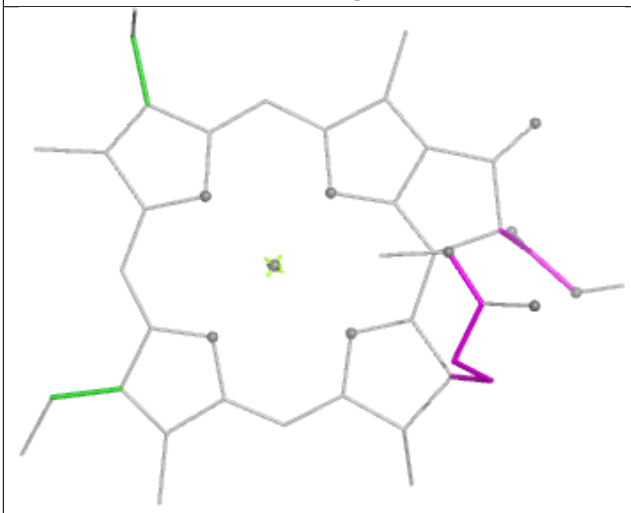
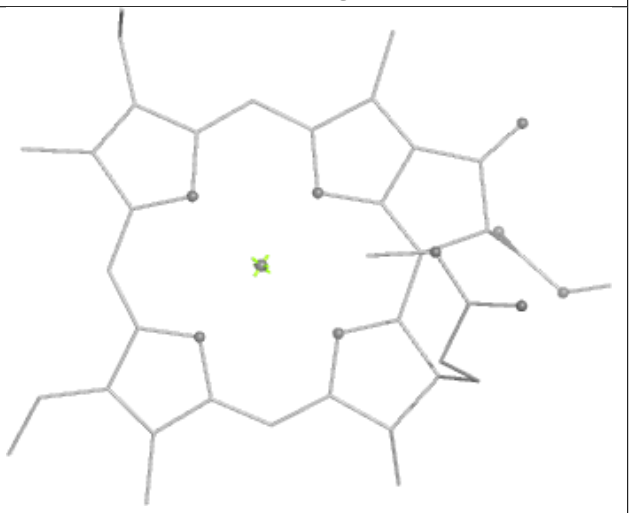
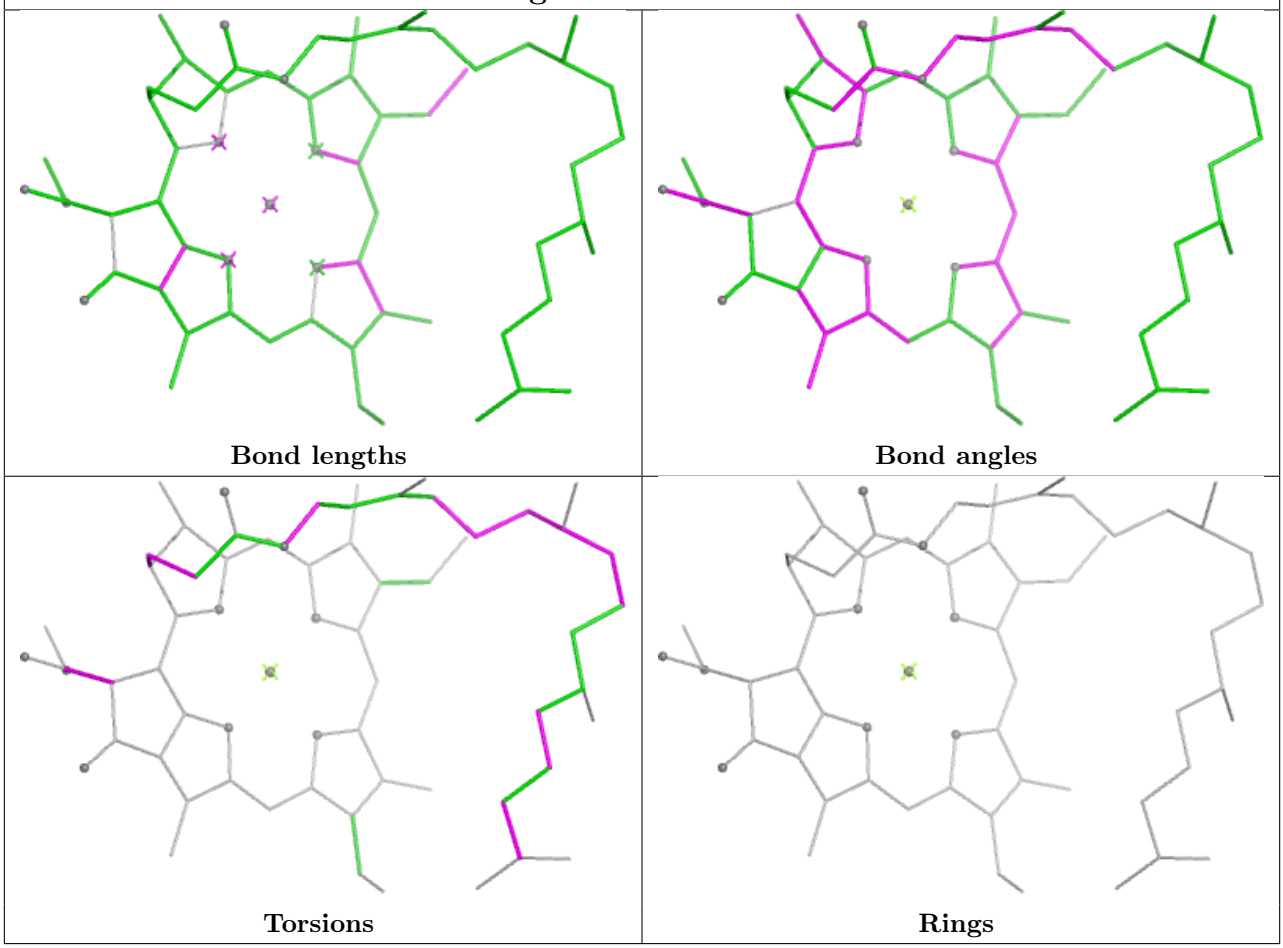
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 602



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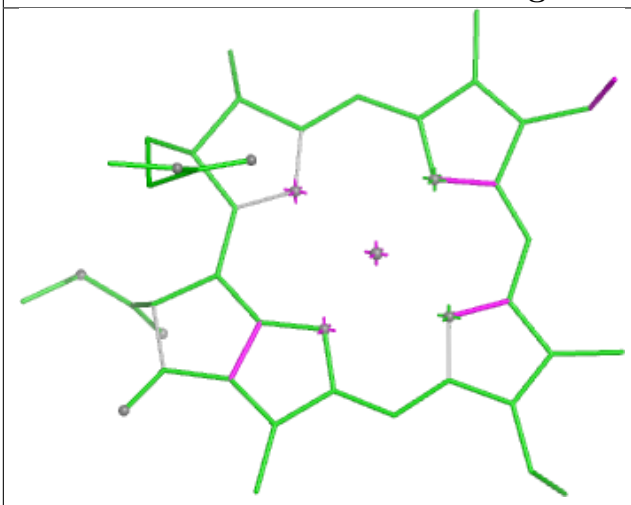

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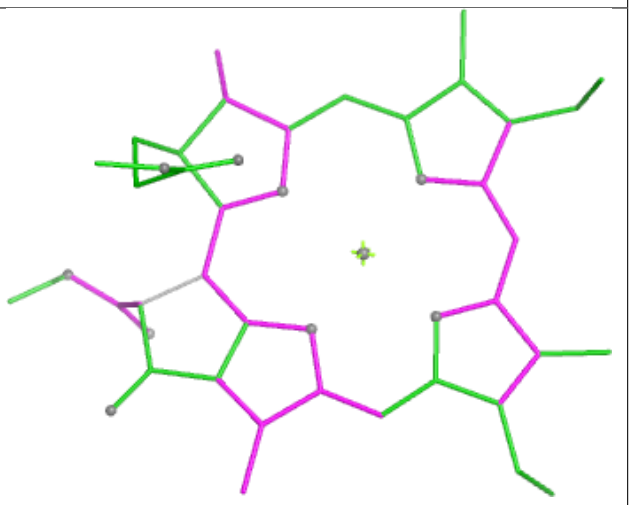
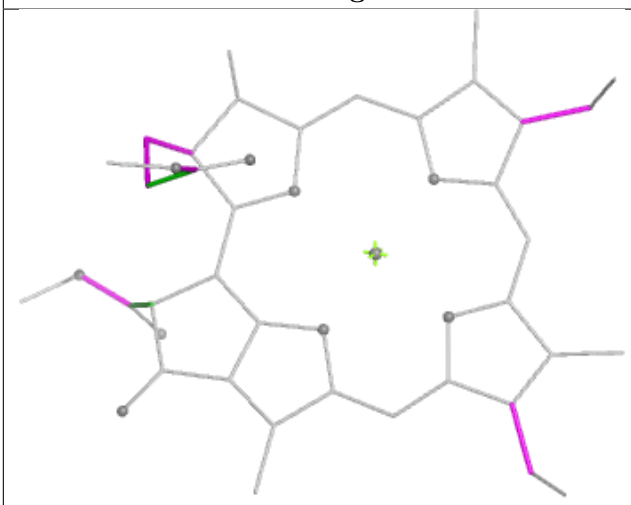


Bond angles



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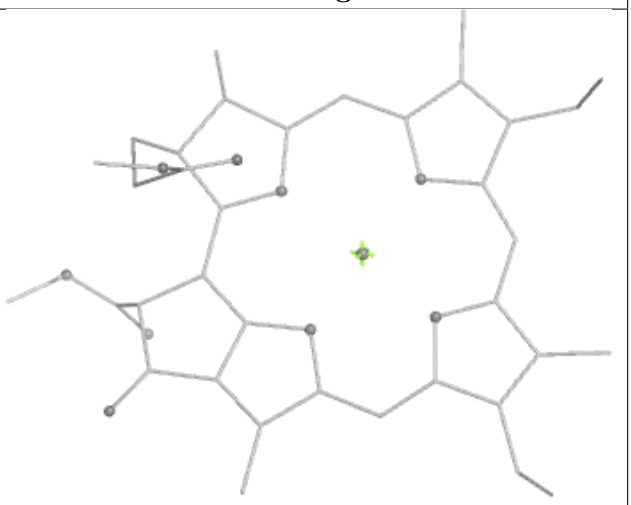
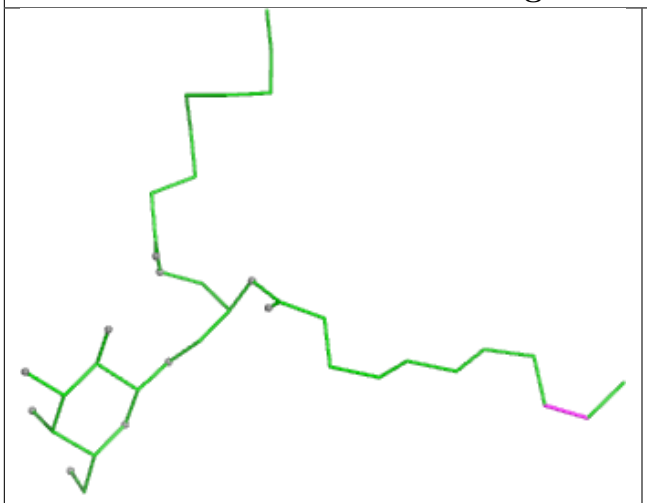


Rings

Ligand LMG 6 322



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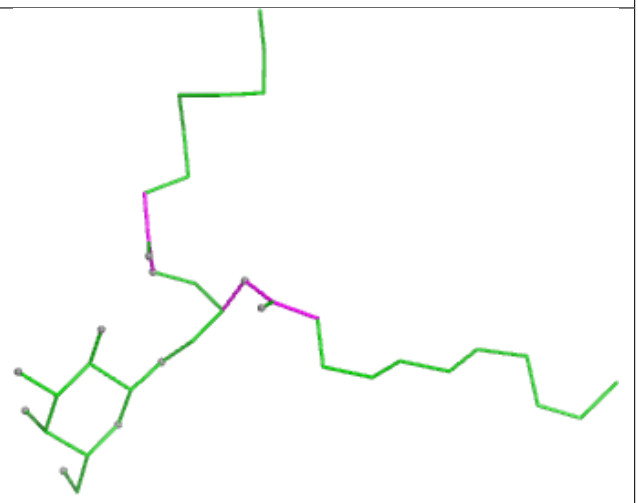

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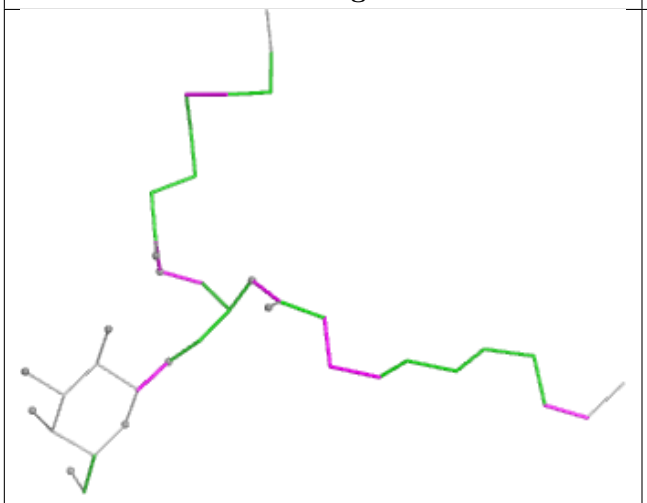

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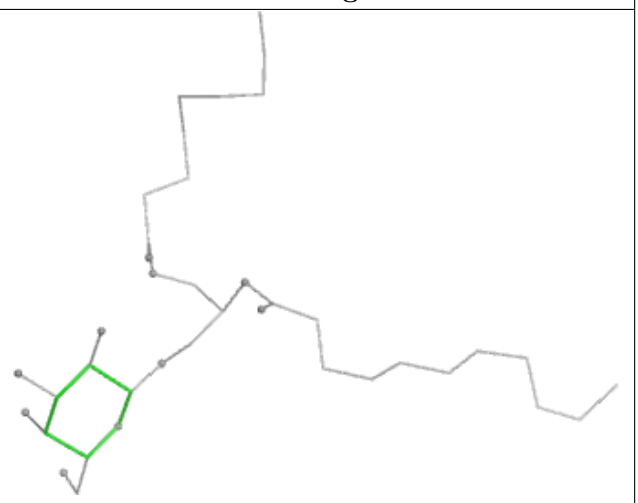

Rings

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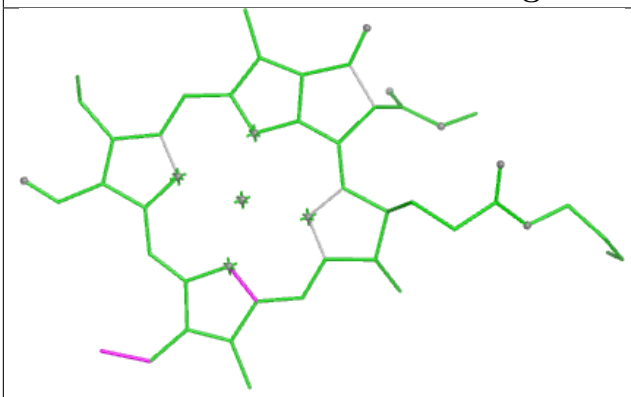
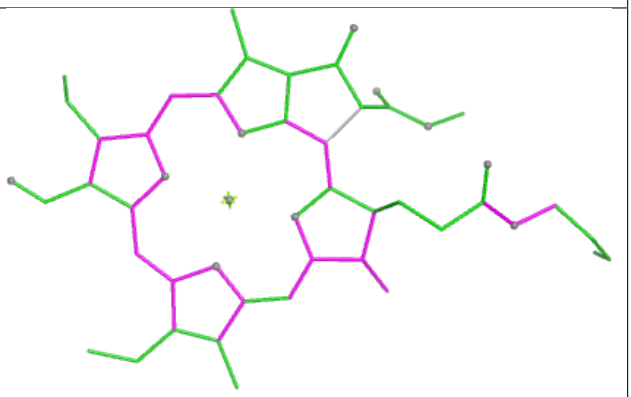
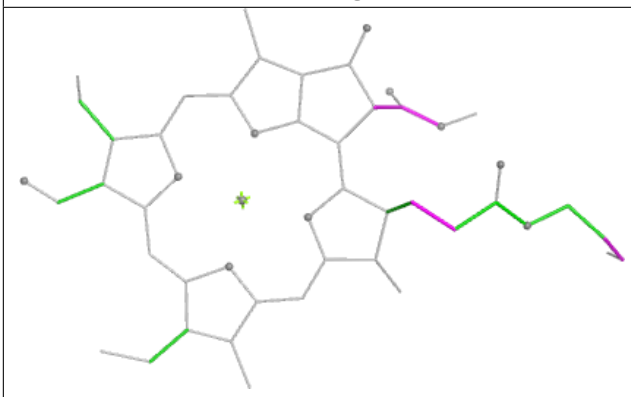
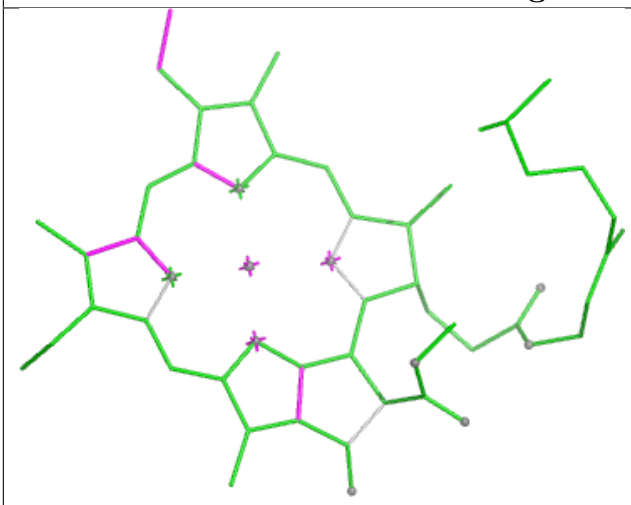
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 3 305



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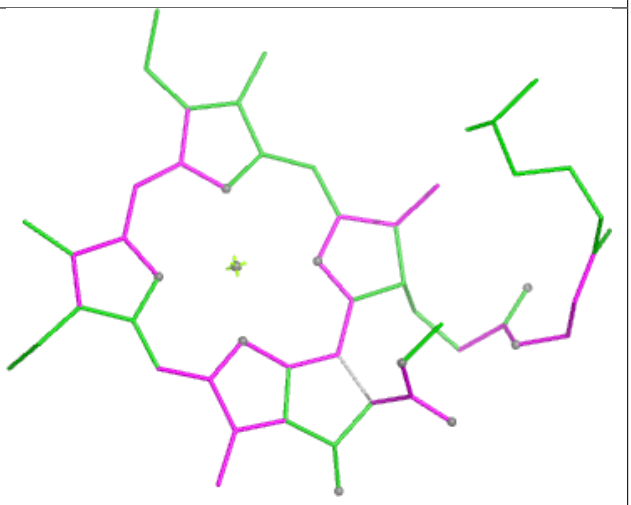
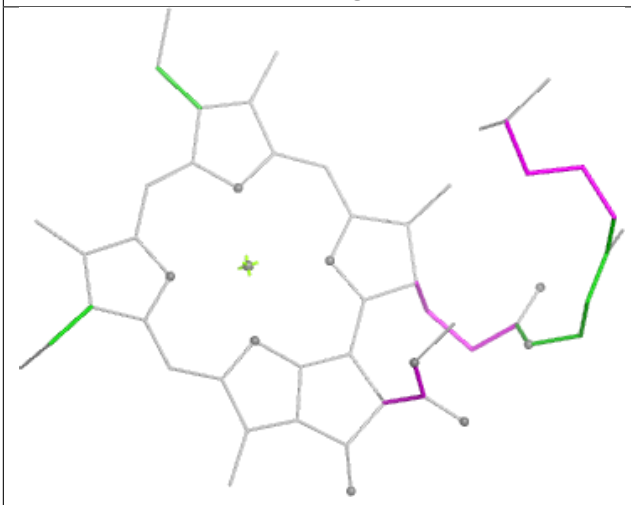


Bond angles



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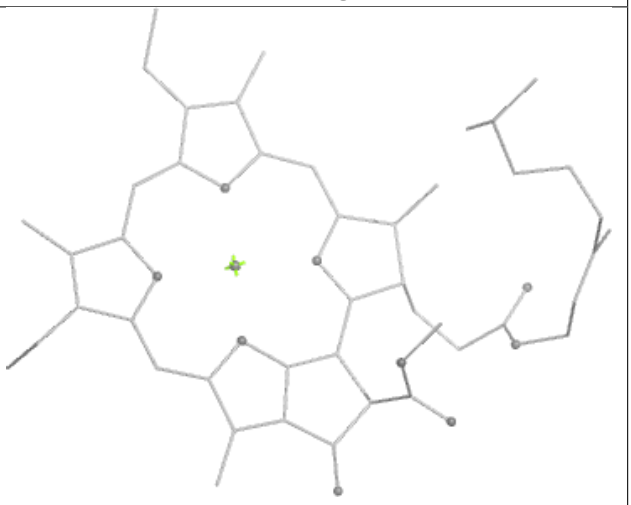

Rings

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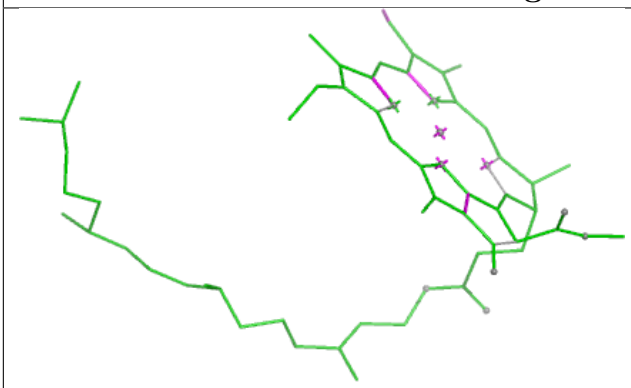
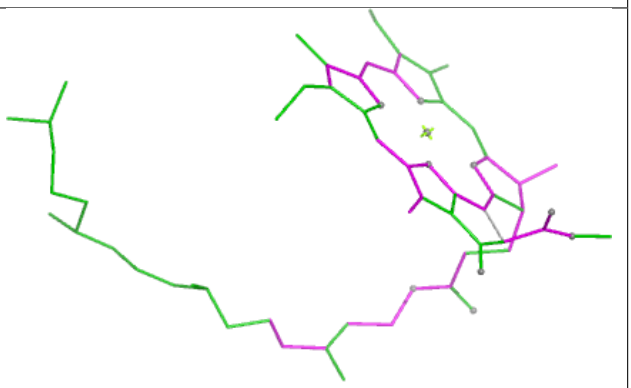
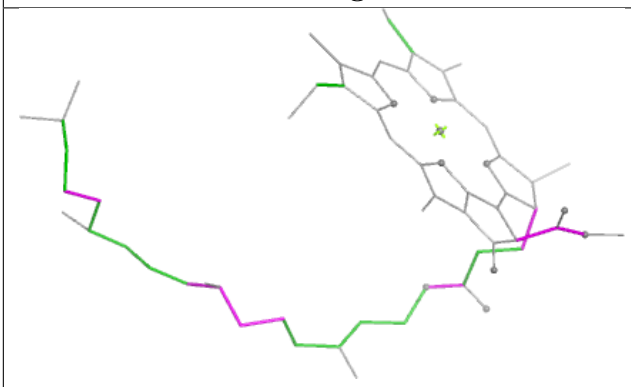
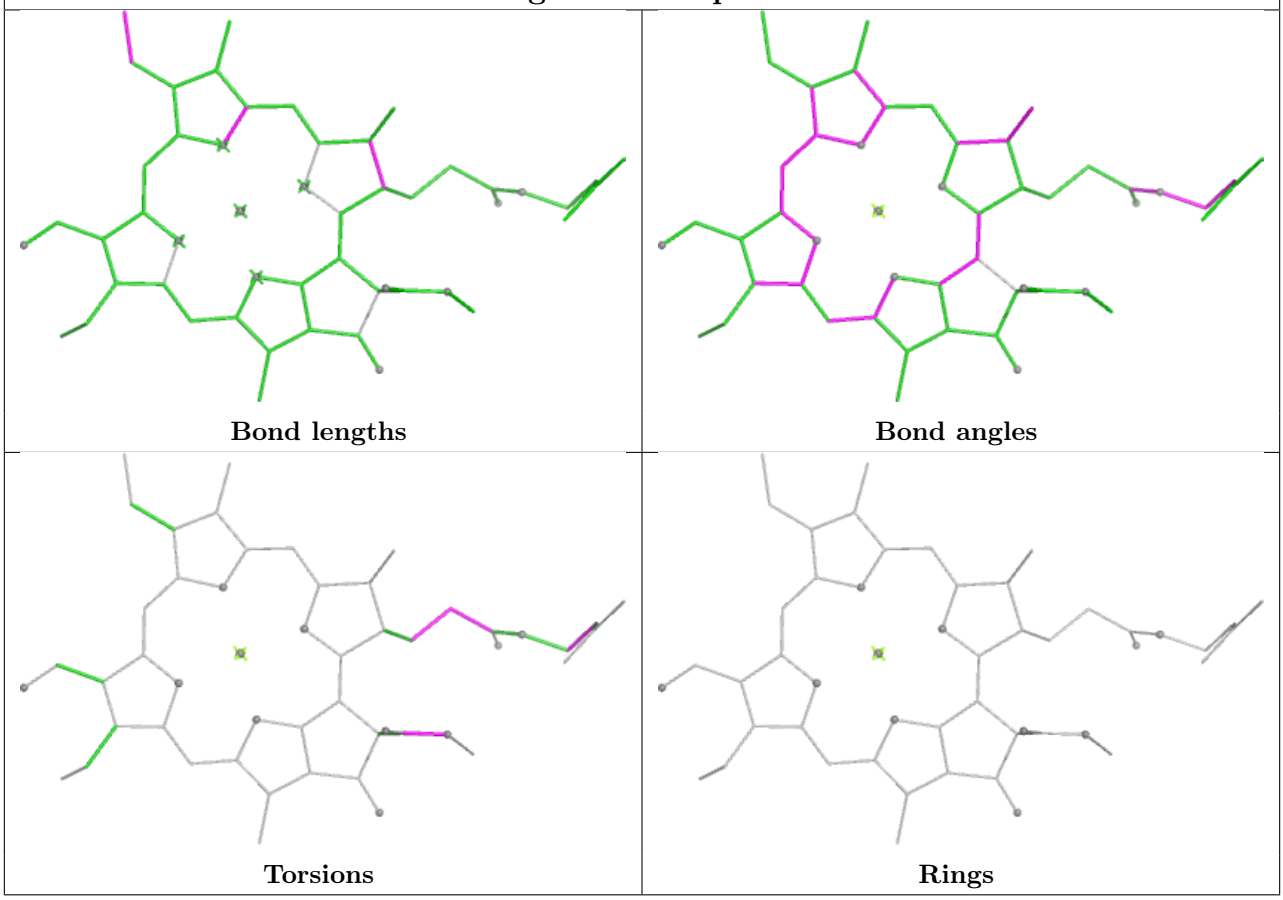
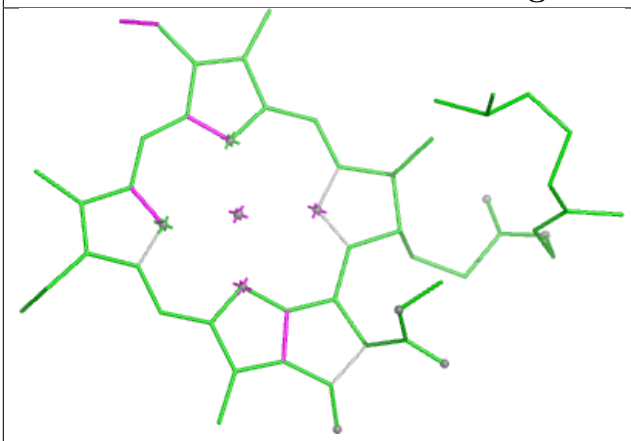
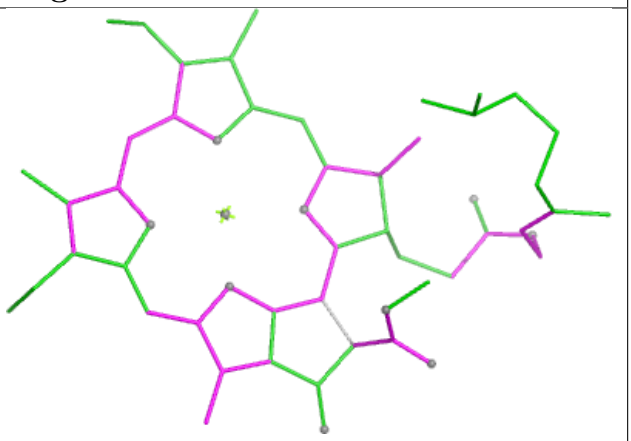
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CHL q 308



Ligand CLA g 304	
	
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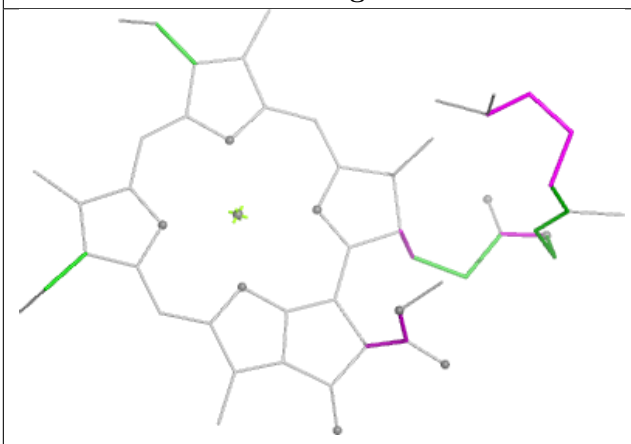
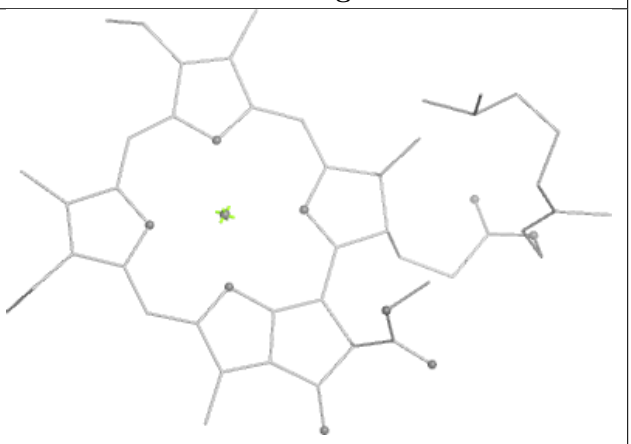
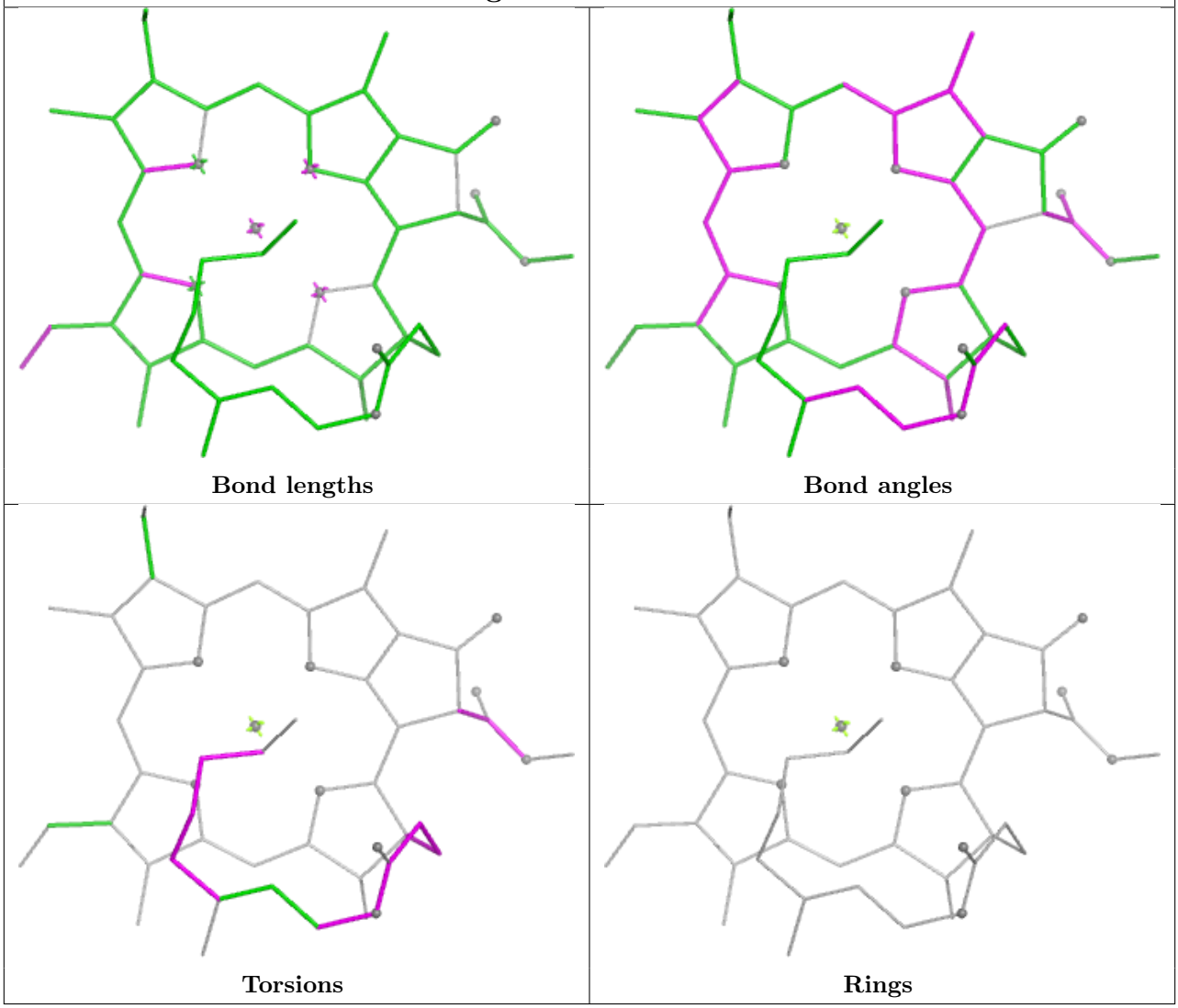
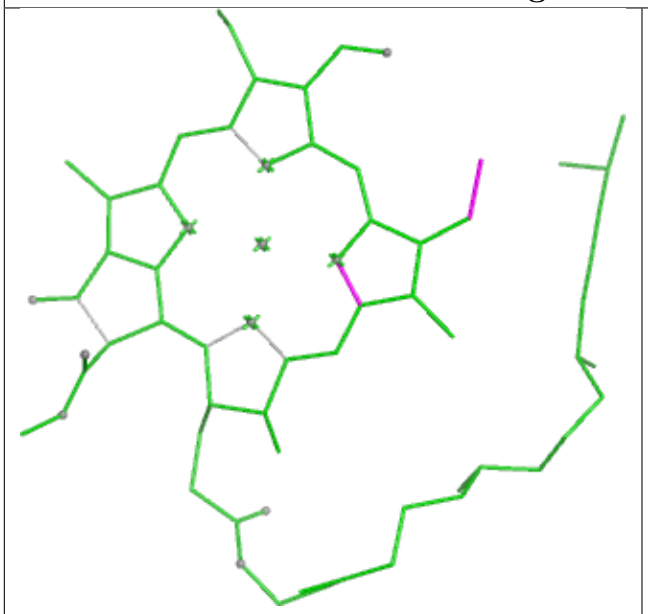
	
Torsions	**Rings**

Ligand CLA 1 614



Ligand CHL y 607



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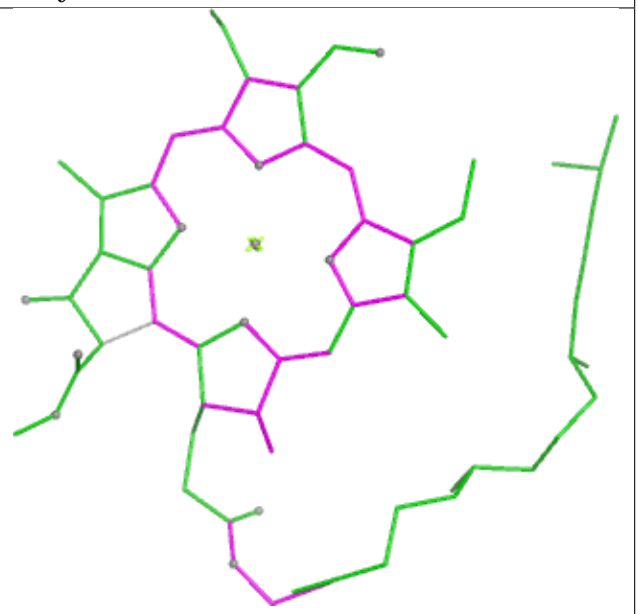
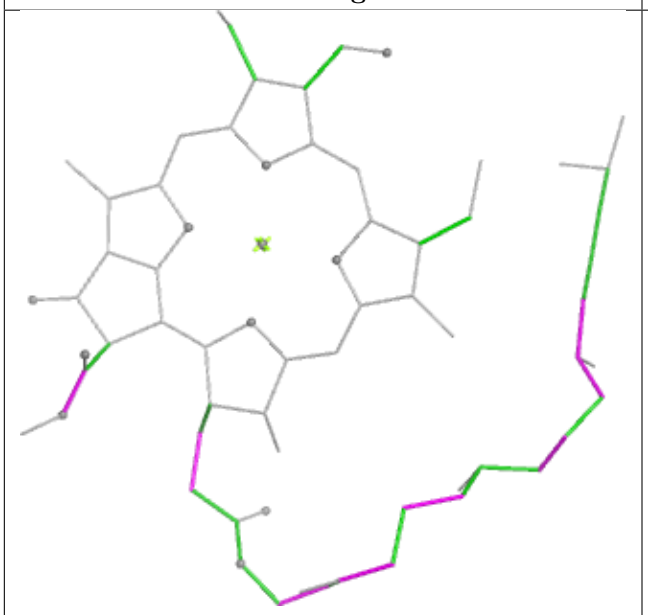


Bond angles



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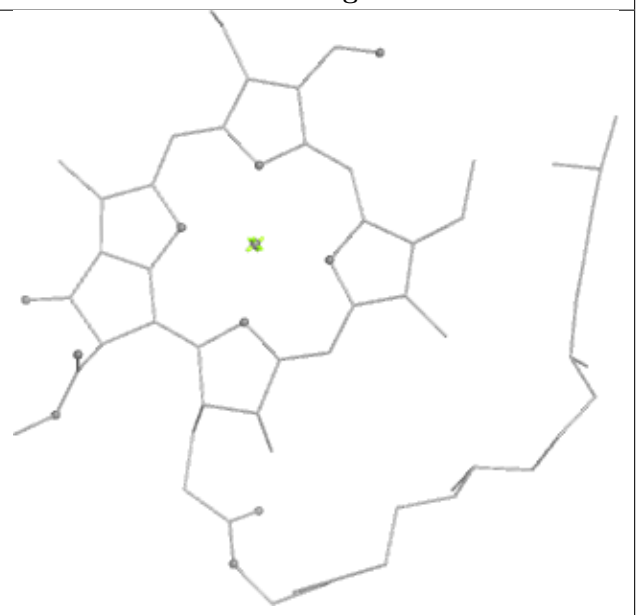
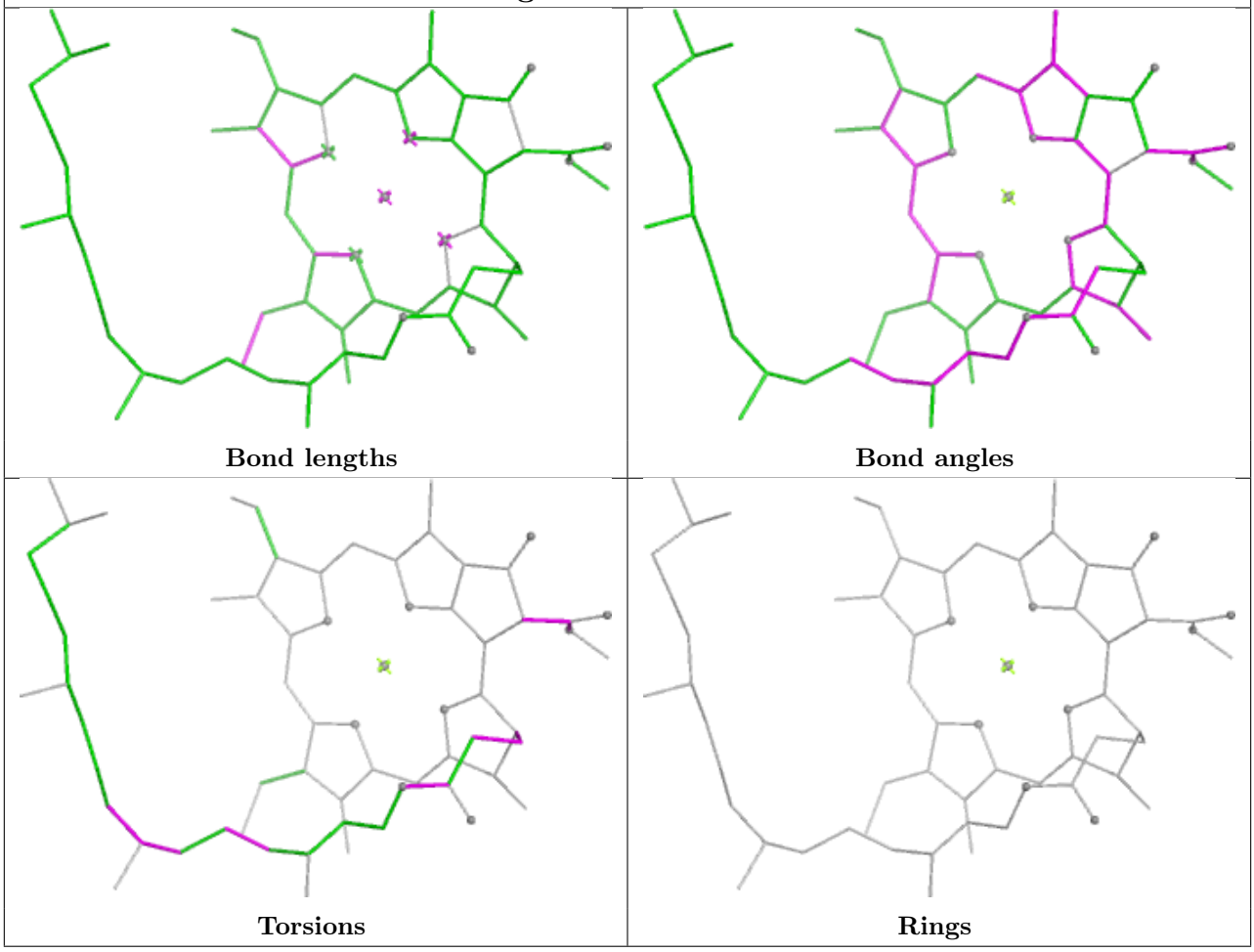
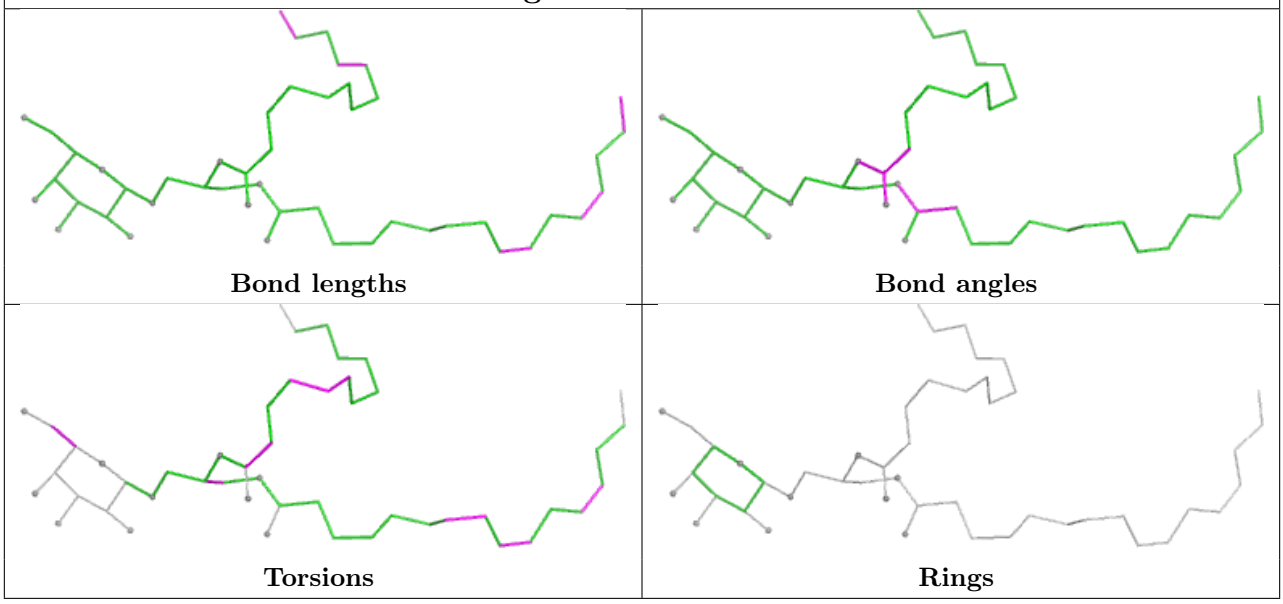


Rings

Ligand CLA 8 602



Ligand LMG d 411



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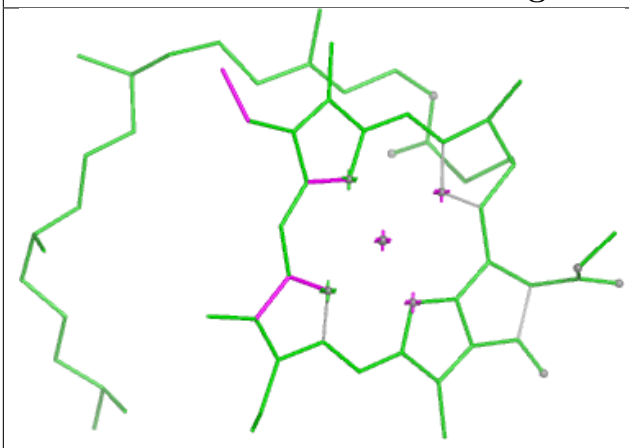
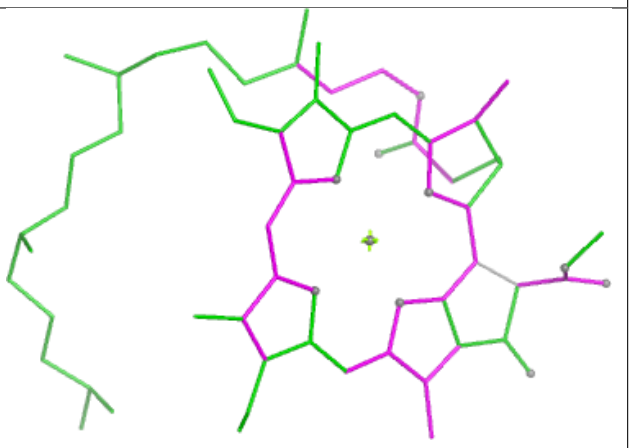
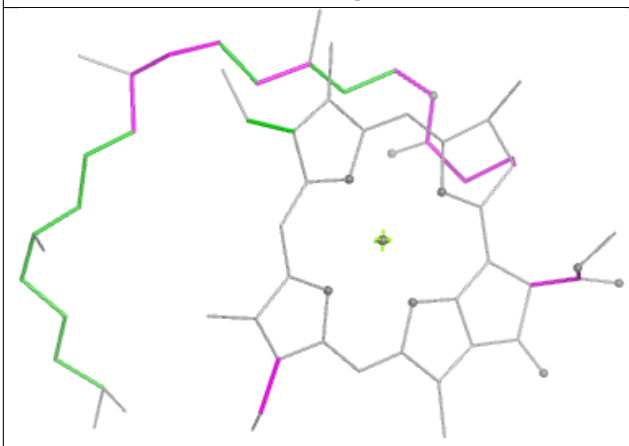
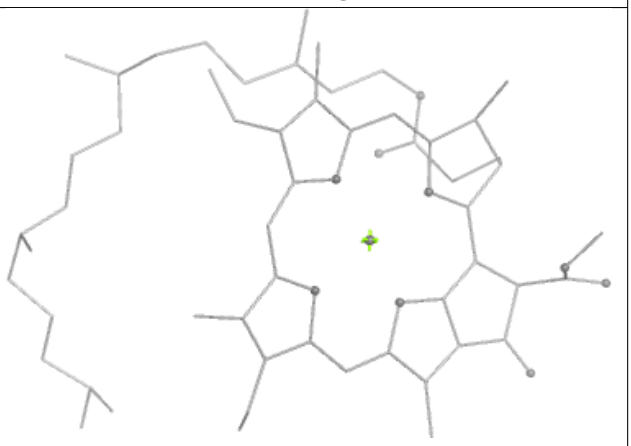
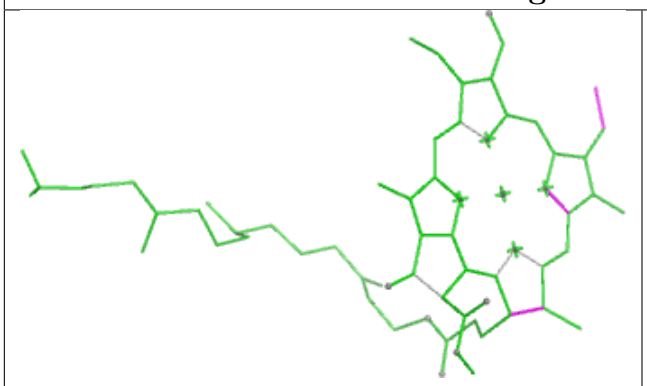
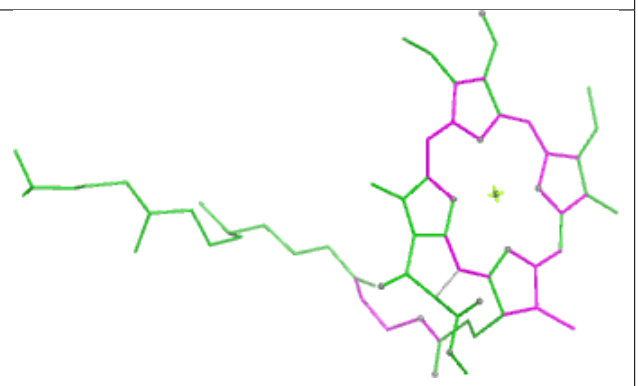
 Bond lengths	 Bond angles
 Torsions	 Rings

