



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:23 AM JST

PDB ID : 5B5E / pdb_00005b5e
Title : Crystal structure analysis of Photosystem II complex
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on : 2016-05-02
Resolution : 1.87 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

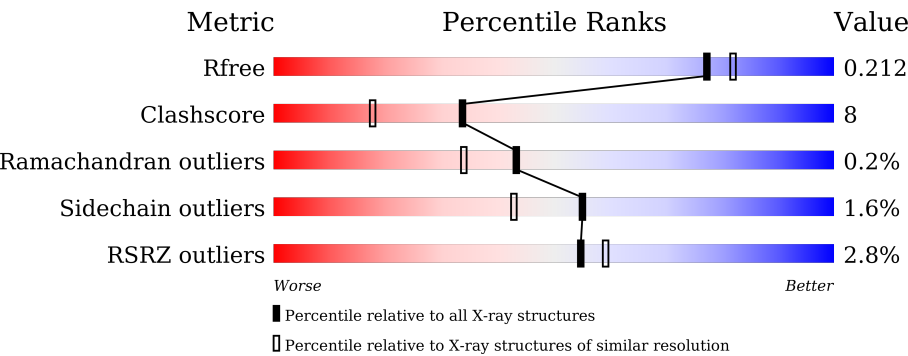
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
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:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	87%10% . .
1	a	344	84%13% .
2	B	505	89%11%
2	b	505	88%11% .
3	C	455	88%11% .
3	c	455	88%12% .

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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

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
29	UNL	M	102	-	-	X	-
29	UNL	U	201	-	-	X	-
31	DMS	A	424	-	-	X	-
31	DMS	B	636	-	-	X	-
31	DMS	B	639	-	-	X	-
31	DMS	B	646	-	-	X	-
31	DMS	D	416	-	-	X	-
31	DMS	F	102	-	-	X	-
31	DMS	H	105	-	-	X	-
31	DMS	O	305	-	-	X	-
31	DMS	O	308	-	-	X	-
31	DMS	U	204	-	-	X	-
31	DMS	V	207	-	-	X	-
31	DMS	V	210	-	-	X	-
31	DMS	a	420	-	-	X	-
31	DMS	b	636	-	-	X	-
31	DMS	b	645	-	-	X	-
31	DMS	c	925	-	-	X	-
31	DMS	d	416	-	-	X	-
31	DMS	l	102	-	-	X	-
31	DMS	v	209	-	-	X	-
40	HEC	V	203	X	-	-	-
40	HEC	v	203	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 55401 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2622	1718	431	458	15			
1	a	334	Total	C	N	O	S	0	4	0
			2633	1727	431	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	4	0
			3992	2619	668	692	13			
2	b	501	Total	C	N	O	S	0	3	0
			3929	2582	653	681	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3511	2297	591	610	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	UNP D0VWR7

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	2	0
			2733	1813	446	462	12			
4	d	342	Total	C	N	O	S	0	2	0
			2733	1813	446	462	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			651	426	103	122			
5	e	79	Total	C	N	O	0	0	0
			637	419	101	117			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			280	190	46	43	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	2	0
			511	341	83	85	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	338	83	83	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			285	195	45	44	1			
8	i	38	Total	C	N	O	S	0	0	0
			303	205	48	49	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			285	190	44	49	2			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			306	205	48	53			
11	l	36	Total	C	N	O	0	1	0
			297	200	47	50			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	2	0
			1861	1164	311	382	4			
13	o	243	Total	C	N	O	S	0	1	0
			1852	1159	310	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	31	Total	C	N	O	S	0	0	0
			261	183	37	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O		0	1	0
			776	493	129	154				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			210	137	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

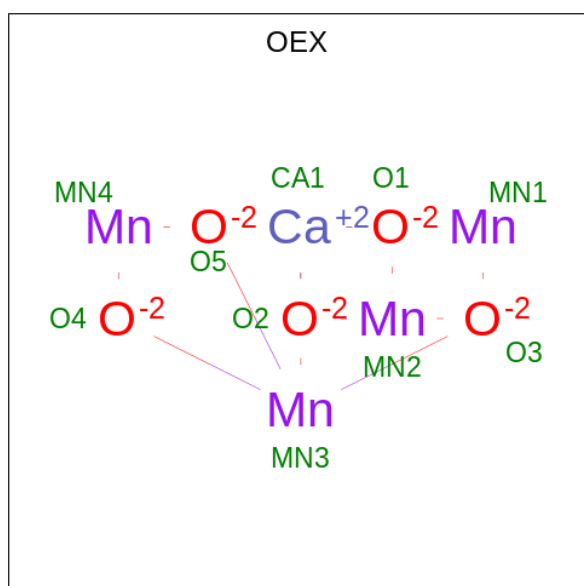
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O		0	0	0
			275	185	44	46				

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			468	320	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			457	312	70	73	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

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

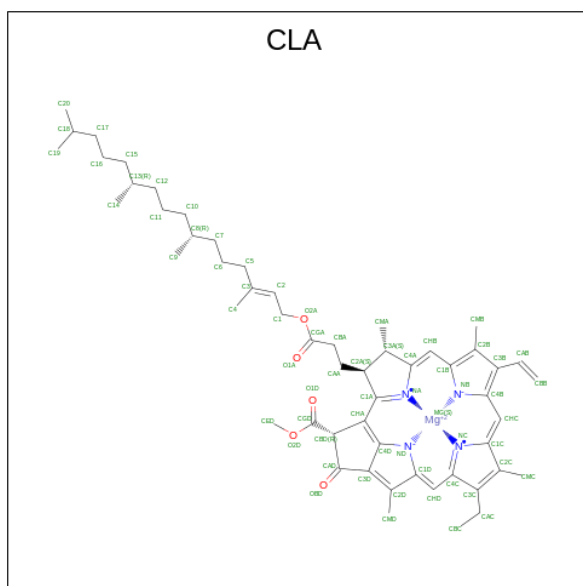
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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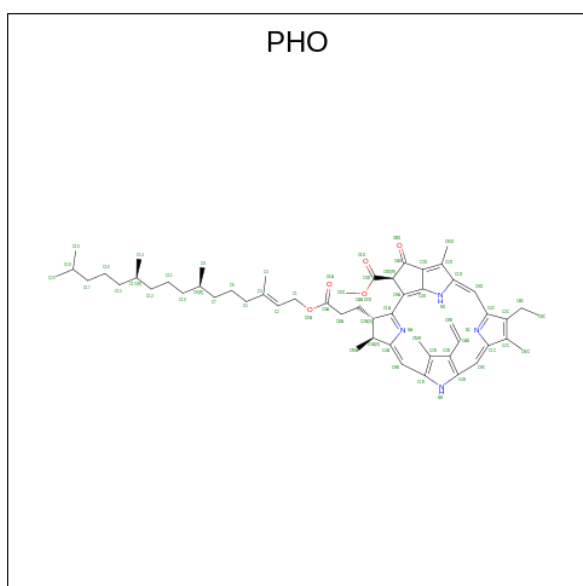
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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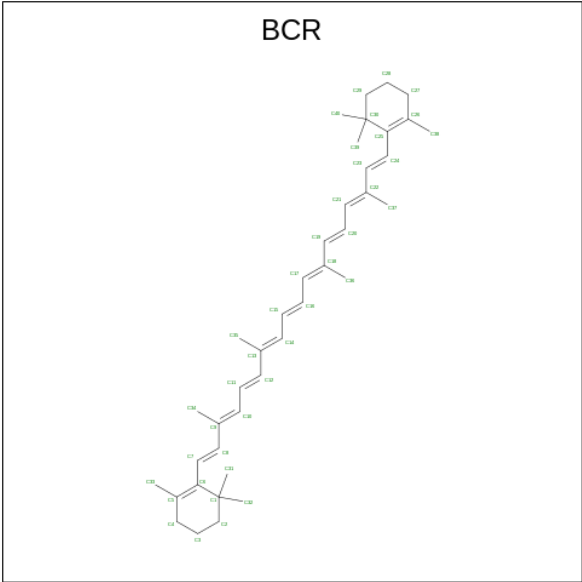
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



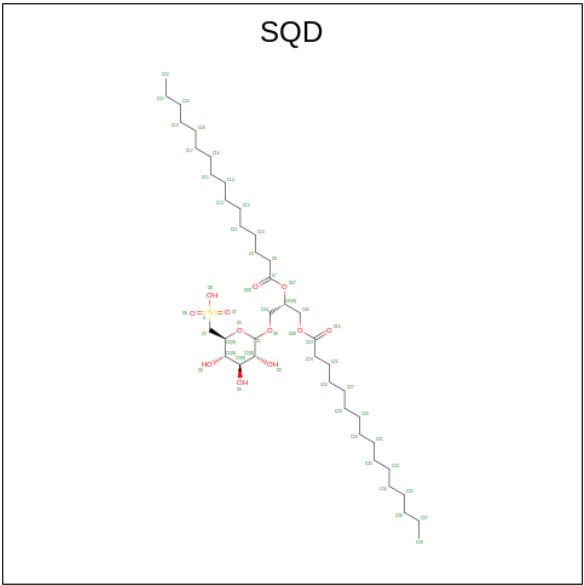
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



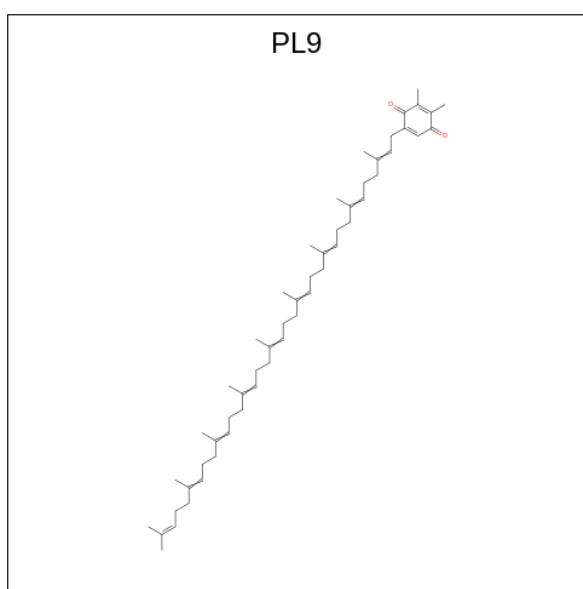
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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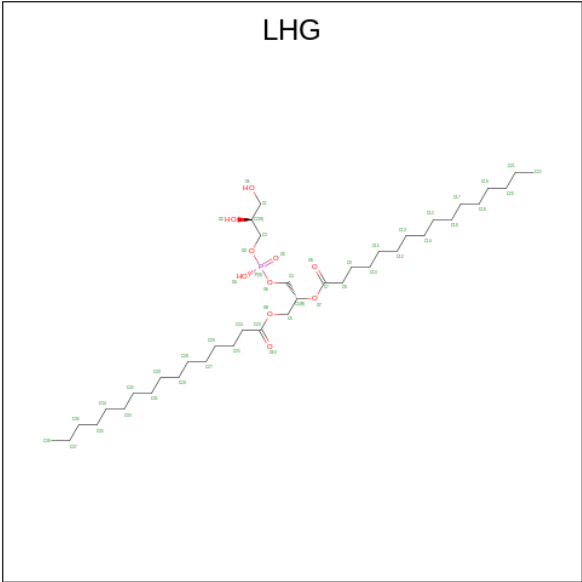
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	x	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 27 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				ZeroOcc	AltConf
27	A	1	Total	C	O		0	0
			55	53	2			
27	D	1	Total	C	O		0	0
			55	53	2			
27	a	1	Total	C	O		0	0
			55	53	2			
27	d	1	Total	C	O		0	0
			55	53	2			

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			46	35	10	1		
28	E	1	Total	C	O	P	0	0
			49	38	10	1		
28	K	1	Total	C	O	P	0	0
			44	35	8	1		
28	L	1	Total	C	O	P	0	0
			49	38	10	1		
28	a	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			44	33	10	1		
28	d	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			46	35	10	1		
28	e	1	Total	C	O	P	0	0
			40	29	10	1		
28	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

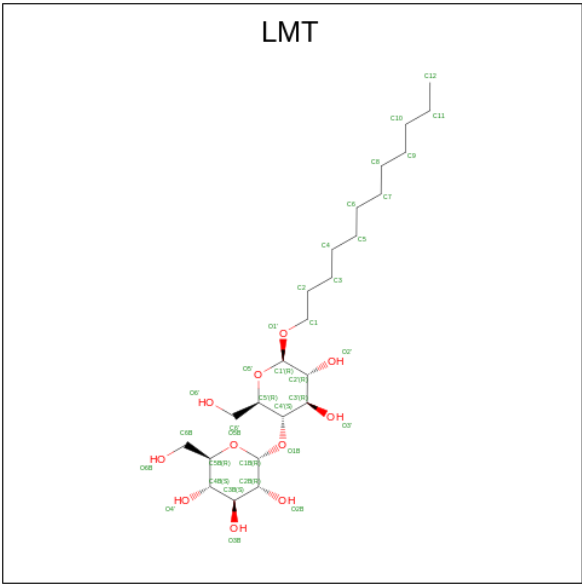
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	3	Total C 33 33	0	0
29	B	7	Total C 97 97	0	0
29	C	1	Total C 11 11	0	0
29	D	1	Total C 16 16	0	0
29	E	3	Total C 45 45	0	0
29	H	1	Total C 14 14	0	0
29	I	3	Total C 45 45	0	0
29	J	3	Total C 43 43	0	0
29	M	1	Total C 11 11	0	0
29	T	1	Total C 13 13	0	0
29	U	1	Total C 14 14	0	0
29	X	1	Total C 16 16	0	0
29	Z	2	Total C 23 23	0	0
29	a	2	Total C 16 16	0	0
29	b	7	Total C 102 102	0	0
29	c	1	Total C 10 10	0	0
29	d	2	Total C 27 27	0	0
29	e	1	Total C 16 16	0	0
29	i	4	Total C 64 64	0	0
29	j	1	Total C 16 16	0	0
29	k	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	m	1	Total	C	0	0
			11	11		
29	t	1	Total	C	0	0
			16	16		
29	u	2	Total	C	0	0
			27	27		
29	x	1	Total	C	0	0
			15	15		
29	z	1	Total	C	0	0
			13	13		

- Molecule 30 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



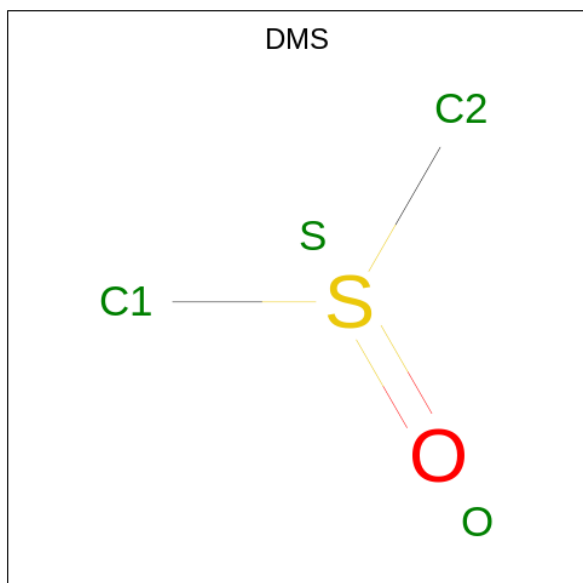
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	1	Total	C O	0	0
			35	24 11		
30	B	1	Total	C O	0	0
			35	24 11		
30	B	1	Total	C O	0	0
			24	18 6		
30	B	1	Total	C O	0	0
			24	18 6		
30	F	1	Total	C O	0	0
			35	24 11		
30	I	1	Total	C O	0	0
			35	24 11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	M	1	Total	C	O	0	0
			35	24	11		
30	T	1	Total	C	O	0	0
			24	18	6		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	e	1	Total	C	O	0	0
			25	19	6		
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0

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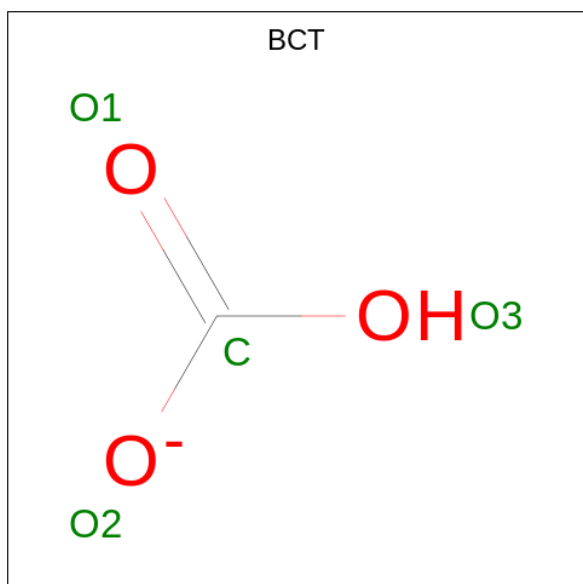
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	e	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	k	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

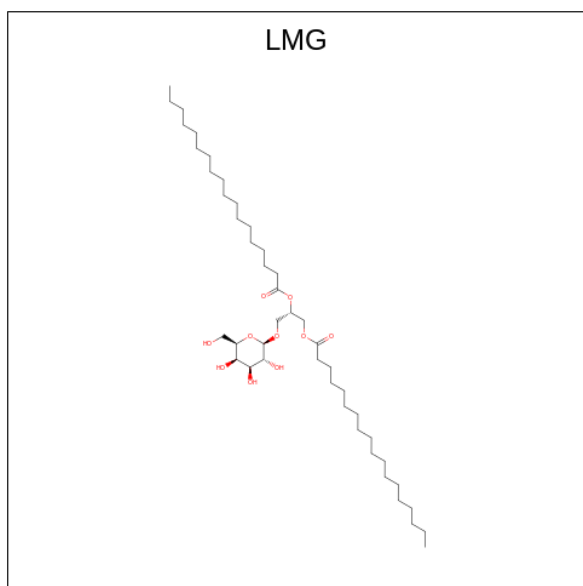
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	O	1	Total 1	Ca 1	0	0
33	b	1	Total 1	Ca 1	0	0
33	c	1	Total 1	Ca 1	0	0
33	o	1	Total 1	Ca 1	0	0

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



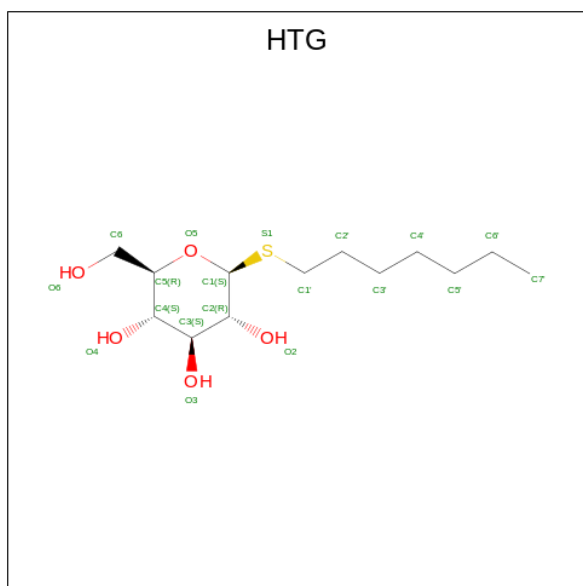
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total 51	C 41	O 10	0	0
34	C	1	Total 51	C 41	O 10	0	0
34	C	1	Total 51	C 41	O 10	0	0
34	C	1	Total 51	C 41	O 10	0	0
34	D	1	Total 51	C 41	O 10	0	0
34	J	1	Total 51	C 41	O 10	0	0
34	a	1	Total 51	C 41	O 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



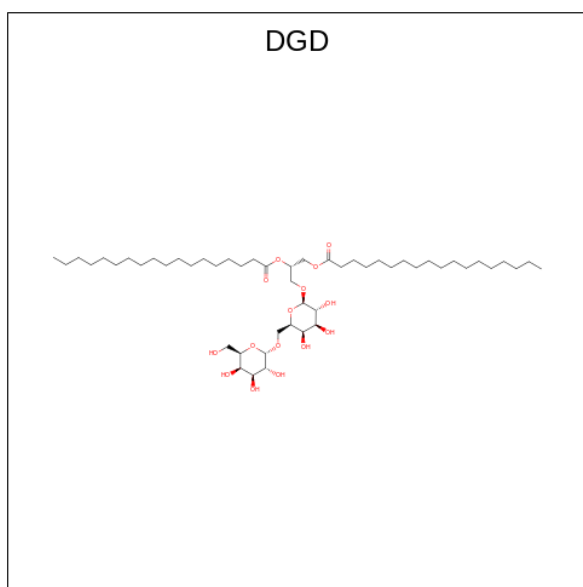
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		

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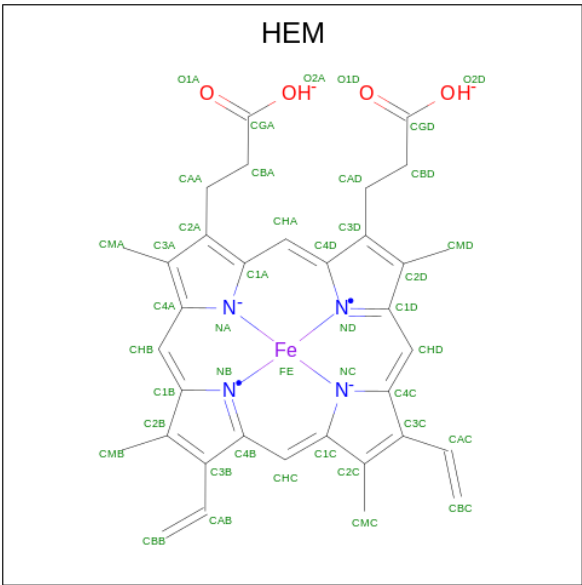
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			14	8	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			13	10	2	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	v	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



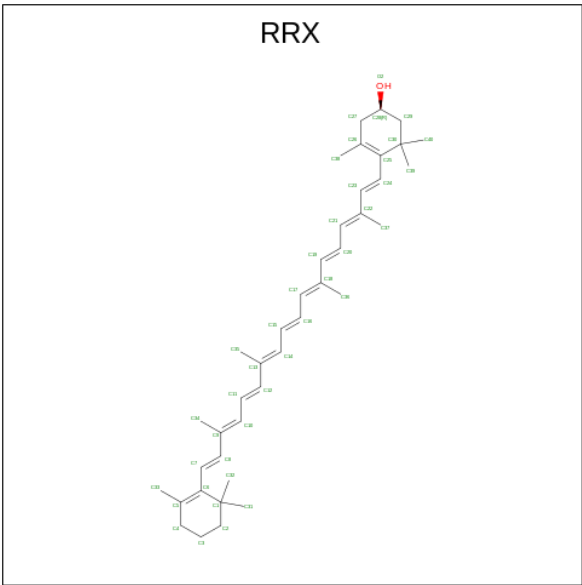
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	D	1	Total	C	O	0	0
			50	41	9		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	d	1	Total	C	O	0	0
			50	41	9		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).

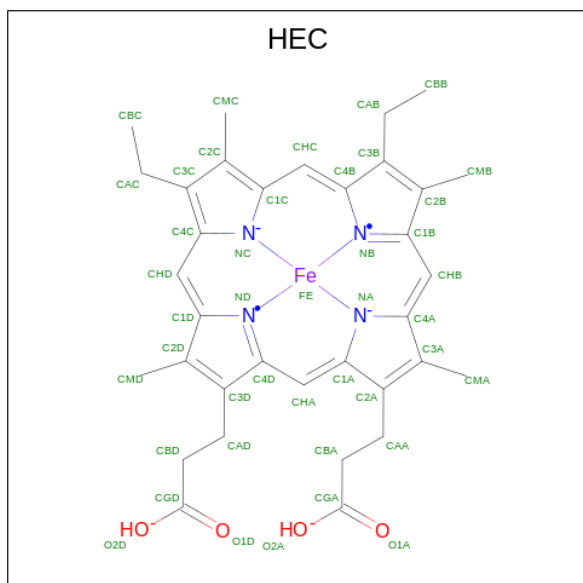


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	x	1	Total	C	O	0	0
			41	40	1		

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	J	1	Total Mg 1 1	0	0
39	j	1	Total Mg 1 1	0	0

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
40	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
40	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	176	Total O 187 187	0	11
41	B	420	Total O 437 437	0	17
41	C	286	Total O 294 294	0	8
41	D	159	Total O 166 166	0	7
41	E	44	Total O 47 47	0	3

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	F	9	Total O 9 9	0	0
41	H	54	Total O 54 54	0	0
41	I	11	Total O 13 13	0	2
41	J	16	Total O 17 17	0	1
41	K	13	Total O 14 14	0	1
41	L	23	Total O 26 26	0	3
41	M	15	Total O 17 17	0	2
41	O	251	Total O 265 265	0	14
41	T	15	Total O 16 16	0	1
41	U	123	Total O 128 128	0	5
41	V	165	Total O 169 169	0	4
41	Y	8	Total O 8 8	0	0
41	X	14	Total O 14 14	0	0
41	Z	8	Total O 10 10	0	2
41	a	172	Total O 175 175	0	3
41	b	405	Total O 423 423	0	18
41	c	300	Total O 320 320	0	20
41	d	177	Total O 185 185	0	8
41	e	52	Total O 56 56	0	4
41	f	9	Total O 9 9	0	0
41	h	56	Total O 57 57	0	1

Continued on next page...

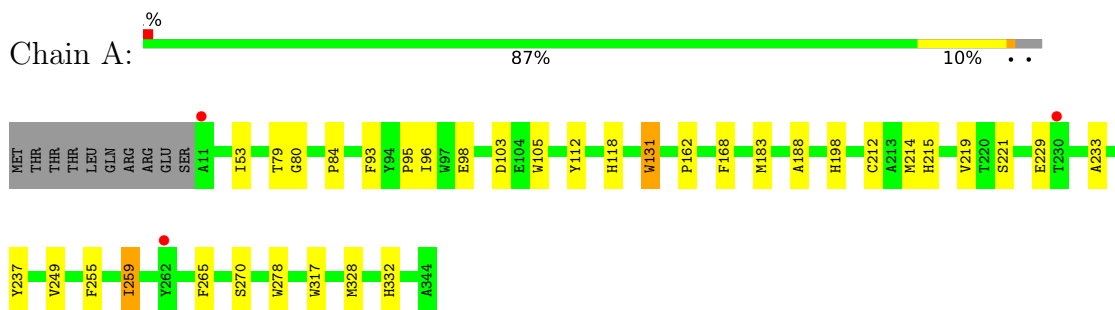
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	i	12	Total 13	O 13	0	1
41	j	13	Total 13	O 13	0	0
41	k	14	Total 14	O 14	0	0
41	l	16	Total 19	O 19	0	3
41	m	14	Total 15	O 15	0	1
41	o	223	Total 240	O 240	0	17
41	t	19	Total 21	O 21	0	2
41	u	146	Total 157	O 157	0	11
41	v	147	Total 154	O 154	0	7
41	y	16	Total 16	O 16	0	0
41	x	18	Total 19	O 19	0	1
41	z	5	Total 5	O 5	0	0

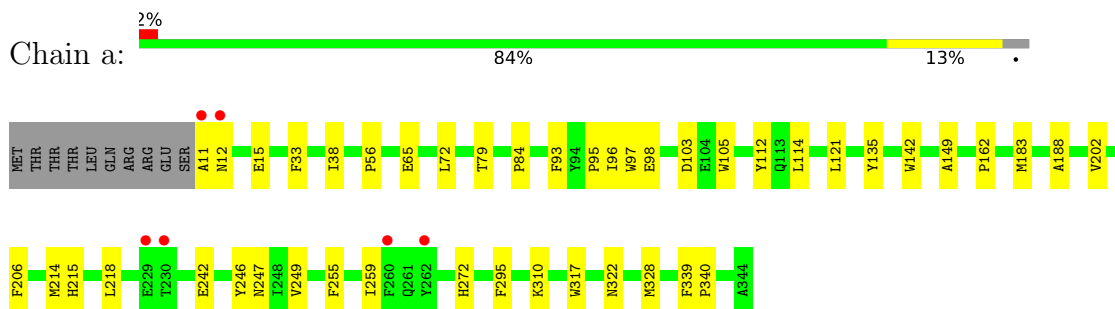
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

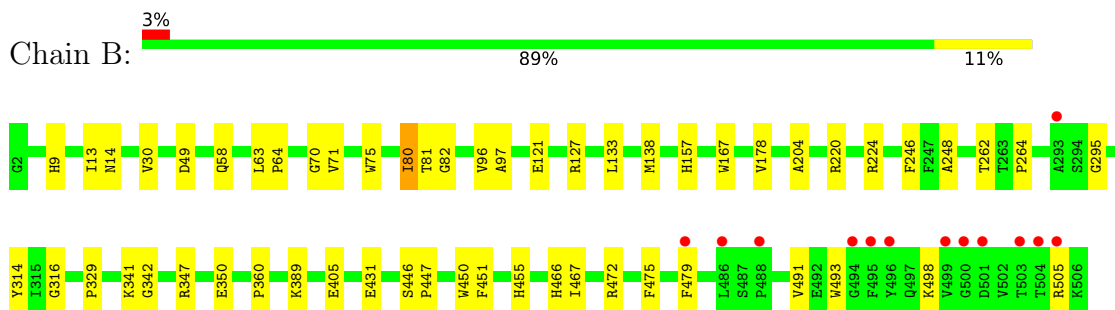
- Molecule 1: Photosystem II protein D1



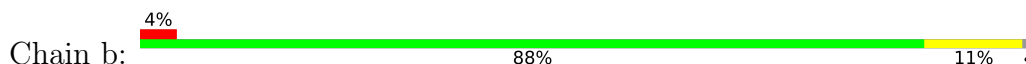
- Molecule 1: Photosystem II protein D1

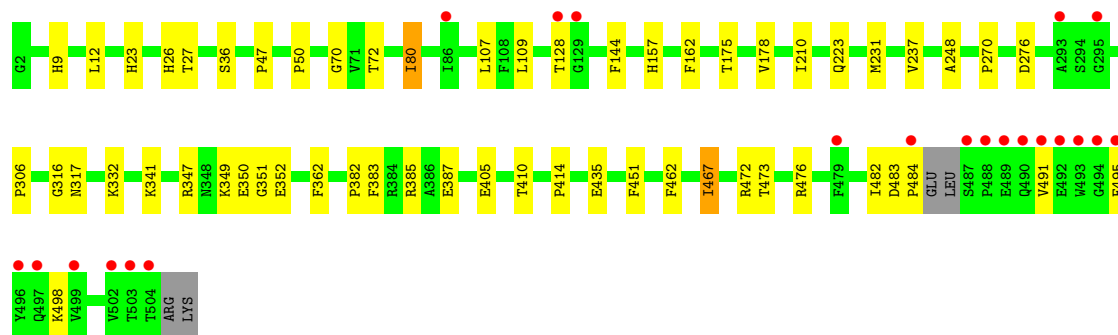


- Molecule 2: Photosystem II CP47 reaction center protein

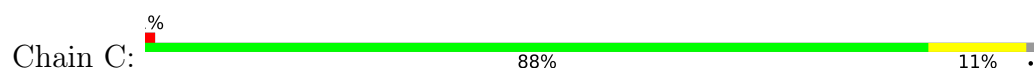


- Molecule 2: Photosystem II CP47 reaction center protein

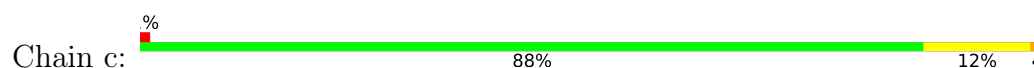




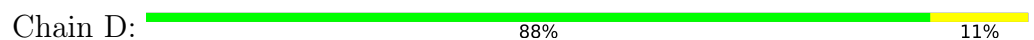
• Molecule 3: Photosystem II CP43 reaction center protein



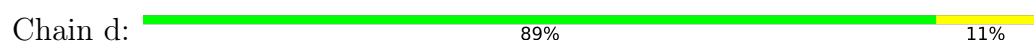
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein

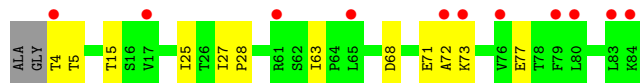
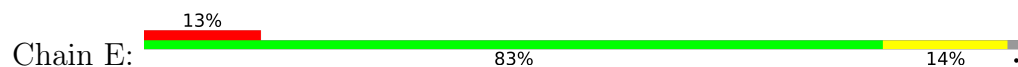


• Molecule 4: Photosystem II D2 protein

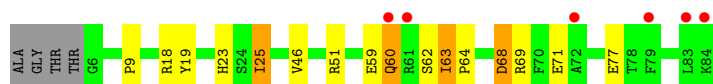
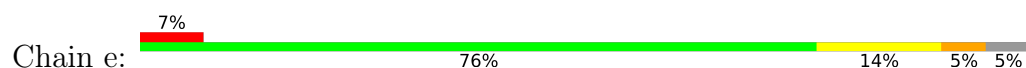




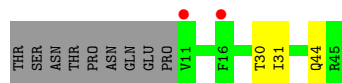
- Molecule 5: Cytochrome b559 subunit alpha



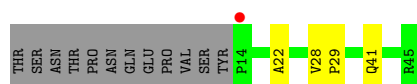
- Molecule 5: Cytochrome b559 subunit alpha



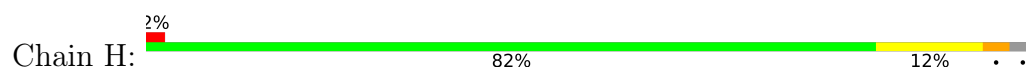
- Molecule 6: Cytochrome b559 subunit beta



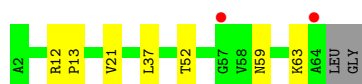
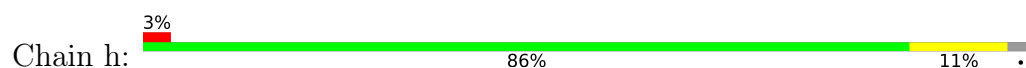
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

Chain I:  89% 8%



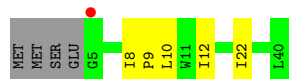
- Molecule 8: Photosystem II reaction center protein I

Chain i:  5% 87% 13%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  2% 78% 12% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  5% 85% 15%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  84% 16%

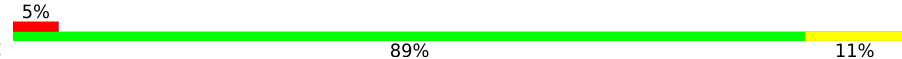


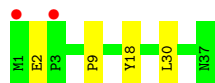
- Molecule 10: Photosystem II reaction center protein K

Chain k:  76% 24%

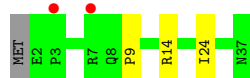
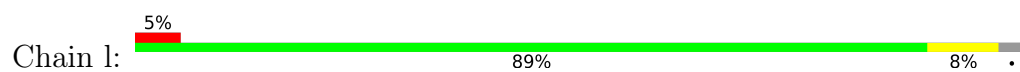


- Molecule 11: Photosystem II reaction center protein L

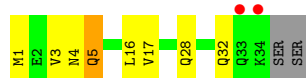
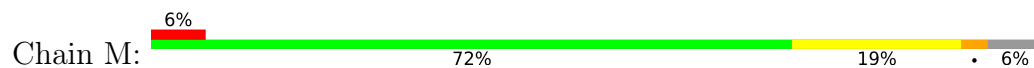
Chain L:  5% 89% 11%



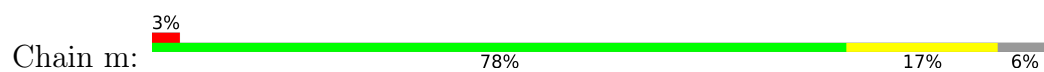
- Molecule 11: Photosystem II reaction center protein L



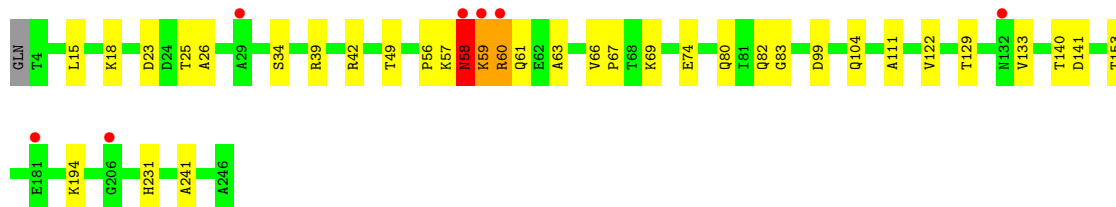
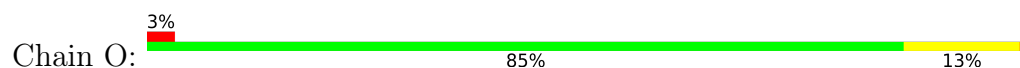
- Molecule 12: Photosystem II reaction center protein M



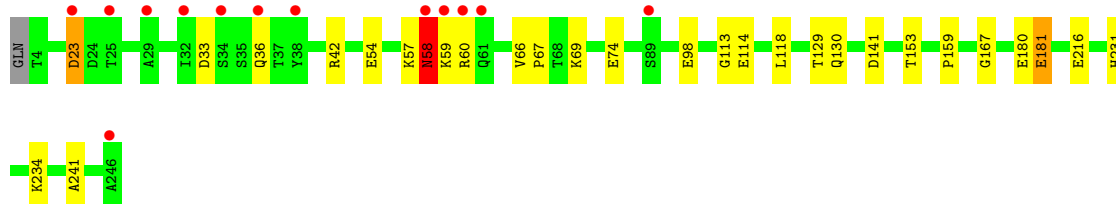
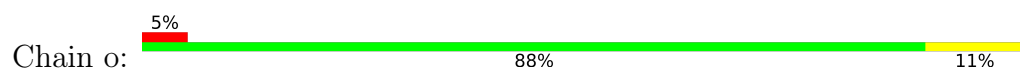
- Molecule 12: Photosystem II reaction center protein M



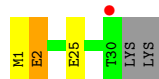
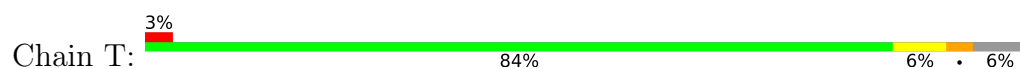
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



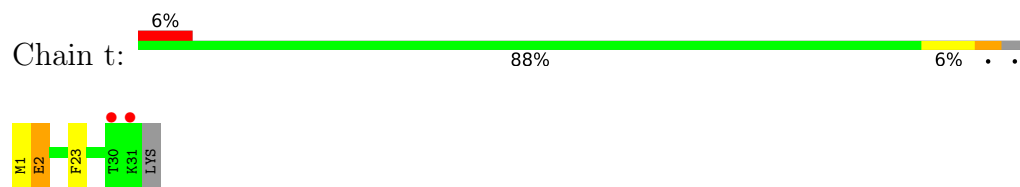
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



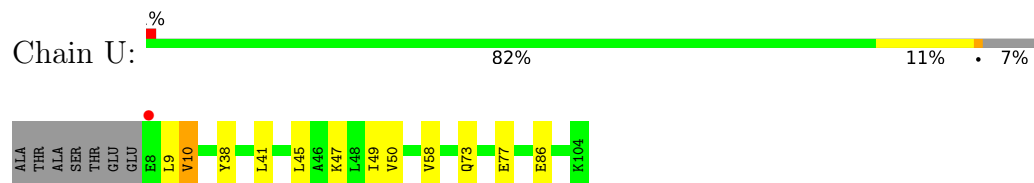
- Molecule 14: Photosystem II reaction center protein T



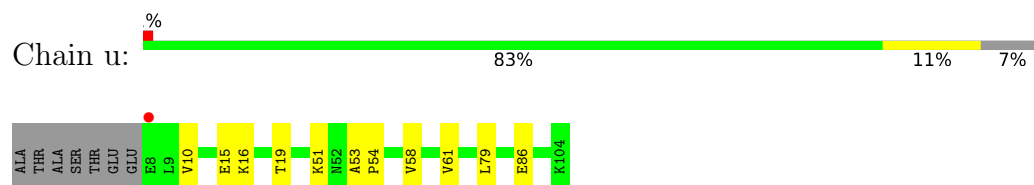
- Molecule 14: Photosystem II reaction center protein T



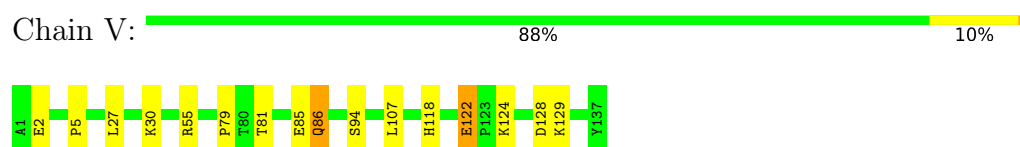
- Molecule 15: Photosystem II 12 kDa extrinsic protein



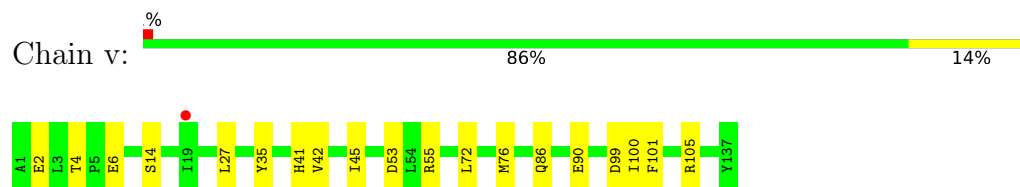
- Molecule 15: Photosystem II 12 kDa extrinsic protein



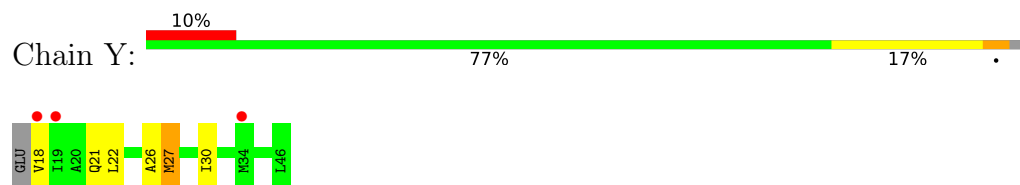
- Molecule 16: Cytochrome c-550



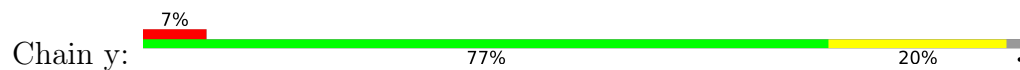
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12

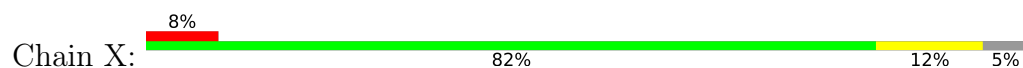


- Molecule 17: Photosystem II reaction center protein Ycf12

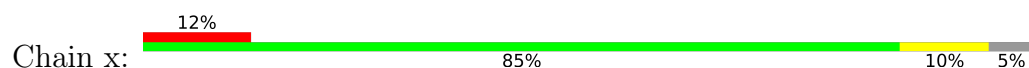




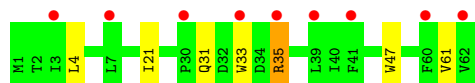
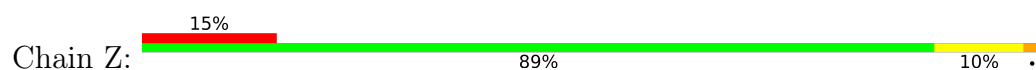
- Molecule 18: Photosystem II reaction center protein X



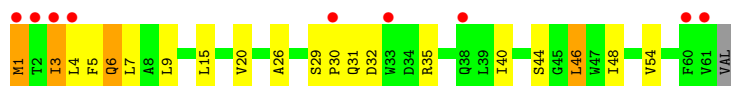
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.40Å 228.22Å 286.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 1.87 48.98 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.98-1.87) 99.8 (48.98-1.87)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.171 , 0.212 0.171 , 0.212	Depositor DCC
R_{free} test set	32518 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55401	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, DGD, LMG, BCR, FME, CL, PL9, BCT, HEM, RRX, LMT, SQD, MG, FE2, PHO, HEC, HTG, CLA, UNL, LHG, OEX, CA

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	A	1.27	5/2710 (0.2%)	1.04	3/3696 (0.1%)
1	a	1.24	4/2730 (0.1%)	1.08	7/3723 (0.2%)
2	B	1.15	5/4144 (0.1%)	1.04	3/5647 (0.1%)
2	b	1.21	6/4076 (0.1%)	1.03	3/5558 (0.1%)
3	C	1.14	6/3633 (0.2%)	0.99	2/4945 (0.0%)
3	c	1.09	1/3638 (0.0%)	1.02	0/4953
4	D	1.25	5/2834 (0.2%)	1.05	5/3861 (0.1%)
4	d	1.24	6/2834 (0.2%)	1.00	0/3861
5	E	0.94	0/670	1.02	0/917
5	e	0.88	0/656	1.03	4/896 (0.4%)
6	F	0.96	0/289	0.92	0/394
6	f	0.97	0/262	0.99	0/356
7	H	0.97	0/530	0.98	0/722
7	h	1.03	0/522	0.95	1/711 (0.1%)
8	I	0.92	0/282	0.89	1/381 (0.3%)
8	i	0.91	0/300	0.92	0/406
9	J	0.91	0/257	0.98	0/349
9	j	0.95	0/291	0.99	2/393 (0.5%)
10	K	0.93	0/303	0.97	0/416
10	k	0.90	0/303	1.05	0/416
11	L	1.10	1/316 (0.3%)	1.00	0/430
11	l	1.12	0/307	1.00	0/418
12	M	1.06	0/270	1.08	2/369 (0.5%)
12	m	0.95	0/270	1.00	0/369
13	O	1.01	1/1898 (0.1%)	1.04	3/2577 (0.1%)
13	o	0.98	0/1886	1.05	4/2562 (0.2%)
14	T	0.97	0/255	1.02	2/346 (0.6%)
14	t	1.05	0/260	0.94	0/353
15	U	1.01	0/777	0.96	0/1055
15	u	1.02	0/790	0.97	0/1071
16	V	1.16	0/1096	1.05	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	1.03	0/1084	1.05	1/1475 (0.1%)
17	Y	0.80	0/211	1.06	0/282
17	y	0.71	0/208	1.08	1/278 (0.4%)
18	X	0.83	0/286	1.13	0/387
18	x	0.86	0/278	1.01	0/376
19	Z	0.76	0/479	1.00	0/656
19	z	0.71	0/468	0.97	0/640
All	All	1.12	40/42403 (0.1%)	1.02	45/57732 (0.1%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	TRP	N-CA	-7.33	1.41	1.46
4	D	87	HIS	ND1-CE1	7.15	1.39	1.32
4	D	87	HIS	CG-CD2	6.80	1.43	1.35
1	A	118	HIS	ND1-CE1	6.73	1.39	1.32
4	D	189	HIS	CG-CD2	6.50	1.43	1.35
3	C	398	HIS	ND1-CE1	6.47	1.39	1.32
1	A	198	HIS	ND1-CE1	6.42	1.39	1.32
2	b	23	HIS	CG-CD2	6.19	1.42	1.35
1	a	38	ILE	CA-CB	6.08	1.57	1.54
2	b	414	PRO	CA-C	6.04	1.57	1.52
4	d	330	ALA	C-O	-6.04	1.18	1.24
2	B	9	HIS	ND1-CE1	5.94	1.38	1.32
4	d	61	HIS	CE1-NE2	5.86	1.38	1.32
1	A	332	HIS	CG-CD2	5.79	1.42	1.35
4	D	189	HIS	ND1-CE1	5.71	1.38	1.32
11	L	30	LEU	CA-C	5.68	1.60	1.52
4	d	189	HIS	ND1-CE1	5.63	1.38	1.32
3	C	53	HIS	CG-CD2	5.62	1.42	1.35
2	b	473	THR	N-CA	5.62	1.53	1.46
3	C	441	HIS	CG-CD2	5.59	1.42	1.35
2	b	9	HIS	ND1-CE1	5.59	1.38	1.32
3	C	91	HIS	CG-CD2	5.58	1.42	1.35
1	a	206	PHE	N-CA	5.57	1.53	1.46
2	B	9	HIS	N-CA	5.47	1.53	1.46
1	a	149	ALA	CA-C	5.45	1.58	1.52
1	a	56	PRO	CA-C	5.43	1.57	1.52
2	B	97	ALA	N-CA	5.43	1.52	1.46
4	d	117	HIS	CG-CD2	5.37	1.41	1.35
4	D	147	SER	C-O	-5.36	1.17	1.24
2	b	9	HIS	CG-CD2	5.29	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	122	VAL	CA-CB	5.28	1.61	1.54
3	C	91	HIS	CE1-NE2	5.20	1.37	1.32
3	c	365	TRP	CD2-CE2	5.14	1.50	1.41
2	B	450	TRP	NE1-CE2	-5.13	1.31	1.37
4	d	330	ALA	CA-C	5.12	1.59	1.52
1	A	80	GLY	N-CA	5.09	1.52	1.45
4	d	158	LEU	CA-C	5.08	1.56	1.52
2	B	466	HIS	ND1-CE1	5.06	1.37	1.32
2	b	26	HIS	CG-CD2	5.02	1.41	1.35
3	C	430	HIS	CG-ND1	-5.02	1.32	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	142	TRP	N-CA-C	7.59	122.57	113.16
2	B	342	GLY	N-CA-C	-7.12	104.89	112.08
1	a	65	GLU	CA-C-N	-6.99	112.44	119.99
1	a	65	GLU	C-N-CA	-6.99	112.44	119.99
4	D	170	ALA	CA-C-N	-6.51	113.25	119.76
4	D	170	ALA	C-N-CA	-6.51	113.25	119.76
3	C	255	THR	CA-C-N	-6.45	113.12	119.76
3	C	255	THR	C-N-CA	-6.45	113.12	119.76
2	b	316	GLY	N-CA-C	-6.38	107.65	114.67
13	O	58	ASN	N-CA-C	6.27	118.95	109.23
5	e	51	ARG	CA-C-N	-6.03	113.41	119.56
5	e	51	ARG	C-N-CA	-6.03	113.41	119.56
4	D	94	GLY	CA-C-N	6.00	126.11	119.87
4	D	94	GLY	C-N-CA	6.00	126.11	119.87
13	o	113	GLY	N-CA-C	5.89	122.58	114.92
12	M	17	VAL	CA-C-N	-5.82	112.57	119.84
12	M	17	VAL	C-N-CA	-5.82	112.57	119.84
9	j	37	GLY	N-CA-C	-5.74	107.41	115.32
1	a	242	GLU	N-CA-C	5.72	117.59	111.36
13	O	104	GLN	CA-C-N	-5.61	114.16	119.76
13	O	104	GLN	C-N-CA	-5.61	114.16	119.76
5	e	63	ILE	N-CA-C	5.48	114.11	109.02
7	h	52	THR	N-CA-C	-5.47	105.73	112.90
1	A	131	TRP	CA-CB-CG	-5.39	103.35	113.60
2	B	479	PHE	N-CA-C	5.31	117.75	111.33
16	V	85	GLU	N-CA-C	5.27	118.87	112.23
13	o	130	GLN	CA-C-N	-5.27	115.31	120.52
13	o	130	GLN	C-N-CA	-5.27	115.31	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	295	PHE	N-CA-C	-5.26	106.17	112.59
2	B	295	GLY	N-CA-C	5.26	121.76	114.92
8	I	34	ARG	N-CA-C	5.24	117.27	109.25
14	T	25	GLU	CA-C-N	-5.23	114.99	120.38
14	T	25	GLU	C-N-CA	-5.23	114.99	120.38
13	o	58	ASN	N-CA-C	5.22	117.96	109.24
1	A	53	ILE	N-CA-C	5.21	115.87	110.82
1	A	233	ALA	N-CA-C	-5.19	106.21	112.54
2	b	175	THR	CB-CA-C	-5.16	102.58	111.45
16	v	105	ARG	N-CA-C	5.10	118.28	111.75
5	e	25	ILE	N-CA-C	5.09	116.51	111.67
4	D	303	ILE	N-CA-C	-5.08	105.59	110.72
2	b	495	PHE	N-CA-C	5.07	116.61	111.14
1	a	33	PHE	CA-C-N	5.03	125.56	119.98
1	a	33	PHE	C-N-CA	5.03	125.56	119.98
17	y	28	ILE	N-CA-C	-5.03	105.64	110.72
9	j	27	LEU	N-CA-C	-5.02	105.88	111.36

There are no chirality outliers.

There are no planarity outliers.

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	A	2622	0	2519	26	0
1	a	2633	0	2540	41	0
2	B	3992	0	3848	48	0
2	b	3929	0	3774	69	0
3	C	3511	0	3440	37	0
3	c	3521	0	3439	50	0
4	D	2733	0	2647	33	0
4	d	2733	0	2647	38	0
5	E	651	0	626	9	0
5	e	637	0	617	12	0
6	F	280	0	284	2	0
6	f	255	0	263	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	511	0	535	12	0
7	h	506	0	531	4	0
8	I	285	0	305	0	0
8	i	303	0	313	6	0
9	J	251	0	257	3	0
9	j	285	0	293	3	0
10	K	293	0	305	4	0
10	k	293	0	305	6	0
11	L	306	0	320	4	0
11	l	297	0	311	3	0
12	M	264	0	283	6	0
12	m	264	0	283	7	0
13	O	1861	0	1825	30	0
13	o	1852	0	1812	20	0
14	T	256	0	256	1	0
14	t	261	0	258	2	0
15	U	766	0	758	11	0
15	u	776	0	775	9	0
16	V	1072	0	1086	19	0
16	v	1060	0	1053	20	0
17	Y	210	0	230	4	0
17	y	207	0	221	3	0
18	X	280	0	312	5	0
18	x	275	0	301	6	0
19	Z	468	0	492	11	0
19	z	457	0	471	10	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	195	0	216	7	0
23	B	1040	0	1152	25	0
23	C	845	0	936	24	0
23	D	195	0	216	5	0
23	a	195	0	216	8	0
23	b	1040	0	1152	34	0
23	c	845	0	936	27	0
23	d	195	0	216	9	0
24	A	64	0	74	1	0
24	D	64	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	128	0	148	4	0
25	A	40	0	56	3	0
25	B	120	0	168	8	0
25	C	120	0	168	7	0
25	D	40	0	56	5	0
25	T	40	0	56	6	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	11	0
25	c	80	0	112	6	0
25	d	40	0	56	2	0
25	j	40	0	56	4	0
25	k	40	0	56	1	0
25	t	40	0	56	7	0
26	A	108	0	155	11	0
26	B	54	0	78	4	0
26	D	45	0	57	2	0
26	L	54	0	78	4	0
26	a	108	0	156	5	0
26	x	41	0	49	2	0
27	A	55	0	80	12	0
27	D	55	0	80	0	0
27	a	55	0	80	14	0
27	d	55	0	80	0	0
28	A	49	0	74	1	0
28	D	144	0	213	7	0
28	E	49	0	74	3	0
28	K	44	0	67	0	0
28	L	49	0	74	1	0
28	a	49	0	74	1	0
28	d	188	0	274	6	0
28	e	40	0	53	5	0
28	l	49	0	74	0	0
29	A	33	0	0	1	0
29	B	97	0	0	1	0
29	C	11	0	0	0	0
29	D	16	0	0	0	0
29	E	45	0	0	0	0
29	H	14	0	0	0	0
29	I	45	0	0	0	0
29	J	43	0	0	1	0
29	M	11	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	T	13	0	0	0	0
29	U	14	0	0	3	0
29	X	16	0	0	0	0
29	Z	23	0	0	0	0
29	a	16	0	0	0	0
29	b	102	0	0	0	0
29	c	10	0	0	0	0
29	d	27	0	0	0	0
29	e	16	0	0	0	0
29	i	64	0	0	0	0
29	j	16	0	0	0	0
29	k	8	0	0	0	0
29	m	11	0	0	0	0
29	t	16	0	0	0	0
29	u	27	0	0	1	0
29	x	15	0	0	0	0
29	z	13	0	0	0	0
30	A	35	0	46	2	0
30	B	83	0	116	3	0
30	F	35	0	46	0	0
30	I	35	0	46	2	0
30	M	35	0	46	1	0
30	T	24	0	35	0	0
30	Z	35	0	46	6	0
30	a	70	0	92	8	0
30	b	25	0	35	4	0
30	e	25	0	35	1	0
30	m	70	0	92	3	0
30	z	32	0	33	1	0
31	A	24	0	36	8	0
31	B	48	0	72	25	0
31	C	28	0	42	6	0
31	D	12	0	18	9	0
31	F	4	0	6	5	0
31	H	8	0	12	7	0
31	O	36	0	54	16	0
31	U	12	0	18	5	0
31	V	36	0	54	16	0
31	a	16	0	24	12	0
31	b	60	0	90	34	0
31	c	48	0	72	17	0
31	d	20	0	30	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	e	4	0	6	1	0
31	h	16	0	24	3	0
31	i	8	0	12	3	0
31	k	4	0	6	0	0
31	l	4	0	6	5	0
31	o	12	0	18	4	0
31	u	16	0	24	5	0
31	v	32	0	48	14	0
32	A	4	0	0	0	0
32	a	4	0	0	1	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	4	0
34	D	51	0	72	5	0
34	J	51	0	72	3	0
34	a	51	0	72	8	0
34	c	102	0	144	4	0
34	d	51	0	72	5	0
34	j	51	0	72	0	0
34	m	51	0	72	3	0
35	B	95	0	130	4	0
35	C	57	0	78	1	0
35	D	19	0	26	3	0
35	O	19	0	26	2	0
35	V	14	0	13	0	0
35	b	76	0	104	5	0
35	c	51	0	70	2	0
35	d	19	0	26	0	0
35	v	19	0	26	4	0
36	C	186	0	246	2	0
36	D	50	0	69	4	0
36	H	62	0	82	0	0
36	c	186	0	246	3	0
36	d	50	0	69	6	0
36	h	62	0	82	0	0
37	E	43	0	30	1	0
37	e	43	0	30	1	0
38	H	41	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	x	41	0	56	4	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	187	0	0	7	0
41	B	437	0	0	10	0
41	C	294	0	0	6	0
41	D	166	0	0	4	0
41	E	47	0	0	0	0
41	F	9	0	0	0	0
41	H	54	0	0	1	0
41	I	13	0	0	0	0
41	J	17	0	0	3	0
41	K	14	0	0	0	0
41	L	26	0	0	1	0
41	M	17	0	0	1	0
41	O	265	0	0	12	0
41	T	16	0	0	0	0
41	U	128	0	0	2	0
41	V	169	0	0	7	0
41	X	14	0	0	0	0
41	Y	8	0	0	0	0
41	Z	10	0	0	2	0
41	a	175	0	0	5	0
41	b	423	0	0	15	0
41	c	320	0	0	2	0
41	d	185	0	0	0	0
41	e	56	0	0	1	0
41	f	9	0	0	0	0
41	h	57	0	0	1	0
41	i	13	0	0	0	0
41	j	13	0	0	0	0
41	k	14	0	0	1	0
41	l	19	0	0	2	0
41	m	15	0	0	2	0
41	o	240	0	0	7	0
41	t	21	0	0	0	0
41	u	157	0	0	7	0
41	v	154	0	0	5	0
41	x	19	0	0	0	0
41	y	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	z	5	0	0	0	0
All	All	55401	0	52590	803	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 8.

All (803) 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)
31:O:311:DMS:H13	41:O:573:HOH:O	1.47	1.14
2:B:347[B]:ARG:NH2	41:B:1034[B]:HOH:O	1.80	1.13
1:A:214:MET:HG2	27:A:411:PL9:H102	1.20	1.12
2:b:347[A]:ARG:NH2	41:b:702[A]:HOH:O	1.81	1.10
1:a:97:TRP:HD1	31:a:420:DMS:H23	1.05	1.09
1:a:97:TRP:CD1	31:a:420:DMS:H23	1.87	1.09
2:B:350:GLU:HG3	31:B:639:DMS:H12	1.26	1.09
1:a:214:MET:HG2	27:a:414:PL9:H102	1.18	1.09
31:a:420:DMS:H21	8:i:5:LYS:HD2	1.19	1.08
19:Z:35:ARG:HG2	19:Z:35:ARG:HH11	1.18	1.04
2:b:350[B]:GLU:HG2	31:b:636:DMS:H12	1.38	1.04
3:c:362:ARG:HD3	31:c:925:DMS:H22	1.37	1.03
13:O:133:VAL:HG22	31:O:305:DMS:H22	1.39	1.01
2:B:350:GLU:H	31:B:639:DMS:H13	1.20	1.00
31:c:925:DMS:H21	41:o:433:HOH:O	1.60	0.99
1:a:97:TRP:HD1	31:a:420:DMS:C2	1.77	0.97
26:A:410:SQD:H162	26:A:410:SQD:H122	1.44	0.95
2:b:350[B]:GLU:HG2	31:b:636:DMS:C1	1.97	0.94
15:U:9:LEU:HA	31:U:204:DMS:S	2.08	0.94
16:v:90:GLU:HB2	31:v:209:DMS:C1	1.98	0.93
1:a:97:TRP:CD1	31:a:420:DMS:C2	2.51	0.92
13:o:74[B]:GLU:OE1	41:o:474[B]:HOH:O	1.85	0.92
31:B:646:DMS:H22	31:D:415:DMS:H11	1.51	0.90
31:B:636:DMS:H12	41:D:553:HOH:O	1.74	0.87
34:a:413:LMG:C25	34:a:413:LMG:H422	2.05	0.86
2:B:350:GLU:H	31:B:639:DMS:C1	1.89	0.86
13:O:23:ASP:HB3	41:O:564:HOH:O	1.74	0.86
16:v:4:THR:HG22	31:v:206:DMS:H23	1.57	0.86
10:k:21:LEU:HD13	17:y:24:MET:HE3	1.56	0.85
2:B:389:LYS:HE3	41:B:1009:HOH:O	1.75	0.85
13:O:82:GLN:NE2	41:O:402:HOH:O	2.08	0.85
2:B:350:GLU:HG3	31:B:639:DMS:C1	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:414:PL9:H251	28:e:101:LHG:H222	1.58	0.84
2:b:350[B]:GLU:CG	31:b:636:DMS:H12	2.06	0.84
3:c:362:ARG:HH11	31:c:925:DMS:H23	1.42	0.84
5:e:9:PRO:HA	28:e:101:LHG:HC2	1.61	0.83
4:d:101:PHE:H	36:d:407:DGD:HA21	1.43	0.83
23:B:615:CLA:H18	34:B:622:LMG:H422	1.61	0.82
13:O:74[B]:GLU:OE1	41:O:401:HOH:O	1.97	0.81
31:a:420:DMS:H21	8:i:5:LYS:CD	2.08	0.81
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.63	0.81
31:b:645:DMS:H23	41:b:1057[A]:HOH:O	1.80	0.80
2:B:360:PRO:HA	31:B:636:DMS:H11	1.64	0.80
16:v:90:GLU:HB2	31:v:209:DMS:H11	1.63	0.80
2:b:472:ARG:HG2	31:d:416:DMS:C1	2.12	0.80
4:D:140:PRO:HD2	31:D:416:DMS:O	1.81	0.80
2:b:472:ARG:HG2	31:d:416:DMS:H13	1.62	0.80
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.47	0.79
4:D:135:LEU:HD23	34:D:412:LMG:HC5	1.66	0.78
2:b:405:GLU:HG2	41:b:995:HOH:O	1.82	0.78
2:B:350:GLU:CG	31:B:639:DMS:H12	2.12	0.77
15:u:15:GLU:OE1	41:u:425[B]:HOH:O	2.02	0.77
1:a:214:MET:CG	27:a:414:PL9:H102	2.07	0.77
23:d:404:CLA:HBB1	23:d:404:CLA:HMB3	1.65	0.77
3:c:362:ARG:NH1	31:c:925:DMS:H23	1.99	0.77
28:D:411:LHG:H141	28:D:411:LHG:C35	2.15	0.76
17:Y:26:ALA:O	17:Y:30:ILE:HG12	1.85	0.76
13:O:15:LEU:HD23	13:O:18:LYS:HD3	1.67	0.76
31:u:205:DMS:H13	41:u:366:HOH:O	1.85	0.76
25:b:620:BCR:C8	25:b:620:BCR:H331	2.16	0.75
1:a:15[B]:GLU:HG3	30:a:422:LMT:C6B	2.16	0.75
4:D:14:TRP:CD1	35:D:414:HTG:H61	2.22	0.75
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.69	0.74
19:Z:35:ARG:HG2	19:Z:35:ARG:NH1	1.94	0.74
31:b:641:DMS:H21	41:b:787:HOH:O	1.87	0.73
2:b:350[A]:GLU:H	31:b:636:DMS:C1	2.01	0.73
30:B:644:LMT:H6E	41:B:914:HOH:O	1.87	0.73
15:U:10:VAL:H	31:U:204:DMS:H21	1.53	0.73
16:v:90:GLU:HB2	31:v:209:DMS:H13	1.69	0.73
2:B:472:ARG:HG2	31:D:416:DMS:C1	2.18	0.73
23:A:405:CLA:HMB3	23:A:405:CLA:HBB1	1.70	0.73
1:A:98:GLU:OE1	41:A:654[B]:HOH:O	2.06	0.72
2:B:350:GLU:N	31:B:639:DMS:H13	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:416:LMT:H6'1	41:A:650:HOH:O	1.90	0.72
1:a:72:LEU:HD11	30:a:418:LMT:H52	1.71	0.72
31:b:638:DMS:H13	41:b:1038:HOH:O	1.89	0.71
4:D:141:TYR:CZ	31:D:416:DMS:H22	2.26	0.71
2:b:223[A]:GLN:NE2	41:b:703[A]:HOH:O	2.24	0.71
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.73	0.71
2:b:350[B]:GLU:H	31:b:636:DMS:C1	2.04	0.70
13:o:33:ASP:HB3	13:o:36:GLN:HE21	1.55	0.70
2:b:467:ILE:HG13	4:d:126:MET:CE	2.22	0.69
2:b:347[A]:ARG:NH1	2:b:351:GLY:O	2.24	0.69
13:O:58:ASN:C	13:O:58:ASN:HD22	1.98	0.69
13:O:111:ALA:HB3	31:O:308:DMS:H11	1.74	0.69
1:a:15[B]:GLU:HG3	30:a:422:LMT:H6'1	1.74	0.69
4:d:332:GLN:HG2	31:d:414:DMS:H23	1.75	0.69
23:C:504:CLA:CHC	34:C:531:LMG:H241	2.22	0.68
4:D:135:LEU:CD2	34:D:412:LMG:HC5	2.22	0.68
26:A:410:SQD:H162	26:A:410:SQD:C12	2.21	0.68
15:U:86:GLU:HG3	29:U:201:UNL:C14	2.23	0.68
23:c:910:CLA:HMB1	23:c:910:CLA:HBB1	1.75	0.68
23:C:507:CLA:H92	30:I:101:LMT:H111	1.74	0.68
1:a:246:TYR:OH	41:a:501[A]:HOH:O	2.12	0.68
31:B:646:DMS:H11	41:B:835:HOH:O	1.92	0.68
2:b:332:LYS:NZ	31:b:647:DMS:H13	2.08	0.68
25:b:620:BCR:H331	25:b:620:BCR:HC8	1.74	0.68
9:j:2:MET:HG3	9:j:4:GLU:H	1.58	0.68
31:o:303:DMS:H21	41:o:478:HOH:O	1.95	0.67
31:O:308:DMS:H22	2:b:47:PRO:HG2	1.76	0.67
31:B:636:DMS:H13	41:D:566:HOH:O	1.93	0.67
1:A:214:MET:HG2	27:A:411:PL9:C10	2.12	0.67
34:D:412:LMG:H352	35:D:414:HTG:H7'2	1.76	0.67
31:h:101:DMS:H12	41:h:234:HOH:O	1.94	0.66
31:C:526:DMS:H11	41:C:749:HOH:O	1.94	0.66
2:B:341:LYS:NZ	35:B:625:HTG:S1	2.62	0.66
16:v:90:GLU:CB	31:v:209:DMS:H13	2.25	0.66
25:c:915:BCR:H382	25:c:915:BCR:H23C	1.78	0.65
5:E:15:THR:HB	9:J:8:ILE:O	1.96	0.65
23:C:513:CLA:H121	23:C:514:CLA:H142	1.78	0.65
31:B:646:DMS:H22	31:D:415:DMS:C1	2.25	0.65
31:B:648:DMS:H21	11:L:2:GLU:HB2	1.78	0.65
13:O:133:VAL:CG2	31:O:305:DMS:H22	2.19	0.65
13:O:194:LYS:HZ1	31:O:303:DMS:H23	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:362:ARG:HH11	31:c:925:DMS:C2	2.08	0.65
16:V:128:ASP:HB3	31:V:210:DMS:H21	1.78	0.65
25:t:101:BCR:HC8	25:t:101:BCR:H311	1.78	0.65
5:e:19:TYR:CE2	5:e:23:HIS:CE1	2.85	0.65
23:b:602:CLA:C9	38:x:102:RRX:H25	2.26	0.65
5:E:68:ASP:OD1	5:E:71:GLU:HB2	1.97	0.65
30:b:621:LMT:H122	34:d:411:LMG:H222	1.79	0.64
34:a:413:LMG:H211	36:c:917:DGD:HA82	1.78	0.64
4:d:332:GLN:HG2	31:d:414:DMS:C2	2.28	0.64
13:O:49[B]:THR:HG22	41:O:530:HOH:O	1.96	0.64
1:a:15[B]:GLU:HG3	30:a:422:LMT:H6'2	1.80	0.64
1:a:214:MET:HG2	27:a:414:PL9:C10	2.12	0.64
31:b:646:DMS:H21	41:b:1057[B]:HOH:O	1.97	0.64
5:E:68:ASP:O	5:E:72:ALA:HB2	1.98	0.64
2:b:347[B]:ARG:HD2	31:b:645:DMS:C2	2.28	0.63
10:K:14:ALA:HB2	19:Z:61:VAL:HG12	1.80	0.63
25:j:104:BCR:H321	25:j:104:BCR:HC8	1.81	0.63
19:z:1:MET:SD	19:z:1:MET:N	2.61	0.63
31:F:102:DMS:C1	41:J:214:HOH:O	2.46	0.63
1:a:121[B]:LEU:HG	34:a:413:LMG:H181	1.78	0.63
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.80	0.63
3:c:148:GLY:O	3:c:156:LYS:NZ	2.31	0.63
2:b:476:ARG:NH1	41:b:704[A]:HOH:O	2.31	0.63
31:F:102:DMS:H11	41:J:214:HOH:O	1.98	0.63
1:a:214:MET:HE2	1:a:255:PHE:CE2	2.34	0.63
23:B:611:CLA:H151	23:B:611:CLA:H203	1.80	0.62
23:B:614:CLA:HBB1	23:B:614:CLA:HMB1	1.80	0.62
1:A:214:MET:CG	27:A:411:PL9:H102	2.13	0.62
23:B:617:CLA:HED2	23:B:617:CLA:H43	1.81	0.62
16:V:5:PRO:HD3	31:V:206:DMS:H13	1.81	0.62
2:b:350[A]:GLU:HG3	31:b:636:DMS:H12	1.81	0.62
15:u:19:THR:HG21	41:u:358:HOH:O	1.98	0.62
3:c:362:ARG:HD3	31:c:925:DMS:C2	2.19	0.62
9:j:2:MET:HE3	9:j:3:SER:H	1.64	0.62
2:b:347[B]:ARG:HH11	31:b:645:DMS:H21	1.65	0.62
25:B:620:BCR:H331	25:B:620:BCR:C8	2.29	0.62
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.81	0.61
4:D:13:GLY:HA3	35:D:414:HTG:H62	1.81	0.61
26:A:410:SQD:H381	9:J:22:ILE:HD11	1.82	0.61
23:C:510:CLA:HMB3	23:C:510:CLA:HBB1	1.81	0.61
31:F:102:DMS:H12	16:V:27:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:74[A]:GLU:OE1	41:O:403:HOH:O	2.16	0.61
41:l:210[B]:HOH:O	12:m:4:ASN:ND2	2.33	0.61
13:O:57:LYS:HD2	41:b:749:HOH:O	2.01	0.61
16:V:55[A]:ARG:NH1	41:V:301:HOH:O	2.34	0.61
2:b:341:LYS:HZ1	35:b:622:HTG:C2	2.13	0.61
23:C:510:CLA:HBB1	23:C:510:CLA:CMB	2.31	0.61
34:a:413:LMG:H232	23:c:906:CLA:H92	1.82	0.61
2:b:350[B]:GLU:CD	31:b:636:DMS:H12	2.26	0.61
3:c:182:PHE:HA	35:c:921:HTG:H61	1.83	0.60
4:d:24:ARG:HE	18:x:37:VAL:HG22	1.66	0.60
1:a:215:HIS:HA	27:a:414:PL9:O1	2.01	0.60
23:b:617:CLA:H142	25:b:620:BCR:H12C	1.83	0.60
3:C:377:LEU:HG	3:C:381[A]:LYS:HE3	1.83	0.60
7:h:12:ARG:HB3	7:h:13:PRO:HD3	1.83	0.60
31:A:424:DMS:H13	35:O:302:HTG:H1'1	1.83	0.60
15:U:47:LYS:NZ	41:U:301:HOH:O	2.34	0.60
7:H:2:ALA:N	41:H:201:HOH:O	2.35	0.59
16:V:55[A]:ARG:HH22	31:V:210:DMS:H23	1.67	0.59
3:c:138:GLU:HG3	31:c:933:DMS:H12	1.84	0.59
30:M:101:LMT:H6D	11:l:9:PRO:HA	1.83	0.59
23:c:909:CLA:H192	34:c:920:LMG:H362	1.84	0.59
2:B:446:SER:HB2	2:B:447:PRO:CD	2.32	0.59
2:b:223[B]:GLN:OE1	7:h:21:VAL:HG21	2.02	0.59
4:D:141:TYR:OH	31:D:416:DMS:H22	2.01	0.59
16:V:55[A]:ARG:NH2	31:V:210:DMS:H23	2.18	0.59
31:u:205:DMS:H12	41:u:302:HOH:O	2.02	0.59
1:A:237:TYR:CZ	4:D:264[B]:LYS:HG3	2.38	0.59
25:C:516:BCR:H331	25:C:516:BCR:C8	2.33	0.58
31:C:529:DMS:H11	41:C:826:HOH:O	2.02	0.58
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.85	0.58
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.83	0.58
35:B:624:HTG:H7'2	30:a:418:LMT:H122	1.85	0.58
23:c:906:CLA:HBB1	23:c:906:CLA:HMB3	1.85	0.58
25:B:619:BCR:H331	25:B:619:BCR:C8	2.32	0.58
3:C:117:VAL:HG12	34:C:531:LMG:H211	1.85	0.58
30:b:621:LMT:C12	34:d:411:LMG:H242	2.34	0.58
1:a:11:ALA:HB1	1:a:15[A]:GLU:OE1	2.03	0.58
30:B:623:LMT:H22	34:D:412:LMG:HC91	1.85	0.58
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.35	0.58
1:A:265:PHE:HE2	27:A:411:PL9:H122	1.68	0.58
26:A:410:SQD:H291	23:C:509:CLA:H71	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:TYR:CE1	2:B:316:GLY:HA3	2.38	0.58
1:a:183:MET:HA	23:a:406:CLA:HMD1	1.86	0.58
2:b:350[B]:GLU:H	31:b:636:DMS:H11	1.68	0.58
4:d:135:LEU:HD21	34:d:411:LMG:HC62	1.85	0.58
2:b:350[A]:GLU:H	31:b:636:DMS:H11	1.68	0.57
3:c:138:GLU:HG3	31:c:933:DMS:C1	2.34	0.57
26:a:417:SQD:H442	41:a:641[B]:HOH:O	2.04	0.57
23:b:608:CLA:H2	34:m:102:LMG:H152	1.85	0.57
4:d:103:ARG:HH21	5:e:77:GLU:HG3	1.69	0.57
25:B:619:BCR:H382	25:t:101:BCR:H11C	1.85	0.57
2:b:349:LYS:HB3	31:b:636:DMS:H13	1.86	0.57
31:F:102:DMS:C1	16:V:27:LEU:HD21	2.35	0.57
15:U:10:VAL:H	31:U:204:DMS:C2	2.15	0.57
2:b:410:THR:H	31:b:639:DMS:H23	1.70	0.57
31:O:308:DMS:H12	41:b:805:HOH:O	2.04	0.57
7:H:30:LEU:H	31:H:105:DMS:H21	1.70	0.56
2:B:220:ARG:HG3	7:H:20:LYS:HG2	1.87	0.56
34:d:411:LMG:C29	34:d:411:LMG:HC8	2.35	0.56
15:U:73:GLN:O	15:U:77:GLU:HG3	2.04	0.56
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.87	0.56
2:b:467:ILE:HG13	4:d:126:MET:HE2	1.87	0.56
23:c:903:CLA:H61	23:c:913:CLA:H42	1.87	0.56
1:a:215:HIS:ND1	27:a:414:PL9:O1	2.33	0.56
27:a:414:PL9:H502	4:d:39:PRO:HG3	1.87	0.56
28:d:402:LHG:HC82	10:k:45:PHE:CD2	2.40	0.56
3:C:60:ILE:HG22	23:C:504:CLA:HHD	1.88	0.56
3:c:163:PHE:CD2	23:c:913:CLA:HAB	2.40	0.56
23:c:913:CLA:H202	23:c:913:CLA:HMB2	1.86	0.56
31:O:308:DMS:H13	41:O:435:HOH:O	2.06	0.56
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.41	0.56
2:B:81:THR:O	31:B:640:DMS:H21	2.05	0.55
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.38	0.55
35:v:204:HTG:H5'1	35:v:204:HTG:H1'2	1.87	0.55
23:D:404:CLA:H192	18:X:15[A]:LEU:HG	1.88	0.55
1:A:183:MET:HA	23:A:405:CLA:HMD1	1.88	0.55
23:A:406:CLA:H152	27:A:411:PL9:H262	1.88	0.55
29:U:201:UNL:C14	41:U:413:HOH:O	2.55	0.55
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.36	0.55
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.89	0.55
16:V:107:LEU:HD23	31:V:209:DMS:H12	1.88	0.55
1:A:215:HIS:HA	27:A:411:PL9:O1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:248:ALA:HA	23:b:604:CLA:H42	1.88	0.55
23:b:615:CLA:H111	23:b:615:CLA:H161	1.88	0.55
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.89	0.54
19:Z:35:ARG:HH11	19:Z:35:ARG:CG	2.07	0.54
1:A:215:HIS:ND1	27:A:411:PL9:O1	2.35	0.54
23:c:902:CLA:H192	23:c:907:CLA:C1B	2.38	0.54
23:c:907:CLA:HMC2	23:c:908:CLA:H102	1.88	0.54
31:O:308:DMS:C2	2:b:47:PRO:HG2	2.37	0.54
23:b:617:CLA:H141	25:b:620:BCR:H10C	1.89	0.54
23:d:404:CLA:HBB1	23:d:404:CLA:CMB	2.34	0.54
16:v:45:ILE:C	16:v:45:ILE:HD12	2.32	0.54
4:d:85:MET:CE	4:d:96:GLU:HG2	2.37	0.54
26:A:410:SQD:H331	23:C:509:CLA:H202	1.88	0.54
2:b:350[B]:GLU:OE2	31:b:636:DMS:H12	2.08	0.54
13:o:58:ASN:ND2	41:o:403:HOH:O	2.41	0.54
26:B:621:SQD:H242	11:l:14:ARG:HD3	1.88	0.54
3:C:150:ASP:OD1	41:C:601:HOH:O	2.18	0.54
23:b:616:CLA:H2	23:b:617:CLA:HBB2	1.89	0.54
3:C:377:LEU:O	3:C:381[A]:LYS:HG3	2.08	0.54
25:d:405:BCR:HC22	36:d:407:DGD:HAF2	1.90	0.54
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.90	0.54
11:L:9:PRO:HA	30:m:104:LMT:H6D	1.90	0.54
31:b:647:DMS:H22	12:m:2:GLU:HB3	1.90	0.54
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.91	0.53
41:A:538:HOH:O	31:V:207:DMS:H13	2.06	0.53
23:b:610:CLA:NC	38:x:102:RRX:H56	2.23	0.53
23:B:606:CLA:C14	23:B:611:CLA:HED2	2.38	0.53
26:A:410:SQD:H383	29:J:104:UNL:C16	2.39	0.53
31:B:645:DMS:H12	41:B:1107:HOH:O	2.08	0.53
31:O:311:DMS:C1	41:O:573:HOH:O	2.27	0.53
16:V:2:GLU:OE2	31:V:207:DMS:H12	2.08	0.53
16:V:128:ASP:OD2	31:V:205:DMS:H12	2.08	0.53
34:c:920:LMG:H292	34:c:920:LMG:H162	1.91	0.53
28:d:408:LHG:H223	12:m:18:PRO:HD3	1.91	0.53
2:B:82:GLY:O	31:B:641:DMS:S	2.66	0.53
2:b:387:GLU:HG2	31:u:206:DMS:H23	1.90	0.53
4:d:192:THR:HG23	23:d:403:CLA:HBC2	1.90	0.53
3:C:318:LEU:C	3:C:318:LEU:HD23	2.34	0.53
31:c:929:DMS:H21	41:c:1291:HOH:O	2.08	0.53
2:b:332:LYS:HZ2	31:b:647:DMS:H13	1.72	0.52
5:e:68:ASP:OD1	5:e:71:GLU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:405:BCR:H313	36:D:407:DGD:HAE1	1.91	0.52
19:z:15:LEU:HD22	19:z:46:LEU:HD23	1.90	0.52
2:B:405:GLU:OE2	2:B:431:GLU:OE1	2.27	0.52
4:d:100:ASP:HA	36:d:407:DGD:HA32	1.91	0.52
31:A:421:DMS:H23	5:E:63:ILE:HD11	1.90	0.52
3:c:213:LEU:HD11	25:c:916:BCR:C20	2.40	0.52
4:D:11:GLU:O	4:D:12:ARG:HB2	2.10	0.52
7:H:62:TRP:O	31:H:101:DMS:H13	2.09	0.52
1:a:98:GLU:OE1	41:a:502:HOH:O	2.18	0.52
1:a:218:LEU:HD12	27:a:414:PL9:C3	2.40	0.52
4:d:269:PHE:CD1	28:d:408:LHG:HC11	2.45	0.52
2:B:451:PHE:CE2	2:B:455:HIS:CE1	2.98	0.52
23:B:606:CLA:HHC	23:B:606:CLA:HBB1	1.91	0.52
41:b:888:HOH:O	31:h:101:DMS:H22	2.08	0.52
26:A:415:SQD:H442	41:A:616[B]:HOH:O	2.10	0.52
4:D:272:LEU:C	4:D:272:LEU:HD23	2.34	0.52
31:a:420:DMS:C2	8:i:5:LYS:HD2	2.14	0.52
23:b:602:CLA:H91	38:x:102:RRX:H25	1.91	0.52
13:o:231:HIS:HD2	31:o:304:DMS:O	1.93	0.52
31:A:424:DMS:C1	35:O:302:HTG:H1'1	2.40	0.52
23:B:602:CLA:CGA	23:B:602:CLA:H72	2.40	0.52
13:o:98:GLU:HG3	41:o:402:HOH:O	2.09	0.52
3:C:364:PRO:HA	31:C:529:DMS:H13	1.92	0.51
5:e:19:TYR:CD2	5:e:23:HIS:CE1	2.97	0.51
16:V:118:HIS:CE1	16:V:122:GLU:HG2	2.45	0.51
31:V:207:DMS:H23	41:V:405:HOH:O	2.10	0.51
2:b:50:PRO:HG2	31:b:637:DMS:H23	1.93	0.51
23:c:905:CLA:H42	36:c:918:DGD:HB31	1.92	0.51
30:b:621:LMT:H122	34:d:411:LMG:H242	1.93	0.51
32:a:424:BCT:O1	4:d:264[B]:LYS:NZ	2.42	0.51
2:b:347[B]:ARG:NH1	31:b:645:DMS:H21	2.25	0.51
10:K:14:ALA:CB	19:Z:61:VAL:HG12	2.41	0.51
19:Z:33:TRP:CZ2	30:Z:101:LMT:O3'	2.64	0.51
34:B:622:LMG:O9	34:B:622:LMG:H132	2.10	0.51
27:a:414:PL9:C51	26:x:101:SQD:H342	2.40	0.51
2:b:276:ASP:O	31:b:633:DMS:H22	2.11	0.51
16:v:90:GLU:CB	31:v:209:DMS:C1	2.78	0.51
35:B:624:HTG:C7'	30:a:418:LMT:H122	2.41	0.51
37:E:105:HEM:HMC2	6:F:31:ILE:HG13	1.91	0.51
16:v:53:ASP:CG	16:v:55[B]:ARG:HG3	2.36	0.51
15:U:10:VAL:N	31:U:204:DMS:H21	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:GLU:CG	31:B:639:DMS:C1	2.81	0.51
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.93	0.51
2:b:27:THR:HG22	2:b:107:LEU:HD13	1.93	0.51
23:B:611:CLA:CBB	23:B:611:CLA:HHC	2.41	0.51
31:O:311:DMS:H11	41:O:477:HOH:O	2.10	0.51
3:C:377:LEU:HB3	13:O:80:GLN:OE1	2.11	0.50
1:A:103:ASP:OD1	31:A:424:DMS:H22	2.11	0.50
31:C:526:DMS:H22	41:C:674:HOH:O	2.10	0.50
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.93	0.50
19:Z:33:TRP:HZ2	30:Z:101:LMT:O3'	1.94	0.50
23:b:611:CLA:HHC	23:b:611:CLA:HBB1	1.93	0.50
23:b:615:CLA:H111	23:b:615:CLA:C16	2.42	0.50
13:o:42:ARG:O	13:o:241:ALA:HA	2.12	0.50
7:H:27:THR:HA	31:H:105:DMS:H23	1.94	0.50
3:c:31:SER:CB	3:c:41:ARG:HG2	2.41	0.50
3:c:257:PHE:CZ	31:c:932:DMS:H11	2.47	0.50
2:B:133:LEU:HD12	31:B:638:DMS:H12	1.91	0.50
2:b:472:ARG:HG2	31:d:416:DMS:H11	1.92	0.50
16:v:99:ASP:O	31:v:202:DMS:H21	2.12	0.50
31:a:420:DMS:H22	41:a:502:HOH:O	2.11	0.50
3:c:257:PHE:CE1	31:c:932:DMS:H11	2.47	0.50
15:u:86:GLU:HG2	41:u:373:HOH:O	2.11	0.50
1:A:221:SER:HB2	4:D:139:ARG:O	2.11	0.50
23:B:605:CLA:H43	23:B:606:CLA:H2	1.93	0.50
3:C:78:GLU:HB3	41:C:758[B]:HOH:O	2.11	0.50
3:C:117:VAL:CG1	34:C:531:LMG:H211	2.41	0.50
24:D:402:PHO:HBC2	24:D:402:PHO:HHD	1.94	0.50
2:b:306:PRO:HG3	31:b:641:DMS:H23	1.94	0.50
23:b:616:CLA:H142	23:b:617:CLA:H201	1.93	0.50
15:U:45:LEU:O	15:U:49:ILE:HG13	2.12	0.50
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.49
7:H:29:PRO:HD2	31:H:105:DMS:H22	1.93	0.49
15:u:51:LYS:HE3	41:u:427[B]:HOH:O	2.12	0.49
13:O:231:HIS:HE1	41:O:527:HOH:O	1.95	0.49
2:b:341:LYS:NZ	35:b:622:HTG:S1	2.73	0.49
2:b:350[B]:GLU:HG2	31:b:636:DMS:H11	1.90	0.49
23:A:405:CLA:CBD	23:D:401:CLA:HAC2	2.43	0.49
16:V:128:ASP:CB	31:V:210:DMS:H21	2.42	0.49
36:d:407:DGD:HB21	5:e:46:VAL:HG13	1.93	0.49
23:B:616:CLA:HBB1	23:B:616:CLA:HMB3	1.93	0.49
25:d:405:BCR:H331	25:d:405:BCR:C8	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:103:LMT:H6E	41:e:229:HOH:O	2.11	0.49
27:A:411:PL9:H502	4:D:39:PRO:HG3	1.93	0.49
26:a:417:SQD:H223	25:t:101:BCR:C32	2.43	0.49
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.12	0.49
13:O:140:THR:OG1	31:O:305:DMS:H23	2.13	0.49
23:c:902:CLA:C4D	23:c:904:CLA:H2	2.43	0.49
4:d:236:ASN:O	4:d:239:GLN:HG2	2.13	0.49
19:z:32:ASP:OD1	19:z:35:ARG:HB3	2.13	0.49
28:D:409:LHG:O9	28:L:101:LHG:HC81	2.13	0.49
2:B:138:MET:HE3	23:B:616:CLA:CHD	2.42	0.49
23:b:603:CLA:HBB1	23:b:603:CLA:CMB	2.43	0.49
3:c:31:SER:HB2	3:c:41:ARG:HG2	1.95	0.49
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.48	0.48
27:a:414:PL9:H511	26:x:101:SQD:H342	1.93	0.48
4:d:141:TYR:CZ	31:d:416:DMS:H22	2.48	0.48
3:C:279:LEU:HA	3:C:282:MET:HE3	1.93	0.48
3:c:373:ASN:HB3	41:o:470:HOH:O	2.14	0.48
5:e:18:ARG:NH1	37:e:105:HEM:O2A	2.45	0.48
1:A:214:MET:HE2	1:A:255:PHE:CE2	2.48	0.48
23:A:405:CLA:CAD	23:D:401:CLA:HAC2	2.44	0.48
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.94	0.48
31:C:526:DMS:H12	41:C:800:HOH:O	2.13	0.48
23:b:605:CLA:H43	23:b:606:CLA:H2	1.95	0.48
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.44	0.48
9:J:9:PRO:HD2	9:J:12:ILE:HD12	1.95	0.48
13:O:133:VAL:HG13	31:O:305:DMS:C2	2.44	0.48
19:Z:47:TRP:CE2	30:Z:101:LMT:H112	2.48	0.48
1:a:339:PHE:HB3	1:a:340:PRO:HD2	1.95	0.48
3:c:409:GLY:HA2	31:c:927:DMS:S	2.53	0.48
26:B:621:SQD:H462	26:B:621:SQD:H1	1.94	0.48
26:D:408:SQD:H461	18:X:31:ILE:HG21	1.96	0.48
31:V:207:DMS:H12	41:V:405:HOH:O	2.14	0.48
2:b:347[B]:ARG:HH11	31:b:645:DMS:C2	2.27	0.48
25:c:915:BCR:H23C	25:c:915:BCR:C38	2.43	0.48
23:A:405:CLA:HBB1	23:A:405:CLA:CMB	2.43	0.48
5:e:60:GLN:HE21	5:e:60:GLN:HB2	1.50	0.48
11:l:24[A]:ILE:CD1	12:m:18:PRO:HB2	2.43	0.48
13:O:56:PRO:HD3	13:O:63:ALA:HB2	1.96	0.48
23:b:611:CLA:H152	23:b:611:CLA:OBD	2.14	0.48
3:c:318:LEU:C	3:c:318:LEU:HD23	2.39	0.48
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.95	0.48
1:a:84:PRO:HA	1:a:112:TYR:CG	2.49	0.48
24:a:409:PHO:HBC2	24:a:409:PHO:HHD	1.96	0.48
2:B:80:ILE:HD11	2:B:167:TRP:CZ3	2.48	0.48
23:B:617:CLA:H142	29:B:634:UNL:C7	2.43	0.48
3:c:179:ALA:O	3:c:184:GLY:HA2	2.14	0.48
10:k:17:ILE:HG23	10:k:18:PHE:CD2	2.48	0.48
34:a:413:LMG:O3	31:a:420:DMS:H22	2.14	0.47
2:b:341:LYS:NZ	35:b:622:HTG:C2	2.77	0.47
2:B:121[B]:GLU:HG3	41:B:1025:HOH:O	2.13	0.47
3:C:406:SER:HA	3:C:420:VAL:HG23	1.95	0.47
15:U:50:VAL:O	31:U:202:DMS:H23	2.14	0.47
36:D:407:DGD:O2D	36:D:407:DGD:HG11	2.15	0.47
23:b:604:CLA:CMD	23:b:607:CLA:HMB2	2.44	0.47
15:u:16:LYS:HD2	41:u:358:HOH:O	2.14	0.47
29:M:102:UNL:C7	31:l:102:DMS:H22	2.45	0.47
3:c:191:PRO:HB2	31:c:936:DMS:H12	1.96	0.47
30:m:103:LMT:H1B	41:m:210:HOH:O	2.14	0.47
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.49	0.47
30:B:623:LMT:H3B	34:D:412:LMG:HC62	1.96	0.47
2:b:350[B]:GLU:CG	31:b:636:DMS:C1	2.77	0.47
4:d:272:LEU:C	4:d:272:LEU:HD23	2.39	0.47
27:A:411:PL9:H152	28:E:101:LHG:H302	1.95	0.47
4:D:27:PHE:HE1	28:E:101:LHG:HC2	1.80	0.47
3:c:201:ASN:ND2	35:c:922:HTG:O6	2.47	0.47
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.47
4:d:264[B]:LYS:HB3	4:d:264[B]:LYS:HE3	1.74	0.47
13:o:66:VAL:HB	13:o:67:PRO:HD2	1.96	0.47
2:B:224:ARG:HG3	7:H:25:TRP:CD2	2.50	0.47
25:T:101:BCR:C23	25:T:101:BCR:H382	2.44	0.47
25:j:104:BCR:C8	25:j:104:BCR:H311	2.45	0.47
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.96	0.47
15:u:58:VAL:O	15:u:61:VAL:HG12	2.15	0.47
16:v:2:GLU:HG3	31:v:206:DMS:H12	1.97	0.47
23:A:408:CLA:H162	23:A:408:CLA:H122	1.58	0.47
2:B:13:ILE:O	31:B:638:DMS:H11	2.14	0.47
15:U:86:GLU:H	29:U:201:UNL:C14	2.27	0.47
19:Z:61:VAL:HG13	41:Z:1605:HOH:O	2.15	0.47
13:o:23:ASP:OD1	13:o:23:ASP:N	2.48	0.47
31:v:210:DMS:H11	41:v:328:HOH:O	2.13	0.47
36:d:407:DGD:HB22	36:d:407:DGD:HBN1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:37:LEU:HD11	31:h:104:DMS:H23	1.96	0.47
3:C:50:LEU:O	3:C:54:VAL:HG23	2.15	0.47
3:C:381[B]:LYS:NZ	13:O:99:ASP:OD2	2.48	0.47
3:c:126:GLY:O	3:c:130:VAL:HG23	2.14	0.47
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.97	0.47
2:b:347[B]:ARG:HD2	31:b:645:DMS:H21	1.96	0.46
19:z:3:ILE:HA	19:z:6:GLN:HB2	1.96	0.46
16:V:128:ASP:CG	31:V:210:DMS:H21	2.40	0.46
12:m:16[B]:LEU:HD21	41:m:214:HOH:O	2.16	0.46
31:A:422:DMS:H22	41:A:546:HOH:O	2.14	0.46
2:B:204:ALA:CB	23:B:603:CLA:HAB	2.46	0.46
12:M:28:GLN:O	12:M:32:GLN:HG3	2.16	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
23:D:403:CLA:HBC3	23:D:403:CLA:HHD	1.98	0.46
26:D:408:SQD:H242	18:X:31:ILE:HD13	1.98	0.46
12:M:5:GLN:H	12:M:5:GLN:HG2	1.36	0.46
2:B:75:TRP:HB3	31:a:423:DMS:H23	1.96	0.46
23:B:611:CLA:HHC	23:B:611:CLA:HBB1	1.98	0.46
25:D:405:BCR:C38	34:J:101:LMG:H231	2.45	0.46
2:b:72:THR:HG22	2:b:80:ILE:HD11	1.98	0.46
23:c:907:CLA:HMB1	23:c:908:CLA:NB	2.29	0.46
4:d:24:ARG:HH22	18:x:35:ASP:CG	2.23	0.46
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.50	0.46
2:B:498:LYS:HD2	4:D:20:ASP:HA	1.98	0.46
1:a:103:ASP:OD2	13:o:69:LYS:HE3	2.15	0.46
23:B:606:CLA:HHC	23:B:606:CLA:CBB	2.45	0.46
26:B:621:SQD:H341	26:B:621:SQD:H311	1.64	0.46
3:C:38:GLY:HA3	23:C:512:CLA:HMD2	1.97	0.46
2:b:162:PHE:O	23:b:607:CLA:HHD	2.16	0.46
23:d:404:CLA:H192	23:d:404:CLA:H161	1.84	0.46
31:l:102:DMS:H11	41:l:201[B]:HOH:O	2.15	0.46
2:B:472:ARG:HG2	31:D:416:DMS:H11	1.97	0.46
23:C:513:CLA:H101	23:C:514:CLA:H141	1.98	0.46
1:a:12:ASN:HB3	1:a:15[B]:GLU:H	1.80	0.46
1:a:202:VAL:HG11	23:a:407:CLA:C3D	2.46	0.46
3:C:409:GLY:HA2	31:V:202:DMS:S	2.56	0.46
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.98	0.46
19:z:26:ALA:HB3	19:z:40:ILE:HD11	1.97	0.46
23:B:614:CLA:H51	28:D:409:LHG:H351	1.97	0.46
31:B:646:DMS:H13	41:B:779:HOH:O	2.15	0.46
23:a:406:CLA:CBD	23:d:401:CLA:HAC2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:9:PRO:HA	28:e:101:LHG:C2	2.41	0.46
30:Z:101:LMT:H82	30:Z:101:LMT:H51	1.80	0.45
25:b:620:BCR:HC8	25:b:620:BCR:C33	2.42	0.45
25:j:104:BCR:HC7	25:j:104:BCR:H331	1.82	0.45
3:C:31:SER:CB	3:C:41:ARG:HG2	2.46	0.45
1:a:135:TYR:OH	31:i:105:DMS:H23	2.16	0.45
3:c:121:SER:HB2	34:c:930:LMG:H241	1.98	0.45
26:A:415:SQD:H272	2:b:109:LEU:HD13	1.97	0.45
35:B:630:HTG:H62	31:a:423:DMS:H12	1.98	0.45
13:O:39:ARG:HB2	13:O:83:GLY:O	2.17	0.45
23:b:617:CLA:C14	25:b:620:BCR:H12C	2.45	0.45
3:c:109:PHE:N	3:c:110:PRO:CD	2.80	0.45
5:e:63:ILE:HG23	5:e:64:PRO:HD2	1.98	0.45
28:e:101:LHG:H212	28:e:101:LHG:H181	1.61	0.45
31:e:104:DMS:H13	31:v:205:DMS:H23	1.97	0.45
13:o:33:ASP:CB	13:o:36:GLN:HE21	2.26	0.45
16:v:27:LEU:HD11	31:v:207:DMS:H12	1.97	0.45
2:B:248:ALA:HA	23:B:604:CLA:H42	1.98	0.45
3:C:377:LEU:CB	13:O:80:GLN:OE1	2.64	0.45
25:T:101:BCR:H382	25:T:101:BCR:H23C	1.98	0.45
31:B:636:DMS:C1	41:B:833:HOH:O	2.64	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.45
31:V:210:DMS:H13	41:V:368:HOH:O	2.16	0.45
1:a:72:LEU:CD1	30:a:418:LMT:H52	2.45	0.45
1:a:218:LEU:HD12	27:a:414:PL9:C4	2.46	0.45
23:c:909:CLA:H122	23:c:909:CLA:H162	1.73	0.45
36:d:407:DGD:HA22	36:d:407:DGD:HA51	1.56	0.45
8:i:28:PRO:C	31:i:105:DMS:H12	2.42	0.45
16:v:14:SER:HB2	35:v:204:HTG:O2	2.16	0.45
16:v:55[A]:ARG:NH1	41:v:306:HOH:O	2.50	0.45
30:z:101:LMT:H1B	30:z:101:LMT:H4B	1.58	0.45
25:B:619:BCR:H363	25:t:101:BCR:H19C	1.99	0.45
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.52	0.45
23:b:617:CLA:H203	23:b:617:CLA:H122	1.99	0.45
23:c:912:CLA:HAA1	23:c:912:CLA:HBD	1.98	0.45
25:t:101:BCR:H23C	25:t:101:BCR:H382	1.97	0.45
25:t:101:BCR:H331	25:t:101:BCR:HC7	1.63	0.45
2:B:63:LEU:N	2:B:64:PRO:HD2	2.31	0.45
23:C:505:CLA:H42	36:C:518:DGD:HB31	1.99	0.45
23:C:514:CLA:C4B	25:C:515:BCR:H383	2.46	0.45
3:c:60:ILE:HG22	23:c:904:CLA:HHD	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:v:204:HTG:H1'2	35:v:204:HTG:C5'	2.35	0.45
17:y:44:GLY:HA2	19:z:30:PRO:HD3	1.99	0.45
31:B:636:DMS:H11	41:B:833:HOH:O	2.16	0.45
2:b:352:GLU:HB2	31:b:644:DMS:H12	1.97	0.45
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.47	0.45
23:C:507:CLA:H151	23:C:507:CLA:H18	1.63	0.45
26:L:102:SQD:H1	26:L:102:SQD:H462	1.99	0.45
25:T:101:BCR:HC7	25:T:101:BCR:H331	1.61	0.45
1:a:114:LEU:C	1:a:114:LEU:HD23	2.42	0.45
1:a:247:ASN:HB3	2:b:482:ILE:HD11	1.98	0.45
2:b:157:HIS:C	2:b:157:HIS:CD2	2.94	0.45
25:b:620:BCR:H24C	25:b:620:BCR:H371	1.77	0.45
3:c:42:LEU:HD21	23:c:912:CLA:H2A	1.99	0.45
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.99	0.45
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.52	0.45
34:a:413:LMG:H382	36:c:917:DGD:HB51	1.98	0.45
23:b:616:CLA:H2	23:b:617:CLA:CBB	2.47	0.45
31:A:421:DMS:H23	5:E:63:ILE:CD1	2.47	0.44
41:A:538:HOH:O	31:V:207:DMS:C1	2.62	0.44
2:B:224:ARG:HG2	7:H:24:GLY:C	2.42	0.44
3:c:147:PHE:CD1	23:c:914:CLA:H3A	2.53	0.44
4:d:141:TYR:CZ	31:d:416:DMS:C2	3.00	0.44
13:o:54:GLU:HA	31:o:304:DMS:H22	1.99	0.44
23:C:511:CLA:H192	23:C:511:CLA:HBC3	2.00	0.44
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.98	0.44
23:b:617:CLA:H91	23:b:617:CLA:H112	1.55	0.44
3:c:84:GLN:OE1	41:c:1001:HOH:O	2.21	0.44
3:c:223:TRP:CG	3:c:224:ILE:H	2.36	0.44
28:d:410:LHG:H341	28:d:410:LHG:H302	1.99	0.44
13:o:59:LYS:O	13:o:60:ARG:CB	2.64	0.44
23:B:614:CLA:HBB1	23:B:614:CLA:CMB	2.46	0.44
31:B:648:DMS:C2	11:L:2:GLU:HB2	2.47	0.44
11:L:18:TYR:OH	26:L:102:SQD:H242	2.18	0.44
17:Y:27:MET:HE3	17:Y:27:MET:HB3	1.65	0.44
28:a:415:LHG:H122	28:a:415:LHG:H242	1.98	0.44
3:c:334:PRO:HA	13:o:153:THR:OG1	2.18	0.44
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.53	0.44
4:D:126:MET:HA	4:D:129:GLN:OE1	2.17	0.44
23:d:401:CLA:H203	23:d:401:CLA:H162	1.68	0.44
25:A:409:BCR:C8	25:A:409:BCR:H331	2.47	0.44
3:C:155[B]:ASN:OD1	3:C:255:THR:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:362:ARG:HD3	31:C:525:DMS:O	2.17	0.44
26:L:102:SQD:O49	31:l:102:DMS:O	2.36	0.44
1:a:12:ASN:HB3	1:a:15[A]:GLU:H	1.81	0.44
16:v:86:GLN:NE2	41:v:302:HOH:O	2.45	0.44
4:D:209:LEU:HD23	4:D:209:LEU:C	2.43	0.44
15:u:53:ALA:HB1	15:u:54:PRO:HA	1.99	0.44
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.77	0.44
23:B:612:CLA:HBB1	23:B:612:CLA:HMB3	1.99	0.44
4:D:24:ARG:NH1	41:D:610[B]:HOH:O	2.50	0.44
28:D:411:LHG:H142	28:D:411:LHG:H322	1.99	0.44
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.44
16:V:2:GLU:OE2	31:V:207:DMS:C1	2.66	0.44
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.99	0.44
3:c:163:PHE:CE2	23:c:913:CLA:HAB	2.53	0.44
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.92	0.44
8:i:34:ARG:O	31:i:105:DMS:H11	2.17	0.44
31:v:209:DMS:H11	41:v:384:HOH:O	2.17	0.44
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.44
1:A:259:ILE:HD12	27:A:411:PL9:H253	2.00	0.44
2:B:262:THR:C	2:B:264:PRO:HD3	2.42	0.44
13:O:133:VAL:HG13	31:O:305:DMS:H22	2.00	0.44
24:a:409:PHO:HMA2	27:a:414:PL9:H221	1.99	0.44
34:a:413:LMG:H201	34:a:413:LMG:H231	1.60	0.44
2:b:144:PHE:CE2	2:b:210:ILE:HG23	2.53	0.44
4:d:23:LYS:HD3	4:d:135:LEU:HD21	2.00	0.44
5:e:59:GLU:OE1	5:e:59:GLU:HA	2.18	0.44
25:C:530:BCR:H11C	25:C:530:BCR:H341	1.92	0.43
16:V:129:LYS:HD2	41:V:410:HOH:O	2.18	0.43
27:a:414:PL9:H403	6:f:22:ALA:HB2	2.00	0.43
4:d:27:PHE:CD2	28:e:101:LHG:HC12	2.53	0.43
16:v:72:LEU:O	16:v:76:MET:HG3	2.17	0.43
23:B:616:CLA:HBB1	23:B:616:CLA:CMB	2.49	0.43
13:O:194:LYS:NZ	31:O:303:DMS:H23	2.33	0.43
23:a:406:CLA:HBB1	23:a:406:CLA:HMB1	2.01	0.43
23:c:909:CLA:C9	28:d:410:LHG:H151	2.48	0.43
26:A:410:SQD:H122	26:A:410:SQD:C16	2.31	0.43
30:A:416:LMT:H123	29:A:417:UNL:C13	2.48	0.43
19:Z:47:TRP:CD2	30:Z:101:LMT:H112	2.54	0.43
2:b:483:ASP:HA	2:b:484:PRO:HD3	1.85	0.43
23:b:602:CLA:H2	23:b:602:CLA:H72	1.99	0.43
23:b:602:CLA:O1D	35:b:623:HTG:H4	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:k:102:BCR:H331	25:k:102:BCR:C8	2.48	0.43
3:C:464:GLU:OE2	4:D:245:SER:OG	2.25	0.43
31:D:415:DMS:H13	41:D:575:HOH:O	2.19	0.43
25:b:619:BCR:H331	25:b:619:BCR:C8	2.49	0.43
41:b:1034:HOH:O	31:u:206:DMS:C2	2.66	0.43
23:c:913:CLA:H203	23:c:913:CLA:H161	1.91	0.43
4:d:24:ARG:NH2	18:x:35:ASP:O	2.51	0.43
13:o:129:THR:HA	13:o:141:ASP:O	2.19	0.43
35:v:204:HTG:H61	41:v:416:HOH:O	2.18	0.43
2:B:30:VAL:HG13	23:B:614:CLA:HMC2	2.00	0.43
2:B:350:GLU:N	31:B:639:DMS:C1	2.69	0.43
23:B:606:CLA:H62	23:B:606:CLA:H41	1.79	0.43
23:C:504:CLA:H72	23:C:504:CLA:H112	1.77	0.43
41:L:208[B]:HOH:O	12:M:4:ASN:ND2	2.41	0.43
16:V:79:PRO:HD3	16:V:94:SER:HB3	1.99	0.43
16:V:124:LYS:NZ	41:V:308:HOH:O	2.51	0.43
4:d:233:ARG:HH11	28:d:402:LHG:HC12	1.82	0.43
16:v:101:PHE:CD1	31:v:201:DMS:H12	2.54	0.43
26:A:410:SQD:H142	28:D:411:LHG:C16	2.49	0.43
28:A:412:LHG:H111	28:A:412:LHG:H242	2.00	0.43
3:C:203:THR:O	3:C:235:GLY:HA3	2.19	0.43
3:c:146:PHE:O	3:c:156:LYS:NZ	2.51	0.43
2:B:493:TRP:HD1	5:E:5:THR:CG2	2.32	0.43
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.01	0.43
28:D:411:LHG:H322	28:D:411:LHG:C14	2.49	0.43
28:D:411:LHG:H302	28:D:411:LHG:H331	1.65	0.43
31:O:304:DMS:H12	41:O:532[B]:HOH:O	2.18	0.43
26:a:412:SQD:H302	23:c:909:CLA:H93	2.00	0.43
23:b:602:CLA:H92	38:x:102:RRX:H25	1.98	0.43
3:c:472:LEU:HD11	4:d:255:GLN:HG3	2.01	0.43
3:C:472:LEU:HD11	4:D:255:GLN:HG3	2.00	0.43
23:C:507:CLA:H92	30:I:101:LMT:C11	2.45	0.43
10:K:19:ASP:HB2	10:K:20:PRO:HD3	2.01	0.43
26:L:102:SQD:H462	26:L:102:SQD:C1	2.48	0.43
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.54	0.43
2:b:350[A]:GLU:H	31:b:636:DMS:H13	1.81	0.43
25:b:619:BCR:H20C	25:b:619:BCR:H361	1.79	0.43
16:v:41:HIS:O	16:v:42:VAL:C	2.59	0.43
3:C:167:VAL:HG13	23:C:513:CLA:H71	2.01	0.43
3:C:308:GLU:HB2	3:C:361:PHE:CE2	2.53	0.43
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.00	0.43
24:A:407:PHO:NC	24:A:407:PHO:ND	2.67	0.43
23:C:503:CLA:H193	35:C:521:HTG:H3'1	2.00	0.43
29:M:102:UNL:C6	31:l:102:DMS:C2	2.96	0.43
1:a:247:ASN:HA	31:a:421:DMS:H23	2.00	0.43
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.43
3:c:470:PRO:HA	31:c:934:DMS:H12	2.00	0.43
31:c:925:DMS:C2	41:o:433:HOH:O	2.41	0.43
4:d:296:TYR:CE1	4:d:319:LEU:HD22	2.53	0.43
16:V:81:THR:CG2	16:V:86:GLN:HG3	2.49	0.42
16:V:129:LYS:CD	41:V:410:HOH:O	2.66	0.42
1:a:322:ASN:OD1	3:c:412:THR:HA	2.19	0.42
23:a:406:CLA:HBB1	23:a:406:CLA:CMB	2.49	0.42
12:m:16[B]:LEU:HD23	12:m:16[B]:LEU:HA	1.81	0.42
13:o:180:GLU:CD	13:o:180:GLU:H	2.27	0.42
25:C:515:BCR:C8	25:C:515:BCR:H331	2.48	0.42
1:a:249:VAL:HG12	2:b:491:VAL:HG23	2.01	0.42
24:a:409:PHO:ND	24:a:409:PHO:NC	2.66	0.42
23:b:603:CLA:HBB1	23:b:603:CLA:HMB1	2.00	0.42
3:c:397:THR:HA	31:c:927:DMS:H13	2.01	0.42
7:h:59:ASN:ND2	7:h:63:LYS:O	2.53	0.42
15:u:10:VAL:HG11	15:u:15:GLU:OE2	2.19	0.42
29:u:201:UNL:C1	29:u:202:UNL:C16	2.97	0.42
19:z:3:ILE:CA	19:z:6:GLN:HB2	2.49	0.42
26:B:621:SQD:H45	14:t:23:PHE:CD1	2.53	0.42
18:X:23:LEU:O	18:X:27:VAL:HG23	2.20	0.42
2:b:435:GLU:CD	41:b:706[A]:HOH:O	2.61	0.42
19:z:44:SER:O	19:z:48:ILE:HG13	2.19	0.42
2:B:58:GLN:C	2:B:329:PRO:HB3	2.44	0.42
25:B:620:BCR:H24C	25:B:620:BCR:H371	1.87	0.42
26:a:417:SQD:H223	25:t:101:BCR:H322	2.01	0.42
1:A:265:PHE:HE2	27:A:411:PL9:C12	2.31	0.42
23:B:602:CLA:H91	23:B:602:CLA:H111	1.61	0.42
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.19	0.42
4:D:27:PHE:CE1	28:E:101:LHG:HC2	2.54	0.42
29:M:102:UNL:C6	31:l:102:DMS:H22	2.50	0.42
25:T:101:BCR:C23	25:T:101:BCR:C38	2.97	0.42
23:b:617:CLA:H92	23:b:617:CLA:H61	1.79	0.42
23:d:404:CLA:H192	18:x:15:LEU:HB2	2.00	0.42
13:o:114:GLU:OE1	31:o:304:DMS:H12	2.19	0.42
2:b:451:PHE:CD1	2:b:451:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:78:GLU:HG2	3:c:79:LYS:N	2.35	0.42
23:c:910:CLA:HBB1	23:c:910:CLA:CMB	2.48	0.42
2:B:157:HIS:C	2:B:157:HIS:CD2	2.97	0.42
25:B:619:BCR:H20C	25:B:619:BCR:H361	1.85	0.42
7:H:30:LEU:H	31:H:105:DMS:C2	2.30	0.42
7:H:59:ASN:ND2	7:H:63:LYS:O	2.53	0.42
24:a:408:PHO:NC	24:a:408:PHO:ND	2.67	0.42
2:b:36:SER:OG	25:b:619:BCR:H362	2.20	0.42
2:b:410:THR:H	31:b:639:DMS:C2	2.32	0.42
3:c:406:SER:HA	3:c:420:VAL:HG23	2.02	0.42
23:c:907:CLA:HMB1	23:c:908:CLA:C4B	2.50	0.42
2:B:49:ASP:OD2	13:o:57:LYS:NZ	2.50	0.42
25:B:618:BCR:H382	25:B:618:BCR:H23C	2.02	0.42
3:C:158:THR:O	3:C:251:HIS:HB3	2.19	0.42
34:C:501:LMG:H221	36:C:517:DGD:HAW1	2.01	0.42
12:M:1:MET:N	41:M:203:HOH:O	2.53	0.42
2:b:467:ILE:HD12	2:b:467:ILE:HA	1.73	0.42
3:c:38:GLY:HA3	23:c:912:CLA:HMD2	2.01	0.42
3:c:79:LYS:HD2	16:v:35:TYR:CE2	2.55	0.42
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.02	0.42
23:C:512:CLA:H191	30:Z:101:LMT:H122	2.01	0.42
1:A:270:SER:OG	26:A:410:SQD:H3	2.19	0.41
17:Y:18:VAL:O	17:Y:22:LEU:HD12	2.20	0.41
34:a:413:LMG:H151	34:a:413:LMG:H182	1.35	0.41
2:b:382:PRO:HG2	2:b:385:ARG:HD2	2.02	0.41
30:b:621:LMT:H6E	4:d:19:ASP:OD2	2.20	0.41
23:C:510:CLA:H141	23:C:513:CLA:HMD3	2.02	0.41
25:D:405:BCR:HC22	36:D:407:DGD:HA92	2.02	0.41
6:F:30:THR:HG21	34:J:101:LMG:H412	2.02	0.41
7:H:30:LEU:N	31:H:105:DMS:H21	2.34	0.41
25:c:916:BCR:C8	25:c:916:BCR:H331	2.50	0.41
1:A:131:TRP:CD2	1:A:131:TRP:C	2.96	0.41
3:C:155[B]:ASN:OD1	3:C:255:THR:OG1	2.26	0.41
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.03	0.41
3:c:367:GLU:HB2	31:c:929:DMS:H22	2.02	0.41
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.96	0.41
31:A:422:DMS:H11	41:A:501:HOH:O	2.19	0.41
2:B:224:ARG:HG2	7:H:24:GLY:O	2.21	0.41
25:B:620:BCR:H20C	25:B:620:BCR:H361	1.93	0.41
25:D:405:BCR:C8	25:D:405:BCR:H331	2.50	0.41
13:O:58:ASN:C	13:O:58:ASN:ND2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:129:THR:HA	13:O:141:ASP:O	2.20	0.41
26:a:412:SQD:O7	3:c:28:GLN:NE2	2.37	0.41
25:c:915:BCR:C38	25:c:915:BCR:C23	2.98	0.41
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.02	0.41
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.41
3:C:215:LYS:HB2	3:C:223:TRP:HA	2.02	0.41
3:c:71:GLU:HB3	3:c:89:ILE:HD12	2.02	0.41
31:F:102:DMS:H13	41:J:214:HOH:O	2.14	0.41
19:Z:35:ARG:NH2	41:Z:1601:HOH:O	2.53	0.41
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.56	0.41
4:d:284:ILE:HD13	34:m:102:LMG:H241	2.03	0.41
2:B:472:ARG:HG2	31:D:416:DMS:H13	2.01	0.41
13:O:61:GLN:O	13:O:61:GLN:HG2	2.21	0.41
23:a:406:CLA:HBD	23:d:401:CLA:HAC2	2.01	0.41
30:a:422:LMT:H71	23:c:907:CLA:H52	2.02	0.41
18:x:23:LEU:HD23	18:x:23:LEU:HA	1.92	0.41
23:B:617:CLA:H41	23:B:617:CLA:H72	2.02	0.41
3:C:31:SER:HB2	3:C:41:ARG:HG2	2.02	0.41
23:C:503:CLA:HBD	23:C:504:CLA:H43	2.02	0.41
25:T:101:BCR:H321	25:T:101:BCR:C8	2.50	0.41
2:b:237:VAL:HG11	23:b:611:CLA:H201	2.02	0.41
2:b:462:PHE:CE1	23:b:614:CLA:HMB3	2.56	0.41
31:b:646:DMS:H11	41:b:1057[B]:HOH:O	2.20	0.41
25:j:104:BCR:C23	25:j:104:BCR:H382	2.51	0.41
24:D:402:PHO:NC	24:D:402:PHO:ND	2.67	0.41
25:D:405:BCR:H383	34:J:101:LMG:H171	2.01	0.41
1:a:79:THR:HG22	4:d:315:TYR:HB2	2.02	0.41
2:b:270:PRO:HG2	2:b:317:ASN:O	2.20	0.41
23:b:611:CLA:HHC	23:b:611:CLA:CBB	2.51	0.41
23:b:614:CLA:OBD	23:b:615:CLA:HHC	2.21	0.41
3:c:155[A]:ASN:HD22	3:c:155[A]:ASN:H	1.69	0.41
3:c:185:LEU:HB2	3:c:230:LEU:HD13	2.03	0.41
3:c:443:TRP:CZ2	23:c:909:CLA:HMD1	2.56	0.41
23:d:404:CLA:C19	18:x:15:LEU:HB2	2.50	0.41
13:o:181:GLU:OE1	13:o:181:GLU:N	2.49	0.41
16:v:90:GLU:HB3	31:v:209:DMS:H13	2.01	0.41
41:B:1104:HOH:O	31:H:101:DMS:H21	2.20	0.41
3:C:124:VAL:HB	25:C:515:BCR:H362	2.03	0.41
3:C:283:GLY:HA3	3:C:434:ALA:HB2	2.03	0.41
25:C:530:BCR:H24C	25:C:530:BCR:H371	1.71	0.41
1:a:310:LYS:NZ	41:a:511:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:407:CLA:H171	27:a:414:PL9:H262	2.03	0.41
23:c:909:CLA:H191	34:c:920:LMG:C25	2.51	0.41
23:C:506:CLA:HMB3	23:C:506:CLA:HBB1	2.02	0.40
36:D:407:DGD:HD2	36:D:407:DGD:HG32	1.87	0.40
13:O:25:THR:HG23	41:O:564:HOH:O	2.19	0.40
23:a:410:CLA:H71	8:i:13:THR:HG23	2.03	0.40
2:b:231:MET:HE2	23:b:611:CLA:HMC1	2.02	0.40
19:z:32:ASP:CG	19:z:35:ARG:HB3	2.46	0.40
23:D:403:CLA:HBC3	23:D:403:CLA:CHD	2.51	0.40
41:b:1034:HOH:O	31:u:206:DMS:H22	2.20	0.40
3:c:168:LEU:HD23	3:c:168:LEU:HA	1.92	0.40
34:m:102:LMG:HC3	30:m:103:LMT:H2'	2.03	0.40
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.46	0.40
3:C:334:PRO:HA	13:O:153:THR:OG1	2.21	0.40
25:c:916:BCR:H24C	25:c:916:BCR:H371	1.77	0.40
10:k:10:LYS:N	41:k:204:HOH:O	2.54	0.40
27:A:411:PL9:H531	27:A:411:PL9:H523	1.88	0.40
31:A:424:DMS:H21	35:b:627:HTG:O6	2.20	0.40
2:B:14:ASN:HA	31:B:638:DMS:H21	2.04	0.40
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.91	0.40
2:b:12:LEU:HB2	23:b:613:CLA:HMC2	2.03	0.40
2:b:498:LYS:HA	4:d:24:ARG:HA	2.02	0.40
23:b:615:CLA:H41	23:b:615:CLA:H62	1.78	0.40
2:B:71:VAL:HG21	2:B:96:VAL:HG21	2.04	0.40
3:C:142:GLU:CD	3:C:142:GLU:H	2.30	0.40
3:C:166:ILE:HB	23:C:513:CLA:H203	2.03	0.40
3:C:221:GLU:O	3:C:226:SER:HB3	2.20	0.40
13:O:59:LYS:O	13:O:60:ARG:CB	2.69	0.40
25:a:411:BCR:H24C	25:a:411:BCR:H371	1.79	0.40
23:b:602:CLA:H141	23:b:602:CLA:H162	1.87	0.40
25:b:620:BCR:C23	25:b:620:BCR:H383	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	333/344 (97%)	325 (98%)	7 (2%)	1 (0%)	36	26
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	36	26
2	B	507/505 (100%)	497 (98%)	10 (2%)	0	100	100
2	b	500/505 (99%)	490 (98%)	10 (2%)	0	100	100
3	C	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	43	34
3	c	454/455 (100%)	441 (97%)	12 (3%)	1 (0%)	43	34
4	D	342/342 (100%)	333 (97%)	8 (2%)	1 (0%)	36	26
4	d	342/342 (100%)	333 (97%)	9 (3%)	0	100	100
5	E	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
5	e	77/83 (93%)	76 (99%)	1 (1%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	229 (94%)	11 (4%)	3 (1%)	10	2
13	o	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	1
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	0
All	All	5210/5350 (97%)	5059 (97%)	140 (3%)	11 (0%)	43	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
19	Z	31	GLN
3	c	416	SER
19	z	31	GLN
3	C	416	SER
19	z	3	ILE
13	O	26	ALA
13	O	59	LYS
13	O	60	ARG
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	269/279 (96%)	268 (100%)	1 (0%)	84	79
1	a	272/279 (98%)	271 (100%)	1 (0%)	84	79
2	B	403/403 (100%)	398 (99%)	5 (1%)	63	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	394/403 (98%)	390 (99%)	4 (1%)	68	60
3	C	355/356 (100%)	353 (99%)	2 (1%)	78	72
3	c	356/356 (100%)	351 (99%)	5 (1%)	59	48
4	D	278/277 (100%)	275 (99%)	3 (1%)	65	56
4	d	278/277 (100%)	277 (100%)	1 (0%)	84	79
5	E	70/72 (97%)	68 (97%)	2 (3%)	37	20
5	e	68/72 (94%)	64 (94%)	4 (6%)	18	5
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	14
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	53 (96%)	2 (4%)	31	14
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	31/34 (91%)	31 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	26	10
9	j	27/28 (96%)	27 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	3
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	16
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	30/33 (91%)	29 (97%)	1 (3%)	33	16
12	m	30/33 (91%)	29 (97%)	1 (3%)	33	16
13	O	205/207 (99%)	202 (98%)	3 (2%)	57	46
13	o	203/207 (98%)	198 (98%)	5 (2%)	42	26
14	T	25/28 (89%)	24 (96%)	1 (4%)	28	11
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	11
15	U	82/89 (92%)	80 (98%)	2 (2%)	43	27
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	115 (98%)	3 (2%)	42	26
16	v	115/117 (98%)	114 (99%)	1 (1%)	70	63
17	Y	20/23 (87%)	19 (95%)	1 (5%)	22	7
17	y	19/23 (83%)	17 (90%)	2 (10%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	49/52 (94%)	46 (94%)	3 (6%)	17	4
19	z	46/52 (88%)	38 (83%)	8 (17%)	2	0
All	All	4255/4376 (97%)	4188 (98%)	67 (2%)	55	43