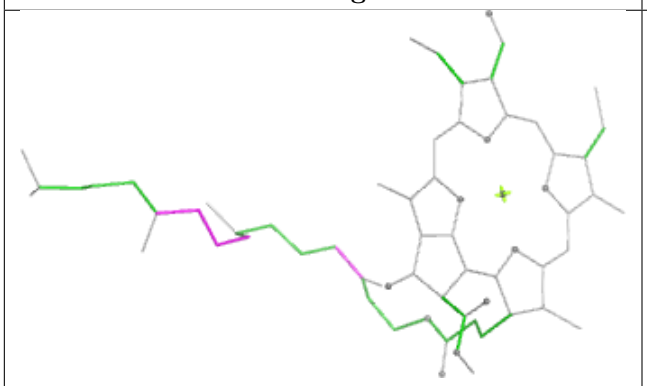
Ligand CHL 1 609



Bond lengths



Bond angles



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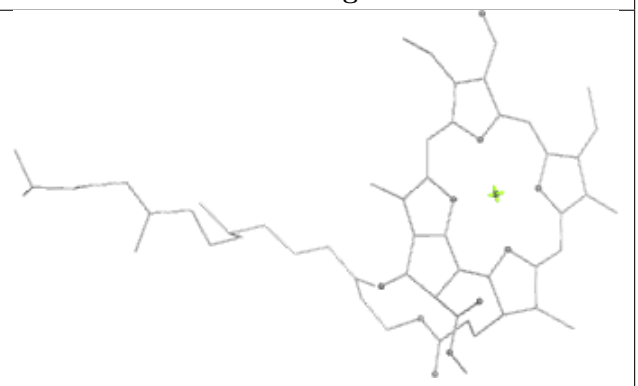
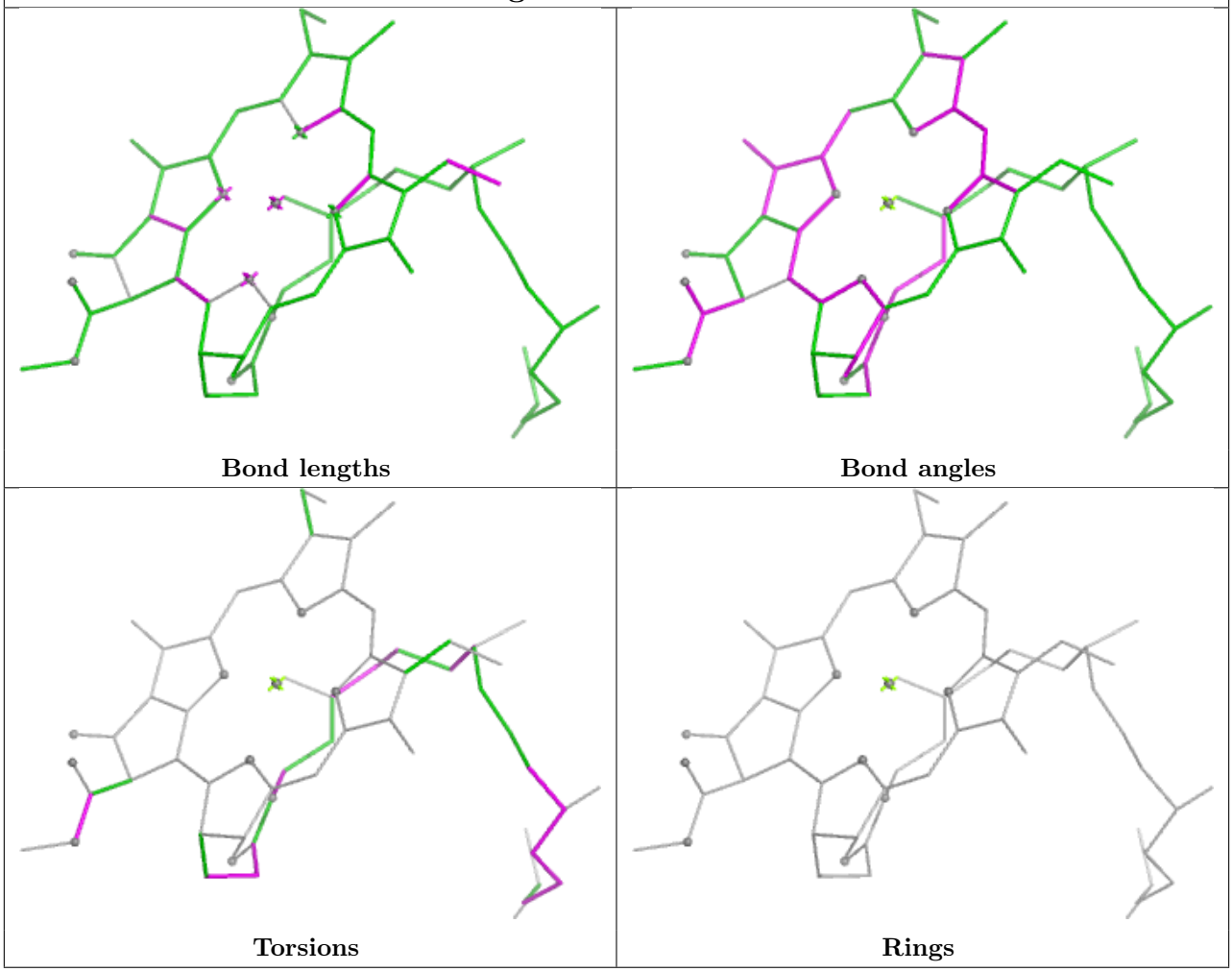
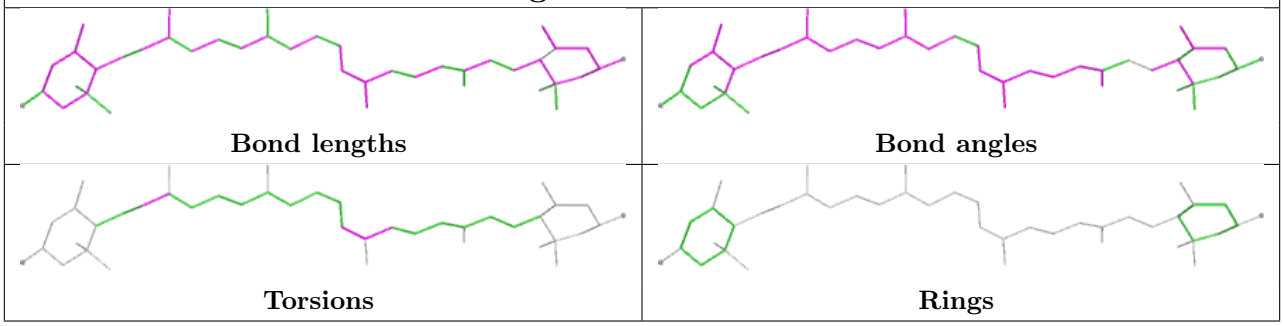


Rings

Ligand CLA 1 613



Ligand LUT 9 318



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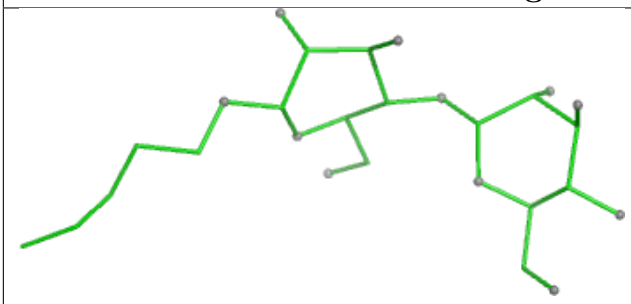
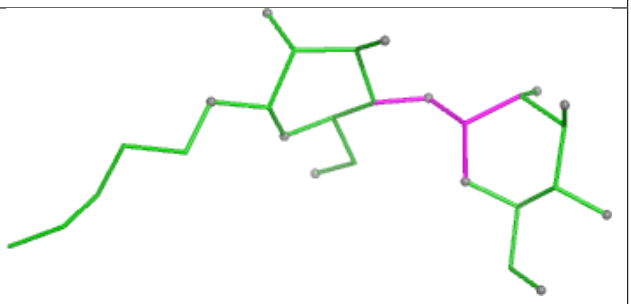
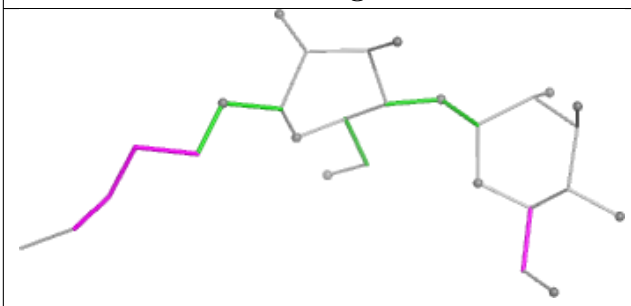
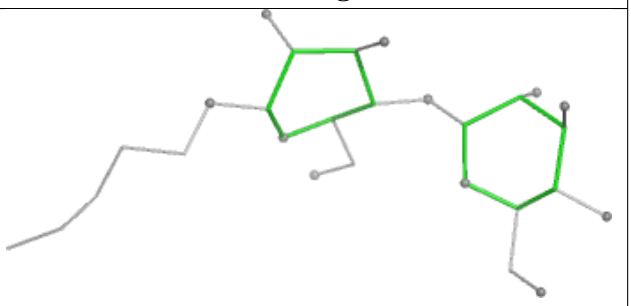
 Bond lengths	 Bond angles
 Torsions	 Rings

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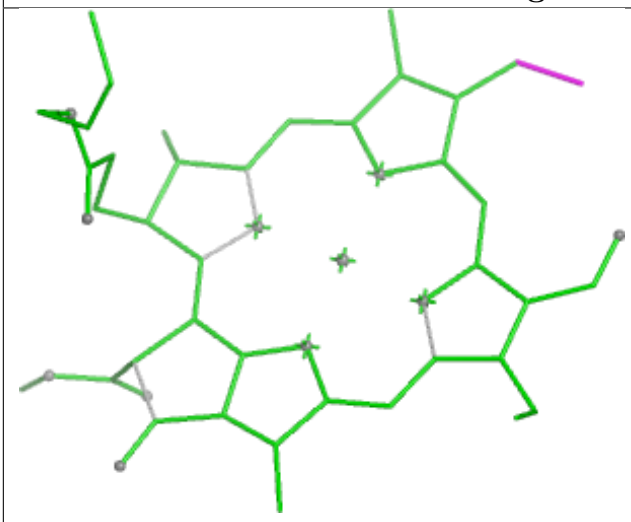
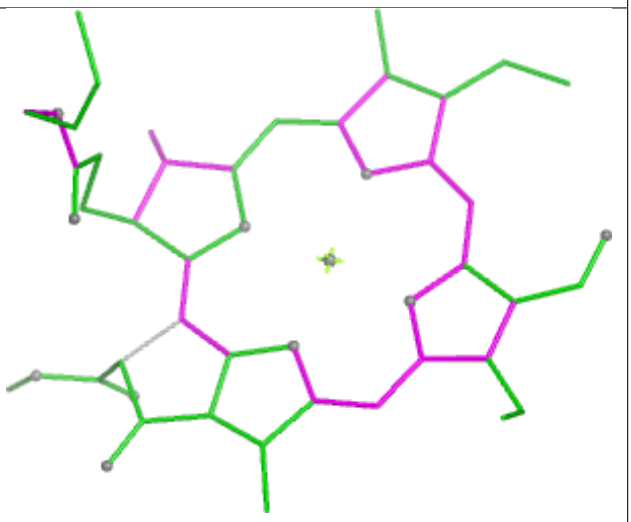
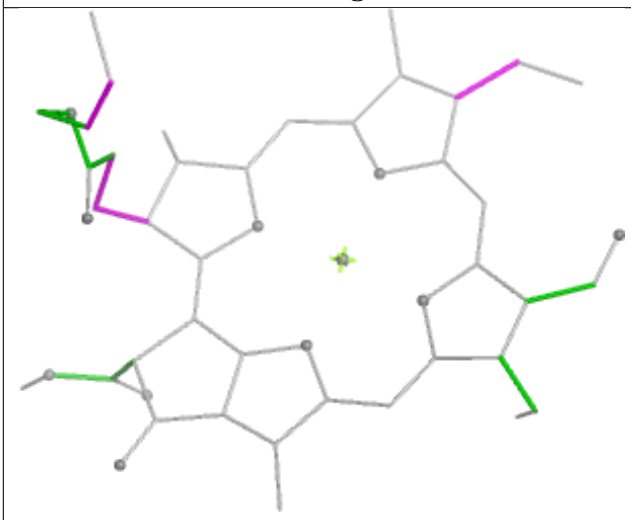
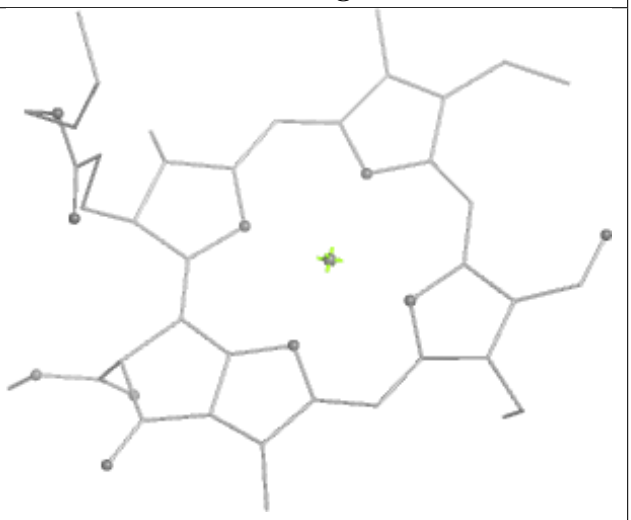
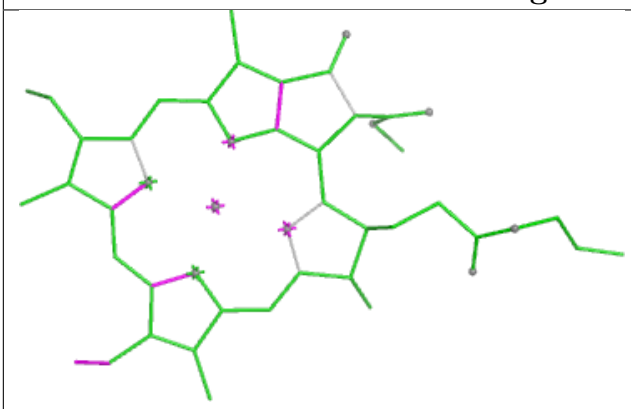
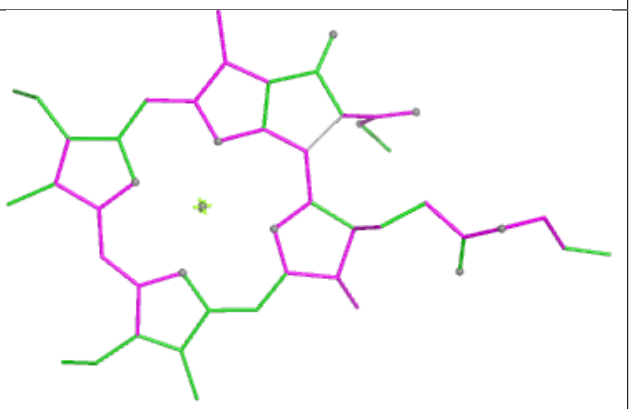
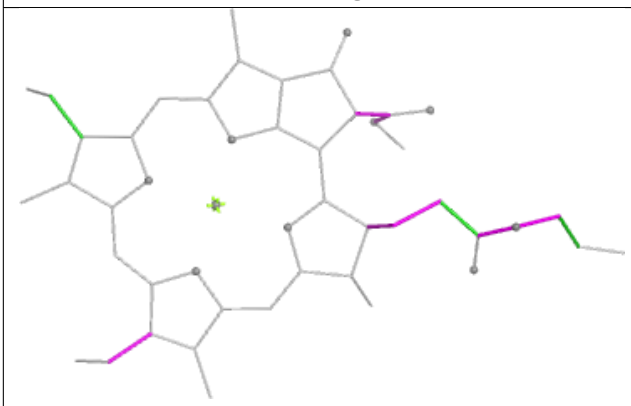
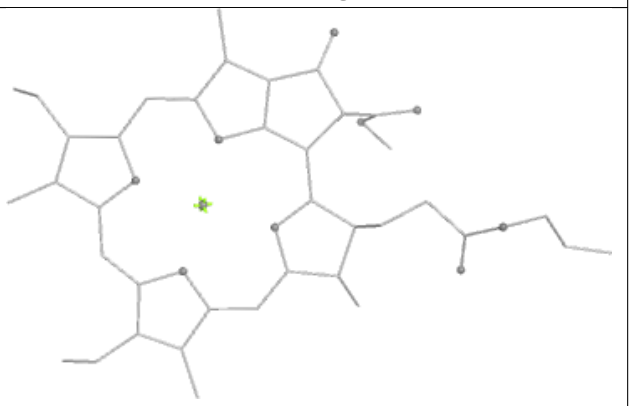
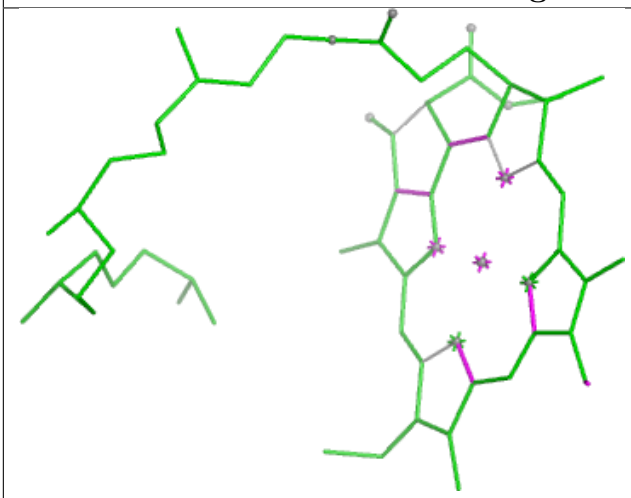
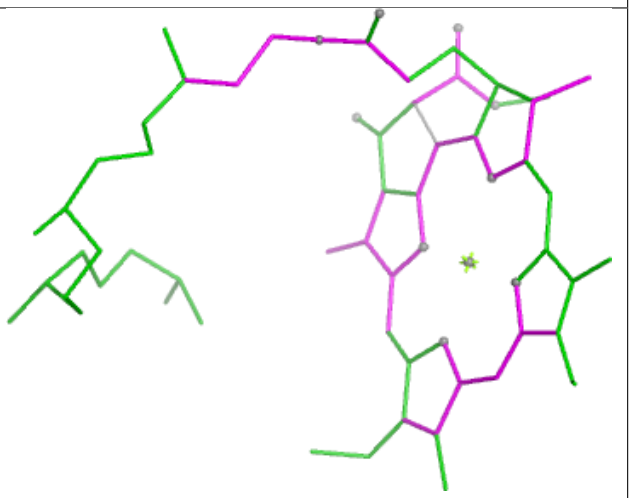
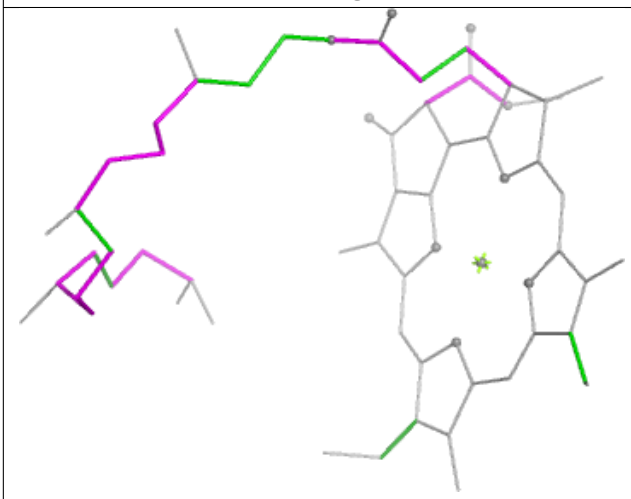
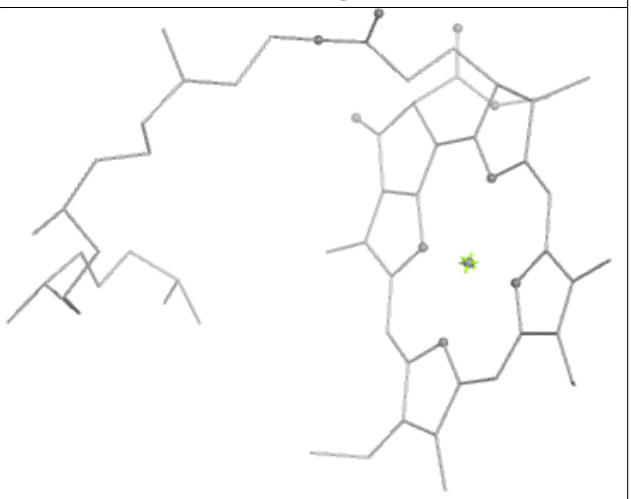
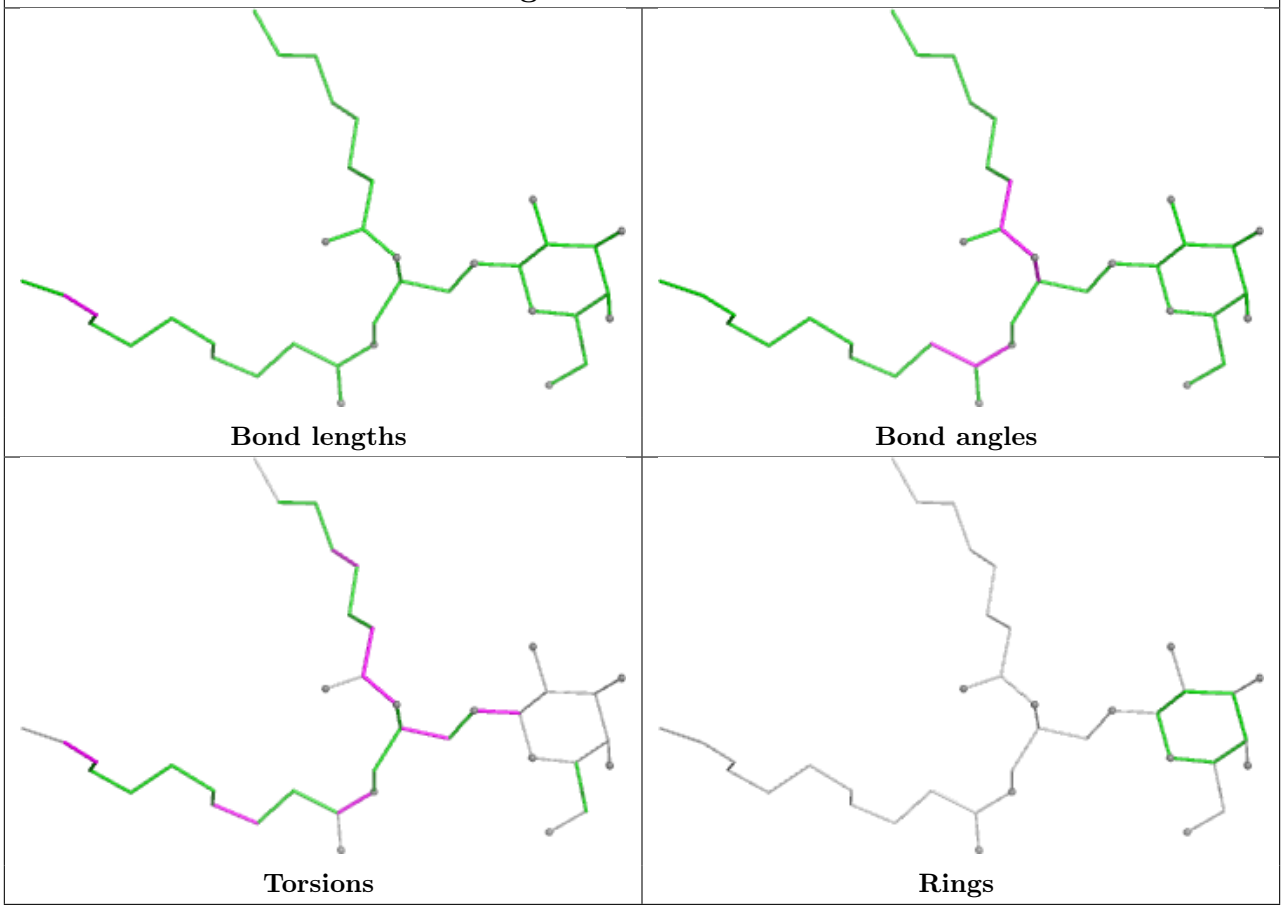
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

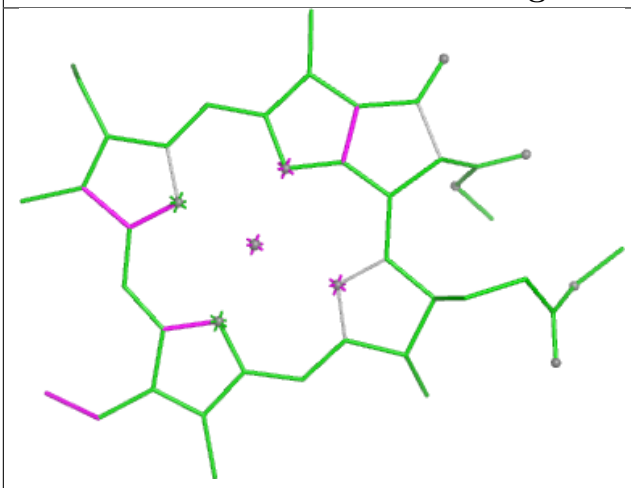
Ligand CLA r 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

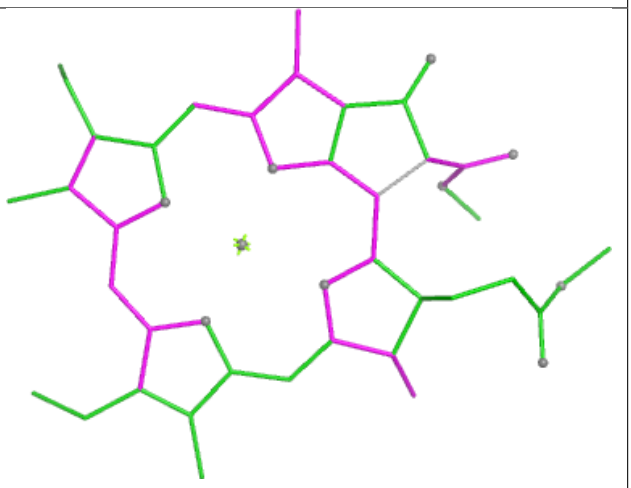
Ligand LMG A 418



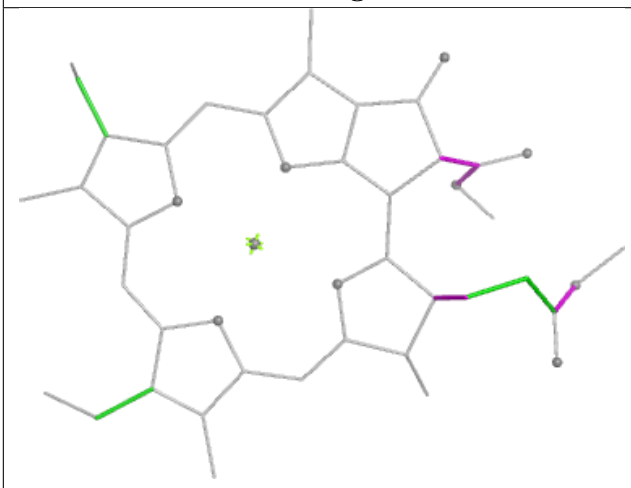
Ligand CLA 0 612



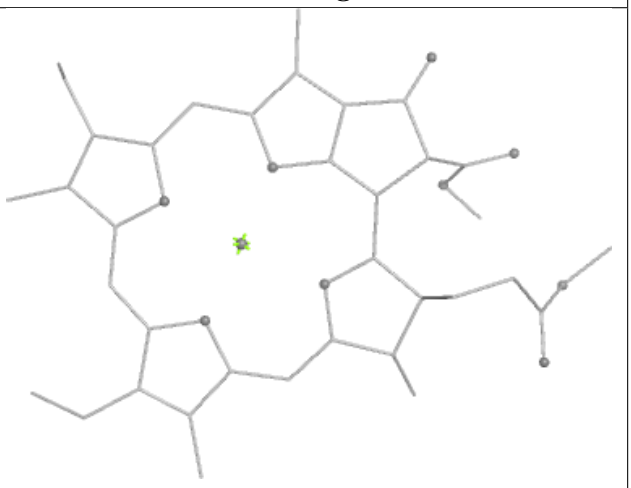
Bond lengths



Bond angles

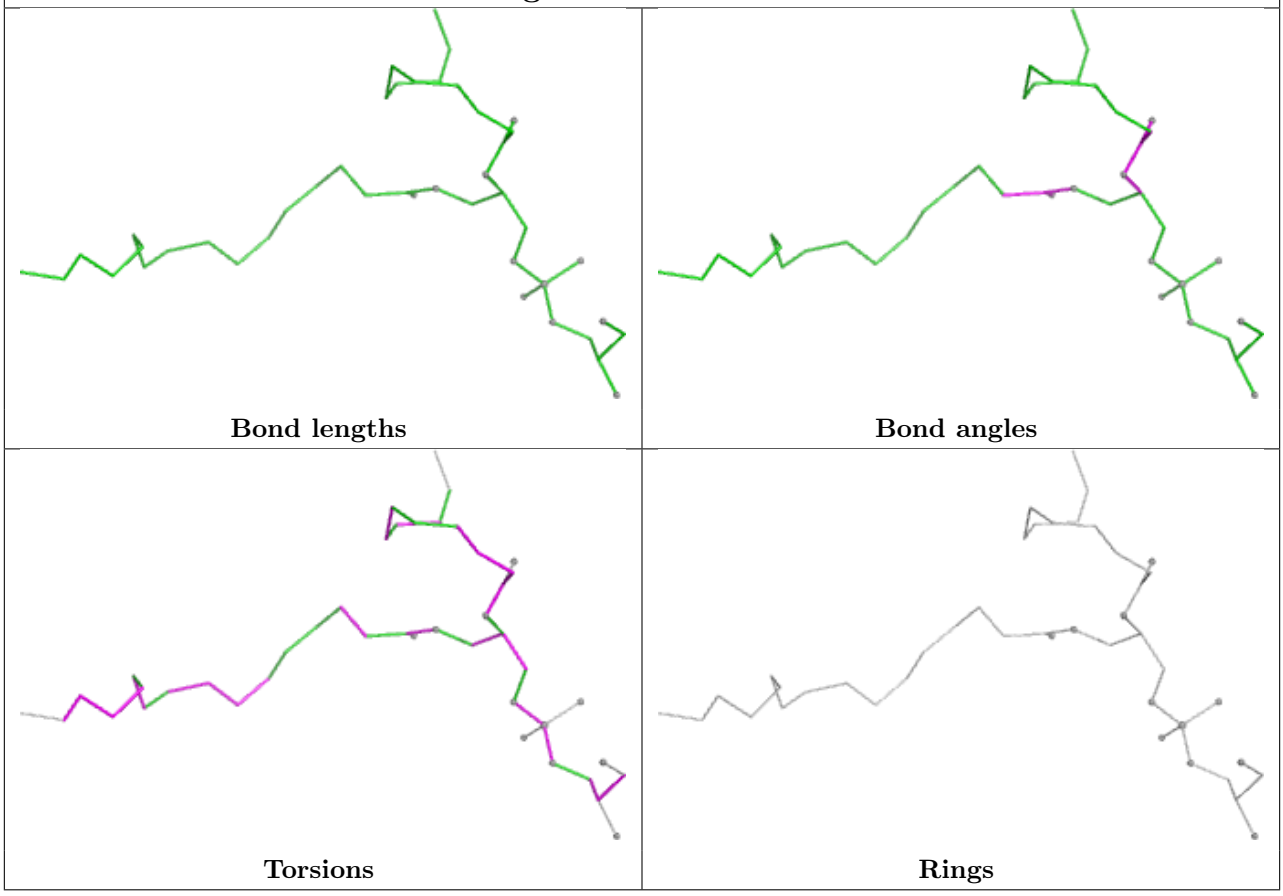


Torsions

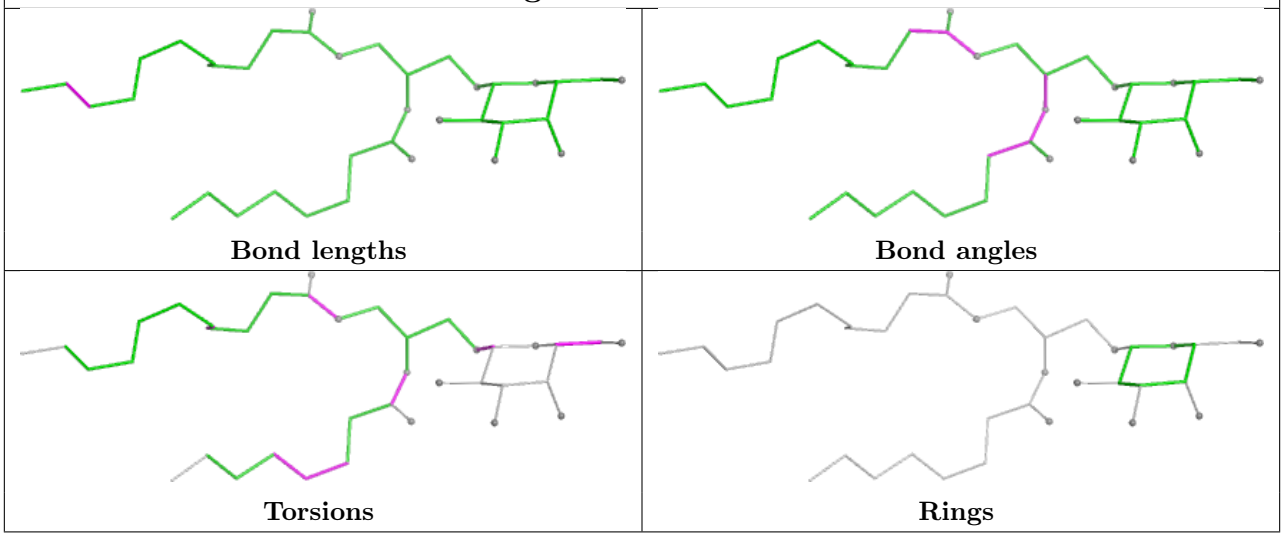


Rings

Ligand LHG A 415



Ligand LMG k 102



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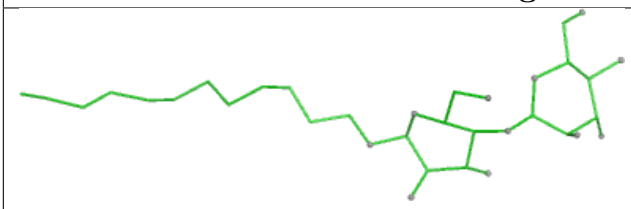
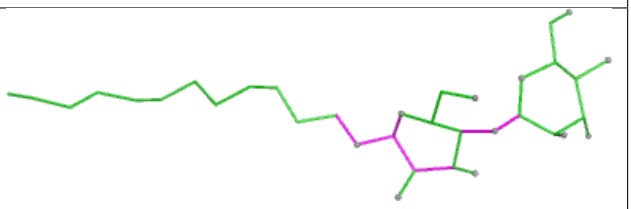
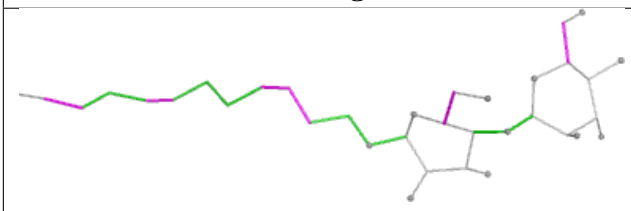
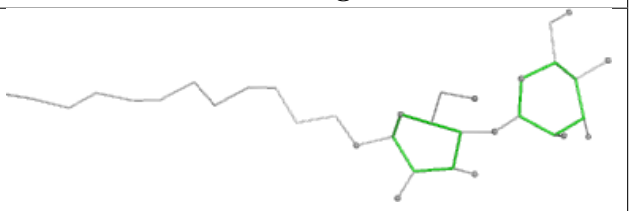
 Bond lengths	 Bond angles
 Torsions	 Rings

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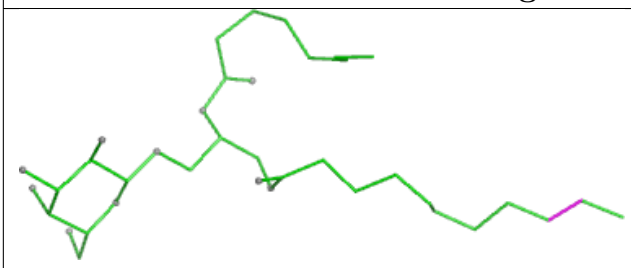
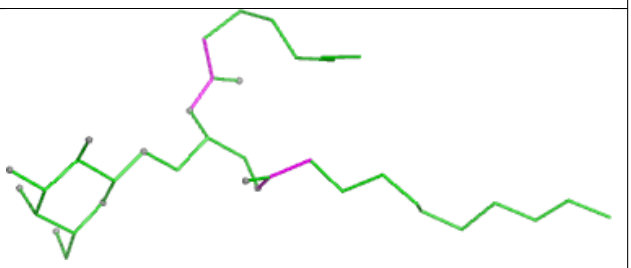
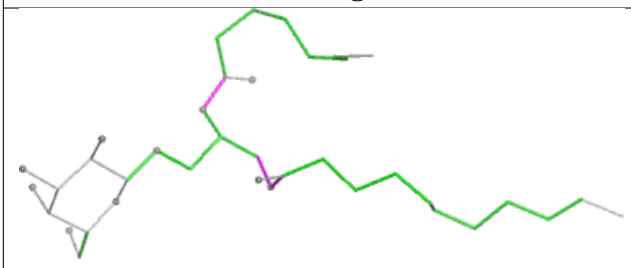
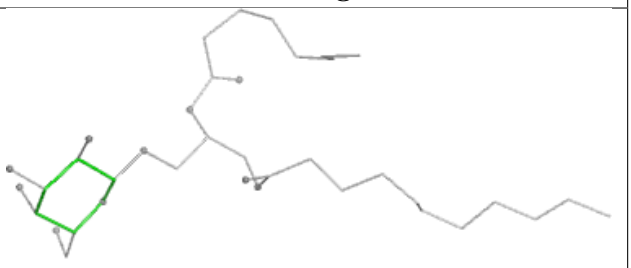
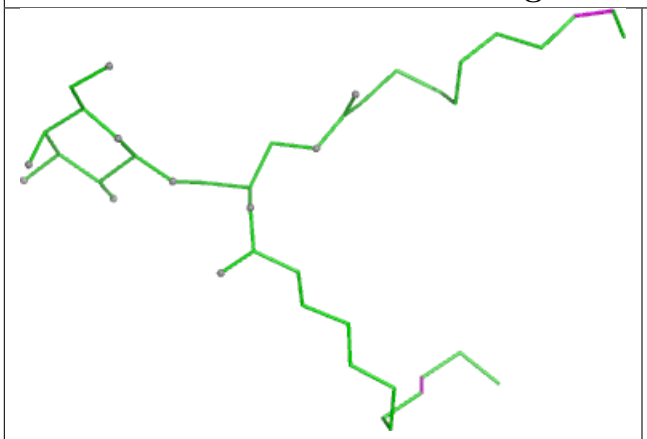
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG 0 620



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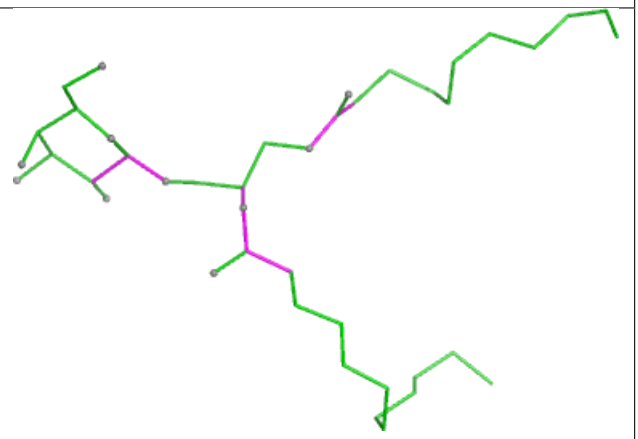
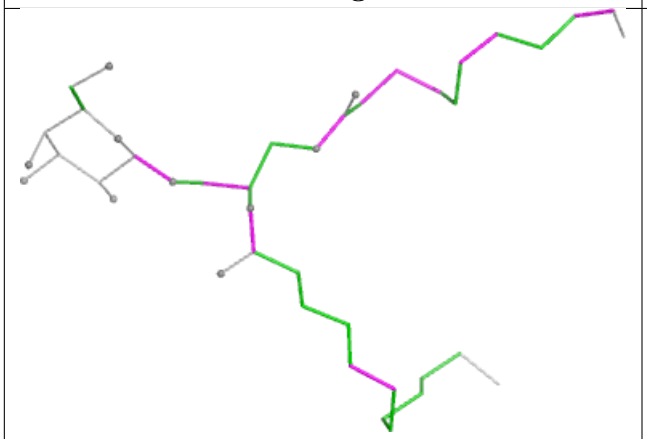


Bond angles



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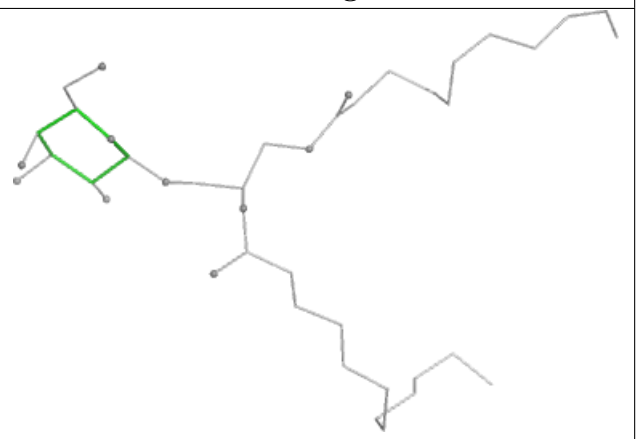
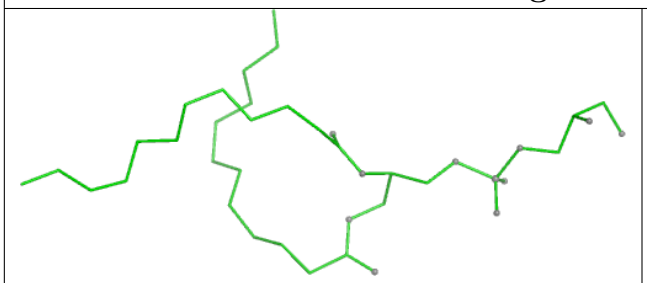


Rings

Ligand LHG s 320



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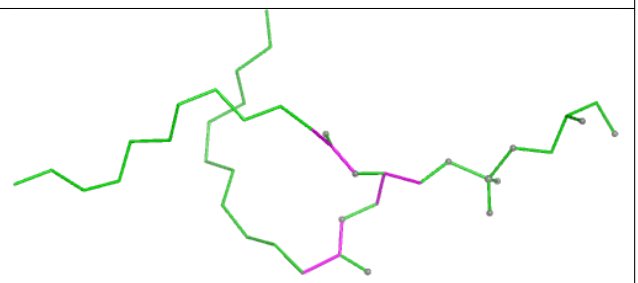
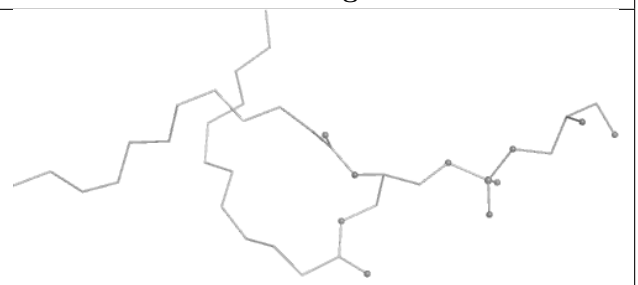
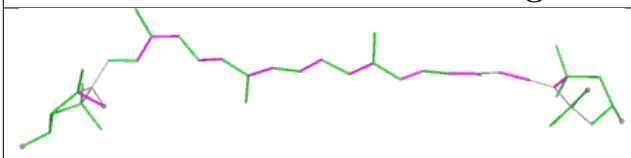
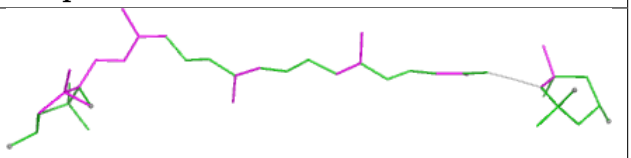
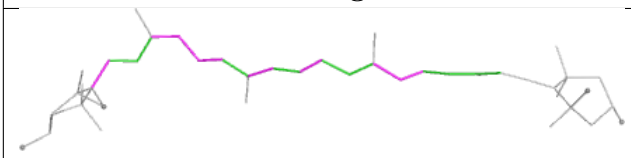
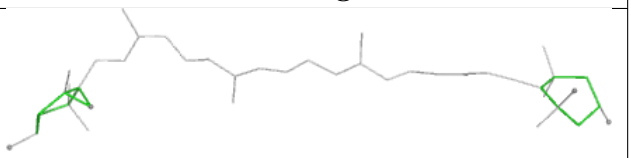