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	GLU
2	B	80	ILE
2	B	127	ARG
2	B	246	PHE
2	B	467	ILE
2	B	505	ARG
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	90	LEU
4	D	329	MET
5	E	4	THR
5	E	25	ILE
6	F	44	GLN
7	H	20	LYS
7	H	63	LYS
9	J	10	LEU
10	K	10	LYS
10	K	17	ILE
12	M	5	GLN
13	O	34	SER
13	O	58	ASN
13	O	69	LYS
14	T	2	GLU
15	U	10	VAL
15	U	58	VAL
16	V	30	LYS
16	V	86	GLN
16	V	122	GLU
17	Y	27	MET
19	Z	4	LEU
19	Z	21	ILE

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Mol	Chain	Res	Type
19	Z	35	ARG
1	a	162	PRO
2	b	80	ILE
2	b	128	THR
2	b	362	PHE
2	b	467	ILE
3	c	78	GLU
3	c	240	ILE
3	c	289	PHE
3	c	355	THR
3	c	416	SER
4	d	24	ARG
5	e	25	ILE
5	e	60	GLN
5	e	62	SER
5	e	68	ASP
10	k	27	VAL
12	m	9	ILE
13	o	23	ASP
13	o	58	ASN
13	o	118	LEU
13	o	159	PRO
13	o	181	GLU
14	t	2	GLU
16	v	6	GLU
17	y	23	THR
17	y	30	ILE
19	z	1	MET
19	z	4	LEU
19	z	5	PHE
19	z	6	GLN
19	z	7	LEU
19	z	20	VAL
19	z	29	SER
19	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
2	B	53	ASN
2	B	179	GLN

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Mol	Chain	Res	Type
2	B	331	ASN
3	C	44	ASN
3	C	415	ASN
3	C	418	ASN
4	D	186	GLN
4	D	255	GLN
11	L	6	ASN
13	O	58	ASN
13	O	82	GLN
13	O	155	ASN
16	V	34	GLN
19	Z	6	GLN
1	a	165	GLN
1	a	234	ASN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	331	ASN
2	b	374	ASN
3	c	44	ASN
3	c	201	ASN
3	c	322	GLN
4	d	186	GLN
4	d	255	GLN
4	d	332	GLN
6	f	44	GLN
7	h	59	ASN
13	o	36	GLN
13	o	82	GLN
13	o	155	ASN
13	o	231	HIS
15	u	73	GLN
16	v	34	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.53	0	7,9,11	1.70	2 (28%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	1.70	3 (42%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.04	0
8	FME	i	1	8	8,9,10	0.73	0	7,9,11	1.54	3 (42%)

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
14	FME	T	1	14	-	3/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CE-SD-CG	2.58	109.25	100.40
14	T	1	FME	O-C-CA	-2.49	118.27	124.78
14	t	1	FME	O-C-CA	-2.36	118.60	124.78
14	t	1	FME	CE-SD-CG	2.29	108.28	100.40
8	i	1	FME	O1-CN-N	-2.24	119.36	125.27
14	t	1	FME	C-CA-N	2.24	113.77	109.73
8	i	1	FME	C-CA-N	2.07	113.47	109.73
8	i	1	FME	O-C-CA	-2.01	119.50	124.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	N-CA-CB-CG
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	C-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE
8	I	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 366 ligands modelled in this entry, 13 are monoatomic and 53 are unknown - leaving 300 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	$\# Z > 2$
28	LHG	d	402	-	43,43,48	1.06	2 (4%)	46,49,54	0.96	3 (6%)
31	DMS	V	207	-	3,3,3	2.84	1 (33%)	3,3,3	1.25	0
28	LHG	d	410	-	45,45,48	1.00	2 (4%)	48,51,54	1.02	3 (6%)
31	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
23	CLA	b	603	2	69,73,73	2.10	22 (31%)	83,113,113	2.48	35 (42%)
31	DMS	B	645	-	3,3,3	2.80	1 (33%)	3,3,3	0.70	0
31	DMS	i	106	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
23	CLA	C	508	41	69,73,73	2.38	20 (28%)	83,113,113	2.48	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	D	405	-	41,41,41	1.10	4 (9%)	56,56,56	1.99	14 (25%)
31	DMS	V	202	-	3,3,3	2.66	1 (33%)	3,3,3	0.81	0
31	DMS	B	639	-	3,3,3	2.77	1 (33%)	3,3,3	0.89	0
36	DGD	c	919	-	63,63,67	0.94	3 (4%)	77,77,81	1.23	10 (12%)
26	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.60	7 (11%)
31	DMS	C	524	-	3,3,3	2.39	1 (33%)	3,3,3	0.94	0
31	DMS	a	420	-	3,3,3	2.65	1 (33%)	3,3,3	0.36	0
24	PHO	a	409	-	58,69,69	2.57	14 (24%)	56,99,99	3.10	17 (30%)
31	DMS	b	639	-	3,3,3	2.77	1 (33%)	3,3,3	1.33	1 (33%)
23	CLA	C	506	3	69,73,73	2.30	21 (30%)	83,113,113	2.19	25 (30%)
30	LMT	e	103	-	25,25,36	0.71	1 (4%)	30,30,47	1.02	3 (10%)
26	SQD	A	415	-	53,54,54	1.03	3 (5%)	62,65,65	1.91	12 (19%)
35	HTG	B	631	-	19,19,19	1.11	1 (5%)	23,24,24	1.25	2 (8%)
35	HTG	C	522	-	19,19,19	1.05	2 (10%)	23,24,24	1.95	4 (17%)
28	LHG	L	101	-	48,48,48	0.97	3 (6%)	51,54,54	1.13	3 (5%)
23	CLA	C	503	3	69,73,73	2.27	19 (27%)	83,113,113	2.14	25 (30%)
23	CLA	B	614	2	69,73,73	1.81	16 (23%)	83,113,113	2.43	27 (32%)
37	HEM	E	105	5,6	50,50,50	2.09	9 (18%)	66,82,82	1.66	11 (16%)
23	CLA	b	607	2	69,73,73	2.31	18 (26%)	83,113,113	2.35	29 (34%)
31	DMS	B	640	-	3,3,3	2.63	1 (33%)	3,3,3	0.77	0
31	DMS	v	202	-	3,3,3	2.60	1 (33%)	3,3,3	0.32	0
23	CLA	C	505	41	69,73,73	2.09	18 (26%)	83,113,113	2.59	28 (33%)
35	HTG	O	302	-	19,19,19	1.45	3 (15%)	23,24,24	1.51	5 (21%)
23	CLA	a	407	41	69,73,73	1.92	20 (28%)	83,113,113	2.37	25 (30%)
28	LHG	l	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.03	3 (5%)
30	LMT	m	104	-	36,36,36	0.56	0	47,47,47	1.24	4 (8%)
23	CLA	B	607	2	69,73,73	2.20	17 (24%)	83,113,113	2.61	26 (31%)
35	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.69	1 (4%)
23	CLA	b	610	2	69,73,73	2.52	19 (27%)	83,113,113	2.14	27 (32%)
25	BCR	b	620	-	41,41,41	0.90	2 (4%)	56,56,56	1.24	5 (8%)
30	LMT	M	101	-	36,36,36	0.64	0	47,47,47	0.92	2 (4%)
31	DMS	d	414	-	3,3,3	2.70	1 (33%)	3,3,3	0.77	0
31	DMS	d	415	-	3,3,3	2.65	1 (33%)	3,3,3	0.88	0
31	DMS	B	642	-	3,3,3	2.92	1 (33%)	3,3,3	1.28	0
31	DMS	H	101	-	3,3,3	2.78	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	c	917	-	63,63,67	0.84	3 (4%)	77,77,81	1.24	8 (10%)
31	DMS	b	644	-	3,3,3	2.78	1 (33%)	3,3,3	0.99	0
31	DMS	V	201	-	3,3,3	2.57	1 (33%)	3,3,3	0.76	0
35	HTG	b	627	-	19,19,19	1.22	2 (10%)	23,24,24	1.49	2 (8%)
24	PHO	D	402	-	58,69,69	2.55	12 (20%)	56,99,99	2.85	16 (28%)
31	DMS	B	641	-	3,3,3	2.82	1 (33%)	3,3,3	0.81	0
34	LMG	j	101	39	51,51,55	0.98	4 (7%)	59,59,63	1.16	7 (11%)
26	SQD	a	412	-	53,54,54	0.93	3 (5%)	62,65,65	2.14	13 (20%)
34	LMG	J	101	39	51,51,55	0.93	2 (3%)	59,59,63	0.97	4 (6%)
34	LMG	c	920	-	51,51,55	0.96	2 (3%)	59,59,63	1.31	7 (11%)
35	HTG	d	413	-	19,19,19	1.18	1 (5%)	23,24,24	2.11	5 (21%)
36	DGD	D	407	-	50,50,67	1.28	3 (6%)	58,58,81	1.74	8 (13%)
23	CLA	B	609	2	69,73,73	2.02	19 (27%)	83,113,113	2.28	27 (32%)
40	HEC	v	203	16	50,50,50	1.80	14 (28%)	68,82,82	1.63	13 (19%)
31	DMS	O	310	-	3,3,3	2.61	1 (33%)	3,3,3	0.71	0
23	CLA	C	507	3	69,73,73	2.15	21 (30%)	83,113,113	2.38	22 (26%)
31	DMS	c	928	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
23	CLA	a	406	1	69,73,73	1.89	17 (24%)	83,113,113	2.31	29 (34%)
27	PL9	D	406	-	55,55,55	1.02	3 (5%)	68,69,69	1.49	13 (19%)
25	BCR	B	618	-	41,41,41	1.06	1 (2%)	56,56,56	1.48	9 (16%)
31	DMS	B	646	-	3,3,3	2.60	1 (33%)	3,3,3	0.71	0
28	LHG	d	409	-	48,48,48	0.79	2 (4%)	51,54,54	1.28	8 (15%)
35	HTG	b	623	-	19,19,19	1.11	2 (10%)	23,24,24	1.79	4 (17%)
25	BCR	c	915	-	41,41,41	0.79	0	56,56,56	1.33	8 (14%)
31	DMS	v	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
40	HEC	V	203	16	50,50,50	1.89	11 (22%)	68,82,82	1.81	14 (20%)
26	SQD	D	408	-	44,45,54	1.22	4 (9%)	53,56,65	2.21	13 (24%)
28	LHG	a	415	-	48,48,48	1.01	2 (4%)	51,54,54	1.07	4 (7%)
31	DMS	b	646	-	3,3,3	2.74	1 (33%)	3,3,3	0.69	0
31	DMS	A	424	-	3,3,3	2.76	1 (33%)	3,3,3	1.08	0
31	DMS	u	206	-	3,3,3	2.79	1 (33%)	3,3,3	0.63	0
31	DMS	O	308	-	3,3,3	2.72	1 (33%)	3,3,3	0.69	0
38	RRX	H	102	-	42,42,42	0.89	1 (2%)	57,58,58	1.57	9 (15%)
35	HTG	c	922	-	19,19,19	1.02	2 (10%)	23,24,24	1.74	3 (13%)
26	SQD	a	417	-	53,54,54	1.10	5 (9%)	62,65,65	1.35	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OEX	A	401	1,41,3	0,14,14	-	-	-		
31	DMS	O	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
31	DMS	U	202	-	3,3,3	2.68	1 (33%)	3,3,3	1.60	1 (33%)
31	DMS	B	637	-	3,3,3	2.27	1 (33%)	3,3,3	0.96	0
31	DMS	b	645	-	3,3,3	2.69	1 (33%)	3,3,3	0.49	0
30	LMT	z	101	-	32,32,36	0.63	1 (3%)	42,42,47	1.19	5 (11%)
31	DMS	c	932	-	3,3,3	2.65	1 (33%)	3,3,3	0.75	0
36	DGD	h	102	-	63,63,67	0.93	3 (4%)	77,77,81	1.23	9 (11%)
31	DMS	o	301	-	3,3,3	2.14	1 (33%)	3,3,3	0.39	0
38	RRX	x	102	-	42,42,42	0.90	0	57,58,58	1.38	7 (12%)
23	CLA	c	909	3	69,73,73	2.27	20 (28%)	83,113,113	2.32	21 (25%)
25	BCR	C	515	-	41,41,41	0.83	0	56,56,56	1.50	10 (17%)
25	BCR	T	101	-	41,41,41	0.90	0	56,56,56	1.81	18 (32%)
35	HTG	B	625	-	19,19,19	1.41	3 (15%)	23,24,24	2.08	8 (34%)
31	DMS	A	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.71	0
31	DMS	C	528	-	3,3,3	2.64	1 (33%)	3,3,3	0.71	0
27	PL9	a	414	-	55,55,55	0.94	3 (5%)	68,69,69	1.65	16 (23%)
31	DMS	U	203	-	3,3,3	2.71	1 (33%)	3,3,3	0.51	0
23	CLA	b	602	41	69,73,73	2.82	21 (30%)	83,113,113	2.67	34 (40%)
31	DMS	c	927	-	3,3,3	2.71	1 (33%)	3,3,3	1.27	1 (33%)
31	DMS	A	418	-	3,3,3	2.73	1 (33%)	3,3,3	0.65	0
31	DMS	d	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
23	CLA	b	611	41	69,73,73	2.16	21 (30%)	83,113,113	2.20	25 (30%)
23	CLA	c	908	41	69,73,73	2.17	17 (24%)	83,113,113	2.43	27 (32%)
31	DMS	A	421	-	3,3,3	2.71	1 (33%)	3,3,3	0.80	0
23	CLA	b	613	2	69,73,73	2.09	18 (26%)	83,113,113	2.32	29 (34%)
31	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	1.00	0
23	CLA	b	608	41	69,73,73	2.16	21 (30%)	83,113,113	2.30	33 (39%)
25	BCR	A	409	-	41,41,41	1.06	4 (9%)	56,56,56	1.44	9 (16%)
23	CLA	D	404	4	69,73,73	2.05	20 (28%)	83,113,113	2.52	34 (40%)
31	DMS	c	934	-	3,3,3	2.70	1 (33%)	3,3,3	0.73	0
25	BCR	d	405	-	41,41,41	0.99	1 (2%)	56,56,56	1.93	19 (33%)
23	CLA	B	615	2	69,73,73	2.22	22 (31%)	83,113,113	2.73	32 (38%)
23	CLA	b	606	2	69,73,73	2.13	20 (28%)	83,113,113	2.44	27 (32%)
23	CLA	B	613	2	69,73,73	2.25	18 (26%)	83,113,113	2.27	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	l	102	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
31	DMS	F	102	-	3,3,3	2.61	1 (33%)	3,3,3	0.25	0
23	CLA	c	903	3	69,73,73	2.05	18 (26%)	83,113,113	2.55	36 (43%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.17	9 (16%)
30	LMT	A	416	-	36,36,36	0.84	1 (2%)	47,47,47	1.19	6 (12%)
31	DMS	v	209	-	3,3,3	2.71	1 (33%)	3,3,3	0.72	0
36	DGD	C	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.13	8 (10%)
31	DMS	a	401	-	3,3,3	2.71	1 (33%)	3,3,3	0.70	0
31	DMS	V	208	-	3,3,3	2.60	1 (33%)	3,3,3	0.41	0
23	CLA	b	614	2	69,73,73	1.97	17 (24%)	83,113,113	2.39	25 (30%)
23	CLA	A	408	1	69,73,73	2.00	16 (23%)	83,113,113	2.90	34 (40%)
25	BCR	Y	101	-	41,41,41	0.85	0	56,56,56	1.66	15 (26%)
23	CLA	D	403	4	69,73,73	2.12	16 (23%)	83,113,113	2.53	30 (36%)
31	DMS	O	309	-	3,3,3	2.88	1 (33%)	3,3,3	0.94	0
23	CLA	b	609	2	69,73,73	2.24	18 (26%)	83,113,113	2.22	29 (34%)
31	DMS	B	648	-	3,3,3	2.49	1 (33%)	3,3,3	1.05	0
35	HTG	b	628	-	19,19,19	0.90	1 (5%)	23,24,24	1.51	1 (4%)
36	DGD	C	518	-	63,63,67	0.95	4 (6%)	77,77,81	1.09	4 (5%)
35	HTG	c	921	-	19,19,19	0.95	2 (10%)	23,24,24	1.45	2 (8%)
23	CLA	C	504	3	69,73,73	2.43	24 (34%)	83,113,113	2.27	28 (33%)
31	DMS	C	525	-	3,3,3	2.62	1 (33%)	3,3,3	0.90	0
31	DMS	C	529	-	3,3,3	2.55	1 (33%)	3,3,3	0.44	0
31	DMS	O	304	-	3,3,3	2.79	1 (33%)	3,3,3	0.87	0
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.22	8 (10%)
23	CLA	B	616	2	69,73,73	2.27	21 (30%)	83,113,113	2.55	26 (31%)
31	DMS	B	636	-	3,3,3	3.09	1 (33%)	3,3,3	0.77	0
31	DMS	i	105	-	3,3,3	2.69	1 (33%)	3,3,3	0.88	0
31	DMS	c	935	-	3,3,3	2.68	1 (33%)	3,3,3	0.74	0
34	LMG	d	411	-	51,51,55	1.13	3 (5%)	59,59,63	1.32	6 (10%)
36	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.18	9 (11%)
31	DMS	u	203	-	3,3,3	2.58	1 (33%)	3,3,3	0.92	0
23	CLA	B	610	2	69,73,73	2.21	18 (26%)	83,113,113	2.23	25 (30%)
35	HTG	b	622	-	19,19,19	1.31	3 (15%)	23,24,24	1.51	4 (17%)
31	DMS	C	527	-	3,3,3	2.56	1 (33%)	3,3,3	0.63	0
23	CLA	c	902	3	69,73,73	2.13	19 (27%)	83,113,113	2.77	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	b	642	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
31	DMS	h	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
31	DMS	u	205	-	3,3,3	2.62	1 (33%)	3,3,3	1.05	0
26	SQD	L	102	-	53,54,54	1.08	3 (5%)	62,65,65	1.68	12 (19%)
31	DMS	e	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
36	DGD	d	407	-	50,50,67	1.11	2 (4%)	58,58,81	1.24	6 (10%)
31	DMS	A	423	-	3,3,3	1.91	1 (33%)	3,3,3	0.64	0
28	LHG	D	411	-	45,45,48	0.98	2 (4%)	48,51,54	1.03	4 (8%)
35	HTG	c	923	-	11,12,19	0.54	0	11,11,24	1.89	2 (18%)
23	CLA	B	603	2	69,73,73	2.21	21 (30%)	83,113,113	2.31	31 (37%)
31	DMS	c	929	-	3,3,3	2.83	1 (33%)	3,3,3	0.69	0
23	CLA	b	604	2	69,73,73	2.33	21 (30%)	83,113,113	2.38	31 (37%)
31	DMS	B	638	-	3,3,3	2.78	1 (33%)	3,3,3	1.01	0
23	CLA	C	512	3	69,73,73	2.43	21 (30%)	83,113,113	2.57	27 (32%)
31	DMS	B	647	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
34	LMG	B	622	-	51,51,55	0.99	3 (5%)	59,59,63	1.31	9 (15%)
35	HTG	B	630	-	19,19,19	0.98	2 (10%)	23,24,24	1.32	2 (8%)
31	DMS	b	643	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
27	PL9	A	411	-	55,55,55	0.90	4 (7%)	68,69,69	1.69	14 (20%)
37	HEM	e	105	5,6	50,50,50	2.06	11 (22%)	66,82,82	1.48	10 (15%)
31	DMS	v	208	-	3,3,3	2.73	1 (33%)	3,3,3	0.73	0
34	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.15	4 (6%)
34	LMG	D	412	-	51,51,55	1.10	2 (3%)	59,59,63	1.34	8 (13%)
23	CLA	c	905	41	69,73,73	2.27	20 (28%)	83,113,113	2.81	31 (37%)
26	SQD	x	101	-	40,41,54	1.26	3 (7%)	49,52,65	1.46	9 (18%)
31	DMS	h	101	-	3,3,3	2.68	1 (33%)	3,3,3	1.34	1 (33%)
23	CLA	A	406	41	69,73,73	1.81	19 (27%)	83,113,113	2.70	27 (32%)
25	BCR	B	620	-	41,41,41	1.00	2 (4%)	56,56,56	1.57	13 (23%)
23	CLA	c	904	3	69,73,73	2.70	21 (30%)	83,113,113	2.36	27 (32%)
31	DMS	c	937	-	3,3,3	2.66	1 (33%)	3,3,3	0.62	0
31	DMS	O	311	-	3,3,3	2.64	1 (33%)	3,3,3	0.85	0
35	HTG	B	624	-	19,19,19	1.52	3 (15%)	23,24,24	1.56	4 (17%)
25	BCR	C	530	-	41,41,41	0.84	0	56,56,56	1.56	8 (14%)
23	CLA	C	513	3	69,73,73	2.59	20 (28%)	83,113,113	2.25	27 (32%)
23	CLA	C	502	3	69,73,73	2.29	19 (27%)	83,113,113	2.29	23 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LHG	K	101	-	43,43,48	1.07	2 (4%)	47,48,54	1.14	5 (10%)
30	LMT	B	643	-	24,24,36	0.39	0	29,29,47	0.88	1 (3%)
30	LMT	I	101	-	36,36,36	0.74	1 (2%)	47,47,47	1.40	5 (10%)
31	DMS	O	305	-	3,3,3	2.66	1 (33%)	3,3,3	0.88	0
31	DMS	D	416	-	3,3,3	2.49	1 (33%)	3,3,3	0.88	0
30	LMT	T	103	-	24,24,36	0.50	0	29,29,47	1.32	4 (13%)
31	DMS	U	204	-	3,3,3	2.88	1 (33%)	3,3,3	0.80	0
30	LMT	Z	101	-	36,36,36	0.70	1 (2%)	47,47,47	0.90	2 (4%)
28	LHG	e	101	-	39,39,48	1.16	2 (5%)	42,45,54	1.02	3 (7%)
31	DMS	O	307	-	3,3,3	2.75	1 (33%)	3,3,3	0.72	0
31	DMS	b	638	-	3,3,3	2.93	1 (33%)	3,3,3	1.08	0
23	CLA	D	401	41	69,73,73	2.12	21 (30%)	83,113,113	2.06	23 (27%)
23	CLA	c	906	3	69,73,73	2.22	24 (34%)	83,113,113	2.22	29 (34%)
34	LMG	C	520	-	51,51,55	1.15	2 (3%)	59,59,63	1.35	9 (15%)
34	LMG	a	413	-	51,51,55	1.00	2 (3%)	59,59,63	1.10	4 (6%)
35	HTG	B	626	-	19,19,19	0.94	1 (5%)	23,24,24	1.59	1 (4%)
31	DMS	v	206	-	3,3,3	2.60	1 (33%)	3,3,3	0.81	0
31	DMS	d	419	-	3,3,3	2.69	1 (33%)	3,3,3	0.71	0
28	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.24	3 (5%)
23	CLA	C	511	3	69,73,73	2.30	17 (24%)	83,113,113	2.19	27 (32%)
28	LHG	D	410	-	48,48,48	0.83	2 (4%)	51,54,54	1.13	2 (3%)
23	CLA	d	404	4	69,73,73	1.97	22 (31%)	83,113,113	2.73	33 (39%)
23	CLA	B	605	2	69,73,73	2.14	21 (30%)	83,113,113	2.13	25 (30%)
28	LHG	E	101	-	48,48,48	1.06	2 (4%)	51,54,54	1.17	5 (9%)
30	LMT	B	623	-	36,36,36	0.59	0	47,47,47	1.05	3 (6%)
31	DMS	b	634	-	3,3,3	2.45	1 (33%)	3,3,3	0.96	0
31	DMS	b	636	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
34	LMG	c	930	-	51,51,55	1.07	3 (5%)	59,59,63	1.26	5 (8%)
34	LMG	m	102	-	51,51,55	0.95	2 (3%)	59,59,63	1.33	6 (10%)
35	HTG	V	204	-	14,14,19	0.67	0	18,19,24	3.10	6 (33%)
23	CLA	A	405	1	69,73,73	1.96	17 (24%)	83,113,113	2.34	29 (34%)
23	CLA	C	509	3	69,73,73	2.28	19 (27%)	83,113,113	2.49	25 (30%)
24	PHO	A	407	-	58,69,69	2.18	14 (24%)	56,99,99	3.07	15 (26%)
31	DMS	v	207	-	3,3,3	2.72	1 (33%)	3,3,3	0.75	0
24	PHO	a	408	-	58,69,69	2.26	14 (24%)	56,99,99	2.59	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	401	41	69,73,73	1.97	14 (20%)	83,113,113	2.42	29 (34%)
23	CLA	B	608	41	69,73,73	2.05	16 (23%)	83,113,113	2.35	30 (36%)
31	DMS	V	211	-	3,3,3	2.97	1 (33%)	3,3,3	1.05	0
31	DMS	C	533	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
23	CLA	B	617	2	69,73,73	2.01	20 (28%)	83,113,113	2.51	34 (40%)
31	DMS	b	640	-	3,3,3	2.70	1 (33%)	3,3,3	0.83	0
30	LMT	B	644	-	24,24,36	0.34	0	29,29,47	1.26	4 (13%)
35	HTG	C	523	-	19,19,19	1.09	2 (10%)	23,24,24	1.74	1 (4%)
25	BCR	t	101	-	41,41,41	1.03	0	56,56,56	1.52	14 (25%)
23	CLA	d	403	4	69,73,73	1.91	17 (24%)	83,113,113	2.14	25 (30%)
31	DMS	v	201	-	3,3,3	2.42	1 (33%)	3,3,3	0.47	0
31	DMS	D	417	-	3,3,3	2.99	1 (33%)	3,3,3	0.77	0
35	HTG	D	414	-	19,19,19	0.94	1 (5%)	23,24,24	1.31	1 (4%)
32	BCT	a	424	21	2,3,3	0.66	0	2,3,3	1.00	0
32	BCT	A	420	21	2,3,3	0.48	0	2,3,3	1.16	0
31	DMS	b	633	-	3,3,3	1.83	1 (33%)	3,3,3	0.60	0
23	CLA	B	602	41	69,73,73	2.38	16 (23%)	83,113,113	2.72	28 (33%)
26	SQD	A	410	-	53,54,54	0.99	3 (5%)	62,65,65	2.00	17 (27%)
31	DMS	c	924	-	3,3,3	2.36	1 (33%)	3,3,3	0.42	0
34	LMG	C	531	-	51,51,55	1.03	2 (3%)	59,59,63	1.08	4 (6%)
31	DMS	a	421	-	3,3,3	2.68	1 (33%)	3,3,3	0.63	0
28	LHG	A	412	-	48,48,48	1.05	2 (4%)	51,54,54	0.96	3 (5%)
31	DMS	b	647	-	3,3,3	2.75	1 (33%)	3,3,3	0.71	0
30	LMT	b	621	-	25,25,36	0.63	1 (4%)	30,30,47	1.30	5 (16%)
31	DMS	C	526	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
31	DMS	D	415	-	3,3,3	2.74	1 (33%)	3,3,3	0.69	0
30	LMT	F	101	-	36,36,36	0.71	1 (2%)	47,47,47	1.19	5 (10%)
23	CLA	B	606	2	69,73,73	2.07	19 (27%)	83,113,113	2.39	26 (31%)
31	DMS	c	933	-	3,3,3	2.67	1 (33%)	3,3,3	0.93	0
31	DMS	u	204	-	3,3,3	2.76	1 (33%)	3,3,3	0.87	0
23	CLA	c	912	3	69,73,73	2.49	21 (30%)	83,113,113	2.39	25 (30%)
31	DMS	V	209	-	3,3,3	2.52	1 (33%)	3,3,3	0.80	0
23	CLA	C	514	3	69,73,73	2.58	22 (31%)	83,113,113	2.32	24 (28%)
23	CLA	a	410	1	69,73,73	2.00	17 (24%)	83,113,113	2.37	30 (36%)
31	DMS	V	205	-	3,3,3	2.63	1 (33%)	3,3,3	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	617	2	69,73,73	2.26	21 (30%)	83,113,113	2.14	27 (32%)
31	DMS	V	210	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
31	DMS	h	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.58	0
31	DMS	B	649	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
31	DMS	V	206	-	3,3,3	2.65	1 (33%)	3,3,3	0.77	0
23	CLA	B	612	2	69,73,73	2.05	16 (23%)	83,113,113	2.38	27 (32%)
23	CLA	C	510	3	69,73,73	2.27	17 (24%)	83,113,113	2.56	30 (36%)
30	LMT	a	418	-	36,36,36	0.71	1 (2%)	47,47,47	1.30	6 (12%)
28	LHG	D	409	-	48,48,48	0.85	1 (2%)	51,54,54	1.27	6 (11%)
23	CLA	b	615	2	69,73,73	2.10	19 (27%)	83,113,113	2.57	30 (36%)
31	DMS	h	105	-	3,3,3	2.74	1 (33%)	3,3,3	0.68	0
31	DMS	b	637	-	3,3,3	2.68	1 (33%)	3,3,3	1.01	0
23	CLA	c	910	3	69,73,73	2.46	20 (28%)	83,113,113	2.78	30 (36%)
20	OEX	a	402	1,41,3	0,14,14	-	-	-	-	-
31	DMS	k	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.78	0
31	DMS	O	306	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
35	HTG	v	204	-	19,19,19	0.90	1 (5%)	23,24,24	2.78	8 (34%)
23	CLA	B	604	2	69,73,73	1.94	18 (26%)	83,113,113	2.68	31 (37%)
25	BCR	c	916	-	41,41,41	0.81	0	56,56,56	1.56	10 (17%)
31	DMS	H	105	-	3,3,3	2.74	1 (33%)	3,3,3	0.65	0
23	CLA	c	913	3	69,73,73	2.46	21 (30%)	83,113,113	2.58	27 (32%)
36	DGD	H	103	-	63,63,67	1.05	3 (4%)	77,77,81	1.32	7 (9%)
25	BCR	C	516	-	41,41,41	0.99	0	56,56,56	1.37	7 (12%)
23	CLA	c	914	3	69,73,73	2.51	21 (30%)	83,113,113	2.37	25 (30%)
23	CLA	b	616	2	69,73,73	2.10	18 (26%)	83,113,113	2.23	27 (32%)
30	LMT	a	422	-	36,36,36	0.65	1 (2%)	47,47,47	0.95	3 (6%)
31	DMS	A	422	-	3,3,3	2.68	1 (33%)	3,3,3	0.84	0
25	BCR	b	618	-	41,41,41	0.95	0	56,56,56	1.75	13 (23%)
31	DMS	c	925	-	3,3,3	2.81	1 (33%)	3,3,3	0.84	0
31	DMS	c	926	-	3,3,3	2.61	1 (33%)	3,3,3	0.30	0
31	DMS	a	423	-	3,3,3	2.80	1 (33%)	3,3,3	0.82	0
31	DMS	c	936	-	3,3,3	2.73	1 (33%)	3,3,3	0.83	0
23	CLA	c	907	3	69,73,73	2.52	19 (27%)	83,113,113	2.41	30 (36%)
23	CLA	c	911	3	69,73,73	2.21	19 (27%)	83,113,113	2.55	30 (36%)
23	CLA	b	612	2	69,73,73	2.09	14 (20%)	83,113,113	2.47	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	611	41	69,73,73	2.32	23 (33%)	83,113,113	2.45	28 (33%)
25	BCR	a	411	-	41,41,41	1.20	3 (7%)	56,56,56	1.35	5 (8%)
31	DMS	o	304	-	3,3,3	2.76	1 (33%)	3,3,3	0.81	0
31	DMS	b	635	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
25	BCR	k	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.21	8 (14%)
31	DMS	b	641	-	3,3,3	2.64	1 (33%)	3,3,3	0.75	0
25	BCR	j	104	-	41,41,41	0.82	0	56,56,56	1.48	11 (19%)
31	DMS	d	418	-	3,3,3	2.75	1 (33%)	3,3,3	0.62	0
30	LMT	m	103	-	36,36,36	0.61	1 (2%)	47,47,47	0.98	3 (6%)
23	CLA	b	605	2	69,73,73	2.08	19 (27%)	83,113,113	2.33	27 (32%)
27	PL9	d	406	-	55,55,55	1.05	4 (7%)	68,69,69	1.59	12 (17%)
25	BCR	b	619	-	41,41,41	1.03	2 (4%)	56,56,56	1.34	7 (12%)

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
28	LHG	d	402	-	-	24/48/48/53	-
28	LHG	d	410	-	-	11/50/50/53	-
23	CLA	b	603	2	-	2/39/115/115	-
23	CLA	C	508	41	-	11/39/115/115	-
25	BCR	D	405	-	-	4/29/63/63	0/2/2/2
36	DGD	c	919	-	-	15/51/91/95	0/2/2/2
26	SQD	B	621	-	-	29/49/69/69	0/1/1/1
24	PHO	a	409	-	-	4/37/103/103	0/5/6/6
23	CLA	C	506	3	-	2/39/115/115	-
30	LMT	e	103	-	-	6/17/37/61	0/1/1/2
26	SQD	A	415	-	-	24/49/69/69	0/1/1/1
35	HTG	B	631	-	-	3/10/30/30	0/1/1/1
35	HTG	C	522	-	-	5/10/30/30	0/1/1/1
28	LHG	L	101	-	-	18/53/53/53	-
23	CLA	C	503	3	-	6/39/115/115	-
23	CLA	B	614	2	-	6/39/115/115	-
37	HEM	E	105	5,6	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	607	2	-	12/39/115/115	-
23	CLA	C	505	41	-	9/39/115/115	-
23	CLA	a	407	41	-	9/39/115/115	-
28	LHG	l	101	-	-	13/53/53/53	-
30	LMT	m	104	-	-	2/21/61/61	0/2/2/2
23	CLA	B	607	2	-	8/39/115/115	-
35	HTG	C	521	-	-	3/10/30/30	0/1/1/1
23	CLA	b	610	2	-	0/39/115/115	-
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
24	PHO	D	402	-	-	2/37/103/103	0/5/6/6
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1
26	SQD	a	412	-	-	23/49/69/69	0/1/1/1
34	LMG	J	101	39	-	15/46/66/70	0/1/1/1
35	HTG	d	413	-	-	7/10/30/30	0/1/1/1
36	DGD	D	407	-	-	24/44/64/95	0/1/1/2
23	CLA	B	609	2	-	1/39/115/115	-
40	HEC	v	203	16	1/1/3/7	4/14/54/54	-
23	CLA	C	507	3	-	16/39/115/115	-
23	CLA	a	406	1	-	6/39/115/115	-
27	PL9	D	406	-	-	3/53/73/73	0/1/1/1
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	LHG	d	409	-	-	10/53/53/53	-
35	HTG	b	623	-	-	8/10/30/30	0/1/1/1
25	BCR	c	915	-	-	1/29/63/63	0/2/2/2
40	HEC	V	203	16	1/1/3/7	6/14/54/54	-
26	SQD	D	408	-	-	19/40/60/69	0/1/1/1
28	LHG	a	415	-	-	20/53/53/53	-
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
35	HTG	c	922	-	-	4/10/30/30	0/1/1/1
26	SQD	a	417	-	-	14/49/69/69	0/1/1/1
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
36	DGD	h	102	-	-	17/51/91/95	0/2/2/2
38	RRX	x	102	-	-	0/29/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	909	3	-	4/39/115/115	-
25	BCR	C	515	-	-	3/29/63/63	0/2/2/2
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
27	PL9	a	414	-	-	11/53/73/73	0/1/1/1
23	CLA	b	602	41	-	18/39/115/115	-
23	CLA	b	611	41	-	7/39/115/115	-
23	CLA	c	908	41	-	10/39/115/115	-
23	CLA	b	613	2	-	3/39/115/115	-
23	CLA	b	608	41	-	2/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	D	404	4	-	11/39/115/115	-
25	BCR	d	405	-	-	4/29/63/63	0/2/2/2
23	CLA	B	615	2	-	9/39/115/115	-
23	CLA	b	606	2	-	6/39/115/115	-
23	CLA	B	613	2	-	2/39/115/115	-
23	CLA	c	903	3	-	8/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	LMT	A	416	-	-	7/21/61/61	0/2/2/2
36	DGD	C	519	-	-	18/51/91/95	0/2/2/2
23	CLA	b	614	2	-	3/39/115/115	-
23	CLA	A	408	1	-	18/39/115/115	-
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
23	CLA	D	403	4	-	7/39/115/115	-
35	HTG	b	628	-	-	1/10/30/30	0/1/1/1
23	CLA	b	609	2	-	1/39/115/115	-
36	DGD	C	518	-	-	14/51/91/95	0/2/2/2
35	HTG	c	921	-	-	5/10/30/30	0/1/1/1
23	CLA	C	504	3	-	3/39/115/115	-
36	DGD	C	517	-	-	13/51/91/95	0/2/2/2
23	CLA	B	616	2	-	5/39/115/115	-
36	DGD	c	918	-	-	16/51/91/95	0/2/2/2
34	LMG	d	411	-	-	25/46/66/70	0/1/1/1
23	CLA	B	610	2	-	2/39/115/115	-
35	HTG	b	622	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	902	3	-	5/39/115/115	-
26	SQD	L	102	-	-	27/49/69/69	0/1/1/1
36	DGD	d	407	-	-	22/44/64/95	0/1/1/2
28	LHG	D	411	-	-	15/50/50/53	-
35	HTG	c	923	-	-	4/8/10/30	-
23	CLA	B	603	2	-	4/39/115/115	-
23	CLA	b	604	2	-	5/39/115/115	-
23	CLA	C	512	3	-	0/39/115/115	-
34	LMG	B	622	-	-	15/46/66/70	0/1/1/1
35	HTG	B	630	-	-	4/10/30/30	0/1/1/1
27	PL9	A	411	-	-	14/53/73/73	0/1/1/1
37	HEM	e	105	5,6	-	3/14/54/54	-
34	LMG	C	501	-	-	24/46/66/70	0/1/1/1
23	CLA	c	905	41	-	9/39/115/115	-
26	SQD	x	101	-	-	19/36/56/69	0/1/1/1
23	CLA	A	406	41	-	11/39/115/115	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
23	CLA	c	904	3	-	4/39/115/115	-
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
25	BCR	C	530	-	-	0/29/63/63	0/2/2/2
23	CLA	C	513	3	-	14/39/115/115	-
23	CLA	C	502	3	-	5/39/115/115	-
28	LHG	K	101	-	-	24/45/45/53	-
30	LMT	B	643	-	-	6/15/35/61	0/1/1/2
30	LMT	I	101	-	-	8/21/61/61	0/2/2/2
34	LMG	c	920	-	-	21/46/66/70	0/1/1/1
36	DGD	c	917	-	-	13/51/91/95	0/2/2/2
30	LMT	T	103	-	-	7/15/35/61	0/1/1/2
34	LMG	C	520	-	-	20/46/66/70	0/1/1/1
30	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
28	LHG	e	101	-	-	18/44/44/53	-
35	HTG	B	626	-	-	7/10/30/30	0/1/1/1
23	CLA	D	401	41	-	4/39/115/115	-
23	CLA	c	906	3	-	4/39/115/115	-
34	LMG	a	413	-	-	24/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	d	408	-	-	14/53/53/53	-
23	CLA	C	511	3	-	2/39/115/115	-
28	LHG	D	410	-	-	10/53/53/53	-
23	CLA	d	404	4	-	13/39/115/115	-
23	CLA	B	605	2	-	8/39/115/115	-
28	LHG	E	101	-	-	28/53/53/53	-
30	LMT	B	623	-	-	15/21/61/61	0/2/2/2
34	LMG	c	930	-	-	7/46/66/70	0/1/1/1
34	LMG	m	102	-	-	18/46/66/70	0/1/1/1
35	HTG	V	204	-	-	1/5/25/30	0/1/1/1
23	CLA	A	405	1	-	2/39/115/115	-
23	CLA	C	509	3	-	6/39/115/115	-
24	PHO	A	407	-	-	3/37/103/103	0/5/6/6
24	PHO	a	408	-	-	6/37/103/103	0/5/6/6
23	CLA	d	401	41	-	7/39/115/115	-
23	CLA	B	608	41	-	3/39/115/115	-
23	CLA	B	617	2	-	11/39/115/115	-
30	LMT	B	644	-	-	8/15/35/61	0/1/1/2
35	HTG	C	523	-	-	4/10/30/30	0/1/1/1
25	BCR	t	101	-	-	4/29/63/63	0/2/2/2
23	CLA	d	403	4	-	3/39/115/115	-
35	HTG	D	414	-	-	3/10/30/30	0/1/1/1
23	CLA	B	602	41	-	21/39/115/115	-
26	SQD	A	410	-	-	20/49/69/69	0/1/1/1
34	LMG	C	531	-	-	18/46/66/70	0/1/1/1
28	LHG	A	412	-	-	29/53/53/53	-
30	LMT	b	621	-	-	12/17/37/61	0/1/1/2
30	LMT	F	101	-	-	11/21/61/61	0/2/2/2
23	CLA	B	606	2	-	6/39/115/115	-
23	CLA	c	912	3	-	1/39/115/115	-
23	CLA	C	514	3	-	9/39/115/115	-
23	CLA	a	410	1	-	8/39/115/115	-
23	CLA	b	617	2	-	19/39/115/115	-
23	CLA	B	612	2	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	510	3	-	9/39/115/115	-
30	LMT	a	418	-	-	12/21/61/61	0/2/2/2
28	LHG	D	409	-	-	9/53/53/53	-
23	CLA	b	615	2	-	13/39/115/115	-
23	CLA	c	910	3	-	9/39/115/115	-
35	HTG	v	204	-	-	7/10/30/30	0/1/1/1
23	CLA	B	604	2	-	3/39/115/115	-
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
23	CLA	c	913	3	-	7/39/115/115	-
36	DGD	H	103	-	-	10/51/91/95	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	c	914	3	-	9/39/115/115	-
23	CLA	b	616	2	-	8/39/115/115	-
30	LMT	a	422	-	-	5/21/61/61	0/2/2/2
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
23	CLA	c	907	3	-	10/39/115/115	-
23	CLA	c	911	3	-	3/39/115/115	-
23	CLA	b	612	2	-	6/39/115/115	-
23	CLA	B	611	41	-	5/39/115/115	-
25	BCR	a	411	-	-	1/29/63/63	0/2/2/2
35	HTG	O	302	-	-	3/10/30/30	0/1/1/1
25	BCR	k	102	-	-	2/29/63/63	0/2/2/2
34	LMG	D	412	-	-	24/46/66/70	0/1/1/1
25	BCR	j	104	-	-	2/29/63/63	0/2/2/2
30	LMT	m	103	-	-	10/21/61/61	0/2/2/2
23	CLA	b	605	2	-	5/39/115/115	-
27	PL9	d	406	-	-	4/53/73/73	0/1/1/1
25	BCR	b	619	-	-	1/29/63/63	0/2/2/2

All (1744) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	914	CLA	MG-NA	12.47	2.35	2.06
23	c	904	CLA	MG-NA	12.19	2.35	2.06
23	b	607	CLA	MG-NA	11.84	2.34	2.06
23	b	610	CLA	MG-NA	11.72	2.34	2.06
23	B	602	CLA	MG-NA	11.01	2.32	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	MG-NB	-10.79	1.84	2.05
23	c	913	CLA	MG-NA	10.78	2.31	2.06
23	C	512	CLA	MG-NA	10.61	2.31	2.06
23	C	513	CLA	MG-NA	10.55	2.31	2.06
23	C	514	CLA	MG-NA	10.20	2.30	2.06
23	c	910	CLA	MG-NA	10.17	2.30	2.06
23	C	510	CLA	MG-NA	9.93	2.29	2.06
23	c	908	CLA	MG-NA	9.90	2.29	2.06
23	c	907	CLA	MG-ND	-9.85	1.86	2.05
23	b	604	CLA	MG-NA	9.77	2.29	2.06
23	C	503	CLA	MG-NA	9.77	2.29	2.06
23	b	602	CLA	MG-ND	9.75	2.25	2.05
23	B	613	CLA	MG-NA	9.62	2.29	2.06
23	c	912	CLA	MG-NC	9.61	2.29	2.06
23	c	905	CLA	MG-NA	9.50	2.28	2.06
23	B	607	CLA	MG-NA	9.46	2.28	2.06
23	c	911	CLA	MG-ND	-9.46	1.87	2.05
23	c	902	CLA	MG-NA	9.36	2.28	2.06
23	B	611	CLA	MG-NA	9.06	2.27	2.06
23	C	509	CLA	MG-NA	8.91	2.27	2.06
24	a	409	PHO	C1D-C2D	8.91	1.49	1.39
23	b	612	CLA	MG-NA	8.74	2.27	2.06
24	A	407	PHO	C1D-C2D	8.72	1.49	1.39
24	D	402	PHO	C1B-C2B	8.70	1.49	1.39
23	c	907	CLA	MG-NB	8.65	2.22	2.05
23	B	612	CLA	MG-NA	8.48	2.26	2.06
23	C	508	CLA	MG-NC	8.44	2.26	2.06
23	B	608	CLA	MG-NA	8.43	2.26	2.06
24	a	409	PHO	C1B-C2B	8.41	1.48	1.39
23	B	605	CLA	MG-NA	8.39	2.26	2.06
37	e	105	HEM	C3D-C2D	8.35	1.54	1.36
23	b	615	CLA	MG-NA	8.33	2.26	2.06
23	d	401	CLA	MG-NA	8.24	2.25	2.06
23	C	511	CLA	MG-NA	8.11	2.25	2.06
23	D	403	CLA	MG-NA	8.11	2.25	2.06
24	a	408	PHO	C1B-C2B	7.95	1.48	1.39
23	B	616	CLA	MG-NA	7.92	2.25	2.06
23	C	504	CLA	MG-NC	7.90	2.25	2.06
23	c	906	CLA	MG-NA	7.85	2.24	2.06
24	D	402	PHO	C1D-C2D	7.83	1.48	1.39
23	B	603	CLA	MG-NA	7.81	2.24	2.06
24	a	408	PHO	C1D-C2D	7.70	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	MG-NA	7.67	2.24	2.06
23	B	606	CLA	MG-NA	7.67	2.24	2.06
23	C	502	CLA	MG-NC	7.66	2.24	2.06
37	E	105	HEM	FE-NC	7.42	2.20	1.95
23	c	903	CLA	MG-NA	7.36	2.23	2.06
23	c	909	CLA	MG-NA	7.31	2.23	2.06
23	B	610	CLA	MG-NA	7.29	2.23	2.06
23	b	605	CLA	MG-NA	7.27	2.23	2.06
37	E	105	HEM	C3D-C2D	7.11	1.51	1.36
23	B	610	CLA	MG-NB	6.89	2.19	2.05
40	v	203	HEC	C3D-C2D	6.88	1.51	1.36
23	C	505	CLA	MG-NA	6.75	2.22	2.06
23	b	613	CLA	MG-NA	6.70	2.22	2.06
23	C	507	CLA	MG-NA	6.68	2.22	2.06
23	b	602	CLA	MG-NC	6.60	2.21	2.06
23	C	513	CLA	MG-NB	6.57	2.18	2.05
23	C	506	CLA	MG-NA	6.55	2.21	2.06
23	D	404	CLA	MG-NC	6.47	2.21	2.06
23	c	904	CLA	MG-NC	6.47	2.21	2.06
23	C	502	CLA	MG-NB	6.44	2.18	2.05
23	A	406	CLA	MG-NA	6.43	2.21	2.06
23	D	401	CLA	CHD-C4C	6.39	1.53	1.39
23	C	508	CLA	MG-NA	6.37	2.21	2.06
23	C	513	CLA	C3C-C2C	6.33	1.50	1.36
23	b	610	CLA	MG-NB	6.27	2.18	2.05
23	c	910	CLA	MG-ND	-6.18	1.93	2.05
23	B	615	CLA	MG-NA	6.18	2.20	2.06
23	c	907	CLA	MG-NA	6.16	2.20	2.06
23	b	609	CLA	MG-NA	6.15	2.20	2.06
23	A	408	CLA	MG-ND	-6.11	1.93	2.05
23	b	617	CLA	MG-NA	6.10	2.20	2.06
23	c	913	CLA	MG-NB	6.10	2.17	2.05
23	A	405	CLA	MG-ND	-6.09	1.93	2.05
24	a	409	PHO	C3B-C4B	6.08	1.48	1.41
23	b	608	CLA	MG-NA	6.08	2.20	2.06
23	b	617	CLA	MG-NC	6.04	2.20	2.06
23	B	614	CLA	MG-NA	6.02	2.20	2.06
23	a	407	CLA	MG-NA	6.00	2.20	2.06
40	V	203	HEC	FE-NB	5.97	2.13	1.94
23	C	514	CLA	MG-ND	5.94	2.17	2.05
24	D	402	PHO	C3B-C2B	5.93	1.48	1.40
24	A	407	PHO	C1B-C2B	5.90	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C4B-NB	-5.88	1.30	1.37
23	b	604	CLA	CHC-C1C	5.87	1.50	1.38
23	a	410	CLA	CHC-C1C	5.84	1.50	1.38
23	B	607	CLA	C3C-C2C	5.82	1.49	1.36
23	b	609	CLA	CHC-C1C	5.81	1.50	1.38
23	c	904	CLA	CHC-C1C	5.81	1.50	1.38
23	c	904	CLA	C3C-C2C	5.79	1.49	1.36
23	C	513	CLA	O2D-CGD	5.78	1.47	1.33
23	B	609	CLA	MG-NC	5.75	2.19	2.06
23	C	511	CLA	MG-NB	5.73	2.17	2.05
23	d	403	CLA	MG-NA	5.72	2.19	2.06
23	c	909	CLA	MG-NC	5.71	2.19	2.06
23	C	504	CLA	CHC-C1C	5.71	1.50	1.38
23	a	406	CLA	MG-NA	5.71	2.19	2.06
23	C	514	CLA	C3C-C2C	5.65	1.48	1.36
23	c	912	CLA	MG-ND	5.64	2.17	2.05
23	b	610	CLA	CHC-C1C	5.63	1.50	1.38
23	b	614	CLA	MG-NA	5.60	2.19	2.06
23	c	910	CLA	OBD-CAD	5.59	1.32	1.22
23	B	616	CLA	O2D-CGD	5.57	1.46	1.33
23	c	913	CLA	C3C-C2C	5.57	1.48	1.36
23	C	512	CLA	MG-NB	-5.56	1.94	2.05
23	C	510	CLA	C3C-C2C	5.56	1.48	1.36
23	B	603	CLA	CHD-C1D	5.55	1.49	1.38
23	b	602	CLA	MG-NA	5.54	2.19	2.06
24	D	402	PHO	C3D-C4D	-5.54	1.33	1.41
23	B	615	CLA	CHD-C1D	5.54	1.49	1.38
23	b	608	CLA	MG-NC	5.52	2.19	2.06
23	d	404	CLA	MG-NA	5.51	2.19	2.06
23	b	602	CLA	O2A-CGA	5.49	1.49	1.33
24	a	409	PHO	C3A-C2A	-5.49	1.49	1.54
23	b	605	CLA	C3C-C2C	5.48	1.48	1.36
23	c	912	CLA	MG-NA	5.46	2.19	2.06
23	c	910	CLA	CHD-C1D	5.45	1.49	1.38
23	C	504	CLA	C3C-C2C	5.43	1.48	1.36
23	c	912	CLA	O2D-CGD	5.41	1.46	1.33
23	b	606	CLA	MG-NB	5.38	2.16	2.05
23	b	617	CLA	C3C-C2C	5.38	1.48	1.36
23	B	615	CLA	CHC-C1C	5.38	1.49	1.38
23	d	403	CLA	CHC-C1C	5.37	1.49	1.38
23	B	603	CLA	CHC-C1C	5.37	1.49	1.38
23	B	617	CLA	CHC-C1C	5.35	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	909	CLA	MG-NB	5.34	2.16	2.05
23	c	903	CLA	CHC-C1C	5.34	1.49	1.38
23	b	603	CLA	C3C-C2C	5.34	1.48	1.36
23	b	609	CLA	C3C-C2C	5.33	1.48	1.36
23	C	514	CLA	CHD-C1D	5.33	1.48	1.38
23	c	904	CLA	MG-ND	5.32	2.16	2.05
23	C	508	CLA	CHD-C1D	5.31	1.48	1.38
23	b	610	CLA	C3C-C2C	5.31	1.48	1.36
23	a	406	CLA	C3C-C2C	5.31	1.48	1.36
31	B	636	DMS	O-S	5.31	1.86	1.50
23	b	611	CLA	O2D-CGD	5.30	1.46	1.33
40	V	203	HEC	C3D-C2D	5.30	1.48	1.36
23	b	606	CLA	MG-NA	5.30	2.18	2.06
23	B	607	CLA	CHC-C1C	5.29	1.49	1.38
23	b	617	CLA	CHC-C1C	5.29	1.49	1.38
23	C	508	CLA	C3C-C2C	5.27	1.47	1.36
23	C	503	CLA	CHB-C1B	5.27	1.51	1.39
23	B	611	CLA	C3C-C2C	5.27	1.47	1.36
23	C	506	CLA	C3C-C2C	5.27	1.47	1.36
23	c	908	CLA	C3C-C2C	5.26	1.47	1.36
37	e	105	HEM	FE-ND	5.26	2.11	1.94
23	B	604	CLA	O2D-CGD	5.25	1.46	1.33
23	c	905	CLA	C3C-C2C	5.25	1.47	1.36
23	b	616	CLA	C3C-C2C	5.24	1.47	1.36
23	C	514	CLA	MG-NC	5.24	2.18	2.06
23	c	914	CLA	C3C-C2C	5.23	1.47	1.36
23	B	616	CLA	CHD-C1D	5.22	1.48	1.38
23	b	607	CLA	CHC-C4B	5.20	1.51	1.39
23	C	508	CLA	MG-ND	5.19	2.16	2.05
23	C	505	CLA	C3C-C2C	5.18	1.47	1.36
23	b	614	CLA	CHC-C1C	5.17	1.49	1.38
23	B	609	CLA	CHD-C1D	5.17	1.48	1.38
23	C	502	CLA	CHC-C1C	5.15	1.49	1.38
23	a	407	CLA	CHC-C1C	5.15	1.49	1.38
23	b	606	CLA	C1B-NB	-5.15	1.31	1.37
23	b	612	CLA	CHB-C1B	5.15	1.51	1.39
23	B	614	CLA	CHC-C1C	5.15	1.49	1.38
23	c	907	CLA	O2D-CGD	5.14	1.45	1.33
23	b	608	CLA	C3C-C2C	5.14	1.47	1.36
35	B	624	HTG	C1'-S1	-5.14	1.74	1.81
23	B	602	CLA	O2A-CGA	5.13	1.48	1.33
23	B	612	CLA	CHC-C1C	5.13	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	O2D-CGD	5.13	1.45	1.33
23	b	602	CLA	C3C-C2C	5.13	1.47	1.36
34	C	520	LMG	O8-C28	5.13	1.48	1.33
23	B	613	CLA	C1D-ND	-5.13	1.31	1.37
23	b	611	CLA	CHC-C1C	5.12	1.48	1.38
23	b	606	CLA	C3C-C2C	5.12	1.47	1.36
23	C	509	CLA	O2D-CGD	5.12	1.45	1.33
23	C	507	CLA	C3C-C2C	5.11	1.47	1.36
23	a	410	CLA	C3C-C2C	5.11	1.47	1.36
23	b	611	CLA	MG-NA	5.09	2.18	2.06
23	b	609	CLA	MG-NB	5.09	2.15	2.05
23	b	606	CLA	CHC-C1C	5.09	1.48	1.38
23	b	609	CLA	C1D-ND	-5.08	1.31	1.37
23	B	606	CLA	CHC-C1C	5.08	1.48	1.38
23	c	909	CLA	C3C-C2C	5.08	1.47	1.36
23	c	912	CLA	CHD-C1D	5.07	1.48	1.38
23	C	514	CLA	O2D-CGD	5.07	1.45	1.33
23	b	605	CLA	CHC-C1C	5.06	1.48	1.38
23	c	907	CLA	CHC-C1C	5.06	1.48	1.38
23	c	914	CLA	O2D-CGD	5.06	1.45	1.33
23	a	410	CLA	MG-NA	5.06	2.18	2.06
23	b	609	CLA	C4B-NB	-5.05	1.31	1.37
23	C	505	CLA	O2D-CGD	5.05	1.45	1.33
23	C	511	CLA	O2D-CGD	5.05	1.45	1.33
36	D	407	DGD	O1G-C1A	5.04	1.48	1.33
23	c	912	CLA	CHC-C1C	5.04	1.48	1.38
23	B	610	CLA	C3C-C2C	5.02	1.47	1.36
23	b	614	CLA	O2D-CGD	5.02	1.45	1.33
23	B	610	CLA	CHC-C1C	5.01	1.48	1.38
34	D	412	LMG	O8-C28	5.01	1.48	1.33
23	C	502	CLA	C3C-C2C	5.01	1.47	1.36
23	c	909	CLA	CHC-C1C	5.00	1.48	1.38
23	C	507	CLA	CHC-C1C	5.00	1.48	1.38
23	C	509	CLA	MG-ND	-4.99	1.95	2.05
31	D	417	DMS	O-S	4.99	1.83	1.50
23	B	615	CLA	C3C-C2C	4.98	1.47	1.36
24	a	409	PHO	C4D-CHA	4.98	1.47	1.39
28	E	101	LHG	O8-C23	4.97	1.47	1.33
23	c	914	CLA	CHC-C1C	4.97	1.48	1.38
23	D	404	CLA	C3C-C2C	4.96	1.47	1.36
23	b	612	CLA	O2D-CGD	4.96	1.45	1.33
23	C	511	CLA	CHC-C1C	4.96	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	909	CLA	CHD-C1D	4.96	1.48	1.38
23	B	617	CLA	C3C-C2C	4.95	1.47	1.36
31	V	211	DMS	O-S	4.95	1.83	1.50
23	A	408	CLA	CHB-C1B	4.95	1.50	1.39
23	C	504	CLA	MG-NA	4.94	2.18	2.06
23	C	504	CLA	CHD-C4C	4.94	1.50	1.39
23	B	609	CLA	MG-NB	-4.93	1.96	2.05
23	D	401	CLA	C4B-NB	-4.93	1.31	1.37
34	C	531	LMG	O7-C10	4.93	1.48	1.34
23	B	603	CLA	C3C-C2C	4.92	1.47	1.36
23	C	513	CLA	CHD-C1D	4.92	1.47	1.38
23	c	912	CLA	C3C-C2C	4.91	1.47	1.36
23	C	513	CLA	CHC-C1C	4.90	1.48	1.38
23	B	607	CLA	O2D-CGD	4.89	1.45	1.33
23	b	613	CLA	C3C-C2C	4.88	1.47	1.36
34	d	411	LMG	O7-C10	4.88	1.48	1.34
23	C	510	CLA	CHD-C1D	4.88	1.47	1.38
31	b	638	DMS	O-S	4.88	1.83	1.50
31	B	642	DMS	O-S	4.88	1.83	1.50
23	C	509	CLA	C3C-C2C	4.87	1.47	1.36
23	B	602	CLA	O2D-CGD	4.87	1.45	1.33
24	D	402	PHO	C4D-CHA	4.85	1.47	1.39
23	C	512	CLA	O2D-CGD	4.85	1.45	1.33
23	b	602	CLA	O2D-CGD	4.85	1.45	1.33
23	b	604	CLA	CHD-C1D	4.85	1.47	1.38
23	B	613	CLA	CHC-C1C	4.84	1.48	1.38
23	C	506	CLA	C1D-ND	-4.84	1.31	1.37
26	L	102	SQD	O47-C7	4.84	1.47	1.34
23	c	913	CLA	CHC-C1C	4.83	1.48	1.38
36	D	407	DGD	O2G-C1B	4.82	1.47	1.34
23	C	506	CLA	CHD-C1D	4.81	1.47	1.38
40	V	203	HEC	FE-ND	4.81	2.09	1.94
34	D	412	LMG	O7-C10	4.81	1.47	1.34
23	b	612	CLA	CHC-C1C	4.81	1.48	1.38
23	b	611	CLA	C1B-NB	-4.80	1.31	1.37
31	O	309	DMS	O-S	4.80	1.82	1.50
23	b	604	CLA	O2D-CGD	4.80	1.44	1.33
31	U	204	DMS	O-S	4.79	1.82	1.50
23	b	616	CLA	O2D-CGD	4.79	1.44	1.33
23	B	615	CLA	CHB-C1B	4.79	1.50	1.39
23	B	604	CLA	C3C-C2C	4.79	1.46	1.36
36	d	407	DGD	O2G-C1B	4.78	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C1D-ND	-4.78	1.31	1.37
34	d	411	LMG	O8-C28	4.78	1.47	1.33
23	b	604	CLA	C3C-C2C	4.78	1.46	1.36
23	C	507	CLA	CHB-C1B	4.76	1.50	1.39
23	C	505	CLA	CHD-C1D	4.76	1.47	1.38
23	b	612	CLA	CHD-C1D	4.75	1.47	1.38
31	c	929	DMS	O-S	4.74	1.82	1.50
31	a	423	DMS	O-S	4.74	1.82	1.50
31	V	207	DMS	O-S	4.74	1.82	1.50
23	C	511	CLA	CHD-C1D	4.73	1.47	1.38
23	B	602	CLA	C3C-C2C	4.73	1.46	1.36
23	c	913	CLA	O2D-CGD	4.73	1.44	1.33
23	C	506	CLA	O2D-CGD	4.73	1.44	1.33
31	B	641	DMS	O-S	4.72	1.82	1.50
23	C	514	CLA	CHC-C1C	4.72	1.48	1.38
23	b	603	CLA	C1B-NB	-4.72	1.32	1.37
23	C	502	CLA	CHD-C1D	4.71	1.47	1.38
31	c	925	DMS	O-S	4.71	1.82	1.50
23	b	605	CLA	O2D-CGD	4.71	1.44	1.33
24	D	402	PHO	C3A-C2A	-4.70	1.50	1.54
23	B	613	CLA	O2D-CGD	4.69	1.44	1.33
23	B	606	CLA	C3C-C2C	4.69	1.46	1.36
23	b	615	CLA	CHC-C1C	4.68	1.48	1.38
31	O	304	DMS	O-S	4.68	1.81	1.50
34	c	930	LMG	O7-C10	4.67	1.47	1.34
28	d	402	LHG	O8-C23	4.67	1.47	1.33
31	B	645	DMS	O-S	4.67	1.81	1.50
23	C	503	CLA	C3C-C2C	4.67	1.46	1.36
23	C	506	CLA	CHC-C1C	4.67	1.48	1.38
31	u	206	DMS	O-S	4.67	1.81	1.50
28	e	101	LHG	O8-C23	4.67	1.47	1.33
23	c	906	CLA	CHD-C1D	4.67	1.47	1.38
23	B	602	CLA	MG-ND	4.67	2.15	2.05
31	B	639	DMS	O-S	4.66	1.81	1.50
23	B	612	CLA	C3C-C2C	4.66	1.46	1.36
31	A	424	DMS	O-S	4.66	1.81	1.50
37	e	105	HEM	FE-NC	4.65	2.10	1.95
23	a	410	CLA	CHB-C1B	4.65	1.49	1.39
23	D	403	CLA	MG-NB	-4.65	1.96	2.05
23	b	602	CLA	CHD-C1D	4.65	1.47	1.38
26	D	408	SQD	O47-C7	4.65	1.47	1.34
23	c	911	CLA	C3C-C2C	4.65	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	413	LMG	O8-C28	4.65	1.46	1.33
23	b	610	CLA	CHB-C1B	4.65	1.49	1.39
23	C	504	CLA	CHC-C4B	4.65	1.49	1.39
23	c	905	CLA	O2D-CGD	4.64	1.44	1.33
23	B	616	CLA	CHC-C1C	4.64	1.48	1.38
31	b	636	DMS	O-S	4.64	1.81	1.50
31	B	638	DMS	O-S	4.64	1.81	1.50
26	x	101	SQD	O47-C7	4.64	1.47	1.34
23	c	902	CLA	CHD-C1D	4.64	1.47	1.38
28	e	101	LHG	O7-C7	4.64	1.47	1.34
23	B	602	CLA	CHC-C1C	4.64	1.47	1.38
23	C	507	CLA	O2D-CGD	4.64	1.44	1.33
23	c	908	CLA	CHC-C1C	4.63	1.47	1.38
23	b	615	CLA	CHC-C4B	4.63	1.49	1.39
24	a	408	PHO	C3D-C2D	4.63	1.47	1.39
23	B	608	CLA	CHC-C1C	4.63	1.47	1.38
31	b	647	DMS	O-S	4.63	1.81	1.50
31	C	526	DMS	O-S	4.63	1.81	1.50
31	H	101	DMS	O-S	4.62	1.81	1.50
31	H	105	DMS	O-S	4.62	1.81	1.50
23	c	904	CLA	CHB-C1B	4.62	1.49	1.39
31	u	204	DMS	O-S	4.61	1.81	1.50
24	A	407	PHO	C3B-C2B	4.61	1.46	1.40
31	o	304	DMS	O-S	4.61	1.81	1.50
23	c	914	CLA	CHB-C1B	4.61	1.49	1.39
23	B	616	CLA	C3C-C2C	4.61	1.46	1.36
31	b	644	DMS	O-S	4.61	1.81	1.50
23	b	607	CLA	O2D-CGD	4.60	1.44	1.33
31	O	308	DMS	O-S	4.60	1.81	1.50
23	C	512	CLA	C3C-C2C	4.60	1.46	1.36
31	O	307	DMS	O-S	4.59	1.81	1.50
31	d	418	DMS	O-S	4.59	1.81	1.50
24	a	408	PHO	C3C-C2C	4.59	1.46	1.36
31	b	639	DMS	O-S	4.59	1.81	1.50
31	D	415	DMS	O-S	4.59	1.81	1.50
23	B	605	CLA	CHC-C1C	4.58	1.47	1.38
31	d	416	DMS	O-S	4.58	1.81	1.50
31	h	105	DMS	O-S	4.58	1.81	1.50
23	d	404	CLA	C3C-C2C	4.58	1.46	1.36
28	a	415	LHG	O8-C23	4.58	1.46	1.33
23	d	403	CLA	C3C-C2C	4.58	1.46	1.36
31	i	106	DMS	O-S	4.58	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	646	DMS	O-S	4.57	1.81	1.50
23	b	614	CLA	C3C-C2C	4.57	1.46	1.36
31	A	418	DMS	O-S	4.57	1.81	1.50
28	A	412	LHG	O7-C7	4.57	1.47	1.34
23	B	613	CLA	C3C-C2C	4.57	1.46	1.36
31	A	419	DMS	O-S	4.57	1.81	1.50
31	V	210	DMS	O-S	4.56	1.81	1.50
31	v	209	DMS	O-S	4.56	1.81	1.50
23	b	612	CLA	C3C-C2C	4.56	1.46	1.36
23	b	606	CLA	C4B-NB	-4.56	1.32	1.37
23	c	905	CLA	MG-NC	4.56	2.17	2.06
34	B	622	LMG	O8-C28	4.56	1.46	1.33
23	C	510	CLA	O2D-CGD	4.56	1.44	1.33
28	A	412	LHG	O8-C23	4.55	1.46	1.33
31	v	208	DMS	O-S	4.55	1.81	1.50
23	c	907	CLA	C3C-C2C	4.55	1.46	1.36
23	B	616	CLA	MG-NC	4.55	2.17	2.06
23	b	617	CLA	O2D-CGD	4.55	1.44	1.33
31	b	635	DMS	O-S	4.55	1.81	1.50
23	B	617	CLA	O2D-CGD	4.55	1.44	1.33
31	B	647	DMS	O-S	4.54	1.80	1.50
23	b	615	CLA	CHD-C1D	4.54	1.47	1.38
31	A	421	DMS	O-S	4.54	1.80	1.50
31	v	207	DMS	O-S	4.54	1.80	1.50
23	c	910	CLA	O2D-CGD	4.54	1.44	1.33
23	d	401	CLA	CHC-C1C	4.53	1.47	1.38
23	c	911	CLA	CHC-C1C	4.53	1.47	1.38
31	h	104	DMS	O-S	4.53	1.80	1.50
23	B	607	CLA	CHC-C4B	4.52	1.49	1.39
31	a	401	DMS	O-S	4.52	1.80	1.50
31	i	105	DMS	O-S	4.52	1.80	1.50
23	B	614	CLA	C3C-C2C	4.52	1.46	1.36
31	U	203	DMS	O-S	4.52	1.80	1.50
23	c	912	CLA	CHB-C1B	4.52	1.49	1.39
31	d	414	DMS	O-S	4.52	1.80	1.50
31	B	649	DMS	O-S	4.52	1.80	1.50
31	c	936	DMS	O-S	4.52	1.80	1.50
31	O	303	DMS	O-S	4.52	1.80	1.50
31	b	645	DMS	O-S	4.52	1.80	1.50
31	O	306	DMS	O-S	4.52	1.80	1.50
23	b	609	CLA	CHB-C1B	4.52	1.49	1.39
23	c	903	CLA	CHD-C1D	4.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	o	303	DMS	O-S	4.52	1.80	1.50
31	b	640	DMS	O-S	4.51	1.80	1.50
23	c	906	CLA	C3C-C2C	4.51	1.46	1.36
23	c	910	CLA	CHC-C1C	4.51	1.47	1.38
31	a	420	DMS	O-S	4.51	1.80	1.50
31	b	642	DMS	O-S	4.51	1.80	1.50
23	D	403	CLA	C4B-NB	-4.51	1.32	1.37
26	D	408	SQD	O48-C23	4.50	1.46	1.33
23	B	611	CLA	CHC-C1C	4.50	1.47	1.38
31	c	934	DMS	O-S	4.50	1.80	1.50
26	B	621	SQD	O47-C7	4.50	1.47	1.34
34	m	102	LMG	O8-C28	4.49	1.46	1.33
31	A	422	DMS	O-S	4.49	1.80	1.50
24	a	409	PHO	O2D-CGD	4.49	1.44	1.33
23	C	513	CLA	CHB-C1B	4.49	1.49	1.39
31	O	305	DMS	O-S	4.49	1.80	1.50
28	E	101	LHG	O7-C7	4.48	1.47	1.34
23	b	611	CLA	CHD-C1D	4.48	1.47	1.38
31	v	210	DMS	O-S	4.48	1.80	1.50
23	b	613	CLA	CHC-C1C	4.48	1.47	1.38
23	C	503	CLA	CHC-C1C	4.48	1.47	1.38
28	K	101	LHG	O7-C7	4.48	1.46	1.34
31	b	643	DMS	O-S	4.48	1.80	1.50
31	a	421	DMS	O-S	4.48	1.80	1.50
31	e	104	DMS	O-S	4.48	1.80	1.50
23	b	603	CLA	CHC-C1C	4.47	1.47	1.38
23	b	611	CLA	C3C-C2C	4.47	1.46	1.36
23	D	403	CLA	CHD-C4C	4.47	1.49	1.39
23	c	904	CLA	CHD-C1D	4.47	1.47	1.38
23	C	503	CLA	CHD-C1D	4.47	1.47	1.38
28	D	409	LHG	O8-C23	4.47	1.46	1.33
23	C	513	CLA	O2A-CGA	4.47	1.46	1.33
23	b	617	CLA	CHB-C1B	4.46	1.49	1.39
31	c	933	DMS	O-S	4.46	1.80	1.50
23	d	404	CLA	CHD-C1D	4.46	1.47	1.38
23	C	504	CLA	MG-ND	4.46	2.14	2.05
31	d	419	DMS	O-S	4.46	1.80	1.50
23	A	405	CLA	C4C-C3C	4.46	1.52	1.45
23	b	608	CLA	O2D-CGD	4.45	1.44	1.33
31	c	935	DMS	O-S	4.45	1.80	1.50
31	C	533	DMS	O-S	4.45	1.80	1.50
24	A	407	PHO	C3B-C4B	4.45	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	l	102	DMS	O-S	4.45	1.80	1.50
23	C	510	CLA	CHC-C1C	4.45	1.47	1.38
23	D	401	CLA	MG-NB	4.45	2.14	2.05
31	F	102	DMS	O-S	4.45	1.80	1.50
31	h	103	DMS	O-S	4.44	1.80	1.50
31	b	641	DMS	O-S	4.44	1.80	1.50
26	x	101	SQD	O48-C23	4.44	1.46	1.33
31	h	101	DMS	O-S	4.44	1.80	1.50
31	c	937	DMS	O-S	4.44	1.80	1.50
23	b	608	CLA	CHC-C1C	4.44	1.47	1.38
24	D	402	PHO	C3C-C2C	4.44	1.46	1.36
31	k	103	DMS	O-S	4.44	1.80	1.50
23	B	613	CLA	CHD-C1D	4.44	1.47	1.38
23	C	509	CLA	CHC-C1C	4.44	1.47	1.38
23	c	905	CLA	CHC-C1C	4.43	1.47	1.38
31	O	311	DMS	O-S	4.43	1.80	1.50
31	c	926	DMS	O-S	4.43	1.80	1.50
31	d	415	DMS	O-S	4.43	1.80	1.50
23	B	611	CLA	CHD-C1D	4.43	1.47	1.38
31	V	206	DMS	O-S	4.43	1.80	1.50
31	c	932	DMS	O-S	4.42	1.80	1.50
24	a	408	PHO	OBD-CAD	4.42	1.28	1.22
23	B	609	CLA	O2D-CGD	4.42	1.44	1.33
23	C	506	CLA	C1B-NB	-4.42	1.32	1.37
31	c	928	DMS	O-S	4.42	1.80	1.50
31	v	205	DMS	O-S	4.42	1.80	1.50
31	c	927	DMS	O-S	4.41	1.80	1.50
23	c	905	CLA	CHD-C1D	4.41	1.47	1.38
31	b	637	DMS	O-S	4.41	1.80	1.50
23	D	401	CLA	CHC-C1C	4.41	1.47	1.38
23	b	608	CLA	CHD-C1D	4.41	1.46	1.38
34	C	501	LMG	O7-C10	4.40	1.46	1.34
31	C	528	DMS	O-S	4.40	1.80	1.50
23	B	602	CLA	CHD-C1D	4.40	1.46	1.38
23	c	907	CLA	CHD-C1D	4.40	1.46	1.38
36	d	407	DGD	O1G-C1A	4.40	1.46	1.33
23	C	508	CLA	O2D-CGD	4.39	1.43	1.33
26	a	417	SQD	O48-C23	4.39	1.46	1.33
34	c	930	LMG	O8-C28	4.39	1.46	1.33
26	a	417	SQD	O47-C7	4.38	1.46	1.34
23	c	911	CLA	O2D-CGD	4.38	1.43	1.33
23	B	608	CLA	C3C-C2C	4.37	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	415	LHG	O7-C7	4.37	1.46	1.34
23	b	602	CLA	CHC-C1C	4.37	1.47	1.38
23	d	401	CLA	CHD-C4C	4.36	1.49	1.39
31	V	205	DMS	O-S	4.36	1.79	1.50
23	C	504	CLA	O2D-CGD	4.36	1.43	1.33
23	b	603	CLA	MG-NA	4.36	2.16	2.06
31	v	206	DMS	O-S	4.36	1.79	1.50
31	B	646	DMS	O-S	4.36	1.79	1.50
23	C	511	CLA	C3C-C2C	4.36	1.46	1.36
31	v	202	DMS	O-S	4.36	1.79	1.50
23	C	510	CLA	OBD-CAD	4.36	1.30	1.22
23	a	406	CLA	CHD-C4C	4.36	1.49	1.39
28	K	101	LHG	O8-C23	4.35	1.46	1.33
23	B	608	CLA	CHD-C1D	4.35	1.46	1.38
34	a	413	LMG	O7-C10	4.35	1.46	1.34
31	V	208	DMS	O-S	4.33	1.79	1.50
23	a	410	CLA	O2D-CGD	4.33	1.43	1.33
31	B	640	DMS	O-S	4.33	1.79	1.50
26	A	415	SQD	O48-C23	4.32	1.46	1.33
23	a	406	CLA	CHC-C1C	4.32	1.47	1.38
23	C	502	CLA	MG-ND	-4.32	1.97	2.05
34	C	520	LMG	O7-C10	4.32	1.46	1.34
31	O	310	DMS	O-S	4.32	1.79	1.50
23	C	505	CLA	CHD-C4C	4.32	1.49	1.39
31	V	201	DMS	O-S	4.32	1.79	1.50
23	C	505	CLA	MG-NC	4.31	2.16	2.06
31	V	202	DMS	O-S	4.31	1.79	1.50
24	a	409	PHO	C3B-C2B	4.31	1.46	1.40
23	C	504	CLA	O2A-CGA	4.31	1.45	1.33
23	D	403	CLA	C3C-C2C	4.30	1.45	1.36
31	U	202	DMS	O-S	4.30	1.79	1.50
23	B	603	CLA	CHB-C1B	4.30	1.49	1.39
23	C	512	CLA	CHB-C1B	4.30	1.49	1.39
23	B	616	CLA	C1B-NB	-4.30	1.32	1.37
24	D	402	PHO	C3D-C2D	4.29	1.47	1.39
31	u	205	DMS	O-S	4.29	1.79	1.50
23	d	401	CLA	CHD-C1D	4.28	1.46	1.38
23	b	611	CLA	MG-NC	4.28	2.16	2.06
23	b	616	CLA	CHD-C4C	4.28	1.49	1.39
23	C	506	CLA	CHD-C4C	4.28	1.49	1.39
31	C	527	DMS	O-S	4.28	1.79	1.50
23	c	910	CLA	CHB-C1B	4.28	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C1C-NC	-4.28	1.31	1.37
24	D	402	PHO	O2D-CGD	4.27	1.43	1.33
31	C	529	DMS	O-S	4.26	1.79	1.50
23	C	514	CLA	CHB-C1B	4.26	1.49	1.39
23	C	510	CLA	O2A-CGA	4.25	1.45	1.33
23	c	902	CLA	CHC-C4B	4.25	1.48	1.39
23	C	512	CLA	CHD-C1D	4.25	1.46	1.38
23	B	611	CLA	MG-NC	4.25	2.16	2.06
23	B	608	CLA	CHB-C1B	4.24	1.48	1.39
36	C	519	DGD	O1G-C1A	4.24	1.45	1.33
23	c	904	CLA	O2D-CGD	4.24	1.43	1.33
23	b	606	CLA	CHD-C4C	4.24	1.48	1.39
24	A	407	PHO	C3C-C2C	4.23	1.45	1.36
23	C	511	CLA	OBD-CAD	4.23	1.29	1.22
23	D	404	CLA	CHC-C1C	4.23	1.47	1.38
23	c	914	CLA	O2A-CGA	4.23	1.45	1.33
31	V	209	DMS	O-S	4.23	1.78	1.50
23	d	401	CLA	C3C-C2C	4.23	1.45	1.36
28	d	402	LHG	O7-C7	4.23	1.46	1.34
23	c	907	CLA	O2A-CGA	4.22	1.45	1.33
31	D	416	DMS	O-S	4.22	1.78	1.50
31	C	525	DMS	O-S	4.22	1.78	1.50
24	a	409	PHO	C3D-C2D	4.22	1.47	1.39
23	B	604	CLA	MG-NA	4.21	2.16	2.06
23	b	607	CLA	CHC-C1C	4.21	1.47	1.38
23	B	605	CLA	C3C-C2C	4.21	1.45	1.36
23	b	607	CLA	CHB-C1B	4.21	1.48	1.39
34	C	531	LMG	O8-C28	4.20	1.45	1.33
23	C	504	CLA	MG-NB	4.20	2.14	2.05
23	C	508	CLA	CHD-C4C	4.20	1.48	1.39
23	C	507	CLA	O2A-CGA	4.20	1.45	1.33
23	b	617	CLA	MG-ND	4.20	2.14	2.05
23	c	903	CLA	O2D-CGD	4.20	1.43	1.33
23	b	604	CLA	C1B-NB	-4.20	1.32	1.37
23	A	408	CLA	C3C-C2C	4.19	1.45	1.36
23	b	607	CLA	C3C-C2C	4.19	1.45	1.36
31	u	203	DMS	O-S	4.19	1.78	1.50
37	E	105	HEM	FE-NA	4.19	2.09	1.95
23	B	603	CLA	CHD-C4C	4.19	1.48	1.39
23	d	403	CLA	CHB-C1B	4.18	1.48	1.39
23	C	505	CLA	CHC-C1C	4.18	1.47	1.38
23	C	509	CLA	CHD-C1D	4.17	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	CHC-C1C	4.17	1.47	1.38
23	c	908	CLA	CHC-C4B	4.15	1.48	1.39
23	b	603	CLA	C1B-C2B	4.15	1.53	1.43
23	C	504	CLA	CHD-C1D	4.15	1.46	1.38
23	C	514	CLA	CHD-C4C	4.15	1.48	1.39
23	A	408	CLA	CHC-C1C	4.14	1.46	1.38
35	O	302	HTG	C1'-S1	-4.14	1.76	1.81
23	c	902	CLA	O2D-CGD	4.14	1.43	1.33
24	D	402	PHO	OBD-CAD	4.13	1.28	1.22
23	b	614	CLA	O2A-CGA	4.13	1.45	1.33
23	b	606	CLA	C1D-ND	-4.13	1.32	1.37
23	b	617	CLA	CHD-C1D	4.13	1.46	1.38
34	c	920	LMG	O7-C10	4.12	1.45	1.34
23	D	401	CLA	CHC-C4B	4.12	1.48	1.39
23	B	604	CLA	CHB-C1B	4.12	1.48	1.39
23	b	607	CLA	CHD-C1D	4.12	1.46	1.38
31	b	634	DMS	O-S	4.12	1.78	1.50
23	B	612	CLA	CHD-C1D	4.12	1.46	1.38
23	c	913	CLA	CHD-C1D	4.12	1.46	1.38
23	D	401	CLA	MG-NA	4.12	2.16	2.06
26	L	102	SQD	O48-C23	4.11	1.45	1.33
23	A	408	CLA	CHD-C1D	4.11	1.46	1.38
34	c	920	LMG	O8-C28	4.11	1.45	1.33
23	b	615	CLA	C4C-C3C	4.11	1.52	1.45
23	c	906	CLA	CHC-C1C	4.11	1.46	1.38
23	B	604	CLA	CHD-C1D	4.11	1.46	1.38
23	c	911	CLA	CHB-C1B	4.11	1.48	1.39
34	j	101	LMG	O8-C28	4.10	1.45	1.33
23	b	602	CLA	CHB-C1B	4.09	1.48	1.39
35	b	627	HTG	C1'-S1	-4.09	1.76	1.81
23	C	506	CLA	OBD-CAD	4.09	1.29	1.22
23	B	612	CLA	C1D-ND	-4.09	1.32	1.37
23	A	405	CLA	O2D-CGD	4.08	1.43	1.33
23	D	404	CLA	CHB-C1B	4.08	1.48	1.39
23	B	603	CLA	OBD-CAD	4.08	1.29	1.22
34	m	102	LMG	O7-C10	4.08	1.45	1.34
23	c	906	CLA	CHD-C4C	4.08	1.48	1.39
23	C	502	CLA	CHD-C4C	4.08	1.48	1.39
23	C	509	CLA	CHC-C4B	4.07	1.48	1.39
23	b	610	CLA	CHD-C1D	4.07	1.46	1.38
23	A	405	CLA	CHC-C1C	4.07	1.46	1.38
23	C	502	CLA	CHC-C4B	4.06	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CHB-C1B	4.06	1.48	1.39
23	B	612	CLA	CHC-C4B	4.06	1.48	1.39
23	b	609	CLA	CHD-C1D	4.06	1.46	1.38
31	v	201	DMS	O-S	4.05	1.77	1.50
23	C	507	CLA	CHD-C4C	4.05	1.48	1.39
23	C	511	CLA	CHB-C1B	4.05	1.48	1.39
23	A	405	CLA	OBD-CAD	4.05	1.29	1.22
23	c	911	CLA	CHD-C1D	4.05	1.46	1.38
23	a	406	CLA	C4B-NB	-4.05	1.32	1.37
23	B	611	CLA	O2D-CGD	4.04	1.43	1.33
23	B	611	CLA	CHD-C4C	4.04	1.48	1.39
37	E	105	HEM	FE-ND	4.04	2.07	1.94
24	a	409	PHO	C3C-C2C	4.04	1.45	1.36
23	c	903	CLA	CHD-C4C	4.03	1.48	1.39
23	c	906	CLA	CHB-C1B	4.03	1.48	1.39
34	J	101	LMG	O7-C10	4.03	1.45	1.34
23	B	616	CLA	CHB-C1B	4.02	1.48	1.39
24	D	402	PHO	C3B-C4B	4.02	1.46	1.41
23	d	403	CLA	C1D-ND	-4.02	1.32	1.37
23	c	903	CLA	CHB-C1B	4.01	1.48	1.39
23	b	617	CLA	CHC-C4B	4.01	1.48	1.39
23	b	616	CLA	OBD-CAD	4.01	1.29	1.22
23	c	906	CLA	C1D-ND	-4.01	1.32	1.37
31	B	648	DMS	O-S	4.01	1.77	1.50
23	A	408	CLA	MG-NA	4.01	2.15	2.06
26	A	410	SQD	O47-C7	4.01	1.45	1.34
23	C	506	CLA	CHC-C4B	4.01	1.48	1.39
23	c	910	CLA	C3C-C2C	4.00	1.45	1.36
23	C	512	CLA	MG-NC	4.00	2.15	2.06
23	b	603	CLA	CHD-C4C	3.99	1.48	1.39
23	b	616	CLA	CHD-C1D	3.99	1.46	1.38
23	b	611	CLA	CHC-C4B	3.99	1.48	1.39
23	d	404	CLA	CHC-C4B	3.99	1.48	1.39
36	H	103	DGD	O5D-C1E	3.99	1.47	1.40
23	c	908	CLA	CHB-C1B	3.98	1.48	1.39
23	c	906	CLA	O2A-CGA	3.98	1.45	1.33
23	A	408	CLA	CHC-C4B	3.98	1.48	1.39
23	d	404	CLA	C4C-C3C	3.98	1.51	1.45
23	B	609	CLA	CHD-C4C	3.98	1.48	1.39
23	c	908	CLA	CHD-C4C	3.98	1.48	1.39
23	D	404	CLA	CHC-C4B	3.97	1.48	1.39
23	b	610	CLA	CHC-C4B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	C4D-CHA	3.97	1.45	1.39
23	B	609	CLA	C3C-C2C	3.97	1.45	1.36
23	B	604	CLA	CHD-C4C	3.97	1.48	1.39
23	d	404	CLA	MG-NB	-3.97	1.97	2.05
23	c	909	CLA	O2D-CGD	3.96	1.42	1.33
23	B	608	CLA	CHC-C4B	3.96	1.48	1.39
23	B	610	CLA	CHD-C1D	3.96	1.46	1.38
23	B	609	CLA	CHC-C1C	3.96	1.46	1.38
23	b	605	CLA	CHD-C1D	3.95	1.46	1.38
31	c	924	DMS	O-S	3.95	1.76	1.50
36	H	103	DGD	O2G-C1B	3.95	1.45	1.34
23	b	610	CLA	O2D-CGD	3.94	1.42	1.33
23	B	615	CLA	C1B-NB	-3.94	1.32	1.37
23	c	902	CLA	CHC-C1C	3.94	1.46	1.38
23	c	904	CLA	MG-NB	3.94	2.13	2.05
23	a	406	CLA	CHB-C1B	3.94	1.48	1.39
26	A	415	SQD	O47-C7	3.94	1.45	1.34
31	C	524	DMS	O-S	3.93	1.76	1.50
23	B	605	CLA	MG-ND	3.93	2.13	2.05
23	B	606	CLA	C3B-C4B	3.93	1.51	1.42
23	C	510	CLA	CHB-C1B	3.92	1.48	1.39
23	B	604	CLA	MG-NB	-3.92	1.98	2.05
23	D	403	CLA	CHD-C1D	3.92	1.46	1.38
23	C	504	CLA	C3B-C4B	3.92	1.51	1.42
23	b	613	CLA	MG-NB	3.92	2.13	2.05
23	A	406	CLA	CHC-C1C	3.92	1.46	1.38
23	D	404	CLA	O2D-CGD	3.90	1.42	1.33
23	b	613	CLA	CHD-C1D	3.90	1.46	1.38
23	B	606	CLA	O2D-CGD	3.90	1.42	1.33
23	a	410	CLA	O2A-CGA	3.89	1.44	1.33
24	a	408	PHO	C3B-C4B	3.89	1.45	1.41
23	C	509	CLA	CHB-C1B	3.89	1.48	1.39
23	C	514	CLA	C3D-C2D	3.88	1.49	1.39
23	C	514	CLA	CHC-C4B	3.88	1.48	1.39
23	c	914	CLA	CHC-C4B	3.88	1.48	1.39
23	C	510	CLA	C3D-C2D	3.88	1.49	1.39
23	d	403	CLA	CHD-C1D	3.88	1.45	1.38
23	b	605	CLA	C4B-NB	-3.87	1.33	1.37
23	b	604	CLA	CHB-C1B	3.87	1.48	1.39
23	b	611	CLA	CHB-C1B	3.86	1.48	1.39
23	C	513	CLA	CHD-C4C	3.86	1.48	1.39
26	a	412	SQD	O48-C23	3.86	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	911	CLA	OBD-CAD	3.86	1.29	1.22
28	L	101	LHG	O7-C7	3.86	1.45	1.34
28	d	408	LHG	O8-C23	3.85	1.44	1.33
34	C	501	LMG	O8-C28	3.85	1.44	1.33
23	b	616	CLA	CHC-C1C	3.85	1.46	1.38
23	c	902	CLA	OBD-CAD	3.85	1.29	1.22
23	B	603	CLA	O2D-CGD	3.84	1.42	1.33
23	B	615	CLA	O2D-CGD	3.84	1.42	1.33
23	c	912	CLA	OBD-CAD	3.84	1.29	1.22
23	A	405	CLA	CHC-C4B	3.84	1.48	1.39
36	c	918	DGD	O1G-C1A	3.84	1.44	1.33
23	D	403	CLA	C3B-C4B	3.84	1.51	1.42
23	B	605	CLA	MG-NB	-3.83	1.98	2.05
23	d	404	CLA	OBD-CAD	3.83	1.29	1.22
23	c	912	CLA	CHD-C4C	3.83	1.48	1.39
23	C	508	CLA	CHB-C1B	3.83	1.48	1.39
23	b	613	CLA	CHB-C1B	3.83	1.48	1.39
23	C	511	CLA	CHC-C4B	3.83	1.48	1.39
23	b	605	CLA	C3B-C4B	3.83	1.51	1.42
23	C	507	CLA	CHC-C4B	3.83	1.48	1.39
23	B	604	CLA	CHC-C1C	3.83	1.46	1.38
23	B	605	CLA	C3B-C4B	3.82	1.51	1.42
23	b	617	CLA	O2A-CGA	3.82	1.44	1.33
23	C	511	CLA	C3D-C2D	3.82	1.49	1.39
35	b	622	HTG	C1-S1	3.82	1.86	1.80
35	C	523	HTG	C1'-S1	-3.82	1.76	1.81
23	c	913	CLA	CHB-C1B	3.82	1.48	1.39
23	c	913	CLA	CHC-C4B	3.82	1.48	1.39
23	c	906	CLA	CHC-C4B	3.82	1.48	1.39
23	c	910	CLA	CHD-C4C	3.81	1.47	1.39
23	B	606	CLA	CHB-C1B	3.81	1.48	1.39
23	B	605	CLA	CHD-C4C	3.81	1.47	1.39
23	c	911	CLA	O2A-CGA	3.81	1.44	1.33
23	C	507	CLA	CHD-C1D	3.81	1.45	1.38
23	d	404	CLA	CHC-C1C	3.80	1.46	1.38
23	C	502	CLA	C3B-C4B	3.80	1.51	1.42
23	b	615	CLA	O2A-CGA	3.80	1.44	1.33
36	c	919	DGD	O1G-C1A	3.80	1.44	1.33
36	C	518	DGD	O1G-C1A	3.79	1.44	1.33
23	B	602	CLA	CHB-C1B	3.79	1.47	1.39
23	c	908	CLA	O2A-CGA	3.79	1.44	1.33
23	B	612	CLA	OBD-CAD	3.79	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	904	CLA	CHC-C4B	3.79	1.47	1.39
26	B	621	SQD	O48-C23	3.79	1.44	1.33
23	C	507	CLA	MG-NC	3.79	2.15	2.06
23	b	610	CLA	O2A-CGA	3.78	1.44	1.33
23	A	406	CLA	C3C-C2C	3.78	1.44	1.36
23	c	914	CLA	CHD-C1D	3.78	1.45	1.38
23	c	905	CLA	OBD-CAD	3.77	1.29	1.22
23	D	401	CLA	C3C-C2C	3.77	1.44	1.36
23	A	408	CLA	O2D-CGD	3.77	1.42	1.33
23	B	612	CLA	O2D-CGD	3.77	1.42	1.33
36	h	102	DGD	O5D-C1E	3.77	1.46	1.40
23	B	614	CLA	CHB-C1B	3.77	1.47	1.39
23	c	906	CLA	C1B-NB	-3.77	1.33	1.37
23	c	912	CLA	C3B-C4B	3.76	1.51	1.42
23	b	609	CLA	CHD-C4C	3.76	1.47	1.39
35	B	631	HTG	C1'-S1	-3.76	1.76	1.81
23	c	912	CLA	O2A-CGA	3.76	1.44	1.33
23	c	914	CLA	CHD-C4C	3.76	1.47	1.39
23	B	611	CLA	C4C-C3C	3.76	1.51	1.45
23	B	608	CLA	C3B-C4B	3.76	1.51	1.42
23	b	602	CLA	OBD-CAD	3.76	1.29	1.22
23	B	602	CLA	CHC-C4B	3.75	1.47	1.39
23	B	610	CLA	CHB-C1B	3.75	1.47	1.39
23	c	911	CLA	MG-NB	3.75	2.13	2.05
23	c	913	CLA	CHD-C4C	3.75	1.47	1.39
35	b	623	HTG	C1'-S1	-3.75	1.76	1.81
23	b	616	CLA	C1D-ND	-3.75	1.33	1.37
31	B	637	DMS	O-S	3.75	1.75	1.50
23	a	407	CLA	C4B-NB	-3.75	1.33	1.37
23	b	606	CLA	C3B-C4B	3.75	1.51	1.42
23	c	909	CLA	CHB-C1B	3.74	1.47	1.39
34	j	101	LMG	O7-C10	3.74	1.44	1.34
23	b	608	CLA	C3D-C2D	3.74	1.49	1.39
23	b	608	CLA	CHB-C1B	3.74	1.47	1.39
28	L	101	LHG	O8-C23	3.74	1.44	1.33
23	B	605	CLA	CHD-C1D	3.74	1.45	1.38
23	b	611	CLA	CHD-C4C	3.73	1.47	1.39
23	c	908	CLA	CHD-C1D	3.73	1.45	1.38
23	b	602	CLA	CHD-C4C	3.72	1.47	1.39
23	b	616	CLA	MG-NB	3.72	2.13	2.05
23	c	902	CLA	CHB-C1B	3.72	1.47	1.39
23	b	615	CLA	C3C-C2C	3.72	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	CHB-C1B	3.72	1.47	1.39
23	C	511	CLA	CHD-C4C	3.71	1.47	1.39
23	C	502	CLA	O2D-CGD	3.71	1.42	1.33
23	B	615	CLA	O2A-CGA	3.71	1.44	1.33
23	C	509	CLA	OBD-CAD	3.71	1.28	1.22
23	D	404	CLA	MG-NA	3.71	2.15	2.06
23	b	607	CLA	MG-NB	3.71	2.13	2.05
23	B	617	CLA	MG-NA	3.71	2.15	2.06
26	A	410	SQD	O48-C23	3.70	1.44	1.33
23	B	607	CLA	CHD-C1D	3.70	1.45	1.38
23	B	617	CLA	C1D-ND	-3.70	1.33	1.37
23	A	405	CLA	CHD-C4C	3.69	1.47	1.39
23	a	410	CLA	CHD-C1D	3.68	1.45	1.38
23	a	410	CLA	MG-ND	3.68	2.13	2.05
23	B	610	CLA	C1B-NB	-3.68	1.33	1.37
23	c	902	CLA	C3C-C2C	3.68	1.44	1.36
23	D	404	CLA	O2A-CGA	3.67	1.44	1.33
23	D	401	CLA	C3B-C4B	3.67	1.51	1.42
24	a	408	PHO	C4D-CHA	3.67	1.45	1.39
23	b	603	CLA	OBD-CAD	3.67	1.28	1.22
23	B	613	CLA	CHD-C4C	3.66	1.47	1.39
23	a	407	CLA	CHB-C1B	3.66	1.47	1.39
23	C	513	CLA	C3B-C4B	3.66	1.51	1.42
23	b	603	CLA	C3B-C4B	3.65	1.51	1.42
23	B	617	CLA	O2A-CGA	3.65	1.44	1.33
23	B	606	CLA	C1D-ND	-3.65	1.33	1.37
23	C	512	CLA	MG-ND	3.65	2.13	2.05
23	B	610	CLA	C3B-C4B	3.65	1.51	1.42
23	c	903	CLA	C3C-C2C	3.65	1.44	1.36
23	C	506	CLA	MG-NB	3.64	2.13	2.05
23	B	613	CLA	C4B-NB	-3.64	1.33	1.37
23	C	505	CLA	O2A-CGA	3.64	1.44	1.33
23	C	512	CLA	CHC-C1C	3.64	1.45	1.38
23	a	410	CLA	CHD-C4C	3.63	1.47	1.39
23	b	614	CLA	CHD-C4C	3.63	1.47	1.39
23	C	503	CLA	C3B-C4B	3.63	1.51	1.42
23	d	403	CLA	CHC-C4B	3.63	1.47	1.39
23	B	609	CLA	CHB-C1B	3.62	1.47	1.39
23	B	617	CLA	MG-NC	3.62	2.14	2.06
35	d	413	HTG	C1'-S1	-3.62	1.76	1.81
23	B	615	CLA	OBD-CAD	3.62	1.28	1.22
23	B	614	CLA	O2A-CGA	3.62	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	O2A-CGA	3.61	1.43	1.33
23	B	602	CLA	OBD-CAD	3.61	1.28	1.22
28	D	411	LHG	O8-C23	3.61	1.43	1.33
23	B	606	CLA	CHD-C1D	3.61	1.45	1.38
23	c	905	CLA	CHB-C1B	3.60	1.47	1.39
23	c	910	CLA	O2A-CGA	3.60	1.43	1.33
24	A	407	PHO	C3D-C4D	-3.60	1.36	1.41
24	a	409	PHO	OBD-CAD	3.60	1.27	1.22
23	C	508	CLA	O2A-CGA	3.59	1.43	1.33
23	a	407	CLA	O2D-CGD	3.59	1.42	1.33
23	B	613	CLA	CHB-C1B	3.59	1.47	1.39
26	a	412	SQD	O47-C7	3.59	1.44	1.34
23	c	905	CLA	CHC-C4B	3.59	1.47	1.39
23	C	513	CLA	CHC-C4B	3.59	1.47	1.39
23	D	403	CLA	O2A-CGA	3.58	1.43	1.33
23	C	514	CLA	C3B-C4B	3.58	1.51	1.42
23	b	609	CLA	O2D-CGD	3.58	1.41	1.33
23	b	608	CLA	C1B-NB	-3.58	1.33	1.37
23	A	405	CLA	C4D-ND	3.56	1.42	1.37
23	C	511	CLA	MG-ND	-3.56	1.98	2.05
23	B	609	CLA	MG-ND	3.56	2.12	2.05
23	C	509	CLA	C3D-C2D	3.56	1.48	1.39
23	C	509	CLA	O2A-CGA	3.56	1.43	1.33
23	b	604	CLA	CHD-C4C	3.55	1.47	1.39
23	C	512	CLA	O2A-CGA	3.55	1.43	1.33
23	b	605	CLA	CHB-C1B	3.54	1.47	1.39
23	a	407	CLA	CHD-C1D	3.54	1.45	1.38
23	c	913	CLA	O2A-CGA	3.54	1.43	1.33
23	C	512	CLA	CHD-C4C	3.54	1.47	1.39
24	a	409	PHO	C3D-C4D	-3.54	1.36	1.41
23	c	909	CLA	C3D-C2D	3.53	1.48	1.39
23	C	505	CLA	MG-ND	3.53	2.12	2.05
23	b	605	CLA	MG-NB	3.53	2.12	2.05
23	B	616	CLA	CHD-C4C	3.53	1.47	1.39
23	b	615	CLA	CHD-C4C	3.53	1.47	1.39
23	D	404	CLA	MG-ND	-3.53	1.98	2.05
23	B	616	CLA	MG-ND	3.53	2.12	2.05
23	C	506	CLA	O2A-CGA	3.52	1.43	1.33
23	B	606	CLA	CHD-C4C	3.52	1.47	1.39
23	C	503	CLA	C4D-CHA	3.52	1.50	1.38
23	b	614	CLA	OBD-CAD	3.52	1.28	1.22
23	B	614	CLA	C4C-C3C	3.51	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C4B-NB	-3.51	1.33	1.37
23	a	407	CLA	C3C-C2C	3.51	1.44	1.36
23	A	406	CLA	C3B-C4B	3.51	1.51	1.42
23	C	503	CLA	O2A-CGA	3.51	1.43	1.33
23	C	503	CLA	C3D-C2D	3.50	1.48	1.39
23	C	514	CLA	O2A-CGA	3.50	1.43	1.33
23	B	617	CLA	CHD-C4C	3.49	1.47	1.39
23	b	608	CLA	MG-ND	3.49	2.12	2.05
23	b	615	CLA	CHB-C1B	3.49	1.47	1.39
23	B	610	CLA	C1D-ND	-3.49	1.33	1.37
23	c	905	CLA	O2A-CGA	3.49	1.43	1.33
23	d	403	CLA	O2A-CGA	3.49	1.43	1.33
23	A	406	CLA	C1B-NB	-3.49	1.33	1.37
28	d	410	LHG	O8-C23	3.48	1.43	1.33
23	A	406	CLA	MG-NB	-3.48	1.98	2.05
23	c	910	CLA	C3D-C2D	3.48	1.48	1.39
24	D	402	PHO	O2A-CGA	3.48	1.43	1.33
23	b	604	CLA	C1D-ND	-3.48	1.33	1.37
23	B	617	CLA	CHD-C1D	3.47	1.45	1.38
23	c	913	CLA	C4C-C3C	3.47	1.51	1.45
34	J	101	LMG	O8-C28	3.47	1.43	1.33
23	A	408	CLA	CHD-C4C	3.46	1.47	1.39
23	B	617	CLA	C4B-NB	-3.46	1.33	1.37
28	D	411	LHG	O7-C7	3.46	1.44	1.34
25	a	411	BCR	C26-C25	3.46	1.40	1.34
23	B	610	CLA	OBD-CAD	3.46	1.28	1.22
23	C	508	CLA	OBD-CAD	3.46	1.28	1.22
23	b	602	CLA	C3B-C4B	3.45	1.50	1.42
23	B	607	CLA	MG-NC	3.45	2.14	2.06
23	c	910	CLA	MG-NB	3.45	2.12	2.05
23	B	615	CLA	MG-NC	3.45	2.14	2.06
23	B	611	CLA	CHC-C4B	3.44	1.47	1.39
31	o	301	DMS	O-S	3.44	1.73	1.50
23	B	602	CLA	CHD-C4C	3.44	1.47	1.39
23	c	909	CLA	CHC-C4B	3.44	1.47	1.39
23	A	408	CLA	O2A-CGA	3.44	1.43	1.33
27	a	414	PL9	C7-C3	3.43	1.54	1.51
23	b	606	CLA	CHD-C1D	3.43	1.45	1.38
40	V	203	HEC	CBC-CAC	-3.43	1.36	1.51
23	c	905	CLA	C4C-C3C	3.43	1.50	1.45
23	C	506	CLA	CHB-C1B	3.43	1.47	1.39
23	c	902	CLA	CHD-C4C	3.43	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	O2D-CGD	3.43	1.41	1.33
23	B	611	CLA	C1B-NB	-3.43	1.33	1.37
23	c	909	CLA	OBD-CAD	3.42	1.28	1.22
23	C	505	CLA	C3B-C4B	3.41	1.50	1.42
23	C	513	CLA	C3D-C2D	3.41	1.48	1.39
23	B	613	CLA	OBD-CAD	3.41	1.28	1.22
23	D	404	CLA	MG-NB	-3.41	1.99	2.05
23	b	606	CLA	CHC-C4B	3.41	1.47	1.39
23	b	605	CLA	CHD-C4C	3.41	1.47	1.39
23	C	502	CLA	O2A-CGA	3.41	1.43	1.33
23	b	612	CLA	O2A-CGA	3.41	1.43	1.33
23	b	615	CLA	O2D-CGD	3.41	1.41	1.33
23	c	909	CLA	CHD-C4C	3.40	1.47	1.39
23	c	913	CLA	C3D-C2D	3.40	1.48	1.39
23	D	403	CLA	C4D-CHA	3.40	1.50	1.38
35	B	625	HTG	C1-S1	3.40	1.86	1.80
23	B	607	CLA	OBD-CAD	3.39	1.28	1.22
23	b	604	CLA	C3B-C4B	3.39	1.50	1.42
35	B	630	HTG	C1'-S1	-3.39	1.77	1.81
23	b	614	CLA	C3B-C4B	3.39	1.50	1.42
23	b	609	CLA	OBD-CAD	3.39	1.28	1.22
23	c	914	CLA	MG-ND	3.39	2.12	2.05
28	D	410	LHG	O7-C7	3.38	1.43	1.34
23	b	609	CLA	C3B-C4B	3.38	1.50	1.42
23	C	512	CLA	CHC-C4B	3.38	1.47	1.39
23	C	506	CLA	C3D-C2D	3.38	1.48	1.39
23	B	613	CLA	C1B-NB	-3.38	1.33	1.37
23	B	603	CLA	CHC-C4B	3.38	1.47	1.39
24	a	409	PHO	O2A-CGA	3.38	1.43	1.33
34	B	622	LMG	O7-C10	3.37	1.43	1.34
23	B	611	CLA	C4D-CHA	3.37	1.50	1.38
23	b	617	CLA	CHD-C4C	3.37	1.46	1.39
23	B	606	CLA	O2A-CGA	3.37	1.43	1.33
23	C	512	CLA	C3D-C2D	3.37	1.48	1.39
23	c	904	CLA	C1B-NB	-3.37	1.33	1.37
40	v	203	HEC	FE-ND	3.36	2.05	1.94
23	B	610	CLA	C3D-C2D	3.36	1.48	1.39
23	d	404	CLA	O2A-CGA	3.36	1.43	1.33
23	B	615	CLA	C4C-C3C	3.36	1.50	1.45
23	b	613	CLA	CHD-C4C	3.36	1.46	1.39
23	B	611	CLA	O2A-CGA	3.36	1.43	1.33
23	A	406	CLA	CHB-C1B	3.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	CHD-C1D	3.35	1.44	1.38
23	b	603	CLA	O2A-CGA	3.35	1.43	1.33
23	c	914	CLA	OBD-CAD	3.35	1.28	1.22
23	c	913	CLA	OBD-CAD	3.35	1.28	1.22
23	b	613	CLA	CHC-C4B	3.34	1.46	1.39
23	C	503	CLA	CHC-C4B	3.34	1.46	1.39
23	D	403	CLA	O2D-CGD	3.34	1.41	1.33
23	b	608	CLA	CHD-C4C	3.34	1.46	1.39
23	D	404	CLA	C3B-C4B	3.34	1.50	1.42
23	b	612	CLA	C3B-C4B	3.34	1.50	1.42
23	b	603	CLA	CHB-C1B	3.34	1.46	1.39
23	D	401	CLA	CHB-C1B	3.33	1.46	1.39
23	c	904	CLA	CHD-C4C	3.33	1.46	1.39
23	B	617	CLA	MG-NB	-3.33	1.99	2.05
36	c	917	DGD	O1G-C1A	3.33	1.43	1.33
23	C	508	CLA	CHC-C4B	3.33	1.46	1.39
23	A	405	CLA	CHB-C1B	3.33	1.46	1.39
23	C	502	CLA	C3D-C2D	3.33	1.48	1.39
23	b	604	CLA	C4B-NB	-3.31	1.33	1.37
23	B	603	CLA	C4C-C3C	3.31	1.50	1.45
23	c	903	CLA	O2A-CGA	3.31	1.43	1.33
23	B	613	CLA	CHC-C4B	3.31	1.46	1.39
23	b	606	CLA	O2D-CGD	3.31	1.41	1.33
23	C	513	CLA	MG-NC	3.30	2.14	2.06
23	d	404	CLA	CHD-C4C	3.30	1.46	1.39
40	v	203	HEC	CBC-CAC	-3.30	1.36	1.51
23	B	607	CLA	C4C-C3C	3.29	1.50	1.45
23	b	613	CLA	O2D-CGD	3.29	1.41	1.33
23	a	410	CLA	OBD-CAD	3.29	1.28	1.22
23	b	617	CLA	C1D-ND	-3.29	1.33	1.37
35	c	922	HTG	C1'-S1	-3.29	1.77	1.81
27	A	411	PL9	C7-C3	3.28	1.54	1.51
23	B	608	CLA	MG-ND	3.28	2.12	2.05
28	l	101	LHG	O8-C23	3.28	1.42	1.33
36	D	407	DGD	O3G-C1D	3.27	1.45	1.40
23	b	617	CLA	C4D-CHA	3.27	1.50	1.38
23	c	905	CLA	C3B-C4B	3.27	1.50	1.42
23	b	611	CLA	C3B-C4B	3.27	1.50	1.42
23	c	906	CLA	C4D-CHA	3.27	1.50	1.38
23	B	613	CLA	O2A-CGA	3.26	1.42	1.33
23	B	605	CLA	C4D-CHA	3.26	1.50	1.38
23	a	410	CLA	C1D-ND	-3.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	911	CLA	C1B-NB	-3.26	1.33	1.37
23	B	617	CLA	CHB-C1B	3.26	1.46	1.39
23	C	505	CLA	C3D-C2D	3.25	1.48	1.39
23	b	603	CLA	O2D-CGD	3.25	1.41	1.33
23	c	909	CLA	C1C-NC	-3.25	1.33	1.37
23	d	401	CLA	C3B-C4B	3.25	1.50	1.42
23	B	609	CLA	O2A-CGA	3.25	1.42	1.33
23	b	610	CLA	CHD-C4C	3.24	1.46	1.39
23	C	512	CLA	C4D-CHA	3.24	1.49	1.38
23	b	610	CLA	C3B-C4B	3.24	1.50	1.42
36	C	517	DGD	O1G-C1A	3.24	1.42	1.33
23	c	909	CLA	O2A-CGA	3.24	1.42	1.33
23	a	406	CLA	O2A-CGA	3.23	1.42	1.33
23	B	614	CLA	CHD-C1D	3.23	1.44	1.38
23	c	912	CLA	C3D-C2D	3.23	1.47	1.39
23	c	904	CLA	C3D-C2D	3.23	1.47	1.39
23	B	608	CLA	C3D-C2D	3.22	1.47	1.39
23	c	908	CLA	C1D-ND	-3.22	1.33	1.37
23	c	907	CLA	CHC-C4B	3.22	1.46	1.39
23	B	611	CLA	OBD-CAD	3.22	1.28	1.22
23	c	909	CLA	C1D-ND	-3.22	1.33	1.37
23	B	614	CLA	CHD-C4C	3.21	1.46	1.39
23	A	408	CLA	MG-NC	3.21	2.13	2.06
23	B	610	CLA	CHC-C4B	3.21	1.46	1.39
36	H	103	DGD	O1G-C1A	3.21	1.42	1.33
24	A	407	PHO	OBD-CAD	3.21	1.26	1.22
23	b	612	CLA	MG-NC	3.20	2.13	2.06
23	B	605	CLA	O2D-CGD	3.20	1.41	1.33
23	b	603	CLA	CHD-C1D	3.20	1.44	1.38
23	B	611	CLA	C3D-C2D	3.20	1.47	1.39
23	B	610	CLA	O2A-CGA	3.20	1.42	1.33
35	B	625	HTG	O5-C1	3.20	1.47	1.42
23	b	608	CLA	CHC-C4B	3.20	1.46	1.39
36	c	918	DGD	O2G-C1B	3.20	1.43	1.34
23	B	611	CLA	CHB-C1B	3.20	1.46	1.39
23	a	406	CLA	CHD-C1D	3.19	1.44	1.38
23	B	616	CLA	CHC-C4B	3.19	1.46	1.39
23	c	906	CLA	C3B-C4B	3.19	1.50	1.42
23	c	907	CLA	CHD-C4C	3.19	1.46	1.39
23	B	607	CLA	CHB-C1B	3.19	1.46	1.39
23	b	617	CLA	C3D-C2D	3.19	1.47	1.39
23	b	614	CLA	CHD-C1D	3.19	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	O2A-CGA	3.19	1.42	1.33
23	c	903	CLA	C3D-C2D	3.19	1.47	1.39
23	D	404	CLA	C4C-C3C	3.19	1.50	1.45
28	D	410	LHG	O8-C23	3.18	1.42	1.33
23	C	513	CLA	OBD-CAD	3.18	1.28	1.22
23	C	508	CLA	C3B-C4B	3.18	1.50	1.42
23	c	905	CLA	C3D-C2D	3.18	1.47	1.39
23	c	910	CLA	C1C-NC	-3.18	1.33	1.37
23	b	609	CLA	C4D-CHA	3.17	1.49	1.38
23	C	514	CLA	C4D-CHA	3.17	1.49	1.38
23	d	404	CLA	CHB-C1B	3.17	1.46	1.39
23	b	609	CLA	O2A-CGA	3.17	1.42	1.33
23	b	612	CLA	C3D-C2D	3.17	1.47	1.39
23	C	504	CLA	OBD-CAD	3.17	1.27	1.22
23	C	509	CLA	C4C-C3C	3.17	1.50	1.45
23	b	608	CLA	C3B-C4B	3.16	1.50	1.42
37	E	105	HEM	CAC-C3C	3.16	1.56	1.47
23	b	613	CLA	C3D-C2D	3.16	1.47	1.39
23	B	605	CLA	O2A-CGA	3.16	1.42	1.33
23	B	616	CLA	C4C-C3C	3.16	1.50	1.45
23	B	617	CLA	C3D-C2D	3.16	1.47	1.39
23	b	613	CLA	C1B-NB	-3.16	1.33	1.37
23	c	903	CLA	C3B-C4B	3.16	1.50	1.42
23	C	507	CLA	C4D-CHA	3.16	1.49	1.38
23	c	907	CLA	C3B-C4B	3.16	1.50	1.42
23	c	910	CLA	MG-NC	3.16	2.13	2.06
23	B	617	CLA	CHC-C4B	3.16	1.46	1.39
23	B	609	CLA	C1D-ND	-3.15	1.33	1.37
24	A	407	PHO	O2D-CGD	3.15	1.40	1.33
23	a	407	CLA	O2A-CGA	3.15	1.42	1.33
24	a	408	PHO	O2D-CGD	3.15	1.40	1.33
23	b	603	CLA	MG-ND	3.15	2.12	2.05
23	b	613	CLA	C1B-C2B	3.15	1.50	1.43
23	c	911	CLA	MG-NA	3.15	2.13	2.06
23	c	908	CLA	O2D-CGD	3.15	1.40	1.33
23	A	406	CLA	C4B-NB	-3.15	1.33	1.37
23	b	602	CLA	CHC-C4B	3.15	1.46	1.39
40	v	203	HEC	FE-NA	3.15	2.05	1.95
23	d	403	CLA	OBD-CAD	3.15	1.27	1.22
23	B	607	CLA	C3D-C2D	3.14	1.47	1.39
23	a	407	CLA	C3D-C2D	3.14	1.47	1.39
23	b	605	CLA	C3D-C2D	3.14	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	CHD-C4C	3.14	1.46	1.39
23	c	907	CLA	OBD-CAD	3.14	1.27	1.22
23	b	610	CLA	C4B-NB	-3.14	1.33	1.37
23	B	608	CLA	O2D-CGD	3.14	1.40	1.33
23	a	407	CLA	CHC-C4B	3.13	1.46	1.39
35	C	522	HTG	C1'-S1	-3.13	1.77	1.81
31	A	423	DMS	O-S	3.13	1.71	1.50
23	B	615	CLA	CHD-C4C	3.13	1.46	1.39
23	c	904	CLA	C1D-ND	-3.13	1.33	1.37
23	B	612	CLA	C3B-C4B	3.12	1.50	1.42
23	D	401	CLA	C1B-NB	-3.12	1.33	1.37
23	B	602	CLA	C3B-C4B	3.12	1.50	1.42
23	b	613	CLA	O2A-CGA	3.11	1.42	1.33
23	B	604	CLA	C3B-C4B	3.11	1.50	1.42
23	c	911	CLA	C1D-ND	-3.10	1.34	1.37
24	A	407	PHO	C4B-NB	-3.10	1.32	1.38
23	D	404	CLA	CHD-C4C	3.10	1.46	1.39
36	C	519	DGD	O2G-C1B	3.10	1.43	1.34
23	b	615	CLA	C3D-C2D	3.10	1.47	1.39
23	D	401	CLA	CHD-C1D	3.10	1.44	1.38
23	B	603	CLA	C1D-ND	-3.09	1.34	1.37
23	C	513	CLA	C4C-C3C	3.09	1.50	1.45
23	C	504	CLA	C3D-C2D	3.09	1.47	1.39
23	B	603	CLA	C1B-C2B	3.09	1.50	1.43
23	D	403	CLA	CHB-C1B	3.09	1.46	1.39
23	A	406	CLA	O2A-CGA	3.09	1.42	1.33
23	C	512	CLA	C4C-C3C	3.08	1.50	1.45
23	A	408	CLA	C4C-C3C	3.08	1.50	1.45
23	b	607	CLA	CHD-C4C	3.08	1.46	1.39
23	C	506	CLA	MG-ND	3.07	2.11	2.05
23	b	613	CLA	C3B-C4B	3.07	1.49	1.42
35	b	627	HTG	C1-S1	-3.07	1.76	1.80
23	C	514	CLA	C4C-C3C	3.07	1.50	1.45
23	C	510	CLA	CHD-C4C	3.07	1.46	1.39
23	c	914	CLA	C1D-ND	-3.07	1.34	1.37
23	A	408	CLA	C4D-CHA	3.07	1.49	1.38
23	D	404	CLA	C3D-C2D	3.07	1.47	1.39
35	v	204	HTG	C1'-S1	-3.07	1.77	1.81
23	c	906	CLA	C3D-C2D	3.07	1.47	1.39
23	a	406	CLA	OBD-CAD	3.07	1.27	1.22
23	B	611	CLA	C3B-C4B	3.07	1.49	1.42
23	B	603	CLA	C1B-NB	-3.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	401	CLA	C1B-C2B	3.06	1.50	1.43
23	C	512	CLA	OBD-CAD	3.06	1.27	1.22
23	C	502	CLA	CHB-C1B	3.06	1.46	1.39
23	C	510	CLA	C4B-NB	-3.06	1.34	1.37
23	B	610	CLA	C4B-NB	-3.06	1.34	1.37
30	A	416	LMT	O1'-C1'	3.06	1.45	1.40
23	c	914	CLA	C3D-C2D	3.06	1.47	1.39
23	c	904	CLA	C4D-CHA	3.05	1.49	1.38
23	B	615	CLA	C3B-C4B	3.05	1.49	1.42
23	a	406	CLA	O2D-CGD	3.05	1.40	1.33
23	b	607	CLA	C3D-C2D	3.05	1.47	1.39
23	b	602	CLA	C4D-CHA	3.04	1.49	1.38
23	C	507	CLA	C3D-C2D	3.04	1.47	1.39
23	D	401	CLA	O2D-CGD	3.04	1.40	1.33
23	b	616	CLA	C1B-C2B	3.04	1.50	1.43
23	b	604	CLA	C4D-ND	-3.03	1.33	1.37
23	C	508	CLA	C4C-C3C	3.03	1.50	1.45
23	b	610	CLA	OBD-CAD	3.03	1.27	1.22
23	A	406	CLA	O2D-CGD	3.03	1.40	1.33
23	d	401	CLA	OBD-CAD	3.03	1.27	1.22
37	E	105	HEM	CAB-C3B	3.03	1.55	1.47
36	h	102	DGD	O2G-C1B	3.03	1.42	1.34
28	d	408	LHG	O7-C7	3.03	1.42	1.34
23	C	508	CLA	C3D-C2D	3.03	1.47	1.39
23	A	406	CLA	CHD-C1D	3.03	1.44	1.38
23	A	405	CLA	MG-NB	3.02	2.11	2.05
23	b	615	CLA	MG-NC	3.02	2.13	2.06
23	b	610	CLA	C3D-C2D	3.02	1.47	1.39
23	B	603	CLA	MG-NC	3.02	2.13	2.06
23	C	506	CLA	C4C-C3C	3.02	1.50	1.45
23	b	603	CLA	C4C-C3C	3.01	1.50	1.45
23	B	603	CLA	C3D-C2D	3.01	1.47	1.39
23	C	512	CLA	C3B-C4B	3.01	1.49	1.42
36	c	919	DGD	O2G-C2G	-3.01	1.39	1.46
23	c	907	CLA	CHB-C1B	3.01	1.46	1.39
23	b	614	CLA	C1D-ND	-3.01	1.34	1.37
23	C	508	CLA	C4D-CHA	3.01	1.49	1.38
23	c	913	CLA	C1B-NB	-3.01	1.34	1.37
23	C	511	CLA	C4D-CHA	3.00	1.49	1.38
23	B	612	CLA	CHD-C4C	3.00	1.46	1.39
23	b	611	CLA	C4D-CHA	3.00	1.49	1.38
23	C	503	CLA	CHD-C4C	3.00	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	906	CLA	O2D-CGD	3.00	1.40	1.33
23	d	403	CLA	O2D-CGD	2.99	1.40	1.33
23	A	405	CLA	C3C-C2C	2.99	1.43	1.36
23	c	904	CLA	C4C-C3C	2.99	1.50	1.45
23	b	614	CLA	C3D-C2D	2.99	1.47	1.39
23	C	514	CLA	OBD-CAD	2.98	1.27	1.22
23	c	908	CLA	OBD-CAD	2.98	1.27	1.22
23	C	507	CLA	C1B-NB	-2.98	1.34	1.37
35	c	921	HTG	C1'-S1	-2.98	1.77	1.81
23	C	505	CLA	C4D-CHA	2.98	1.49	1.38
37	e	105	HEM	FE-NA	2.98	2.05	1.95
23	c	902	CLA	O2A-CGA	2.98	1.42	1.33
23	C	513	CLA	C1D-ND	-2.98	1.34	1.37
23	B	606	CLA	OBD-CAD	2.98	1.27	1.22
40	v	203	HEC	CAB-C3B	2.97	1.58	1.51
23	b	602	CLA	C3D-C2D	2.97	1.47	1.39
23	c	908	CLA	C3B-C4B	2.97	1.49	1.42
23	B	616	CLA	O2A-CGA	2.97	1.42	1.33
23	C	507	CLA	C3B-C4B	2.97	1.49	1.42
23	A	406	CLA	OBD-CAD	2.97	1.27	1.22
23	c	908	CLA	C4D-CHA	2.96	1.48	1.38
23	C	504	CLA	C1B-NB	-2.96	1.34	1.37
25	A	409	BCR	C19-C18	2.96	1.52	1.45
23	B	610	CLA	C1B-C2B	2.96	1.50	1.43
23	b	615	CLA	C1C-C2C	2.96	1.50	1.44
23	D	403	CLA	OBD-CAD	2.96	1.27	1.22
23	B	611	CLA	C1C-NC	-2.96	1.33	1.37
23	a	407	CLA	C4D-ND	-2.96	1.33	1.37
23	B	612	CLA	C4D-CHA	2.96	1.48	1.38
23	C	509	CLA	C3B-C4B	2.95	1.49	1.42
23	B	606	CLA	C1B-NB	-2.95	1.34	1.37
23	b	616	CLA	O2A-CGA	2.95	1.42	1.33
23	d	401	CLA	CHB-C1B	2.94	1.46	1.39
23	C	502	CLA	C1B-NB	-2.94	1.34	1.37
23	b	602	CLA	C4D-ND	2.94	1.41	1.37
23	b	603	CLA	MG-NB	-2.94	2.00	2.05
23	d	401	CLA	C1B-C2B	2.94	1.50	1.43
23	B	607	CLA	O2A-CGA	2.94	1.41	1.33
23	C	504	CLA	C1C-C2C	2.94	1.50	1.44
23	C	511	CLA	C1C-NC	-2.93	1.33	1.37
35	O	302	HTG	O5-C1	2.93	1.47	1.42
23	c	903	CLA	C1D-ND	-2.93	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	CHC-C4B	2.93	1.46	1.39
23	b	614	CLA	C1C-NC	-2.93	1.33	1.37
25	b	619	BCR	C5-C6	2.93	1.39	1.34
23	c	906	CLA	MG-NB	2.92	2.11	2.05
30	Z	101	LMT	O1'-C1'	2.92	1.45	1.40
23	b	613	CLA	OBD-CAD	2.92	1.27	1.22
23	C	513	CLA	C4D-CHA	2.92	1.48	1.38
23	c	911	CLA	CHC-C4B	2.92	1.46	1.39
23	c	903	CLA	C3D-C4D	-2.92	1.37	1.44
24	a	408	PHO	C3D-C4D	-2.91	1.37	1.41
23	c	914	CLA	C1C-C2C	2.91	1.50	1.44
23	D	403	CLA	CHC-C4B	2.91	1.45	1.39
23	d	404	CLA	C3D-C2D	2.91	1.47	1.39
23	b	607	CLA	OBD-CAD	2.91	1.27	1.22
23	a	407	CLA	C1D-ND	-2.91	1.34	1.37
30	I	101	LMT	O1'-C1'	2.91	1.45	1.40
23	b	610	CLA	C1B-C2B	2.91	1.50	1.43
35	C	521	HTG	C1'-S1	-2.91	1.77	1.81
23	C	507	CLA	C1D-ND	-2.91	1.34	1.37
23	c	904	CLA	O2A-CGA	2.90	1.41	1.33
23	b	616	CLA	C3D-C2D	2.90	1.47	1.39
23	C	510	CLA	CHC-C4B	2.90	1.45	1.39
23	c	902	CLA	C3D-C2D	2.90	1.47	1.39
23	c	909	CLA	C3B-C4B	2.90	1.49	1.42
37	e	105	HEM	CMC-C2C	2.90	1.56	1.50
23	d	401	CLA	O2A-CGA	2.90	1.41	1.33
26	A	415	SQD	C6-S	-2.90	1.66	1.77
24	a	408	PHO	CBD-CGD	-2.90	1.48	1.52
23	c	903	CLA	OBD-CAD	2.89	1.27	1.22
35	B	626	HTG	C1'-S1	-2.89	1.77	1.81
23	a	407	CLA	C4C-C3C	2.89	1.50	1.45
23	c	902	CLA	C4C-C3C	2.89	1.50	1.45
23	C	509	CLA	MG-NC	2.89	2.13	2.06
23	C	504	CLA	C4D-CHA	2.89	1.48	1.38
23	A	405	CLA	O2A-CGA	2.89	1.41	1.33
23	c	912	CLA	C4C-C3C	2.88	1.50	1.45
26	a	417	SQD	C6-S	-2.88	1.66	1.77
23	c	912	CLA	CHC-C4B	2.88	1.45	1.39
23	D	401	CLA	C4D-ND	-2.88	1.33	1.37
23	c	910	CLA	CHC-C4B	2.88	1.45	1.39
23	C	509	CLA	C4D-ND	2.88	1.41	1.37
23	B	614	CLA	MG-ND	-2.87	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C3B-C4B	2.87	1.49	1.42
23	c	914	CLA	C3B-C4B	2.87	1.49	1.42
23	C	509	CLA	CHD-C4C	2.87	1.45	1.39
23	b	614	CLA	MG-NC	2.87	2.13	2.06
36	c	917	DGD	O2G-C1B	2.86	1.42	1.34
35	D	414	HTG	C1'-S1	-2.86	1.77	1.81
23	b	608	CLA	C1D-ND	-2.86	1.34	1.37
23	b	609	CLA	C1B-NB	-2.86	1.34	1.37
24	A	407	PHO	O2A-CGA	2.85	1.41	1.33
23	c	912	CLA	C4D-CHA	2.85	1.48	1.38
25	B	618	BCR	C14-C13	2.85	1.39	1.35
40	V	203	HEC	CBB-CAB	-2.85	1.38	1.51
23	B	605	CLA	C4B-NB	-2.85	1.34	1.37
27	a	414	PL9	C2-C3	2.84	1.42	1.34
23	C	505	CLA	C4B-NB	-2.84	1.34	1.37
23	B	603	CLA	C3B-C4B	2.84	1.49	1.42
23	C	514	CLA	MG-NB	2.84	2.11	2.05
31	b	633	DMS	O-S	2.84	1.69	1.50
23	c	906	CLA	OBD-CAD	2.84	1.27	1.22
23	B	614	CLA	CHC-C4B	2.83	1.45	1.39
23	B	608	CLA	OBD-CAD	2.83	1.27	1.22
28	l	101	LHG	O7-C7	2.82	1.42	1.34
23	b	614	CLA	CHB-C1B	2.82	1.45	1.39
36	C	517	DGD	O2G-C1B	2.82	1.42	1.34
23	B	615	CLA	C3D-C2D	2.82	1.46	1.39
23	B	615	CLA	CHC-C4B	2.82	1.45	1.39
23	b	603	CLA	CHC-C4B	2.82	1.45	1.39
23	C	506	CLA	C3B-C4B	2.82	1.49	1.42
23	C	510	CLA	C1B-C2B	2.82	1.49	1.43
23	b	610	CLA	C1B-NB	-2.82	1.34	1.37
28	d	409	LHG	O7-C7	2.82	1.42	1.34
23	B	608	CLA	CHD-C4C	2.82	1.45	1.39
23	b	604	CLA	C1B-C2B	2.81	1.49	1.43
23	b	617	CLA	OBD-CAD	2.81	1.27	1.22
40	v	203	HEC	CMC-C2C	2.81	1.56	1.50
23	a	410	CLA	C1B-C2B	2.81	1.49	1.43
23	a	406	CLA	C3B-C4B	2.81	1.49	1.42
40	V	203	HEC	CMC-C2C	2.81	1.56	1.50
23	c	905	CLA	C1C-NC	-2.81	1.33	1.37
23	A	408	CLA	C1C-NC	-2.81	1.33	1.37
37	e	105	HEM	CAB-C3B	2.80	1.55	1.47
23	B	616	CLA	C4D-ND	2.80	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	910	CLA	C1D-ND	-2.80	1.34	1.37
23	B	602	CLA	C4D-CHA	2.80	1.48	1.38
23	b	611	CLA	C3D-C4D	-2.79	1.37	1.44
23	a	410	CLA	C3D-C2D	2.79	1.46	1.39
23	C	512	CLA	C1D-ND	-2.79	1.34	1.37
23	b	611	CLA	C4C-C3C	2.79	1.49	1.45
23	D	401	CLA	C4D-CHA	2.79	1.48	1.38
23	C	502	CLA	C1C-NC	-2.79	1.33	1.37
23	B	616	CLA	C3D-C2D	2.78	1.46	1.39
23	B	617	CLA	C4D-CHA	2.78	1.48	1.38
23	B	609	CLA	CHC-C4B	2.77	1.45	1.39
23	B	612	CLA	O2A-CGA	2.77	1.41	1.33
23	a	410	CLA	CHC-C4B	2.77	1.45	1.39
23	C	505	CLA	CHB-C1B	2.77	1.45	1.39
23	b	607	CLA	C3B-C4B	2.77	1.49	1.42
23	C	502	CLA	C4D-CHA	2.76	1.48	1.38
23	C	512	CLA	C4D-ND	2.76	1.41	1.37
28	d	410	LHG	O7-C7	2.76	1.42	1.34
23	C	504	CLA	CHB-C1B	2.76	1.45	1.39
23	c	911	CLA	CHD-C4C	2.76	1.45	1.39
23	d	401	CLA	CHC-C4B	2.76	1.45	1.39
23	a	410	CLA	C4D-CHA	2.76	1.48	1.38
23	d	401	CLA	C1B-NB	-2.76	1.34	1.37
25	D	405	BCR	C12-C13	2.75	1.51	1.45
23	d	404	CLA	O2D-CGD	2.75	1.39	1.33
36	h	102	DGD	O1G-C1A	2.75	1.41	1.33
23	c	903	CLA	C4D-CHA	2.75	1.48	1.38
23	b	606	CLA	O2A-CGA	2.75	1.41	1.33
23	C	510	CLA	C4D-CHA	2.74	1.48	1.38
23	c	907	CLA	C1C-NC	-2.74	1.33	1.37
37	e	105	HEM	CMA-C3A	2.74	1.56	1.50
23	c	903	CLA	CHC-C4B	2.74	1.45	1.39
23	d	403	CLA	CHD-C4C	2.74	1.45	1.39
30	a	422	LMT	O1'-C1'	2.74	1.44	1.40
23	b	605	CLA	MG-NC	2.74	2.12	2.06
36	c	919	DGD	O2G-C1B	2.74	1.42	1.34
23	B	616	CLA	OBD-CAD	2.74	1.27	1.22
23	c	906	CLA	C4B-NB	-2.74	1.34	1.37
23	C	503	CLA	C4B-NB	-2.73	1.34	1.37
23	B	615	CLA	C4D-CHA	2.73	1.48	1.38
23	b	604	CLA	CHC-C4B	2.73	1.45	1.39
23	b	608	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C1D-ND	-2.73	1.34	1.37
23	c	913	CLA	C1D-ND	-2.73	1.34	1.37
23	b	605	CLA	C1B-C2B	2.72	1.49	1.43
23	c	902	CLA	MG-ND	-2.72	2.00	2.05
23	C	504	CLA	C1D-ND	-2.72	1.34	1.37
23	C	506	CLA	C4D-CHA	2.72	1.48	1.38
23	c	902	CLA	C4D-CHA	2.72	1.48	1.38
23	C	508	CLA	C1B-C2B	2.72	1.49	1.43
23	C	514	CLA	C1D-ND	-2.72	1.34	1.37
23	B	604	CLA	C1D-ND	-2.71	1.34	1.37
23	b	611	CLA	OBD-CAD	2.71	1.27	1.22
23	b	617	CLA	C3B-C4B	2.71	1.49	1.42
23	b	605	CLA	O2A-CGA	2.71	1.41	1.33
23	b	606	CLA	MG-NC	-2.71	1.99	2.06
23	c	902	CLA	C1B-NB	-2.70	1.34	1.37
23	c	912	CLA	C1B-C2B	2.70	1.49	1.43
23	b	610	CLA	C4D-CHA	2.70	1.48	1.38
23	c	906	CLA	C1B-C2B	2.70	1.49	1.43
23	c	913	CLA	C4D-CHA	2.70	1.48	1.38
35	B	624	HTG	O5-C1	2.70	1.46	1.42
37	E	105	HEM	CMC-C2C	2.70	1.56	1.50
23	b	605	CLA	C4D-CHA	2.70	1.48	1.38
23	B	608	CLA	O2A-CGA	2.69	1.41	1.33
23	B	617	CLA	C3B-C4B	2.69	1.49	1.42
23	c	913	CLA	C3B-C4B	2.69	1.49	1.42
23	a	407	CLA	C4D-CHA	2.69	1.48	1.38
24	a	408	PHO	C3B-C2B	2.69	1.44	1.40
35	B	624	HTG	C1-C2	2.69	1.58	1.53
35	b	628	HTG	C1'-S1	-2.68	1.78	1.81
23	B	616	CLA	C4D-CHA	2.68	1.47	1.38
26	a	412	SQD	C6-S	-2.68	1.67	1.77
23	b	605	CLA	C4C-C3C	2.68	1.49	1.45
23	b	616	CLA	C3B-C4B	2.68	1.49	1.42
40	v	203	HEC	CAC-C3C	2.68	1.58	1.51
23	B	606	CLA	C1B-C2B	2.67	1.49	1.43
23	A	405	CLA	C4D-CHA	2.67	1.47	1.38
23	C	506	CLA	C1B-C2B	2.67	1.49	1.43
23	B	615	CLA	C1B-C2B	2.67	1.49	1.43
23	b	609	CLA	C3D-C2D	2.67	1.46	1.39
23	C	502	CLA	C4B-NB	-2.67	1.34	1.37
23	D	401	CLA	O2A-CGA	2.67	1.41	1.33
23	b	616	CLA	CHC-C4B	2.66	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	617	CLA	C1C-NC	-2.66	1.33	1.37
23	d	403	CLA	C3B-C4B	2.66	1.49	1.42
23	B	609	CLA	C3D-C4D	-2.66	1.38	1.44
23	b	611	CLA	C1B-C2B	2.66	1.49	1.43
23	B	607	CLA	C1D-ND	-2.66	1.34	1.37
23	b	616	CLA	C4C-C3C	2.66	1.49	1.45
35	C	521	HTG	C1-S1	-2.65	1.76	1.80
23	c	914	CLA	C4D-CHA	2.65	1.47	1.38
23	a	406	CLA	C4D-CHA	2.65	1.47	1.38
23	B	603	CLA	C3D-C4D	-2.64	1.38	1.44
23	d	404	CLA	C4D-CHA	2.64	1.47	1.38
23	b	606	CLA	C4D-CHA	2.64	1.47	1.38
23	B	602	CLA	C1D-ND	-2.64	1.34	1.37
23	B	605	CLA	MG-NC	2.64	2.12	2.06
23	C	503	CLA	C1B-C2B	2.64	1.49	1.43
23	B	609	CLA	OBD-CAD	2.64	1.27	1.22
23	B	607	CLA	C4D-CHA	2.63	1.47	1.38
37	e	105	HEM	CAC-C3C	2.63	1.54	1.47
23	b	606	CLA	MG-ND	2.63	2.11	2.05
23	b	615	CLA	OBD-CAD	2.63	1.27	1.22
23	B	614	CLA	C3B-C4B	2.63	1.48	1.42
23	c	907	CLA	C1D-ND	-2.63	1.34	1.37
23	b	607	CLA	C4D-CHA	2.63	1.47	1.38
23	B	611	CLA	MG-ND	-2.63	2.00	2.05
23	b	604	CLA	MG-ND	2.63	2.11	2.05
23	b	615	CLA	C4D-CHA	2.62	1.47	1.38
23	b	603	CLA	C4D-CHA	2.62	1.47	1.38
23	c	908	CLA	C1C-C2C	2.62	1.49	1.44
23	B	617	CLA	OBD-CAD	2.61	1.27	1.22
23	C	511	CLA	C4C-C3C	2.61	1.49	1.45
23	b	611	CLA	C1D-ND	-2.61	1.34	1.37
23	b	606	CLA	C1B-C2B	2.61	1.49	1.43
23	C	509	CLA	C1C-C2C	2.61	1.49	1.44
23	a	406	CLA	CHC-C4B	2.60	1.45	1.39
23	B	602	CLA	C3D-C2D	2.60	1.46	1.39
23	b	614	CLA	CHC-C4B	2.60	1.45	1.39
30	e	103	LMT	O1'-C1'	2.59	1.44	1.40
23	B	609	CLA	C3B-C4B	2.59	1.48	1.42
23	c	905	CLA	C1B-NB	-2.59	1.34	1.37
23	b	602	CLA	C1C-C2C	2.59	1.49	1.44
23	b	617	CLA	C4B-NB	-2.59	1.34	1.37
23	c	910	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	911	CLA	C3D-C2D	2.58	1.46	1.39
23	C	503	CLA	OBD-CAD	2.58	1.26	1.22
23	b	609	CLA	CHC-C4B	2.58	1.45	1.39
23	b	607	CLA	O2A-CGA	2.58	1.40	1.33
23	B	616	CLA	C1C-NC	-2.58	1.34	1.37
23	b	615	CLA	C3D-C4D	-2.57	1.38	1.44
23	b	604	CLA	C4D-CHA	2.57	1.47	1.38
23	c	910	CLA	C4C-C3C	2.57	1.49	1.45
23	b	604	CLA	C3D-C2D	2.56	1.46	1.39
23	C	510	CLA	C3B-C4B	2.56	1.48	1.42
23	B	613	CLA	MG-ND	2.56	2.10	2.05
23	D	404	CLA	OBD-CAD	2.56	1.26	1.22
27	a	414	PL9	C6-C5	2.56	1.48	1.35
23	c	907	CLA	C3D-C2D	2.56	1.46	1.39
23	A	406	CLA	C3D-C2D	2.56	1.46	1.39
23	D	401	CLA	C4C-C3C	2.56	1.49	1.45
23	c	903	CLA	C1B-C2B	2.55	1.49	1.43
23	C	503	CLA	MG-ND	-2.55	2.00	2.05
23	b	617	CLA	C1C-C2C	2.55	1.49	1.44
23	c	911	CLA	C4D-CHA	2.55	1.47	1.38
23	a	407	CLA	C1B-C2B	2.55	1.49	1.43
23	A	405	CLA	C3D-C2D	2.55	1.46	1.39
27	D	406	PL9	C6-C5	2.55	1.48	1.35
23	c	909	CLA	C4C-C3C	2.54	1.49	1.45
23	c	904	CLA	C1B-C2B	2.54	1.49	1.43
23	A	405	CLA	CHD-C1D	2.54	1.43	1.38
27	D	406	PL9	C2-C3	2.54	1.41	1.34
23	b	603	CLA	MG-NC	2.53	2.12	2.06
23	D	403	CLA	MG-ND	2.53	2.10	2.05
23	b	612	CLA	C4D-CHA	2.53	1.47	1.38
23	b	612	CLA	C3D-C4D	-2.53	1.38	1.44
23	b	608	CLA	O2A-CGA	2.53	1.40	1.33
27	A	411	PL9	C2-C3	2.53	1.41	1.34
23	B	612	CLA	C3D-C2D	2.52	1.46	1.39
23	b	604	CLA	OBD-CAD	2.52	1.26	1.22
23	b	612	CLA	CHC-C4B	2.52	1.45	1.39
23	B	613	CLA	C3B-C4B	2.52	1.48	1.42
37	E	105	HEM	CMB-C2B	2.52	1.56	1.50
35	b	622	HTG	C1-C2	2.51	1.57	1.53
23	D	401	CLA	C1D-ND	-2.51	1.34	1.37
34	d	411	LMG	O1-C1	2.51	1.44	1.40
23	d	403	CLA	C3D-C2D	2.51	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	PHO	C4B-NB	-2.50	1.33	1.38
23	B	606	CLA	CHC-C4B	2.50	1.45	1.39
23	d	404	CLA	C3B-C4B	2.50	1.48	1.42
23	C	502	CLA	OBD-CAD	2.50	1.26	1.22
40	v	203	HEC	CBB-CAB	-2.50	1.40	1.51
36	C	518	DGD	O2G-C1B	2.50	1.41	1.34
25	b	620	BCR	C26-C25	2.49	1.38	1.34
36	c	917	DGD	O5D-C1E	2.49	1.44	1.40
23	C	513	CLA	C1C-C2C	2.49	1.49	1.44
23	b	616	CLA	C4D-CHA	2.48	1.47	1.38
23	d	404	CLA	C1C-NC	-2.48	1.34	1.37
23	c	907	CLA	C4D-CHA	2.48	1.47	1.38
23	c	905	CLA	C4D-CHA	2.48	1.47	1.38
23	c	911	CLA	MG-NC	2.48	2.12	2.06
23	c	912	CLA	C1B-NB	-2.48	1.34	1.37
27	A	411	PL9	C6-C5	2.48	1.48	1.35
23	c	910	CLA	C3B-C4B	2.47	1.48	1.42
37	e	105	HEM	FE-NB	2.47	2.02	1.94
23	c	906	CLA	C1D-C2D	2.47	1.50	1.45
23	B	605	CLA	C1D-ND	-2.47	1.34	1.37
23	C	510	CLA	C4C-C3C	2.47	1.49	1.45
23	d	403	CLA	C1B-NB	-2.47	1.34	1.37
23	b	606	CLA	C3D-C2D	2.47	1.45	1.39
23	d	401	CLA	C4C-C3C	2.46	1.49	1.45
23	C	509	CLA	C4D-CHA	2.46	1.47	1.38
23	B	604	CLA	CAA-C2A	2.46	1.58	1.54
23	B	604	CLA	C1B-C2B	2.46	1.49	1.43
23	B	608	CLA	C1D-ND	-2.46	1.34	1.37
23	B	612	CLA	C1B-NB	-2.46	1.34	1.37
23	b	604	CLA	C4C-C3C	2.45	1.49	1.45
23	a	407	CLA	OBD-CAD	2.45	1.26	1.22
38	H	102	RRX	C5-C6	2.45	1.38	1.34
24	a	409	PHO	C4D-ND	2.44	1.41	1.38
23	c	904	CLA	C3B-C4B	2.44	1.48	1.42
23	B	614	CLA	O2D-CGD	2.44	1.39	1.33
26	x	101	SQD	C6-S	-2.44	1.68	1.77
23	b	608	CLA	MG-NB	2.44	2.10	2.05
23	c	910	CLA	C4D-CHA	2.43	1.47	1.38
23	B	604	CLA	CHC-C4B	2.43	1.44	1.39
23	b	612	CLA	CHD-C4C	2.43	1.44	1.39
26	L	102	SQD	C6-S	-2.43	1.68	1.77
23	B	611	CLA	C4D-ND	2.43	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	406	PL9	C23-C24	2.43	1.38	1.33
30	z	101	LMT	O1'-C1'	2.42	1.44	1.40
23	c	913	CLA	C1C-C2C	2.42	1.49	1.44
23	a	406	CLA	CMD-C2D	-2.42	1.45	1.50
23	B	602	CLA	C1C-C2C	2.42	1.49	1.44
25	A	409	BCR	C8-C9	2.42	1.51	1.45
23	B	612	CLA	CHB-C1B	2.42	1.44	1.39
27	d	406	PL9	C6-C5	2.41	1.47	1.35
23	B	614	CLA	C4D-CHA	2.41	1.47	1.38
23	b	605	CLA	C1B-NB	-2.41	1.34	1.37
23	C	508	CLA	C1C-C2C	2.41	1.49	1.44
23	C	503	CLA	C4C-C3C	2.41	1.49	1.45
23	b	607	CLA	C1C-C2C	2.41	1.49	1.44
23	b	604	CLA	O2A-CGA	2.40	1.40	1.33
23	b	608	CLA	C4D-CHA	2.40	1.46	1.38
23	b	614	CLA	MG-NB	2.40	2.10	2.05
23	B	604	CLA	OBD-CAD	2.40	1.26	1.22
27	D	406	PL9	C23-C24	2.39	1.38	1.33
23	B	617	CLA	MG-ND	2.39	2.10	2.05
23	b	611	CLA	C3D-C2D	2.39	1.45	1.39
23	D	401	CLA	MG-ND	2.39	2.10	2.05
23	b	615	CLA	C4B-NB	-2.38	1.34	1.37
23	B	606	CLA	C4C-C3C	2.38	1.49	1.45
23	C	507	CLA	C4B-NB	-2.38	1.34	1.37
23	A	406	CLA	C4D-CHA	2.37	1.46	1.38
23	A	406	CLA	C3D-C4D	-2.37	1.38	1.44
23	d	401	CLA	C4D-CHA	2.37	1.46	1.38
23	B	616	CLA	C1B-C2B	2.37	1.48	1.43
23	C	513	CLA	C1B-C2B	2.37	1.48	1.43
23	b	607	CLA	C4C-C3C	2.37	1.49	1.45
37	E	105	HEM	CMD-C2D	2.37	1.55	1.50
40	V	203	HEC	CAC-C3C	2.37	1.57	1.51
23	b	610	CLA	C1C-C2C	2.37	1.49	1.44
23	B	606	CLA	O1D-CGD	2.37	1.27	1.21
23	c	914	CLA	MG-NB	2.37	2.10	2.05
23	A	405	CLA	C1B-NB	-2.36	1.34	1.37
23	B	605	CLA	C1B-C2B	2.36	1.48	1.43
23	B	607	CLA	C3B-C4B	2.36	1.48	1.42
23	a	406	CLA	O2A-C1	-2.36	1.39	1.46
23	A	406	CLA	CHC-C4B	2.36	1.44	1.39
23	c	907	CLA	C1B-C2B	2.35	1.48	1.43
23	d	404	CLA	C3D-C4D	-2.35	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406	CLA	C3D-C2D	2.35	1.45	1.39
23	C	506	CLA	MG-NC	2.35	2.11	2.06
23	C	514	CLA	C1C-C2C	2.35	1.49	1.44
26	A	410	SQD	C6-S	-2.34	1.68	1.77
23	B	606	CLA	O2A-C1	-2.34	1.39	1.46
23	B	613	CLA	C3D-C2D	2.34	1.45	1.39
23	b	617	CLA	C1B-NB	-2.34	1.34	1.37
23	c	908	CLA	C3D-C2D	2.34	1.45	1.39
23	C	504	CLA	C4C-C3C	2.34	1.49	1.45
23	c	905	CLA	C1C-C2C	2.33	1.49	1.44
23	B	614	CLA	OBD-CAD	2.33	1.26	1.22
23	c	911	CLA	C4D-ND	2.33	1.40	1.37
23	a	407	CLA	C3B-C4B	2.33	1.48	1.42
23	B	606	CLA	C4D-CHA	2.33	1.46	1.38
23	C	504	CLA	C4B-NB	-2.33	1.34	1.37
23	A	408	CLA	C3D-C4D	-2.33	1.38	1.44
35	c	922	HTG	C1-S1	-2.33	1.77	1.80
24	A	407	PHO	CBD-CGD	-2.33	1.49	1.52
23	B	607	CLA	CHD-C4C	2.32	1.44	1.39
23	c	904	CLA	C1C-C2C	2.32	1.49	1.44
23	D	401	CLA	OBD-CAD	2.32	1.26	1.22
34	c	930	LMG	O1-C1	2.32	1.44	1.40
23	B	612	CLA	C4C-C3C	2.31	1.49	1.45
23	B	605	CLA	OBD-CAD	2.31	1.26	1.22
23	c	909	CLA	C4D-CHA	2.31	1.46	1.38
23	d	404	CLA	C1B-NB	-2.31	1.34	1.37
23	a	410	CLA	C3B-C4B	2.31	1.48	1.42
23	A	406	CLA	CHD-C4C	2.30	1.44	1.39
23	C	512	CLA	C1B-C2B	2.30	1.48	1.43
23	b	617	CLA	C4C-C3C	2.30	1.49	1.45
23	B	609	CLA	C3D-C2D	2.29	1.45	1.39
24	A	407	PHO	C3D-C2D	2.29	1.43	1.39
23	c	905	CLA	CHD-C4C	2.29	1.44	1.39
23	C	505	CLA	CHC-C4B	2.29	1.44	1.39
35	c	921	HTG	C1-S1	-2.29	1.77	1.80
23	B	605	CLA	C1B-NB	-2.28	1.35	1.37
23	B	604	CLA	MG-NC	2.28	2.11	2.06
40	V	203	HEC	CAB-C3B	2.28	1.57	1.51
23	C	513	CLA	C3B-C2B	2.28	1.48	1.41
23	b	607	CLA	C3B-C2B	2.28	1.48	1.41
23	b	613	CLA	C4D-CHA	2.28	1.46	1.38
26	B	621	SQD	O6-C1	2.28	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	523	HTG	C1-S1	-2.28	1.77	1.80
23	B	609	CLA	MG-NA	2.28	2.11	2.06
23	C	510	CLA	C1B-NB	-2.28	1.35	1.37
25	D	405	BCR	C30-C25	-2.28	1.50	1.53
34	B	622	LMG	O7-C8	-2.27	1.40	1.46
23	b	604	CLA	MG-NB	2.27	2.10	2.05
23	D	404	CLA	C1C-C2C	2.27	1.49	1.44
23	C	503	CLA	MG-NB	2.27	2.10	2.05
23	B	604	CLA	C3D-C2D	2.27	1.45	1.39
23	b	608	CLA	OBD-CAD	2.26	1.26	1.22
23	C	514	CLA	C1B-C2B	2.26	1.48	1.43
23	c	905	CLA	C4B-NB	-2.25	1.35	1.37
30	m	103	LMT	O1'-C1'	2.25	1.44	1.40
23	B	616	CLA	C3B-C4B	2.25	1.48	1.42
23	B	616	CLA	C1D-ND	-2.25	1.35	1.37
26	D	408	SQD	O6-C1	2.25	1.44	1.40
28	L	101	LHG	O7-C5	-2.25	1.41	1.46
23	C	512	CLA	C3D-C4D	-2.25	1.39	1.44
23	C	504	CLA	C1B-C2B	2.24	1.48	1.43
23	c	906	CLA	MG-ND	2.24	2.10	2.05
24	a	408	PHO	O2A-CGA	2.24	1.39	1.33
23	b	616	CLA	C3B-C2B	2.24	1.48	1.41
23	c	905	CLA	C1B-C2B	2.24	1.48	1.43
23	b	611	CLA	C4B-NB	-2.24	1.35	1.37
23	B	614	CLA	C4D-ND	-2.24	1.34	1.37
23	C	514	CLA	C4B-NB	-2.24	1.35	1.37
23	b	608	CLA	C4C-C3C	2.23	1.48	1.45
23	c	907	CLA	C1C-C2C	2.22	1.48	1.44
40	v	203	HEC	CMD-C2D	2.22	1.55	1.50
25	B	620	BCR	C20-C21	2.22	1.50	1.43
23	c	902	CLA	C1B-C2B	2.22	1.48	1.43
23	c	903	CLA	C4D-ND	2.22	1.40	1.37
23	C	507	CLA	C4C-C3C	2.22	1.48	1.45
23	C	508	CLA	C3B-C2B	2.22	1.48	1.41
23	C	509	CLA	C3B-C2B	2.22	1.48	1.41
23	a	407	CLA	C3D-C4D	-2.21	1.39	1.44
23	c	908	CLA	C1C-NC	-2.21	1.34	1.37
23	C	504	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	608	CLA	C4D-CHA	2.21	1.46	1.38
23	D	404	CLA	C4D-CHA	2.21	1.46	1.38
23	B	610	CLA	CHD-C4C	2.21	1.44	1.39
23	b	608	CLA	C4B-NB	-2.21	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	CAA-C2A	2.21	1.58	1.54
23	c	914	CLA	C1B-NB	-2.21	1.35	1.37
23	b	617	CLA	C3D-C4D	-2.21	1.39	1.44
23	D	401	CLA	C3D-C2D	2.21	1.45	1.39
23	b	614	CLA	C4D-CHA	2.21	1.46	1.38
23	B	617	CLA	C4C-C3C	2.21	1.48	1.45
23	b	615	CLA	C1C-NC	-2.20	1.34	1.37
23	b	611	CLA	O2A-CGA	2.20	1.39	1.33
23	B	603	CLA	O2A-CGA	2.20	1.39	1.33
23	B	606	CLA	C1C-C2C	2.20	1.48	1.44
40	V	203	HEC	FE-NC	2.20	2.02	1.95
23	c	902	CLA	C3B-C4B	2.20	1.47	1.42
23	b	602	CLA	C1C-NC	-2.20	1.34	1.37
23	D	403	CLA	CHC-C1C	2.19	1.43	1.38
23	B	611	CLA	C4B-NB	-2.19	1.35	1.37
40	v	203	HEC	FE-NB	2.19	2.01	1.94
23	D	404	CLA	C1B-C2B	2.19	1.48	1.43
27	d	406	PL9	C7-C3	2.19	1.53	1.51
36	C	518	DGD	O2G-C2G	-2.19	1.41	1.46
23	b	603	CLA	CAB-C3B	2.19	1.53	1.47
25	D	405	BCR	C20-C21	2.19	1.50	1.43
23	b	602	CLA	C4C-C3C	2.18	1.48	1.45
23	c	913	CLA	C1B-C2B	2.18	1.48	1.43
26	D	408	SQD	C6-S	-2.18	1.69	1.77
30	b	621	LMT	O1'-C1'	2.18	1.43	1.40
25	a	411	BCR	C5-C6	2.18	1.38	1.34
23	d	404	CLA	C4B-NB	-2.18	1.35	1.37
23	c	902	CLA	C1C-C2C	2.18	1.48	1.44
23	B	611	CLA	C1C-C2C	2.17	1.48	1.44
23	c	906	CLA	MG-NC	2.17	2.11	2.06
24	a	408	PHO	C1B-NB	-2.17	1.34	1.38
30	F	101	LMT	O1'-C1'	2.17	1.43	1.40
35	b	622	HTG	O5-C1	2.17	1.45	1.42
23	a	410	CLA	C1B-NB	-2.17	1.35	1.37
37	e	105	HEM	CMB-C2B	2.17	1.55	1.50
23	D	404	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	606	CLA	CHB-C1B	2.17	1.44	1.39
23	c	911	CLA	C3B-C4B	2.17	1.47	1.42
23	C	507	CLA	C4D-ND	2.16	1.40	1.37
23	C	504	CLA	C3B-C2B	2.16	1.48	1.41
23	B	615	CLA	C4D-ND	2.16	1.40	1.37
40	v	203	HEC	CBD-CAD	2.16	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	409	LHG	O8-C23	2.16	1.39	1.33
25	b	619	BCR	C24-C25	2.16	1.52	1.45
23	b	605	CLA	C1C-C2C	2.15	1.48	1.44
23	b	603	CLA	C4D-ND	2.15	1.40	1.37
30	a	418	LMT	O1'-C1'	2.15	1.43	1.40
35	B	630	HTG	C1-S1	-2.14	1.77	1.80
23	c	902	CLA	C3D-C4D	-2.14	1.39	1.44
23	c	914	CLA	C4C-C3C	2.14	1.48	1.45
23	d	404	CLA	MG-NC	2.14	2.11	2.06
23	b	613	CLA	C3D-C4D	-2.14	1.39	1.44
40	V	203	HEC	C4B-NB	-2.14	1.36	1.40
25	k	102	BCR	C19-C18	2.14	1.50	1.45
24	a	408	PHO	C4B-NB	-2.13	1.34	1.38
23	d	404	CLA	C1C-C2C	2.13	1.48	1.44
23	a	406	CLA	C1B-C2B	2.13	1.48	1.43
23	B	605	CLA	C1D-C2D	2.13	1.49	1.45
23	B	609	CLA	C4D-CHA	2.13	1.46	1.38
34	j	101	LMG	O7-C8	-2.12	1.41	1.46
23	B	604	CLA	C4D-CHA	2.12	1.45	1.38
25	d	405	BCR	C19-C18	2.12	1.50	1.45
23	C	514	CLA	C3B-C2B	2.12	1.48	1.41
34	j	101	LMG	O1-C1	2.12	1.43	1.40
23	b	610	CLA	C4C-C3C	2.12	1.48	1.45
40	v	203	HEC	CMB-C2B	2.12	1.55	1.50
23	C	505	CLA	C4C-C3C	2.11	1.48	1.45
23	B	608	CLA	MG-NC	2.11	2.11	2.06
35	O	302	HTG	C1-S1	2.11	1.84	1.80
23	c	906	CLA	C1C-C2C	2.11	1.48	1.44
23	a	407	CLA	C1B-NB	-2.11	1.35	1.37
23	c	912	CLA	C1D-ND	-2.11	1.35	1.37
23	d	403	CLA	C1D-C2D	2.11	1.49	1.45
23	c	914	CLA	C4D-ND	2.10	1.40	1.37
23	B	614	CLA	C1C-C2C	2.10	1.48	1.44
23	B	605	CLA	C1C-NC	-2.10	1.34	1.37
23	b	605	CLA	C1D-ND	-2.10	1.35	1.37
40	v	203	HEC	FE-NC	2.10	2.02	1.95
23	c	912	CLA	C3B-C2B	2.10	1.48	1.41
23	c	912	CLA	C1C-C2C	2.10	1.48	1.44
23	b	609	CLA	C3D-C4D	-2.10	1.39	1.44
23	c	904	CLA	C1C-NC	-2.10	1.34	1.37
23	c	914	CLA	C4B-NB	-2.09	1.35	1.37
35	B	625	HTG	C1-C2	2.09	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	OBD-CAD	2.09	1.26	1.22
25	B	619	BCR	C24-C25	2.09	1.52	1.45
23	c	908	CLA	C4B-NB	-2.09	1.35	1.37
23	b	611	CLA	CAA-C2A	2.09	1.58	1.54
40	v	203	HEC	O2D-CGD	-2.09	1.23	1.30
23	B	603	CLA	MG-ND	2.09	2.09	2.05
23	B	613	CLA	C1B-C2B	2.09	1.48	1.43
23	A	406	CLA	C1C-NC	-2.09	1.34	1.37
23	C	511	CLA	C3D-C4D	-2.08	1.39	1.44
23	b	606	CLA	OBD-CAD	2.08	1.26	1.22
26	a	417	SQD	O7-S	2.08	1.51	1.45
23	A	406	CLA	C1B-C2B	2.08	1.48	1.43
23	d	403	CLA	C4D-CHA	2.08	1.45	1.38
23	c	906	CLA	C4C-C3C	2.08	1.48	1.45
23	B	603	CLA	C4D-CHA	2.08	1.45	1.38
23	C	505	CLA	C1D-ND	-2.07	1.35	1.37
35	b	623	HTG	C1-S1	-2.07	1.77	1.80
40	V	203	HEC	CMB-C2B	2.07	1.55	1.50
23	C	502	CLA	C1B-C2B	2.07	1.48	1.43
27	A	411	PL9	C6-C1	2.07	1.52	1.48
37	e	105	HEM	CMD-C2D	2.06	1.55	1.50
23	B	615	CLA	CHB-C4A	-2.06	1.32	1.37
23	B	613	CLA	MG-NB	2.06	2.09	2.05
23	c	909	CLA	C1C-C2C	2.06	1.48	1.44
35	C	522	HTG	O5-C1	2.06	1.45	1.42
23	C	507	CLA	C1A-CHA	2.06	1.51	1.43
23	B	615	CLA	C3D-C4D	-2.06	1.39	1.44
23	c	909	CLA	C3D-C4D	-2.06	1.39	1.44
23	d	404	CLA	CHB-C4A	-2.05	1.32	1.37
23	B	615	CLA	C4B-NB	-2.05	1.35	1.37
23	c	913	CLA	C3B-C2B	2.05	1.48	1.41
23	B	610	CLA	C4D-CHA	2.05	1.45	1.38
23	C	503	CLA	C3B-C2B	2.05	1.48	1.41
23	b	615	CLA	C3B-C4B	2.04	1.47	1.42
23	C	508	CLA	C1D-C2D	2.04	1.49	1.45
23	c	903	CLA	MG-ND	-2.04	2.01	2.05
25	A	409	BCR	C23-C22	2.04	1.50	1.45
23	B	611	CLA	MG-NB	2.04	2.09	2.05
23	B	611	CLA	C1-C2	2.04	1.55	1.49
25	D	405	BCR	C19-C18	2.04	1.50	1.45
25	b	620	BCR	C30-C25	-2.03	1.51	1.53
23	b	603	CLA	C3D-C2D	2.03	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	913	CLA	C4D-ND	2.03	1.40	1.37
23	B	609	CLA	O2A-C1	-2.03	1.40	1.46
23	C	507	CLA	C1B-C2B	2.02	1.48	1.43
25	B	620	BCR	C19-C18	2.02	1.50	1.45
36	C	518	DGD	O3G-C1D	2.02	1.43	1.40
25	a	411	BCR	C8-C9	2.02	1.50	1.45
23	B	603	CLA	C3B-C2B	2.02	1.48	1.41
24	A	407	PHO	C4D-ND	-2.01	1.35	1.38
23	d	403	CLA	C1B-C2B	2.01	1.48	1.43
23	C	505	CLA	OBD-CAD	2.01	1.25	1.22
23	c	906	CLA	C1C-NC	-2.01	1.34	1.37
23	B	607	CLA	C1C-C2C	2.01	1.48	1.44
23	b	607	CLA	MG-ND	-2.01	2.01	2.05
23	b	602	CLA	C3B-C2B	2.01	1.48	1.41
27	d	406	PL9	C13-C14	2.00	1.37	1.33
25	A	409	BCR	C26-C25	2.00	1.37	1.34
26	a	417	SQD	O9-S	2.00	1.50	1.45