Bond angles

Torsions



Rings

Ligand NEX q 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

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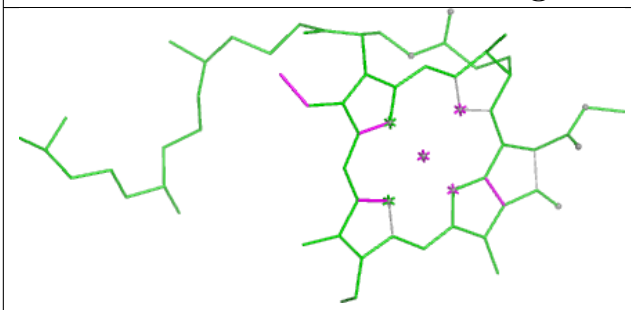
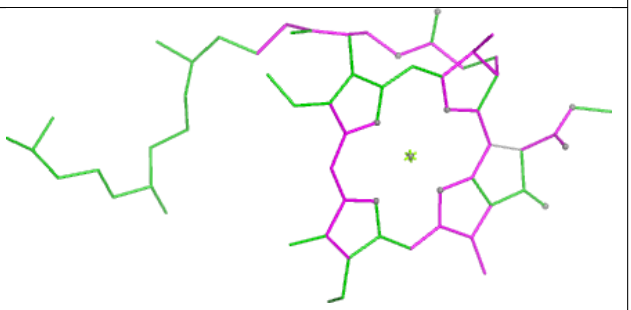
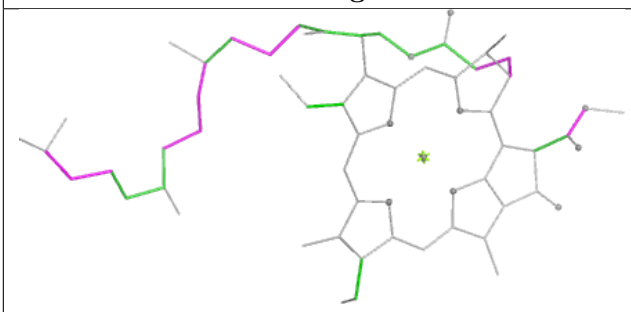
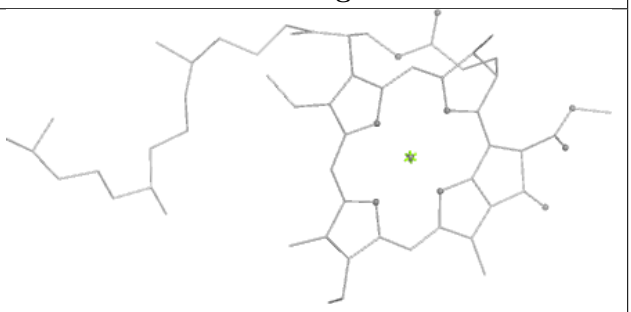
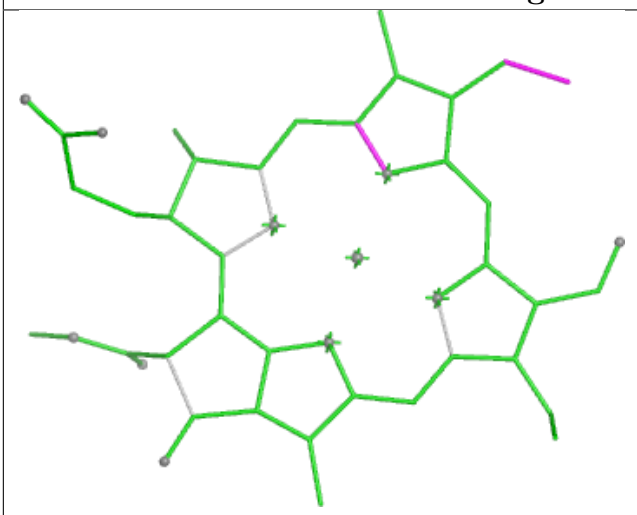
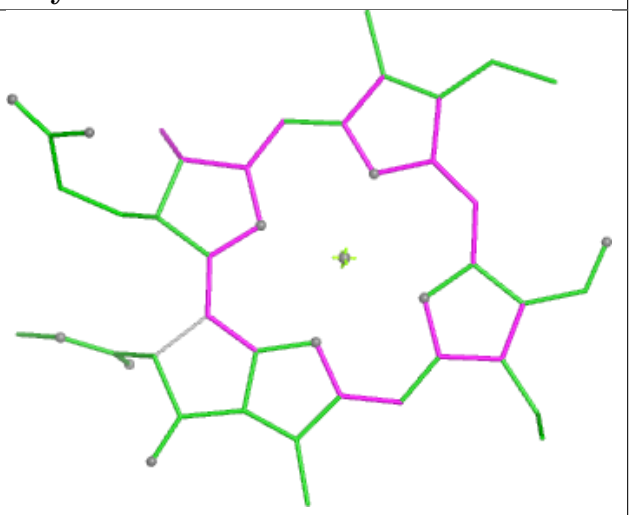
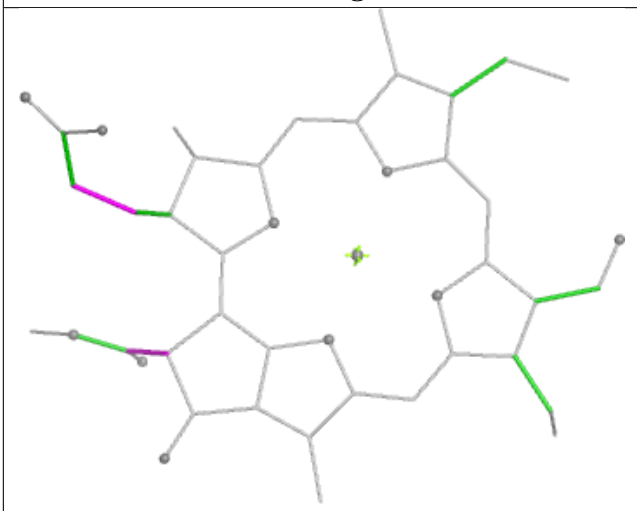
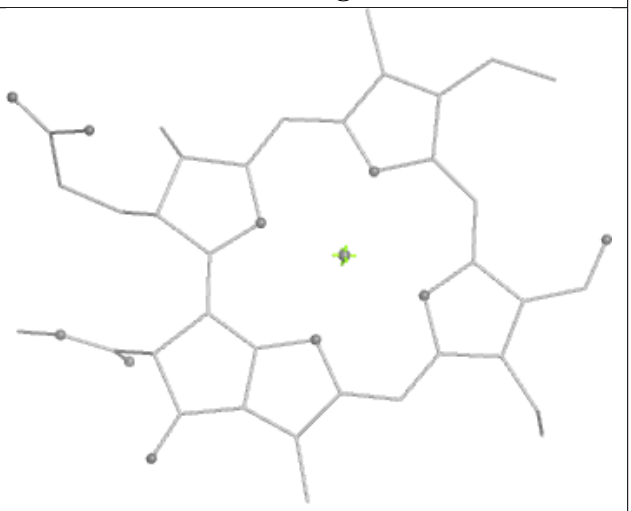
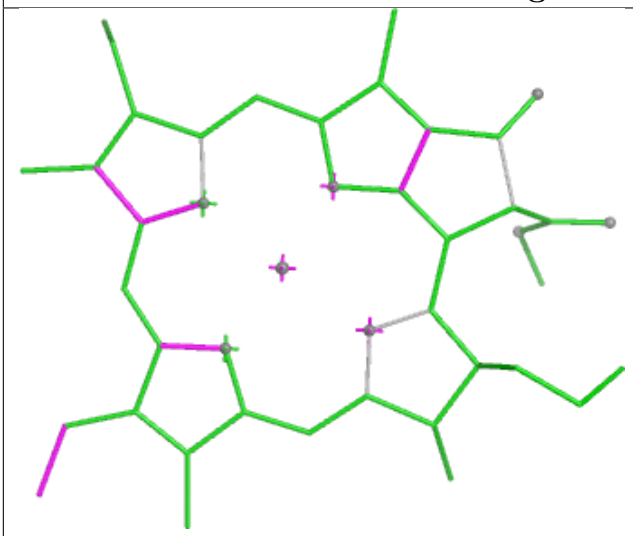
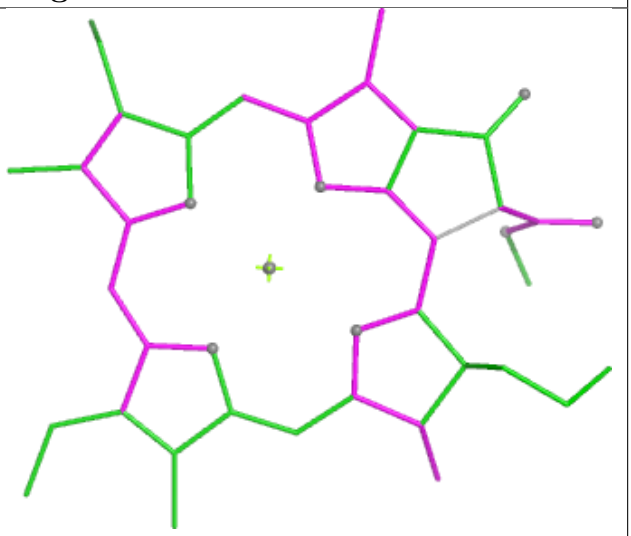
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL y 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

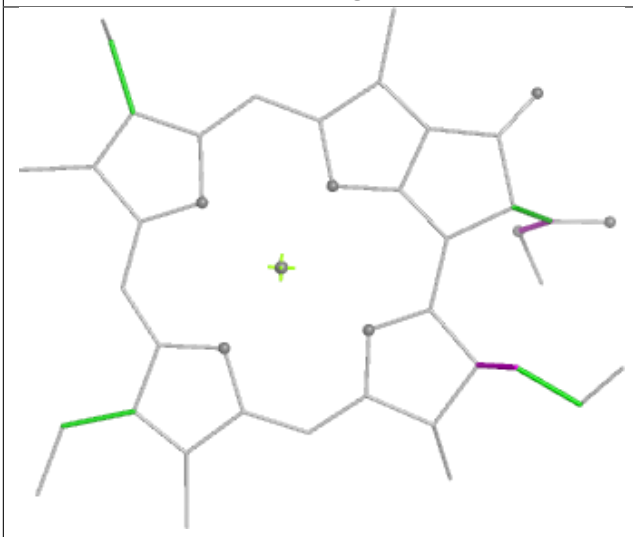
Ligand CLA g 312



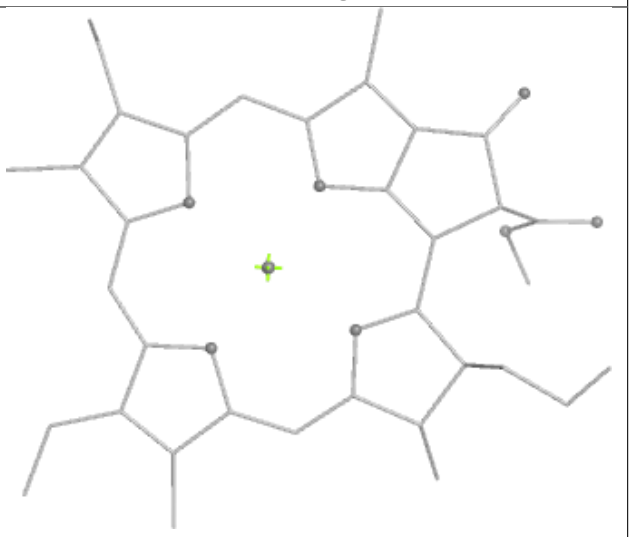
Bond lengths



Bond angles

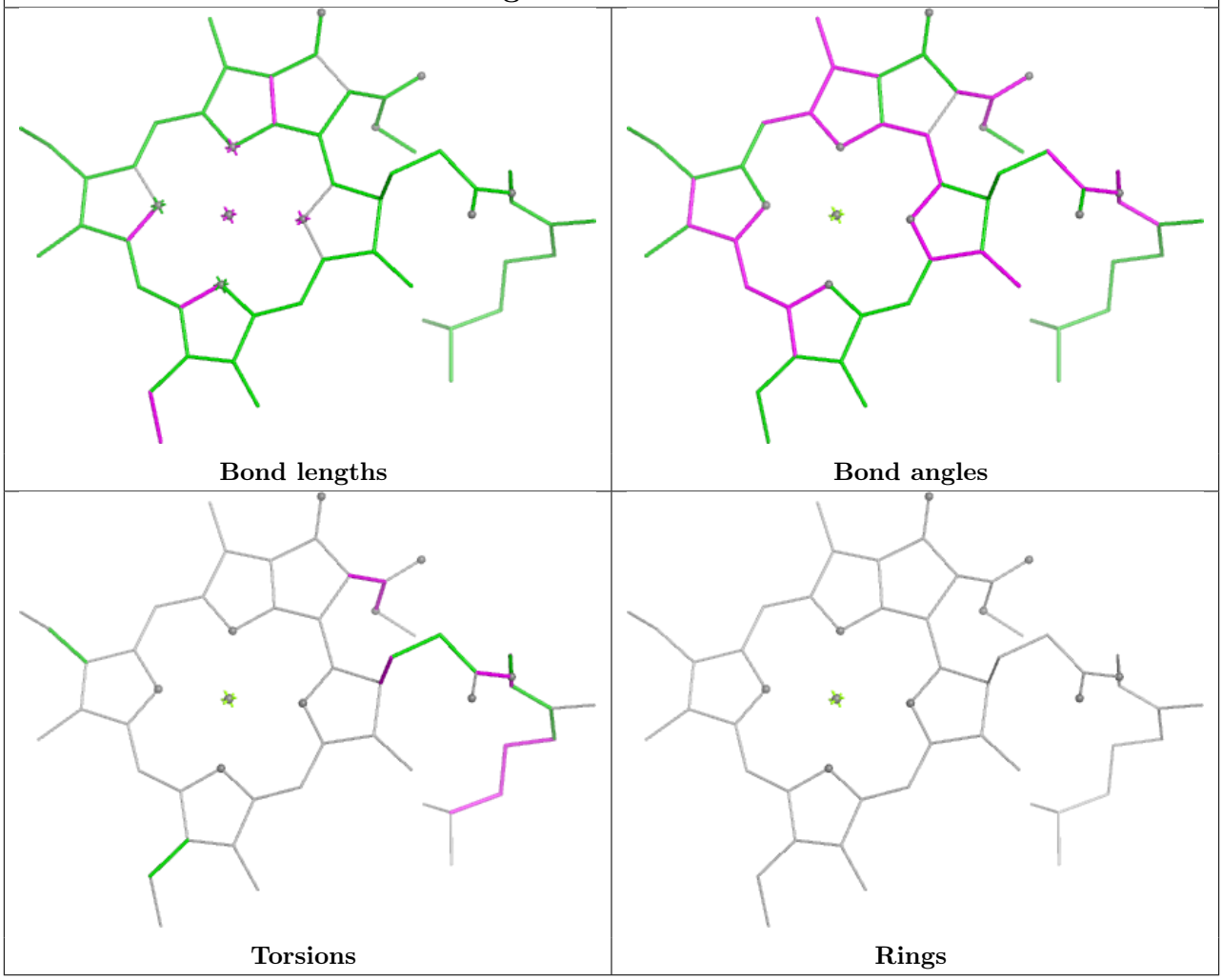


Torsions

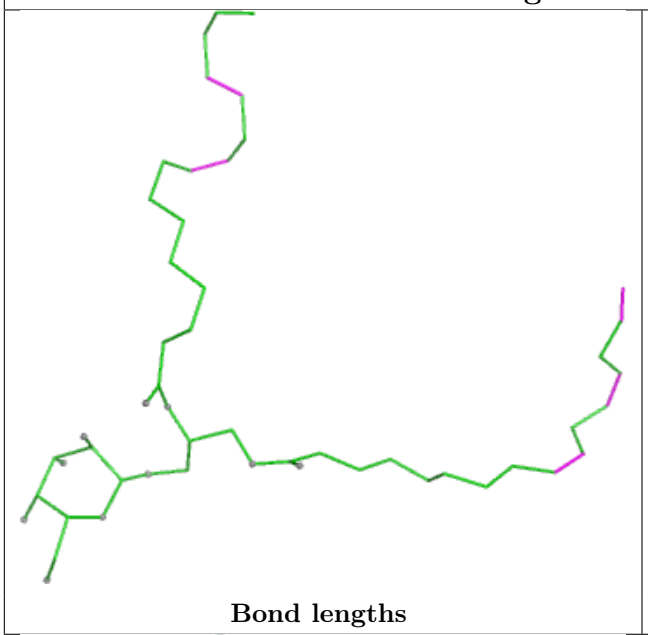


Rings

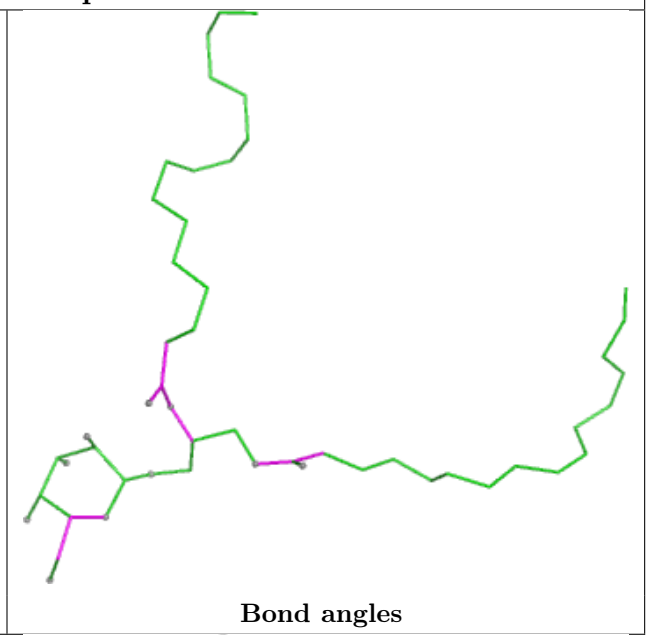
Ligand CLA n 304



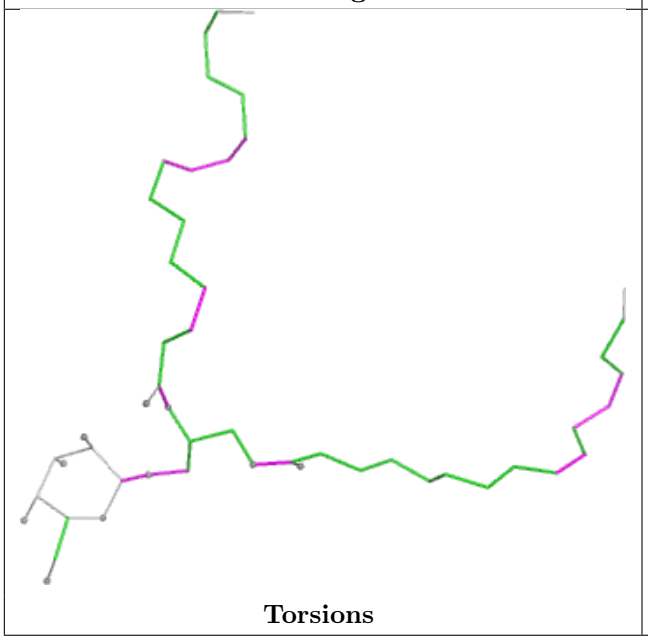
Ligand LMG q 301



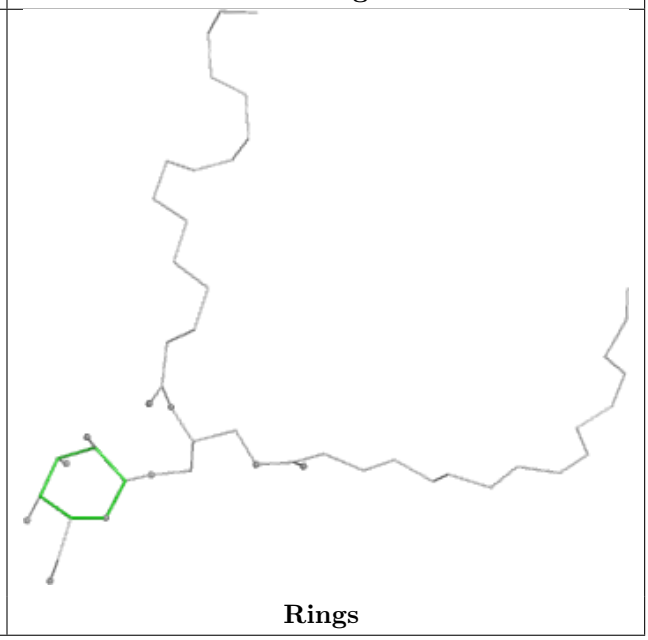
Bond lengths



Bond angles

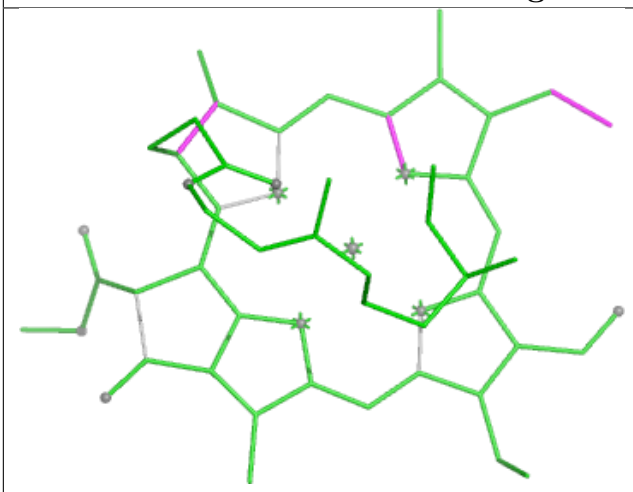


Torsions



Rings

Ligand CHL q 309



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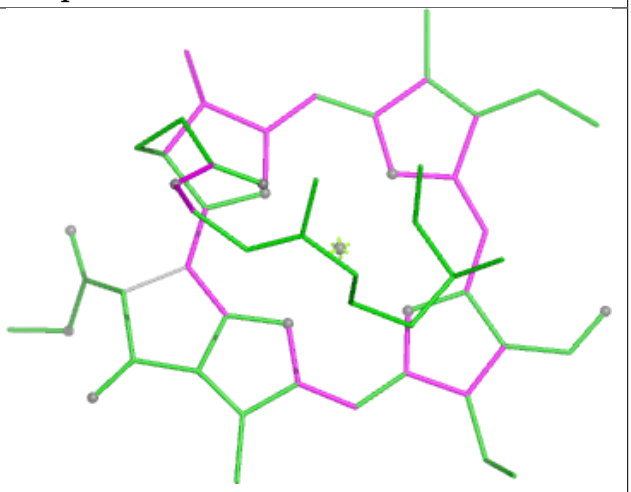
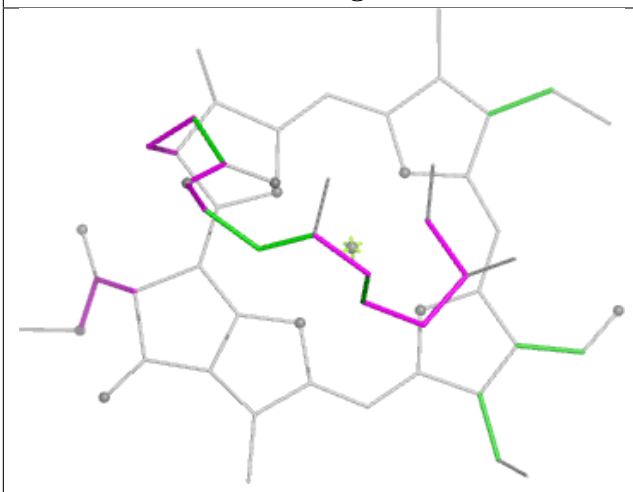


Bond angles



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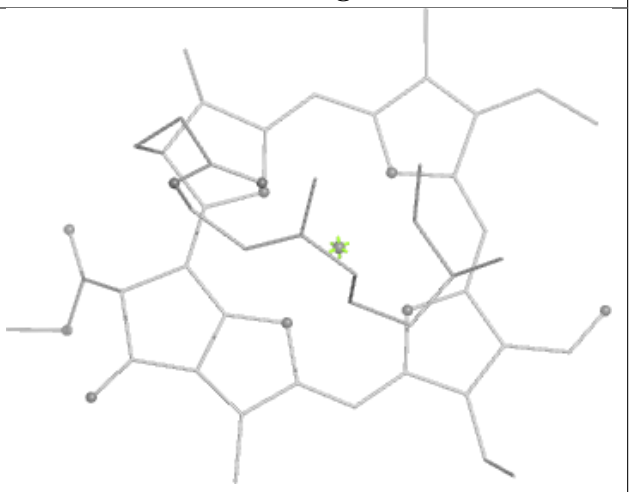
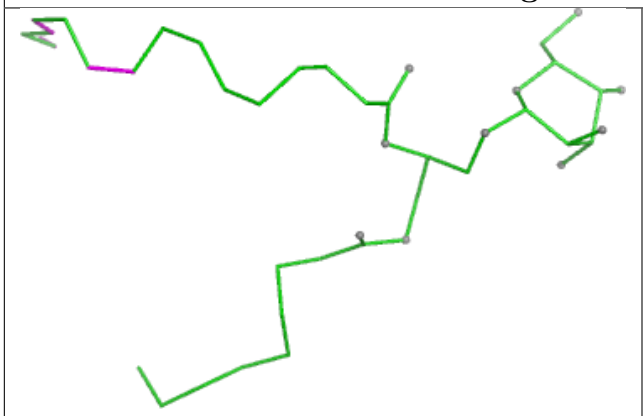
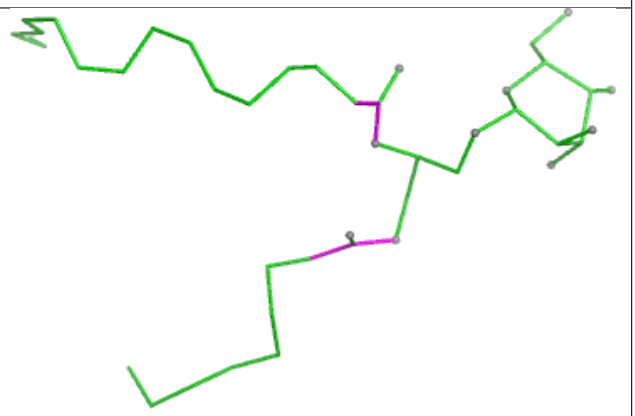
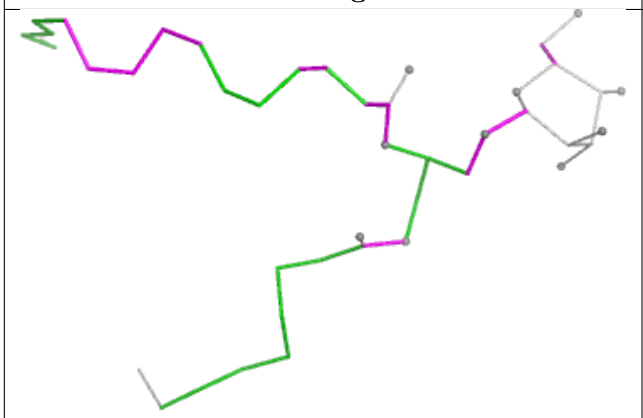
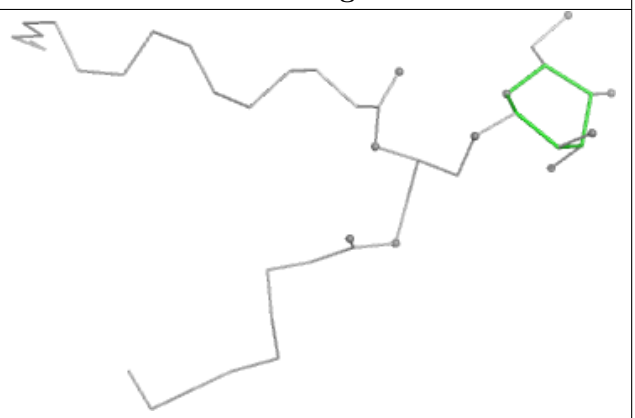
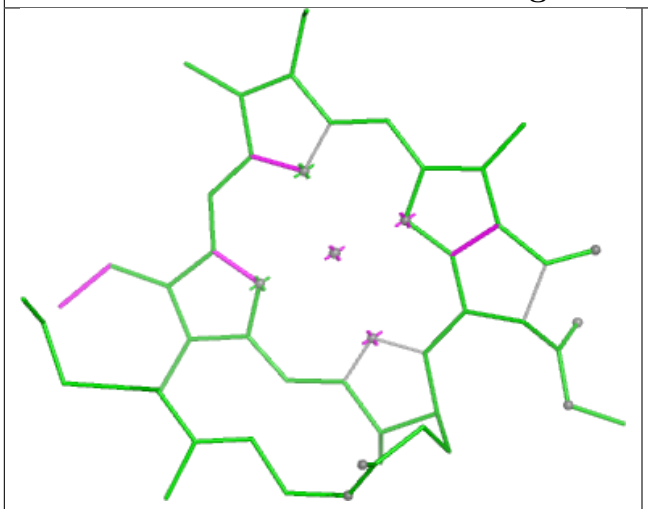


Rings

Ligand LMG C 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 312



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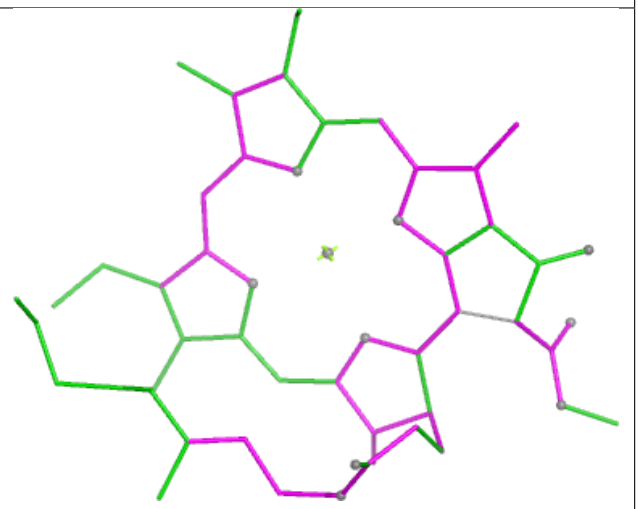
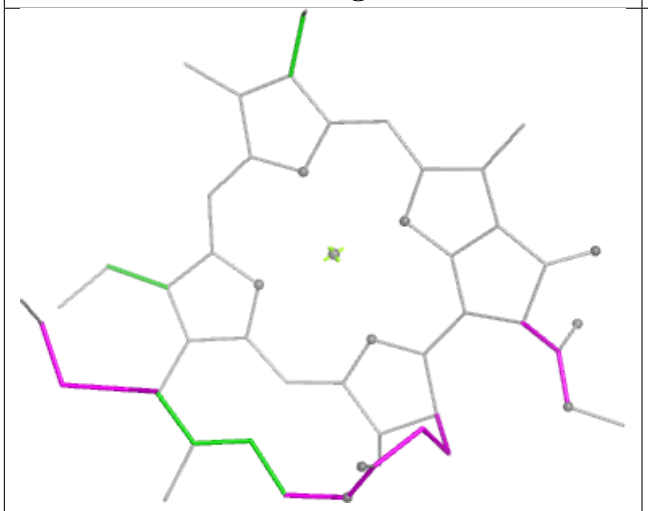


Bond angles



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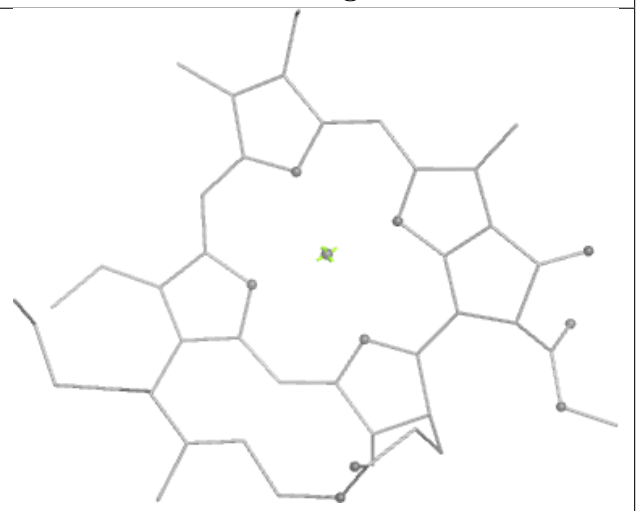
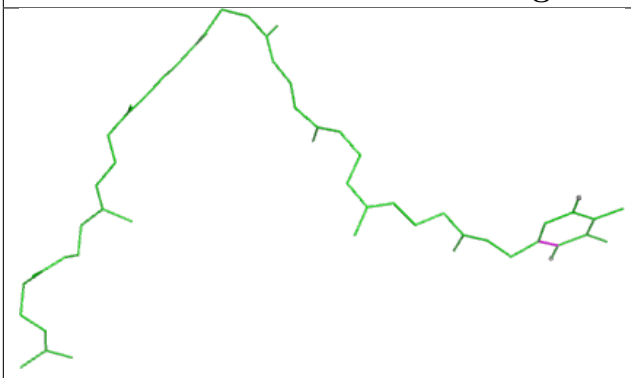
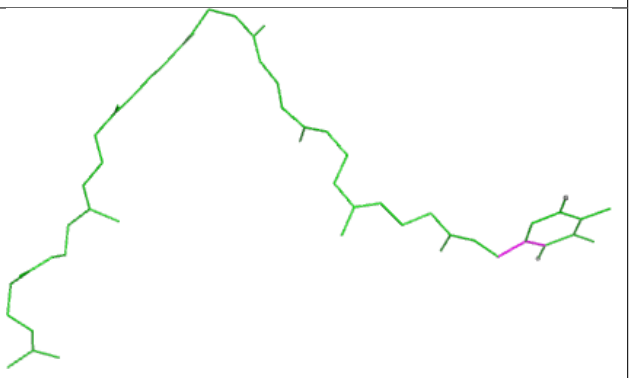


Rings

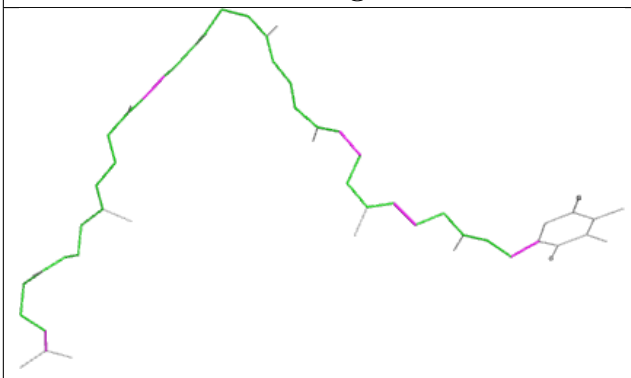
Ligand PL9 d 407



Bond lengths



Bond angles



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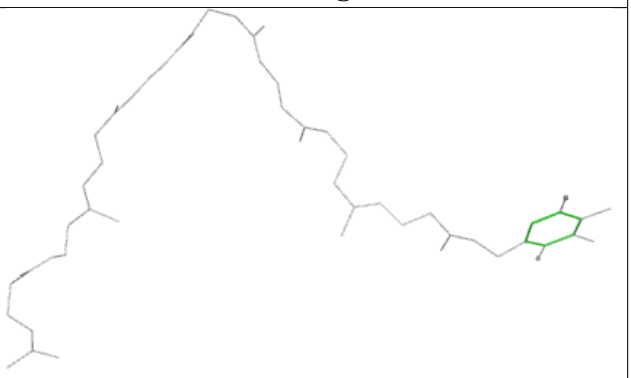
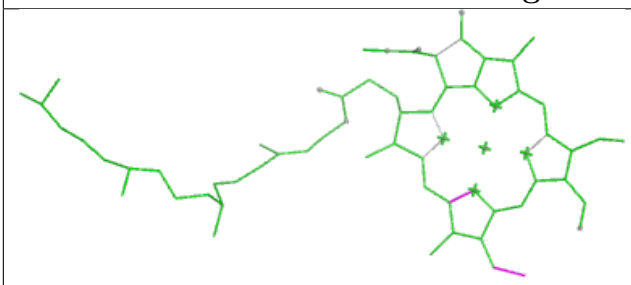


Rings

Ligand CHL G 601



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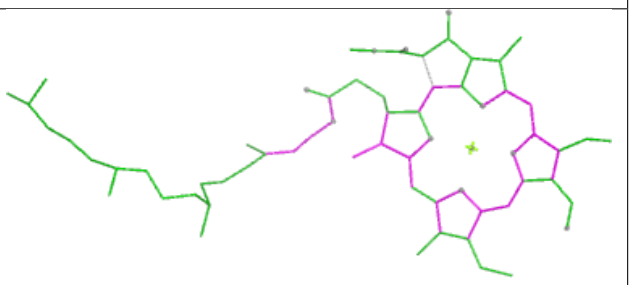
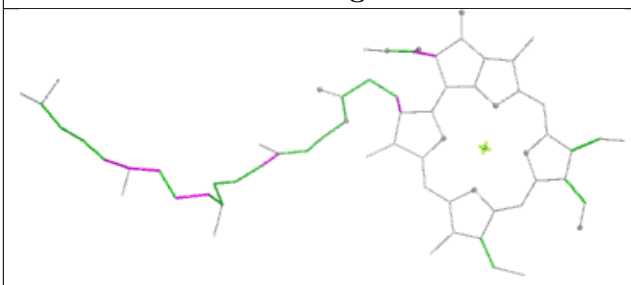


Bond angles



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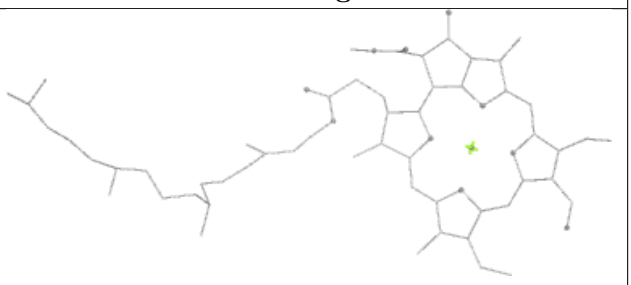
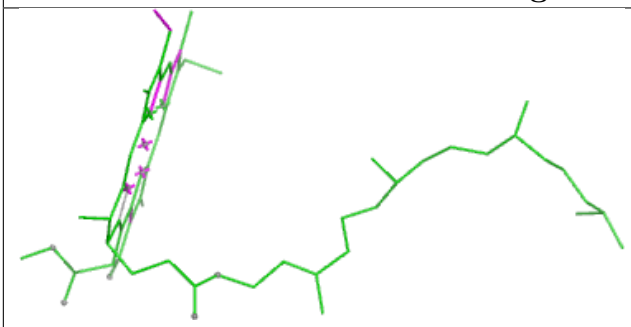
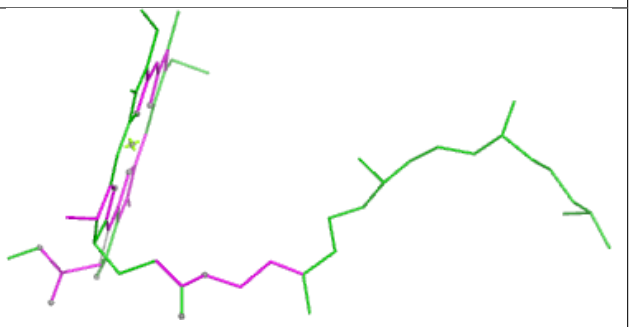
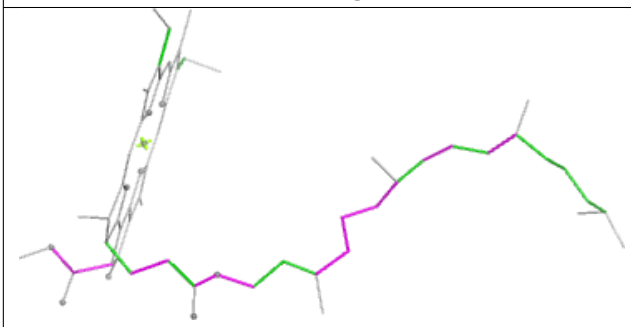
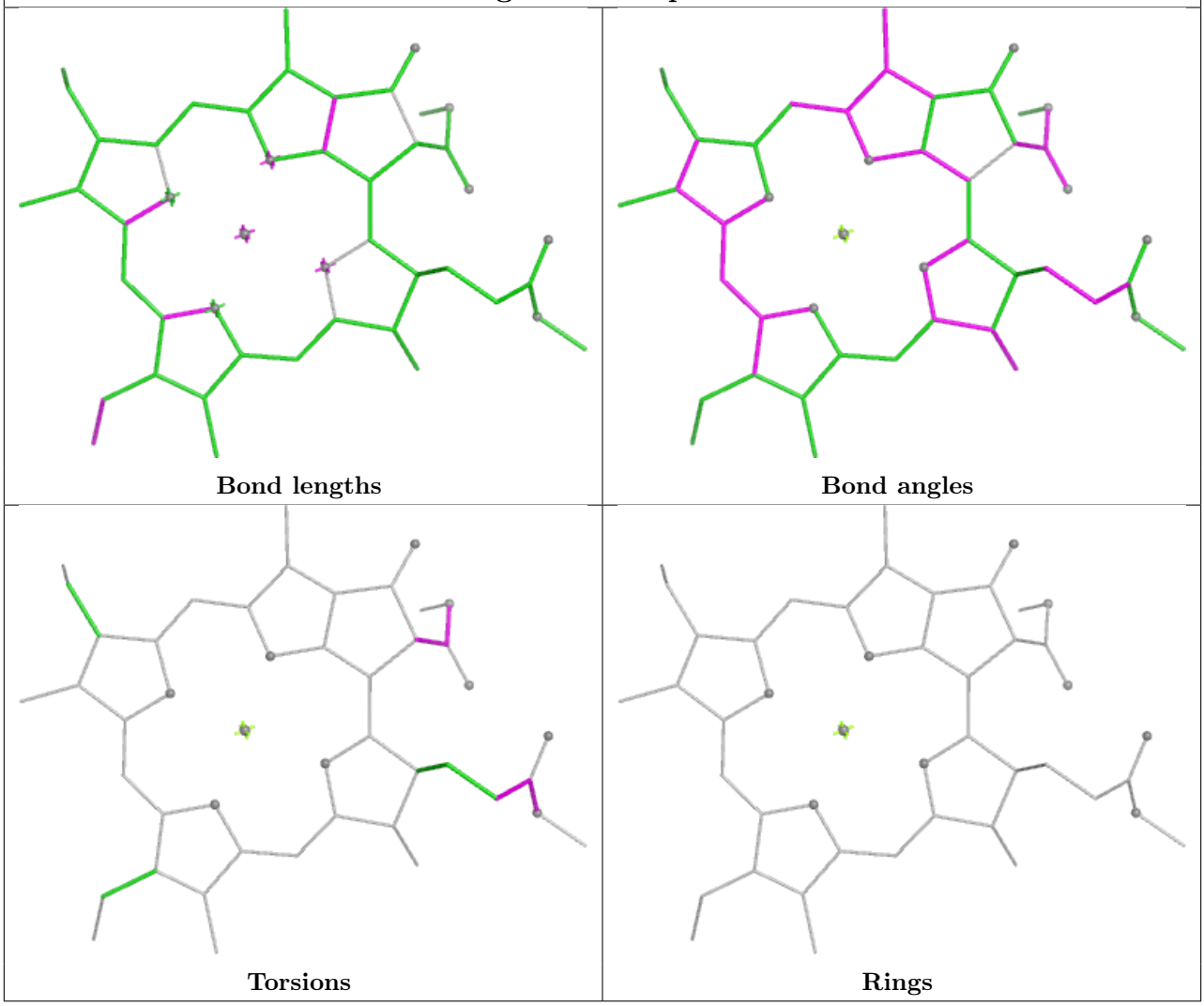


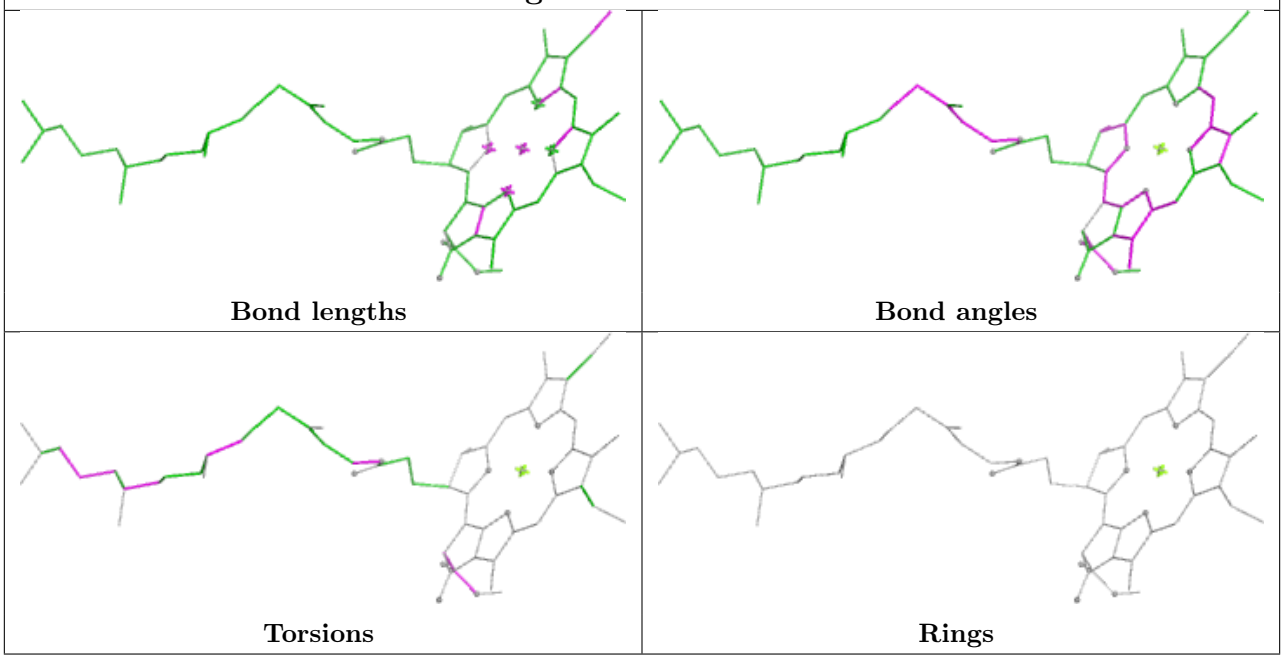
Rings

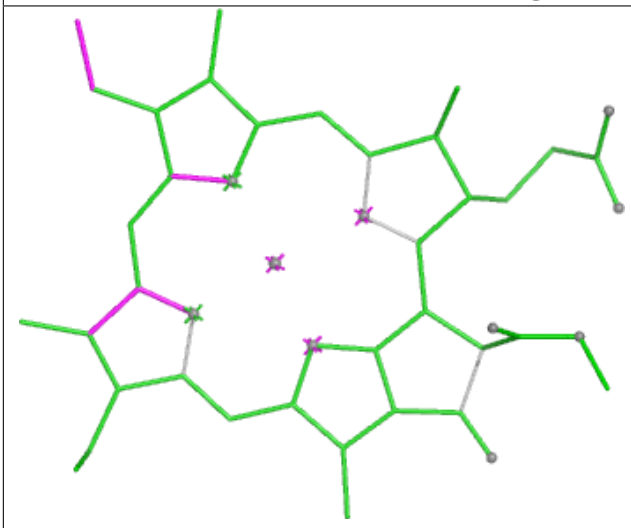
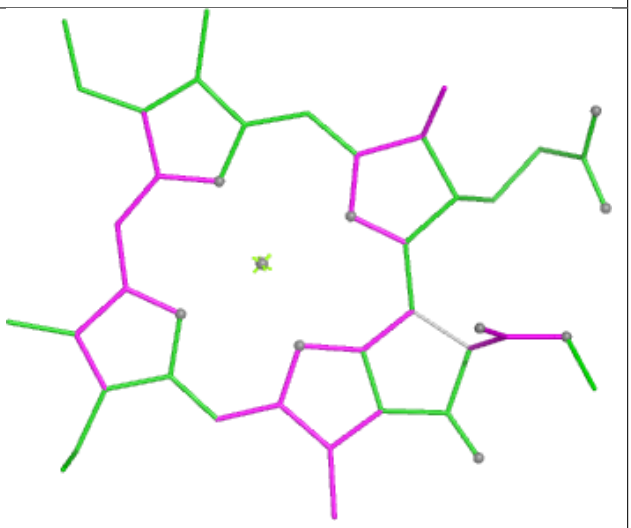
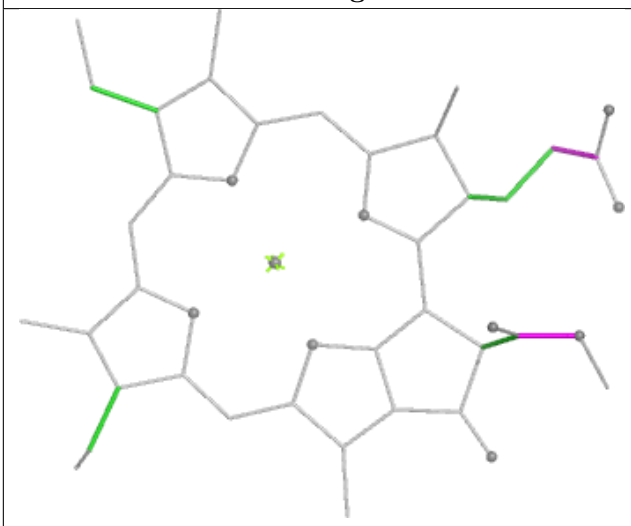
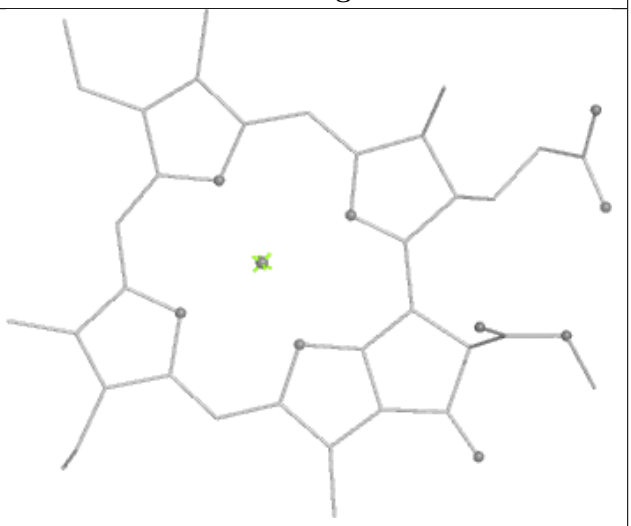
Ligand CLA s 305	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA q 314