All (2780) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	905	CLA	C4A-NA-C1A	12.36	112.26	106.71
23	c	910	CLA	C4A-NA-C1A	12.30	112.23	106.71
23	C	512	CLA	C4A-NA-C1A	11.20	111.74	106.71
23	c	902	CLA	C4A-NA-C1A	11.01	111.66	106.71
24	A	407	PHO	C2D-C1D-ND	10.97	117.10	109.53
23	b	612	CLA	C4A-NA-C1A	10.40	111.38	106.71
23	d	404	CLA	C2B-C1B-NB	10.22	117.09	110.23
23	c	904	CLA	C4A-NA-C1A	9.94	111.18	106.71
23	c	913	CLA	C4A-NA-C1A	9.90	111.16	106.71
24	a	408	PHO	C2D-C1D-ND	9.80	116.30	109.53
23	A	408	CLA	C2D-C1D-ND	9.74	117.28	110.10
24	a	409	PHO	C2B-C1B-NB	9.66	116.20	109.53
23	C	508	CLA	C4A-NA-C1A	9.48	110.97	106.71
24	a	409	PHO	C2D-C1D-ND	9.32	115.96	109.53
35	v	204	HTG	C1'-S1-C1	9.28	117.46	100.09
24	D	402	PHO	C2D-C1D-ND	9.26	115.92	109.53
23	D	404	CLA	C2B-C1B-NB	9.20	116.40	110.23
24	A	407	PHO	C4D-ND-C1D	-9.20	99.47	108.83
23	A	408	CLA	C2B-C1B-NB	9.11	116.34	110.23
26	D	408	SQD	O6-C1-C2	9.05	122.43	108.30
23	B	616	CLA	C4A-NA-C1A	8.93	110.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	C2B-C1B-NB	8.90	116.20	110.23
23	b	602	CLA	C4A-NA-C1A	8.89	110.70	106.71
23	c	909	CLA	C2B-C1B-NB	8.84	116.16	110.23
23	A	406	CLA	C4A-NA-C1A	8.75	110.64	106.71
24	D	402	PHO	C2B-C1B-NB	8.67	115.51	109.53
23	c	911	CLA	C2D-C1D-ND	8.60	116.44	110.10
23	B	604	CLA	C2C-C1C-NC	8.55	117.98	109.97
23	A	408	CLA	C1D-ND-C4D	-8.47	100.31	106.33
23	C	505	CLA	C2B-C1B-NB	8.46	115.90	110.23
23	c	912	CLA	C4A-NA-C1A	8.44	110.50	106.71
23	C	510	CLA	C4A-NA-C1A	8.40	110.48	106.71
23	a	407	CLA	C2C-C1C-NC	8.39	117.83	109.97
23	b	611	CLA	C2B-C1B-NB	8.32	115.81	110.23
23	B	616	CLA	C2B-C1B-NB	8.30	115.80	110.23
24	D	402	PHO	C4D-ND-C1D	-8.28	100.41	108.83
23	B	608	CLA	C2B-C1B-NB	8.25	115.76	110.23
23	B	617	CLA	C2B-C1B-NB	8.25	115.76	110.23
23	B	614	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	B	604	CLA	C2B-C1B-NB	8.21	115.74	110.23
23	C	513	CLA	C4A-NA-C1A	8.20	110.39	106.71
23	C	507	CLA	C4A-NA-C1A	8.19	110.39	106.71
24	a	409	PHO	C4D-ND-C1D	-8.16	100.53	108.83
23	d	401	CLA	C2B-C1B-NB	8.11	115.67	110.23
23	C	509	CLA	C2D-C1D-ND	8.10	116.07	110.10
23	b	615	CLA	C2D-C1D-ND	8.09	116.06	110.10
24	A	407	PHO	C1C-C2C-C3C	-8.08	101.89	108.61
23	b	605	CLA	C4A-NA-C1A	8.05	110.33	106.71
23	B	607	CLA	C2B-C1B-NB	8.05	115.63	110.23
40	V	203	HEC	C1D-ND-C4D	8.05	113.39	105.07
23	C	505	CLA	C4A-NA-C1A	8.04	110.32	106.71
26	a	412	SQD	O6-C1-C2	8.03	120.85	108.30
23	c	903	CLA	C2B-C1B-NB	8.01	115.60	110.23
23	c	905	CLA	C2B-C1B-NB	7.99	115.59	110.23
23	C	514	CLA	C4A-NA-C1A	7.97	110.29	106.71
23	c	905	CLA	C2D-C1D-ND	7.91	115.93	110.10
23	b	603	CLA	C2D-C1D-ND	7.90	115.92	110.10
35	V	204	HTG	O5-C1-C2	-7.89	100.39	110.31
23	B	602	CLA	C2B-C1B-NB	7.89	115.52	110.23
24	a	408	PHO	C2B-C1B-NB	7.88	114.97	109.53
23	b	602	CLA	C2B-C1B-NB	7.81	115.47	110.23
23	B	606	CLA	C2B-C1B-NB	7.81	115.47	110.23
23	c	910	CLA	C2B-C1B-NB	7.81	115.47	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	909	CLA	C4A-NA-C1A	7.79	110.21	106.71
24	A	407	PHO	C2B-C1B-NB	7.78	114.90	109.53
23	D	403	CLA	C2C-C1C-NC	7.74	117.22	109.97
23	b	615	CLA	C2B-C1B-NB	7.73	115.42	110.23
23	B	612	CLA	C2B-C1B-NB	7.73	115.41	110.23
23	B	609	CLA	C2B-C1B-NB	7.72	115.41	110.23
23	D	404	CLA	C2D-C1D-ND	7.61	115.71	110.10
35	d	413	HTG	C1'-S1-C1	7.60	114.30	100.09
23	B	616	CLA	C2D-C1D-ND	7.59	115.70	110.10
23	c	903	CLA	C4A-NA-C1A	7.58	110.12	106.71
24	a	408	PHO	C1C-C2C-C3C	-7.58	102.31	108.61
23	B	607	CLA	CHC-C4B-NB	7.56	132.26	124.26
23	C	509	CLA	C1D-ND-C4D	-7.56	100.97	106.33
23	D	403	CLA	C4A-NA-C1A	7.54	110.10	106.71
23	C	509	CLA	C4A-NA-C1A	7.48	110.07	106.71
24	a	409	PHO	O2D-CGD-CBD	7.48	120.48	111.00
35	C	523	HTG	C1'-S1-C1	7.46	114.04	100.09
23	c	914	CLA	C4A-NA-C1A	7.44	110.05	106.71
23	b	609	CLA	C2B-C1B-NB	7.42	115.21	110.23
23	A	405	CLA	C2B-C1B-NB	7.38	115.18	110.23
23	B	602	CLA	C4A-NA-C1A	7.36	110.02	106.71
23	C	514	CLA	C2B-C1B-NB	7.35	115.16	110.23
23	c	911	CLA	C2B-C1B-NB	7.35	115.16	110.23
23	b	612	CLA	C2B-C1B-NB	7.31	115.13	110.23
26	a	412	SQD	O9-S-C6	7.30	115.62	106.94
23	c	902	CLA	C2D-C1D-ND	7.28	115.47	110.10
23	B	607	CLA	C4A-NA-C1A	7.28	109.98	106.71
23	C	512	CLA	C2B-C1B-NB	7.27	115.10	110.23
23	B	611	CLA	C4A-NA-C1A	7.26	109.97	106.71
23	B	602	CLA	O2D-CGD-CBD	7.25	124.15	111.27
23	B	615	CLA	C2B-C1B-NB	7.19	115.05	110.23
23	b	614	CLA	C4A-NA-C1A	7.19	109.94	106.71
23	B	606	CLA	C2D-C1D-ND	7.16	115.38	110.10
23	B	602	CLA	C2D-C1D-ND	7.16	115.38	110.10
35	C	521	HTG	C1'-S1-C1	7.15	113.47	100.09
23	B	611	CLA	C2B-C1B-NB	7.13	115.01	110.23
23	c	914	CLA	C2D-C1D-ND	7.10	115.33	110.10
23	B	615	CLA	C4A-NA-C1A	7.08	109.89	106.71
23	c	903	CLA	C2D-C1D-ND	7.03	115.29	110.10
23	A	406	CLA	C2C-C1C-NC	6.98	116.52	109.97
35	b	623	HTG	C1'-S1-C1	6.96	113.11	100.09
23	a	410	CLA	C2D-C1D-ND	6.96	115.23	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	CLA	C2D-C1D-ND	6.91	115.19	110.10
23	b	606	CLA	C2D-C1D-ND	6.89	115.18	110.10
23	c	907	CLA	C2B-C1B-NB	6.87	114.84	110.23
23	b	607	CLA	C2D-C1D-ND	6.86	115.16	110.10
23	B	613	CLA	C4A-NA-C1A	6.83	109.78	106.71
23	d	404	CLA	C2C-C1C-NC	6.81	116.35	109.97
23	d	404	CLA	C2D-C1D-ND	6.81	115.12	110.10
23	C	506	CLA	C2C-C1C-NC	6.80	116.34	109.97
23	b	604	CLA	C2C-C1C-NC	6.80	116.34	109.97
23	C	504	CLA	C2B-C1B-NB	6.80	114.79	110.23
24	A	407	PHO	C3D-C4D-ND	6.78	116.97	107.72
23	D	404	CLA	C4A-NA-C1A	6.76	109.75	106.71
23	c	908	CLA	C2D-C1D-ND	6.76	115.09	110.10
25	D	405	BCR	C7-C8-C9	-6.74	116.05	126.23
35	V	204	HTG	C1'-S1-C1	6.73	113.03	100.16
23	b	602	CLA	C2D-C1D-ND	6.71	115.05	110.10
23	b	605	CLA	C2D-C1D-ND	6.68	115.03	110.10
24	D	402	PHO	C3D-C4D-ND	6.68	116.83	107.72
23	B	602	CLA	CHD-C1D-ND	-6.67	118.32	124.45
23	B	604	CLA	C2D-C1D-ND	6.67	115.02	110.10
23	c	902	CLA	C2B-C1B-NB	6.66	114.70	110.23
23	a	410	CLA	CHD-C1D-ND	-6.63	118.36	124.45
23	B	615	CLA	C2D-C1D-ND	6.62	114.98	110.10
23	C	505	CLA	CHD-C1D-ND	-6.61	118.38	124.45
23	C	511	CLA	CHD-C4C-C3C	-6.60	115.15	124.84
23	C	506	CLA	C4A-NA-C1A	6.58	109.67	106.71
23	b	606	CLA	CHD-C4C-C3C	-6.57	115.18	124.84
23	c	908	CLA	CHD-C1D-ND	-6.56	118.43	124.45
23	c	912	CLA	C2B-C1B-NB	6.55	114.63	110.23
23	C	502	CLA	O2D-CGD-CBD	6.50	122.83	111.27
23	B	609	CLA	C2D-C1D-ND	6.50	114.90	110.10
23	c	913	CLA	C2D-C1D-ND	6.48	114.88	110.10
23	C	505	CLA	C2C-C1C-NC	6.48	116.04	109.97
23	c	910	CLA	C2D-C1D-ND	6.45	114.86	110.10
23	d	401	CLA	C2C-C1C-NC	6.45	116.01	109.97
23	B	615	CLA	C4D-CHA-C1A	-6.44	113.41	121.25
35	B	626	HTG	C1'-S1-C1	6.40	112.07	100.09
23	B	611	CLA	C2D-C1D-ND	6.39	114.81	110.10
23	C	507	CLA	C2D-C1D-ND	6.38	114.80	110.10
24	a	408	PHO	C4D-ND-C1D	-6.38	102.34	108.83
23	B	602	CLA	CHD-C4C-C3C	-6.36	115.49	124.84
26	A	415	SQD	O6-C1-C2	6.36	118.23	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C2B-C1B-NB	6.36	114.50	110.23
23	B	612	CLA	C2D-C1D-ND	6.36	114.79	110.10
23	b	602	CLA	O2D-CGD-CBD	6.36	122.56	111.27
23	C	511	CLA	C4A-NA-C1A	6.35	109.56	106.71
23	B	608	CLA	C2D-C1D-ND	6.35	114.78	110.10
23	B	606	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	c	911	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
23	b	613	CLA	C2C-C1C-NC	6.31	115.88	109.97
23	B	603	CLA	C4A-NA-C1A	6.29	109.53	106.71
35	c	922	HTG	C1'-S1-C1	6.27	111.82	100.09
23	b	615	CLA	C4A-NA-C1A	6.27	109.53	106.71
23	C	509	CLA	C2B-C1B-NB	6.26	114.43	110.23
23	b	614	CLA	CHD-C1D-ND	-6.25	118.71	124.45
35	b	628	HTG	C1'-S1-C1	6.23	111.75	100.09
23	c	908	CLA	C4A-NA-C1A	6.23	109.51	106.71
23	b	610	CLA	CHC-C4B-NB	6.22	130.84	124.26
23	C	508	CLA	C2B-C1B-NB	6.22	114.40	110.23
23	d	403	CLA	C2C-C1C-NC	6.21	115.79	109.97
23	B	615	CLA	O2D-CGD-O1D	-6.18	111.76	123.84
23	A	405	CLA	C2D-C1D-ND	6.17	114.65	110.10
23	d	404	CLA	CHD-C1D-ND	-6.15	118.80	124.45
35	C	522	HTG	C1'-S1-C1	6.15	111.58	100.09
23	C	511	CLA	C2C-C1C-NC	6.13	115.71	109.97
23	d	401	CLA	C2D-C1D-ND	6.13	114.62	110.10
26	A	415	SQD	C1-O5-C5	-6.12	101.68	113.69
23	C	510	CLA	C2D-C1D-ND	6.11	114.61	110.10
23	C	510	CLA	C2C-C1C-NC	6.11	115.69	109.97
23	b	616	CLA	C2D-C1D-ND	6.10	114.60	110.10
23	c	909	CLA	C2D-C1D-ND	6.10	114.60	110.10
23	B	608	CLA	C2C-C1C-NC	6.10	115.68	109.97
23	B	615	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
23	B	613	CLA	CAC-C3C-C4C	6.09	132.71	124.81
23	B	610	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
26	a	412	SQD	C1-O5-C5	-6.07	101.77	113.69
23	b	614	CLA	C2C-C1C-NC	6.07	115.65	109.97
23	C	502	CLA	CHD-C1D-ND	-6.06	118.88	124.45
23	C	513	CLA	C2B-C1B-NB	6.06	114.29	110.23
23	A	408	CLA	C4D-CHA-C1A	-6.05	113.89	121.25
23	B	604	CLA	C1C-C2C-C3C	-6.04	100.60	106.96
23	C	512	CLA	C2D-C1D-ND	6.04	114.56	110.10
23	B	605	CLA	C2C-C1C-NC	6.02	115.62	109.97
24	D	402	PHO	C1C-C2C-C3C	-6.02	103.61	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C4A-NA-C1A	6.00	109.41	106.71
23	c	906	CLA	C2B-C1B-NB	6.00	114.25	110.23
23	A	406	CLA	C2D-C1D-ND	5.99	114.52	110.10
23	b	613	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
23	c	907	CLA	CHD-C1D-ND	-5.98	118.96	124.45
23	B	604	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	C	502	CLA	O2D-CGD-O1D	-5.96	112.19	123.84
23	B	616	CLA	C2C-C1C-NC	5.94	115.54	109.97
23	c	902	CLA	C2C-C1C-NC	5.94	115.54	109.97
24	a	409	PHO	C3D-C4D-ND	5.92	115.80	107.72
23	c	907	CLA	C2D-C1D-ND	5.91	114.46	110.10
26	B	621	SQD	O7-S-C6	5.91	113.97	106.94
23	b	611	CLA	C2D-C1D-ND	5.90	114.45	110.10
23	B	604	CLA	O2D-CGD-CBD	5.90	121.75	111.27
23	c	913	CLA	CHD-C1D-ND	-5.90	119.03	124.45
24	A	407	PHO	O2D-CGD-CBD	5.89	118.45	111.00
23	c	914	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
23	C	509	CLA	C4D-CHA-C1A	-5.88	114.09	121.25
23	C	507	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	b	613	CLA	C2D-C1D-ND	5.86	114.42	110.10
23	b	608	CLA	C2B-C1B-NB	5.85	114.15	110.23
23	b	615	CLA	C1D-ND-C4D	-5.84	102.19	106.33
23	B	614	CLA	CHD-C1D-ND	-5.83	119.09	124.45
23	a	407	CLA	C1C-C2C-C3C	-5.81	100.85	106.96
23	C	512	CLA	C2C-C1C-NC	5.81	115.41	109.97
23	c	904	CLA	C2D-C1D-ND	5.80	114.38	110.10
23	b	614	CLA	C2D-C1D-ND	5.79	114.37	110.10
23	B	613	CLA	C2C-C1C-NC	5.77	115.38	109.97
23	a	407	CLA	C2B-C1B-NB	5.77	114.10	110.23
23	c	905	CLA	CHD-C1D-ND	-5.77	119.16	124.45
23	b	612	CLA	C2D-C1D-ND	5.76	114.35	110.10
23	c	903	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
23	B	612	CLA	C2C-C1C-NC	5.75	115.36	109.97
25	b	618	BCR	C7-C8-C9	-5.74	117.56	126.23
23	C	503	CLA	C2D-C1D-ND	5.74	114.33	110.10
23	B	617	CLA	C2C-C1C-NC	5.74	115.34	109.97
23	b	613	CLA	C4D-CHA-C1A	-5.72	114.28	121.25
26	A	410	SQD	C1-C2-C3	-5.72	98.08	110.00
35	v	204	HTG	O5-C1-C2	-5.72	103.12	110.31
26	A	415	SQD	O9-S-C6	5.71	113.73	106.94
23	C	502	CLA	C2D-C1D-ND	5.70	114.31	110.10
23	B	609	CLA	C2C-C1C-NC	5.70	115.31	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CHC-C4B-NB	5.68	130.28	124.26
23	C	502	CLA	C2B-C1B-NB	5.68	114.04	110.23
23	c	912	CLA	C2D-C1D-ND	5.68	114.29	110.10
23	a	410	CLA	CAC-C3C-C4C	5.67	132.17	124.81
23	b	605	CLA	C2C-C1C-NC	5.67	115.28	109.97
23	C	504	CLA	CHC-C4B-NB	5.66	130.25	124.26
23	C	503	CLA	C2C-C1C-NC	5.64	115.26	109.97
23	B	610	CLA	C2C-C1C-NC	5.64	115.25	109.97
23	A	408	CLA	C4A-NA-C1A	5.64	109.24	106.71
23	b	606	CLA	CHD-C1D-ND	-5.64	119.28	124.45
30	I	101	LMT	O1B-C4'-C3'	5.63	122.27	107.28
23	b	603	CLA	C2C-C1C-NC	5.63	115.25	109.97
23	b	609	CLA	C2C-C1C-NC	5.63	115.24	109.97
23	c	914	CLA	CHD-C1D-ND	-5.62	119.29	124.45
23	c	902	CLA	C1D-ND-C4D	-5.61	102.35	106.33
23	A	406	CLA	CAC-C3C-C4C	5.60	132.08	124.81
23	C	505	CLA	C1C-C2C-C3C	-5.60	101.07	106.96
23	c	914	CLA	C2B-C1B-NB	5.58	113.98	110.23
23	B	616	CLA	CHD-C1D-ND	-5.58	119.33	124.45
35	c	923	HTG	C1'-S1-C1	5.58	108.98	101.40
23	c	906	CLA	CHD-C1D-ND	-5.58	119.33	124.45
23	B	614	CLA	C2B-C1B-NB	5.56	113.96	110.23
23	B	607	CLA	C2D-C1D-ND	5.56	114.20	110.10
23	B	604	CLA	CHD-C1D-ND	-5.55	119.35	124.45
23	B	603	CLA	CHC-C4B-NB	5.54	130.12	124.26
23	D	401	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	b	606	CLA	C2B-C1B-NB	5.54	113.94	110.23
23	c	908	CLA	CHC-C4B-NB	5.54	130.12	124.26
23	c	908	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
23	b	617	CLA	C4A-NA-C1A	5.53	109.19	106.71
23	c	906	CLA	C2C-C1C-NC	5.52	115.15	109.97
23	D	403	CLA	C3C-C4C-NC	5.52	116.76	110.57
23	d	401	CLA	CHC-C4B-NB	5.49	130.07	124.26
23	B	612	CLA	C4A-NA-C1A	5.49	109.18	106.71
23	B	611	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
25	d	405	BCR	C24-C23-C22	-5.48	117.95	126.23
23	b	615	CLA	C4D-CHA-C1A	-5.48	114.58	121.25
23	c	906	CLA	C4A-NA-C1A	5.48	109.17	106.71
40	V	203	HEC	C4B-NB-C1B	5.47	110.73	105.07
35	D	414	HTG	C1'-S1-C1	5.47	110.31	100.09
23	B	610	CLA	C2D-C1D-ND	5.46	114.13	110.10
23	C	511	CLA	C2B-C1B-NB	5.46	113.89	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	PHO	C1C-C2C-C3C	-5.46	104.07	108.61
23	b	603	CLA	CHD-C1D-ND	-5.46	119.44	124.45
23	D	403	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
23	B	614	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
23	C	504	CLA	C3B-C2B-C1B	-5.42	100.62	107.16
23	b	617	CLA	C2B-C1B-NB	5.42	113.86	110.23
23	b	609	CLA	CAC-C3C-C4C	5.42	131.84	124.81
23	A	405	CLA	C2C-C1C-NC	5.41	115.04	109.97
23	B	603	CLA	C2B-C1B-NB	5.39	113.84	110.23
26	A	410	SQD	O9-S-C6	5.39	113.34	106.94
23	B	607	CLA	C2C-C1C-NC	5.38	115.01	109.97
23	b	604	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	c	909	CLA	C4D-CHA-C1A	-5.36	114.73	121.25
23	C	508	CLA	C2C-C1C-NC	5.36	114.99	109.97
36	D	407	DGD	O3G-C1D-C2D	5.36	116.67	108.30
23	b	606	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	B	611	CLA	C2C-C1C-NC	5.35	114.99	109.97
23	c	902	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
23	B	614	CLA	CMD-C2D-C1D	5.34	134.13	124.71
23	c	905	CLA	C1D-ND-C4D	-5.34	102.54	106.33
23	a	410	CLA	C2C-C1C-NC	5.34	114.97	109.97
23	C	505	CLA	C2D-C1D-ND	5.34	114.04	110.10
23	B	617	CLA	CHC-C4B-NB	5.34	129.91	124.26
23	c	908	CLA	C2B-C1B-NB	5.33	113.81	110.23
23	d	401	CLA	C4A-NA-C1A	5.33	109.10	106.71
23	B	610	CLA	C4D-CHA-C1A	-5.33	114.76	121.25
23	a	406	CLA	C2D-C1D-ND	5.33	114.03	110.10
23	C	504	CLA	CHD-C1D-ND	-5.33	119.56	124.45
23	B	607	CLA	CHD-C4C-C3C	-5.32	117.03	124.84
23	b	615	CLA	CHD-C1D-ND	-5.31	119.57	124.45
23	b	608	CLA	C2D-C1D-ND	5.31	114.02	110.10
35	C	522	HTG	C1-O5-C5	5.31	122.37	112.58
23	C	512	CLA	CHC-C4B-NB	5.31	129.87	124.26
23	c	902	CLA	C4D-CHA-C1A	-5.31	114.79	121.25
23	c	911	CLA	C1D-ND-C4D	-5.31	102.57	106.33
23	C	508	CLA	O2D-CGD-CBD	5.29	120.67	111.27
23	c	912	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
23	b	614	CLA	C2B-C1B-NB	5.28	113.77	110.23
23	b	608	CLA	CHC-C4B-NB	5.25	129.81	124.26
23	A	405	CLA	C1D-CHD-C4C	-5.24	114.75	126.06
23	b	605	CLA	C2B-C1B-NB	5.24	113.74	110.23
23	b	603	CLA	C4A-NA-C1A	-5.23	104.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C2D-C1D-ND	5.23	113.96	110.10
23	B	615	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	A	406	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
23	c	904	CLA	CHD-C1D-ND	-5.23	119.65	124.45
23	C	507	CLA	O2D-CGD-CBD	5.22	120.55	111.27
23	D	403	CLA	CHC-C4B-NB	5.22	129.78	124.26
26	A	410	SQD	O47-C7-C8	5.22	122.75	111.50
23	C	510	CLA	CHC-C4B-NB	5.22	129.78	124.26
23	c	910	CLA	CHC-C4B-NB	5.21	129.78	124.26
23	D	403	CLA	CMC-C2C-C1C	5.21	132.97	125.04
23	b	606	CLA	CAC-C3C-C4C	5.20	131.56	124.81
36	D	407	DGD	O2G-C1B-C2B	5.20	122.71	111.50
26	D	408	SQD	C1-O5-C5	-5.20	103.48	113.69
25	c	916	BCR	C24-C23-C22	-5.19	118.39	126.23
23	a	406	CLA	C1D-CHD-C4C	-5.18	114.89	126.06
23	C	508	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
23	B	617	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
37	e	105	HEM	C4D-ND-C1D	5.17	110.41	105.07
23	C	506	CLA	CHC-C4B-NB	5.16	129.72	124.26
23	c	906	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
23	A	408	CLA	CHD-C1D-ND	-5.16	119.71	124.45
23	A	406	CLA	CMD-C2D-C1D	5.15	133.79	124.71
25	C	530	BCR	C24-C23-C22	-5.15	118.45	126.23
23	b	607	CLA	C2B-C1B-NB	5.14	113.68	110.23
23	b	610	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	B	603	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	C	507	CLA	CHD-C1D-ND	-5.11	119.76	124.45
23	d	403	CLA	C2B-C1B-NB	5.11	113.66	110.23
23	b	613	CLA	CHC-C4B-NB	5.11	129.66	124.26
23	b	610	CLA	C2D-C1D-ND	5.10	113.86	110.10
23	B	617	CLA	CAC-C3C-C4C	5.09	131.41	124.81
23	b	604	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
23	c	907	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
23	D	403	CLA	C2B-C1B-NB	5.08	113.64	110.23
23	b	616	CLA	C2C-C1C-NC	5.07	114.72	109.97
37	E	105	HEM	C4C-NC-C1C	5.07	110.31	105.35
23	c	913	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
23	B	615	CLA	CHD-C1D-ND	-5.06	119.80	124.45
23	A	408	CLA	C2C-C1C-NC	5.06	114.72	109.97
23	c	902	CLA	CHD-C1D-ND	-5.05	119.81	124.45
23	c	913	CLA	C2B-C1B-NB	5.05	113.61	110.23
23	C	502	CLA	CHD-C4C-C3C	-5.04	117.43	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	913	CLA	CHC-C4B-NB	5.03	129.58	124.26
23	b	615	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
23	b	614	CLA	CHD-C4C-C3C	-5.03	117.45	124.84
36	d	407	DGD	O2G-C1B-C2B	5.03	122.33	111.50
23	b	613	CLA	C3C-C4C-NC	5.02	116.20	110.57
23	d	403	CLA	C2D-C1D-ND	5.02	113.80	110.10
23	b	608	CLA	C2C-C1C-NC	5.02	114.67	109.97
24	a	409	PHO	C4D-CHA-CBD	5.01	110.78	108.52
25	C	515	BCR	C38-C26-C25	-5.01	118.90	124.53
23	D	403	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
23	a	410	CLA	O2D-CGD-CBD	5.00	120.15	111.27
23	C	502	CLA	C2C-C1C-NC	5.00	114.65	109.97
23	C	514	CLA	CHC-C4B-NB	4.99	129.54	124.26
26	L	102	SQD	O47-C7-C8	4.99	122.26	111.50
23	D	403	CLA	C2D-C1D-ND	4.99	113.78	110.10
23	a	406	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
23	a	410	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
23	D	401	CLA	CAC-C3C-C4C	4.98	131.27	124.81
23	B	617	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
23	B	606	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	B	607	CLA	CMB-C2B-C1B	4.98	132.95	125.37
23	B	612	CLA	CAC-C3C-C4C	4.97	131.26	124.81
23	B	605	CLA	CHC-C4B-NB	4.97	129.52	124.26
23	b	603	CLA	C2B-C1B-NB	4.96	113.56	110.23
23	B	613	CLA	CHD-C1D-ND	-4.96	119.89	124.45
23	C	506	CLA	C1C-C2C-C3C	-4.96	101.74	106.96
23	B	605	CLA	C4D-CHA-C1A	-4.96	115.22	121.25
28	E	101	LHG	O7-C7-C8	4.95	122.18	111.50
23	B	614	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	B	613	CLA	CHC-C4B-NB	4.95	129.50	124.26
23	B	602	CLA	CHD-C4C-NC	4.93	131.97	124.20
23	c	905	CLA	C4D-CHA-C1A	-4.92	115.26	121.25
23	a	406	CLA	C4A-NA-C1A	4.92	108.92	106.71
23	b	604	CLA	C1C-C2C-C3C	-4.90	101.80	106.96
23	C	511	CLA	CHD-C1D-ND	-4.90	119.95	124.45
23	B	603	CLA	C2D-C1D-ND	4.89	113.71	110.10
23	b	604	CLA	C2D-C1D-ND	4.89	113.71	110.10
37	E	105	HEM	CBD-CAD-C3D	-4.89	99.05	112.63
23	c	913	CLA	C2C-C1C-NC	4.88	114.55	109.97
23	b	614	CLA	C1-C2-C3	-4.88	117.60	126.04
23	D	404	CLA	C3B-C2B-C1B	-4.88	101.28	107.16
23	b	607	CLA	CHD-C4C-C3C	-4.87	117.68	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	C1C-C2C-C3C	-4.87	101.84	106.96
23	b	617	CLA	C2D-C1D-ND	4.87	113.69	110.10
23	b	606	CLA	C4-C3-C5	4.86	123.45	115.27
23	c	913	CLA	O2D-CGD-CBD	4.86	119.91	111.27
26	A	410	SQD	O6-C1-C2	4.85	115.88	108.30
26	a	412	SQD	O47-C7-C8	4.85	121.94	111.50
23	d	404	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	b	602	CLA	C4D-CHA-C1A	-4.84	115.36	121.25
23	C	514	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
23	B	615	CLA	CHD-C4C-NC	4.83	131.81	124.20
23	C	504	CLA	C4A-NA-C1A	4.83	108.88	106.71
23	a	410	CLA	CHC-C4B-NB	4.83	129.37	124.26
26	D	408	SQD	C1-C2-C3	-4.83	99.94	110.00
23	c	907	CLA	CHC-C4B-NB	4.82	129.36	124.26
23	C	507	CLA	C2C-C1C-NC	4.82	114.48	109.97
23	c	910	CLA	C2C-C1C-NC	4.82	114.48	109.97
23	c	911	CLA	C4D-CHA-C1A	-4.81	115.39	121.25
40	v	203	HEC	C1D-ND-C4D	4.81	110.04	105.07
23	C	507	CLA	C2B-C1B-NB	4.81	113.46	110.23
23	d	404	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
23	d	404	CLA	C4D-CHA-C1A	-4.81	115.40	121.25
23	B	616	CLA	CHB-C1B-NB	-4.81	119.17	124.26
28	a	415	LHG	O7-C7-C8	4.81	121.86	111.50
23	b	602	CLA	CHD-C4C-C3C	-4.81	117.78	124.84
23	A	405	CLA	CAC-C3C-C4C	4.80	131.04	124.81
23	C	504	CLA	CHD-C4C-C3C	-4.80	117.78	124.84
27	D	406	PL9	C40-C39-C41	4.80	123.35	115.27
23	b	616	CLA	CHD-C4C-C3C	-4.80	117.79	124.84
23	C	510	CLA	CMB-C2B-C1B	4.79	132.66	125.37
23	a	407	CLA	C3B-C2B-C1B	-4.79	101.39	107.16
23	B	609	CLA	CHD-C1D-ND	-4.78	120.06	124.45
23	B	608	CLA	C1C-C2C-C3C	-4.77	101.94	106.96
26	L	102	SQD	O7-S-C6	4.77	112.61	106.94
23	B	606	CLA	CAC-C3C-C4C	4.76	130.99	124.81
23	C	506	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
23	A	408	CLA	C4-C3-C5	4.75	123.25	115.27
23	c	902	CLA	C1C-C2C-C3C	-4.74	101.97	106.96
35	b	627	HTG	C1'-S1-C1	4.74	108.96	100.09
23	c	907	CLA	C4A-NA-C1A	4.74	108.83	106.71
34	d	411	LMG	O7-C10-C11	4.73	121.69	111.50
23	b	602	CLA	C2C-C1C-NC	4.72	114.40	109.97
23	C	511	CLA	CHD-C4C-NC	4.72	131.64	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	930	LMG	O7-C10-C11	4.72	121.68	111.50
23	c	907	CLA	C2C-C1C-NC	4.72	114.39	109.97
23	a	406	CLA	C2C-C1C-NC	4.72	114.39	109.97
23	c	912	CLA	C2C-C1C-NC	4.71	114.39	109.97
26	B	621	SQD	O6-C1-C2	4.71	115.66	108.30
26	a	412	SQD	C1-C2-C3	-4.71	100.18	110.00
23	C	510	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	C	510	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
23	B	612	CLA	CHD-C4C-C3C	-4.71	117.92	124.84
23	b	608	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	B	605	CLA	CMD-C2D-C1D	4.70	133.00	124.71
23	A	406	CLA	CHC-C4B-NB	4.70	129.23	124.26
23	b	615	CLA	O2D-CGD-CBD	4.70	119.61	111.27
25	T	101	BCR	C38-C26-C25	-4.69	119.26	124.53
23	d	404	CLA	C3B-C4B-NB	4.69	114.87	110.52
27	A	411	PL9	C53-C6-C1	4.69	124.57	114.99
23	c	907	CLA	O2D-CGD-CBD	4.68	119.59	111.27
23	B	616	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
23	c	908	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	B	612	CLA	C1-C2-C3	-4.67	117.96	126.04
23	b	617	CLA	CHD-C4C-C3C	-4.67	117.98	124.84
23	b	604	CLA	O2D-CGD-O1D	-4.66	114.72	123.84
23	b	607	CLA	C4D-CHA-C1A	-4.66	115.57	121.25
35	B	630	HTG	C1'-S1-C1	4.66	108.80	100.09
23	c	903	CLA	CHC-C4B-NB	4.65	129.18	124.26
23	b	607	CLA	C2C-C1C-NC	4.65	114.33	109.97
35	c	921	HTG	C1'-S1-C1	4.65	108.79	100.09
36	D	407	DGD	C4D-C3D-C2D	4.65	118.94	110.82
23	c	905	CLA	CAC-C3C-C4C	4.65	130.84	124.81
23	C	508	CLA	CHC-C4B-NB	4.64	129.17	124.26
23	b	613	CLA	CAC-C3C-C4C	4.64	130.83	124.81
25	D	405	BCR	C24-C23-C22	-4.64	119.23	126.23
23	c	911	CLA	C2C-C1C-NC	4.63	114.31	109.97
23	b	602	CLA	C1-O2A-CGA	4.63	128.60	116.44
23	c	904	CLA	CHC-C4B-NB	4.63	129.16	124.26
23	B	607	CLA	CHD-C1D-ND	-4.63	120.20	124.45
23	c	904	CLA	CHD-C4C-C3C	-4.62	118.04	124.84
36	D	407	DGD	O1G-C1A-C2A	4.62	126.40	111.91
23	b	614	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
25	B	618	BCR	C15-C14-C13	-4.60	120.74	127.31
23	C	505	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
23	A	406	CLA	C4D-CHA-C1A	-4.60	115.65	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406	CLA	C4D-CHA-C1A	-4.59	115.66	121.25
23	b	611	CLA	C2C-C1C-NC	4.58	114.27	109.97
23	D	401	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
23	B	607	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
36	H	103	DGD	O1G-C1A-O1A	-4.58	112.04	123.59
23	C	503	CLA	C4A-NA-C1A	4.58	108.76	106.71
23	b	608	CLA	CHD-C1D-ND	-4.57	120.25	124.45
23	C	512	CLA	C1C-C2C-C3C	-4.57	102.16	106.96
25	B	620	BCR	C38-C26-C25	-4.56	119.40	124.53
23	b	612	CLA	CHC-C4B-NB	4.56	129.09	124.26
23	b	612	CLA	C4D-CHA-C1A	-4.56	115.69	121.25
23	c	904	CLA	C2C-C1C-NC	4.56	114.25	109.97
23	B	606	CLA	C4D-CHA-C1A	-4.56	115.70	121.25
23	c	912	CLA	O2D-CGD-O1D	-4.56	114.93	123.84
37	E	105	HEM	C4A-NA-C1A	4.56	109.81	105.35
23	a	407	CLA	CHC-C4B-NB	4.55	129.08	124.26
23	c	907	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
23	b	606	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	B	610	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	b	616	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
23	d	403	CLA	CHD-C4C-C3C	-4.53	118.18	124.84
23	b	604	CLA	O2D-CGD-CBD	4.53	119.32	111.27
24	A	407	PHO	CBC-CAC-C3C	-4.53	106.25	112.88
23	A	405	CLA	C1D-ND-C4D	-4.52	103.12	106.33
23	d	401	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
36	C	517	DGD	O3G-C3G-C2G	-4.52	99.98	110.90
23	C	514	CLA	C1C-C2C-C3C	-4.52	102.21	106.96
23	d	404	CLA	CMB-C2B-C1B	4.52	132.25	125.37
25	C	516	BCR	C7-C8-C9	-4.51	119.41	126.23
23	c	904	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
23	b	616	CLA	C1D-CHD-C4C	-4.51	116.33	126.06
23	b	605	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
23	b	610	CLA	CHD-C4C-C3C	-4.50	118.22	124.84
24	a	409	PHO	C1-C2-C3	-4.50	118.26	126.04
23	b	612	CLA	C2C-C1C-NC	4.50	114.19	109.97
23	d	404	CLA	C1D-ND-C4D	-4.50	103.14	106.33
23	d	403	CLA	O2D-CGD-O1D	-4.50	115.04	123.84
23	C	508	CLA	CHD-C1D-ND	-4.49	120.33	124.45
23	c	910	CLA	CAC-C3C-C4C	4.49	130.63	124.81
23	B	603	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	B	610	CLA	CHC-C4B-NB	4.49	129.01	124.26
23	B	608	CLA	C4A-NA-C1A	4.49	108.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	CLA	C1D-ND-C4D	-4.49	103.15	106.33
23	C	503	CLA	O2D-CGD-CBD	4.48	119.22	111.27
25	D	405	BCR	C40-C30-C25	-4.48	103.04	110.30
34	C	531	LMG	O7-C10-C11	4.47	121.14	111.50
23	C	504	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	a	407	CLA	CAC-C3C-C4C	4.46	130.60	124.81
23	c	903	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
23	a	406	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
23	b	603	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
23	C	510	CLA	CHD-C1D-ND	-4.45	120.36	124.45
23	b	612	CLA	CHD-C1D-ND	-4.45	120.36	124.45
23	B	613	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	b	607	CLA	C1-C2-C3	-4.44	118.36	126.04
23	C	504	CLA	CHA-C4D-ND	4.44	141.79	132.50
23	C	514	CLA	C2C-C1C-NC	4.44	114.13	109.97
23	C	505	CLA	O2D-CGD-CBD	4.44	119.15	111.27
23	b	607	CLA	CHD-C1D-ND	-4.43	120.38	124.45
35	V	204	HTG	C1-C2-C3	-4.43	101.84	110.59
25	Y	101	BCR	C33-C5-C6	-4.42	119.56	124.53
23	C	510	CLA	O2D-CGD-CBD	4.42	119.12	111.27
26	A	410	SQD	C1-O5-C5	-4.41	105.03	113.69
23	B	617	CLA	CHD-C1D-ND	-4.41	120.40	124.45
23	C	513	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
23	b	604	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
23	B	614	CLA	C1D-ND-C4D	-4.40	103.21	106.33
23	B	613	CLA	C4D-CHA-C1A	-4.40	115.89	121.25
26	a	417	SQD	C1-O5-C5	-4.40	105.05	113.69
35	v	204	HTG	O5-C1-S1	4.39	120.33	109.82
23	b	605	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
30	F	101	LMT	C1B-O5B-C5B	4.39	122.30	113.69
35	B	624	HTG	C1'-S1-C1	4.39	108.29	100.09
23	b	615	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
23	d	401	CLA	C4D-CHA-C1A	-4.38	115.92	121.25
23	B	608	CLA	CHD-C1D-ND	-4.38	120.43	124.45
23	D	403	CLA	O2D-CGD-O1D	-4.38	115.28	123.84
24	D	402	PHO	C1-C2-C3	-4.37	118.48	126.04
23	C	505	CLA	CHC-C4B-NB	4.37	128.88	124.26
23	C	512	CLA	CMB-C2B-C1B	4.37	132.02	125.37
23	A	408	CLA	O2D-CGD-CBD	4.36	119.02	111.27
23	D	401	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
23	b	605	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	b	613	CLA	C4A-NA-C1A	4.36	108.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C1C-C2C-C3C	-4.36	102.38	106.96
23	D	401	CLA	C2D-C1D-ND	4.34	113.31	110.10
23	B	615	CLA	CMD-C2D-C1D	4.34	132.37	124.71
23	b	614	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
23	b	610	CLA	C4D-CHA-C1A	-4.34	115.97	121.25
23	B	611	CLA	O2D-CGD-CBD	4.34	118.97	111.27
26	D	408	SQD	O47-C7-C8	4.34	120.84	111.50
23	c	907	CLA	CMD-C2D-C1D	4.33	132.35	124.71
23	B	607	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
23	c	903	CLA	C2C-C1C-NC	4.32	114.02	109.97
24	a	408	PHO	C3D-C4D-ND	4.32	113.61	107.72
36	c	918	DGD	O2G-C1B-C2B	4.32	120.80	111.50
23	c	910	CLA	C3B-C4B-NB	4.32	114.52	110.52
23	C	513	CLA	C3B-C2B-C1B	-4.31	101.95	107.16
23	c	903	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
23	C	503	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
37	E	105	HEM	C4D-ND-C1D	4.30	109.52	105.07
23	b	609	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
23	B	605	CLA	CHA-C4D-ND	4.30	141.50	132.50
23	c	912	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
23	b	616	CLA	O2D-CGD-O1D	-4.30	115.44	123.84
23	b	611	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
23	B	611	CLA	C1D-CHD-C4C	-4.30	116.79	126.06
23	b	607	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
23	b	604	CLA	C2B-C1B-NB	4.30	113.11	110.23
23	b	607	CLA	O2D-CGD-CBD	4.30	118.90	111.27
23	B	611	CLA	O2D-CGD-O1D	-4.30	115.44	123.84
23	c	910	CLA	C4D-CHA-C1A	-4.29	116.02	121.25
34	m	102	LMG	C9-C8-C7	-4.29	101.64	111.79
23	c	909	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
23	c	902	CLA	CMD-C2D-C1D	4.29	132.27	124.71
28	A	412	LHG	O7-C7-C8	4.29	120.74	111.50
28	K	101	LHG	O7-C7-C8	4.29	120.74	111.50
23	c	913	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
23	b	608	CLA	CHD-C4C-C3C	-4.27	118.56	124.84
23	B	615	CLA	CHC-C4B-NB	4.27	128.78	124.26
23	C	514	CLA	CHD-C1D-ND	-4.27	120.53	124.45
23	B	615	CLA	CHB-C4A-NA	4.27	130.42	124.51
23	b	602	CLA	C1C-C2C-C3C	-4.26	102.47	106.96
23	c	914	CLA	CHC-C4B-NB	4.26	128.77	124.26
23	b	612	CLA	CHD-C4C-C3C	-4.26	118.58	124.84
23	D	403	CLA	CHA-C4D-ND	4.26	141.40	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CHD-C4C-C3C	-4.25	118.59	124.84
23	a	407	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
23	B	602	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	b	616	CLA	C2B-C1B-NB	4.25	113.08	110.23
27	d	406	PL9	O1-C4-C3	-4.25	116.04	120.72
23	b	615	CLA	CHC-C4B-NB	4.23	128.74	124.26
23	a	407	CLA	C3C-C4C-NC	4.23	115.32	110.57
28	D	409	LHG	O8-C23-O10	-4.23	112.91	123.59
23	b	605	CLA	CHA-C4D-ND	4.23	141.35	132.50
23	B	603	CLA	C4D-CHA-C1A	-4.23	116.10	121.25
23	c	911	CLA	CHC-C4B-NB	4.23	128.73	124.26
38	H	102	RRX	C24-C23-C22	-4.23	119.85	126.23
23	c	906	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
23	B	607	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
23	B	612	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
23	c	914	CLA	O2D-CGD-CBD	4.21	118.75	111.27
23	A	408	CLA	CHD-C4C-C3C	-4.21	118.65	124.84
23	B	616	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
40	v	203	HEC	CBC-CAC-C3C	4.20	124.02	112.43
23	c	914	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
23	B	616	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
23	C	510	CLA	C4D-CHA-C1A	-4.20	116.14	121.25
23	c	910	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
23	b	606	CLA	C4D-CHA-C1A	-4.20	116.14	121.25
23	c	913	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
23	c	910	CLA	CMB-C2B-C1B	4.19	131.76	125.37
23	a	407	CLA	C2D-C1D-ND	4.19	113.19	110.10
26	L	102	SQD	C3-C4-C5	4.19	117.72	110.24
26	a	417	SQD	O47-C7-C8	4.19	120.53	111.50
23	c	908	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
23	B	608	CLA	CHD-C4C-C3C	-4.19	118.69	124.84
23	B	604	CLA	CHC-C4B-NB	4.18	128.68	124.26
23	B	615	CLA	CMB-C2B-C1B	4.18	131.73	125.37
23	C	503	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
28	D	409	LHG	O8-C23-C24	4.17	124.99	111.91
23	b	607	CLA	CMB-C2B-C1B	4.16	131.71	125.37
23	C	508	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
23	a	407	CLA	O2D-CGD-CBD	4.16	118.66	111.27
23	b	603	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
23	c	902	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
23	c	905	CLA	C2C-C1C-NC	4.16	113.86	109.97
38	x	102	RRX	C33-C5-C6	-4.15	119.87	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
23	b	609	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
23	c	908	CLA	C2C-C1C-NC	4.15	113.86	109.97
23	a	406	CLA	C4-C3-C5	4.15	122.24	115.27
30	T	103	LMT	C1'-C2'-C3'	4.14	118.63	110.00
23	b	608	CLA	CAC-C3C-C4C	4.14	130.19	124.81
23	b	615	CLA	CMB-C2B-C1B	4.13	131.66	125.37
23	c	908	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
23	c	902	CLA	O2D-CGD-O1D	-4.13	115.76	123.84
23	c	911	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
23	D	404	CLA	C2C-C1C-NC	4.13	113.84	109.97
35	B	625	HTG	C1'-S1-C1	4.13	107.81	100.09
26	A	410	SQD	O3-C3-C4	4.13	119.89	110.35
25	B	618	BCR	C7-C8-C9	-4.13	120.00	126.23
23	a	410	CLA	C2B-C1B-NB	4.12	113.00	110.23
27	d	406	PL9	C40-C39-C41	4.12	122.21	115.27
23	a	406	CLA	CHC-C4B-NB	4.12	128.62	124.26
23	A	406	CLA	CHD-C1D-ND	-4.12	120.67	124.45
23	b	607	CLA	C4A-NA-C1A	4.12	108.56	106.71
26	A	415	SQD	C1-C2-C3	-4.12	101.42	110.00
23	B	605	CLA	O2D-CGD-O1D	-4.12	115.79	123.84
23	d	403	CLA	C4-C3-C5	4.12	122.20	115.27
23	B	610	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	b	609	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
23	c	911	CLA	O2D-CGD-CBD	4.11	118.57	111.27
23	B	602	CLA	C2C-C1C-NC	4.11	113.82	109.97
23	c	911	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
27	a	414	PL9	C53-C6-C1	4.10	123.37	114.99
28	d	408	LHG	O8-C23-O10	-4.10	113.25	123.59
23	B	608	CLA	C3D-C2D-C1D	-4.09	100.24	105.83
34	m	102	LMG	O7-C10-C11	4.09	120.32	111.50
23	c	911	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
23	C	510	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
23	C	504	CLA	C2C-C1C-NC	4.09	113.80	109.97
23	B	617	CLA	C4D-CHA-C1A	-4.09	116.27	121.25
23	c	903	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
23	C	513	CLA	C1-O2A-CGA	4.08	127.15	116.44
23	b	607	CLA	CHC-C4B-NB	4.08	128.57	124.26
23	d	403	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
23	c	902	CLA	C3B-C2B-C1B	-4.07	102.24	107.16
23	b	602	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
23	b	615	CLA	O2D-CGD-O1D	-4.07	115.88	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C3C-C4C-NC	4.07	115.14	110.57
23	C	514	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	b	606	CLA	CHA-C4D-ND	4.07	141.01	132.50
23	A	405	CLA	C4D-CHA-C1A	-4.07	116.30	121.25
23	C	509	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
23	c	904	CLA	C2B-C1B-NB	4.06	112.96	110.23
23	C	505	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
23	a	407	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
27	A	411	PL9	C30-C29-C31	4.06	122.11	115.27
23	A	406	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
23	c	906	CLA	CBC-CAC-C3C	-4.06	101.25	112.43
23	B	609	CLA	C4D-CHA-C1A	-4.06	116.31	121.25
23	d	401	CLA	CHD-C4C-C3C	-4.05	118.88	124.84
23	b	604	CLA	CAC-C3C-C4C	4.05	130.06	124.81
25	b	619	BCR	C29-C30-C25	4.05	116.71	110.48
23	B	610	CLA	CAC-C3C-C4C	4.05	130.06	124.81
23	b	606	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
28	d	408	LHG	O8-C23-C24	4.04	124.58	111.91
23	D	401	CLA	CMD-C2D-C3D	4.04	136.90	127.61
23	C	509	CLA	C2C-C1C-NC	4.04	113.75	109.97
23	a	406	CLA	CAC-C3C-C4C	4.03	130.04	124.81
23	D	404	CLA	C4D-CHA-C1A	-4.03	116.34	121.25
23	B	602	CLA	CMC-C2C-C1C	4.03	131.17	125.04
23	b	604	CLA	C4A-NA-C1A	4.02	108.52	106.71
23	b	609	CLA	C2D-C1D-ND	4.01	113.06	110.10
25	A	409	BCR	C38-C26-C25	-4.01	120.02	124.53
23	c	910	CLA	CHD-C1D-ND	-4.01	120.77	124.45
23	c	912	CLA	CHD-C1D-ND	-4.01	120.77	124.45
23	B	609	CLA	CHD-C4C-C3C	-4.01	118.95	124.84
25	D	405	BCR	C38-C26-C25	-4.01	120.03	124.53
23	A	405	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	C	508	CLA	CHD-C4C-C3C	-4.00	118.96	124.84
23	b	607	CLA	C1-O2A-CGA	4.00	126.94	116.44
23	c	910	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
23	a	407	CLA	CMD-C2D-C1D	4.00	131.76	124.71
23	B	612	CLA	CHC-C4B-NB	4.00	128.49	124.26
34	C	520	LMG	O7-C10-C11	4.00	120.11	111.50
23	b	611	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	b	603	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
27	d	406	PL9	C7-C8-C9	-3.98	120.16	126.79
23	B	609	CLA	C1D-ND-C4D	-3.98	103.50	106.33
35	B	625	HTG	C1-C2-C3	3.98	118.45	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
23	b	617	CLA	CHD-C1D-ND	-3.97	120.81	124.45
23	b	603	CLA	CHA-C4D-ND	3.97	140.80	132.50
35	V	204	HTG	C1-O5-C5	-3.97	105.27	112.58
23	B	606	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
23	D	401	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
23	b	606	CLA	CMC-C2C-C1C	3.96	131.08	125.04
23	D	404	CLA	CHC-C4B-NB	3.96	128.45	124.26
23	c	912	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
23	A	405	CLA	C4-C3-C5	3.96	121.93	115.27
30	a	418	LMT	C1-O1'-C1'	3.96	120.41	113.84
23	c	906	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
23	B	615	CLA	O2D-CGD-CBD	3.96	118.30	111.27
23	A	408	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
23	d	401	CLA	CHD-C1D-ND	-3.95	120.83	124.45
23	c	910	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
23	B	614	CLA	C4D-CHA-C1A	-3.94	116.45	121.25
23	A	406	CLA	CHD-C4C-C3C	-3.94	119.05	124.84
23	c	903	CLA	O2D-CGD-CBD	3.94	118.27	111.27
23	B	615	CLA	CAC-C3C-C4C	3.94	129.92	124.81
23	b	616	CLA	CHC-C4B-NB	3.93	128.42	124.26
23	B	603	CLA	CHD-C1D-ND	-3.93	120.84	124.45
23	c	912	CLA	C4D-CHA-C1A	-3.93	116.47	121.25
23	b	606	CLA	CHD-C4C-NC	3.93	130.39	124.20
23	B	614	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	C	502	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	b	608	CLA	O2D-CGD-CBD	3.92	118.24	111.27
30	b	621	LMT	O5'-C5'-C4'	3.92	118.02	109.75
23	B	604	CLA	C3D-C2D-C1D	-3.92	100.48	105.83
23	B	608	CLA	CED-O2D-CGD	3.92	124.79	115.94
23	C	512	CLA	C3B-C2B-C1B	-3.92	102.44	107.16
23	b	603	CLA	CHC-C4B-NB	3.92	128.40	124.26
23	C	505	CLA	C3D-C2D-C1D	-3.91	100.49	105.83
23	a	406	CLA	C3D-C2D-C1D	-3.91	100.49	105.83
23	C	507	CLA	C3D-C2D-C1D	-3.91	100.50	105.83
23	C	513	CLA	O2D-CGD-CBD	3.91	118.21	111.27
23	C	507	CLA	CHA-C4D-ND	3.90	140.66	132.50
23	B	604	CLA	C3B-C4B-NB	3.90	114.13	110.52
23	B	605	CLA	C2D-C1D-ND	3.90	112.98	110.10
38	H	102	RRX	C38-C26-C25	-3.90	120.15	124.53
23	D	403	CLA	CAC-C3C-C4C	3.90	129.86	124.81
23	B	602	CLA	C3D-C2D-C1D	-3.89	100.52	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C2B-C1B-NB	3.89	112.84	110.23
23	c	912	CLA	CHC-C4B-NB	3.89	128.38	124.26
28	D	411	LHG	O4-P-O5	3.89	131.47	112.24
23	b	608	CLA	C4D-CHA-C1A	-3.89	116.52	121.25
23	C	509	CLA	CAC-C3C-C4C	3.89	129.86	124.81
23	c	906	CLA	CHC-C4B-NB	3.89	128.37	124.26
23	c	907	CLA	C4D-CHA-C1A	-3.89	116.52	121.25
23	C	509	CLA	C3D-C4D-ND	3.88	116.52	110.24
23	d	404	CLA	CMD-C2D-C1D	3.88	131.56	124.71
23	b	602	CLA	C3B-C2B-C1B	-3.88	102.48	107.16
23	c	905	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
23	c	906	CLA	C2D-C1D-ND	3.88	112.96	110.10
25	A	409	BCR	C7-C8-C9	-3.87	120.38	126.23
23	a	406	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
26	L	102	SQD	O6-C1-C2	3.87	114.35	108.30
25	b	618	BCR	C33-C5-C6	-3.87	120.18	124.53
26	a	412	SQD	O5-C1-C2	-3.87	102.17	110.35
23	b	608	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
27	a	414	PL9	C37-C38-C39	-3.86	118.36	127.66
23	c	905	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
36	C	518	DGD	O2G-C1B-C2B	3.86	119.82	111.50
23	b	608	CLA	C4-C3-C5	3.86	121.76	115.27
23	d	401	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
23	b	617	CLA	O2D-CGD-CBD	3.86	118.12	111.27
23	C	510	CLA	C1-C2-C3	-3.85	119.38	126.04
23	C	514	CLA	C4D-CHA-C1A	-3.85	116.56	121.25
23	B	617	CLA	O2D-CGD-CBD	3.85	118.11	111.27
25	b	618	BCR	C24-C23-C22	-3.85	120.42	126.23
23	A	405	CLA	C3B-C4B-NB	3.85	114.08	110.52
35	B	631	HTG	C1'-S1-C1	3.84	107.28	100.09
23	C	506	CLA	CAC-C3C-C4C	3.84	129.79	124.81
28	e	101	LHG	O7-C7-C8	3.84	119.78	111.50
23	B	609	CLA	O2D-CGD-CBD	3.84	118.09	111.27
23	c	905	CLA	C4-C3-C5	3.84	121.73	115.27
23	b	614	CLA	CAC-C3C-C4C	3.84	129.79	124.81
23	B	612	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	b	609	CLA	O2D-CGD-CBD	3.84	118.08	111.27
23	B	616	CLA	CHC-C4B-NB	3.84	128.32	124.26
23	B	611	CLA	C3D-C2D-C1D	-3.84	100.60	105.83
23	b	602	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
23	b	604	CLA	C4-C3-C5	3.83	121.72	115.27
23	b	609	CLA	C1D-CHD-C4C	-3.83	117.80	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	905	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
27	A	411	PL9	C7-C3-C4	3.83	119.99	116.88
23	B	607	CLA	C4D-CHA-C1A	-3.83	116.59	121.25
23	B	606	CLA	C4-C3-C5	3.83	121.71	115.27
23	c	907	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
23	C	510	CLA	CHD-C4C-C3C	-3.82	119.23	124.84
35	V	204	HTG	O5-C1-S1	3.82	118.95	109.82
23	C	503	CLA	C3D-C2D-C1D	-3.81	100.62	105.83
23	D	404	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	A	406	CLA	C3B-C4B-NB	3.81	114.05	110.52
23	c	914	CLA	C2C-C1C-NC	3.81	113.54	109.97
23	B	603	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
23	c	902	CLA	CMB-C2B-C1B	3.81	131.17	125.37
26	B	621	SQD	O47-C7-C8	3.81	119.70	111.50
36	c	917	DGD	O5D-C6D-C5D	-3.80	102.01	109.05
23	B	604	CLA	CHC-C1C-NC	-3.80	118.43	124.20
23	B	611	CLA	CAA-CBA-CGA	-3.80	102.15	113.25
23	D	403	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
25	t	101	BCR	C28-C27-C26	-3.80	107.30	114.08
23	C	508	CLA	C4-C3-C5	3.80	121.66	115.27
23	c	908	CLA	CHD-C4C-NC	3.80	130.18	124.20
23	a	410	CLA	C3B-C2B-C1B	-3.79	102.58	107.16
23	D	401	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
23	c	909	CLA	C2A-C1A-CHA	-3.79	117.23	123.86
23	C	511	CLA	C2D-C1D-ND	3.79	112.90	110.10
23	B	603	CLA	O2D-CGD-CBD	3.79	118.00	111.27
23	B	603	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
23	c	904	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	b	604	CLA	CHC-C4B-NB	3.78	128.26	124.26
23	B	602	CLA	CMD-C2D-C1D	3.78	131.38	124.71
23	A	408	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
23	b	609	CLA	CHA-C4D-ND	3.78	140.41	132.50
23	c	913	CLA	CHD-C4C-NC	3.78	130.16	124.20
23	b	613	CLA	C3B-C2B-C1B	-3.78	102.60	107.16
23	d	404	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
23	d	404	CLA	CHC-C4B-NB	3.78	128.26	124.26
34	D	412	LMG	O7-C10-C11	3.78	119.64	111.50
34	C	520	LMG	O8-C28-C29	3.78	123.75	111.91
35	B	625	HTG	C1-O5-C5	3.77	119.54	112.58
23	A	406	CLA	C3D-C2D-C1D	-3.77	100.68	105.83
23	D	403	CLA	C3D-C2D-C1D	-3.77	100.69	105.83
23	c	911	CLA	CHD-C1D-ND	-3.77	120.99	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	O2D-CGD-CBD	3.76	117.96	111.27
23	B	607	CLA	C4B-CHC-C1C	-3.76	117.41	126.34
23	B	607	CLA	O2D-CGD-CBD	3.76	117.95	111.27
23	B	611	CLA	CHA-C4D-ND	3.76	140.36	132.50
23	B	605	CLA	CHD-C4C-C3C	-3.76	119.32	124.84
23	D	401	CLA	O2D-CGD-CBD	3.76	117.94	111.27
23	c	909	CLA	CHD-C4C-C3C	-3.75	119.32	124.84
23	b	610	CLA	CAC-C3C-C4C	3.75	129.68	124.81
23	b	616	CLA	C3D-C2D-C1D	-3.75	100.72	105.83
26	B	621	SQD	C1-O5-C5	-3.75	106.33	113.69
24	a	409	PHO	CMB-C2B-C3B	3.75	131.69	124.68
23	c	913	CLA	C3B-C2B-C1B	-3.75	102.64	107.16
23	C	513	CLA	C4D-CHA-C1A	-3.74	116.69	121.25
23	b	609	CLA	C3D-C2D-C1D	-3.74	100.72	105.83
23	c	912	CLA	CHD-C4C-NC	3.74	130.10	124.20
24	D	402	PHO	O2D-CGD-CBD	3.74	115.73	111.00
23	b	610	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	C	507	CLA	C3B-C2B-C1B	-3.73	102.65	107.16
23	B	613	CLA	C2B-C1B-NB	3.73	112.73	110.23
23	b	602	CLA	CHA-C4D-ND	3.73	140.30	132.50
23	C	512	CLA	C3D-C2D-C1D	-3.73	100.75	105.83
23	b	617	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
23	b	611	CLA	CHB-C1B-NB	-3.73	120.31	124.26
26	L	102	SQD	O9-S-C6	3.72	111.36	106.94
23	B	607	CLA	CMD-C2D-C1D	3.72	131.27	124.71
23	C	502	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
36	D	407	DGD	C3D-C4D-C5D	3.72	115.56	109.77
24	a	409	PHO	O2D-CGD-O1D	-3.72	116.57	123.84
23	C	508	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
23	B	604	CLA	C3C-C4C-NC	3.72	114.74	110.57
23	b	603	CLA	CHD-C4C-C3C	-3.71	119.38	124.84
23	b	612	CLA	CMD-C2D-C1D	3.71	131.25	124.71
23	B	605	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	d	401	CLA	C3D-C2D-C1D	-3.71	100.77	105.83
23	c	910	CLA	O2D-CGD-CBD	3.71	117.86	111.27
23	A	408	CLA	CMB-C2B-C1B	3.71	131.02	125.37
23	D	404	CLA	CHD-C1D-ND	-3.71	121.05	124.45
25	B	619	BCR	C29-C30-C25	3.71	116.19	110.48
23	C	506	CLA	C3B-C2B-C1B	-3.71	102.69	107.16
23	A	408	CLA	CHB-C4A-NA	3.71	129.64	124.51
23	b	603	CLA	C1-C2-C3	-3.71	119.63	126.04
23	B	610	CLA	O2D-CGD-CBD	3.70	117.85	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	405	BCR	C38-C26-C25	-3.70	120.37	124.53
23	d	404	CLA	CHD-C4C-NC	3.70	130.03	124.20
23	a	406	CLA	C2A-C1A-CHA	-3.70	117.40	123.86
23	c	909	CLA	C3D-C2D-C1D	-3.69	100.79	105.83
25	a	411	BCR	C38-C26-C25	-3.69	120.38	124.53
23	c	903	CLA	CHD-C4C-NC	3.69	130.02	124.20
34	c	920	LMG	O8-C28-C29	3.69	123.48	111.91
28	d	402	LHG	O7-C7-C8	3.69	119.45	111.50
23	B	610	CLA	C2A-C1A-CHA	-3.68	117.42	123.86
23	B	603	CLA	C3B-C2B-C1B	-3.68	102.72	107.16
23	b	616	CLA	CHA-C4D-ND	3.68	140.20	132.50
30	m	104	LMT	C1'-O5'-C5'	-3.68	106.46	113.69
23	b	607	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
34	B	622	LMG	O7-C10-C11	3.68	119.43	111.50
23	c	911	CLA	CHD-C4C-NC	3.67	129.99	124.20
23	C	506	CLA	C2B-C1B-NB	3.67	112.69	110.23
23	C	509	CLA	C4-C3-C5	3.66	121.43	115.27
23	C	509	CLA	CHD-C4C-C3C	-3.66	119.46	124.84
23	C	503	CLA	CMB-C2B-C1B	3.66	130.95	125.37
23	B	606	CLA	CHD-C1D-ND	-3.66	121.09	124.45
25	Y	101	BCR	C38-C26-C25	-3.65	120.42	124.53
23	c	905	CLA	CHD-C4C-C3C	-3.65	119.47	124.84
23	C	513	CLA	CED-O2D-CGD	3.65	124.20	115.94
34	c	930	LMG	O1-C1-C2	3.65	114.00	108.30
23	b	609	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
23	A	408	CLA	CAC-C3C-C4C	3.65	129.54	124.81
23	B	615	CLA	C3D-C2D-C1D	-3.65	100.85	105.83
23	b	606	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	c	914	CLA	C3D-C2D-C1D	-3.65	100.86	105.83
23	c	909	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
23	B	613	CLA	C2D-C1D-ND	3.64	112.79	110.10
23	c	905	CLA	C3B-C4B-NB	3.64	113.89	110.52
30	F	101	LMT	C2'-C3'-C4'	3.64	118.00	109.68
23	D	404	CLA	CAC-C3C-C4C	3.64	129.53	124.81
23	C	509	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
23	B	610	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	C	513	CLA	CHA-C4D-ND	3.63	140.10	132.50
26	D	408	SQD	C3-C4-C5	3.63	116.72	110.24
23	b	616	CLA	C4A-NA-C1A	3.63	108.34	106.71
23	C	503	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
26	A	415	SQD	O47-C7-C8	3.63	119.32	111.50
23	b	605	CLA	C3B-C2B-C1B	-3.63	102.78	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	105	HEM	CMD-C2D-C1D	3.63	130.56	125.04
23	A	406	CLA	O2D-CGD-CBD	3.62	117.71	111.27
23	B	602	CLA	C3B-C2B-C1B	-3.62	102.79	107.16
23	b	602	CLA	O2A-CGA-CBA	3.62	123.28	111.91
23	c	913	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	B	617	CLA	C3D-C2D-C1D	-3.62	100.89	105.83
23	b	605	CLA	CAC-C3C-C4C	3.62	129.51	124.81
34	c	920	LMG	C8-O7-C10	-3.62	108.88	117.79
23	B	602	CLA	C1D-ND-C4D	-3.62	103.76	106.33
23	c	902	CLA	CHD-C4C-NC	3.62	129.90	124.20
23	b	605	CLA	O2D-CGD-CBD	3.62	117.70	111.27
23	b	616	CLA	C2A-C1A-CHA	-3.62	117.54	123.86
23	b	612	CLA	C3B-C2B-C1B	-3.62	102.80	107.16
23	C	506	CLA	CHA-C4D-ND	3.61	140.06	132.50
25	b	620	BCR	C24-C23-C22	-3.61	120.78	126.23
36	h	102	DGD	O2G-C1B-C2B	3.61	119.28	111.50
23	c	914	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	B	610	CLA	C2B-C1B-NB	3.61	112.65	110.23
23	C	504	CLA	CMC-C2C-C1C	3.60	130.53	125.04
23	b	617	CLA	O1D-CGD-CBD	-3.60	117.11	124.48
23	C	507	CLA	CHC-C4B-NB	3.60	128.07	124.26
23	C	511	CLA	O2D-CGD-CBD	3.60	117.67	111.27
23	b	613	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
23	c	910	CLA	CMC-C2C-C1C	3.59	130.51	125.04
34	D	412	LMG	O1-C1-C2	3.59	113.91	108.30
23	a	410	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
23	b	611	CLA	CHA-C4D-ND	3.59	140.00	132.50
23	B	607	CLA	C3D-C2D-C1D	-3.59	100.94	105.83
25	c	915	BCR	C7-C8-C9	-3.58	120.82	126.23
23	b	603	CLA	O2D-CGD-CBD	3.58	117.63	111.27
23	C	512	CLA	CHA-C4D-ND	3.58	139.99	132.50
23	b	617	CLA	CAC-C3C-C4C	3.58	129.45	124.81
23	b	614	CLA	CMD-C2D-C1D	3.58	131.02	124.71
40	v	203	HEC	CBD-CAD-C3D	-3.58	102.69	112.63
23	b	604	CLA	CMC-C2C-C1C	3.57	130.48	125.04
23	B	615	CLA	CHA-C4D-ND	3.57	139.97	132.50
23	B	611	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
23	b	603	CLA	C4-C3-C5	3.57	121.27	115.27
23	B	608	CLA	C3B-C2B-C1B	-3.57	102.86	107.16
23	a	410	CLA	C3D-C2D-C1D	-3.56	100.97	105.83
27	d	406	PL9	C15-C14-C16	3.56	121.27	115.27
23	B	608	CLA	CBC-CAC-C3C	-3.56	102.61	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	913	CLA	C1-C2-C3	-3.56	119.88	126.04
23	b	608	CLA	C3B-C2B-C1B	-3.56	102.86	107.16
23	b	605	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	c	907	CLA	C3B-C2B-C1B	-3.56	102.87	107.16
23	b	613	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
23	c	908	CLA	C3B-C2B-C1B	-3.56	102.87	107.16
23	a	406	CLA	CHC-C1C-C2C	-3.56	116.85	126.73
23	b	610	CLA	C2B-C1B-NB	3.56	112.62	110.23
23	C	507	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
37	e	105	HEM	C4C-NC-C1C	3.55	108.83	105.35
23	b	610	CLA	C3B-C2B-C1B	-3.55	102.88	107.16
23	C	513	CLA	C3D-C2D-C1D	-3.55	100.99	105.83
23	C	513	CLA	C2C-C1C-NC	3.55	113.30	109.97
23	C	508	CLA	CHA-C4D-ND	3.55	139.92	132.50
23	B	615	CLA	C3B-C2B-C1B	-3.55	102.88	107.16
23	b	611	CLA	C4D-CHA-C1A	-3.54	116.94	121.25
23	a	410	CLA	C4-C3-C5	3.54	121.23	115.27
23	c	904	CLA	C4-C3-C5	3.54	121.22	115.27
23	B	602	CLA	C1-O2A-CGA	3.53	125.72	116.44
25	d	405	BCR	C39-C30-C25	-3.53	104.57	110.30
23	b	615	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
23	b	611	CLA	C3D-C2D-C1D	-3.53	101.01	105.83
23	b	616	CLA	CHD-C1D-ND	-3.53	121.21	124.45
23	b	617	CLA	C3B-C4B-NB	3.53	113.79	110.52
23	C	502	CLA	C3B-C2B-C1B	-3.53	102.90	107.16
26	x	101	SQD	O48-C23-C24	3.53	122.97	111.91
36	H	103	DGD	O2G-C1B-C2B	3.52	119.10	111.50
23	D	401	CLA	C4-C3-C5	3.52	121.20	115.27
35	d	413	HTG	O5-C1-C2	3.52	114.75	110.31
23	B	609	CLA	CHA-C4D-ND	3.52	139.87	132.50
23	b	611	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	A	408	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	C	508	CLA	C4D-CHA-C1A	-3.52	116.97	121.25
23	c	902	CLA	O2D-CGD-CBD	3.52	117.52	111.27
25	T	101	BCR	C15-C16-C17	-3.52	116.27	123.47
26	x	101	SQD	C1-O5-C5	3.52	120.59	113.69
23	d	403	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
37	e	105	HEM	CBA-CAA-C2A	-3.51	102.86	112.63
26	L	102	SQD	O48-C23-C24	3.51	122.93	111.91
23	b	615	CLA	O2A-CGA-O1A	-3.51	114.73	123.59
23	C	506	CLA	CMC-C2C-C1C	3.51	130.38	125.04
23	B	605	CLA	C3C-C4C-NC	3.50	114.50	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C15-C16-C17	-3.50	116.30	123.47
26	A	415	SQD	O48-C23-C24	3.50	122.89	111.91
34	a	413	LMG	O8-C28-C29	3.50	122.89	111.91
23	B	609	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
23	b	603	CLA	C3B-C2B-C1B	-3.49	102.94	107.16
23	C	514	CLA	C2D-C1D-ND	3.49	112.68	110.10
23	A	405	CLA	C3B-C2B-C1B	-3.49	102.95	107.16
23	B	605	CLA	C2B-C1B-NB	3.49	112.57	110.23
23	C	511	CLA	CHC-C4B-NB	3.49	127.95	124.26
23	B	613	CLA	O2D-CGD-CBD	3.48	117.46	111.27
23	B	610	CLA	C1-C2-C3	-3.48	120.02	126.04
23	B	606	CLA	C1D-ND-C4D	-3.48	103.86	106.33
23	B	609	CLA	C3B-C4B-NB	3.48	113.74	110.52
23	B	605	CLA	C3D-C2D-C1D	-3.48	101.08	105.83
23	B	617	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	b	606	CLA	O2D-CGD-CBD	3.48	117.45	111.27
23	C	506	CLA	O2D-CGD-CBD	3.48	117.44	111.27
23	B	614	CLA	CHC-C4B-NB	3.48	127.94	124.26
23	b	604	CLA	C3C-C4C-NC	3.47	114.47	110.57
23	c	911	CLA	C3C-C4C-NC	3.47	114.47	110.57
23	b	612	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
23	b	603	CLA	CHC-C1C-NC	-3.47	118.94	124.20
34	a	413	LMG	O7-C10-C11	3.47	118.98	111.50
25	T	101	BCR	C23-C24-C25	-3.47	117.46	127.20
23	b	617	CLA	C4-C3-C5	3.47	121.11	115.27
25	T	101	BCR	C35-C13-C12	3.47	123.54	118.08
23	B	602	CLA	CMB-C2B-C1B	3.46	130.65	125.37
23	B	612	CLA	C3B-C2B-C1B	-3.46	102.98	107.16
23	a	410	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
23	B	604	CLA	C1D-ND-C4D	-3.46	103.88	106.33
23	c	905	CLA	CMD-C2D-C1D	3.46	130.81	124.71
23	a	406	CLA	C5-C3-C2	-3.46	114.12	121.12
23	c	903	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
23	b	609	CLA	O2A-CGA-O1A	-3.46	114.87	123.59
23	c	904	CLA	CHA-C4D-ND	3.46	139.73	132.50
23	c	914	CLA	O2A-CGA-CBA	3.46	122.75	111.91
23	c	912	CLA	C1-O2A-CGA	3.45	125.51	116.44
23	B	614	CLA	CAC-C3C-C4C	3.45	129.29	124.81
23	B	610	CLA	CHA-C4D-ND	3.45	139.72	132.50
23	B	607	CLA	CHD-C4C-NC	3.45	129.64	124.20
26	B	621	SQD	O5-C5-C4	-3.45	103.43	109.69
23	C	513	CLA	C1C-C2C-C3C	-3.45	103.33	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E	101	LHG	O8-C23-C24	3.45	122.73	111.91
23	D	404	CLA	C3D-C2D-C1D	-3.45	101.12	105.83
23	B	616	CLA	CHA-C4D-ND	3.45	139.71	132.50
23	C	509	CLA	C3B-C2B-C1B	-3.45	103.00	107.16
23	b	603	CLA	CMC-C2C-C1C	3.45	130.29	125.04
25	a	411	BCR	C24-C23-C22	-3.45	121.03	126.23
38	H	102	RRX	C7-C8-C9	-3.45	121.03	126.23
23	B	606	CLA	CHA-C4D-ND	3.44	139.70	132.50
36	h	102	DGD	O1G-C1A-O1A	-3.44	114.91	123.59
23	B	602	CLA	CHB-C1B-NB	-3.44	120.61	124.26
23	b	606	CLA	C3C-C4C-NC	3.44	114.43	110.57
23	d	403	CLA	C3B-C4B-NB	3.44	113.71	110.52
23	c	904	CLA	C3B-C2B-C1B	-3.44	103.01	107.16
23	b	610	CLA	O2D-CGD-CBD	3.44	117.38	111.27
23	b	611	CLA	CHD-C4C-C3C	-3.44	119.79	124.84
23	c	907	CLA	CHA-C4D-ND	3.44	139.69	132.50
23	C	507	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
23	C	512	CLA	CHD-C1D-ND	-3.44	121.30	124.45
28	L	101	LHG	O4-P-O5	3.44	129.22	112.24
26	D	408	SQD	O9-S-C6	3.43	111.02	106.94
23	B	606	CLA	CHC-C4B-NB	3.43	127.89	124.26
23	b	616	CLA	CAC-C3C-C4C	3.43	129.26	124.81
23	C	505	CLA	CMB-C2B-C1B	3.43	130.60	125.37
23	b	602	CLA	C3D-C2D-C1D	-3.43	101.15	105.83
23	B	614	CLA	C3B-C4B-NB	3.43	113.70	110.52
23	b	610	CLA	C4A-NA-C1A	3.43	108.25	106.71
38	H	102	RRX	C10-C11-C12	-3.43	112.52	123.22
23	C	514	CLA	CHA-C4D-ND	3.43	139.67	132.50
23	c	908	CLA	C4D-CHA-C1A	-3.43	117.08	121.25
23	c	907	CLA	CHD-C4C-NC	3.42	129.60	124.20
23	C	508	CLA	CBC-CAC-C3C	-3.42	103.00	112.43
23	C	506	CLA	C4D-CHA-C1A	-3.42	117.09	121.25
23	B	617	CLA	C3C-C4C-NC	3.42	114.41	110.57
23	C	503	CLA	CMD-C2D-C1D	3.42	130.74	124.71
35	b	622	HTG	C1-C2-C3	3.42	117.34	110.59
23	b	613	CLA	C1D-ND-C4D	-3.42	103.91	106.33
23	C	507	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
23	c	903	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
23	b	605	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
35	b	622	HTG	C1-O5-C5	3.41	118.86	112.58
23	b	602	CLA	C1D-ND-C4D	-3.41	103.92	106.33
23	b	616	CLA	C3B-C2B-C1B	-3.40	103.06	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	408	SQD	C44-O6-C1	-3.40	107.09	113.74
23	C	509	CLA	C5-C3-C2	-3.40	114.24	121.12
23	b	605	CLA	C4D-CHA-C1A	-3.40	117.11	121.25
23	A	405	CLA	CHD-C4C-C3C	-3.40	119.85	124.84
23	C	503	CLA	CHD-C1D-ND	-3.39	121.34	124.45
23	b	612	CLA	C3D-C2D-C1D	-3.39	101.20	105.83
23	B	617	CLA	CHA-C4D-ND	3.39	139.59	132.50
23	C	504	CLA	O2D-CGD-CBD	3.39	117.28	111.27
36	D	407	DGD	C3G-O3G-C1D	3.39	120.35	113.74
23	b	611	CLA	C4A-NA-C1A	3.39	108.23	106.71
23	a	407	CLA	C1-C2-C3	-3.39	120.19	126.04
23	B	613	CLA	CAC-C3C-C2C	-3.38	121.74	127.53
23	B	603	CLA	CHA-C4D-ND	3.38	139.57	132.50
38	x	102	RRX	C16-C17-C18	-3.38	122.49	127.31
36	C	518	DGD	O2G-C1B-O1B	-3.37	115.55	123.70
28	L	101	LHG	O7-C7-C8	3.37	118.77	111.50
24	A	407	PHO	CMB-C2B-C3B	3.37	130.99	124.68
23	B	606	CLA	C1-C2-C3	-3.37	120.21	126.04
23	B	612	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
23	B	605	CLA	CAC-C3C-C4C	3.37	129.19	124.81
23	b	612	CLA	O2D-CGD-CBD	3.37	117.26	111.27
23	c	913	CLA	C1-O2A-CGA	3.37	125.28	116.44
23	c	909	CLA	CMB-C2B-C1B	3.37	130.50	125.37
23	b	611	CLA	O2D-CGD-CBD	3.37	117.25	111.27
26	x	101	SQD	O47-C7-C8	3.37	120.19	110.80
23	c	914	CLA	CHD-C4C-NC	3.36	129.50	124.20
23	c	910	CLA	CHB-C1B-NB	-3.36	120.70	124.26
23	D	404	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
23	c	911	CLA	C3D-C2D-C1D	-3.36	101.25	105.83
23	a	410	CLA	CHA-C4D-ND	3.36	139.53	132.50
23	C	504	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
23	c	911	CLA	C4A-NA-C1A	3.36	108.22	106.71
23	d	403	CLA	C2A-C1A-CHA	-3.36	117.99	123.86
23	C	507	CLA	CHD-C4C-NC	3.35	129.49	124.20
23	b	613	CLA	O2D-CGD-CBD	3.35	117.23	111.27
23	C	504	CLA	C4-C3-C5	3.35	120.91	115.27
23	B	602	CLA	C4D-CHA-C1A	-3.35	117.17	121.25
23	c	913	CLA	CBC-CAC-C3C	-3.35	103.20	112.43
23	C	509	CLA	CHB-C4A-NA	3.35	129.14	124.51
23	C	502	CLA	C4D-CHA-C1A	-3.34	117.18	121.25
26	A	410	SQD	O47-C7-O49	-3.34	115.62	123.70
23	b	610	CLA	C3C-C4C-NC	3.34	114.32	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	C3B-C4B-NB	3.34	113.62	110.52
23	B	609	CLA	C4A-NA-C1A	3.34	108.21	106.71
23	B	604	CLA	C2A-C1A-CHA	-3.34	118.02	123.86
23	C	502	CLA	C2A-C1A-CHA	-3.34	118.02	123.86
23	C	506	CLA	CHD-C1D-ND	-3.34	121.39	124.45
23	C	514	CLA	C2A-C1A-CHA	-3.34	118.02	123.86
23	B	608	CLA	C1-C2-C3	-3.34	120.27	126.04
23	A	406	CLA	C1D-ND-C4D	-3.33	103.97	106.33
23	b	616	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	c	914	CLA	C3C-C4C-NC	3.33	114.31	110.57
24	A	407	PHO	O2D-CGD-O1D	-3.33	117.33	123.84
23	B	604	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	C	507	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	b	607	CLA	CAC-C3C-C4C	3.33	129.13	124.81
23	c	909	CLA	C2C-C1C-NC	3.33	113.09	109.97
23	b	607	CLA	C3B-C2B-C1B	-3.32	103.15	107.16
23	C	507	CLA	C3C-C4C-NC	3.32	114.30	110.57
23	c	904	CLA	C1-C2-C3	-3.32	120.30	126.04
23	B	616	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
23	B	604	CLA	C3B-C2B-C1B	-3.32	103.15	107.16
23	A	408	CLA	CHB-C1B-NB	-3.32	120.74	124.26
23	c	903	CLA	CHD-C1D-ND	-3.32	121.40	124.45
24	a	409	PHO	C4-C3-C5	3.32	120.85	115.27
23	B	604	CLA	C4A-NA-C1A	3.32	108.20	106.71
23	d	401	CLA	CHA-C4D-ND	3.32	139.44	132.50
23	c	908	CLA	CBC-CAC-C3C	-3.32	103.29	112.43
23	b	612	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
23	B	612	CLA	O2D-CGD-CBD	3.32	117.16	111.27
25	D	405	BCR	C36-C18-C19	3.31	123.30	118.08
23	b	613	CLA	CMC-C2C-C1C	3.31	130.09	125.04
23	c	907	CLA	C2A-C1A-CHA	-3.31	118.07	123.86
23	b	613	CLA	C3D-C2D-C1D	-3.31	101.31	105.83
27	a	414	PL9	C3-C4-C5	3.31	122.91	118.60
23	C	514	CLA	O2D-CGD-CBD	3.31	117.15	111.27
23	C	514	CLA	CHD-C4C-C3C	-3.31	119.98	124.84
23	A	405	CLA	CMD-C2D-C3D	3.31	135.22	127.61
23	C	503	CLA	C16-C17-C18	-3.30	100.41	115.98
23	B	611	CLA	C3B-C2B-C1B	-3.30	103.17	107.16
36	d	407	DGD	C3D-C4D-C5D	3.30	114.92	109.77
23	B	611	CLA	CHB-C1B-NB	-3.30	120.76	124.26
23	C	503	CLA	CHA-C4D-ND	3.30	139.40	132.50
23	c	910	CLA	C3D-C2D-C1D	-3.30	101.33	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	410	CLA	C3C-C4C-NC	3.30	114.27	110.57
23	B	605	CLA	CED-O2D-CGD	3.30	123.39	115.94
25	d	405	BCR	C15-C14-C13	-3.30	122.61	127.31
23	c	912	CLA	C3D-C2D-C1D	-3.29	101.33	105.83
23	b	615	CLA	C2C-C1C-NC	3.29	113.06	109.97
23	A	406	CLA	CHB-C1B-NB	-3.29	120.78	124.26
26	L	102	SQD	C4-C3-C2	3.29	116.56	110.82
23	b	614	CLA	CHD-C4C-NC	3.29	129.38	124.20
23	C	512	CLA	CHD-C4C-C3C	-3.29	120.01	124.84
35	v	204	HTG	O3-C3-C2	3.28	117.94	110.35
23	C	508	CLA	CMC-C2C-C1C	3.28	130.04	125.04
23	B	615	CLA	C3B-C4B-NB	3.28	113.56	110.52
25	D	405	BCR	C29-C30-C25	3.28	115.53	110.48
23	b	610	CLA	CHA-C4D-ND	3.28	139.36	132.50
36	c	919	DGD	O3G-C3G-C2G	-3.27	103.00	110.90
23	B	615	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	C	510	CLA	CAC-C3C-C4C	3.26	129.04	124.81
25	B	620	BCR	C23-C24-C25	-3.26	118.04	127.20
23	B	613	CLA	C4-C3-C5	3.26	120.76	115.27
23	b	617	CLA	C2C-C1C-NC	3.26	113.03	109.97
36	H	103	DGD	O1G-C1A-C2A	3.26	122.14	111.91
25	C	530	BCR	C11-C10-C9	-3.26	122.66	127.31
23	C	509	CLA	CHD-C1D-ND	-3.26	121.46	124.45
23	C	511	CLA	CMB-C2B-C1B	3.25	130.33	125.37
25	b	619	BCR	C38-C26-C25	-3.25	120.87	124.53
23	c	913	CLA	CMD-C2D-C1D	3.25	130.44	124.71
23	b	608	CLA	CHD-C4C-NC	3.25	129.32	124.20
34	C	501	LMG	O1-C1-C2	3.25	113.38	108.30
25	B	620	BCR	C33-C5-C6	-3.25	120.88	124.53
23	C	505	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
28	D	409	LHG	O4-P-O5	3.25	128.28	112.24
25	j	104	BCR	C38-C26-C25	-3.24	120.89	124.53
23	B	617	CLA	C4A-NA-C1A	3.24	108.16	106.71
23	B	602	CLA	CHC-C4B-NB	3.24	127.69	124.26
23	B	603	CLA	CHD-C4C-NC	3.24	129.30	124.20
23	C	511	CLA	C3B-C2B-C1B	-3.23	103.26	107.16
23	b	615	CLA	CMD-C2D-C1D	3.23	130.41	124.71
34	c	920	LMG	O7-C10-C11	3.23	118.47	111.50
24	a	409	PHO	CMA-C3A-C4A	-3.23	107.30	114.38
23	C	504	CLA	CHD-C4C-NC	3.23	129.30	124.20
40	v	203	HEC	C2A-C1A-NA	-3.23	107.18	110.32
23	b	612	CLA	C1D-ND-C4D	-3.23	104.04	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	406	PL9	C3-C4-C5	3.23	122.80	118.60
23	B	607	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
25	A	409	BCR	C15-C16-C17	-3.23	116.86	123.47
23	C	510	CLA	C4-C3-C5	3.23	120.70	115.27
23	B	609	CLA	C1D-CHD-C4C	-3.23	119.10	126.06
23	A	408	CLA	C5-C3-C2	-3.22	114.59	121.12
25	a	411	BCR	C15-C16-C17	-3.22	116.87	123.47
23	a	407	CLA	O2A-CGA-CBA	3.22	122.02	111.91
23	C	505	CLA	C4-C3-C5	3.22	120.69	115.27
23	b	607	CLA	C1D-ND-C4D	-3.22	104.05	106.33
25	C	530	BCR	C33-C5-C6	-3.22	120.91	124.53
23	d	403	CLA	CHC-C4B-NB	3.22	127.66	124.26
23	C	502	CLA	CHC-C4B-NB	3.22	127.66	124.26
23	B	605	CLA	CHD-C1D-ND	-3.22	121.50	124.45
23	c	903	CLA	C1D-ND-C4D	-3.22	104.05	106.33
23	b	602	CLA	CMB-C2B-C1B	3.22	130.27	125.37
23	D	404	CLA	CBC-CAC-C3C	-3.22	103.57	112.43
23	b	615	CLA	C2A-C1A-CHA	-3.21	118.25	123.86
23	B	608	CLA	CAC-C3C-C4C	3.21	128.97	124.81
25	d	405	BCR	C29-C30-C25	3.21	115.42	110.48
23	B	602	CLA	O1D-CGD-CBD	-3.20	117.93	124.48
23	C	505	CLA	CHA-C4D-ND	3.20	139.20	132.50
23	B	611	CLA	O2A-CGA-O1A	-3.20	115.51	123.59
23	C	502	CLA	CHD-C4C-NC	3.20	129.25	124.20
25	T	101	BCR	C7-C8-C9	-3.20	121.41	126.23
23	C	508	CLA	C2D-C1D-ND	3.19	112.46	110.10
23	B	604	CLA	C4D-CHA-C1A	-3.19	117.36	121.25
23	C	508	CLA	C3D-C2D-C1D	-3.19	101.47	105.83
24	D	402	PHO	CMA-C3A-C4A	-3.19	107.39	114.38
40	V	203	HEC	CMD-C2D-C1D	3.19	129.90	125.04
23	b	615	CLA	CHD-C4C-C3C	-3.19	120.15	124.84
24	D	402	PHO	CED-O2D-CGD	3.19	123.15	115.94
23	b	603	CLA	C1-O2A-CGA	3.19	124.81	116.44
25	d	405	BCR	C11-C10-C9	-3.19	122.76	127.31
25	C	530	BCR	C38-C26-C25	-3.19	120.95	124.53
23	d	401	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
23	A	408	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
23	C	506	CLA	C1D-ND-C4D	3.18	108.60	106.33
23	B	606	CLA	CMC-C2C-C1C	3.18	129.89	125.04
23	c	911	CLA	CHA-C4D-ND	3.18	139.15	132.50
23	B	605	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	B	611	CLA	CAC-C3C-C2C	3.18	132.97	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	PL9	C37-C36-C34	-3.18	102.53	112.98
23	c	909	CLA	C7-C6-C5	-3.17	104.74	113.36
23	b	611	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
23	C	512	CLA	CHB-C1B-NB	-3.17	120.90	124.26
23	B	610	CLA	C3B-C2B-C1B	-3.17	103.33	107.16
24	a	408	PHO	O2D-CGD-O1D	-3.17	117.64	123.84
23	A	405	CLA	C2A-C1A-CHA	-3.17	118.32	123.86
37	E	105	HEM	CHC-C4B-NB	3.17	127.86	124.42
28	e	101	LHG	O8-C23-C24	3.17	121.85	111.91
23	B	617	CLA	CMB-C2B-C1B	3.17	130.19	125.37
24	a	409	PHO	C4B-NB-C1B	-3.16	103.93	108.83
23	B	612	CLA	CHA-C4D-ND	3.16	139.12	132.50
23	b	602	CLA	CHD-C1D-ND	-3.16	121.55	124.45
23	c	903	CLA	CMB-C2B-C1B	3.16	130.19	125.37
23	C	502	CLA	CMD-C2D-C1D	3.16	130.29	124.71
35	b	627	HTG	C2'-C1'-S1	-3.16	102.19	112.40
23	b	611	CLA	CMC-C2C-C1C	3.16	129.85	125.04
23	c	908	CLA	CMB-C2B-C1B	3.16	130.18	125.37
23	c	905	CLA	O2D-CGD-CBD	3.16	116.88	111.27
23	a	407	CLA	C4D-CHA-C1A	-3.16	117.41	121.25
23	B	611	CLA	C3C-C4C-NC	3.16	114.11	110.57
23	B	617	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	B	609	CLA	CAC-C3C-C4C	3.16	128.91	124.81
23	b	617	CLA	C3D-C2D-C1D	-3.16	101.53	105.83
23	C	502	CLA	CHA-C4D-ND	3.15	139.10	132.50
23	C	510	CLA	C3C-C4C-NC	3.15	114.11	110.57
23	C	505	CLA	CHD-C4C-NC	3.15	129.17	124.20
23	B	604	CLA	CHD-C4C-NC	3.15	129.17	124.20
36	D	407	DGD	O1G-C1A-O1A	-3.15	115.64	123.59
23	B	606	CLA	CHD-C4C-NC	3.15	129.16	124.20
23	A	408	CLA	CHC-C4B-NB	3.15	127.59	124.26
23	a	406	CLA	O2A-CGA-CBA	3.14	121.78	111.91
23	B	613	CLA	CMC-C2C-C1C	3.14	129.83	125.04
23	c	910	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
23	C	506	CLA	O2A-CGA-O1A	-3.14	115.66	123.59
23	c	914	CLA	CMC-C2C-C1C	3.14	129.82	125.04
25	C	515	BCR	C15-C14-C13	-3.14	122.83	127.31
25	c	915	BCR	C20-C21-C22	-3.14	122.83	127.31
23	B	614	CLA	O2A-CGA-CBA	3.14	121.76	111.91
23	b	616	CLA	CHD-C4C-NC	3.14	129.15	124.20
23	b	603	CLA	C1D-ND-C4D	-3.13	104.11	106.33
23	C	514	CLA	C3D-C2D-C1D	-3.13	101.56	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	412	LMG	C1-C2-C3	-3.13	103.47	110.00
27	A	411	PL9	C3-C4-C5	3.13	122.67	118.60
23	d	404	CLA	O2D-CGD-CBD	3.13	116.83	111.27
25	Y	101	BCR	C7-C8-C9	-3.13	121.51	126.23
23	b	606	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	D	404	CLA	C2A-C1A-CHA	-3.13	118.39	123.86
23	C	505	CLA	CMD-C2D-C1D	3.13	130.22	124.71
23	d	404	CLA	C4A-NA-C1A	3.13	108.11	106.71
23	d	401	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	c	913	CLA	C4D-CHA-C1A	-3.12	117.45	121.25
23	b	617	CLA	CHA-C4D-ND	3.12	139.03	132.50
23	d	401	CLA	CBC-CAC-C3C	-3.12	103.83	112.43
23	b	617	CLA	O2A-CGA-CBA	3.11	121.68	111.91
23	B	614	CLA	CHD-C4C-NC	3.11	129.11	124.20
34	B	622	LMG	C9-C8-C7	-3.11	104.42	111.79
23	b	606	CLA	C1D-CHD-C4C	-3.11	119.34	126.06
23	B	613	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
24	D	402	PHO	C4B-NB-C1B	-3.11	104.01	108.83
25	B	620	BCR	C2-C1-C6	3.11	115.27	110.48
23	d	403	CLA	CAC-C3C-C4C	3.11	128.85	124.81
23	B	610	CLA	CED-O2D-CGD	3.11	122.97	115.94
23	b	616	CLA	C4-C3-C5	3.11	120.50	115.27
23	D	403	CLA	C4D-CHA-C1A	-3.11	117.47	121.25
23	c	911	CLA	CMB-C2B-C1B	3.11	130.10	125.37
23	c	909	CLA	CHB-C1B-NB	-3.11	120.97	124.26
25	T	101	BCR	C12-C13-C14	-3.10	114.18	118.94
23	A	406	CLA	C3C-C4C-NC	3.10	114.05	110.57
23	C	508	CLA	CMD-C2D-C1D	3.10	130.18	124.71
23	c	914	CLA	C1D-ND-C4D	-3.10	104.13	106.33
34	c	920	LMG	O1-C7-C8	-3.10	103.42	110.90
23	b	605	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	C	513	CLA	C4-C3-C5	3.10	120.48	115.27
23	C	511	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
23	b	604	CLA	CMD-C2D-C1D	3.10	130.17	124.71
34	C	520	LMG	O6-C5-C6	3.10	114.14	106.44
30	A	416	LMT	O1'-C1'-C2'	3.10	113.14	108.30
37	e	105	HEM	C4A-NA-C1A	3.09	108.38	105.35
23	b	610	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
35	B	625	HTG	C4-C3-C2	3.09	116.22	110.82
23	C	509	CLA	CHC-C4B-NB	3.09	127.53	124.26
23	C	503	CLA	C3B-C4B-NB	3.09	113.38	110.52
36	c	917	DGD	O3G-C3G-C2G	-3.09	103.45	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C3D-C2D-C1D	-3.09	101.62	105.83
23	c	906	CLA	CHA-C4D-ND	3.08	138.95	132.50
23	D	401	CLA	CHA-C4D-ND	3.08	138.95	132.50
23	C	514	CLA	O2A-CGA-CBA	3.08	121.58	111.91
26	B	621	SQD	O9-S-C6	3.08	110.60	106.94
23	C	503	CLA	CAC-C3C-C4C	3.08	128.80	124.81
23	B	611	CLA	CHD-C4C-NC	3.08	129.05	124.20
23	B	611	CLA	CHC-C4B-NB	3.07	127.51	124.26
23	c	903	CLA	C4D-CHA-C1A	-3.07	117.51	121.25
35	B	625	HTG	O4-C4-C5	3.07	116.92	109.30
23	B	606	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
23	C	508	CLA	CHD-C4C-NC	3.07	129.04	124.20
23	B	615	CLA	C1D-ND-C4D	-3.07	104.16	106.33
23	d	403	CLA	C4D-CHA-C1A	-3.07	117.52	121.25
23	c	907	CLA	CHB-C1B-NB	-3.07	121.01	124.26
23	c	910	CLA	CHD-C4C-NC	3.07	129.03	124.20
23	B	602	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	b	611	CLA	CHD-C1D-ND	-3.06	121.64	124.45
23	b	616	CLA	CMD-C2D-C3D	3.06	134.66	127.61
36	c	917	DGD	O2G-C1B-C2B	3.06	118.10	111.50
23	c	906	CLA	CHD-C4C-NC	3.06	129.03	124.20
23	b	609	CLA	C4A-NA-C1A	3.06	108.08	106.71
23	C	510	CLA	O2A-CGA-CBA	3.06	121.51	111.91
23	b	603	CLA	CMB-C2B-C3B	3.06	133.99	126.59
28	d	409	LHG	O7-C7-O9	-3.06	116.31	123.70
34	d	411	LMG	O6-C5-C6	3.05	114.03	106.44
23	b	606	CLA	C1-C2-C3	-3.05	120.77	126.04
23	d	403	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
37	E	105	HEM	C3B-C2B-C1B	3.05	108.75	106.49
25	C	515	BCR	C32-C1-C6	-3.05	105.36	110.30
23	C	507	CLA	C1-C2-C3	-3.05	120.77	126.04
23	c	902	CLA	C3B-C4B-NB	3.05	113.34	110.52
23	B	608	CLA	C3B-C4B-NB	3.05	113.34	110.52
23	c	906	CLA	C3D-C2D-C1D	-3.04	101.68	105.83
23	B	613	CLA	C3B-C2B-C1B	-3.04	103.49	107.16
23	c	904	CLA	CHD-C4C-NC	3.04	129.00	124.20
23	C	512	CLA	O2D-CGD-CBD	3.04	116.67	111.27
23	c	902	CLA	CMC-C2C-C1C	3.04	129.67	125.04
23	D	404	CLA	CHA-C4D-ND	3.04	138.86	132.50
23	B	602	CLA	C1D-CHD-C4C	-3.04	119.51	126.06
36	C	517	DGD	O5D-C6D-C5D	-3.03	103.43	109.05
23	C	514	CLA	CHB-C1B-NB	-3.03	121.05	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	CBC-CAC-C3C	-3.03	104.07	112.43
23	A	408	CLA	C2A-C1A-CHA	-3.03	118.56	123.86
24	a	408	PHO	O2D-CGD-CBD	3.03	114.84	111.00
23	D	404	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	B	603	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
23	a	407	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
23	b	605	CLA	C6-C5-C3	-3.03	105.52	113.45
23	B	609	CLA	CMC-C2C-C1C	3.03	129.65	125.04
23	C	513	CLA	C3C-C4C-NC	3.02	113.96	110.57
40	V	203	HEC	CBC-CAC-C3C	3.02	120.76	112.43
26	L	102	SQD	O5-C1-C2	-3.02	103.95	110.35
23	c	911	CLA	CHB-C1B-NB	-3.02	121.06	124.26
23	B	603	CLA	C3D-C2D-C1D	-3.02	101.71	105.83
40	V	203	HEC	CBD-CAD-C3D	-3.02	104.23	112.63
23	a	406	CLA	C3B-C2B-C1B	-3.02	103.52	107.16
25	j	104	BCR	C33-C5-C6	-3.02	121.14	124.53
28	d	409	LHG	O7-C7-C8	3.02	118.01	111.50
36	h	102	DGD	O3G-C1D-C2D	3.02	113.02	108.30
23	D	401	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
23	b	608	CLA	CHA-C4D-ND	3.02	138.81	132.50
23	c	906	CLA	O2D-CGD-CBD	3.02	116.63	111.27
25	Y	101	BCR	C24-C23-C22	-3.02	121.68	126.23
23	D	403	CLA	O2D-CGD-CBD	3.02	116.63	111.27
23	C	509	CLA	CMD-C2D-C1D	3.02	130.03	124.71
23	B	609	CLA	C3B-C2B-C1B	-3.02	103.52	107.16
23	B	613	CLA	C3D-C2D-C1D	-3.01	101.72	105.83
23	a	406	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	b	602	CLA	C5-C3-C2	-3.01	115.03	121.12
23	C	512	CLA	C4D-CHA-C1A	-3.01	117.59	121.25
23	D	401	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
28	d	409	LHG	O8-C23-O10	-3.00	116.02	123.59
23	b	604	CLA	C3B-C2B-C1B	-3.00	103.54	107.16
37	e	105	HEM	CBD-CAD-C3D	-3.00	104.30	112.63
23	B	610	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
25	C	516	BCR	C37-C22-C23	3.00	122.80	118.08
23	c	909	CLA	CHC-C4B-NB	2.99	127.42	124.26
23	c	908	CLA	CHA-C4D-ND	2.99	138.76	132.50
23	B	613	CLA	CHD-C4C-C3C	-2.99	120.45	124.84
30	a	422	LMT	C1B-O5B-C5B	2.99	119.55	113.69
23	D	404	CLA	CMD-C2D-C1D	2.99	129.98	124.71
23	b	610	CLA	CHB-C1B-NB	-2.98	121.10	124.26
36	c	918	DGD	O2G-C1B-O1B	-2.98	116.49	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Z	101	LMT	C1'-O5'-C5'	2.98	119.55	113.69
23	B	617	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
23	b	617	CLA	C4D-CHA-C1A	-2.98	117.62	121.25
27	A	411	PL9	C25-C24-C26	2.98	120.29	115.27
23	a	407	CLA	CHD-C1D-ND	-2.98	121.71	124.45
40	V	203	HEC	C3B-C4B-NB	-2.98	106.85	110.17
23	C	505	CLA	C4D-CHA-C1A	-2.98	117.62	121.25
23	d	404	CLA	CHB-C1B-NB	-2.98	121.10	124.26
23	a	406	CLA	CHC-C1C-NC	2.98	128.72	124.20
23	d	403	CLA	C3C-C4C-NC	2.97	113.91	110.57
34	C	520	LMG	O8-C28-O10	-2.97	116.09	123.59
23	d	403	CLA	C3D-C2D-C1D	-2.97	101.78	105.83
23	c	912	CLA	CHA-C4D-ND	2.97	138.71	132.50
25	c	916	BCR	C36-C18-C19	2.97	122.76	118.08
23	B	616	CLA	C1-O2A-CGA	2.97	124.23	116.44
23	B	615	CLA	O2A-CGA-O1A	-2.97	116.11	123.59
23	D	403	CLA	C3B-C2B-C1B	-2.97	103.58	107.16
23	a	410	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
25	k	102	BCR	C7-C8-C9	-2.96	121.76	126.23
23	b	617	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
23	d	404	CLA	C2A-C1A-CHA	-2.96	118.69	123.86
23	c	913	CLA	CHB-C1B-NB	-2.96	121.13	124.26
23	A	408	CLA	CHD-C4C-NC	2.96	128.86	124.20
35	O	302	HTG	C1-O5-C5	2.96	118.03	112.58
23	C	507	CLA	CAC-C3C-C4C	2.95	128.64	124.81
23	b	617	CLA	CED-O2D-CGD	2.95	122.62	115.94
23	c	908	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
23	d	403	CLA	CHA-C4D-ND	2.95	138.68	132.50
23	B	608	CLA	CHD-C4C-NC	2.95	128.85	124.20
30	I	101	LMT	O3'-C3'-C4'	2.95	117.77	109.94
23	C	510	CLA	O2A-CGA-O1A	-2.95	116.15	123.59
23	c	908	CLA	CMD-C2D-C1D	2.95	129.91	124.71
23	c	902	CLA	CAC-C3C-C4C	2.95	128.63	124.81
23	B	611	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
23	D	401	CLA	CMC-C2C-C1C	2.94	129.52	125.04
23	b	617	CLA	C3B-C2B-C1B	-2.94	103.61	107.16
23	C	510	CLA	CHA-C4D-ND	2.94	138.65	132.50
23	b	607	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	c	905	CLA	CHC-C4B-NB	2.94	127.37	124.26
23	c	912	CLA	O2D-CGD-CBD	2.94	116.49	111.27
24	D	402	PHO	CBA-CAA-C2A	-2.94	105.22	113.81
25	d	405	BCR	C16-C15-C14	-2.94	117.45	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	520	LMG	O8-C9-C8	2.94	116.99	108.43
28	d	408	LHG	C6-O8-C23	2.94	128.00	117.12
23	C	510	CLA	CMD-C2D-C1D	2.94	129.89	124.71
23	c	912	CLA	CBC-CAC-C3C	-2.94	104.34	112.43
40	v	203	HEC	CHB-C1B-NB	2.93	127.61	124.42
23	b	615	CLA	CAC-C3C-C4C	2.93	128.62	124.81
23	c	906	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	c	913	CLA	CBA-CAA-C2A	-2.93	105.22	113.86
25	c	916	BCR	C7-C8-C9	-2.93	121.81	126.23
35	B	625	HTG	O2-C2-C3	-2.93	103.59	110.35
23	C	511	CLA	CAC-C3C-C4C	2.92	128.60	124.81
23	b	603	CLA	CBB-CAB-C3B	-2.92	113.08	127.62
23	c	914	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
23	B	603	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
23	c	912	CLA	CMC-C2C-C1C	2.92	129.48	125.04
23	b	602	CLA	CHD-C4C-NC	2.92	128.80	124.20
23	B	611	CLA	C4D-CHA-C1A	-2.91	117.70	121.25
27	a	414	PL9	C20-C19-C21	2.91	120.17	115.27
23	b	609	CLA	CMC-C2C-C1C	2.91	129.47	125.04
36	C	518	DGD	C2G-O2G-C1B	-2.91	110.62	117.79
23	b	604	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
34	c	920	LMG	O3-C3-C4	-2.91	103.63	110.35
23	b	604	CLA	O2A-C1-C2	-2.91	101.00	108.64
23	B	611	CLA	O2A-CGA-CBA	2.91	121.03	111.91
23	B	614	CLA	C2A-C1A-CHA	-2.91	118.78	123.86
23	D	404	CLA	CED-O2D-CGD	2.90	122.50	115.94
23	B	614	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
23	B	603	CLA	C1-C2-C3	-2.90	121.03	126.04
23	b	605	CLA	CHC-C4B-NB	2.90	127.33	124.26
40	V	203	HEC	CHD-C1D-ND	2.89	127.94	124.37
25	b	619	BCR	C8-C7-C6	-2.89	119.08	127.20
26	A	410	SQD	O48-C23-O10	-2.89	116.29	123.59
26	A	415	SQD	O6-C44-C45	-2.89	103.92	110.90
23	B	607	CLA	CHC-C4B-C3B	-2.89	114.85	127.71
30	A	416	LMT	O2'-C2'-C1'	2.89	117.07	110.05
38	x	102	RRX	C24-C23-C22	-2.89	121.87	126.23
23	b	616	CLA	O2D-CGD-CBD	2.89	116.40	111.27
23	c	903	CLA	CMC-C2C-C1C	2.89	129.44	125.04
27	A	411	PL9	C10-C9-C11	2.89	120.13	115.27
23	B	610	CLA	CHD-C1D-ND	-2.89	121.80	124.45
23	c	905	CLA	CHB-C4A-NA	2.88	128.50	124.51
23	B	617	CLA	CED-O2D-CGD	2.88	122.45	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	903	CLA	CMD-C2D-C3D	2.88	134.23	127.61
23	B	617	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
23	B	612	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	B	616	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	C	509	CLA	C3D-C2D-C1D	-2.87	101.91	105.83
23	c	910	CLA	O2A-CGA-CBA	2.87	120.92	111.91
23	A	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
36	C	517	DGD	O1G-C1A-O1A	-2.87	116.35	123.59
24	a	409	PHO	CED-O2D-CGD	2.87	122.43	115.94
34	j	101	LMG	C9-C8-C7	-2.87	105.00	111.79
23	D	403	CLA	CHD-C1D-ND	-2.87	121.82	124.45
23	C	511	CLA	C3D-C2D-C1D	-2.87	101.92	105.83
23	c	914	CLA	CHA-C4D-ND	2.86	138.49	132.50
23	C	512	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
23	c	902	CLA	CHB-C1B-NB	-2.86	121.23	124.26
24	A	407	PHO	C7-C6-C5	-2.86	105.59	113.36
23	B	613	CLA	CAA-CBA-CGA	-2.86	104.90	113.25
28	L	101	LHG	C6-C5-C4	-2.86	105.03	111.79
23	c	910	CLA	CHA-C4D-ND	2.86	138.48	132.50
23	d	404	CLA	C1-C2-C3	-2.86	121.10	126.04
30	m	103	LMT	C1'-O5'-C5'	2.86	119.30	113.69
23	d	401	CLA	CMD-C2D-C1D	2.86	129.75	124.71
23	b	608	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
23	A	405	CLA	C7-C6-C5	-2.85	105.61	113.36
38	H	102	RRX	C16-C17-C18	-2.85	123.24	127.31
23	a	407	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	B	606	CLA	C1D-CHD-C4C	-2.85	119.91	126.06
36	c	918	DGD	O1G-C1A-O1A	-2.85	116.41	123.59
23	a	407	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
27	D	406	PL9	C10-C9-C11	2.85	120.06	115.27
23	b	608	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	A	405	CLA	CHC-C1C-C2C	-2.85	118.83	126.73
23	c	911	CLA	O2A-CGA-O1A	-2.85	116.41	123.59
23	c	908	CLA	C4-C3-C5	2.85	120.06	115.27
25	C	515	BCR	C11-C10-C9	-2.84	123.25	127.31
23	B	614	CLA	O1D-CGD-CBD	2.84	130.30	124.48
23	c	903	CLA	CHA-C4D-ND	2.84	138.44	132.50
30	m	103	LMT	C1B-O1B-C4'	-2.84	110.93	117.96
38	x	102	RRX	C38-C26-C25	-2.84	121.34	124.53
23	B	614	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
35	d	413	HTG	C1-O5-C5	2.84	117.82	112.58
35	c	922	HTG	C4-C3-C2	2.84	115.78	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CED-O2D-CGD	2.84	122.35	115.94
34	d	411	LMG	O8-C28-C29	2.84	120.81	111.91
23	C	514	CLA	CBC-CAC-C3C	-2.84	104.61	112.43
23	A	405	CLA	C3D-C2D-C1D	-2.84	101.96	105.83
27	a	414	PL9	C25-C24-C26	2.83	120.04	115.27
23	B	610	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
23	D	404	CLA	CHB-C1B-NB	-2.83	121.26	124.26
25	D	405	BCR	C28-C27-C26	-2.83	109.02	114.08
23	b	610	CLA	CMB-C2B-C1B	2.83	129.68	125.37
23	a	410	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
23	b	611	CLA	O2A-CGA-O1A	-2.83	116.46	123.59
30	e	103	LMT	C1-O1'-C1'	2.83	118.53	113.84
23	C	506	CLA	C1-O2A-CGA	2.83	123.86	116.44
23	b	606	CLA	C2A-C1A-CHA	-2.83	118.92	123.86
23	b	616	CLA	C1-O2A-CGA	2.83	123.86	116.44
26	D	408	SQD	O48-C23-C24	2.82	120.77	111.91
26	A	410	SQD	O48-C23-C24	2.82	120.76	111.91
23	b	611	CLA	C3B-C4B-NB	2.82	113.13	110.52
23	D	401	CLA	C3B-C2B-C1B	-2.82	103.76	107.16
23	B	611	CLA	C3B-C4B-NB	2.82	113.13	110.52
23	d	401	CLA	CED-O2D-CGD	2.82	122.31	115.94
23	c	906	CLA	CMC-C2C-C1C	2.82	129.33	125.04
25	b	620	BCR	C7-C8-C9	-2.82	121.98	126.23
25	Y	101	BCR	C21-C20-C19	-2.82	114.43	123.22
23	a	406	CLA	CHA-C4D-ND	2.82	138.39	132.50
23	a	406	CLA	C4B-CHC-C1C	-2.82	119.66	126.34
26	a	417	SQD	O6-C1-C2	2.82	112.70	108.30
23	c	914	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
23	C	508	CLA	CHB-C1B-NB	-2.81	121.28	124.26
24	a	408	PHO	CMC-C2C-C1C	2.81	130.04	124.73
27	D	406	PL9	C12-C13-C14	-2.81	120.89	127.66
23	b	612	CLA	CBC-CAC-C3C	-2.81	104.68	112.43
23	c	911	CLA	C4-C3-C5	2.81	120.00	115.27
34	C	531	LMG	O8-C28-C29	2.81	120.73	111.91
25	C	516	BCR	C33-C5-C6	-2.81	121.37	124.53
23	c	913	CLA	CAC-C3C-C4C	2.81	128.46	124.81
23	C	512	CLA	C3B-C4B-NB	2.81	113.12	110.52
26	D	408	SQD	O7-S-C6	2.81	110.28	106.94
23	b	610	CLA	CHD-C1D-ND	-2.81	121.87	124.45
26	x	101	SQD	O8-S-C6	2.81	110.21	105.74
23	c	907	CLA	C1D-CHD-C4C	-2.81	120.00	126.06
25	T	101	BCR	C20-C21-C22	-2.81	123.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	V	203	HEC	CHA-C4D-ND	2.81	127.47	124.42
23	A	408	CLA	CED-O2D-CGD	2.81	122.28	115.94
35	O	302	HTG	C4-C3-C2	2.81	115.72	110.82
26	x	101	SQD	O5-C5-C4	2.81	114.79	109.69
28	a	415	LHG	O8-C23-C24	2.80	120.71	111.91
23	b	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	c	912	CLA	CHB-C1B-NB	-2.80	121.29	124.26
23	C	503	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
27	A	411	PL9	C45-C44-C46	2.80	119.98	115.27
23	c	912	CLA	CMB-C2B-C1B	2.80	129.63	125.37
34	c	920	LMG	O8-C28-O10	-2.80	116.53	123.59
23	C	506	CLA	C3D-C2D-C1D	-2.80	102.01	105.83
23	c	904	CLA	O2A-CGA-CBA	2.79	120.68	111.91
23	c	903	CLA	CAC-C3C-C4C	2.79	128.44	124.81
35	B	624	HTG	O3-C3-C2	2.79	116.81	110.35
23	a	406	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
23	b	608	CLA	O2A-C1-C2	-2.79	101.30	108.64
23	b	602	CLA	C1-C2-C3	2.79	130.87	126.04
23	d	404	CLA	C6-C5-C3	-2.79	106.14	113.45
23	B	608	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
27	a	414	PL9	C7-C8-C9	-2.79	122.16	126.79
34	m	102	LMG	O7-C10-O9	-2.78	116.97	123.70
25	t	101	BCR	C38-C26-C25	-2.78	121.40	124.53
23	a	407	CLA	C4A-NA-C1A	2.78	107.96	106.71
23	b	611	CLA	CAC-C3C-C4C	2.78	128.42	124.81
23	B	602	CLA	O2A-CGA-CBA	2.78	120.63	111.91
23	B	608	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
23	B	615	CLA	CHB-C1B-NB	-2.78	121.32	124.26
23	B	609	CLA	C3C-C4C-NC	2.78	113.69	110.57
23	C	506	CLA	CHD-C4C-NC	2.77	128.58	124.20
23	B	612	CLA	CBC-CAC-C3C	-2.77	104.78	112.43
23	C	504	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	D	404	CLA	C3B-C4B-NB	2.77	113.09	110.52
35	C	522	HTG	O5-C5-C4	2.77	114.73	109.69
25	t	101	BCR	C35-C13-C12	2.77	122.44	118.08
23	c	909	CLA	CMA-C3A-C4A	-2.77	104.33	111.77
28	A	412	LHG	O8-C23-C24	2.77	120.59	111.91
23	C	511	CLA	C4B-CHC-C1C	-2.77	119.78	126.34
27	A	411	PL9	C51-C49-C50	2.77	120.71	114.60
25	D	405	BCR	C29-C28-C27	-2.76	105.20	111.38
26	A	410	SQD	O9-S-O7	-2.76	104.38	113.95
23	b	614	CLA	C3B-C2B-C1B	-2.76	103.83	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	418	LMT	O5'-C5'-C4'	2.76	115.57	109.75
25	c	916	BCR	C16-C17-C18	-2.76	123.37	127.31
25	B	618	BCR	C33-C5-C6	-2.76	121.43	124.53
34	d	411	LMG	O6-C1-O1	2.76	116.50	109.97
23	b	602	CLA	CHB-C1B-NB	-2.76	121.34	124.26
23	c	905	CLA	O2A-C1-C2	-2.75	101.40	108.64
23	b	610	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
23	d	401	CLA	C1D-ND-C4D	-2.75	104.38	106.33
23	b	613	CLA	C4-C3-C5	2.75	119.90	115.27
23	c	909	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	C	511	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
36	C	517	DGD	C1E-O6E-C5E	2.75	119.08	113.69
30	m	103	LMT	O1'-C1'-C2'	2.75	112.59	108.30
36	c	919	DGD	C6B-C5B-C4B	-2.75	100.48	114.42
23	b	609	CLA	C1D-ND-C4D	2.75	108.29	106.33
25	d	405	BCR	C2-C1-C6	2.75	114.71	110.48
23	c	904	CLA	CBC-CAC-C3C	-2.74	104.86	112.43
23	B	606	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
23	c	904	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	C	513	CLA	CHC-C4B-NB	2.74	127.16	124.26
23	c	907	CLA	C3B-C4B-NB	2.74	113.06	110.52
23	b	615	CLA	CHB-C1B-NB	-2.74	121.36	124.26
25	D	405	BCR	C33-C5-C6	-2.74	121.45	124.53
23	c	912	CLA	C4-C3-C5	2.74	119.88	115.27
23	B	615	CLA	C1-C2-C3	-2.73	121.31	126.04
23	D	401	CLA	CHD-C4C-NC	2.73	128.51	124.20
34	j	101	LMG	O7-C10-C11	2.73	117.39	111.50
23	B	608	CLA	CMB-C2B-C3B	2.73	133.21	126.59
23	b	606	CLA	C5-C3-C2	-2.73	115.59	121.12
36	d	407	DGD	O1G-C1A-O1A	-2.73	116.70	123.59
23	B	604	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
23	D	403	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
23	c	906	CLA	C3C-C4C-NC	2.73	113.63	110.57
23	C	512	CLA	C1-O2A-CGA	2.73	123.59	116.44
23	B	612	CLA	C4D-CHA-C1A	-2.72	117.93	121.25
23	C	513	CLA	C1D-CHD-C4C	-2.72	120.18	126.06
30	a	418	LMT	C1B-O1B-C4'	-2.72	111.23	117.96
23	c	902	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	a	410	CLA	CMD-C2D-C3D	2.72	133.87	127.61
23	b	617	CLA	CHD-C4C-NC	2.72	128.49	124.20
38	H	102	RRX	C40-C30-C25	-2.72	105.89	110.30
23	b	612	CLA	CHA-C4D-ND	2.72	138.18	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	904	CLA	CMD-C2D-C1D	2.71	129.50	124.71
23	B	609	CLA	C3D-C2D-C1D	-2.71	102.13	105.83
40	V	203	HEC	C3D-C4D-ND	-2.71	107.73	110.36
23	c	908	CLA	O2A-CGA-CBA	2.71	120.42	111.91
28	d	402	LHG	O8-C23-C24	2.71	120.41	111.91
25	B	620	BCR	C24-C23-C22	-2.71	122.14	126.23
23	B	604	CLA	C1D-CHD-C4C	-2.71	120.22	126.06
23	c	903	CLA	OBD-CAD-C3D	-2.70	122.02	128.52
27	D	406	PL9	C36-C37-C38	-2.70	103.00	111.88
23	B	602	CLA	CHA-C4D-ND	2.70	138.15	132.50
36	C	519	DGD	O1G-C1A-C2A	2.70	120.38	111.91
23	c	910	CLA	CHC-C4B-C3B	-2.70	115.70	127.71
23	C	513	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
23	c	909	CLA	CHB-C4A-NA	2.69	128.24	124.51
23	b	604	CLA	CHA-C4D-ND	2.69	138.13	132.50
27	A	411	PL9	C7-C8-C9	-2.69	122.31	126.79
23	B	616	CLA	C3B-C4B-NB	2.69	113.01	110.52
23	c	905	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	c	913	CLA	CMC-C2C-C1C	2.69	129.13	125.04
23	C	506	CLA	C2D-C1D-ND	2.69	112.08	110.10
24	a	408	PHO	C4D-CHA-CBD	-2.69	107.30	108.52
23	c	905	CLA	CHB-C1B-NB	-2.69	121.41	124.26
35	b	622	HTG	O2-C2-C1	2.69	115.20	110.27
23	c	910	CLA	C1-C2-C3	-2.69	121.40	126.04
23	d	403	CLA	O2A-CGA-CBA	2.68	120.33	111.91
35	v	204	HTG	C1-C2-C3	-2.68	105.29	110.59
25	t	101	BCR	C2-C3-C4	-2.68	105.38	111.38
23	A	408	CLA	CMD-C2D-C1D	2.68	129.44	124.71
27	a	414	PL9	C15-C14-C16	2.68	119.78	115.27
34	d	411	LMG	C8-O7-C10	-2.68	111.19	117.79
23	B	610	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	c	903	CLA	C3B-C4B-NB	2.68	113.00	110.52
40	v	203	HEC	CAD-CBD-CGD	-2.68	107.84	113.60
23	c	910	CLA	C6-C5-C3	-2.68	106.43	113.45
25	C	515	BCR	C33-C5-C6	-2.68	121.52	124.53
25	A	409	BCR	C28-C27-C26	-2.68	109.30	114.08
23	C	512	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	b	614	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
23	c	904	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
25	j	104	BCR	C35-C13-C12	2.67	122.28	118.08
23	b	613	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
34	m	102	LMG	C30-C29-C28	-2.67	103.92	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	917	DGD	O2G-C1B-O1B	-2.67	117.26	123.70
23	C	506	CLA	C3C-C4C-NC	2.67	113.56	110.57
30	I	101	LMT	C3'-C4'-C5'	-2.66	104.82	110.93
27	D	406	PL9	C36-C34-C33	-2.66	115.73	121.12
23	b	602	CLA	CED-O2D-CGD	2.66	121.96	115.94
24	a	408	PHO	C4B-NB-C1B	-2.66	104.71	108.83
23	B	606	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
38	H	102	RRX	C34-C9-C8	2.66	122.27	118.08
25	D	405	BCR	C2-C3-C4	2.66	117.32	111.38
30	B	643	LMT	C1-O1'-C1'	-2.66	109.43	113.84
26	a	412	SQD	O9-S-O7	-2.66	104.75	113.95
25	C	530	BCR	C20-C21-C22	-2.66	123.52	127.31
23	c	913	CLA	CHA-C4D-ND	2.66	138.05	132.50
28	d	410	LHG	O7-C7-O9	-2.65	117.29	123.70
35	c	922	HTG	C1-C2-C3	2.65	115.83	110.59
23	C	508	CLA	C1D-CHD-C4C	-2.65	120.34	126.06
23	B	615	CLA	CHC-C1C-NC	-2.65	120.18	124.20
23	A	405	CLA	C4A-NA-C1A	-2.65	105.51	106.71
25	C	530	BCR	C7-C8-C9	-2.65	122.23	126.23
23	b	609	CLA	C3C-C4C-NC	2.65	113.54	110.57
23	B	602	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	a	406	CLA	C3C-C4C-NC	2.65	113.54	110.57
23	c	906	CLA	CAC-C3C-C4C	2.65	128.25	124.81
34	m	102	LMG	O8-C28-C29	2.65	120.22	111.91
23	c	909	CLA	CHD-C1D-ND	-2.65	122.02	124.45
34	C	520	LMG	O5-C6-C5	-2.65	102.21	111.29
23	B	611	CLA	CMB-C2B-C1B	2.65	129.40	125.37
23	C	503	CLA	CHC-C4B-NB	2.64	127.06	124.26
36	d	407	DGD	O1G-C1A-C2A	2.64	120.20	111.91
23	C	503	CLA	C3B-C2B-C1B	-2.64	103.97	107.16
23	C	507	CLA	C4-C3-C5	2.64	119.71	115.27
26	A	410	SQD	C45-O47-C7	-2.64	111.29	117.79
23	A	408	CLA	C1D-CHD-C4C	-2.64	120.36	126.06
23	C	504	CLA	CHB-C1B-NB	-2.64	121.46	124.26
23	A	405	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	b	617	CLA	C4-C3-C2	-2.64	116.91	123.68
23	b	607	CLA	CMD-C2D-C1D	2.63	129.35	124.71
23	b	617	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
25	d	405	BCR	C32-C1-C6	2.63	114.57	110.30
23	a	407	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	C	511	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
30	B	644	LMT	C1-O1'-C1'	-2.63	109.48	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	408	SQD	O4-C4-C3	-2.63	104.27	110.35
34	B	622	LMG	O7-C10-O9	-2.63	117.35	123.70
25	b	618	BCR	C28-C27-C26	-2.63	109.38	114.08
23	B	604	CLA	CBA-CAA-C2A	2.63	121.62	113.86
34	C	501	LMG	O7-C10-C11	2.63	117.16	111.50
23	b	602	CLA	C4-C3-C5	2.62	119.69	115.27
37	e	105	HEM	C4C-C3C-C2C	2.62	108.91	106.75
35	O	302	HTG	C1'-S1-C1	2.62	105.00	100.09
26	a	412	SQD	O5-C1-O6	2.62	116.19	109.97
23	b	603	CLA	C3C-C4C-NC	2.62	113.51	110.57
23	b	611	CLA	CHC-C4B-NB	2.62	127.03	124.26
23	B	604	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	b	608	CLA	CMB-C2B-C1B	2.62	129.36	125.37
23	C	507	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	C	509	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
30	z	101	LMT	C1B-C2B-C3B	-2.62	104.55	110.00
23	c	911	CLA	C2A-C1A-CHA	-2.62	119.29	123.86
23	b	613	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
23	D	404	CLA	O2D-CGD-CBD	2.61	115.91	111.27
23	b	611	CLA	CHD-C4C-NC	2.61	128.32	124.20
23	B	617	CLA	C1-O2A-CGA	2.61	123.29	116.44
35	c	921	HTG	C3-C4-C5	2.61	114.89	110.24
25	b	618	BCR	C23-C22-C21	-2.61	114.94	118.94
40	v	203	HEC	C1D-C2D-C3D	-2.61	104.21	106.96
23	c	904	CLA	CMB-C2B-C1B	2.61	129.34	125.37
28	D	410	LHG	O7-C7-O9	-2.61	117.41	123.70
25	t	101	BCR	C2-C1-C6	2.61	114.49	110.48
23	B	603	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	x	101	SQD	O7-S-C6	2.60	110.03	106.94
23	D	404	CLA	C1D-CHD-C4C	-2.60	120.44	126.06
23	D	404	CLA	CMA-C3A-C4A	-2.60	104.78	111.77
23	B	607	CLA	CMC-C2C-C3C	2.60	133.18	126.12
35	B	625	HTG	O5-C1-C2	-2.60	107.04	110.31
23	C	503	CLA	CHD-C4C-NC	2.60	128.30	124.20
23	C	502	CLA	CHC-C1C-NC	-2.60	120.26	124.20
25	B	620	BCR	C32-C1-C6	-2.60	106.09	110.30
35	V	204	HTG	O2-C2-C1	2.60	115.04	110.27
23	B	613	CLA	CHA-C4D-ND	2.60	137.93	132.50
26	x	101	SQD	O48-C23-O10	-2.60	117.04	123.59
36	h	102	DGD	O5D-C1E-C2E	2.59	112.35	108.30
28	K	101	LHG	O8-C23-C24	2.59	120.05	111.91
30	m	104	LMT	O1'-C1-C2	-2.59	100.47	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	CHD-C4C-NC	2.59	128.29	124.20
25	c	915	BCR	C11-C10-C9	-2.59	123.61	127.31
25	B	619	BCR	C11-C10-C9	-2.59	123.61	127.31
23	C	513	CLA	CHB-C1B-NB	-2.59	121.52	124.26
23	B	613	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
25	t	101	BCR	C29-C28-C27	-2.59	105.59	111.38
23	b	608	CLA	CMC-C2C-C1C	2.59	128.98	125.04
23	c	908	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	c	907	CLA	CMB-C2B-C1B	2.59	129.31	125.37
23	a	410	CLA	CED-O2D-CGD	2.59	121.79	115.94
23	C	504	CLA	C1D-ND-C4D	2.58	108.17	106.33
30	A	416	LMT	O5'-C5'-C4'	2.58	115.19	109.75
23	c	907	CLA	C4-C3-C5	2.58	119.61	115.27
24	A	407	PHO	CED-O2D-CGD	2.58	121.77	115.94
25	Y	101	BCR	C15-C16-C17	-2.58	118.20	123.47
23	b	602	CLA	CBC-CAC-C3C	-2.57	105.33	112.43
23	b	605	CLA	C3C-C4C-NC	2.57	113.46	110.57
23	b	617	CLA	C3C-C4C-NC	2.57	113.46	110.57