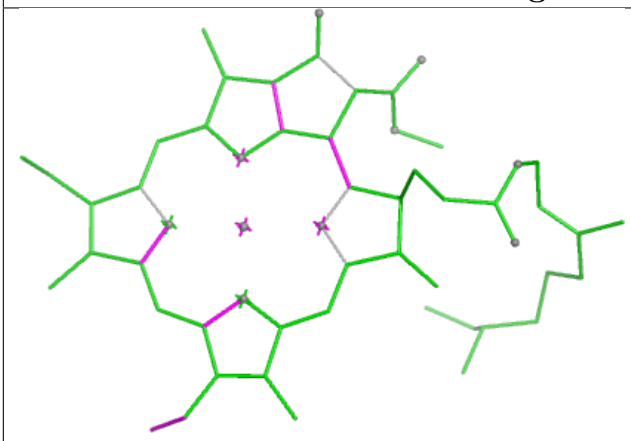


Ligand CLA C 602

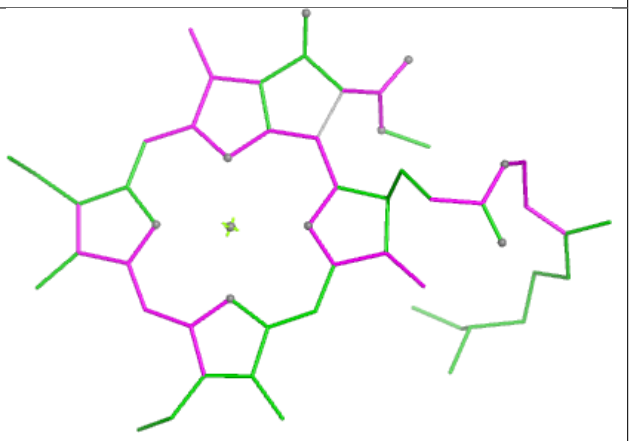


Ligand CLA n 313	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

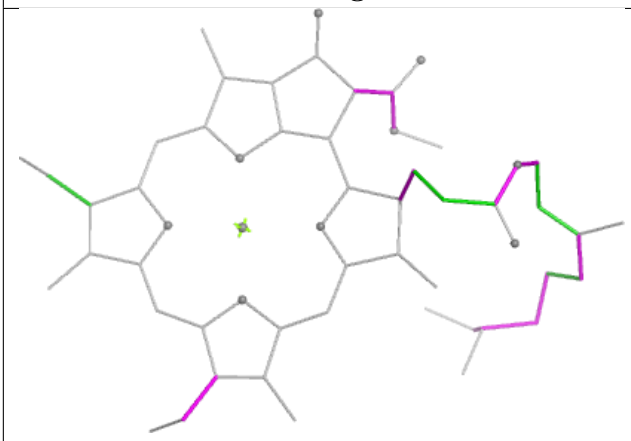
Ligand CLA 0 603



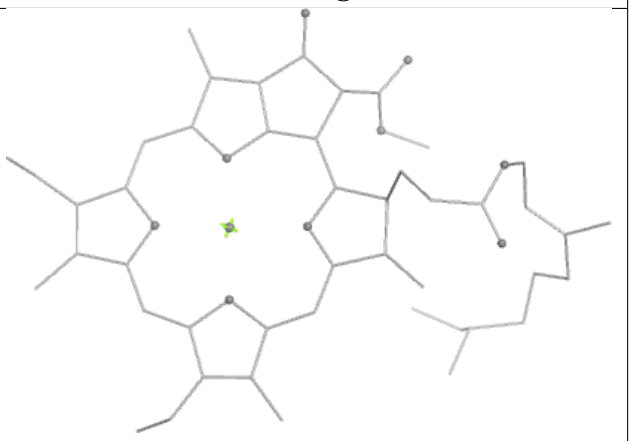
Bond lengths



Bond angles

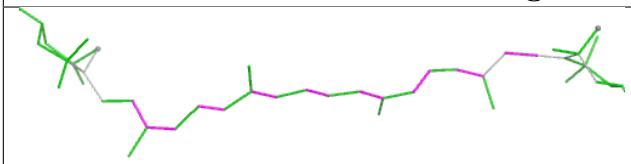


Torsions



Rings

Ligand NEX n 319



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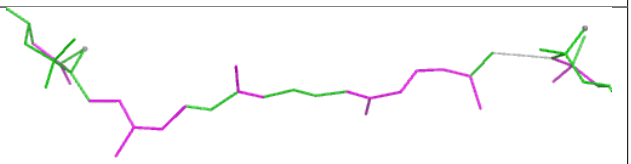
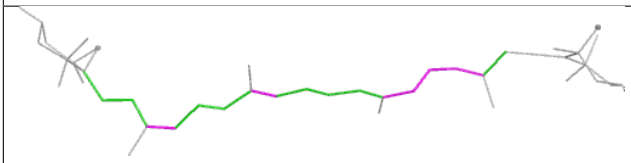


Bond angles



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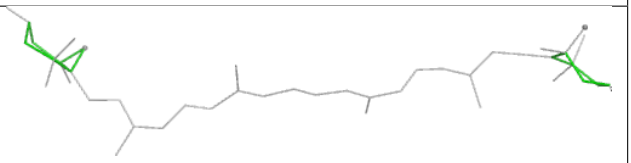
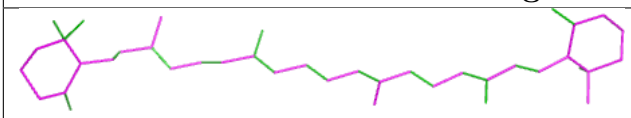


Rings

Ligand BCR B 619



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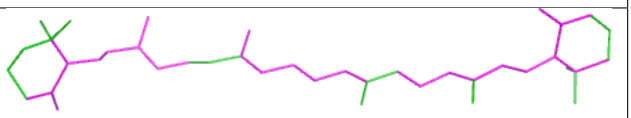
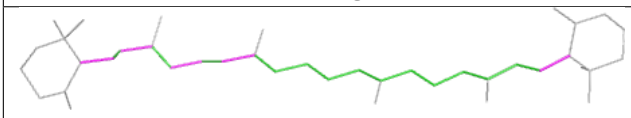


Bond angles



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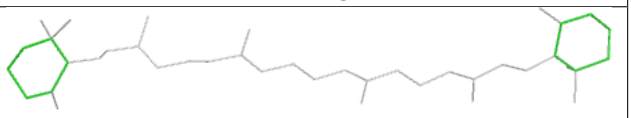
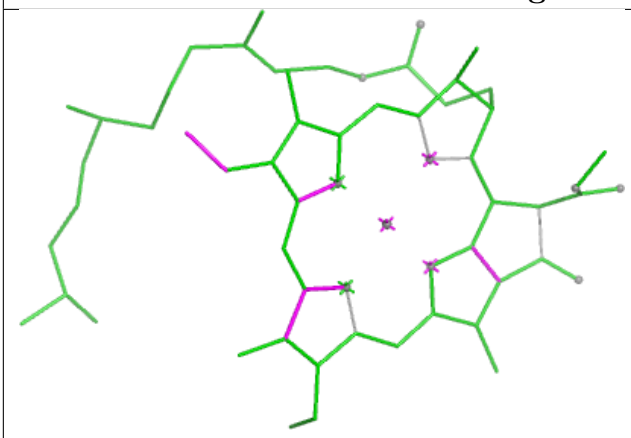


Rings

Ligand CLA 1 602



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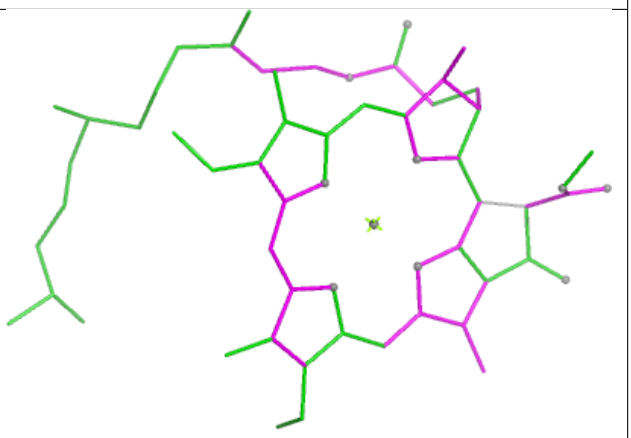
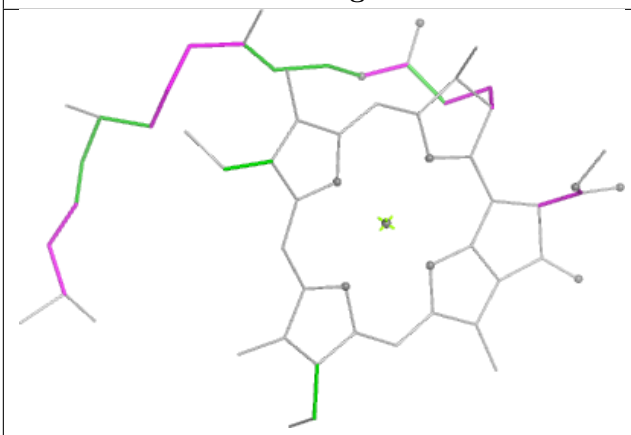


Bond angles



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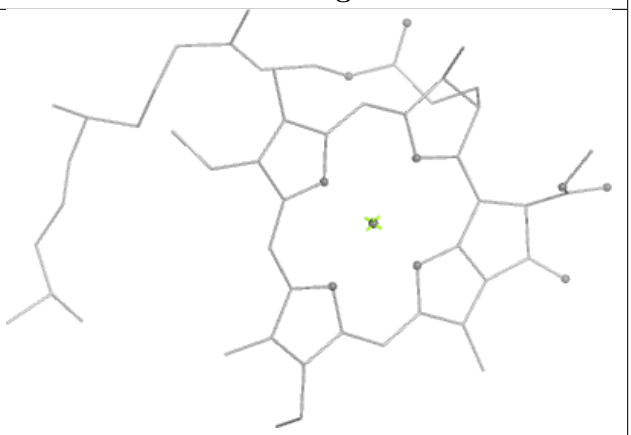
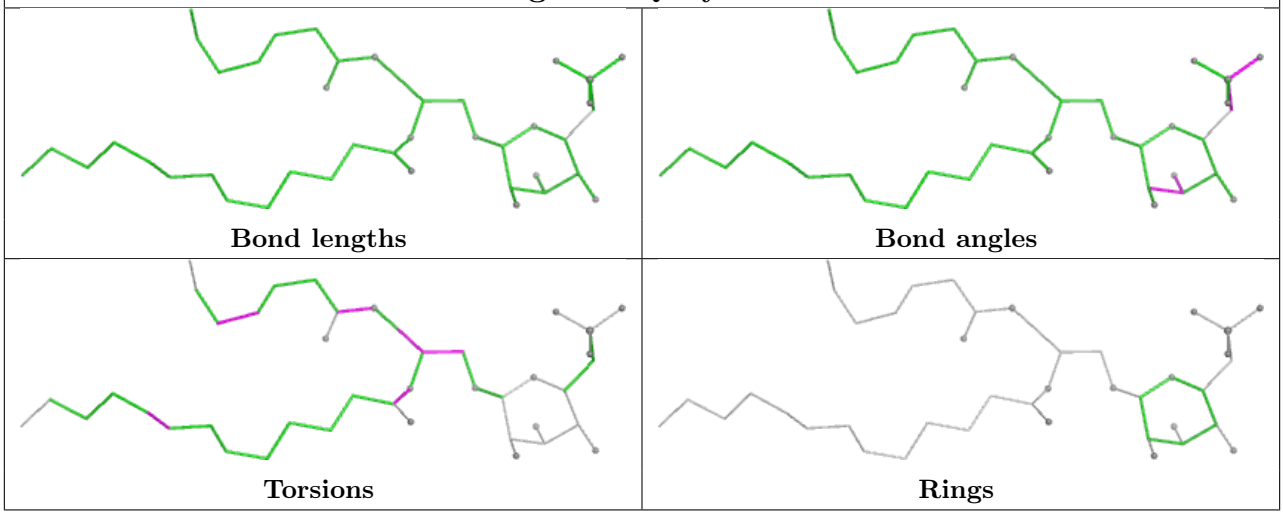
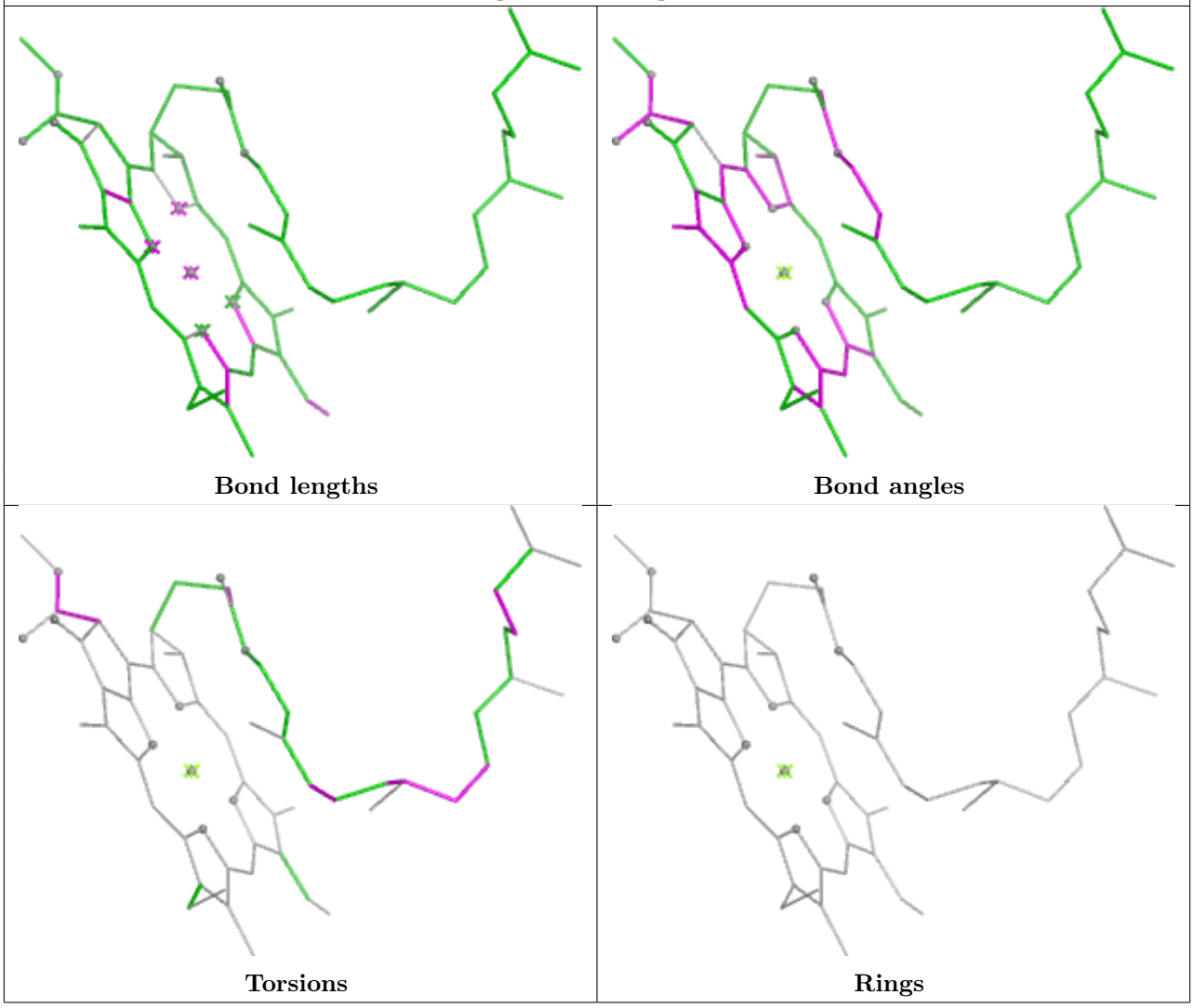


Rings

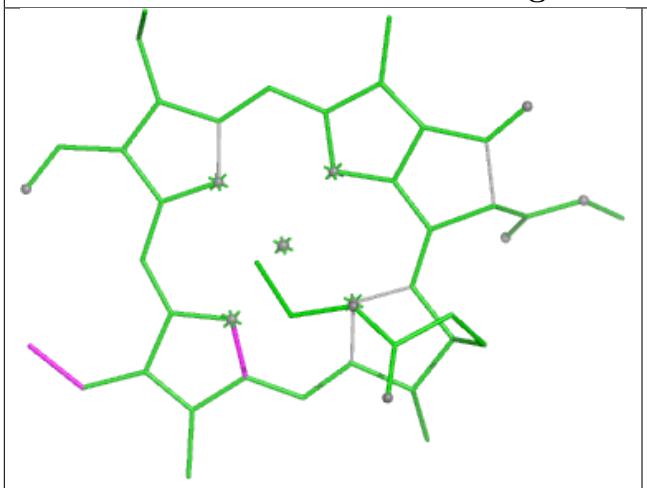
Ligand SQD y 621



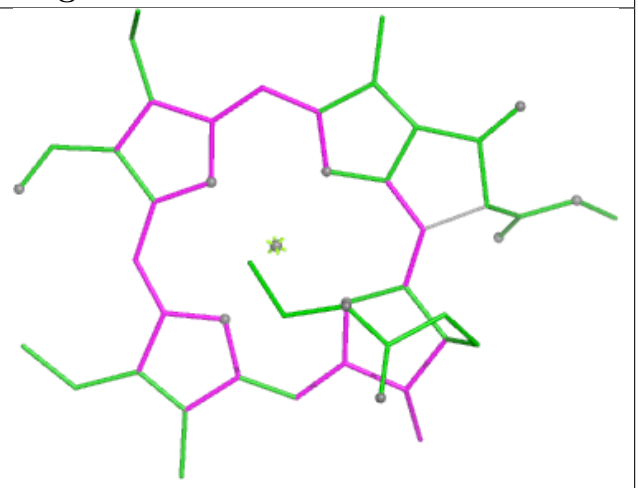
Ligand CLA g 313



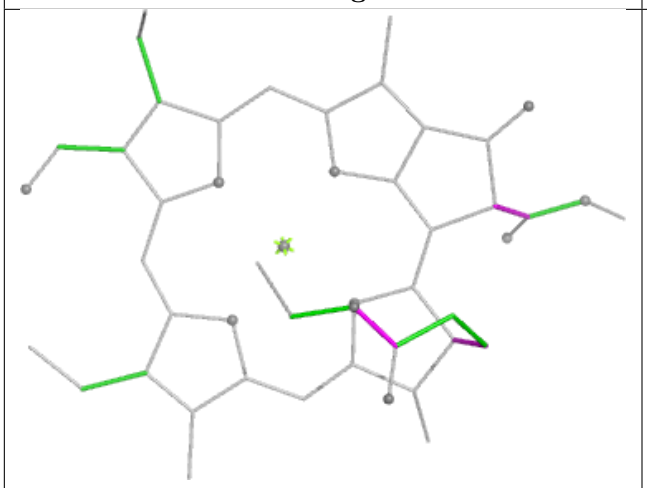
Ligand CHL g 306



Bond lengths



Bond angles



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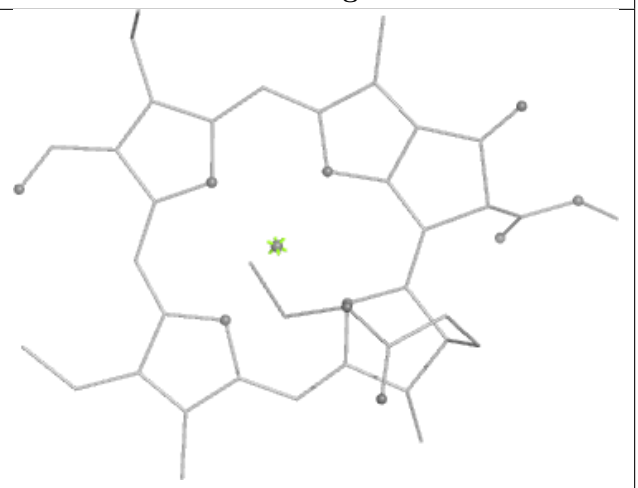
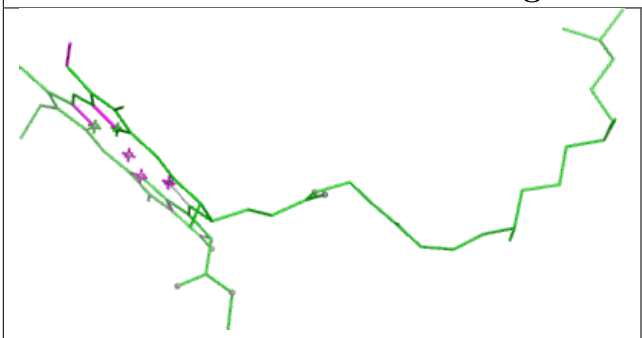
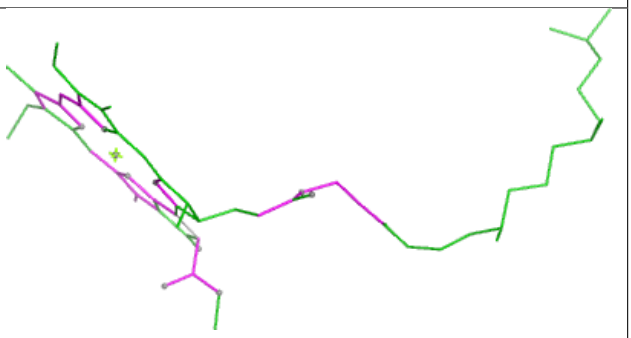
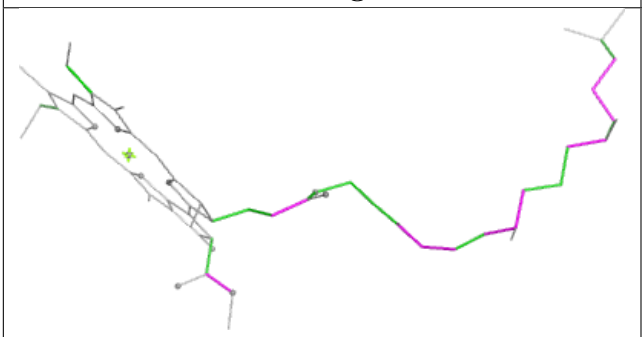
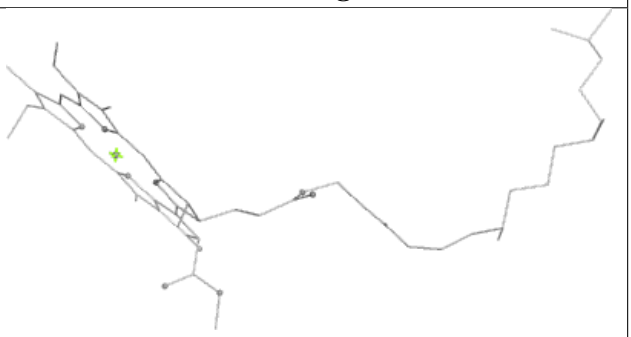
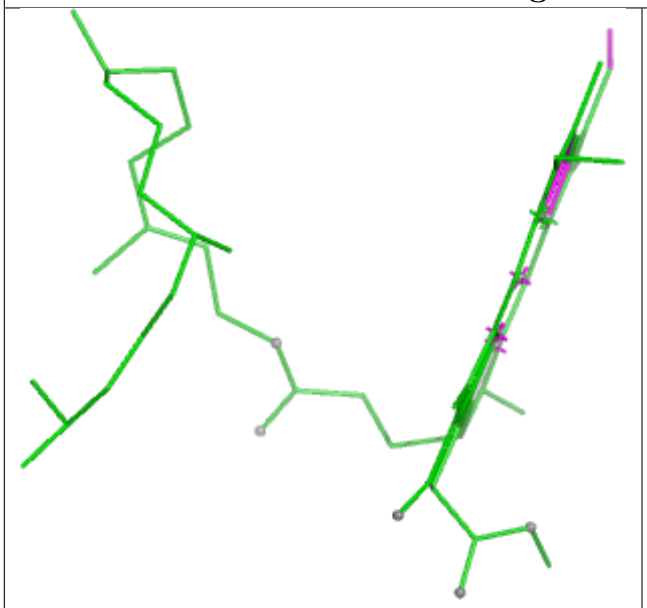


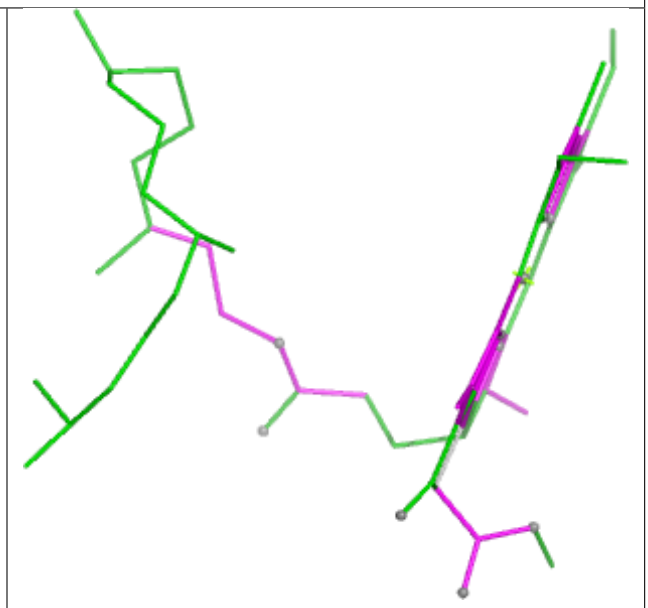
Rings

Ligand CLA D 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

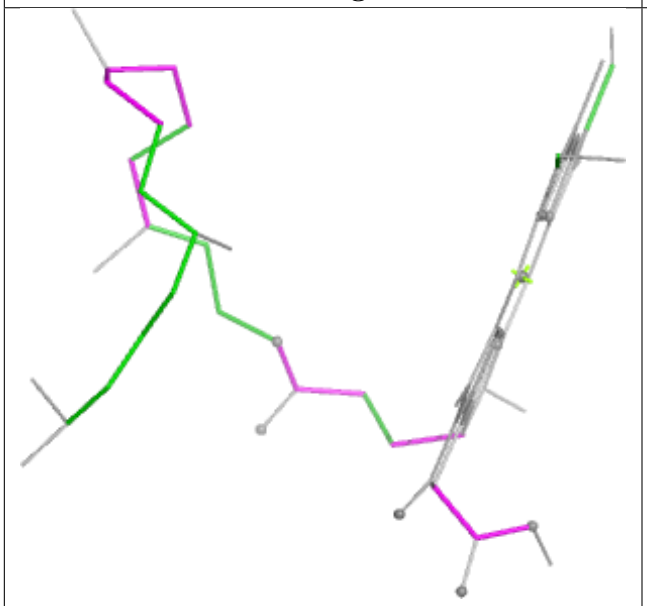
Ligand CLA 9 306



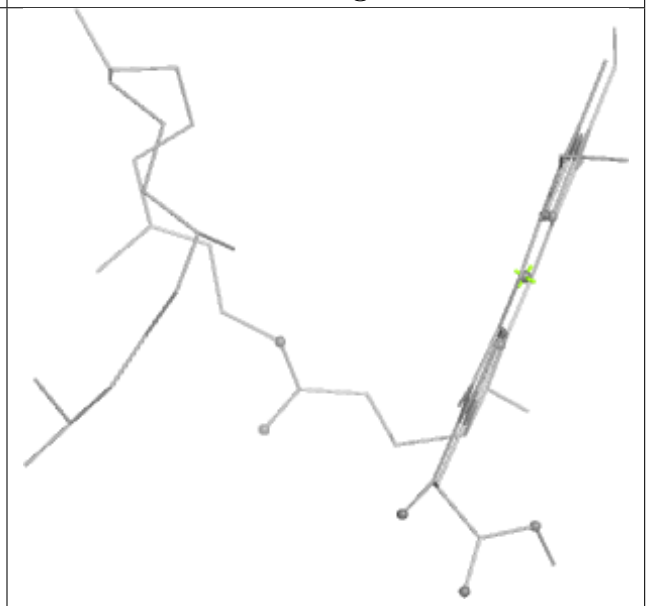
Bond lengths



Bond angles

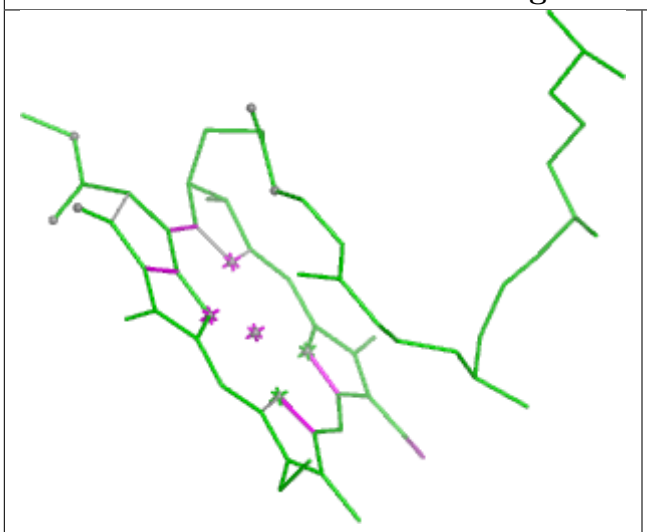


Torsions

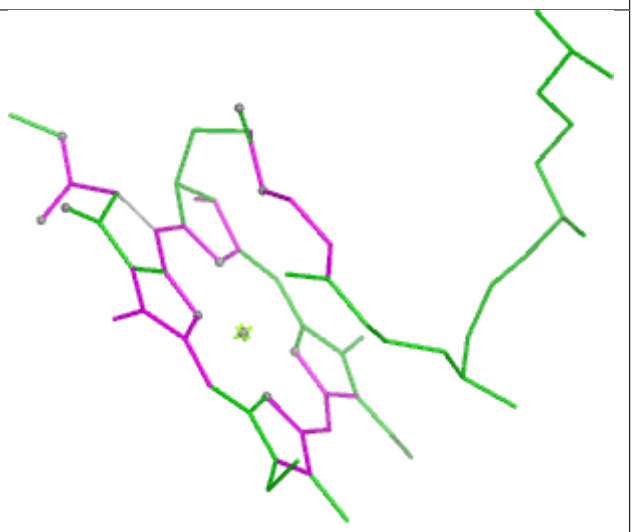


Rings

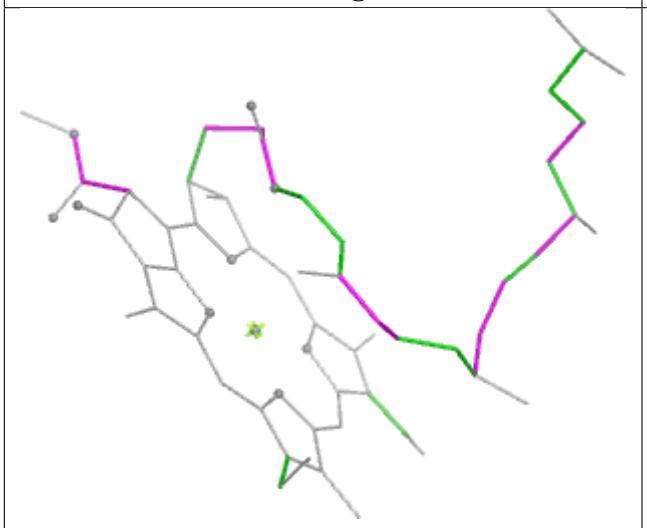
Ligand CLA 7 314



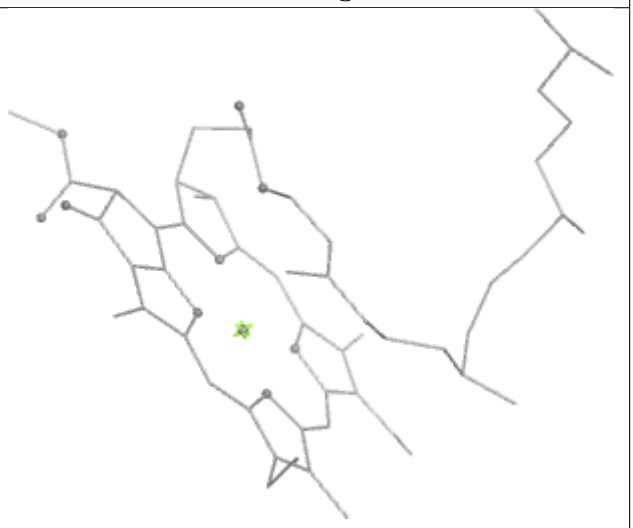
Bond lengths



Bond angles

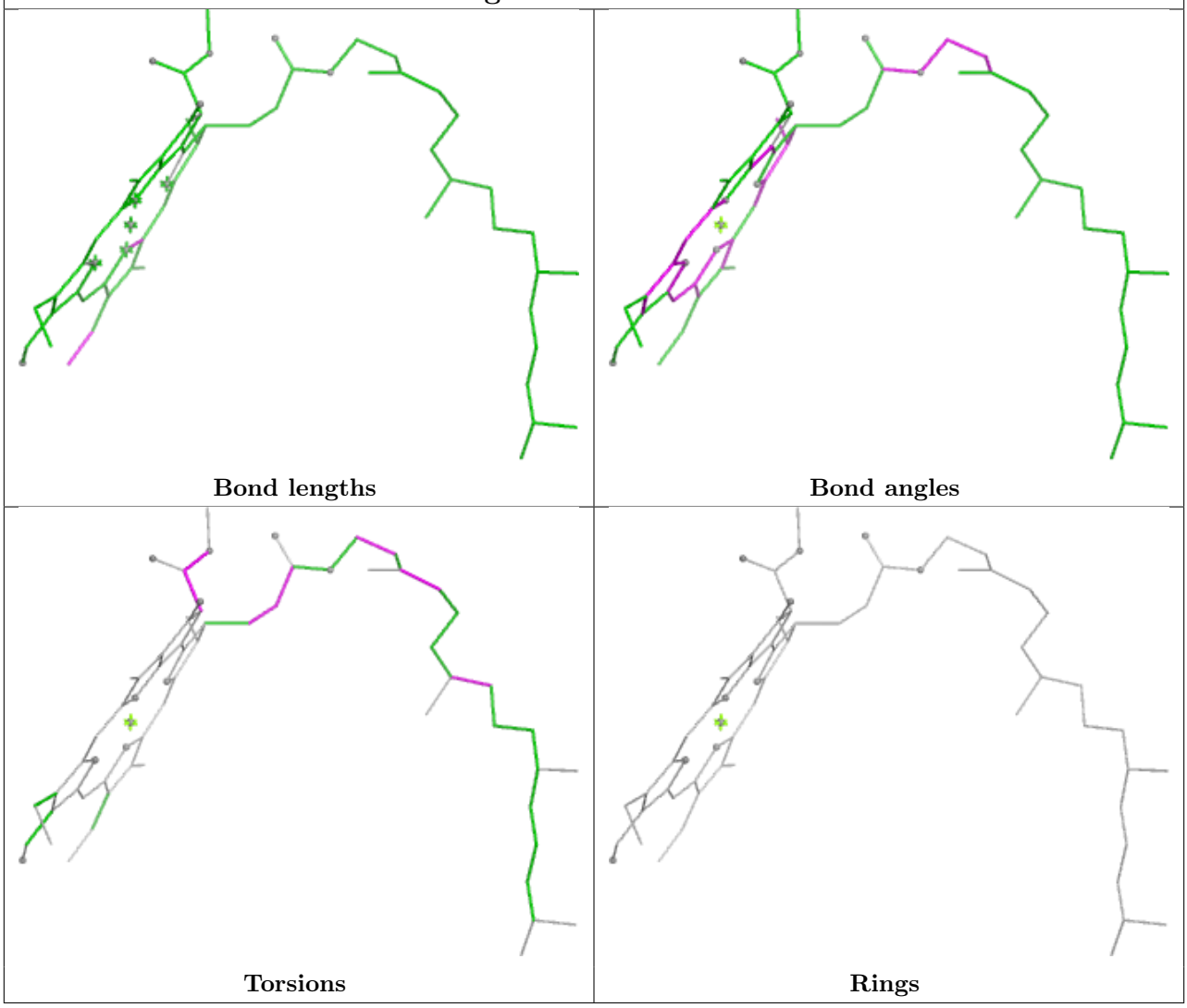


Torsions

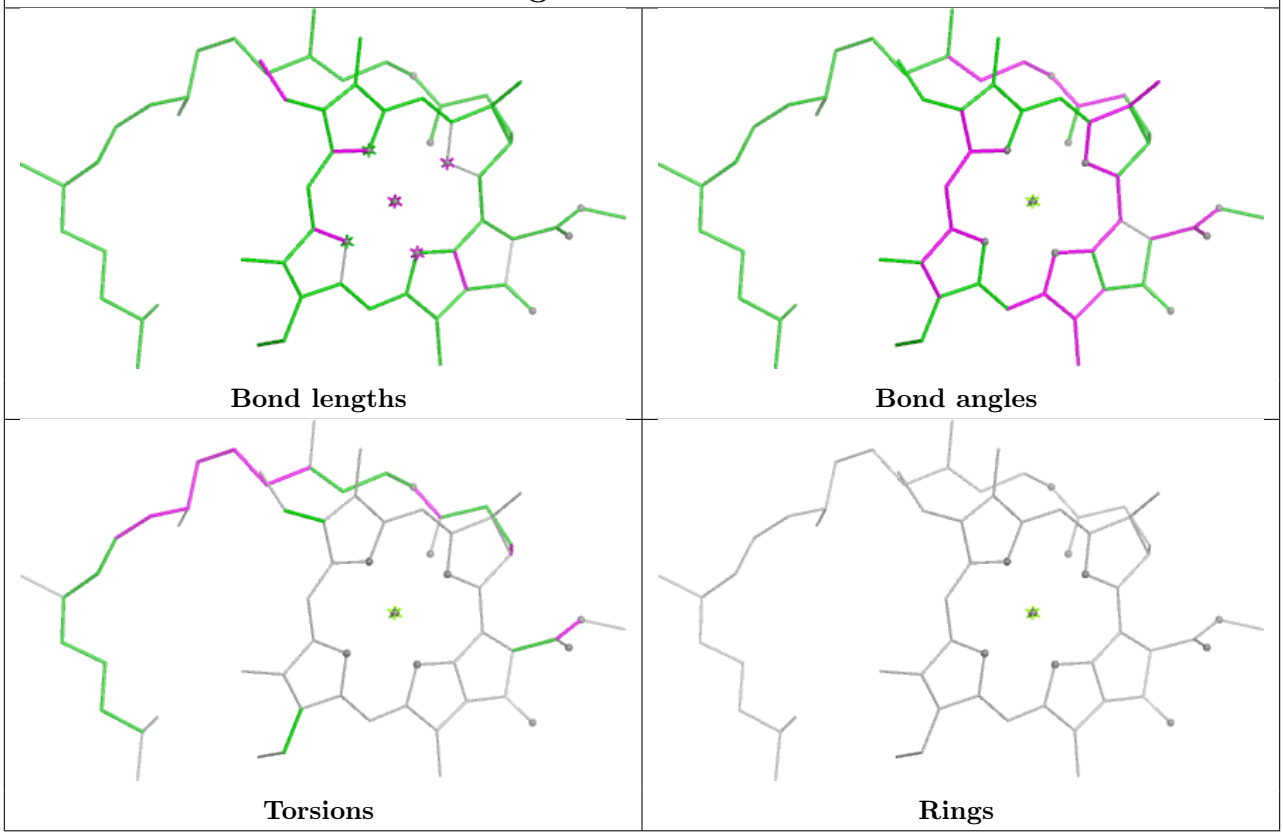


Rings

Ligand CHL N 306



Ligand CLA 0 610



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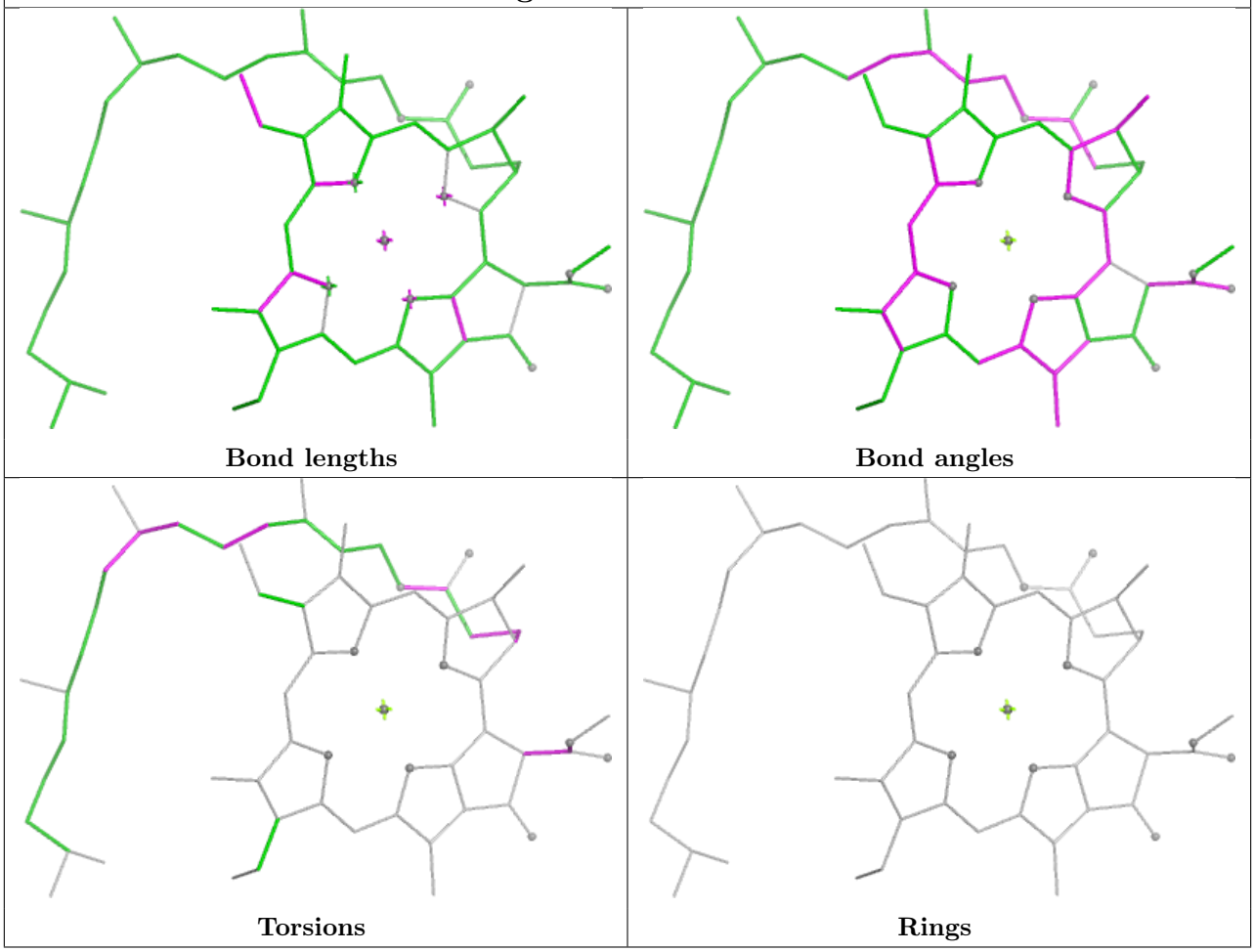
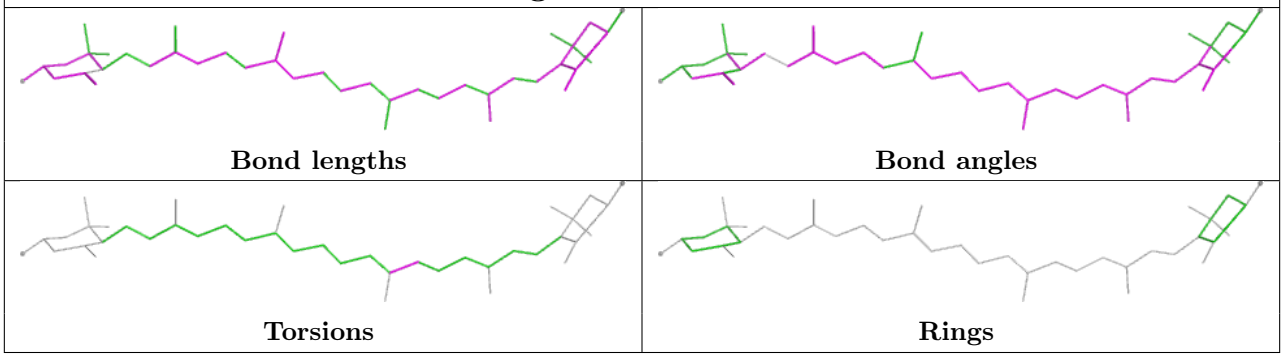
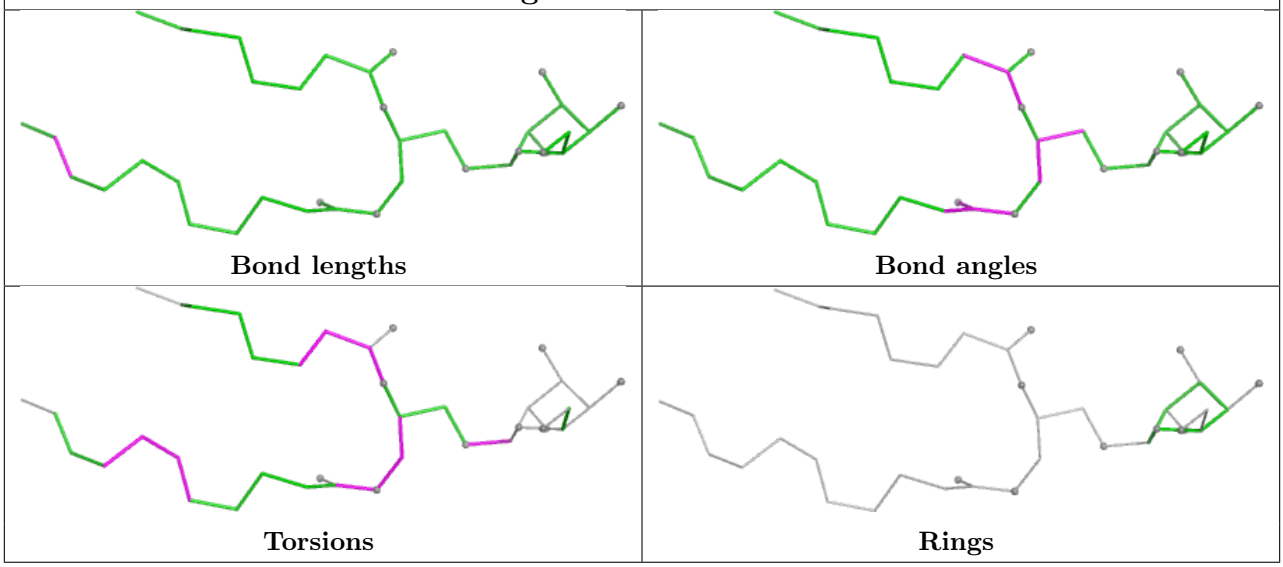


Ligand LUT 0 616



Ligand LMG B 625



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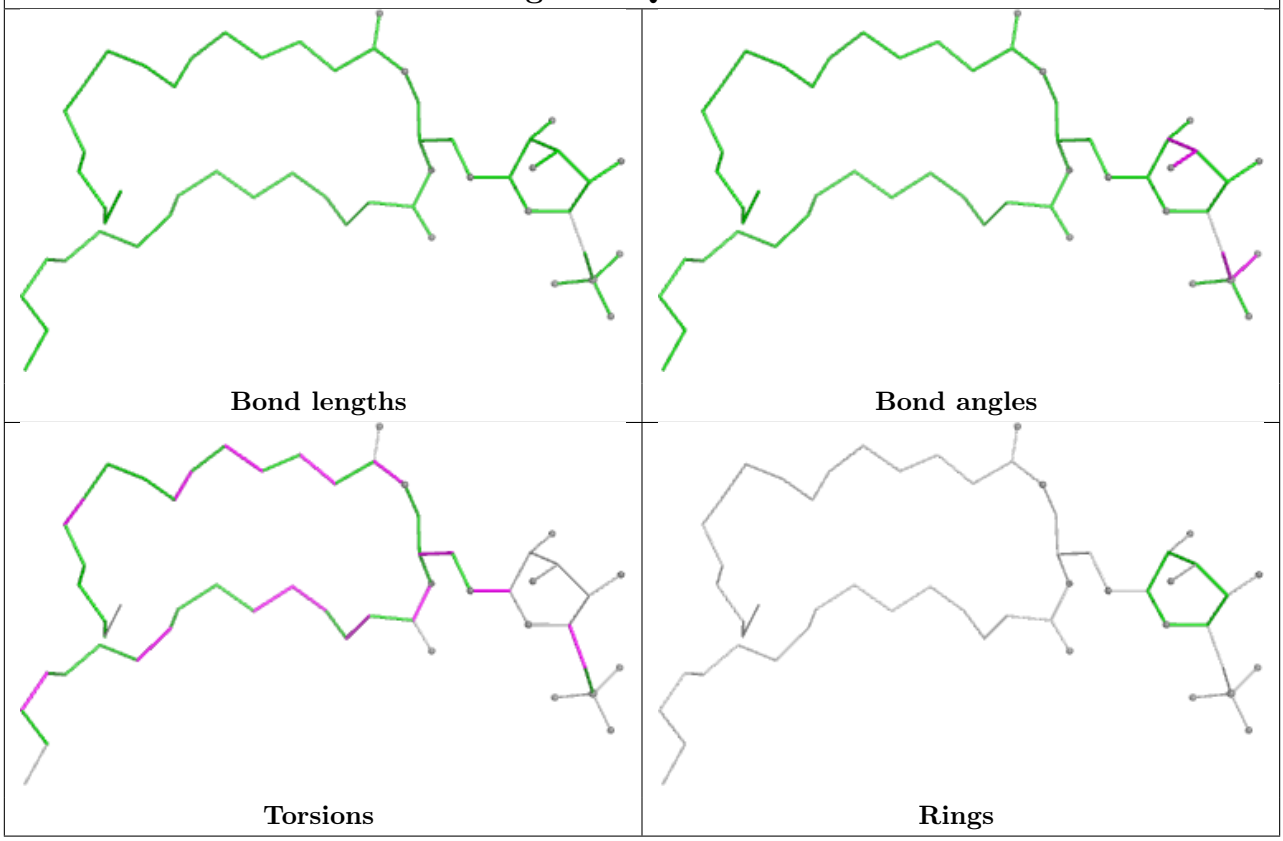