23	D	404	CLA	C4-C3-C5	2.57	119.60	115.27
23	b	610	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
35	B	631	HTG	C1-O5-C5	2.57	117.31	112.58
23	C	505	CLA	C3B-C4B-NB	2.57	112.89	110.52
23	C	505	CLA	CAC-C3C-C4C	2.56	128.14	124.81
23	b	608	CLA	C4A-NA-C1A	2.56	107.86	106.71
23	A	406	CLA	CAC-C3C-C2C	-2.56	123.14	127.53
23	b	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	c	905	CLA	C3D-C4D-ND	2.56	114.38	110.24
25	c	916	BCR	C29-C30-C25	2.56	114.42	110.48
24	D	402	PHO	C4D-CHA-CBD	2.56	109.67	108.52
23	A	408	CLA	CHA-C4D-ND	2.56	137.85	132.50
23	b	615	CLA	CHB-C4A-NA	2.56	128.05	124.51
36	C	517	DGD	CDB-CCB-CBB	-2.56	101.43	114.42
23	B	608	CLA	O2D-CGD-CBD	2.56	115.81	111.27
28	A	412	LHG	O8-C23-O10	-2.56	117.14	123.59
23	c	911	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
36	c	918	DGD	O3D-C3D-C2D	-2.56	104.44	110.35
25	j	104	BCR	C15-C14-C13	-2.56	123.66	127.31
36	H	103	DGD	O4D-C4D-C3D	-2.56	104.44	110.35
23	A	405	CLA	CHA-C4D-ND	2.55	137.84	132.50
23	B	607	CLA	C3B-C4B-NB	2.55	112.88	110.52
23	D	403	CLA	C3B-C4B-NB	2.55	112.88	110.52
30	B	644	LMT	C4'-C3'-C2'	-2.55	106.37	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C2D-C1D-ND	2.55	111.98	110.10
24	a	408	PHO	C7-C6-C5	-2.55	106.43	113.36
34	B	622	LMG	C30-C29-C28	-2.55	104.34	113.62
23	d	404	CLA	C6-C7-C8	-2.55	107.67	115.92
23	B	606	CLA	C3D-C2D-C1D	-2.55	102.35	105.83
23	B	608	CLA	C4D-CHA-C1A	-2.55	118.15	121.25
23	b	605	CLA	CHD-C1D-ND	-2.55	122.11	124.45
23	b	615	CLA	CHD-C4C-NC	2.54	128.21	124.20
27	a	414	PL9	C10-C9-C11	2.54	119.55	115.27
23	B	612	CLA	CMB-C2B-C1B	2.54	129.24	125.37
23	b	610	CLA	C1-O2A-CGA	2.54	123.11	116.44
25	j	104	BCR	C16-C15-C14	-2.54	118.27	123.47
27	A	411	PL9	C17-C18-C19	-2.54	121.54	127.66
23	B	616	CLA	C1D-ND-C4D	-2.54	104.53	106.33
23	B	612	CLA	CMD-C2D-C1D	2.54	129.19	124.71
23	b	602	CLA	C3C-C4C-NC	2.54	113.42	110.57
25	d	405	BCR	C36-C18-C19	2.54	122.08	118.08
36	c	919	DGD	O1G-C1G-C2G	-2.54	101.05	108.43
23	B	615	CLA	CMC-C2C-C1C	2.54	128.90	125.04
34	J	101	LMG	O8-C28-O10	-2.54	117.19	123.59
24	D	402	PHO	OBD-CAD-C3D	-2.54	123.77	127.98
23	b	607	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
23	b	603	CLA	CMD-C2D-C3D	2.54	133.45	127.61
23	b	614	CLA	O2A-CGA-CBA	2.54	119.87	111.91
23	b	612	CLA	CAC-C3C-C4C	2.54	128.10	124.81
25	k	102	BCR	C11-C10-C9	-2.54	123.69	127.31
30	A	416	LMT	O5B-C5B-C6B	2.53	112.73	106.44
23	B	604	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
23	c	914	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
23	a	410	CLA	CHD-C4C-NC	2.53	128.19	124.20
27	D	406	PL9	C53-C6-C1	2.53	120.17	114.99
23	C	514	CLA	CHD-C4C-NC	2.53	128.19	124.20
36	c	917	DGD	CDB-CCB-CBB	-2.53	101.58	114.42
23	b	615	CLA	C3D-C4D-ND	2.53	114.33	110.24
23	B	603	CLA	C4-C3-C5	2.53	119.52	115.27
23	c	906	CLA	CMD-C2D-C1D	2.53	129.17	124.71
23	C	509	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	B	605	CLA	C6-C5-C3	-2.52	106.84	113.45
25	C	516	BCR	C3-C4-C5	-2.52	109.57	114.08
36	c	919	DGD	O1G-C1A-C2A	2.52	119.82	111.91
23	d	401	CLA	O2A-C1-C2	-2.52	102.01	108.64
23	b	614	CLA	CHC-C1C-NC	-2.52	120.38	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C1-C2-C3	-2.52	121.69	126.04
23	C	508	CLA	C1-O2A-CGA	2.52	123.05	116.44
23	C	504	CLA	CMD-C2D-C1D	2.52	129.15	124.71
23	C	511	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
27	D	406	PL9	C40-C39-C38	-2.51	117.23	123.68
28	d	410	LHG	O7-C7-C8	2.51	116.92	111.50
25	T	101	BCR	C37-C22-C21	2.51	126.44	122.92
23	b	605	CLA	CMD-C2D-C3D	2.51	133.39	127.61
23	d	403	CLA	C4A-NA-C1A	2.51	107.83	106.71
25	k	102	BCR	C3-C4-C5	-2.51	109.59	114.08
23	b	607	CLA	C3C-C4C-NC	2.51	113.39	110.57
25	D	405	BCR	C10-C11-C12	-2.51	115.39	123.22
34	a	413	LMG	O8-C28-O10	-2.51	117.26	123.59
23	b	607	CLA	CHA-C4D-ND	2.51	137.75	132.50
37	e	105	HEM	C1B-NB-C4B	2.51	107.66	105.07
23	B	609	CLA	C3D-C4D-CHA	-2.51	106.99	112.72
36	c	917	DGD	C6D-O5D-C1E	-2.51	108.84	113.74
23	c	914	CLA	CED-O2D-CGD	2.50	121.60	115.94
23	c	903	CLA	C16-C17-C18	-2.50	104.19	115.98
23	C	502	CLA	C1-O2A-CGA	2.50	123.01	116.44
23	c	904	CLA	CAC-C3C-C4C	2.50	128.06	124.81
23	C	514	CLA	C4-C3-C5	2.50	119.48	115.27
23	B	605	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
23	c	907	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
35	B	624	HTG	O3-C3-C4	-2.50	104.57	110.35
23	b	606	CLA	C4A-NA-C1A	-2.50	105.58	106.71
26	A	415	SQD	O5-C1-C2	-2.50	105.06	110.35
25	B	619	BCR	C30-C25-C26	-2.50	119.10	122.61
30	z	101	LMT	C1B-O1B-C4'	-2.50	111.78	117.96
26	A	415	SQD	O48-C23-O10	-2.50	117.29	123.59
30	m	104	LMT	C3'-C4'-C5'	-2.50	105.20	110.93
23	b	604	CLA	C5-C3-C2	-2.49	116.07	121.12
23	c	902	CLA	C3D-C4D-ND	2.49	114.27	110.24
23	B	611	CLA	CMD-C2D-C1D	2.49	129.10	124.71
28	l	101	LHG	O8-C23-O10	-2.49	117.31	123.59
23	c	903	CLA	CHB-C1B-NB	-2.49	121.62	124.26
23	b	605	CLA	CHD-C4C-NC	2.49	128.12	124.20
25	t	101	BCR	C34-C9-C8	2.49	121.99	118.08
23	c	914	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
30	z	101	LMT	O1'-C1'-C2'	2.48	111.06	108.15
27	D	406	PL9	C27-C28-C29	-2.48	121.68	127.66
25	a	411	BCR	C8-C7-C6	-2.48	120.23	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	PHO	CMB-C2B-C3B	2.48	129.32	124.68
40	v	203	HEC	CMB-C2B-C1B	-2.48	121.26	125.04
23	b	612	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
25	T	101	BCR	C21-C20-C19	-2.48	115.48	123.22
23	B	613	CLA	CMD-C2D-C1D	2.48	129.08	124.71
23	C	510	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	D	401	CLA	C3B-C4B-NB	2.48	112.81	110.52
36	C	517	DGD	C3D-C4D-C5D	-2.48	105.82	110.24
23	B	610	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
23	c	904	CLA	C4C-C3C-C2C	-2.48	103.29	106.90
23	a	406	CLA	C2B-C1B-NB	2.48	111.89	110.23
23	C	510	CLA	C3B-C4B-NB	2.48	112.81	110.52
25	b	620	BCR	C23-C24-C25	-2.47	120.25	127.20
23	B	612	CLA	C3C-C4C-NC	2.47	113.34	110.57
23	D	404	CLA	C6-C7-C8	-2.47	107.92	115.92
27	A	411	PL9	O2-C1-C2	-2.47	116.11	121.78
23	b	613	CLA	C3D-C4D-ND	2.47	114.24	110.24
23	A	406	CLA	CHC-C4B-C3B	-2.47	116.72	127.71
25	c	916	BCR	C11-C10-C9	-2.47	123.78	127.31
23	b	612	CLA	C3C-C4C-NC	2.47	113.34	110.57
25	k	102	BCR	C38-C26-C25	-2.47	121.76	124.53
23	b	606	CLA	CHB-C1B-NB	-2.47	121.65	124.26
23	C	505	CLA	CHB-C1B-NB	-2.46	121.65	124.26
25	c	916	BCR	C21-C20-C19	-2.46	115.53	123.22
25	B	620	BCR	C37-C22-C21	2.46	126.37	122.92
23	C	513	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
23	C	505	CLA	CMC-C2C-C1C	2.46	128.79	125.04
23	c	911	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	b	610	CLA	CMD-C2D-C1D	2.46	129.05	124.71
23	b	609	CLA	CHB-C1B-C2B	-2.46	120.29	127.24
36	c	919	DGD	O3D-C3D-C4D	2.46	116.04	110.35
23	C	512	CLA	C4-C3-C5	2.46	119.41	115.27
23	b	604	CLA	CMB-C2B-C1B	2.46	129.12	125.37
23	B	613	CLA	C4B-CHC-C1C	-2.46	120.50	126.34
23	D	401	CLA	C3C-C4C-NC	2.46	113.33	110.57
23	A	405	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
23	D	403	CLA	CAA-CBA-CGA	-2.46	106.07	113.25
25	A	409	BCR	C24-C23-C22	-2.46	122.52	126.23
23	c	902	CLA	C4-C3-C5	2.46	119.40	115.27
23	B	617	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	b	604	CLA	CHD-C4C-NC	2.46	128.07	124.20
40	v	203	HEC	CHA-C4D-ND	2.46	127.09	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	910	CLA	C12-C11-C10	-2.46	101.96	113.24
23	c	906	CLA	C11-C10-C8	-2.45	107.99	115.92
23	B	610	CLA	CMD-C2D-C3D	2.45	133.26	127.61
23	c	903	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
28	E	101	LHG	O7-C7-O9	-2.45	117.77	123.70
23	a	410	CLA	CBC-CAC-C3C	-2.45	105.67	112.43
34	c	930	LMG	C3-C4-C5	2.45	114.61	110.24
23	B	607	CLA	C3C-C4C-NC	2.45	113.32	110.57
23	c	912	CLA	C1D-CHD-C4C	-2.45	120.78	126.06
23	C	502	CLA	C3C-C4C-NC	2.45	113.31	110.57
23	a	406	CLA	O2D-CGD-CBD	2.45	115.61	111.27
23	b	607	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	b	617	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	c	912	CLA	O2A-CGA-CBA	2.44	119.57	111.91
25	Y	101	BCR	C4-C5-C6	2.44	126.27	122.73
34	C	531	LMG	O6-C5-C6	2.44	112.50	106.44
30	a	418	LMT	O2'-C2'-C3'	-2.44	104.71	110.35
23	b	602	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	d	404	CLA	CHC-C4B-C3B	-2.44	116.86	127.71
34	C	501	LMG	O8-C28-C29	2.44	119.56	111.91
23	B	603	CLA	CHB-C1B-NB	-2.44	121.68	124.26
26	a	412	SQD	O8-S-C6	2.44	109.62	105.74
23	b	613	CLA	O2A-CGA-CBA	2.44	119.55	111.91
23	A	408	CLA	O2A-C1-C2	-2.44	102.23	108.64
24	a	408	PHO	CMD-C2D-C3D	2.43	129.23	124.68
27	d	406	PL9	C22-C23-C24	-2.43	121.80	127.66
23	c	903	CLA	C16-C15-C13	-2.43	108.05	115.92
23	c	904	CLA	C1D-CHD-C4C	-2.43	120.81	126.06
26	a	412	SQD	O47-C7-O49	-2.43	117.82	123.70
28	D	409	LHG	C11-C10-C9	-2.43	102.07	114.42
34	C	531	LMG	O8-C28-O10	-2.43	117.45	123.59
23	b	612	CLA	C2A-C1A-CHA	-2.43	119.60	123.86
23	b	608	CLA	CMD-C2D-C1D	2.43	129.00	124.71
36	H	103	DGD	C2G-O2G-C1B	-2.43	111.81	117.79
27	d	406	PL9	C7-C3-C4	2.43	118.85	116.88
23	d	404	CLA	CAC-C3C-C4C	2.43	127.96	124.81
28	d	410	LHG	O4-P-O5	2.43	124.25	112.24
23	C	508	CLA	C11-C10-C8	-2.43	108.07	115.92
35	b	623	HTG	C4-C3-C2	2.43	115.06	110.82
23	B	612	CLA	CHB-C1B-C2B	-2.43	120.38	127.24
28	D	409	LHG	O7-C7-O9	-2.43	117.84	123.70
23	B	606	CLA	O2D-CGD-O1D	-2.42	119.10	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C11-C10-C8	-2.42	108.08	115.92
36	h	102	DGD	C6D-C5D-C4D	2.42	117.15	112.09
23	B	617	CLA	CHD-C4C-NC	2.42	128.02	124.20
25	T	101	BCR	C2-C1-C6	2.42	114.21	110.48
23	b	607	CLA	C11-C10-C8	-2.42	108.09	115.92
25	t	101	BCR	C7-C8-C9	-2.42	122.58	126.23
23	b	609	CLA	CMD-C2D-C3D	2.42	133.18	127.61
23	b	608	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
23	d	404	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
34	c	930	LMG	O8-C28-C29	2.42	119.49	111.91
30	B	644	LMT	C1'-C2'-C3'	-2.42	104.97	110.00
25	d	405	BCR	C34-C9-C10	-2.41	119.54	122.92
25	c	916	BCR	C32-C1-C6	-2.41	106.38	110.30
25	t	101	BCR	C33-C5-C6	-2.41	121.82	124.53
26	L	102	SQD	O47-C7-O49	-2.41	117.87	123.70
25	A	409	BCR	C10-C11-C12	-2.41	115.69	123.22
34	C	520	LMG	O7-C10-O9	-2.41	117.87	123.70
23	c	906	CLA	C4D-CHA-C1A	-2.41	118.31	121.25
26	D	408	SQD	O48-C23-O10	-2.41	117.50	123.59
26	D	408	SQD	O5-C1-O6	2.41	115.69	109.97
23	b	608	CLA	C3B-C4B-NB	2.41	112.75	110.52
34	c	920	LMG	O5-C6-C5	-2.41	103.02	111.29
23	B	606	CLA	O2D-CGD-CBD	2.41	115.55	111.27
23	C	513	CLA	CMD-C2D-C3D	2.41	133.16	127.61
23	C	512	CLA	CHC-C4B-C3B	-2.41	117.00	127.71
38	x	102	RRX	C16-C15-C14	-2.41	118.54	123.47
23	b	614	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
23	D	404	CLA	CMB-C2B-C1B	2.41	129.04	125.37
24	A	407	PHO	CBA-CAA-C2A	-2.41	106.78	113.81
23	c	906	CLA	C1-O2A-CGA	2.41	122.76	116.44
25	t	101	BCR	C1-C6-C7	2.41	122.58	115.78
30	z	101	LMT	O1B-C1B-C2B	2.40	114.33	108.10
23	b	613	CLA	C5-C3-C2	-2.40	116.25	121.12
23	C	512	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
31	U	202	DMS	O-S-C1	2.40	118.80	106.54
23	C	504	CLA	C5-C3-C2	-2.40	116.26	121.12
28	d	409	LHG	C34-C33-C32	-2.40	102.23	114.42
23	D	401	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
23	B	616	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
27	a	414	PL9	C45-C44-C46	2.40	119.30	115.27
23	c	903	CLA	O2A-CGA-CBA	2.40	119.43	111.91
23	b	603	CLA	C4B-CHC-C1C	2.40	132.02	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	PL9	C17-C18-C19	-2.40	121.89	127.66
25	Y	101	BCR	C39-C30-C25	-2.40	106.41	110.30
23	B	611	CLA	CHD-C1D-ND	-2.40	122.25	124.45
30	B	623	LMT	C1B-O5B-C5B	2.39	118.39	113.69
23	C	511	CLA	C3B-C4B-NB	2.39	112.73	110.52
23	C	506	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
23	C	511	CLA	C4-C3-C5	2.39	119.29	115.27
23	c	906	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
23	b	616	CLA	OBD-CAD-C3D	-2.39	122.77	128.52
23	d	401	CLA	CHC-C4B-C3B	-2.39	117.08	127.71
23	c	910	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	d	401	CLA	C3C-C4C-NC	2.39	113.25	110.57
25	k	102	BCR	C24-C23-C22	-2.39	122.63	126.23
23	b	604	CLA	CMA-C3A-C4A	2.39	118.19	111.77
23	c	911	CLA	C3D-C4D-CHA	-2.39	107.26	112.72
23	C	510	CLA	CHB-C1B-NB	-2.39	121.73	124.26
23	b	606	CLA	CMD-C2D-C3D	2.39	133.10	127.61
24	a	409	PHO	C16-C15-C13	-2.39	108.21	115.92
23	b	609	CLA	C4-C3-C5	2.38	119.28	115.27
23	b	608	CLA	C1D-ND-C4D	2.38	108.03	106.33
23	b	611	CLA	C1D-ND-C4D	-2.38	104.64	106.33
23	D	403	CLA	C14-C13-C15	-2.38	102.66	111.29
23	c	910	CLA	C1-O2A-CGA	2.38	122.69	116.44
36	h	102	DGD	O2G-C1B-O1B	-2.38	117.94	123.70
25	C	515	BCR	C24-C23-C22	-2.38	122.64	126.23
40	v	203	HEC	C1B-C2B-C3B	2.38	109.46	106.96
25	B	618	BCR	C24-C23-C22	-2.38	122.64	126.23
24	A	407	PHO	C1-C2-C3	-2.38	121.93	126.04
23	d	404	CLA	CHA-C4D-ND	2.38	137.48	132.50
23	D	401	CLA	CHC-C4B-NB	2.38	126.78	124.26
23	B	617	CLA	C1D-CHD-C4C	-2.38	120.93	126.06
23	B	603	CLA	OBD-CAD-C3D	-2.38	122.80	128.52
23	b	613	CLA	CHD-C1D-ND	-2.38	122.27	124.45
26	x	101	SQD	C3-C4-C5	2.38	114.48	110.24
34	d	411	LMG	O8-C28-O10	-2.38	117.59	123.59
26	A	410	SQD	C3-C4-C5	2.38	114.48	110.24
23	c	905	CLA	CMB-C2B-C1B	2.38	128.99	125.37
23	b	612	CLA	C7-C6-C5	-2.38	106.91	113.36
23	b	609	CLA	C5-C3-C2	-2.38	116.31	121.12
25	B	620	BCR	C7-C8-C9	-2.38	122.64	126.23
23	b	604	CLA	C4D-CHA-C1A	-2.38	118.36	121.25
28	d	409	LHG	C32-C31-C30	-2.38	102.37	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	CHC-C4B-C3B	-2.37	117.15	127.71
23	D	401	CLA	C2B-C1B-NB	2.37	111.82	110.23
23	C	511	CLA	C4D-CHA-C1A	-2.37	118.36	121.25
23	c	914	CLA	C4D-CHA-C1A	-2.37	118.36	121.25
23	c	905	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
23	c	908	CLA	C16-C17-C18	-2.37	104.81	115.98
40	V	203	HEC	C2D-C1D-ND	-2.37	107.03	109.84
23	B	604	CLA	CHC-C4B-C3B	-2.37	117.17	127.71
23	a	407	CLA	CHA-C4D-ND	2.37	137.46	132.50
23	c	903	CLA	C3C-C4C-NC	2.37	113.22	110.57
23	d	404	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
27	a	414	PL9	C42-C43-C44	-2.37	121.96	127.66
23	C	510	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
30	a	422	LMT	O1'-C1'-C2'	2.36	112.00	108.30
25	d	405	BCR	C16-C17-C18	-2.36	123.94	127.31
27	D	406	PL9	C35-C34-C36	2.36	119.25	115.27
23	B	617	CLA	C3B-C4B-NB	2.36	112.71	110.52
23	c	909	CLA	C4C-C3C-C2C	-2.36	103.45	106.90
23	A	405	CLA	OBD-CAD-C3D	-2.36	122.84	128.52
23	C	504	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	B	617	CLA	C4B-CHC-C1C	-2.36	120.74	126.34
25	Y	101	BCR	C29-C30-C25	2.36	114.11	110.48
23	a	410	CLA	O2A-CGA-CBA	2.36	119.31	111.91
23	b	606	CLA	C4C-C3C-C2C	-2.36	103.46	106.90
23	B	608	CLA	CHC-C4B-NB	2.36	126.75	124.26
23	C	511	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
25	b	618	BCR	C29-C28-C27	-2.35	106.12	111.38
27	A	411	PL9	C15-C14-C16	2.35	119.23	115.27
23	B	608	CLA	CHB-C1B-C2B	-2.35	120.59	127.24
27	d	406	PL9	C36-C34-C33	-2.35	116.36	121.12
23	B	616	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
23	c	910	CLA	CAA-CBA-CGA	-2.35	106.38	113.25
26	A	410	SQD	O5-C1-C2	-2.35	105.37	110.35
23	C	511	CLA	C3C-C4C-NC	2.35	113.21	110.57
23	B	603	CLA	C4D-C3D-CAD	2.35	110.87	108.10
23	B	613	CLA	C14-C13-C15	-2.35	102.78	111.29
23	b	617	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
23	B	610	CLA	OBD-CAD-C3D	-2.35	122.87	128.52
23	C	511	CLA	CHA-C4D-ND	2.35	137.41	132.50
28	K	101	LHG	O4-P-O5	2.35	119.87	110.68
30	T	103	LMT	C4'-C3'-C2'	2.35	114.92	110.82
26	A	415	SQD	O7-S-C6	-2.35	104.15	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CHA-C4D-ND	2.35	137.41	132.50
23	C	510	CLA	C1-O2A-CGA	2.35	122.60	116.44
25	C	516	BCR	C24-C23-C22	-2.34	122.69	126.23
34	B	622	LMG	O8-C28-O10	-2.34	117.68	123.59
23	A	406	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
25	D	405	BCR	C2-C1-C6	2.34	114.09	110.48
28	d	409	LHG	O8-C23-C24	2.34	119.26	111.91
26	x	101	SQD	O6-C1-C2	2.34	111.96	108.30
36	C	517	DGD	O2G-C1B-O1B	-2.34	118.04	123.70
23	C	502	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
23	b	612	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	C	506	CLA	O2A-CGA-CBA	2.34	119.25	111.91
23	b	605	CLA	CHC-C1C-C2C	-2.34	120.23	126.73
23	a	406	CLA	C1D-ND-C4D	-2.34	104.67	106.33
23	B	615	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
23	C	512	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	d	403	CLA	CED-O2D-CGD	2.34	121.22	115.94
23	C	514	CLA	CED-O2D-CGD	2.34	121.22	115.94
23	b	614	CLA	CHA-C4D-ND	2.34	137.38	132.50
23	C	502	CLA	C4C-C3C-C2C	-2.33	103.49	106.90
23	B	608	CLA	CMC-C2C-C3C	2.33	132.46	126.12
23	b	609	CLA	C11-C10-C8	-2.33	108.37	115.92
24	D	402	PHO	C3D-CAD-CBD	2.33	110.68	107.61
23	A	405	CLA	O2A-CGA-CBA	2.33	119.23	111.91
36	d	407	DGD	O6D-C5D-C4D	2.33	113.70	109.52
28	D	410	LHG	O4-P-O5	2.33	123.76	112.24
23	B	616	CLA	CMD-C2D-C1D	2.33	128.82	124.71
23	B	608	CLA	CHA-C4D-ND	2.33	137.37	132.50
23	c	912	CLA	CMD-C2D-C1D	2.33	128.82	124.71
23	b	608	CLA	C1-C2-C3	-2.33	122.01	126.04
36	d	407	DGD	O2G-C1B-O1B	-2.33	118.07	123.70
23	b	603	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
23	B	614	CLA	C7-C6-C5	-2.33	107.04	113.36
27	d	406	PL9	C31-C32-C33	-2.33	104.23	111.88
25	T	101	BCR	C33-C5-C6	-2.33	121.92	124.53
40	V	203	HEC	CHB-C4A-NA	2.33	126.95	124.44
34	m	102	LMG	O8-C28-O10	-2.33	117.72	123.59
23	B	615	CLA	C4-C3-C5	2.33	119.18	115.27
23	B	602	CLA	C4-C3-C5	2.32	119.18	115.27
25	C	530	BCR	C39-C30-C25	-2.32	106.53	110.30
23	b	609	CLA	C4C-C3C-C2C	-2.32	103.51	106.90
36	c	919	DGD	O2G-C2G-C1G	-2.32	100.00	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	CLA	CHC-C4B-C3B	-2.32	117.39	127.71
23	c	905	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
25	B	619	BCR	C29-C28-C27	-2.32	106.19	111.38
23	C	510	CLA	CHC-C4B-C3B	-2.32	117.39	127.71
23	c	905	CLA	CMC-C2C-C1C	2.32	128.57	125.04
25	c	916	BCR	C15-C14-C13	-2.32	124.00	127.31
27	d	406	PL9	C36-C37-C38	-2.32	104.26	111.88
23	b	612	CLA	C1-C2-C3	-2.32	122.03	126.04
26	L	102	SQD	O48-C23-O10	-2.32	117.75	123.59
23	c	906	CLA	CHB-C1B-NB	-2.32	121.81	124.26
23	b	602	CLA	O1A-CGA-CBA	-2.32	114.70	123.73
23	B	607	CLA	C4-C3-C5	2.32	119.17	115.27
23	B	607	CLA	C4C-C3C-C2C	-2.31	103.52	106.90
23	b	603	CLA	CMA-C3A-C4A	-2.31	105.55	111.77
25	T	101	BCR	C3-C4-C5	-2.31	109.94	114.08
23	b	602	CLA	C3D-C4D-CHA	-2.31	107.43	112.72
23	b	602	CLA	C4D-C3D-CAD	2.31	110.82	108.10
40	v	203	HEC	CMD-C2D-C1D	2.31	128.56	125.04
36	c	917	DGD	O1G-C1G-C2G	-2.31	101.70	108.43
28	d	409	LHG	O2-C2-C3	-2.31	101.45	109.56
23	C	506	CLA	C1D-CHD-C4C	-2.31	121.07	126.06
23	B	608	CLA	C1-O2A-CGA	2.31	122.51	116.44
23	b	608	CLA	CHC-C4B-C3B	-2.31	117.43	127.71
23	b	614	CLA	C3C-C4C-NC	2.31	113.16	110.57
34	B	622	LMG	O8-C28-C29	2.31	119.15	111.91
23	a	410	CLA	C1D-ND-C4D	-2.31	104.69	106.33
35	c	923	HTG	O5-C1-S1	-2.31	107.51	113.87
23	c	909	CLA	CHA-C4D-ND	2.31	137.33	132.50
23	C	503	CLA	C3C-C4C-NC	2.31	113.16	110.57
23	b	615	CLA	C3B-C4B-NB	2.31	112.65	110.52
23	d	401	CLA	C3B-C4B-NB	2.31	112.65	110.52
23	C	508	CLA	OBD-CAD-C3D	-2.30	122.97	128.52
23	b	610	CLA	CHC-C4B-C3B	-2.30	117.46	127.71
23	B	606	CLA	O2A-C1-C2	-2.30	102.58	108.64
23	c	913	CLA	C1D-ND-C4D	-2.30	104.70	106.33
23	B	616	CLA	CMB-C2B-C1B	2.30	128.88	125.37
25	k	102	BCR	C8-C7-C6	-2.30	120.74	127.20
25	Y	101	BCR	C10-C11-C12	-2.30	116.03	123.22
28	a	415	LHG	O8-C23-O10	-2.30	117.78	123.59
30	b	621	LMT	C6'-C5'-C4'	-2.30	106.63	113.33
25	c	916	BCR	C35-C13-C14	-2.30	119.70	122.92
38	H	102	RRX	C16-C15-C14	-2.30	118.76	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	CLA	O2D-CGD-CBD	2.30	115.35	111.27
40	V	203	HEC	O2D-CGD-CBD	2.30	121.41	114.03
23	d	404	CLA	C1D-CHD-C4C	-2.30	121.10	126.06
23	c	905	CLA	CHA-C4D-ND	2.30	137.30	132.50
23	c	902	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
35	B	625	HTG	C3-C4-C5	-2.30	106.14	110.24
25	C	516	BCR	C15-C14-C13	-2.30	124.03	127.31
23	d	404	CLA	C4-C3-C5	2.29	119.13	115.27
28	E	101	LHG	O8-C23-O10	-2.29	117.80	123.59
23	d	404	CLA	CBA-CAA-C2A	-2.29	107.09	113.86
23	A	405	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
25	b	618	BCR	C35-C13-C12	2.29	121.69	118.08
26	B	621	SQD	O9-S-O7	-2.29	106.02	113.95
23	B	613	CLA	O2A-CGA-CBA	2.29	119.09	111.91
23	b	614	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
23	d	401	CLA	CHD-C4C-NC	2.29	127.81	124.20
23	c	911	CLA	O2A-CGA-CBA	2.29	119.09	111.91
25	d	405	BCR	C15-C16-C17	-2.29	118.79	123.47
35	b	623	HTG	C1-O5-C5	-2.29	108.36	112.58
23	b	608	CLA	C4B-CHC-C1C	-2.28	120.92	126.34
23	b	615	CLA	CED-O2D-CGD	2.28	121.10	115.94
23	b	603	CLA	C3D-C4D-CHA	-2.28	107.50	112.72
25	C	515	BCR	C16-C17-C18	-2.28	124.05	127.31
27	a	414	PL9	C22-C23-C24	-2.28	122.16	127.66
34	J	101	LMG	O7-C10-O9	-2.28	118.19	123.70
25	b	620	BCR	C38-C26-C25	-2.28	121.97	124.53
31	b	639	DMS	C2-S-C1	2.28	110.18	98.44
25	b	618	BCR	C23-C24-C25	-2.28	120.80	127.20
23	C	505	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
23	c	907	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
23	b	614	CLA	CMB-C2B-C1B	2.28	128.84	125.37
23	c	907	CLA	CHC-C4B-C3B	-2.28	117.57	127.71
23	b	605	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
40	V	203	HEC	C2B-C1B-NB	-2.28	107.15	109.88
25	a	411	BCR	C7-C8-C9	-2.28	122.80	126.23
38	x	102	RRX	C7-C8-C9	-2.28	122.80	126.23
23	b	613	CLA	C1D-CHD-C4C	-2.28	121.15	126.06
23	A	408	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
25	B	619	BCR	C2-C1-C6	2.27	113.98	110.48
36	c	918	DGD	O1G-C1A-C2A	2.27	119.04	111.91
23	b	604	CLA	C1-C2-C3	-2.27	122.11	126.04
23	c	902	CLA	C3C-C4C-NC	2.27	113.12	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C16-C15-C14	-2.27	118.82	123.47
23	c	913	CLA	O2A-CGA-CBA	2.27	119.03	111.91
25	Y	101	BCR	C37-C22-C23	2.27	121.65	118.08
25	b	619	BCR	C15-C16-C17	-2.27	118.82	123.47
23	c	905	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
23	b	610	CLA	CED-O2D-CGD	2.27	121.07	115.94
27	a	414	PL9	C27-C28-C29	-2.27	122.19	127.66
23	B	603	CLA	C16-C15-C13	-2.27	108.58	115.92
23	B	603	CLA	C1-O2A-CGA	2.27	122.40	116.44
30	Z	101	LMT	O5'-C5'-C4'	2.27	114.53	109.75
23	B	614	CLA	C3B-C2B-C1B	-2.27	104.43	107.16
23	B	612	CLA	C4-C3-C5	2.27	119.08	115.27
36	C	519	DGD	C3D-C4D-C5D	-2.27	106.20	110.24
36	C	519	DGD	O3D-C3D-C2D	-2.26	105.11	110.35
25	c	915	BCR	C33-C5-C6	-2.26	121.99	124.53
23	b	608	CLA	C7-C6-C5	-2.26	107.21	113.36
25	B	619	BCR	C8-C7-C6	-2.26	120.85	127.20
23	A	405	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
26	A	410	SQD	O2-C2-C1	2.26	115.54	110.05
25	j	104	BCR	C15-C16-C17	-2.26	118.84	123.47
35	O	302	HTG	C1-C2-C3	2.26	115.05	110.59
23	B	615	CLA	CHC-C4B-C3B	-2.26	117.66	127.71
23	C	504	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
23	B	613	CLA	CED-O2D-CGD	2.26	121.04	115.94
23	c	903	CLA	C4-C3-C5	2.26	119.07	115.27
35	b	623	HTG	O5-C5-C6	2.26	112.05	106.44
23	C	503	CLA	CHC-C1C-C2C	-2.26	120.46	126.73
23	b	614	CLA	C7-C6-C5	-2.26	107.23	113.36
23	B	607	CLA	CHA-C4D-ND	2.26	137.22	132.50
34	j	101	LMG	C1-O6-C5	2.25	118.11	113.69
23	a	410	CLA	C1D-CHD-C4C	-2.25	121.19	126.06
28	d	402	LHG	O8-C23-O10	-2.25	117.90	123.59
23	A	408	CLA	C3D-C4D-ND	2.25	113.88	110.24
25	A	409	BCR	C8-C7-C6	-2.25	120.88	127.20
23	b	603	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
23	C	510	CLA	CMC-C2C-C3C	2.25	132.22	126.12
23	b	617	CLA	CMB-C2B-C3B	2.25	132.03	126.59
28	D	411	LHG	O7-C7-C8	2.25	116.35	111.50
40	V	203	HEC	CBB-CAB-C3B	2.25	118.63	112.43
35	b	622	HTG	O2-C2-C3	-2.25	105.15	110.35
27	d	406	PL9	C40-C39-C38	-2.25	117.92	123.68
23	b	605	CLA	CGD-CBD-CAD	-2.25	103.46	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	C4-C3-C5	2.25	119.05	115.27
23	b	611	CLA	C6-C5-C3	-2.25	107.57	113.45
34	D	412	LMG	O1-C7-C8	-2.24	105.48	110.90
23	c	903	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
23	B	609	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
30	F	101	LMT	O4'-C4B-C5B	2.24	114.86	109.30
23	A	406	CLA	CHC-C1C-C2C	-2.24	120.51	126.73
23	b	606	CLA	CHB-C4A-NA	2.24	127.61	124.51
25	A	409	BCR	C20-C19-C18	-2.24	120.12	126.42
23	b	614	CLA	CHC-C4B-C3B	-2.24	117.75	127.71
27	a	414	PL9	C40-C39-C41	2.24	119.04	115.27
23	d	403	CLA	C5-C3-C2	-2.24	116.59	121.12
23	B	605	CLA	C3B-C2B-C1B	-2.24	104.46	107.16
27	d	406	PL9	C35-C34-C36	2.24	119.03	115.27
30	M	101	LMT	C1'-O5'-C5'	-2.24	109.30	113.69
23	B	615	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
36	h	102	DGD	C6E-C5E-C4E	2.24	118.24	113.00
34	a	413	LMG	O1-C1-C2	2.24	111.79	108.30
30	B	623	LMT	C3B-C4B-C5B	2.23	114.22	110.24
23	b	609	CLA	CHC-C1C-C2C	-2.23	120.52	126.73
23	B	615	CLA	O2A-CGA-CBA	2.23	118.92	111.91
25	j	104	BCR	C40-C30-C25	-2.23	106.68	110.30
25	c	915	BCR	C28-C27-C26	-2.23	110.09	114.08
38	x	102	RRX	O2-C28-C27	-2.23	104.90	109.68
23	b	610	CLA	C4-C3-C5	2.23	119.02	115.27
34	j	101	LMG	C31-C30-C29	-2.23	105.18	113.19
23	c	903	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
23	B	605	CLA	C3D-C4D-CHA	-2.23	107.63	112.72
23	b	602	CLA	CMD-C2D-C1D	2.23	128.64	124.71
36	c	917	DGD	C1E-O6E-C5E	2.23	118.06	113.69
23	C	512	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
23	B	614	CLA	C4B-CHC-C1C	-2.22	121.06	126.34
25	Y	101	BCR	C8-C9-C10	-2.22	115.53	118.94
26	A	415	SQD	C3-C4-C5	2.22	114.20	110.24
27	a	414	PL9	C16-C14-C13	-2.22	116.62	121.12
27	D	406	PL9	C11-C9-C8	-2.22	116.62	121.12
25	j	104	BCR	C34-C9-C8	2.22	121.58	118.08
23	C	504	CLA	CHC-C1C-NC	-2.22	120.83	124.20
23	C	507	CLA	C2A-C3A-C4A	-2.22	98.28	101.87
36	h	102	DGD	CDA-CCA-CBA	-2.22	103.16	114.42
23	b	612	CLA	O2A-C1-C2	-2.22	102.80	108.64
23	a	410	CLA	C1-C2-C3	-2.22	122.21	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	912	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
36	C	519	DGD	C3G-C2G-C1G	-2.22	106.54	111.79
26	L	102	SQD	O6-C44-C45	2.22	116.25	110.90
25	B	620	BCR	C8-C7-C6	-2.22	120.98	127.20
23	C	513	CLA	CHD-C1D-ND	-2.22	122.42	124.45
23	B	608	CLA	CBB-CAB-C3B	-2.22	116.60	127.62
23	D	404	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
36	c	919	DGD	O1G-C1A-O1A	-2.21	118.00	123.59
23	B	604	CLA	CED-O2D-CGD	2.21	120.94	115.94
23	b	608	CLA	CGD-CBD-CAD	-2.21	103.57	110.73
23	c	914	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
34	C	501	LMG	O6-C1-C2	-2.21	105.67	110.35
23	C	509	CLA	O2D-CGD-CBD	2.21	115.20	111.27
25	c	915	BCR	C29-C28-C27	-2.21	106.44	111.38
23	B	606	CLA	CHC-C1C-NC	-2.21	120.85	124.20
25	b	619	BCR	C37-C22-C21	-2.21	119.83	122.92
23	B	603	CLA	C3D-C4D-CHA	-2.21	107.67	112.72
23	b	616	CLA	C3C-C4C-NC	2.21	113.05	110.57
23	c	908	CLA	C3C-C4C-NC	2.21	113.05	110.57
23	b	602	CLA	CHC-C4B-NB	2.21	126.59	124.26
23	B	605	CLA	CGD-CBD-CAD	-2.21	103.59	110.73
23	d	401	CLA	CHB-C1B-NB	-2.21	121.92	124.26
23	c	907	CLA	C1D-ND-C4D	-2.20	104.77	106.33
23	c	904	CLA	CMC-C2C-C1C	2.20	128.40	125.04
23	B	604	CLA	C6-C5-C3	2.20	119.23	113.45
23	C	504	CLA	O2A-CGA-CBA	2.20	118.82	111.91
25	B	620	BCR	C10-C11-C12	-2.20	116.35	123.22
25	Y	101	BCR	C38-C26-C27	2.20	117.84	113.62
28	D	411	LHG	O8-C23-O10	-2.20	118.04	123.59
23	C	502	CLA	C1-C2-C3	-2.20	122.24	126.04
23	A	406	CLA	CMC-C2C-C1C	2.20	128.39	125.04
28	d	409	LHG	C13-C12-C11	-2.20	103.26	114.42
23	A	405	CLA	C5-C3-C2	-2.20	116.67	121.12
25	d	405	BCR	C7-C8-C9	-2.20	122.91	126.23
25	b	619	BCR	C30-C25-C26	-2.20	119.52	122.61
36	C	519	DGD	C4E-C3E-C2E	-2.20	106.99	110.82
25	C	530	BCR	C16-C17-C18	-2.20	124.18	127.31
23	d	404	CLA	O2A-C1-C2	-2.20	102.86	108.64
23	C	511	CLA	CMD-C2D-C1D	2.20	128.58	124.71
23	B	616	CLA	C3C-C4C-NC	2.20	113.03	110.57
23	a	407	CLA	CMC-C2C-C3C	2.20	132.08	126.12
23	C	508	CLA	CED-O2D-CGD	2.20	120.90	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	CAC-C3C-C4C	2.19	127.66	124.81
28	K	101	LHG	P-O6-C4	2.19	124.34	118.30
23	b	603	CLA	C4D-CHA-C1A	-2.19	118.58	121.25
23	c	903	CLA	C6-C5-C3	-2.19	107.71	113.45
34	D	412	LMG	O8-C28-C29	2.19	118.79	111.91
23	B	612	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	c	904	CLA	CHB-C1B-NB	-2.19	121.94	124.26
30	M	101	LMT	O1'-C1-C2	-2.19	101.89	109.56
23	C	505	CLA	C1D-CHD-C4C	-2.19	121.33	126.06
23	B	603	CLA	CHC-C4B-C3B	-2.19	117.97	127.71
34	C	520	LMG	O1-C7-C8	-2.19	105.61	110.90
25	B	618	BCR	C20-C21-C22	-2.19	124.19	127.31
34	j	101	LMG	O2-C2-C1	-2.19	104.73	110.05
23	B	617	CLA	C1D-ND-C4D	-2.19	104.78	106.33
25	d	405	BCR	C2-C3-C4	2.19	116.27	111.38
23	b	617	CLA	C1D-CHD-C4C	-2.19	121.34	126.06
23	D	404	CLA	CHD-C4C-NC	2.19	127.65	124.20
24	a	409	PHO	C11-C12-C13	-2.19	108.85	115.92
23	b	609	CLA	CHD-C4C-NC	2.19	127.65	124.20
23	B	603	CLA	CAC-C3C-C4C	2.19	127.65	124.81
23	b	614	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
25	T	101	BCR	C40-C30-C25	-2.19	106.75	110.30
30	B	644	LMT	C1'-O5'-C5'	2.19	117.98	113.69
23	b	603	CLA	O2A-CGA-CBA	2.19	118.77	111.91
23	C	513	CLA	CHD-C4C-NC	2.19	127.65	124.20
23	B	617	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	c	908	CLA	C11-C12-C13	-2.18	108.86	115.92
23	d	401	CLA	C6-C7-C8	-2.18	108.86	115.92
23	b	612	CLA	C6-C5-C3	2.18	119.18	113.45
23	d	401	CLA	CHC-C1C-C2C	-2.18	120.67	126.73
25	k	102	BCR	C34-C9-C10	-2.18	119.87	122.92
25	B	618	BCR	C21-C20-C19	-2.18	116.41	123.22
23	D	403	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
23	b	613	CLA	CHD-C4C-NC	2.18	127.64	124.20
24	a	409	PHO	CBC-CAC-C3C	2.18	116.07	112.88
23	b	604	CLA	C7-C6-C5	-2.18	107.44	113.36
35	v	204	HTG	O5-C5-C4	2.18	113.65	109.69
30	z	101	LMT	C1B-O5B-C5B	-2.18	109.42	113.69
36	C	519	DGD	O2G-C1B-O1B	-2.18	118.44	123.70
23	c	905	CLA	C4C-C3C-C2C	-2.18	103.73	106.90
23	a	410	CLA	CMC-C2C-C1C	2.17	128.35	125.04
23	C	514	CLA	O2A-CGA-O1A	-2.17	118.11	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	j	101	LMG	C6-C5-C4	2.17	118.10	113.00
25	t	101	BCR	C8-C9-C10	-2.17	115.61	118.94
23	C	511	CLA	C1D-CHD-C4C	-2.17	121.37	126.06
25	d	405	BCR	C30-C25-C24	2.17	121.92	115.78
34	c	930	LMG	O7-C10-O9	-2.17	118.45	123.70
26	a	412	SQD	C44-O6-C1	-2.17	109.50	113.74
23	C	513	CLA	CHB-C4A-NA	2.17	127.52	124.51
23	b	615	CLA	C1-O2A-CGA	2.17	122.14	116.44
23	b	616	CLA	C3B-C4B-NB	2.17	112.53	110.52
28	l	101	LHG	C6-C5-C4	-2.17	106.65	111.79
23	c	908	CLA	C1D-ND-C4D	-2.17	104.79	106.33
23	c	907	CLA	C3C-C4C-NC	2.17	113.00	110.57
23	D	403	CLA	CMD-C2D-C1D	2.17	128.53	124.71
23	a	410	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	B	609	CLA	C4D-C3D-CAD	2.17	110.65	108.10
23	b	606	CLA	OBD-CAD-C3D	-2.17	123.31	128.52
40	v	203	HEC	CAA-C2A-C3A	-2.17	123.84	127.88
23	a	410	CLA	OBD-CAD-C3D	-2.17	123.31	128.52
25	T	101	BCR	C34-C9-C8	2.17	121.49	118.08
25	t	101	BCR	C12-C13-C14	-2.17	115.62	118.94
23	b	615	CLA	O2A-CGA-CBA	2.16	118.70	111.91
23	B	608	CLA	CHC-C1C-NC	-2.16	120.92	124.20
23	A	406	CLA	C4-C3-C5	2.16	118.91	115.27
23	d	403	CLA	CHD-C4C-NC	2.16	127.61	124.20
36	H	103	DGD	O5E-C6E-C5E	-2.16	103.87	111.29
23	c	907	CLA	CMC-C2C-C1C	2.16	128.33	125.04
23	a	407	CLA	CMB-C2B-C1B	2.16	128.66	125.37
23	B	604	CLA	CMD-C2D-C1D	2.16	128.52	124.71
23	C	513	CLA	OBD-CAD-C3D	-2.16	123.32	128.52
30	b	621	LMT	C1-O1'-C1'	-2.16	110.26	113.84
23	C	505	CLA	C7-C6-C5	-2.16	107.50	113.36
36	C	517	DGD	O5D-C1E-C2E	-2.16	104.93	108.30
23	B	605	CLA	CHC-C4B-C3B	-2.16	118.11	127.71
30	F	101	LMT	C1'-C2'-C3'	2.16	114.49	110.00
24	A	407	PHO	O2A-CGA-O1A	-2.16	118.15	123.59
28	E	101	LHG	C6-O8-C23	2.16	125.10	117.12
23	b	607	CLA	C7-C6-C5	-2.16	107.51	113.36
28	K	101	LHG	O8-C23-O10	-2.15	118.15	123.59
26	a	412	SQD	O48-C23-C24	2.15	118.67	111.91
25	B	620	BCR	C16-C17-C18	-2.15	124.24	127.31
23	C	509	CLA	C3C-C4C-NC	2.15	112.98	110.57
37	e	105	HEM	C2A-C1A-NA	-2.15	107.74	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	BCR	C39-C30-C25	-2.15	106.81	110.30
26	A	410	SQD	O8-S-C6	2.15	109.16	105.74
25	j	104	BCR	C8-C9-C10	-2.15	115.64	118.94
23	C	506	CLA	C7-C6-C5	-2.15	107.53	113.36
23	A	406	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
30	B	623	LMT	O5B-C5B-C4B	2.15	113.59	109.69
30	e	103	LMT	O5'-C5'-C4'	2.15	114.28	109.75
23	C	511	CLA	CHC-C1C-C2C	-2.14	120.77	126.73
30	e	103	LMT	O1'-C1'-C2'	2.14	111.65	108.30
23	c	908	CLA	C7-C6-C5	-2.14	107.54	113.36
23	A	408	CLA	CBA-CAA-C2A	-2.14	107.54	113.86
23	c	907	CLA	CGD-CBD-CAD	-2.14	103.79	110.73
23	B	610	CLA	C1D-CHD-C4C	-2.14	121.44	126.06
25	b	618	BCR	C8-C7-C6	-2.14	121.19	127.20
36	c	919	DGD	O3G-C1D-C2D	-2.14	104.96	108.30
23	B	614	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
23	C	505	CLA	CHC-C4B-C3B	-2.14	118.20	127.71
23	C	508	CLA	C3B-C4B-NB	2.14	112.50	110.52
25	C	515	BCR	C34-C9-C8	2.14	121.44	118.08
36	c	918	DGD	O6E-C5E-C6E	2.14	111.75	106.44
30	a	418	LMT	O2'-C2'-C1'	2.14	115.23	110.05
24	A	407	PHO	OBD-CAD-CBD	-2.14	122.69	125.82
23	b	608	CLA	O2A-CGA-CBA	2.14	118.61	111.91
25	d	405	BCR	C34-C9-C8	2.13	121.44	118.08
25	t	101	BCR	C7-C6-C5	-2.13	116.29	121.46
34	B	622	LMG	O1-C7-C8	-2.13	105.75	110.90
25	b	618	BCR	C11-C10-C9	-2.13	124.27	127.31
30	I	101	LMT	C1B-O1B-C4'	2.13	123.24	117.96
37	E	105	HEM	C1B-NB-C4B	2.13	107.28	105.07
23	b	604	CLA	O2A-CGA-CBA	2.13	118.60	111.91
34	J	101	LMG	O6-C1-C2	2.13	114.86	110.35
23	A	408	CLA	CMC-C2C-C3C	2.13	131.90	126.12
23	B	605	CLA	C4-C3-C5	2.13	118.85	115.27
23	c	904	CLA	C3C-C4C-NC	2.13	112.96	110.57
38	H	102	RRX	C32-C1-C6	2.13	113.75	110.30
23	C	509	CLA	C4C-C3C-C2C	-2.13	103.80	106.90
25	k	102	BCR	C34-C9-C8	2.13	121.43	118.08
23	D	404	CLA	O2A-CGA-CBA	2.13	118.58	111.91
23	b	604	CLA	CHC-C1C-NC	-2.13	120.98	124.20
36	c	918	DGD	O4E-C4E-C3E	-2.13	105.43	110.35
30	b	621	LMT	C3'-C4'-C5'	2.13	115.80	110.93
36	C	519	DGD	O2G-C1B-C2B	2.12	116.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C29-C28-C27	-2.12	106.63	111.38
23	B	606	CLA	CMB-C2B-C1B	2.12	128.60	125.37
24	a	408	PHO	CMB-C2B-C3B	2.12	128.65	124.68
25	b	618	BCR	C32-C1-C6	-2.12	106.85	110.30
25	d	405	BCR	C32-C1-C2	-2.12	100.41	108.91
25	j	104	BCR	C29-C30-C25	2.12	113.75	110.48
23	b	613	CLA	CMD-C2D-C1D	2.12	128.45	124.71
23	C	509	CLA	CHD-C4C-NC	2.12	127.55	124.20
25	B	618	BCR	C34-C9-C10	-2.12	119.95	122.92
23	A	405	CLA	CBB-CAB-C3B	-2.12	117.06	127.62
23	B	612	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
25	c	915	BCR	C15-C16-C17	-2.12	119.13	123.47
23	c	908	CLA	CHC-C4B-C3B	-2.12	118.28	127.71
35	d	413	HTG	C2'-C1'-S1	-2.12	105.56	112.40
23	B	612	CLA	CHD-C1D-ND	-2.12	122.51	124.45
36	C	519	DGD	C3A-C2A-C1A	-2.12	105.92	113.62
23	C	510	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
23	D	403	CLA	CBA-CAA-C2A	-2.12	107.62	113.86
23	C	505	CLA	C1-O2A-CGA	2.12	122.00	116.44
23	D	403	CLA	C3D-C4D-CHA	-2.11	107.89	112.72
23	A	405	CLA	C16-C15-C13	-2.11	109.09	115.92
25	t	101	BCR	C21-C20-C19	-2.11	116.62	123.22
23	B	608	CLA	CMD-C2D-C1D	2.11	128.44	124.71
25	b	619	BCR	C8-C9-C10	-2.11	115.70	118.94
23	C	505	CLA	OBD-CAD-C3D	-2.11	123.44	128.52
23	B	614	CLA	CHC-C4B-C3B	-2.11	118.31	127.71
23	C	508	CLA	CHC-C4B-C3B	-2.11	118.32	127.71
23	b	605	CLA	O2A-CGA-CBA	2.11	118.53	111.91
25	B	619	BCR	C39-C30-C25	-2.11	106.88	110.30
23	b	605	CLA	C3B-C4B-NB	2.11	112.47	110.52
35	B	630	HTG	O5-C5-C6	2.11	111.68	106.44
26	L	102	SQD	O9-S-O7	-2.11	106.65	113.95
27	D	406	PL9	O2-C1-C6	-2.11	116.94	120.59
23	b	609	CLA	C6-C5-C3	-2.11	107.93	113.45
23	B	616	CLA	C11-C10-C8	-2.11	109.11	115.92
25	T	101	BCR	C28-C27-C26	-2.11	110.31	114.08
23	B	613	CLA	CHC-C4B-C3B	-2.11	118.33	127.71
25	c	915	BCR	C37-C22-C23	2.11	121.40	118.08
23	B	602	CLA	CAC-C3C-C4C	2.11	127.54	124.81
23	a	406	CLA	C1-C2-C3	-2.11	122.40	126.04
23	B	603	CLA	CMB-C2B-C3B	2.11	131.69	126.59
30	A	416	LMT	C1B-O5B-C5B	2.11	117.82	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	CLA	C4-C3-C2	-2.11	118.28	123.68
30	T	103	LMT	O5'-C1'-C2'	2.10	114.80	110.35
25	B	618	BCR	C37-C22-C23	2.10	121.39	118.08
23	C	502	CLA	CMB-C2B-C1B	2.10	128.57	125.37
23	B	611	CLA	CMC-C2C-C3C	2.10	131.82	126.12
23	A	408	CLA	C4B-CHC-C1C	-2.10	121.35	126.34
37	e	105	HEM	CAD-CBD-CGD	2.10	118.12	113.60
34	J	101	LMG	O7-C10-C11	2.10	116.03	111.50
23	b	603	CLA	C7-C6-C5	-2.10	107.66	113.36
36	c	919	DGD	CEA-CDA-CCA	-2.10	103.77	114.42
23	b	604	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
23	C	514	CLA	CMB-C2B-C1B	2.10	128.56	125.37
25	T	101	BCR	C1-C6-C7	2.10	121.70	115.78
24	D	402	PHO	CAC-C3C-C4C	2.09	129.58	124.27
23	b	611	CLA	C1-O2A-CGA	2.09	121.94	116.44
23	d	404	CLA	CMC-C2C-C3C	2.09	131.80	126.12
23	B	617	CLA	O2A-C1-C2	2.09	114.14	108.64
25	T	101	BCR	C7-C6-C5	-2.09	116.39	121.46
23	b	603	CLA	C2A-C3A-C4A	-2.09	98.49	101.87
23	b	608	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
23	a	410	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
23	C	504	CLA	C3C-C4C-NC	2.09	112.92	110.57
28	a	415	LHG	O7-C7-O9	-2.09	118.65	123.70
34	B	622	LMG	C18-C17-C16	-2.09	103.82	114.42
23	C	512	CLA	O2A-C1-C2	-2.09	103.14	108.64
23	b	608	CLA	CED-O2D-CGD	2.09	120.66	115.94
23	c	906	CLA	CED-O2D-CGD	2.09	120.66	115.94
23	c	907	CLA	C3D-C4D-CHA	-2.09	107.94	112.72
23	c	904	CLA	C7-C6-C5	-2.09	107.69	113.36
23	B	612	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
23	b	604	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
37	E	105	HEM	CAD-C3D-C4D	2.09	128.30	124.66
30	m	104	LMT	C1-O1'-C1'	2.09	117.30	113.84
26	D	408	SQD	O5-C5-C4	2.08	113.48	109.69
25	B	619	BCR	C33-C5-C6	-2.08	122.19	124.53
23	a	406	CLA	CBB-CAB-C3B	-2.08	117.25	127.62
28	e	101	LHG	O8-C23-O10	-2.08	118.33	123.59
23	b	602	CLA	OBD-CAD-C3D	-2.08	123.51	128.52
23	c	913	CLA	CMB-C2B-C1B	2.08	128.54	125.37
36	h	102	DGD	O3G-C3G-C2G	-2.08	105.88	110.90
23	B	617	CLA	CHB-C1B-C2B	-2.08	121.36	127.24
23	b	610	CLA	C1-C2-C3	-2.08	122.44	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	O2A-CGA-CBA	2.08	118.44	111.91
23	D	404	CLA	CHC-C4B-C3B	-2.08	118.46	127.71
23	c	906	CLA	O2A-CGA-CBA	2.08	118.43	111.91
35	v	204	HTG	O4-C4-C3	-2.08	105.54	110.35
23	c	906	CLA	C4C-C3C-C2C	-2.08	103.87	106.90
23	B	604	CLA	CHA-C4D-ND	2.08	136.85	132.50
23	B	609	CLA	C1-O2A-CGA	2.08	121.90	116.44
34	B	622	LMG	C38-C37-C36	-2.08	103.88	114.42
36	c	918	DGD	C2G-O2G-C1B	-2.08	112.68	117.79
23	b	607	CLA	C4B-CHC-C1C	-2.07	121.42	126.34
23	C	506	CLA	CHC-C4B-C3B	-2.07	118.48	127.71
23	c	911	CLA	C4D-C3D-CAD	2.07	110.54	108.10
23	D	403	CLA	C4C-C3C-C2C	-2.07	103.88	106.90
37	e	105	HEM	C4D-C3D-C2D	-2.07	103.88	106.90
25	b	618	BCR	C20-C19-C18	-2.07	120.59	126.42
23	b	602	CLA	C4C-C3C-C2C	-2.07	103.88	106.90
26	A	410	SQD	O3-C3-C2	-2.07	105.56	110.35
34	D	412	LMG	C3-C4-C5	2.07	113.93	110.24
23	c	903	CLA	C1-C2-C3	-2.07	122.46	126.04
25	B	620	BCR	C38-C26-C27	2.07	117.59	113.62
36	D	407	DGD	O2G-C1B-O1B	-2.07	118.70	123.70
23	b	616	CLA	C4D-CHA-C1A	-2.07	118.73	121.25
26	A	410	SQD	C44-O6-C1	-2.07	109.70	113.74
23	C	508	CLA	CAC-C3C-C4C	2.07	127.49	124.81
26	A	415	SQD	C46-O48-C23	2.07	124.77	117.12
25	C	516	BCR	C38-C26-C25	-2.06	122.21	124.53
23	B	609	CLA	CBB-CAB-C3B	-2.06	117.35	127.62
40	v	203	HEC	C4A-CHB-C1B	-2.06	121.61	126.06
27	A	411	PL9	C16-C14-C13	-2.06	116.94	121.12
30	F	101	LMT	O5B-C5B-C6B	2.06	111.56	106.44
23	C	504	CLA	CBB-CAB-C3B	-2.06	117.36	127.62
23	A	405	CLA	CED-O2D-CGD	2.06	120.60	115.94
23	B	609	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	b	609	CLA	CMB-C2B-C3B	2.06	131.58	126.59
23	c	902	CLA	CHA-C4D-ND	2.06	136.81	132.50
23	c	911	CLA	C3D-C4D-ND	2.06	113.57	110.24
23	D	404	CLA	C3D-C4D-CHA	-2.06	108.02	112.72
35	d	413	HTG	O5-C1-S1	-2.06	104.91	109.82
23	B	605	CLA	O2A-CGA-CBA	2.06	118.36	111.91
25	j	104	BCR	C10-C11-C12	-2.06	116.80	123.22
23	B	614	CLA	C1-C2-C3	-2.05	122.49	126.04
23	c	907	CLA	O2A-CGA-CBA	2.05	118.35	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	I	101	LMT	C2'-C3'-C4'	-2.05	104.99	109.68
23	D	404	CLA	CMC-C2C-C1C	2.05	128.16	125.04
23	b	610	CLA	CHD-C4C-NC	2.05	127.44	124.20
23	B	611	CLA	C1D-ND-C4D	-2.05	104.88	106.33
23	c	903	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
23	c	910	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
28	D	409	LHG	C6-O8-C23	2.05	124.72	117.12
23	c	905	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
28	l	101	LHG	O4-P-O5	2.05	122.38	112.24
23	b	615	CLA	CHC-C4B-C3B	-2.05	118.59	127.71
23	c	911	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
23	b	603	CLA	C4D-C3D-CAD	2.05	110.51	108.10
23	B	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
27	D	406	PL9	C27-C26-C24	-2.05	106.24	112.98
23	d	403	CLA	CHC-C4B-C3B	-2.05	118.60	127.71
23	a	406	CLA	CMC-C2C-C3C	2.05	131.68	126.12
23	C	503	CLA	C4-C3-C5	2.05	118.72	115.27
25	D	405	BCR	C36-C18-C17	-2.05	120.06	122.92
23	b	612	CLA	CHB-C4A-NA	2.05	127.34	124.51
31	h	101	DMS	O-S-C2	2.05	116.99	106.54
23	B	609	CLA	C11-C10-C8	-2.05	109.30	115.92
35	v	204	HTG	O5-C5-C6	2.05	111.53	106.44
25	C	515	BCR	C8-C7-C6	-2.05	121.46	127.20
25	B	619	BCR	C28-C27-C26	-2.04	110.43	114.08
36	c	919	DGD	C3E-C4E-C5E	-2.04	106.59	110.24
23	C	514	CLA	C1D-CHD-C4C	-2.04	121.65	126.06
27	A	411	PL9	C20-C19-C21	2.04	118.71	115.27
34	D	412	LMG	O6-C5-C4	2.04	113.41	109.69
23	B	616	CLA	CHC-C4B-C3B	-2.04	118.62	127.71
23	a	410	CLA	CHC-C4B-C3B	-2.04	118.62	127.71
35	C	522	HTG	O5-C1-C2	2.04	112.88	110.31
23	B	607	CLA	O2A-CGA-CBA	2.04	118.32	111.91
23	B	617	CLA	O2A-CGA-CBA	2.04	118.31	111.91
23	b	603	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
23	d	403	CLA	O1D-CGD-CBD	2.04	128.66	124.48
23	c	906	CLA	CHC-C1C-NC	-2.04	121.11	124.20
23	b	607	CLA	C1D-CHD-C4C	-2.04	121.66	126.06
23	a	407	CLA	CHC-C4B-C3B	-2.04	118.64	127.71
23	C	503	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
25	d	405	BCR	C10-C11-C12	-2.04	116.86	123.22
26	a	417	SQD	O6-C44-C45	-2.04	105.98	110.90
23	B	617	CLA	C3D-C4D-CHA	-2.04	108.06	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	418	LMT	O5B-C5B-C4B	2.04	113.39	109.69
23	c	909	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	c	913	CLA	CHC-C4B-C3B	-2.03	118.66	127.71
23	c	906	CLA	C1D-CHD-C4C	-2.03	121.67	126.06
30	T	103	LMT	O6'-C6'-C5'	-2.03	104.32	111.29
23	B	615	CLA	C3D-C4D-CHA	-2.03	108.07	112.72
23	b	613	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	D	403	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
23	B	603	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
23	b	613	CLA	CMB-C2B-C1B	2.03	128.46	125.37
23	d	401	CLA	CGD-CBD-CAD	-2.03	104.16	110.73
23	b	605	CLA	C6-C7-C8	-2.03	109.35	115.92
23	d	403	CLA	C3B-C2B-C1B	-2.03	104.71	107.16
23	c	914	CLA	CAC-C3C-C4C	2.03	127.44	124.81
23	B	616	CLA	C4D-CHA-C1A	-2.03	118.78	121.25
23	b	612	CLA	C14-C13-C15	-2.03	103.95	111.29
23	c	911	CLA	O2A-C1-C2	-2.03	103.31	108.64
23	b	609	CLA	C3B-C4B-NB	2.03	112.40	110.52
23	D	401	CLA	CAC-C3C-C2C	-2.03	124.06	127.53
34	j	101	LMG	O1-C7-C8	-2.03	106.01	110.90
28	D	411	LHG	O7-C7-O9	-2.03	118.81	123.70
23	B	608	CLA	C7-C6-C5	-2.03	107.86	113.36
23	B	602	CLA	CHB-C4A-NA	2.02	127.31	124.51
23	C	512	CLA	CHD-C4C-NC	2.02	127.39	124.20
23	C	504	CLA	CMB-C2B-C1B	2.02	128.45	125.37
37	E	105	HEM	C2A-C1A-NA	-2.02	107.89	110.15
23	c	903	CLA	CHB-C4A-NA	2.02	127.31	124.51
34	D	412	LMG	C8-O7-C10	-2.02	112.81	117.79
36	c	918	DGD	O5D-C1E-C2E	-2.02	105.15	108.30
25	b	620	BCR	C16-C15-C14	-2.02	119.34	123.47
23	c	905	CLA	CHC-C4B-C3B	-2.02	118.72	127.71
23	b	612	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
36	H	103	DGD	O4D-C4D-C5D	2.02	114.31	109.30
23	B	614	CLA	CHA-C4D-ND	2.02	136.72	132.50
34	C	520	LMG	C9-C8-C7	-2.02	107.01	111.79
23	B	608	CLA	C1D-CHD-C4C	-2.02	121.70	126.06
30	A	416	LMT	O3B-C3B-C4B	2.02	115.02	110.35
23	d	404	CLA	C3D-C4D-ND	2.02	113.50	110.24
23	b	616	CLA	C1-C2-C3	-2.02	122.55	126.04
35	O	302	HTG	O2-C2-C3	-2.02	105.69	110.35
23	D	404	CLA	C4C-C3C-C2C	-2.02	103.96	106.90
23	b	615	CLA	C4-C3-C5	2.02	118.66	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	927	DMS	O-S-C1	2.01	116.82	106.54
23	C	503	CLA	C4B-CHC-C1C	-2.01	121.56	126.34
25	C	515	BCR	C23-C24-C25	-2.01	121.55	127.20
23	d	401	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
25	Y	101	BCR	C2-C1-C6	-2.01	107.38	110.48
23	C	510	CLA	CBB-CAB-C3B	-2.01	117.61	127.62
36	C	518	DGD	O5D-C6D-C5D	2.01	112.77	109.05
25	B	620	BCR	C16-C15-C14	-2.01	119.36	123.47
37	E	105	HEM	C3A-C4A-NA	-2.01	107.02	110.08
26	a	412	SQD	O48-C23-O10	-2.01	118.52	123.59
23	B	604	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
23	b	613	CLA	C4B-CHC-C1C	-2.01	121.58	126.34
30	a	422	LMT	O2'-C2'-C1'	2.01	114.92	110.05
35	B	624	HTG	O2-C2-C3	-2.01	105.71	110.35
23	B	604	CLA	O2A-CGA-CBA	2.01	118.20	111.91
23	B	610	CLA	C7-C6-C5	-2.01	107.91	113.36
27	D	406	PL9	C31-C32-C33	-2.01	105.29	111.88
23	c	910	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
25	Y	101	BCR	C20-C21-C22	-2.01	124.45	127.31
23	D	401	CLA	CBA-CAA-C2A	-2.01	107.94	113.86
23	C	513	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
23	A	408	CLA	CHC-C4B-C3B	-2.00	118.79	127.71
23	b	613	CLA	CHC-C4B-C3B	-2.00	118.79	127.71
23	B	609	CLA	CHD-C4C-NC	2.00	127.36	124.20
25	D	405	BCR	C38-C26-C27	2.00	117.46	113.62
30	b	621	LMT	C1'-O5'-C5'	2.00	117.62	113.69
23	B	612	CLA	C15-C13-C12	-2.00	101.61	112.13
24	a	408	PHO	CMA-C3A-C4A	-2.00	110.00	114.38
23	D	403	CLA	CED-O2D-CGD	2.00	120.46	115.94