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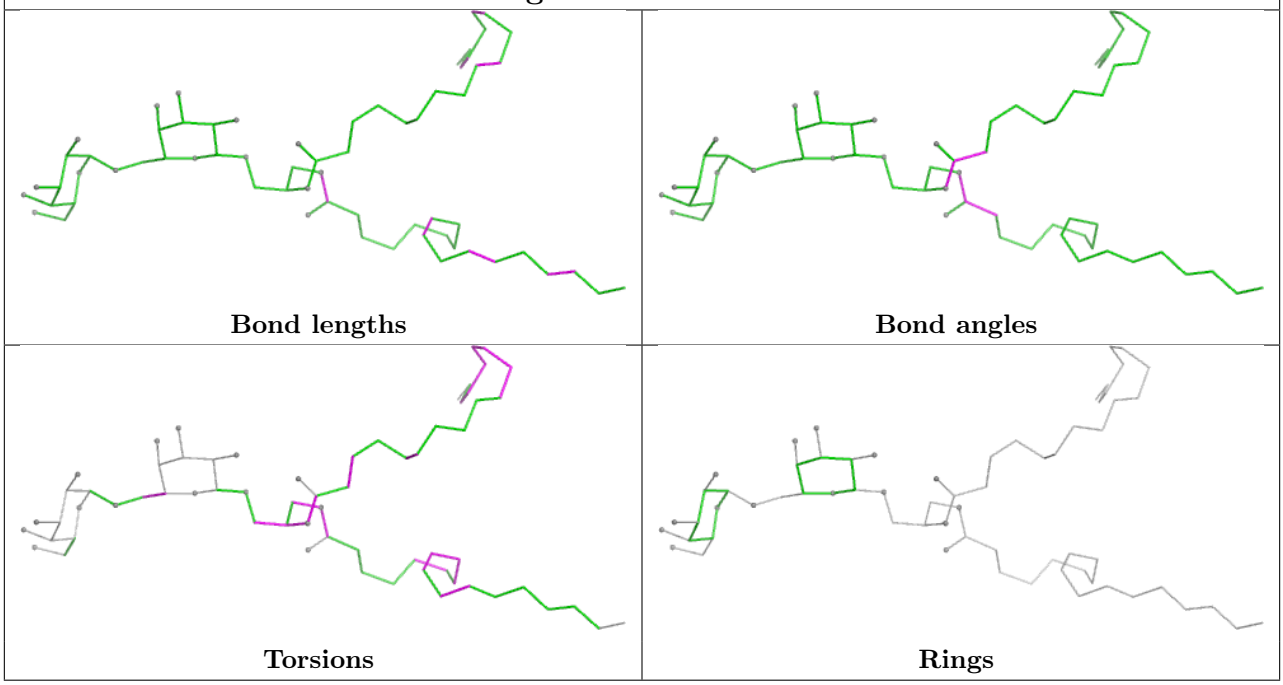

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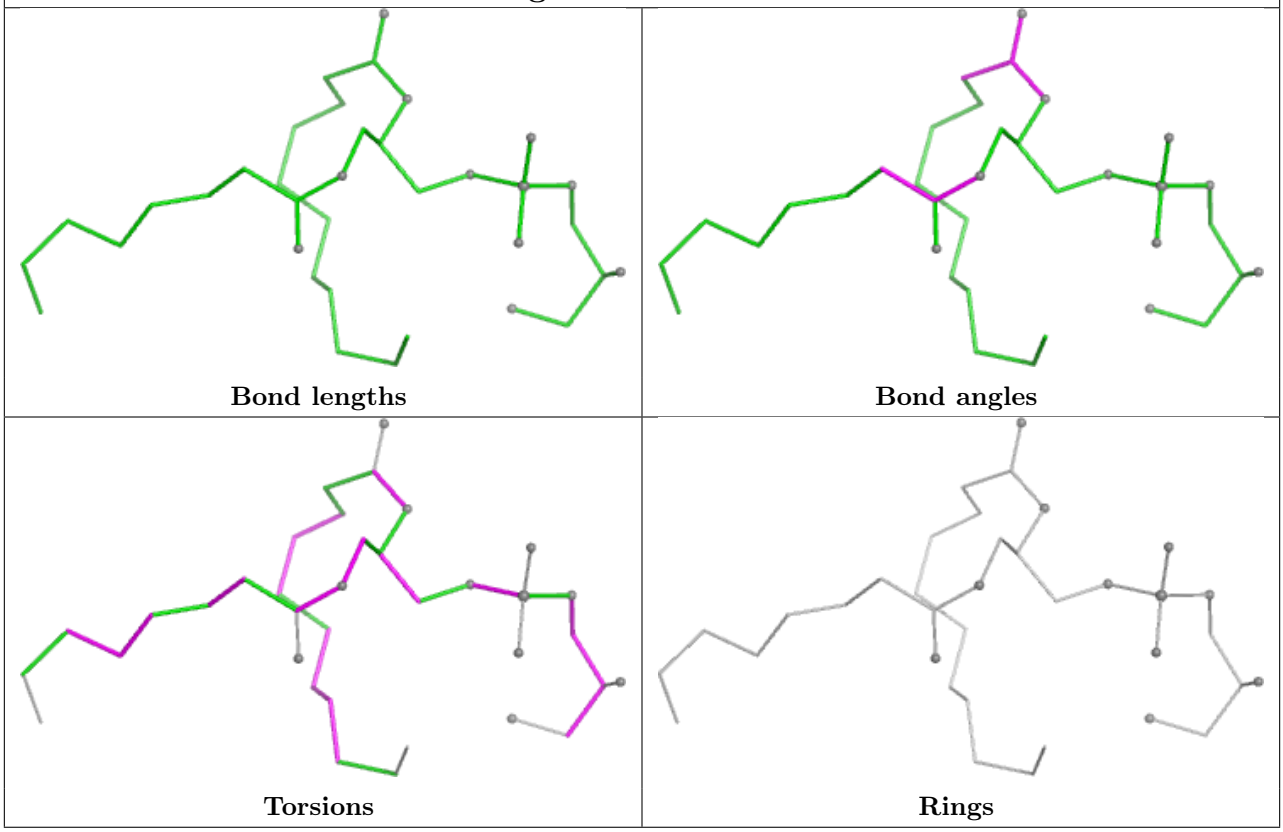

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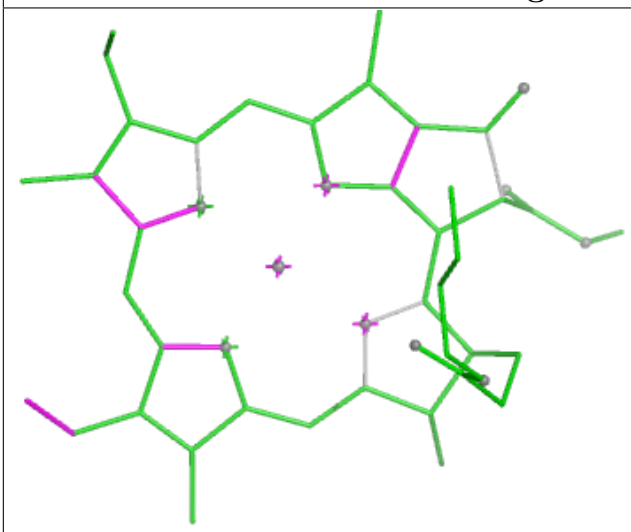
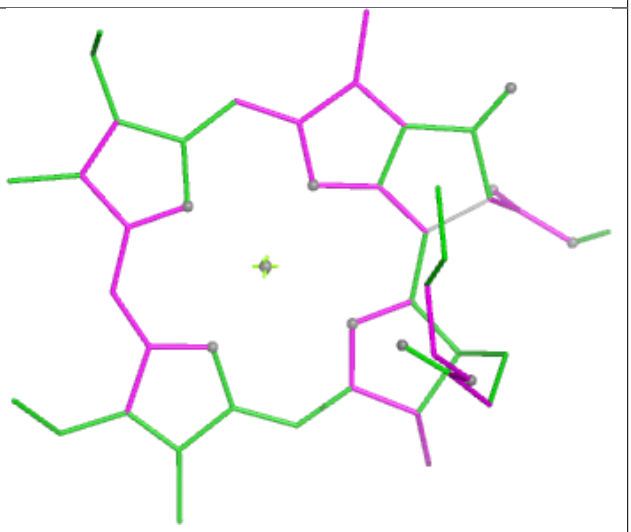
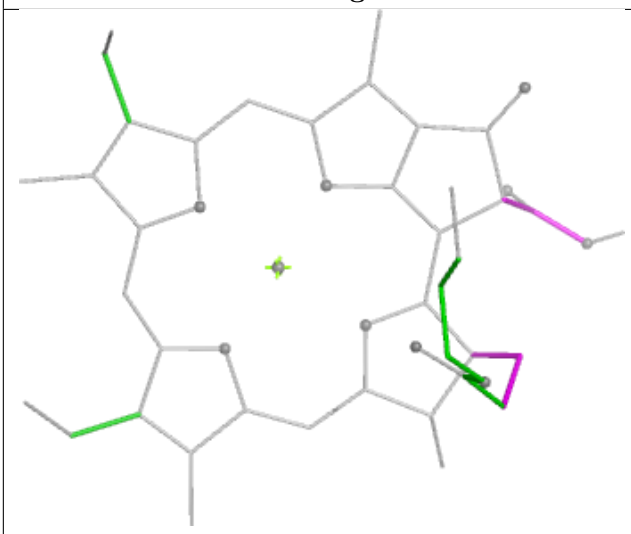


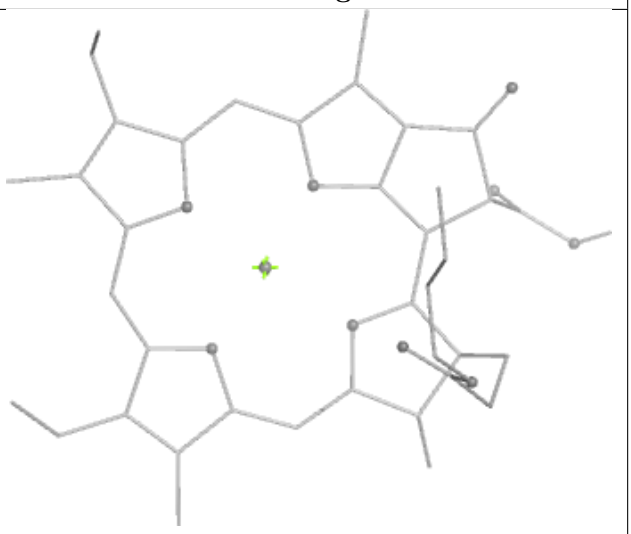
Bond lengths



Bond angles

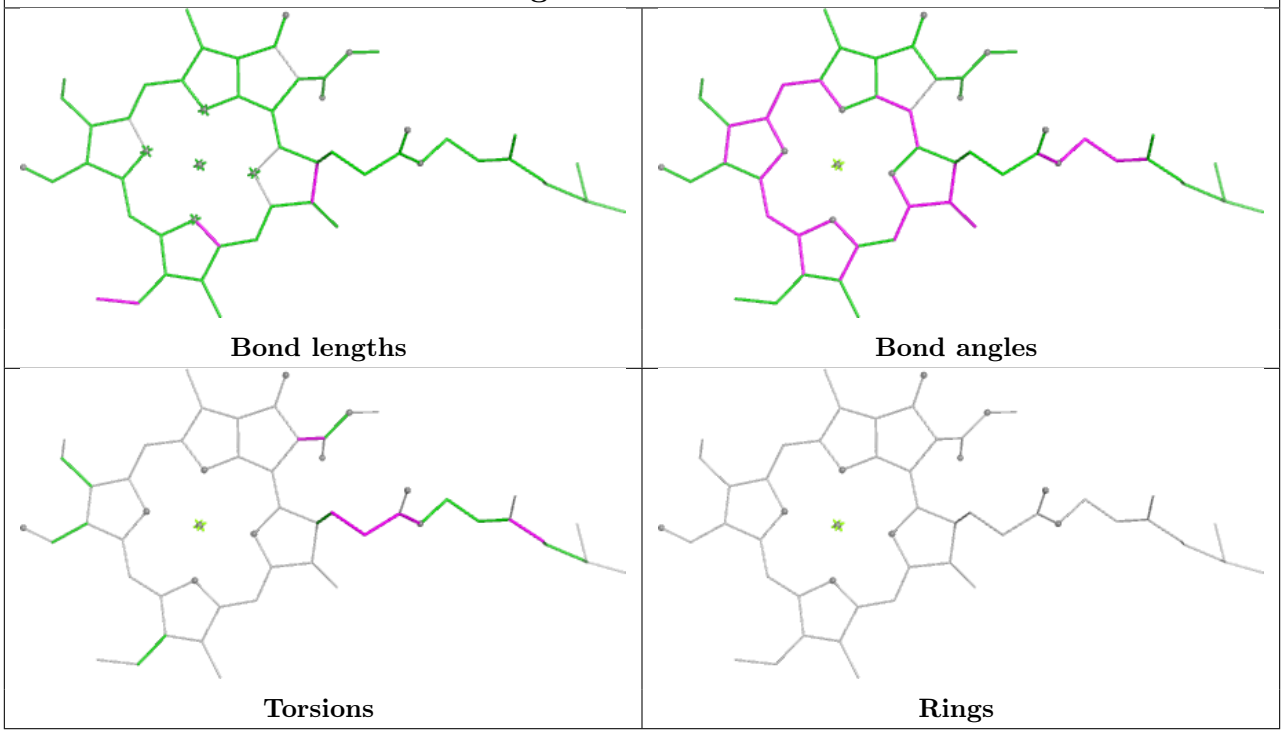


Torsions

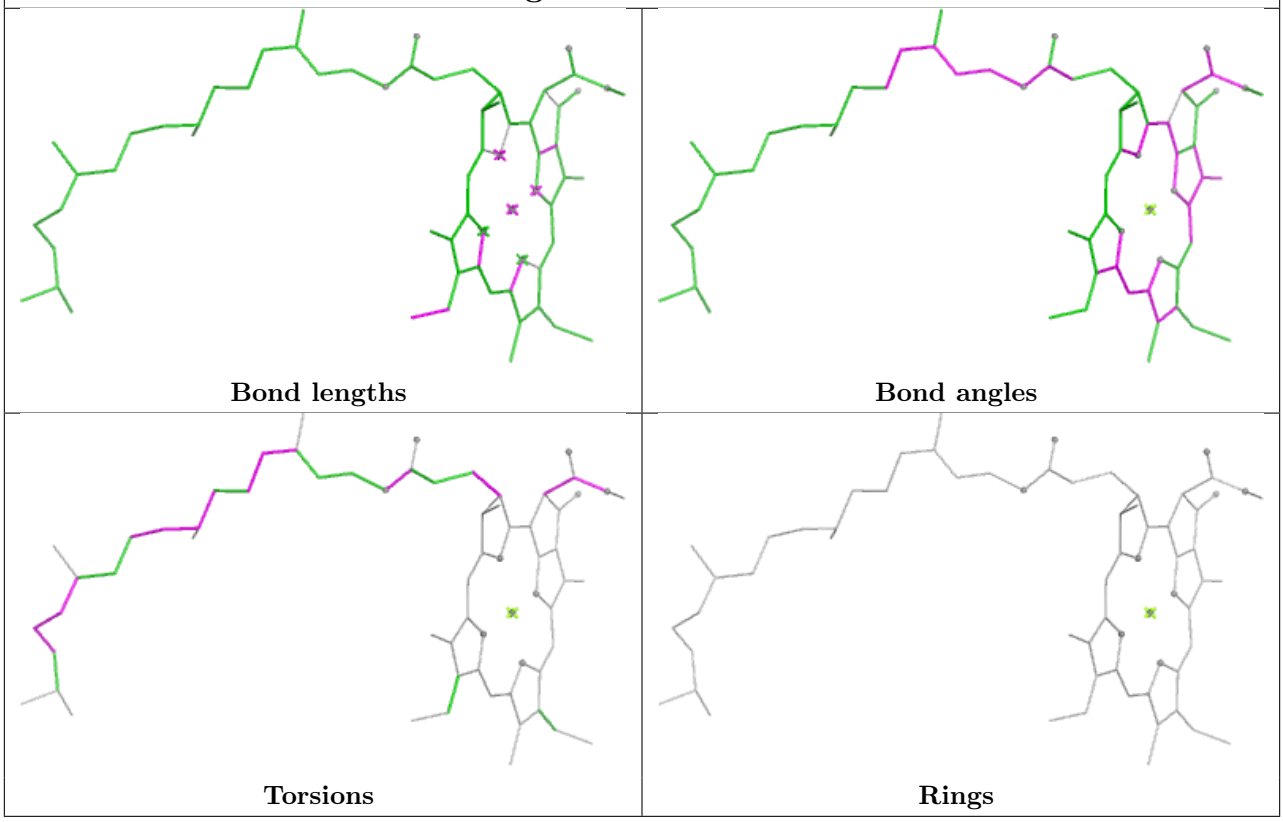


Rings

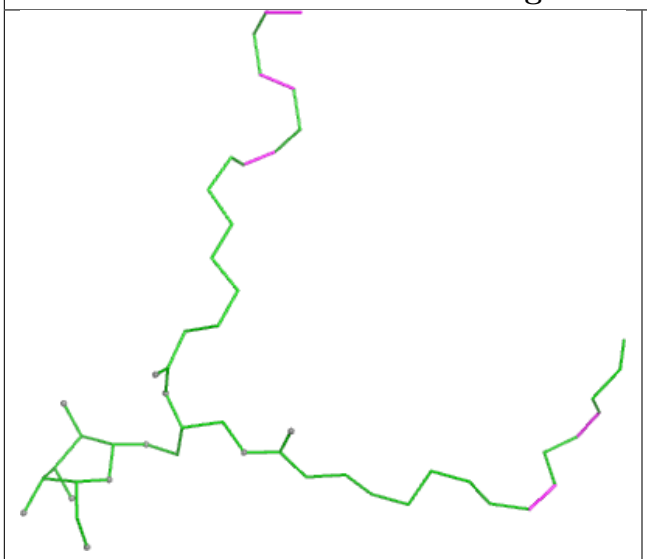
Ligand CHL r 308



Ligand CLA B 609



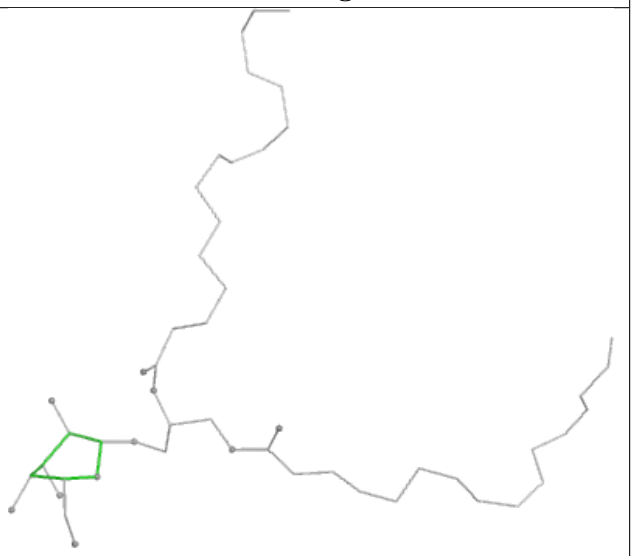
Ligand LMG 2 620



Bond lengths

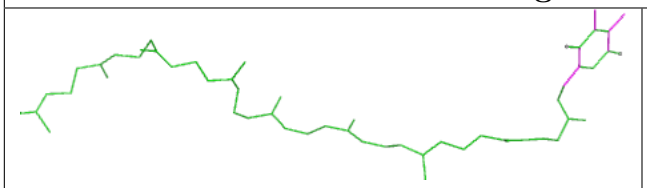
Bond angles

Torsions

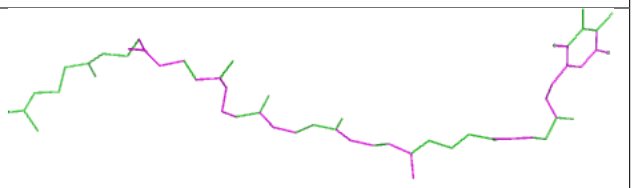


Rings

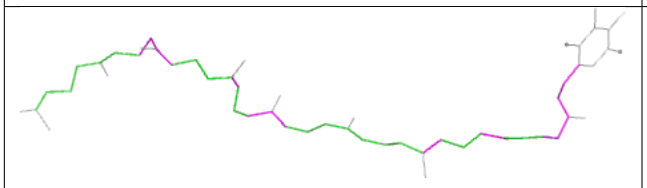
Ligand PL9 a 414



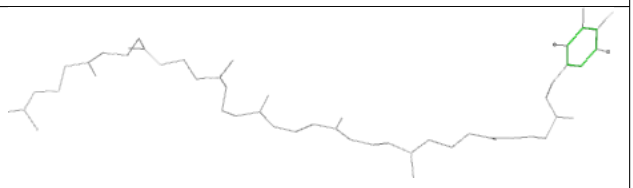
Bond lengths



Bond angles

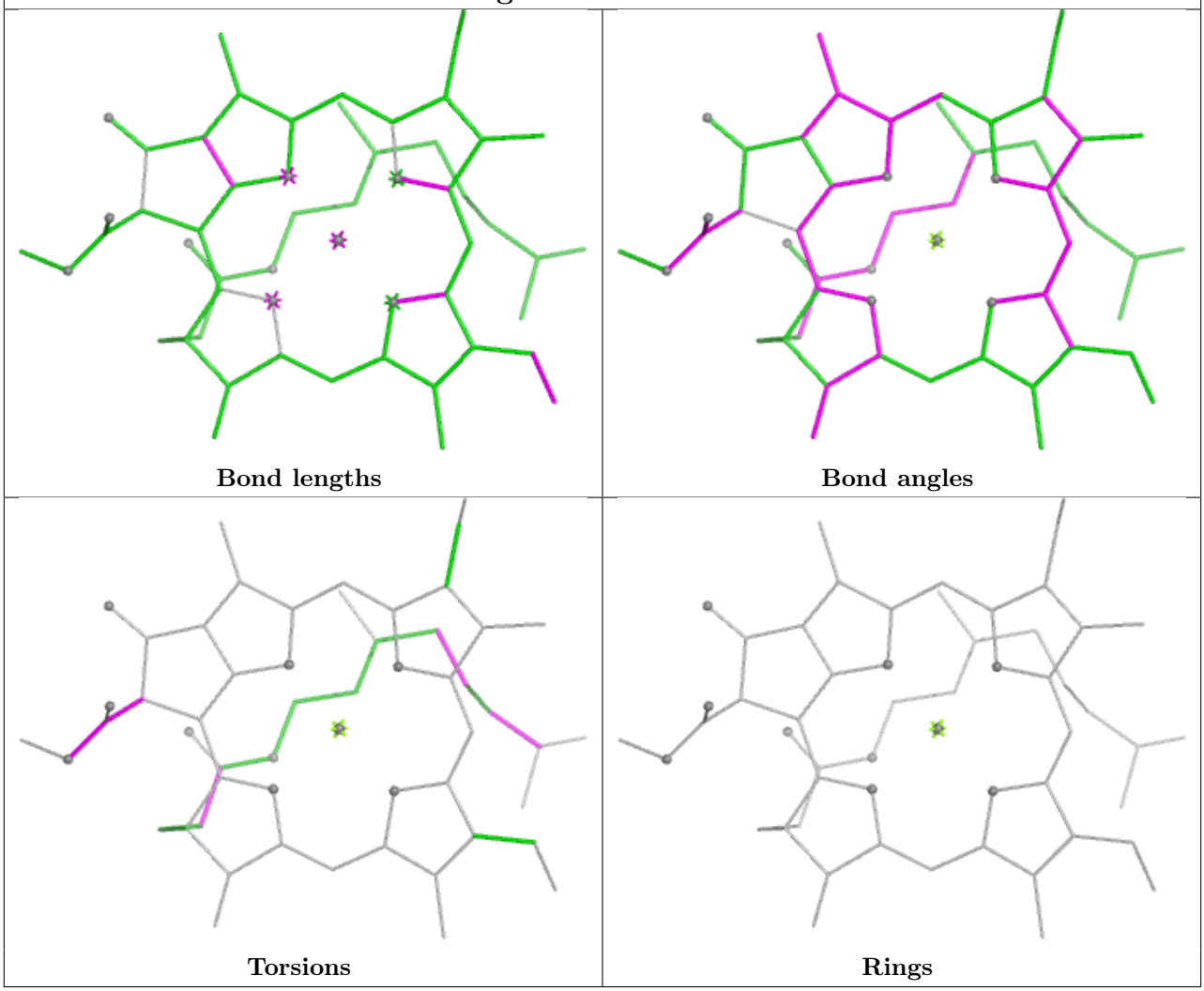


Torsions

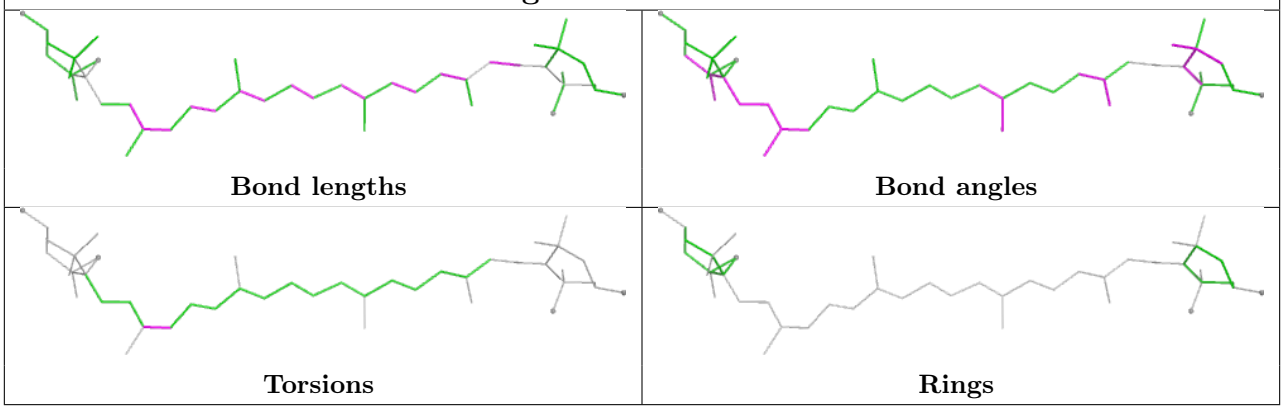


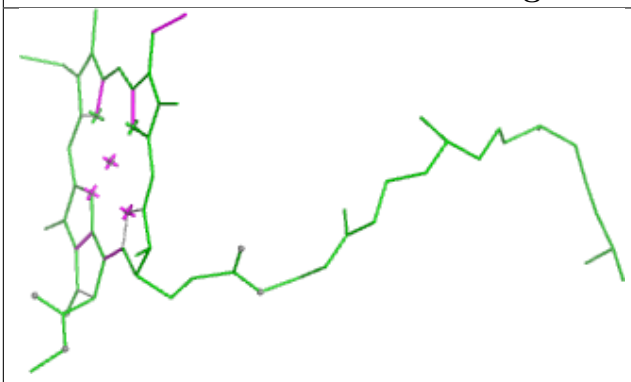
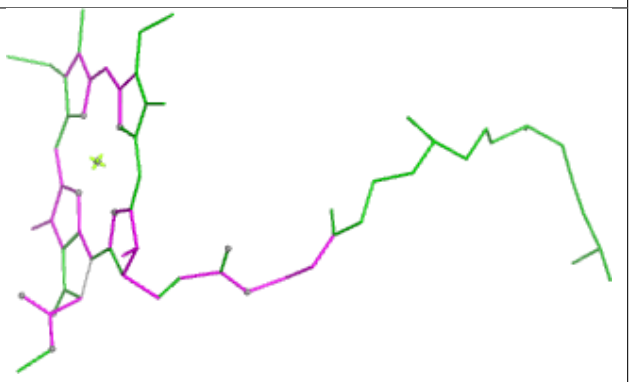
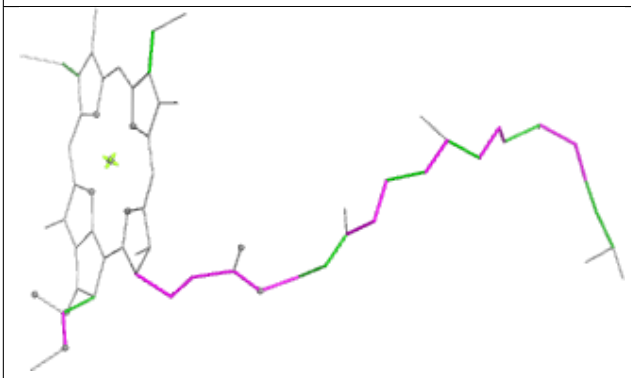
Rings

Ligand CLA 9 315

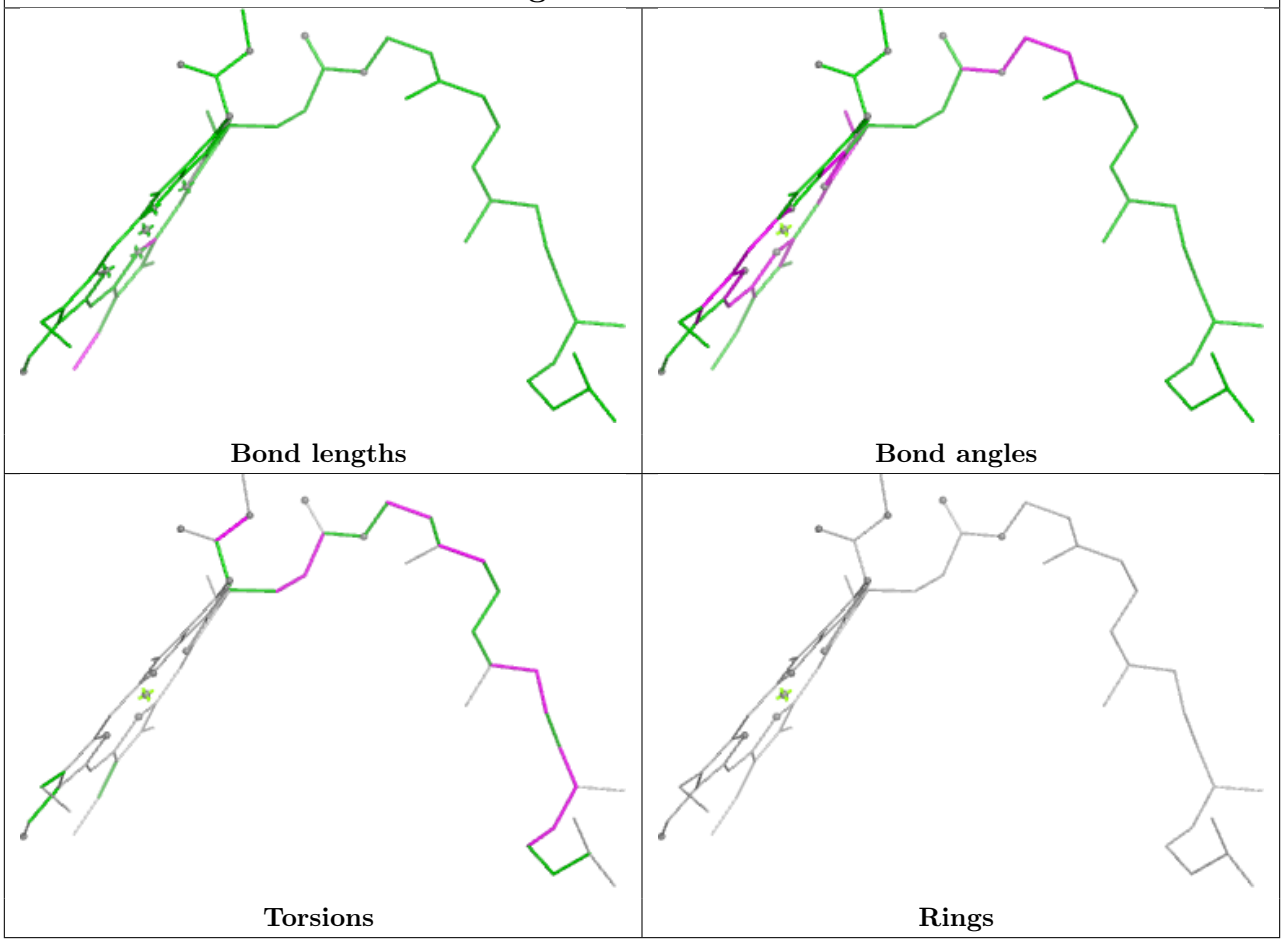


Ligand NEX G 616

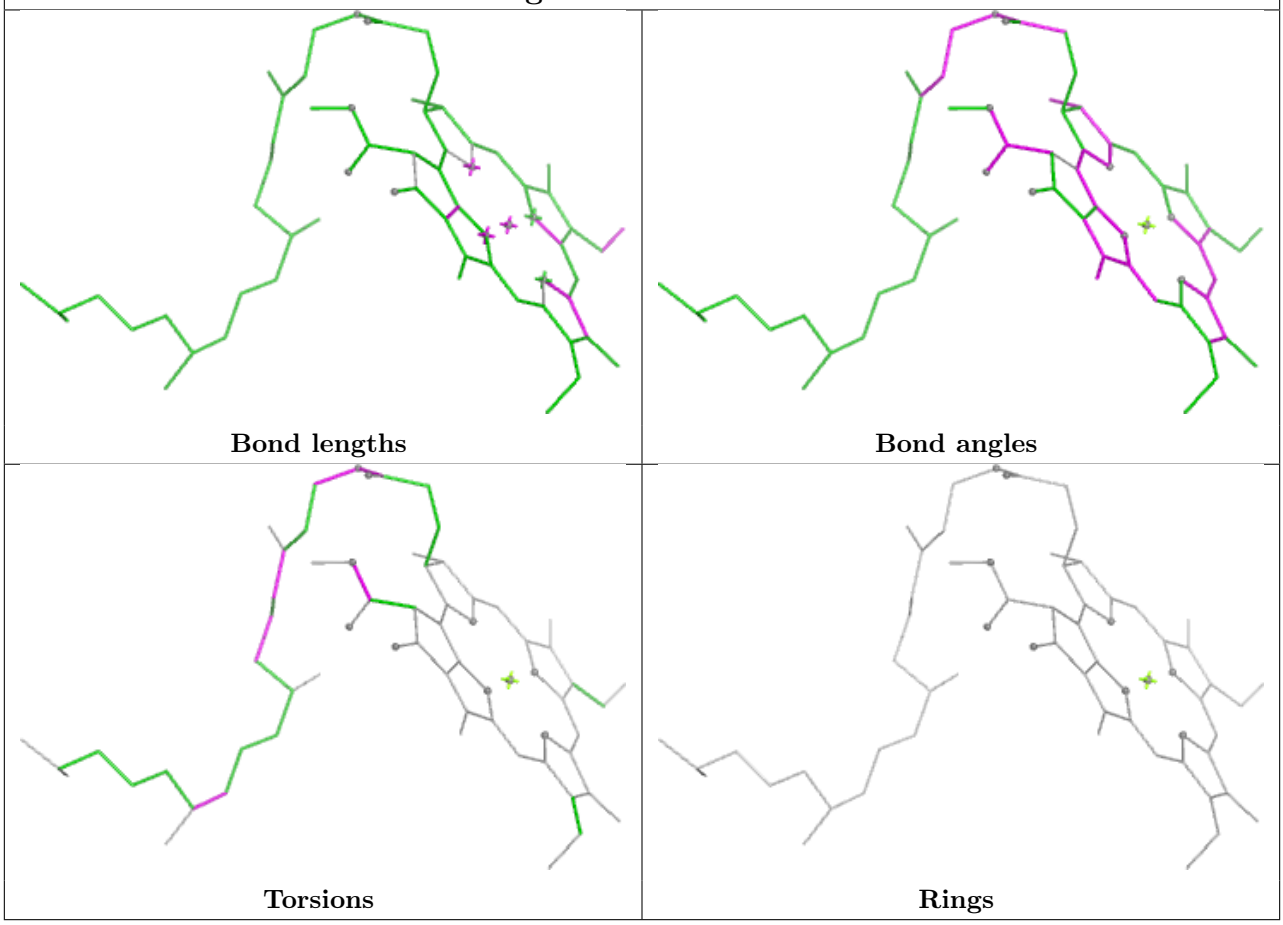


Ligand CLA D 404	
 Bond lengths	 Bond angles
 Torsions	Rings

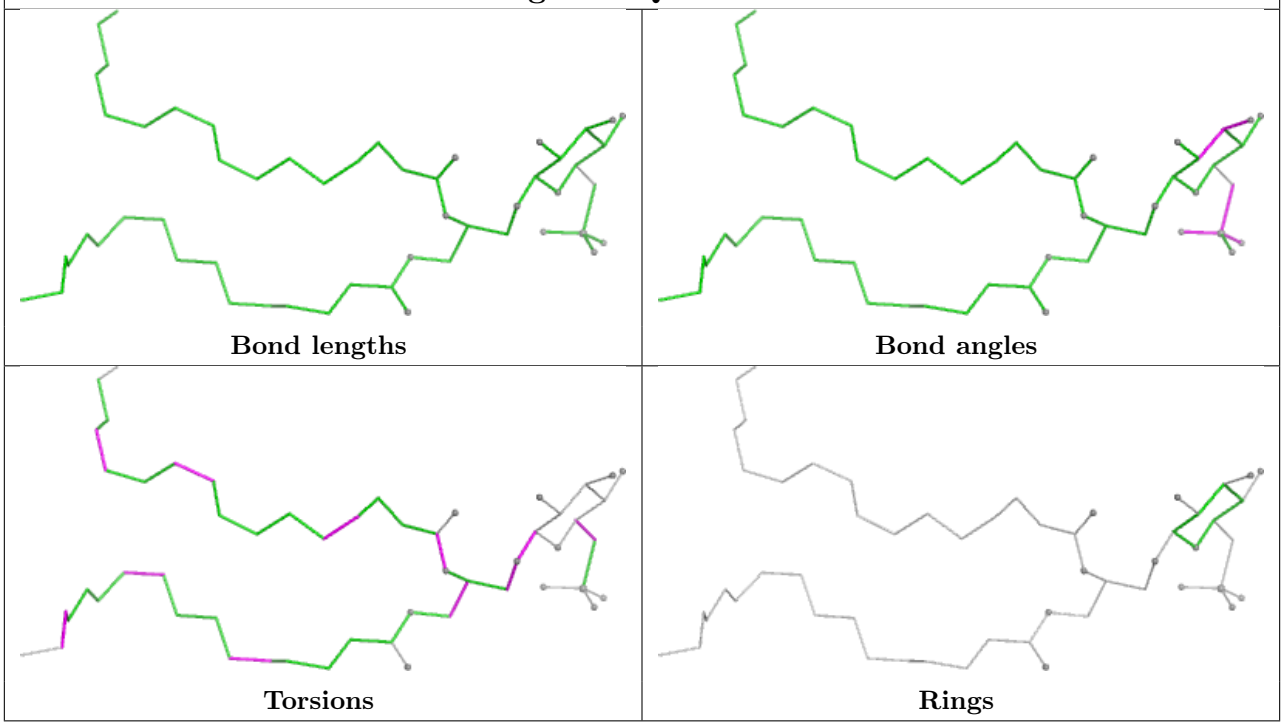
Ligand CHL 8 605



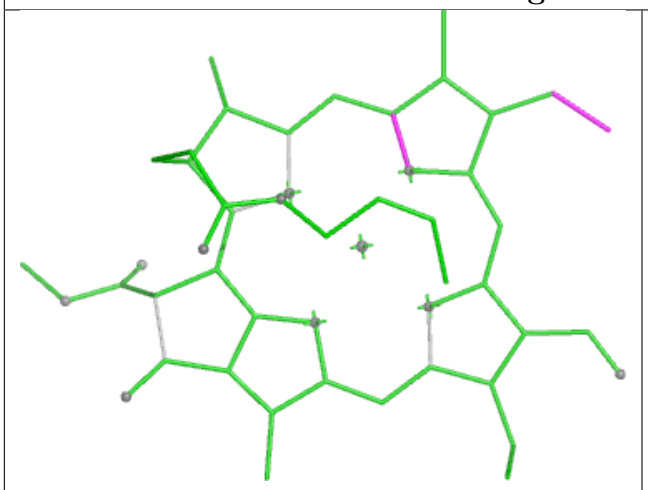
Ligand CLA B 613



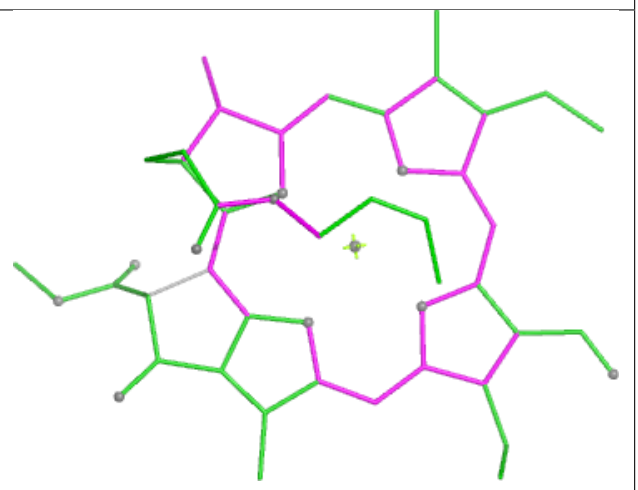
Ligand SQD b 621



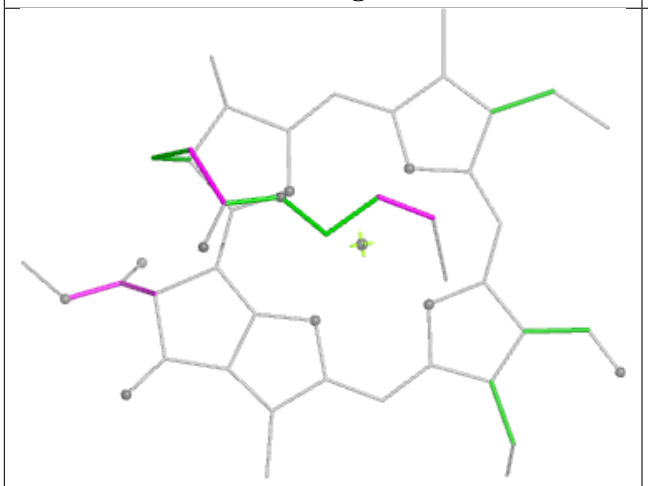
Ligand CHL n 301



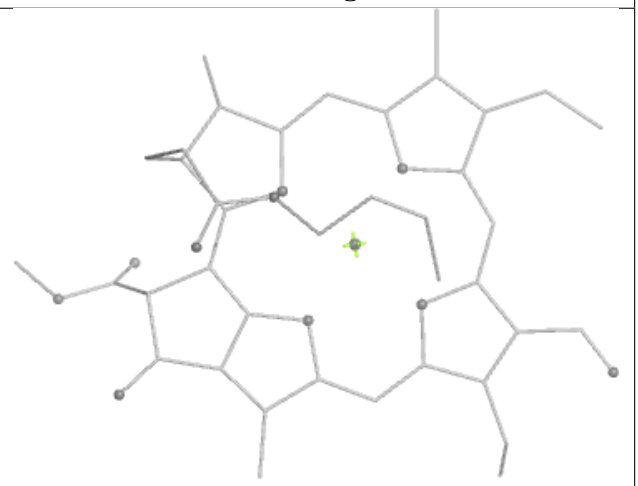
Bond lengths



Bond angles

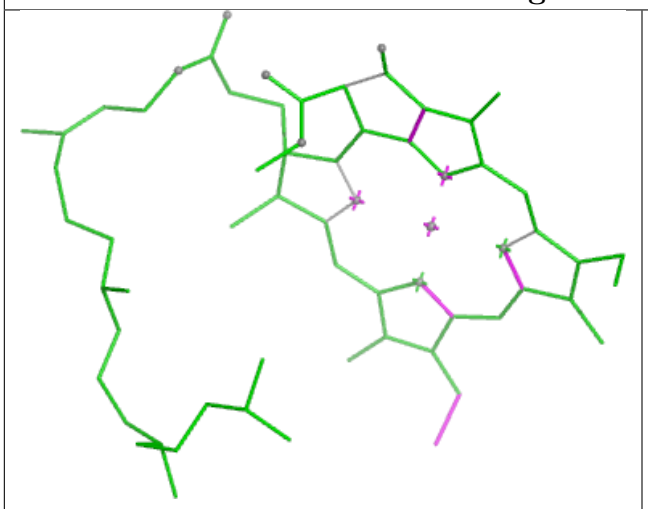


Torsions

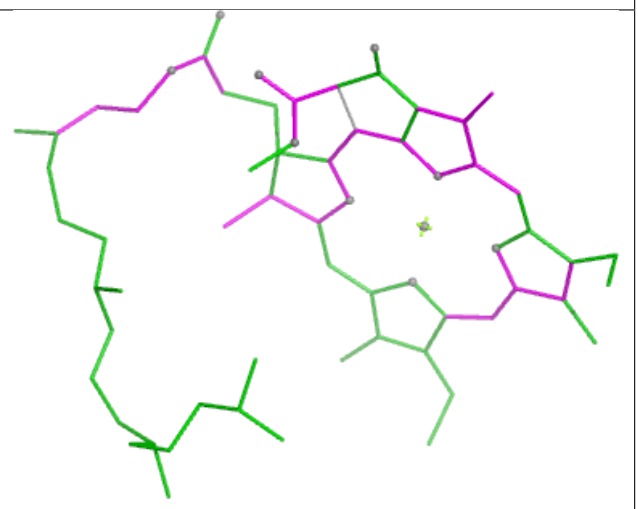


Rings

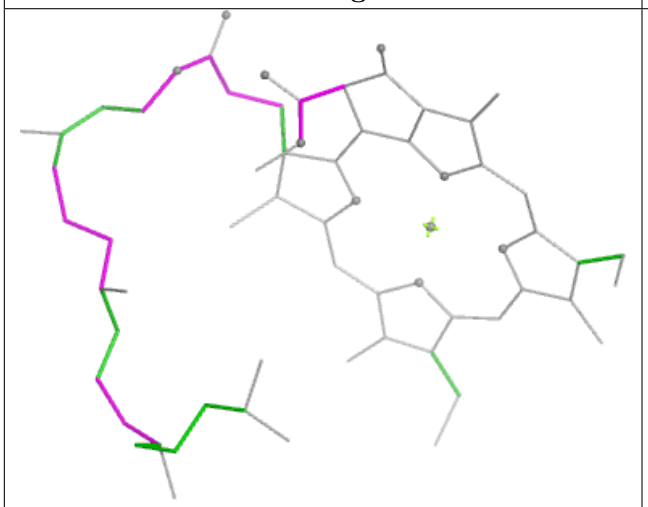
Ligand CLA b 617



Bond lengths



Bond angles



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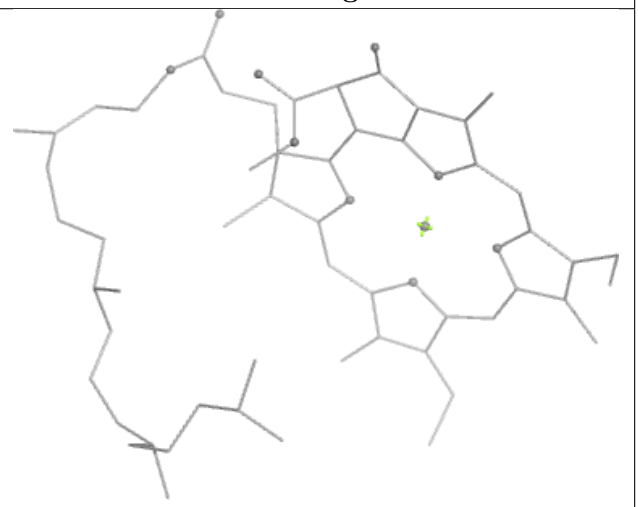
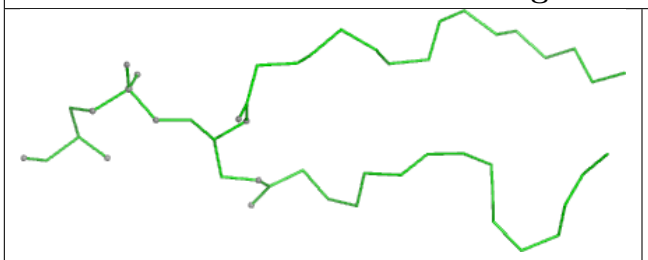
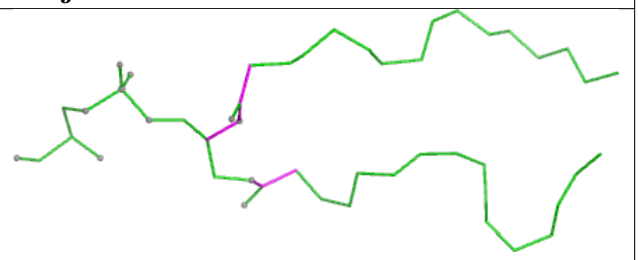


Rings

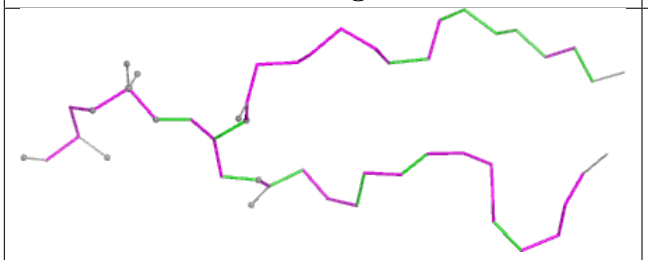
Ligand LHG j 102



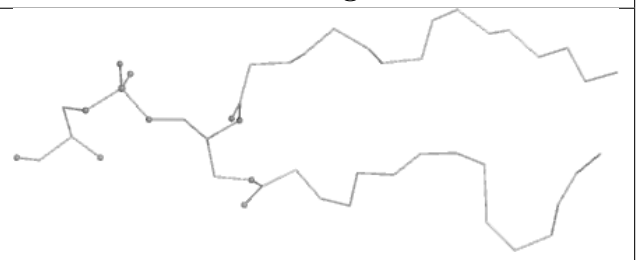
Bond lengths



Bond angles

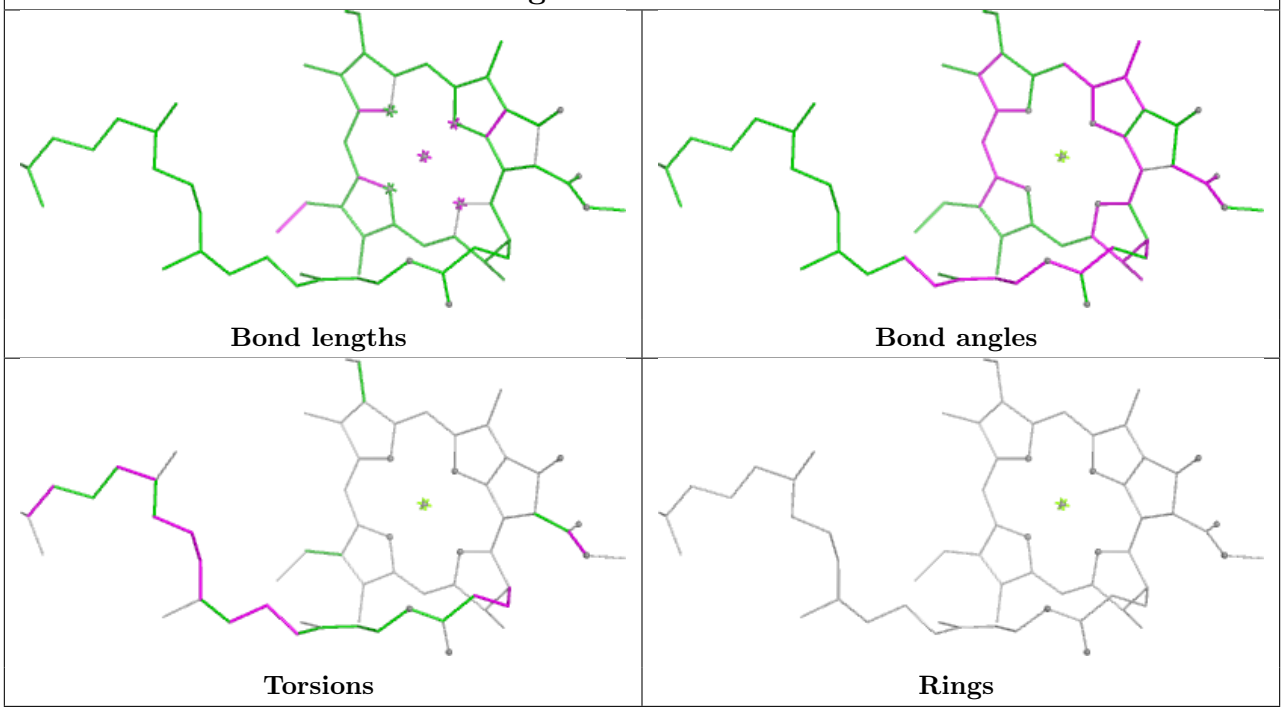


Torsions

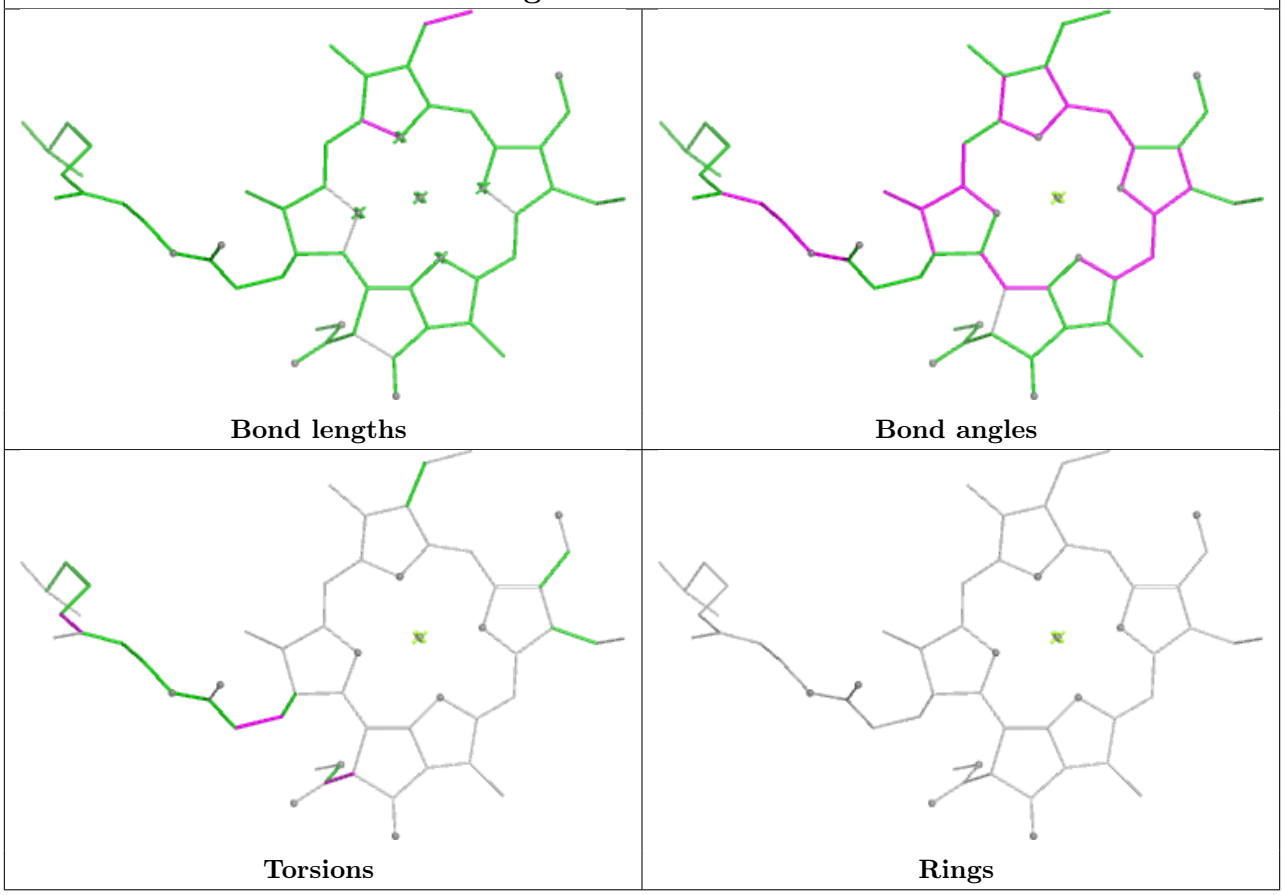


Rings

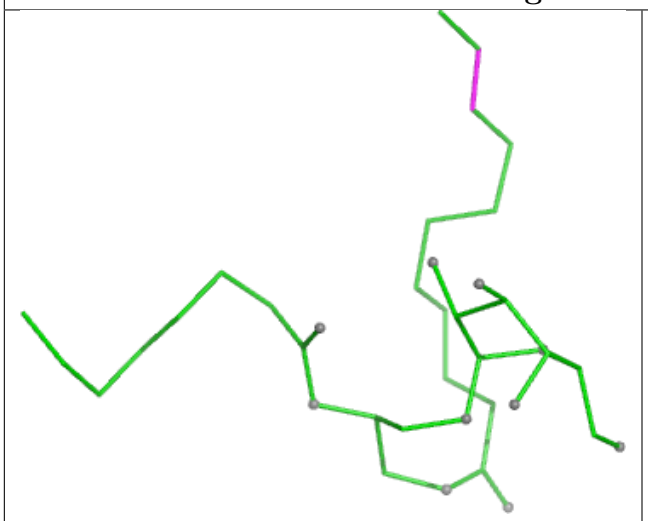
Ligand CLA S 311



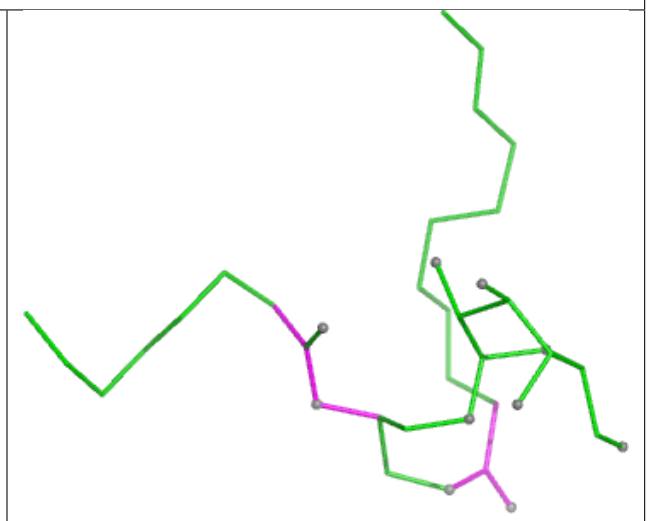
Ligand CHL N 302



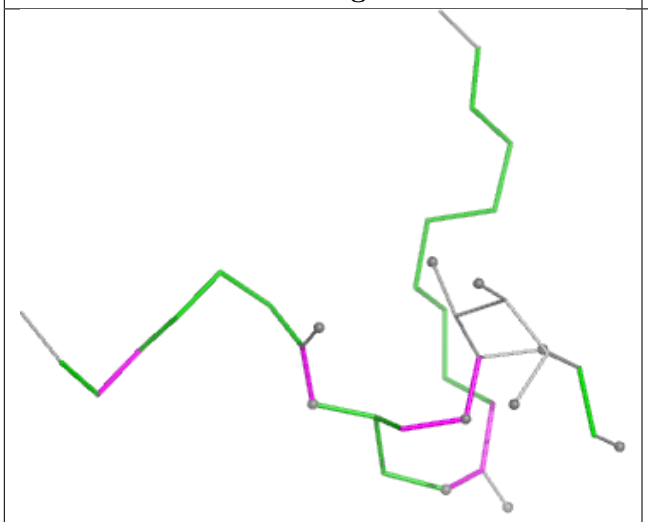
Ligand LMG 9 321



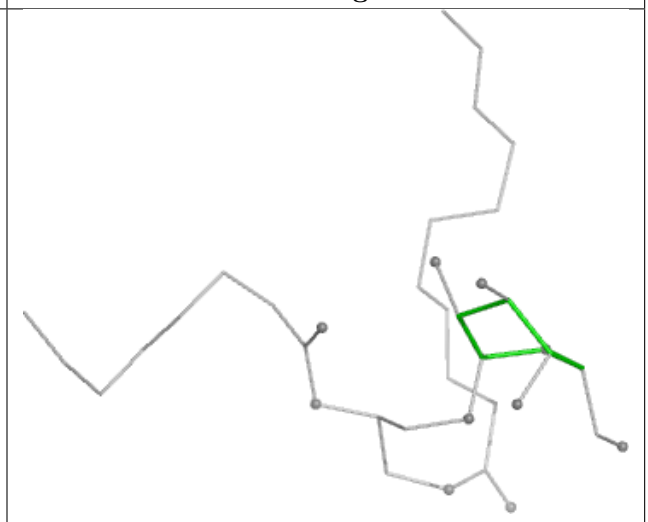
Bond lengths



Bond angles

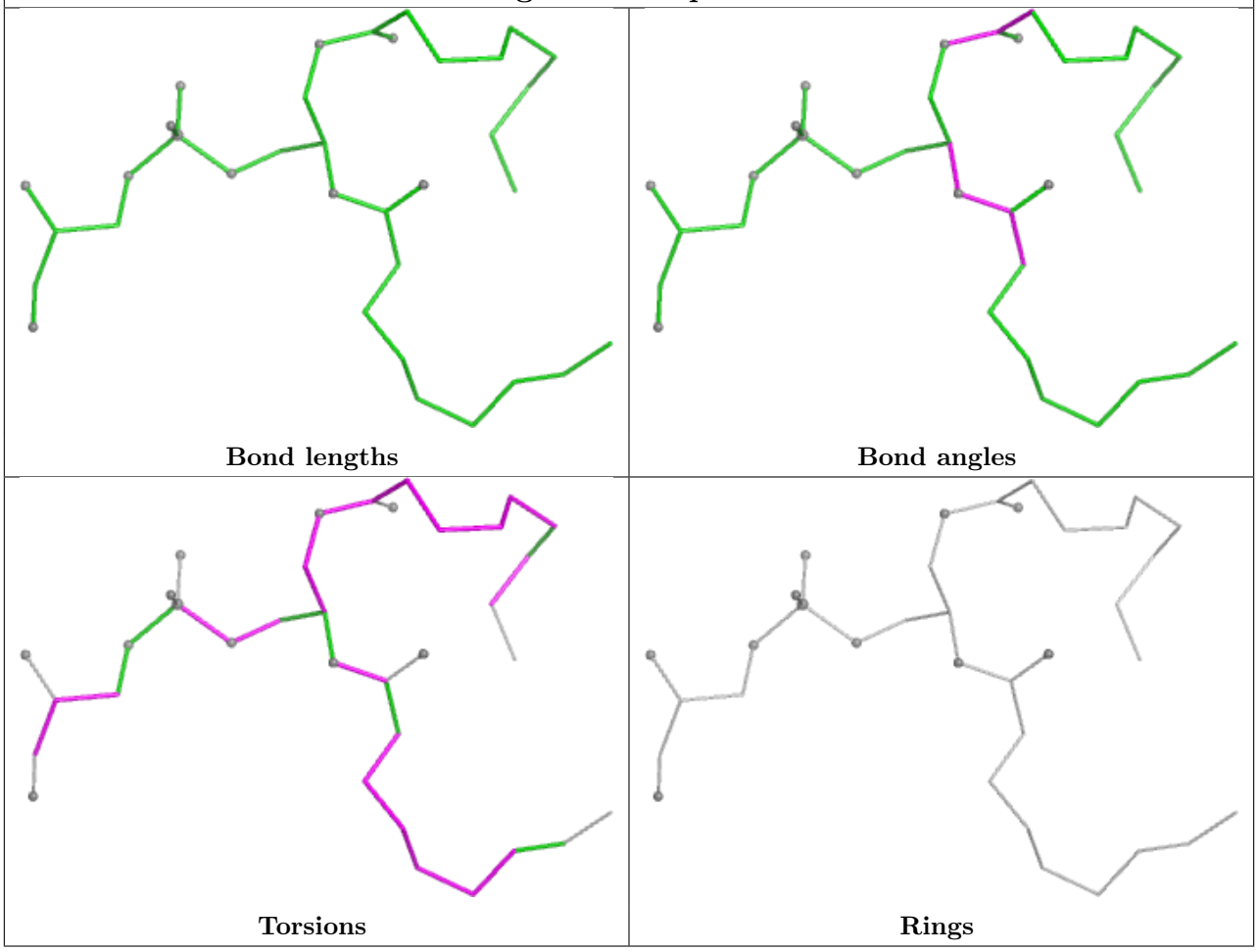


Torsions

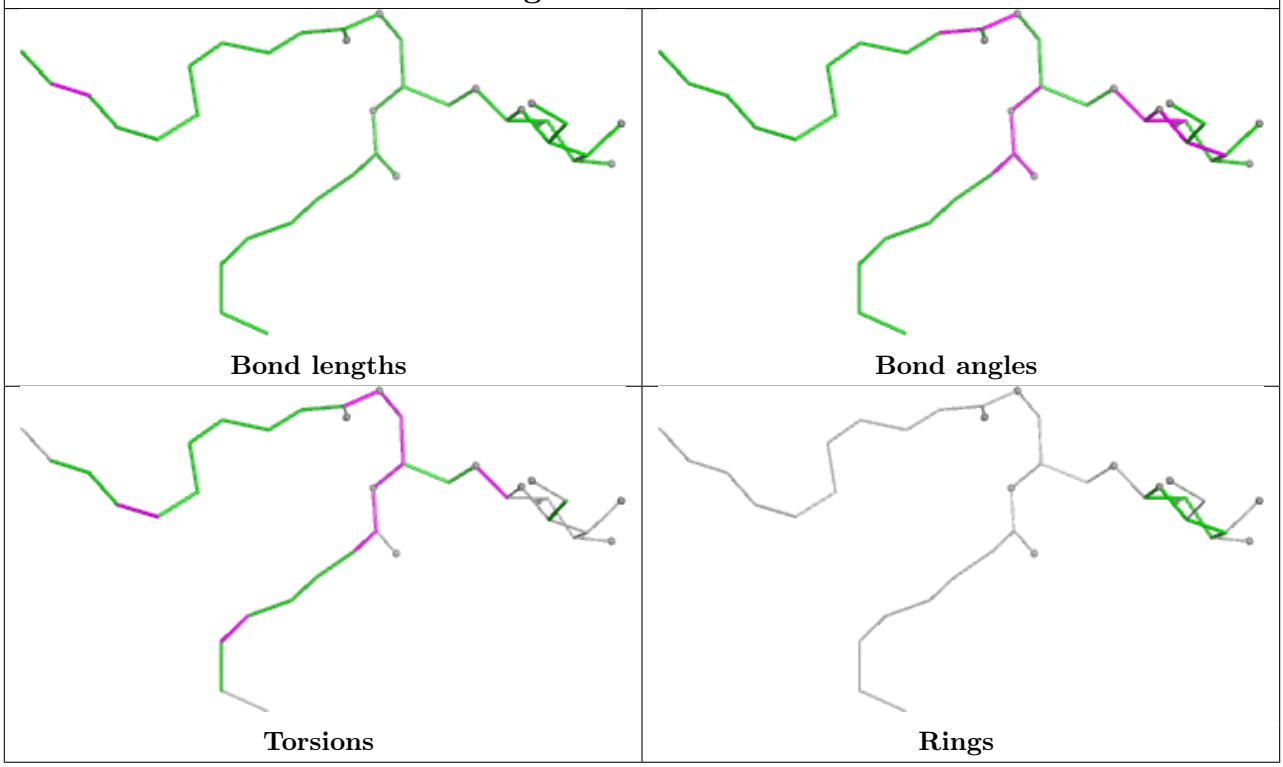


Rings

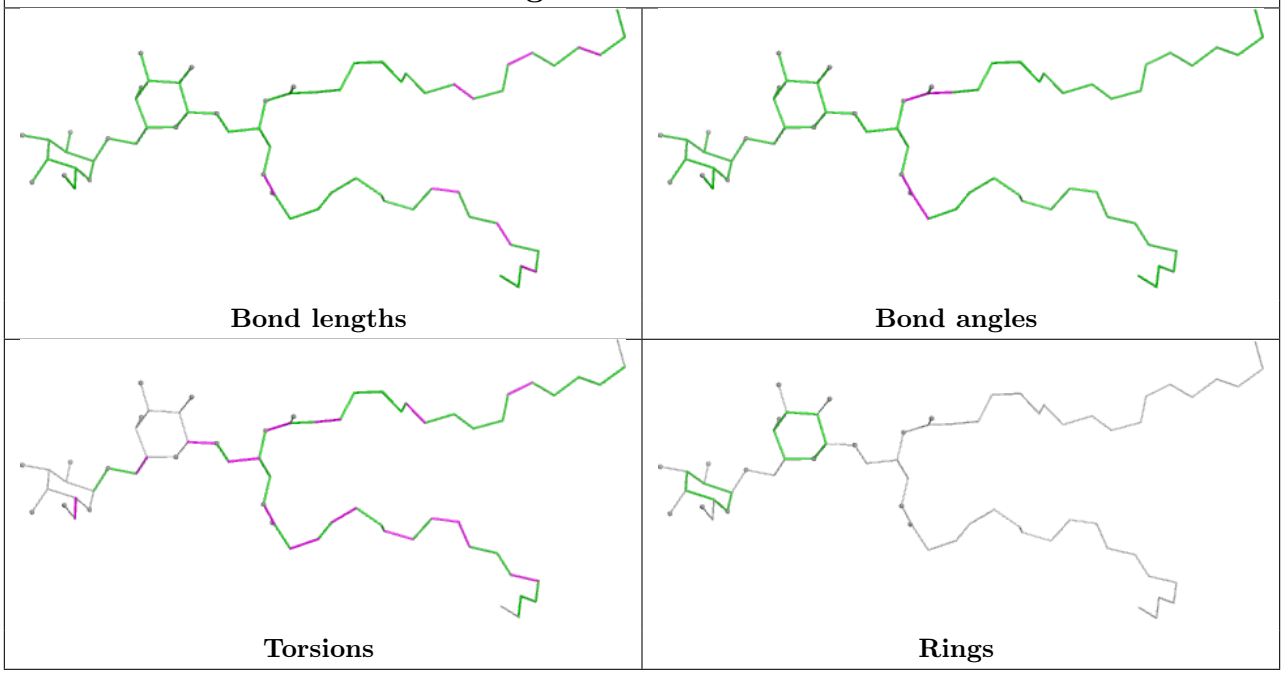
Ligand LHG p 619



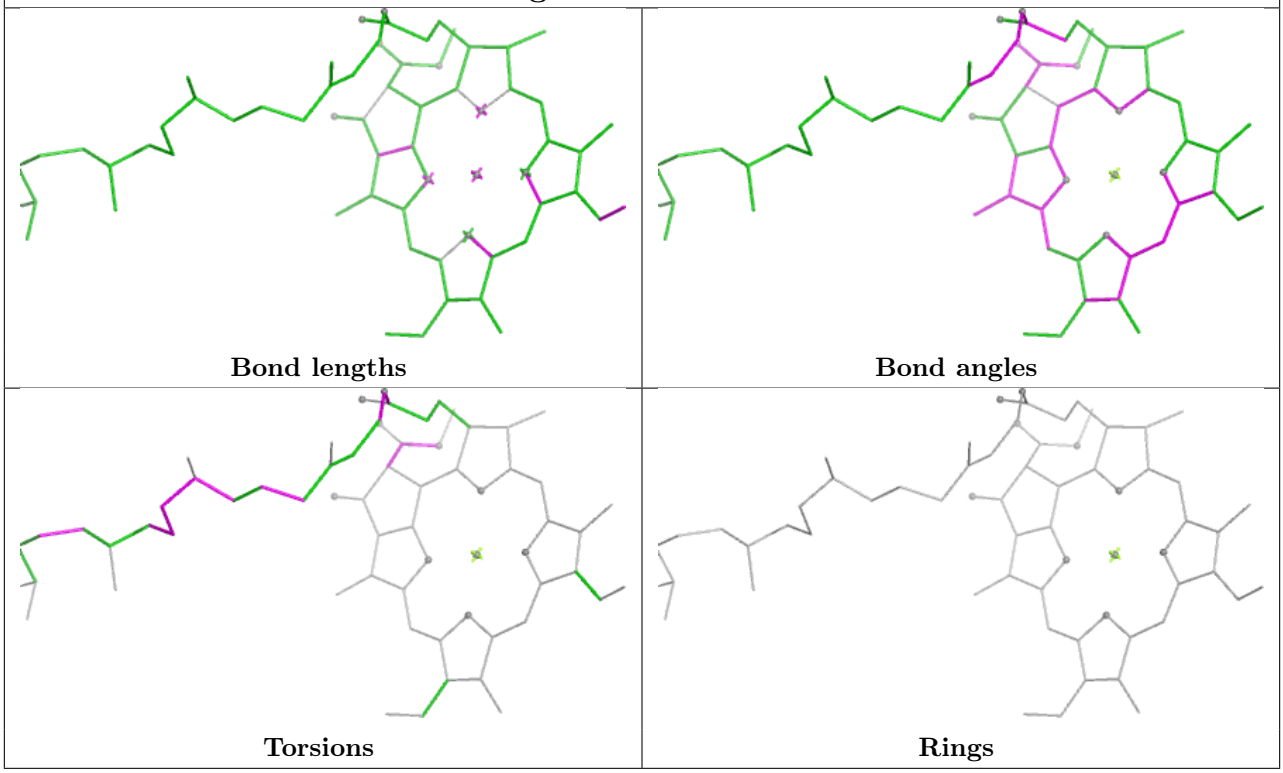
Ligand LMG b 624

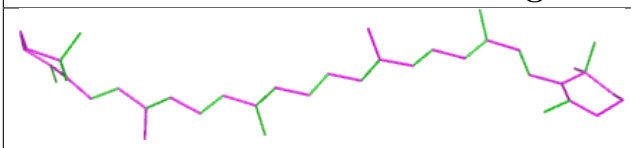
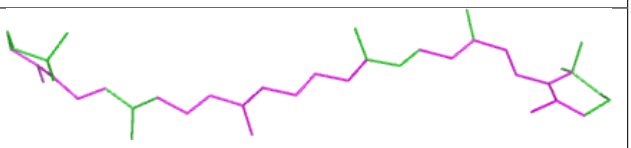
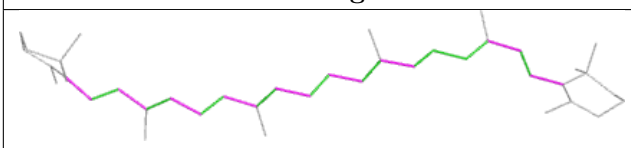
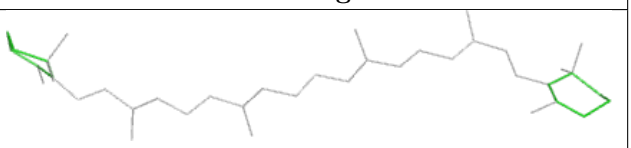


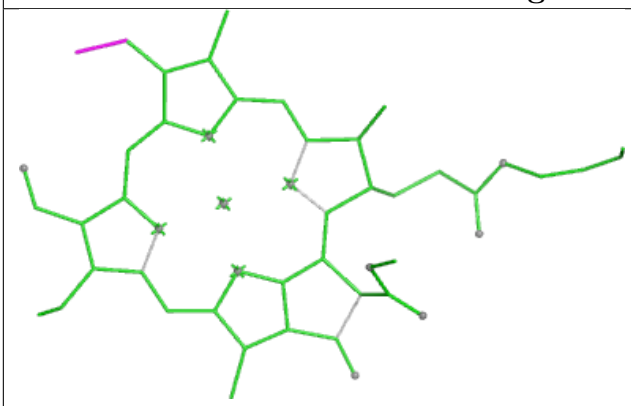
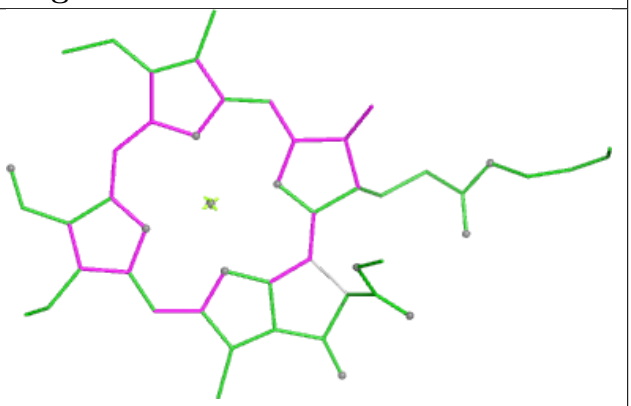
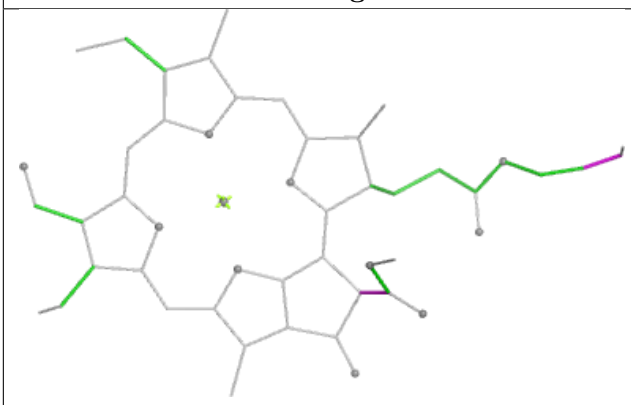
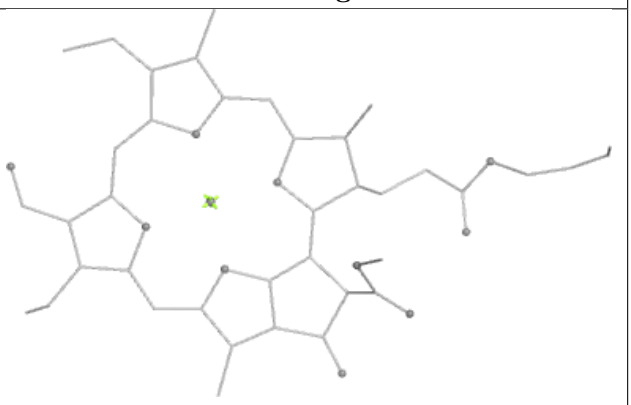
Ligand DGD c 618



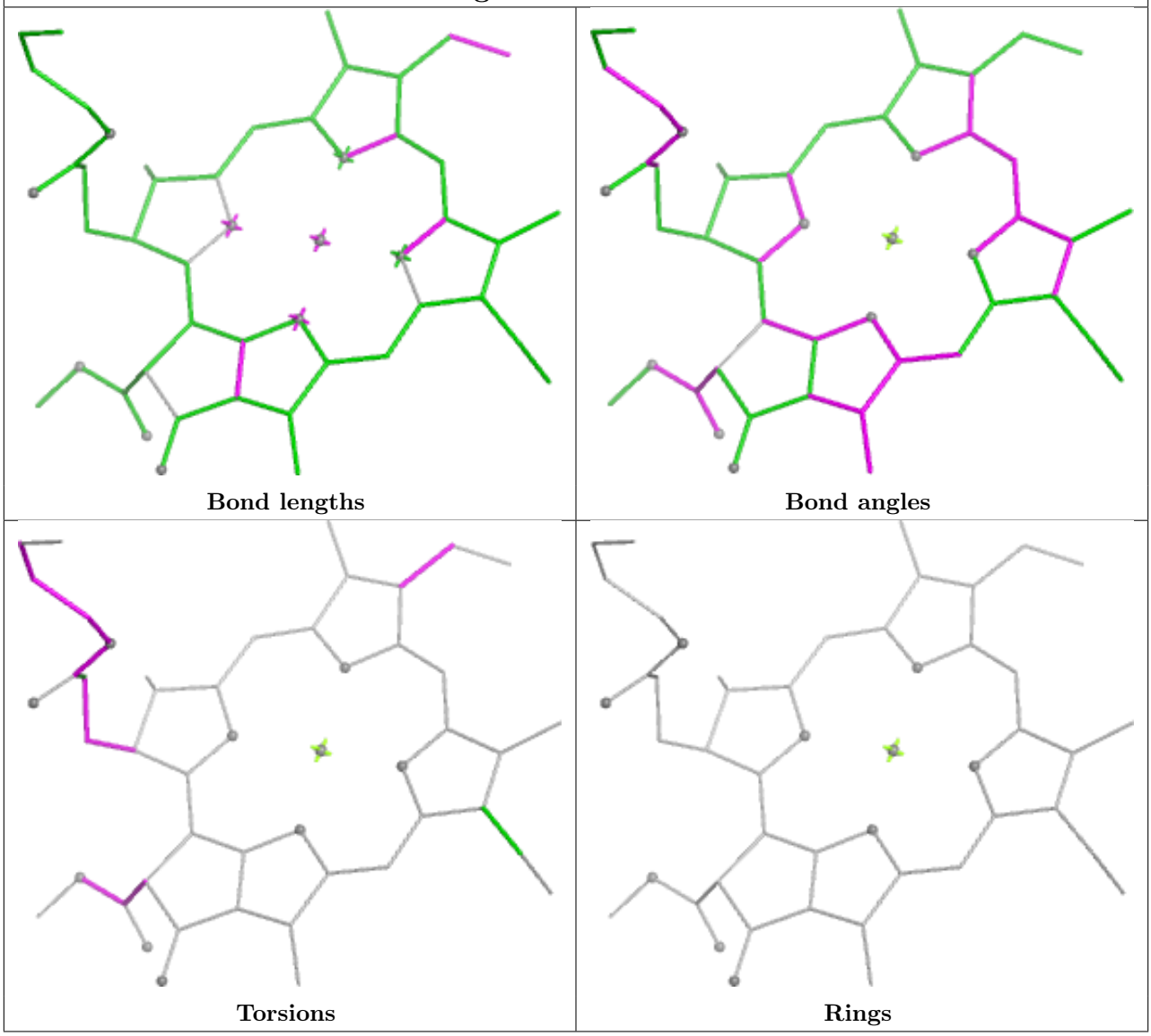
Ligand CLA 1 604



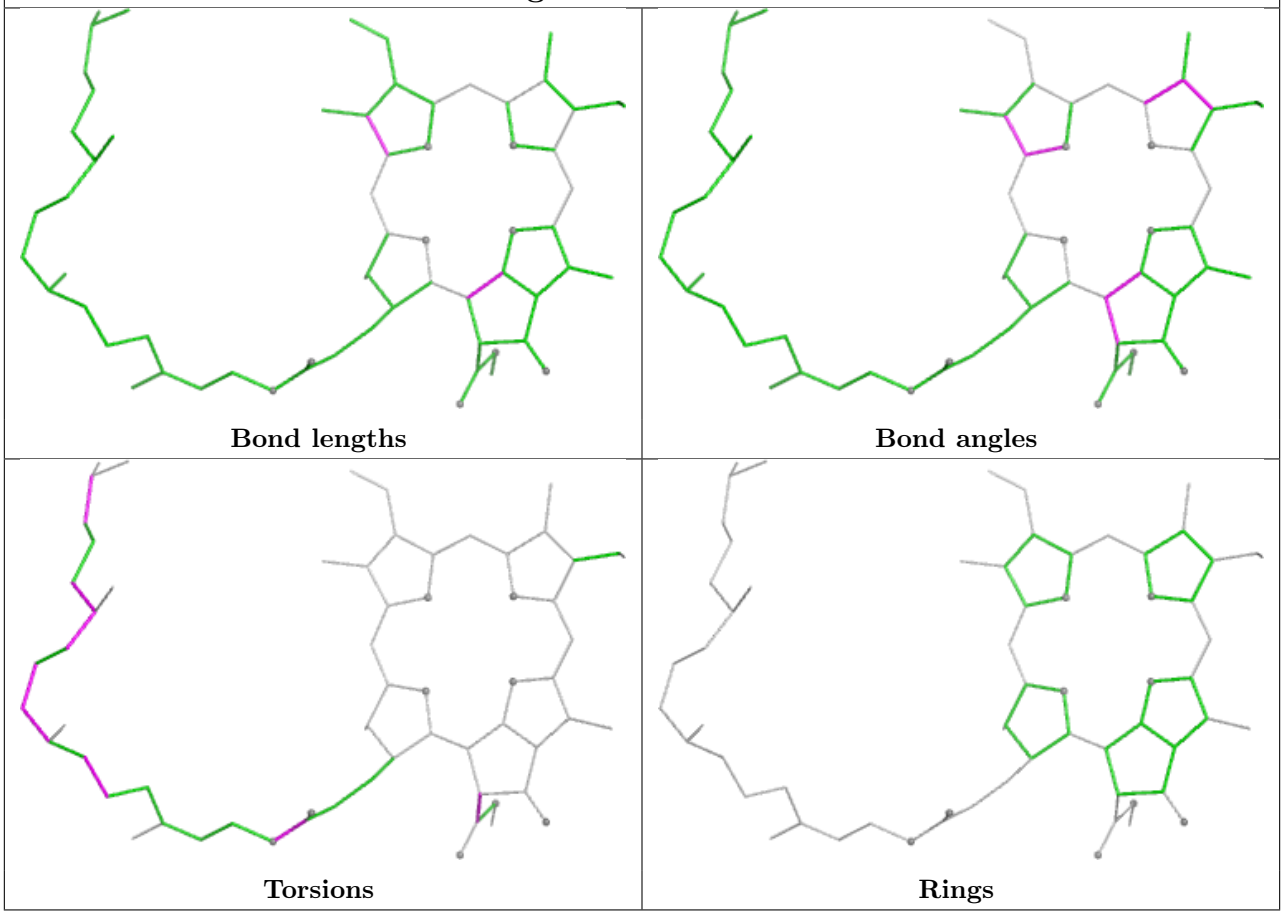
Ligand BCR v 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL g 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

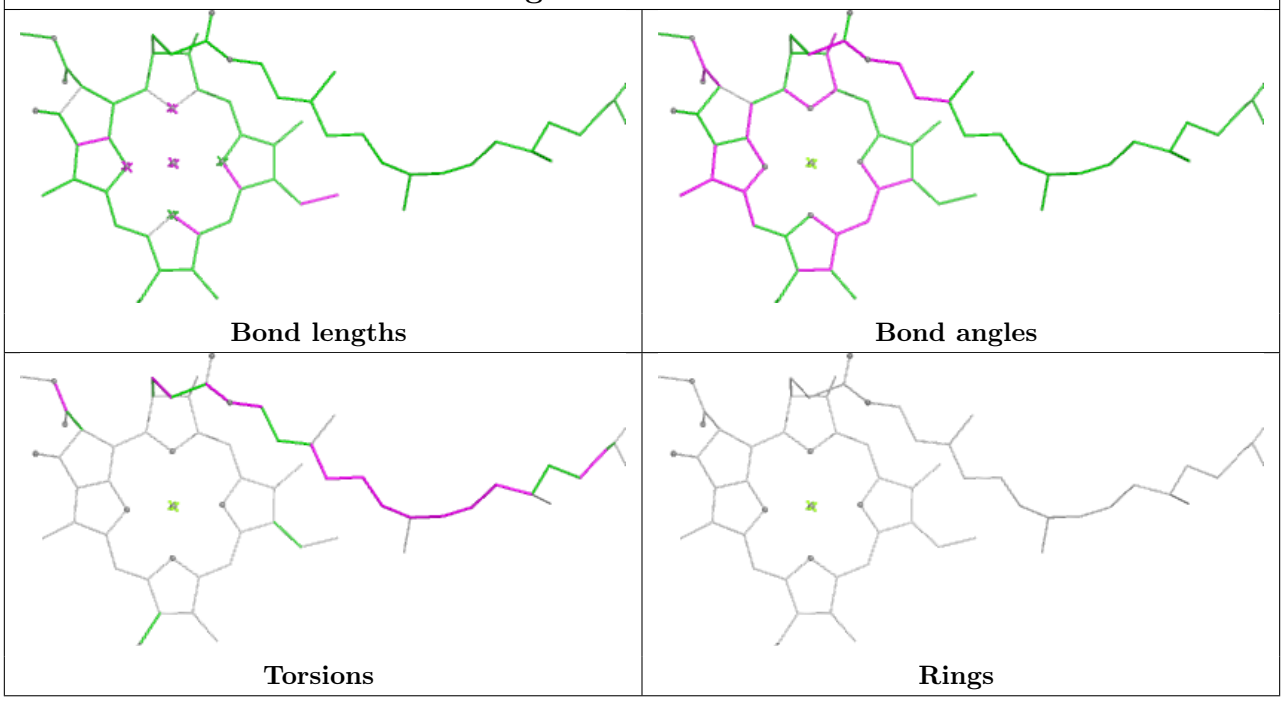
Ligand CLA b 602



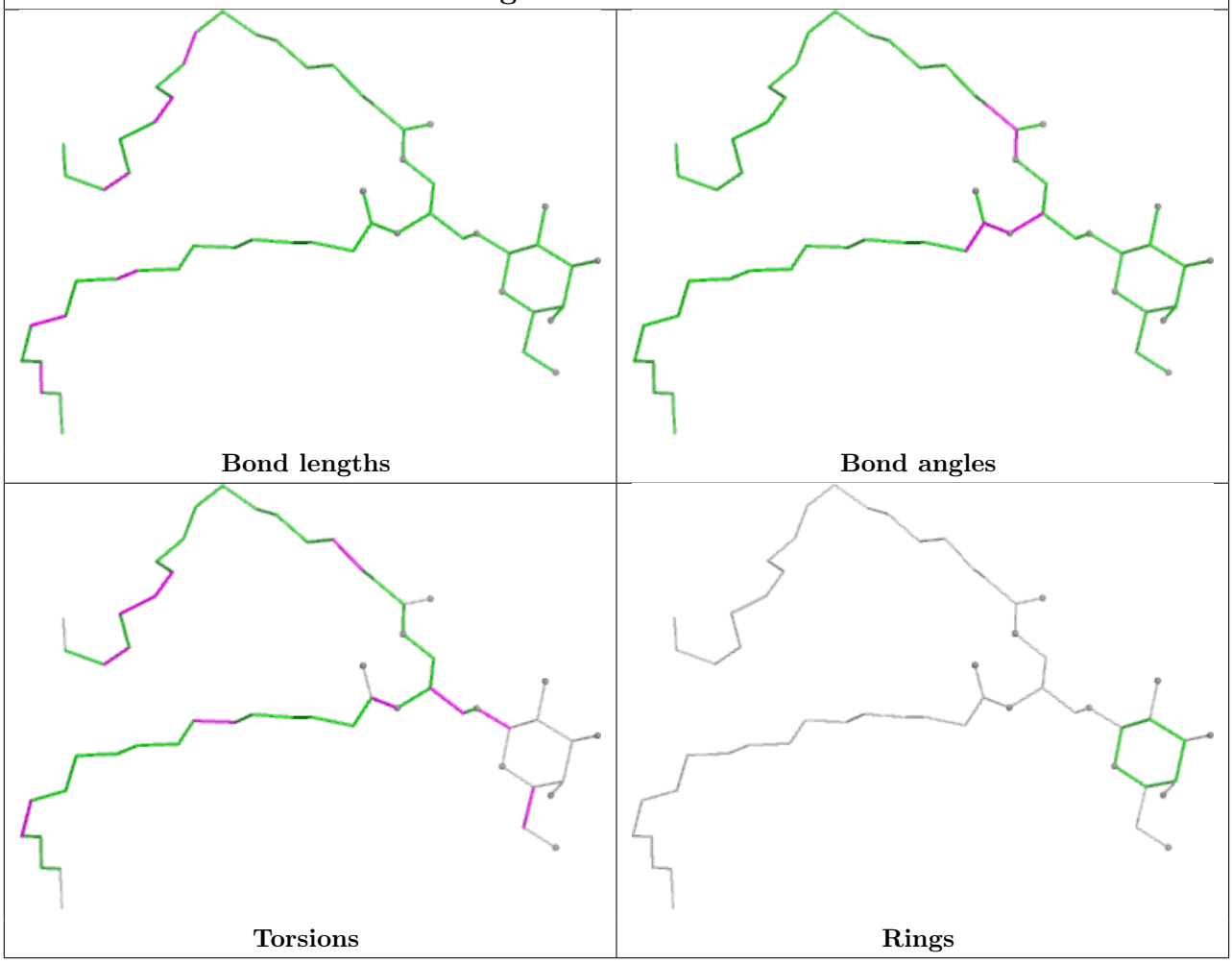
Ligand PHO a 408



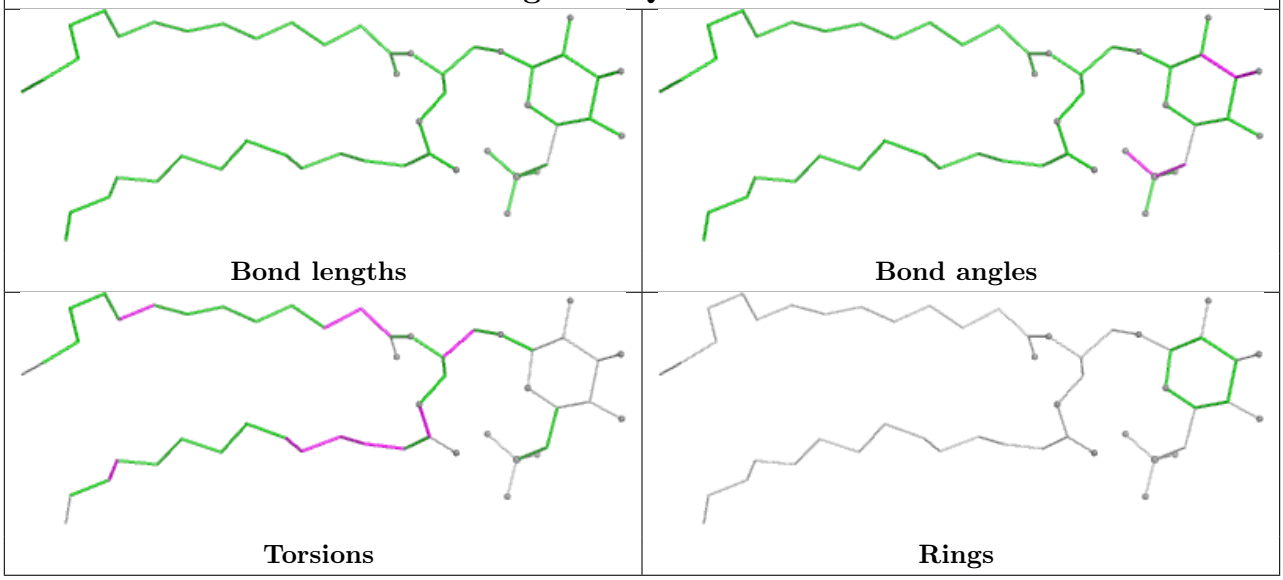
Ligand CLA B 603



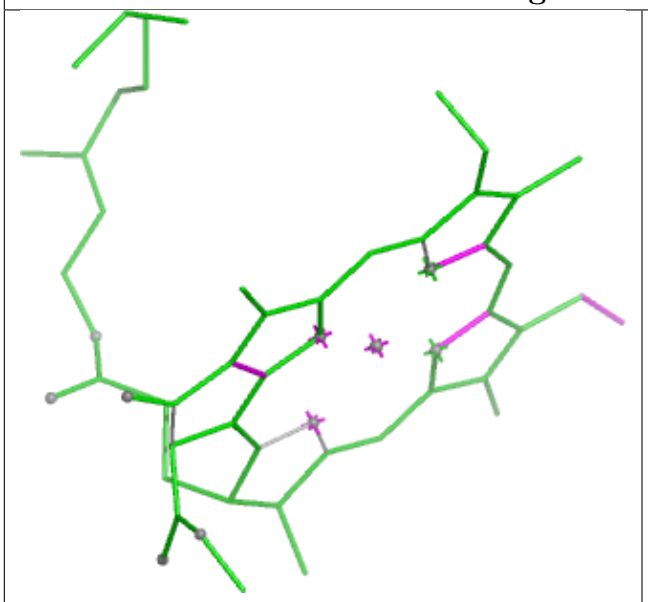
Ligand LMG w 202



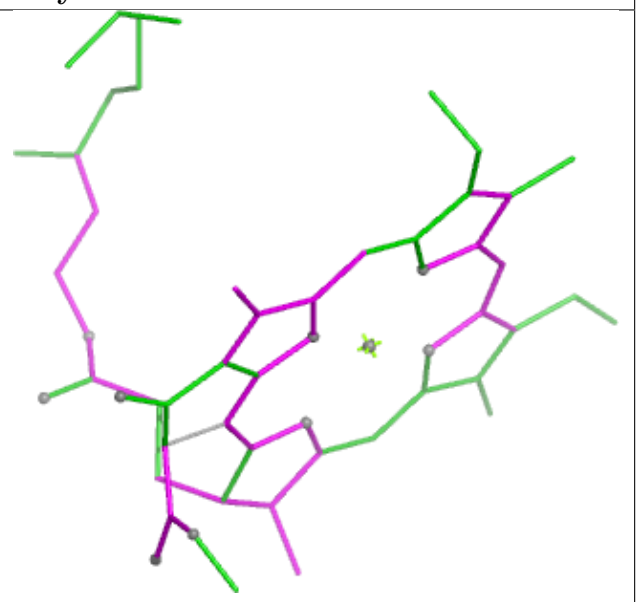
Ligand SQD m 101



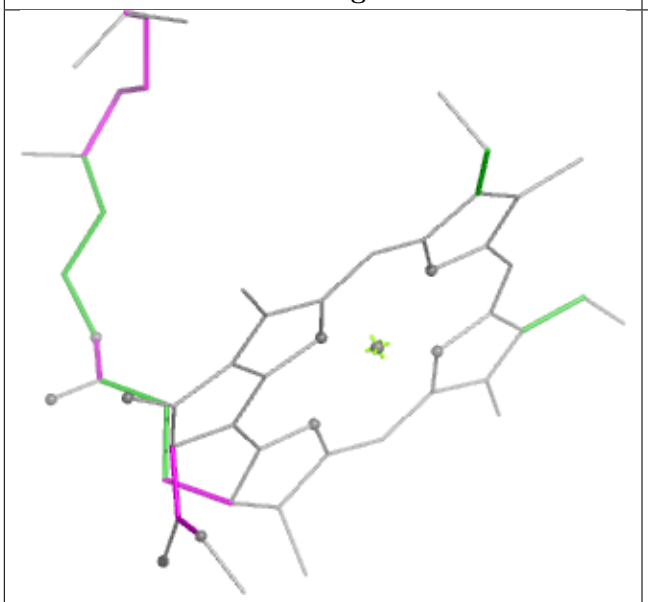
Ligand CLA y 604



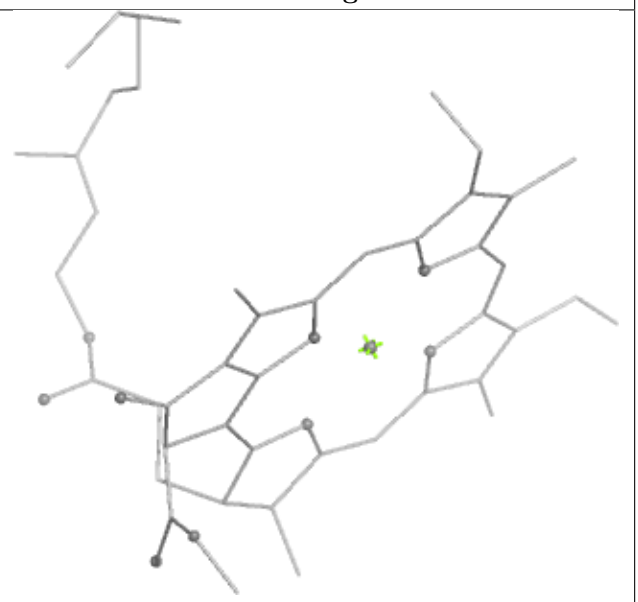
Bond lengths



Bond angles

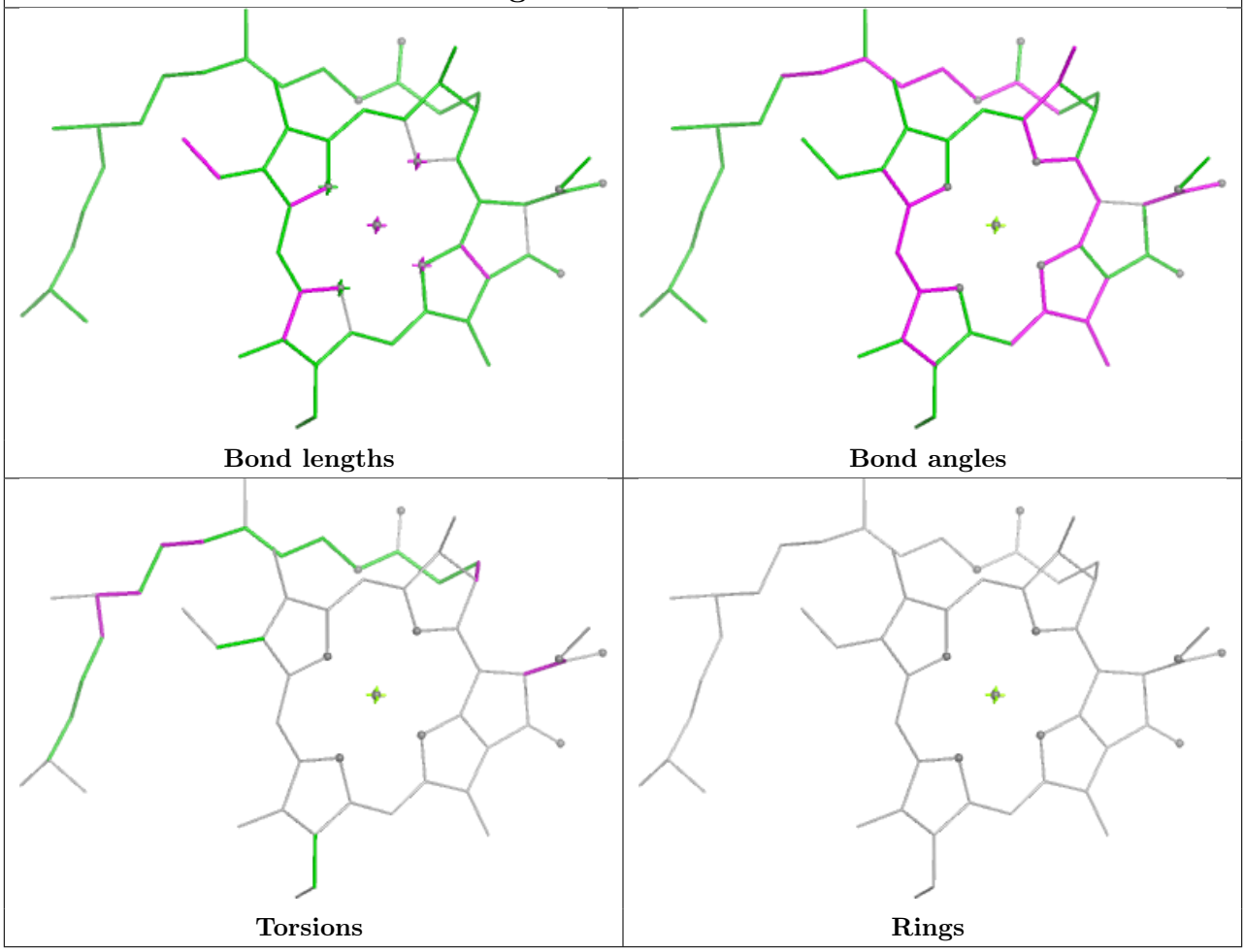


Torsions

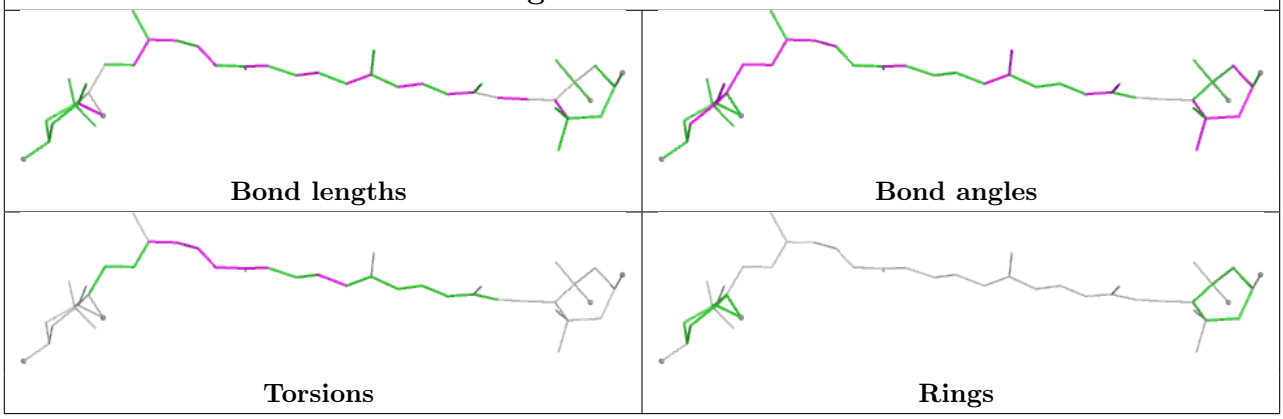


Rings

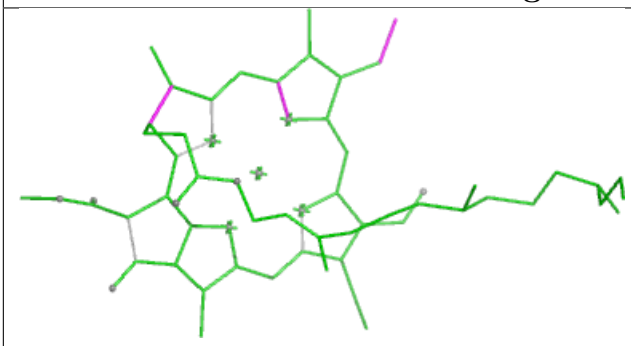
Ligand CLA Y 303



Ligand NEX 6 319



Ligand CHL Y 301



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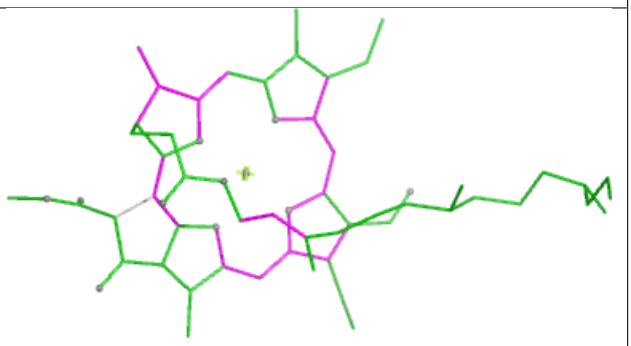
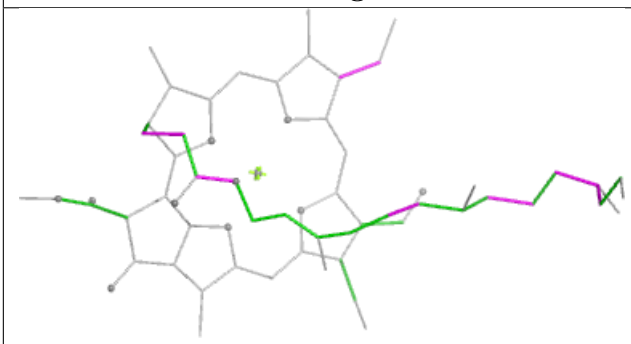


Bond angles



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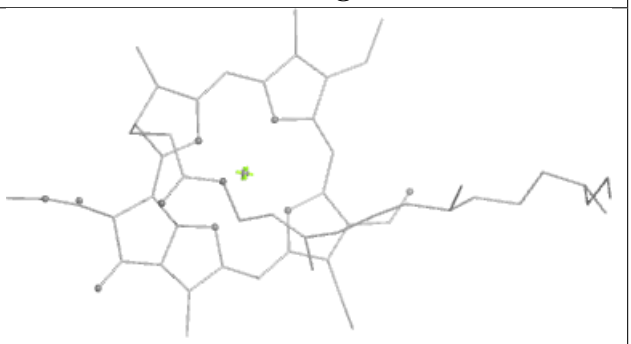
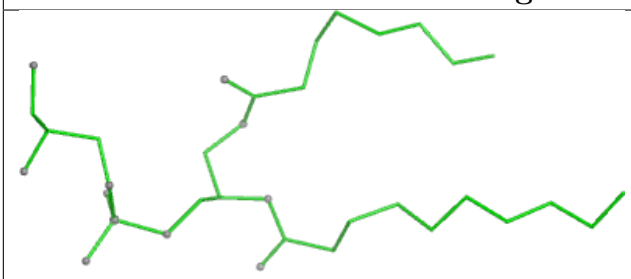
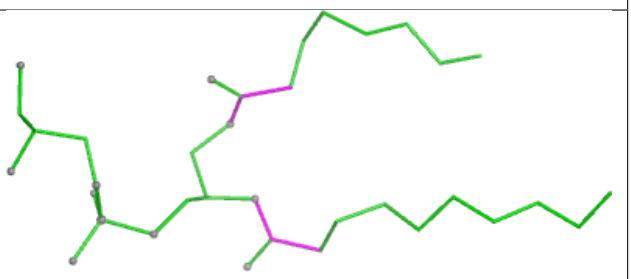


Rings

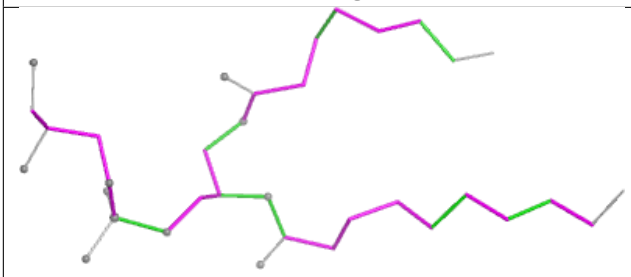
Ligand LHG F1 301



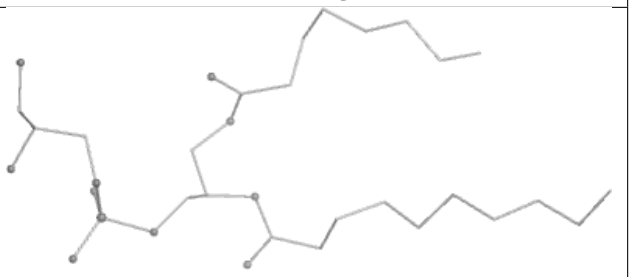
Bond lengths



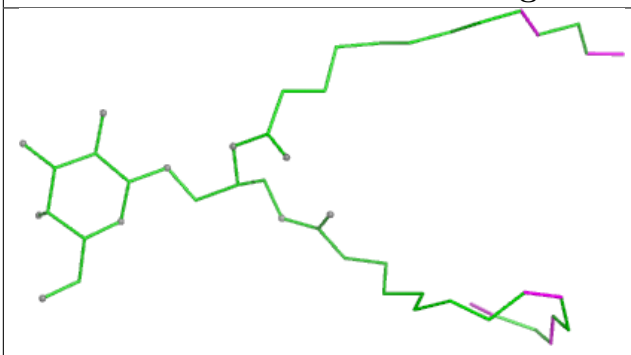
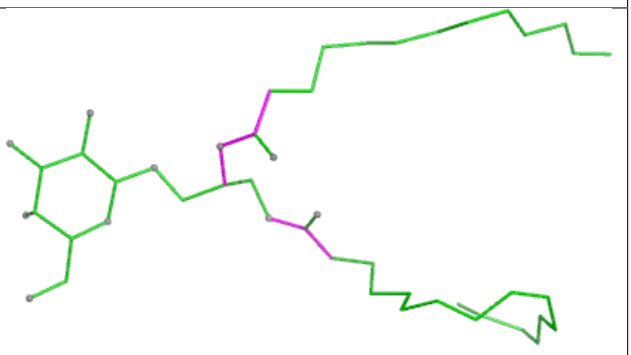
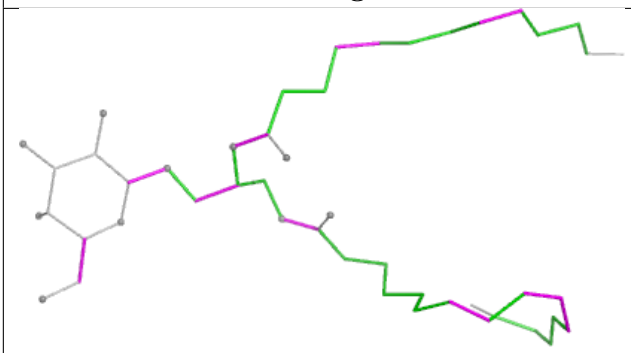
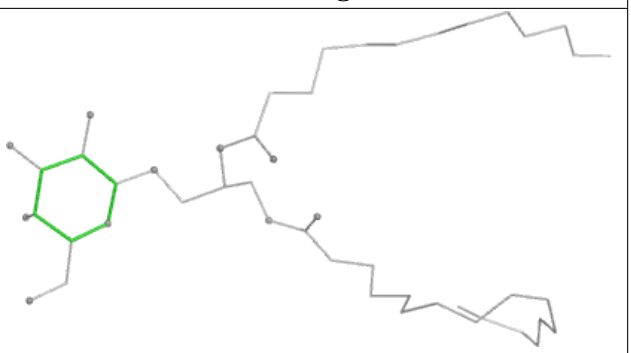
Bond angles



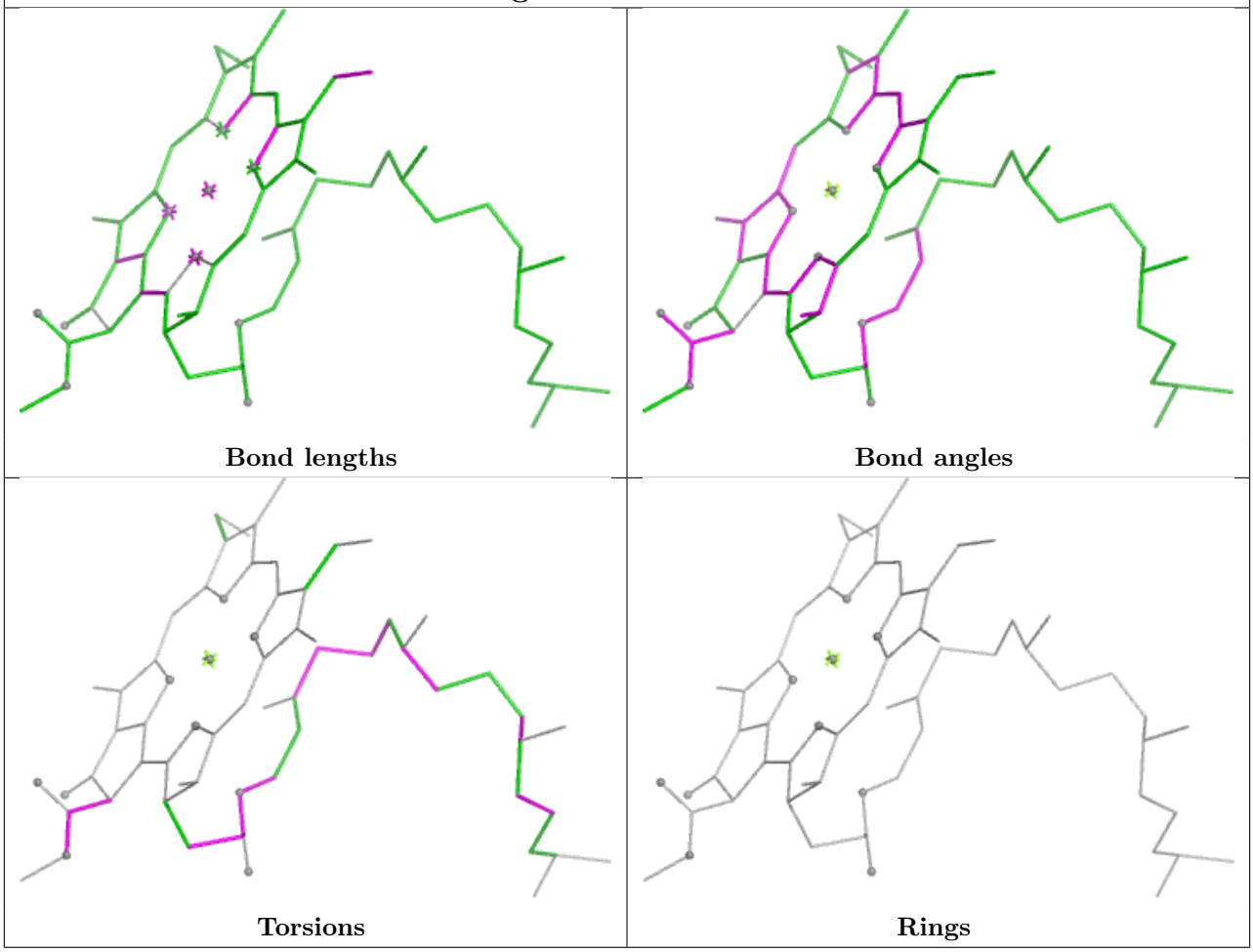
Torsions



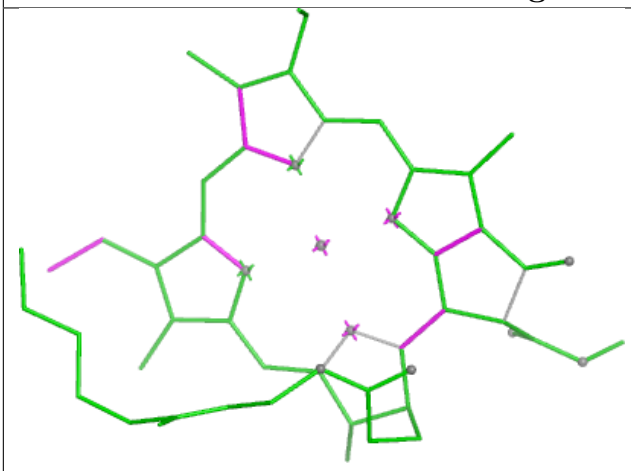
Rings

Ligand LMG w 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

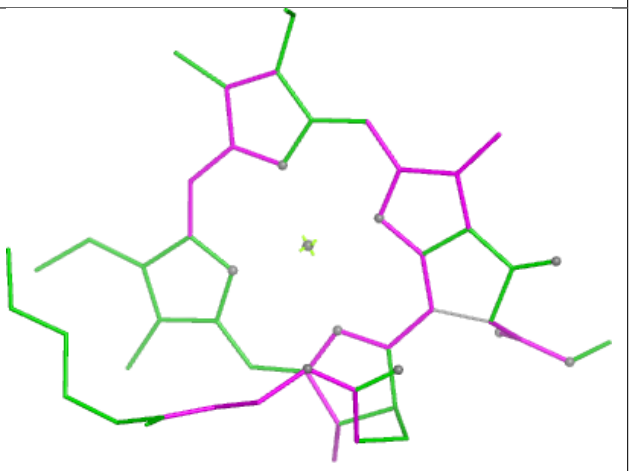
Ligand CLA G 612



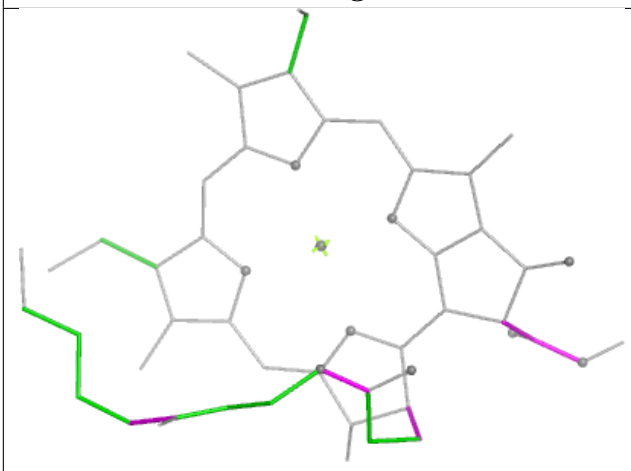
Ligand CLA 4 614



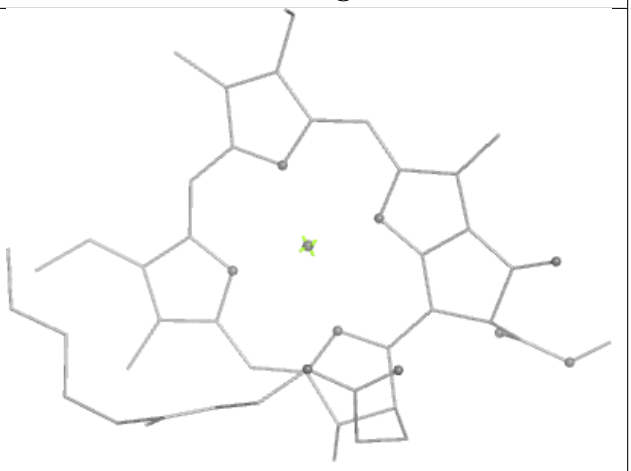
Bond lengths



Bond angles

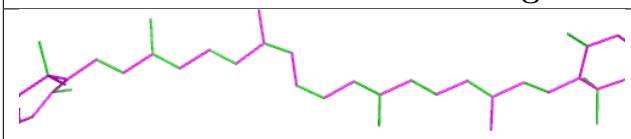


Torsions



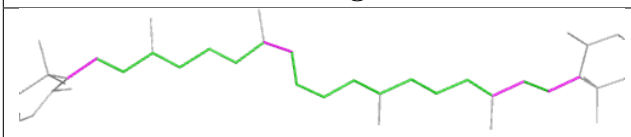
Rings

Ligand BCR A 410



Bond lengths

Bond angles



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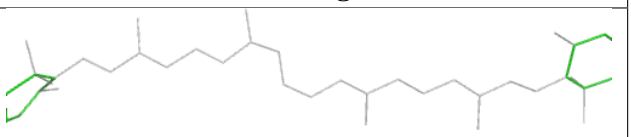
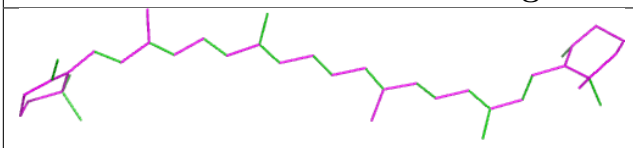
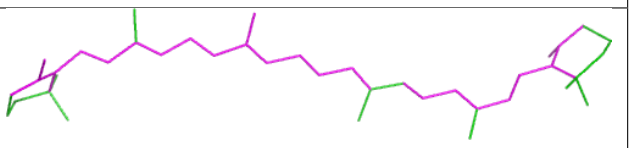


Rings

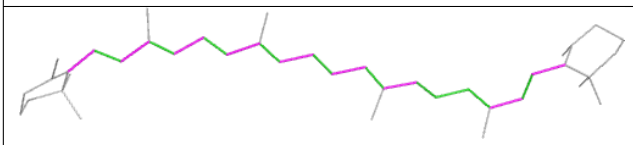
Ligand BCR V 101



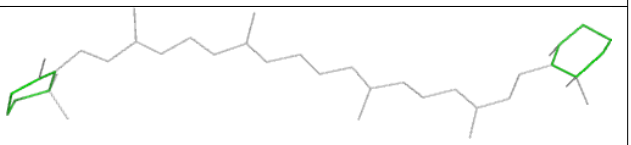
Bond lengths



Bond angles

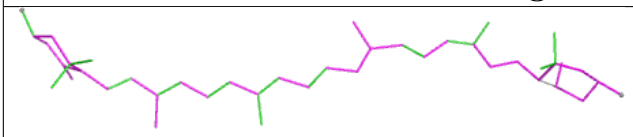


Torsions



Rings

Ligand LUT 2 615



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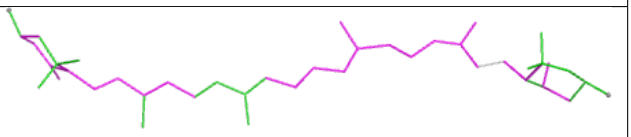
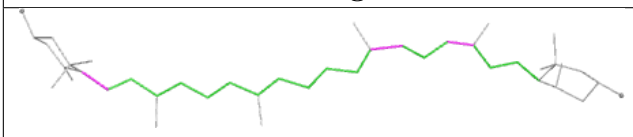
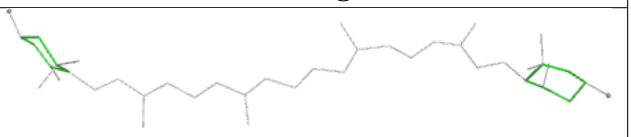


Bond angles

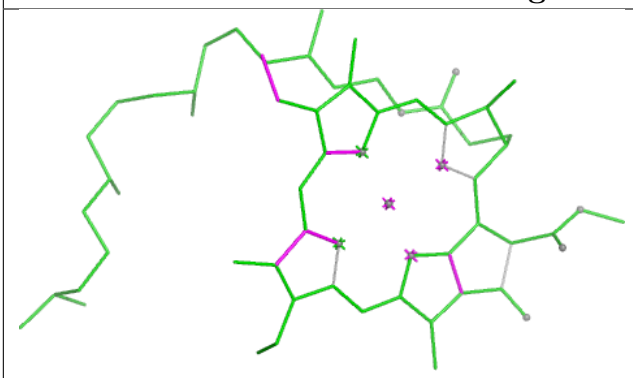


Torsions

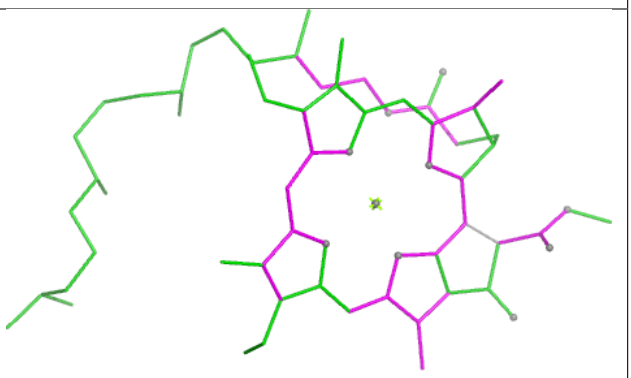


Rings

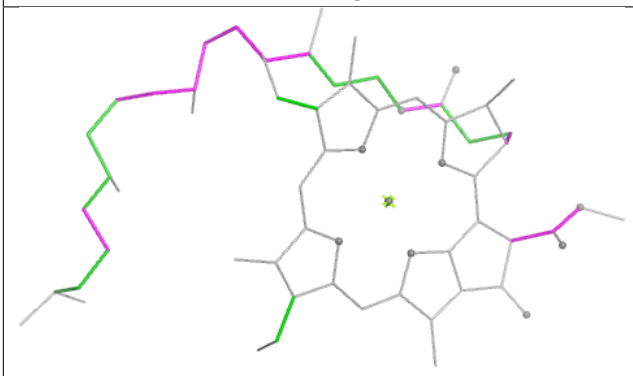
Ligand CLA 7 311



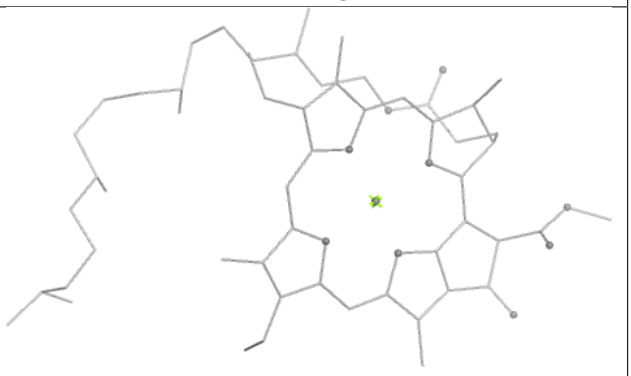
Bond lengths



Bond angles

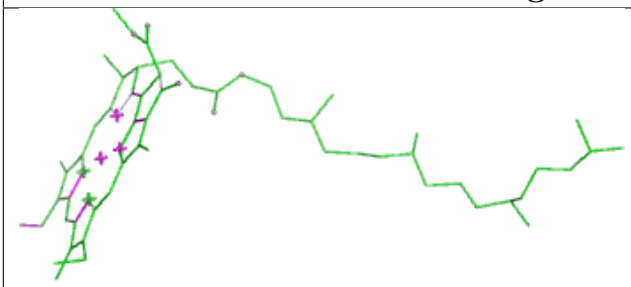


Torsions

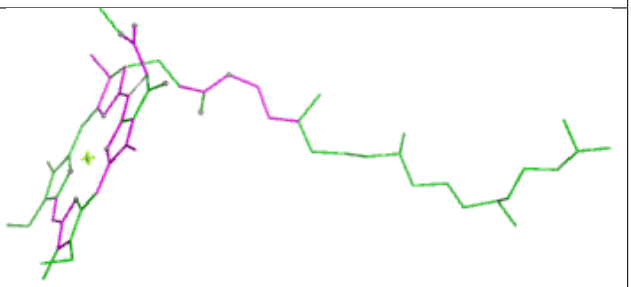


Rings

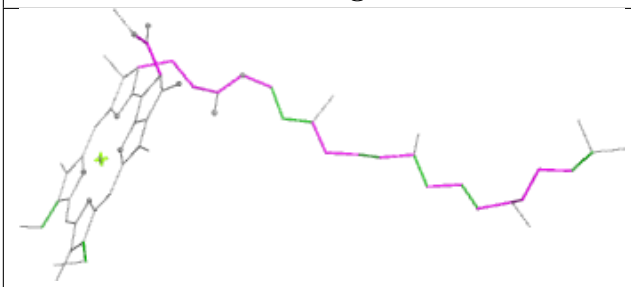
Ligand CLA b 605



Bond lengths



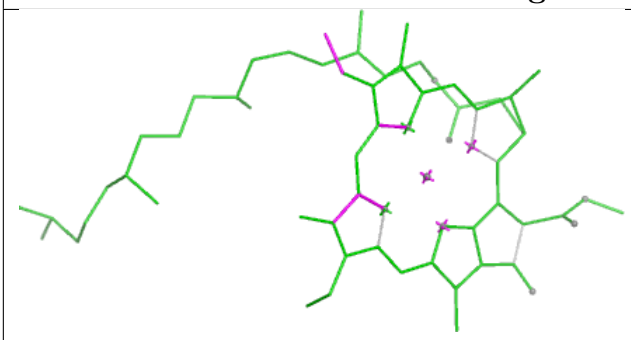
Bond angles



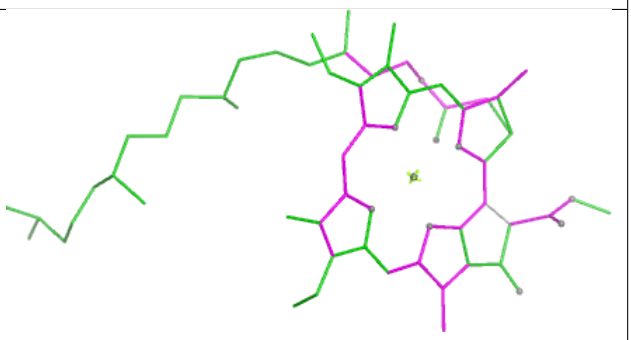
Torsions

Rings

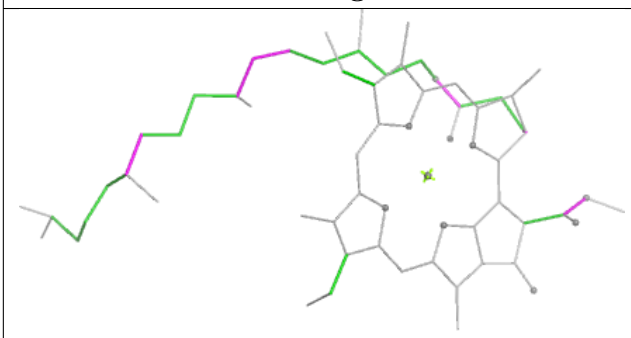
Ligand CLA 8 609



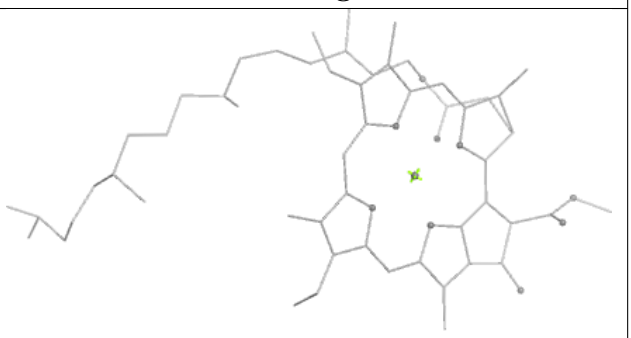
Bond lengths



Bond angles

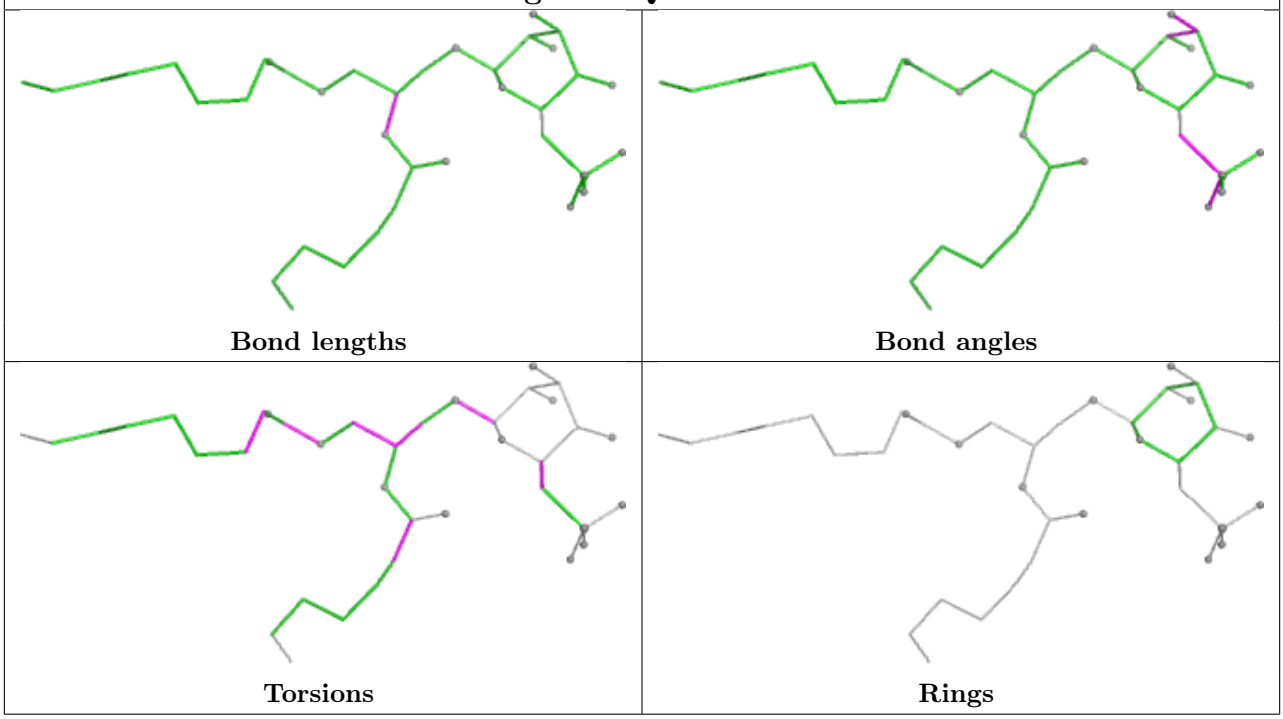


Torsions

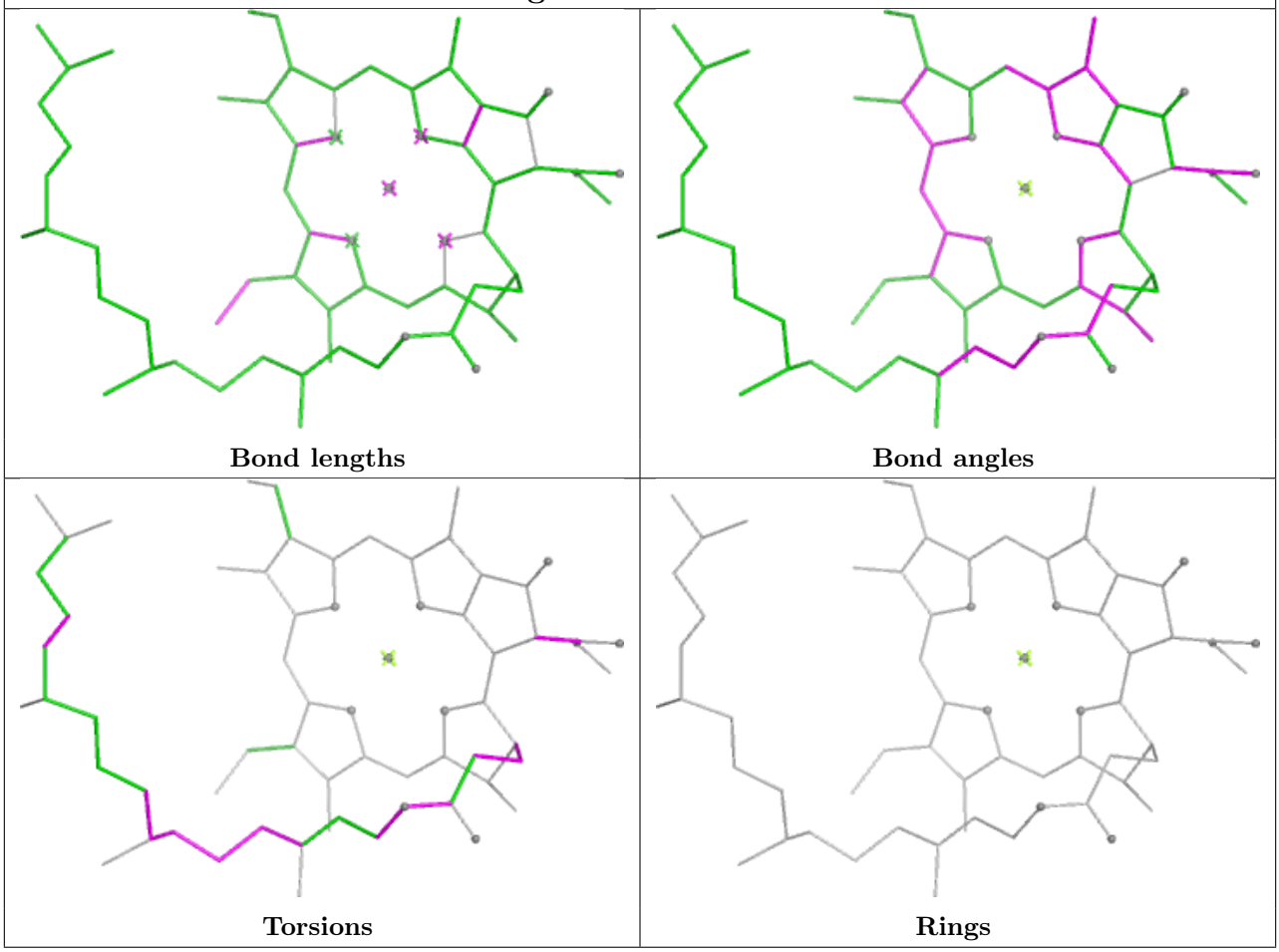


Rings

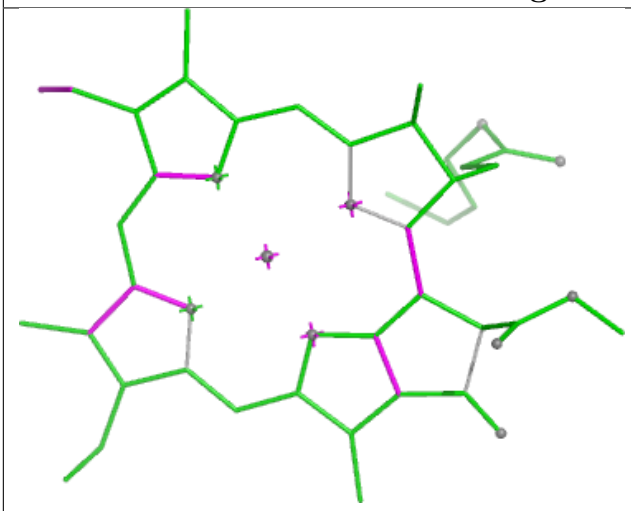
Ligand SQD G 624



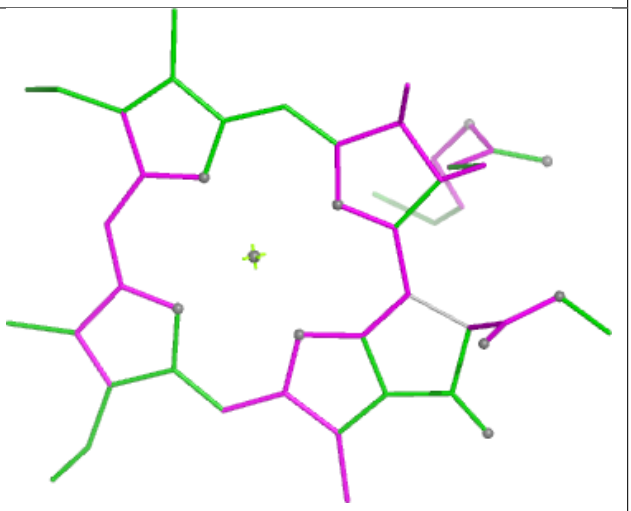
Ligand CLA 0 602



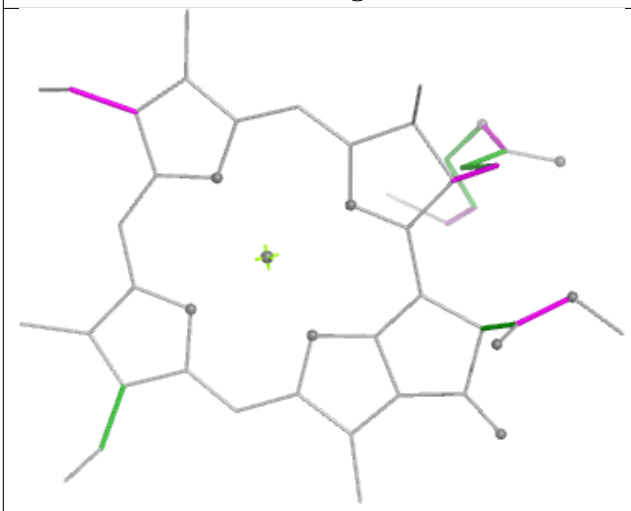
Ligand CLA r 313



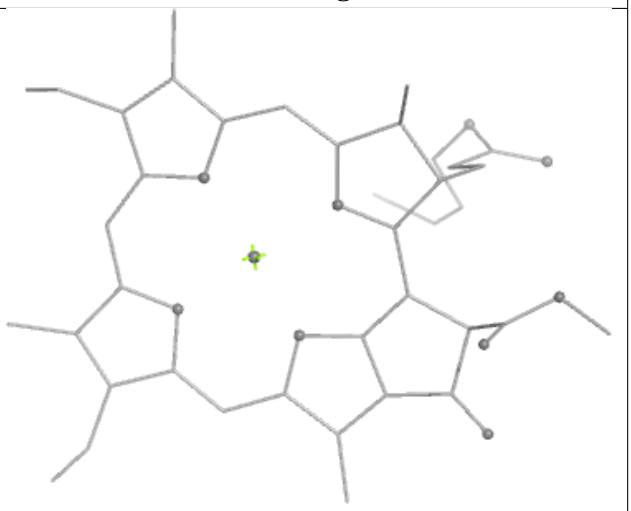
Bond lengths



Bond angles

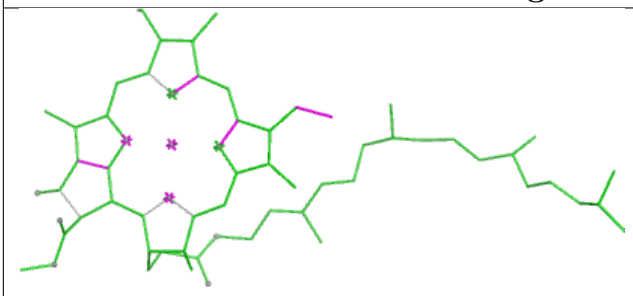


Torsions

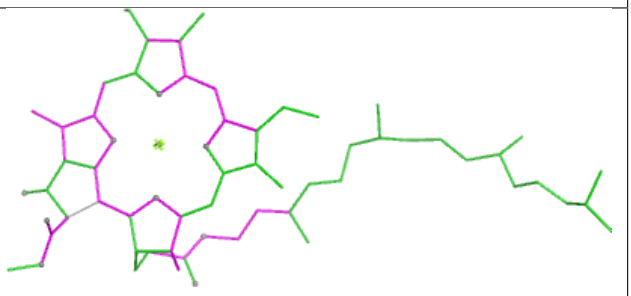


Rings

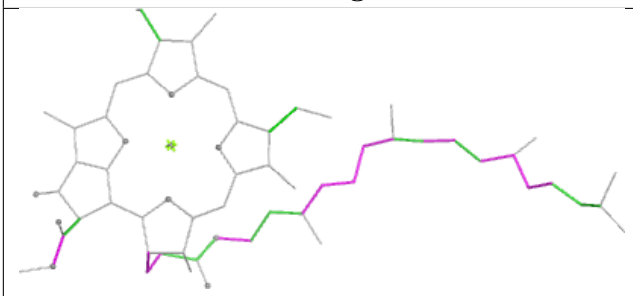
Ligand CLA b 604



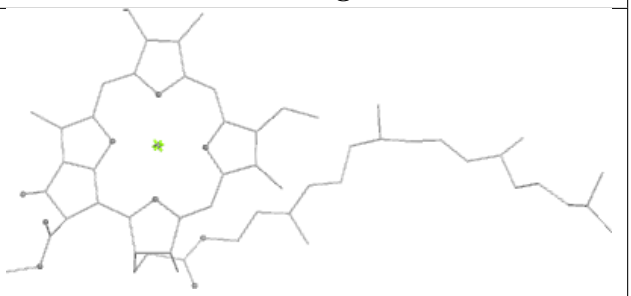
Bond lengths



Bond angles

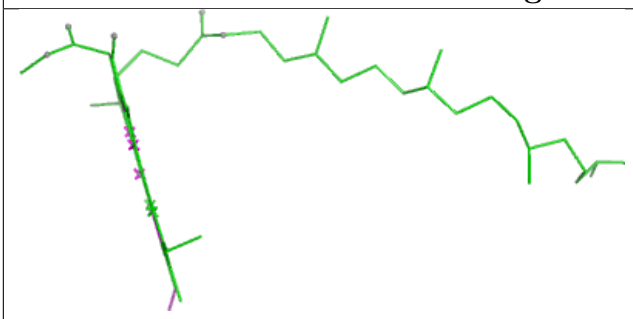


Torsions

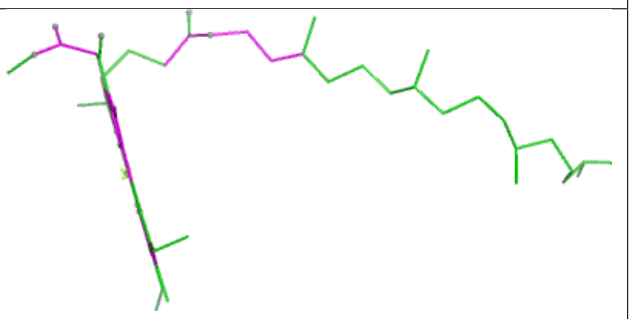


Rings

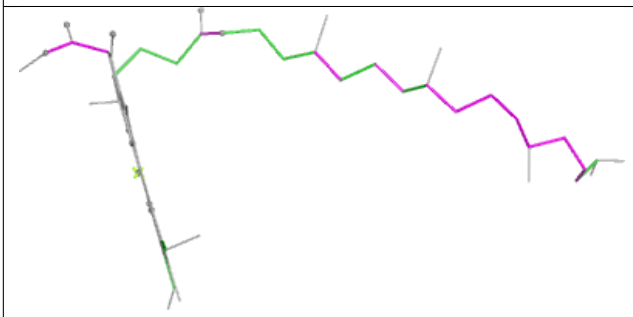
Ligand CLA B 605



Bond lengths

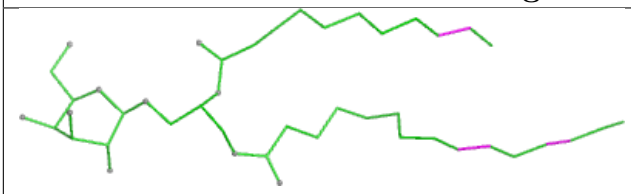
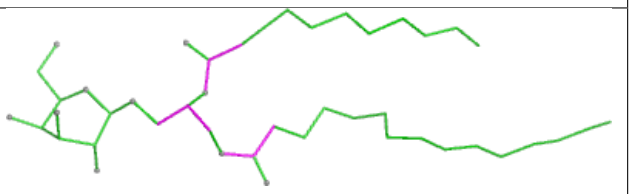
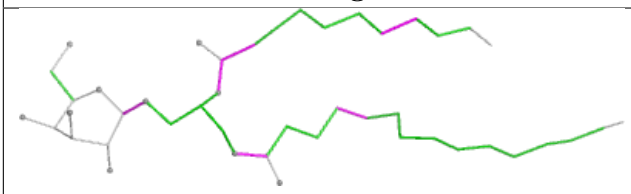
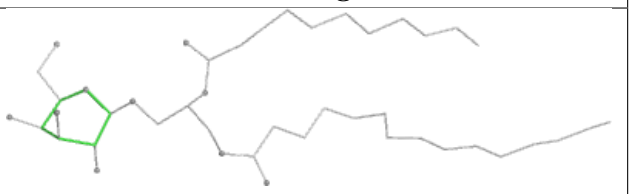


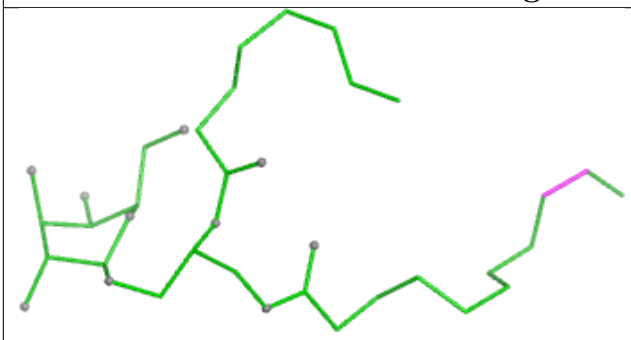
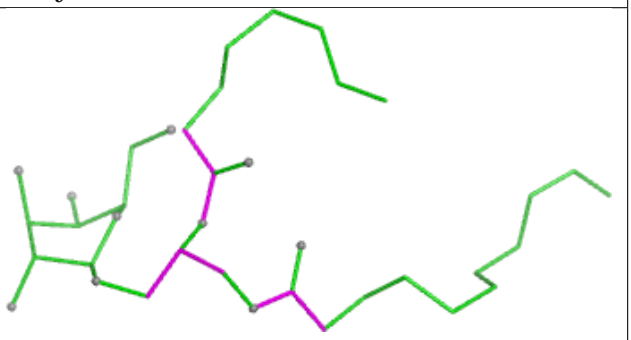
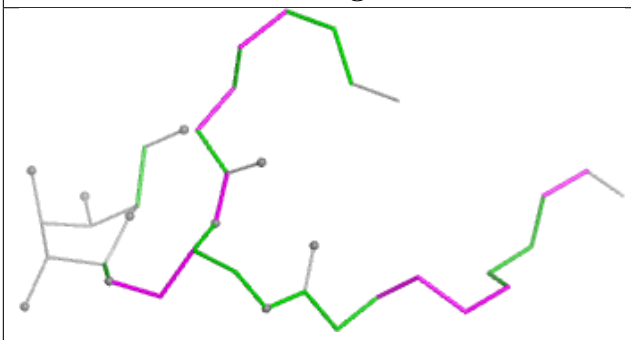
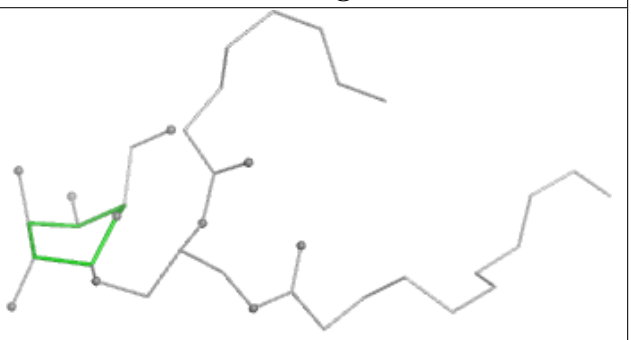
Bond angles



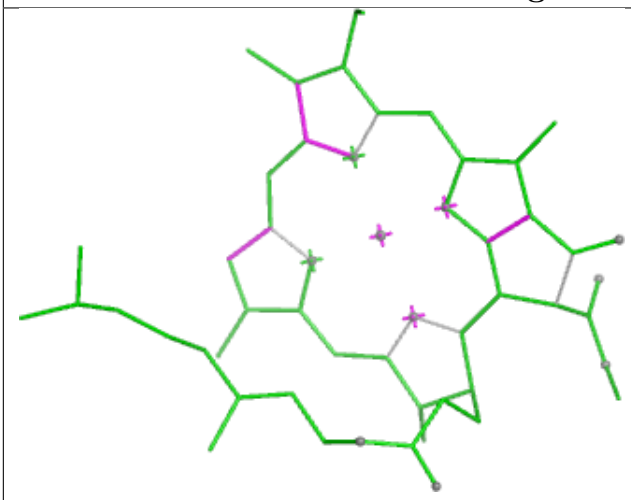
Torsions

Rings

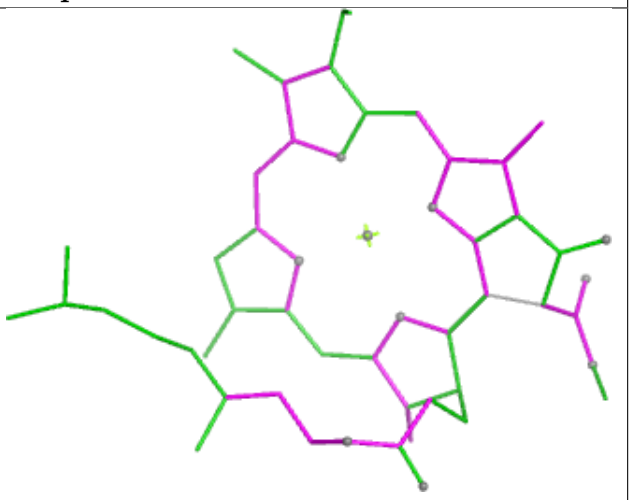
Ligand LMG b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG y 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

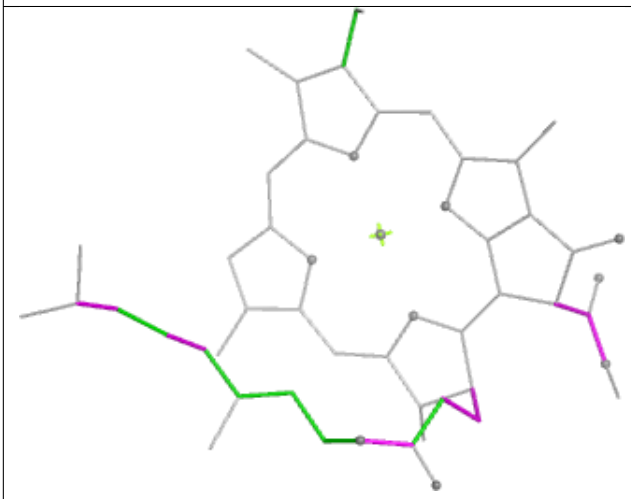
Ligand CLA q 312



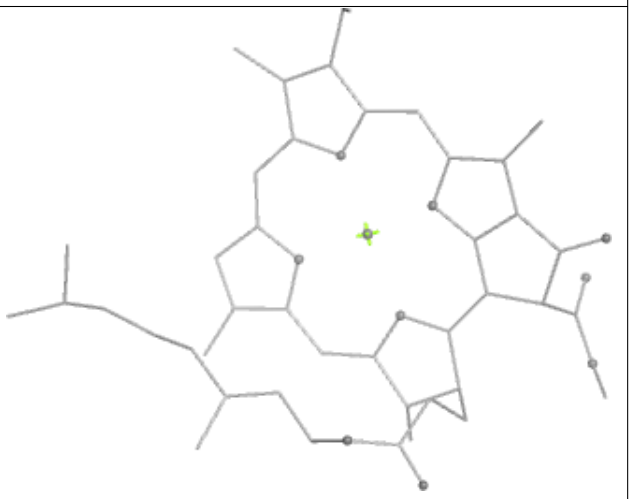
Bond lengths



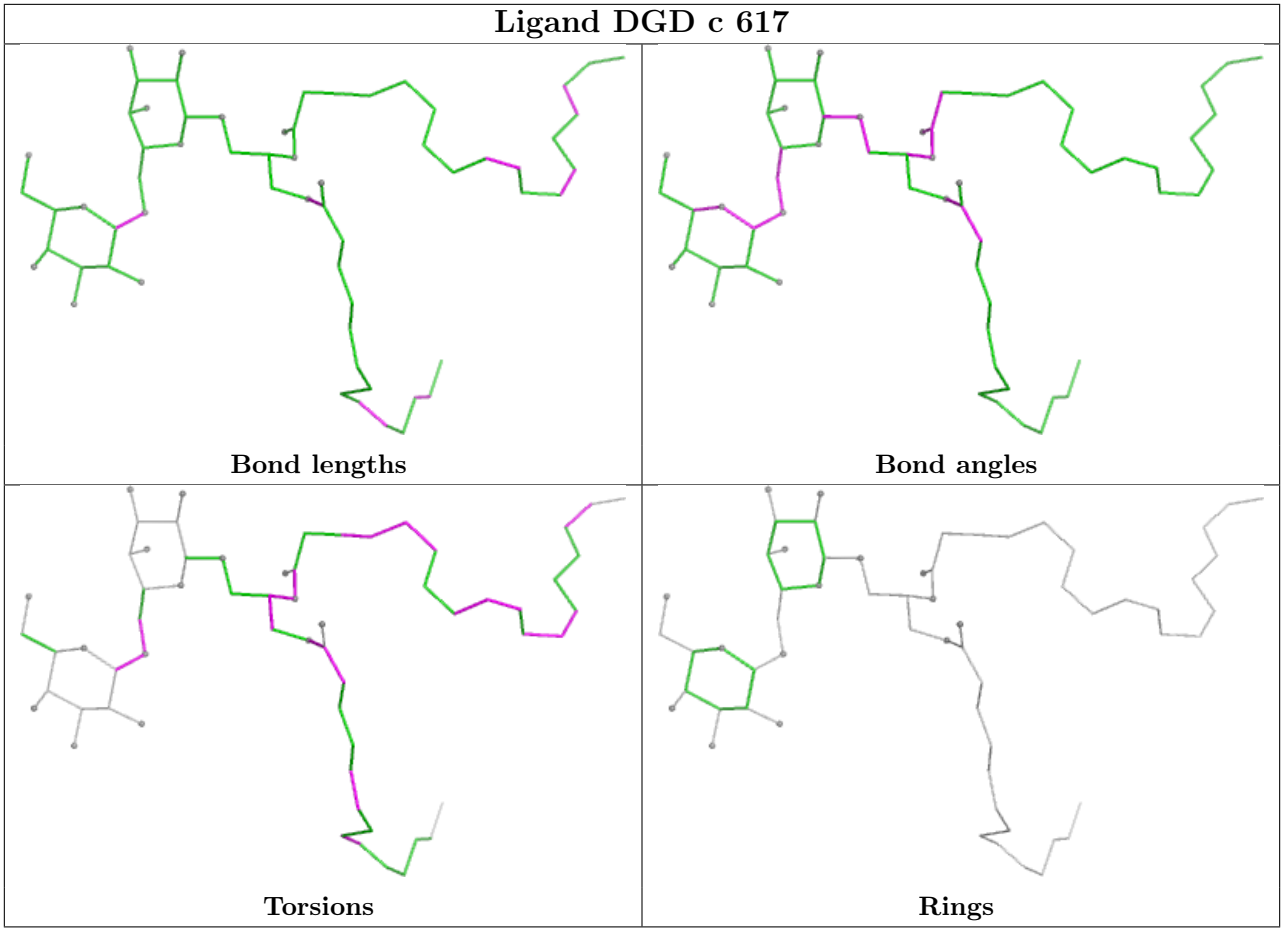
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

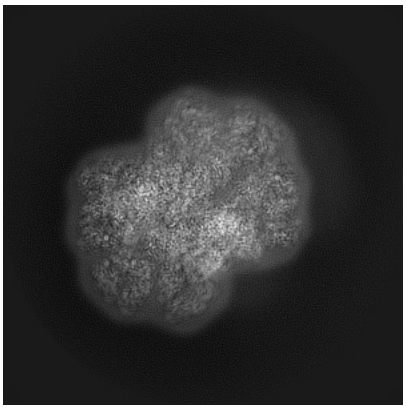
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15973. These allow visual inspection of the internal detail of the map and identification of artifacts.

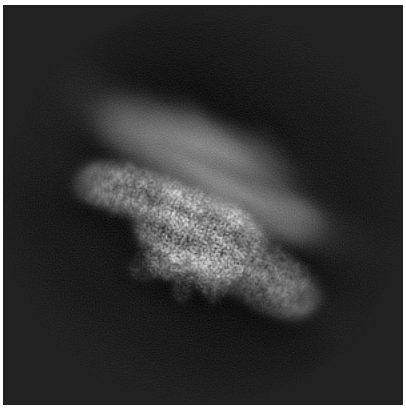
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

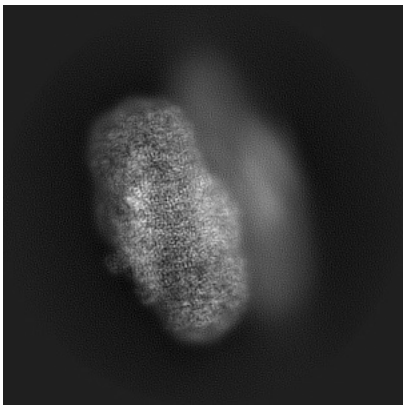
6.1.1 Primary map



X

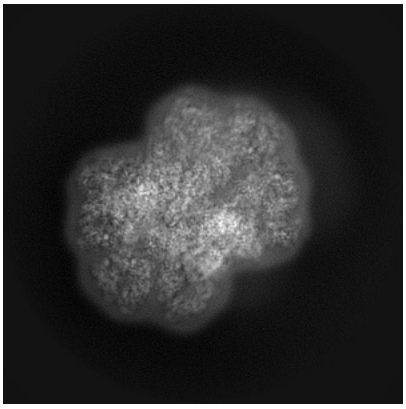


Y

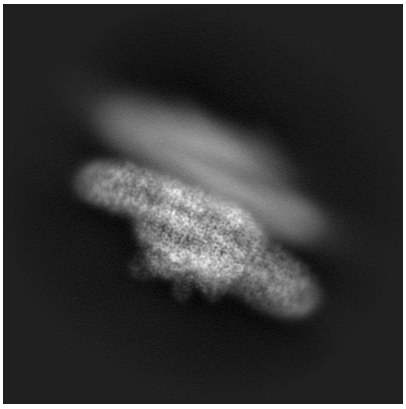


Z

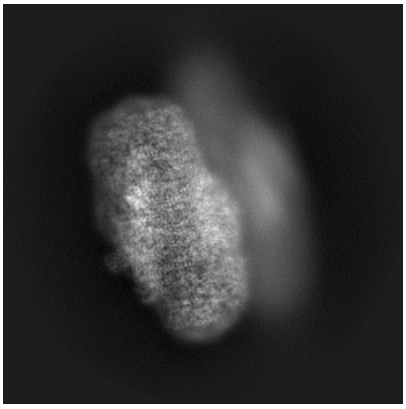
6.1.2 Raw map



X



Y

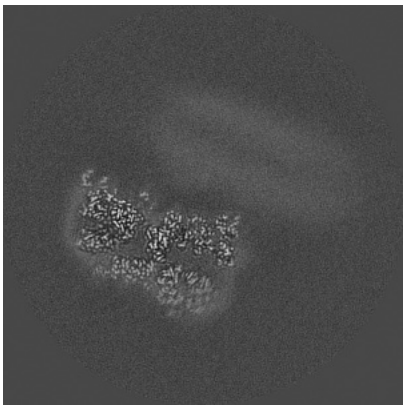


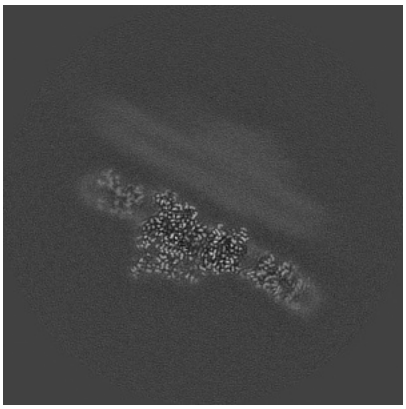
Z

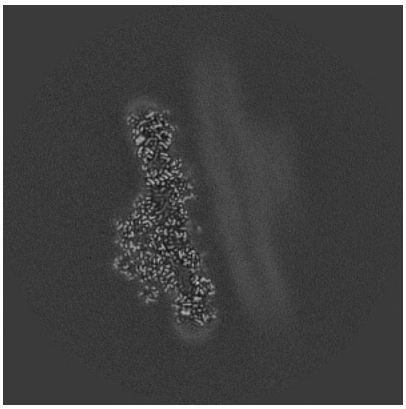
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

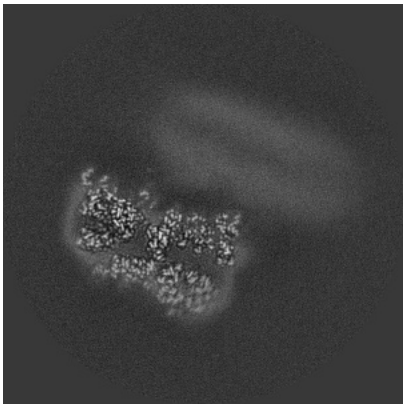
6.2.1 Primary map

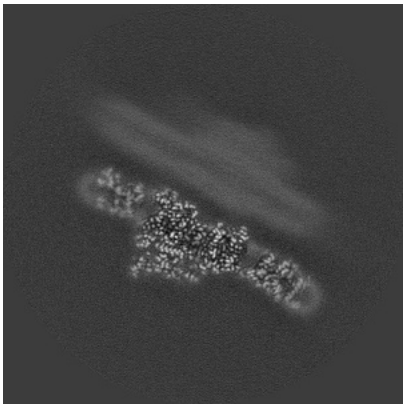

X Index: 250

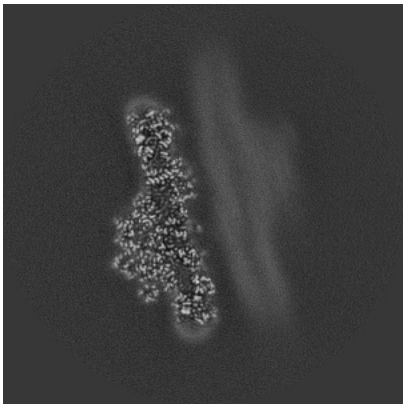

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250

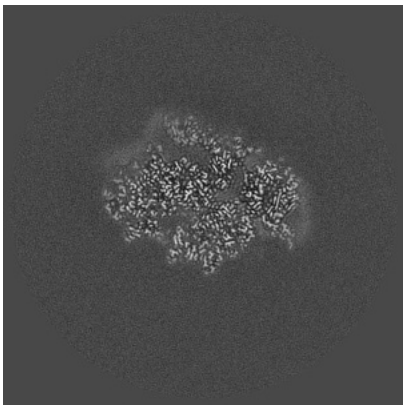

Y Index: 250

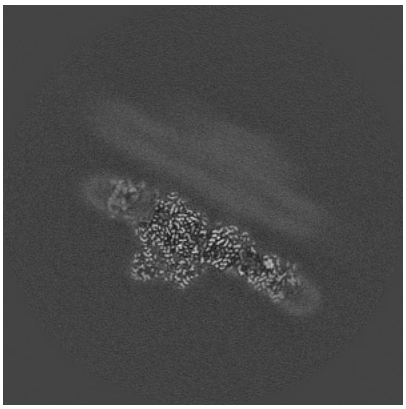

Z Index: 250

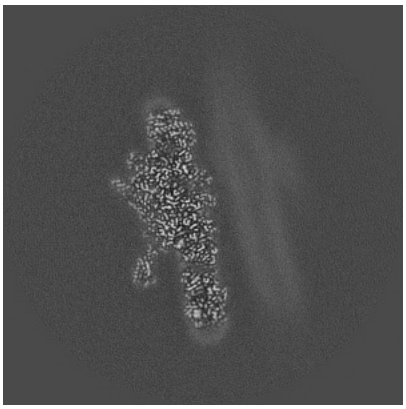
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

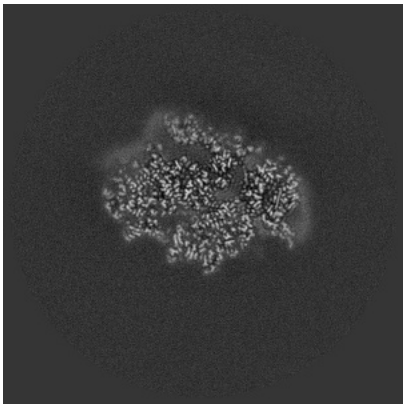
6.3.1 Primary map

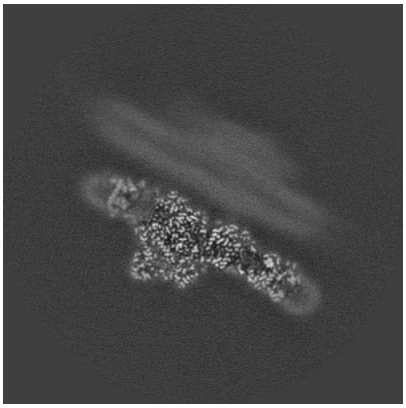

X Index: 183

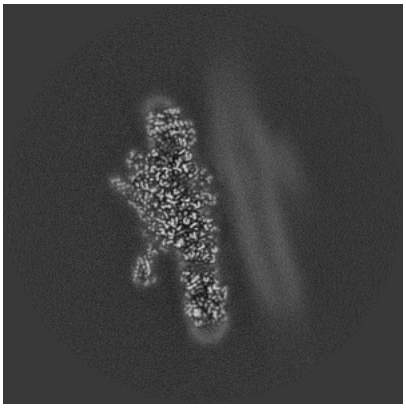

Y Index: 257


Z Index: 213

6.3.2 Raw map


X Index: 183

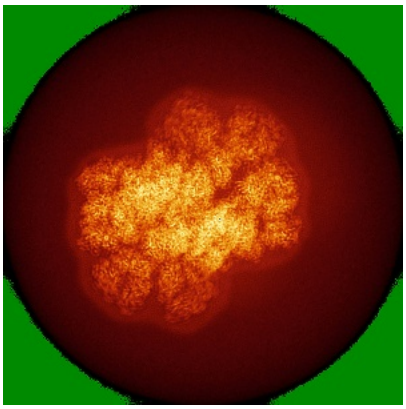

Y Index: 257

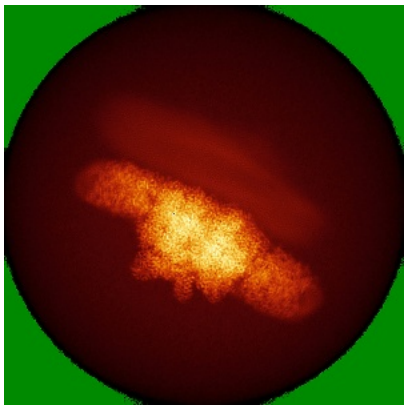

Z Index: 213

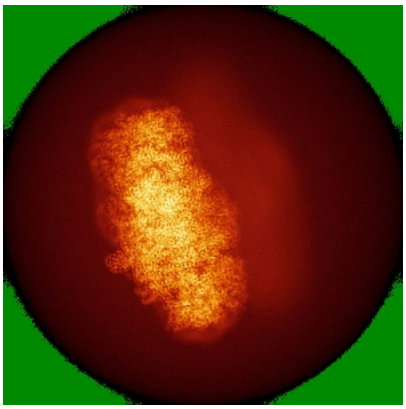
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

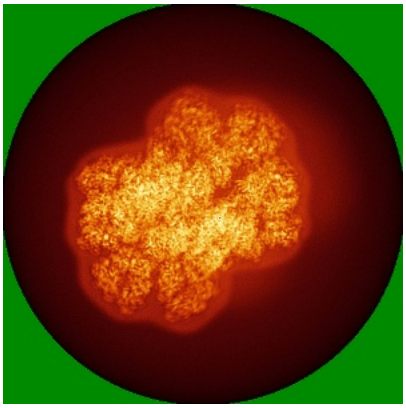
6.4.1 Primary map

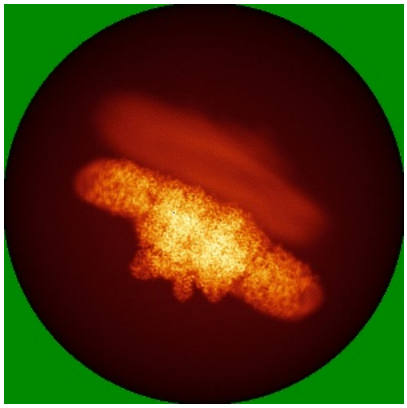

X

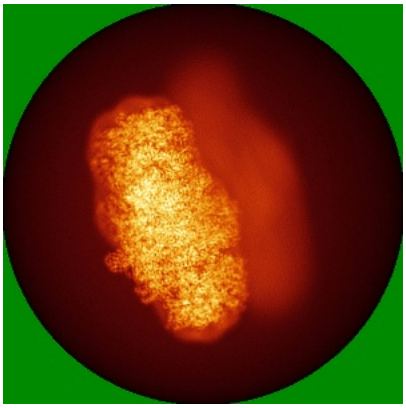

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

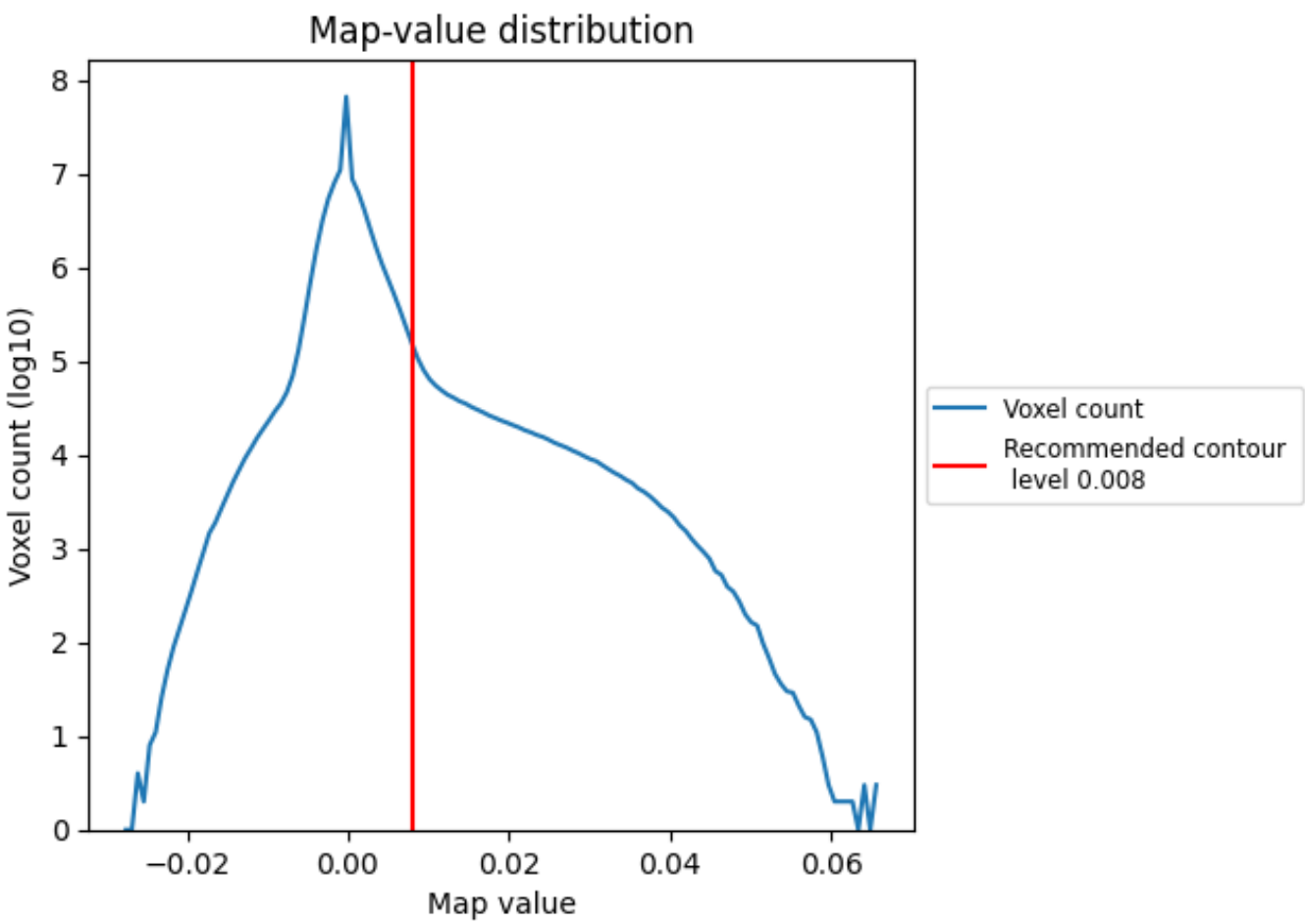
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

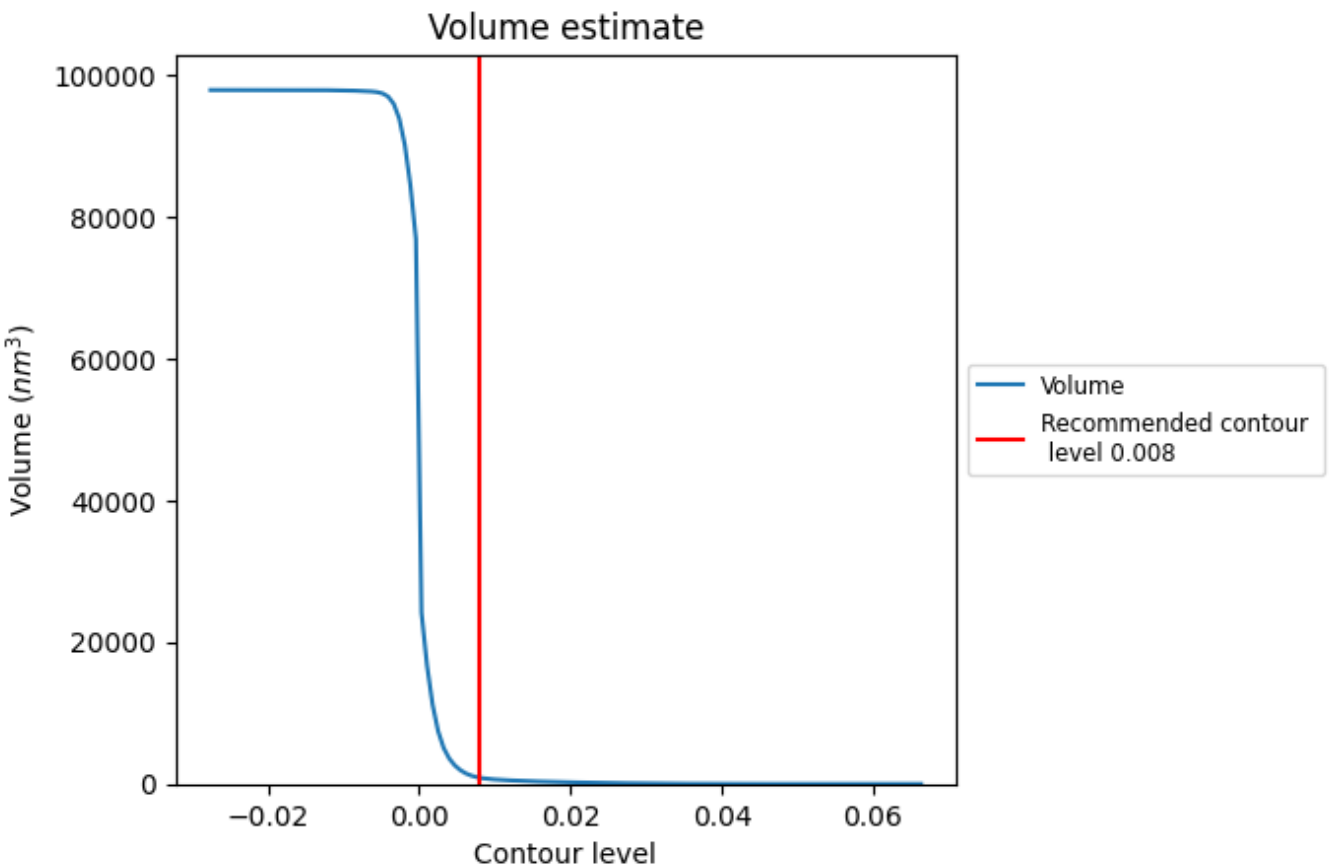
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

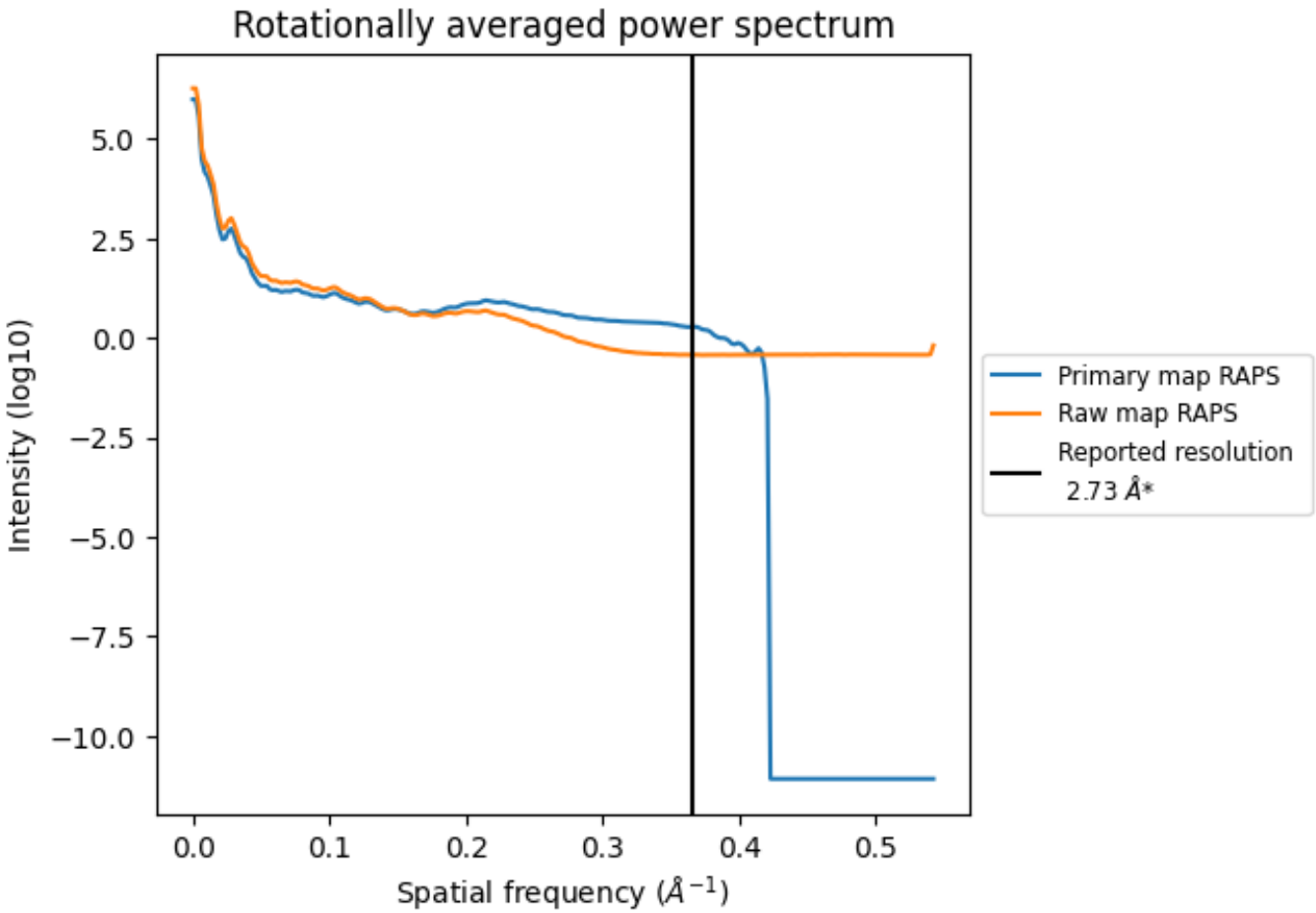
7.2 Volume estimate (i)



The volume at the recommended contour level is 885 nm^3; this corresponds to an approximate mass of 799 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

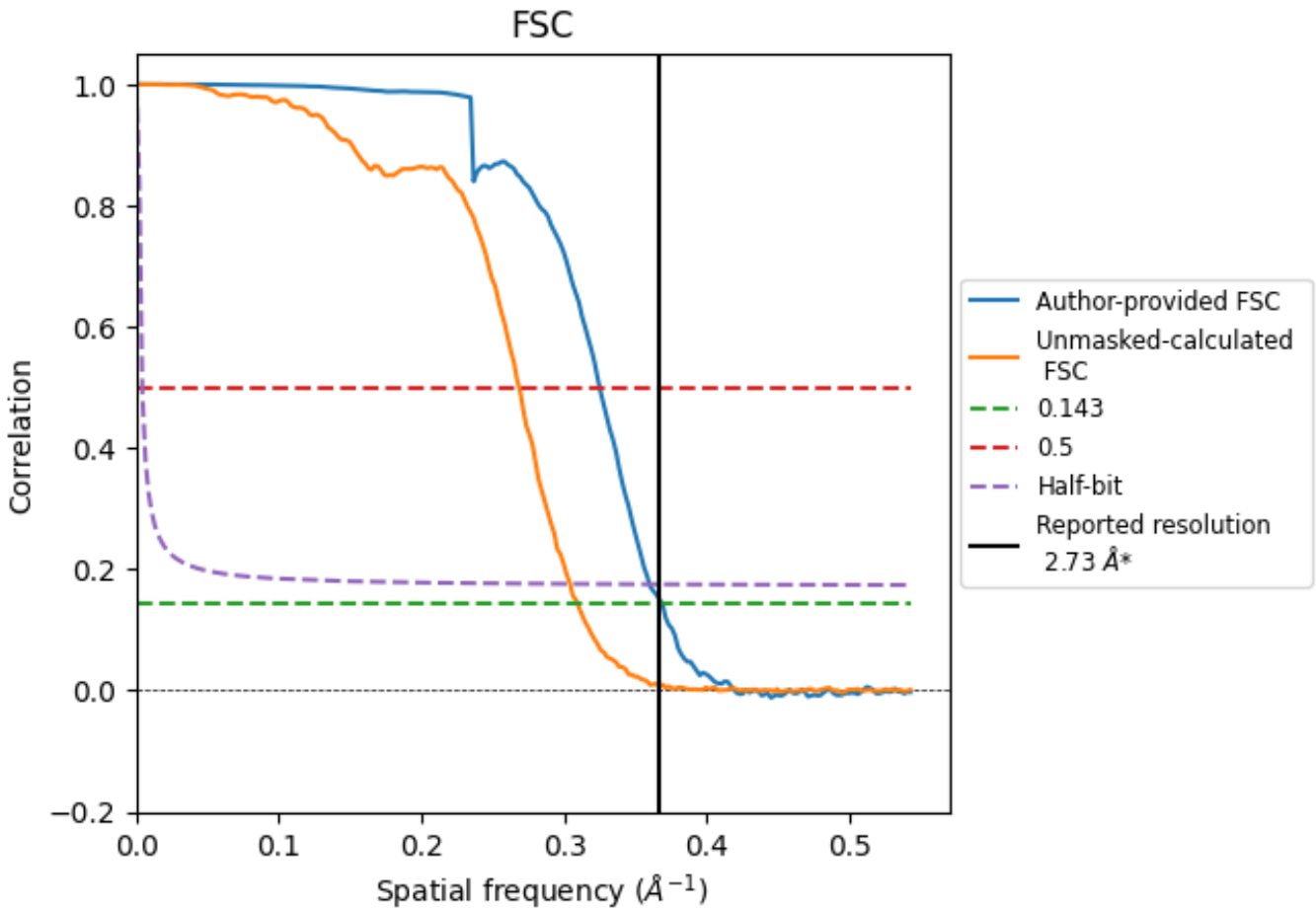


*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8.2 Resolution estimates (i)

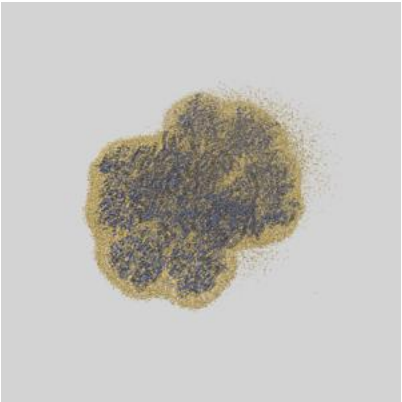
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.71	3.08	2.78
Unmasked-calculated*	3.23	3.73	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.73 by more than 10 %

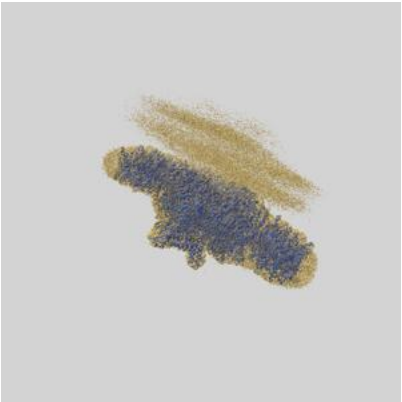
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15973 and PDB model 8BD3. Per-residue inclusion information can be found in section 3 on page 56.

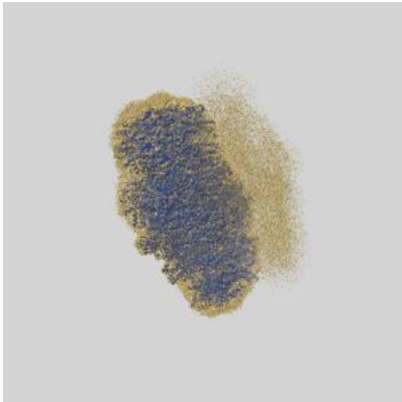
9.1 Map-model overlay (i)



X



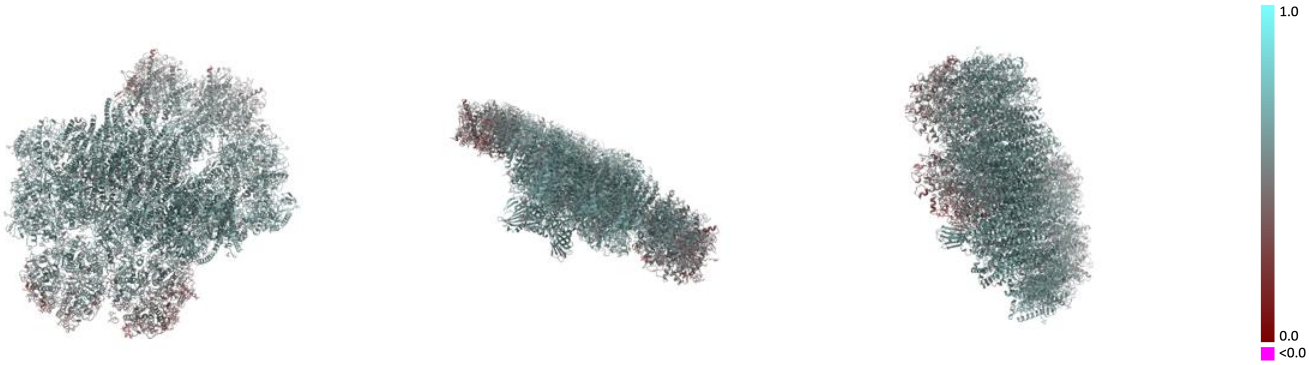
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

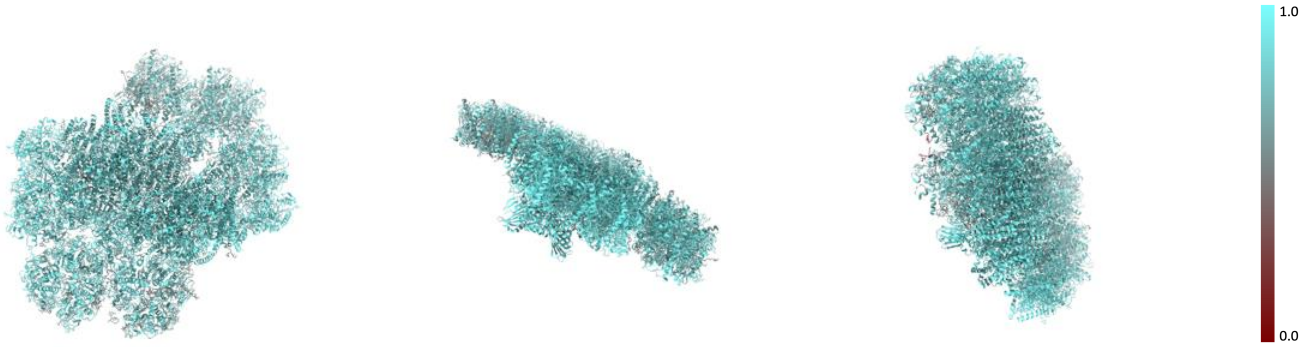
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

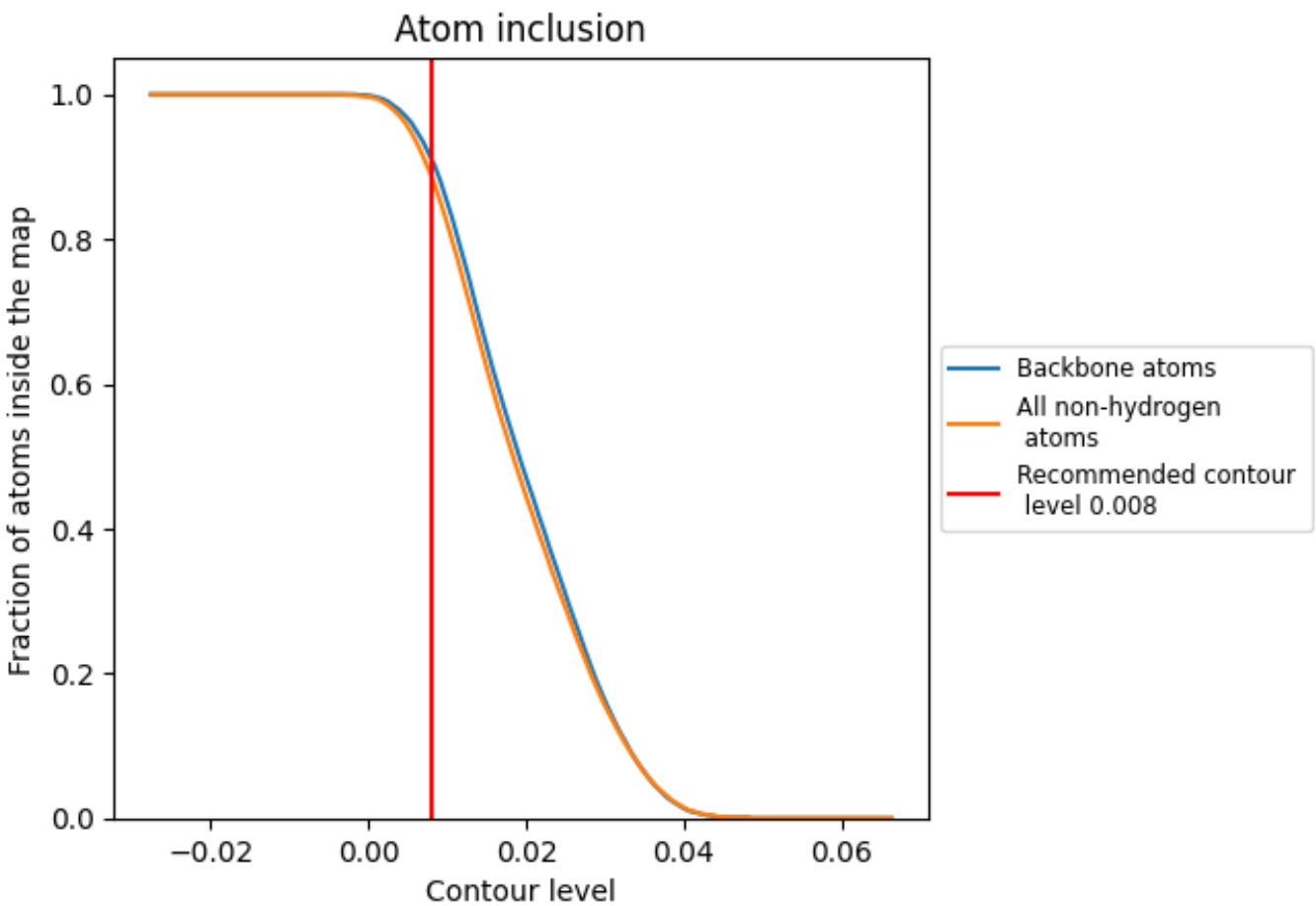
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.5740
0	0.8560	0.5540
1	0.8750	0.5670
2	0.8000	0.5010
3	0.8160	0.4830
4	0.7510	0.4600
5	0.7340	0.4100
6	0.8510	0.5480
7	0.8590	0.5610
8	0.7870	0.4560
9	0.7940	0.4860
A	0.9550	0.6360
B	0.9450	0.6280
C	0.9450	0.6240
D	0.9590	0.6370
E	0.9350	0.6170
F	0.9590	0.6310
F1	0.9210	0.5910
G	0.8990	0.5780
H	0.9560	0.6210
I	0.9350	0.6110
J	0.8950	0.6030
K	0.8510	0.5810
L	0.9280	0.6150
M	0.7890	0.5400
N	0.9150	0.5880
O	0.8970	0.5770
P1	0.8790	0.5930
Q1	0.7590	0.5390
R	0.9020	0.6000
S	0.8980	0.5830
T	0.9070	0.6020
U	0.8870	0.5770
V	0.8380	0.5670
W	0.8310	0.5780

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Chain	Atom inclusion	Q-score
X	0.8580	0.5780
Y	0.9280	0.6150
Z	0.9200	0.5810
a	0.9540	0.6320
b	0.9410	0.6240
c	0.9370	0.6190
d	0.9640	0.6400
e	0.9260	0.6050
f	0.9310	0.6210
f1	0.9180	0.5860
g	0.8950	0.5790
h	0.9580	0.6240
i	0.9740	0.6400
j	0.8940	0.5880
k	0.9420	0.6090
l	0.9340	0.6190
m	0.8210	0.5590
n	0.9170	0.5890
o	0.8930	0.5850
p	0.7040	0.4150
p1	0.8800	0.5840
q	0.7420	0.4650
q1	0.7490	0.5230
r	0.9090	0.6030
s	0.9000	0.5820
t	0.8760	0.5990
u	0.8940	0.5850
v	0.8520	0.5680
w	0.8480	0.5680
x	0.8280	0.5630
y	0.9350	0.6170
z	0.8880	0.5610