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	203	HEC	NA
40	v	203	HEC	NA

All (1594) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	603	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	C2-C3-C5-C6
23	B	606	CLA	C4-C3-C5-C6
23	B	610	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C4B-C3B-CAB-CBB
23	B	615	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	C1A-C2A-CAA-CBA
23	C	509	CLA	CHA-CBD-CGD-O1D
23	D	401	CLA	CHA-CBD-CGD-O1D
23	b	602	CLA	C2-C1-O2A-CGA
23	b	602	CLA	CHA-CBD-CGD-O1D
23	b	602	CLA	CHA-CBD-CGD-O2D
23	b	602	CLA	CAD-CBD-CGD-O1D
23	b	603	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O1D
23	b	617	CLA	O2A-C1-C2-C3
23	b	617	CLA	C2-C3-C5-C6
23	b	617	CLA	C4-C3-C5-C6
23	c	909	CLA	CHA-CBD-CGD-O2D
25	D	405	BCR	C21-C22-C23-C24
25	D	405	BCR	C37-C22-C23-C24
25	d	405	BCR	C37-C22-C23-C24
25	d	405	BCR	C23-C24-C25-C30
25	t	101	BCR	C11-C12-C13-C14
25	t	101	BCR	C11-C12-C13-C35
26	A	415	SQD	C2-C1-O6-C44
26	A	415	SQD	O6-C44-C45-O47
26	L	102	SQD	O5-C1-O6-C44
26	L	102	SQD	O49-C7-O47-C45
26	a	417	SQD	C2-C1-O6-C44
26	a	417	SQD	O5-C1-O6-C44
26	a	417	SQD	O6-C44-C45-O47
26	x	101	SQD	C5-C6-S-O8
26	x	101	SQD	C5-C6-S-O9
27	A	411	PL9	C9-C11-C12-C13
27	A	411	PL9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
27	A	411	PL9	C28-C29-C31-C32
27	A	411	PL9	C30-C29-C31-C32
28	A	412	LHG	C4-O6-P-O4
28	A	412	LHG	C4-O6-P-O5
28	A	412	LHG	C8-C7-O7-C5
28	D	410	LHG	C4-O6-P-O4
28	E	101	LHG	C3-O3-P-O4
28	E	101	LHG	O6-C4-C5-O7
28	K	101	LHG	C4-O6-P-O4
28	K	101	LHG	O9-C7-O7-C5
28	K	101	LHG	C8-C7-O7-C5
28	L	101	LHG	C4-O6-P-O3
28	L	101	LHG	C4-O6-P-O4
28	L	101	LHG	C4-O6-P-O5
28	a	415	LHG	C4-O6-P-O3
28	a	415	LHG	C4-O6-P-O4
28	d	402	LHG	O1-C1-C2-C3
28	d	409	LHG	O1-C1-C2-C3
28	e	101	LHG	C4-O6-P-O3
28	l	101	LHG	C4-O6-P-O4
30	Z	101	LMT	C2'-C1'-O1'-C1
30	e	103	LMT	C2'-C1'-O1'-C1
30	e	103	LMT	O5'-C1'-O1'-C1
30	m	103	LMT	C2-C1-O1'-C1'
34	C	501	LMG	C2-C1-O1-C7
34	C	501	LMG	O6-C1-O1-C7
34	D	412	LMG	C11-C10-O7-C8
34	d	411	LMG	C2-C1-O1-C7
34	d	411	LMG	O6-C1-O1-C7
34	d	411	LMG	C8-C9-O8-C28
34	d	411	LMG	C11-C10-O7-C8
35	B	625	HTG	C2'-C1'-S1-C1
35	B	626	HTG	O5-C1-S1-C1'
35	C	521	HTG	C2'-C1'-S1-C1
35	C	522	HTG	C2-C1-S1-C1'
35	C	522	HTG	O5-C1-S1-C1'
35	C	523	HTG	O5-C1-S1-C1'
35	b	623	HTG	C2-C1-S1-C1'
35	b	623	HTG	O5-C1-S1-C1'
35	c	921	HTG	C2-C1-S1-C1'
35	c	921	HTG	O5-C1-S1-C1'
35	d	413	HTG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
35	d	413	HTG	C2'-C1'-S1-C1
35	v	204	HTG	C2'-C1'-S1-C1
36	D	407	DGD	C2A-C1A-O1G-C1G
36	D	407	DGD	O1A-C1A-O1G-C1G
36	D	407	DGD	C2B-C1B-O2G-C2G
36	D	407	DGD	C2D-C1D-O3G-C3G
36	d	407	DGD	C2B-C1B-O2G-C2G
36	d	407	DGD	O1B-C1B-O2G-C2G
30	b	621	LMT	C3'-C4'-O1B-C1B
28	E	101	LHG	O10-C23-O8-C6
34	d	411	LMG	O10-C28-O8-C9
30	m	103	LMT	C4B-C5B-C6B-O6B
30	I	101	LMT	C3'-C4'-O1B-C1B
28	E	101	LHG	C24-C23-O8-C6
23	b	602	CLA	O1A-CGA-O2A-C1
26	D	408	SQD	O10-C23-O48-C46
28	d	402	LHG	O10-C23-O8-C6
23	B	611	CLA	C15-C16-C17-C18
23	C	514	CLA	CBD-CGD-O2D-CED
28	A	412	LHG	O9-C7-O7-C5
34	D	412	LMG	O9-C10-O7-C8
34	d	411	LMG	O9-C10-O7-C8
36	D	407	DGD	O1B-C1B-O2G-C2G
35	v	204	HTG	C1'-C2'-C3'-C4'
23	B	602	CLA	C3-C5-C6-C7
23	B	605	CLA	C3-C5-C6-C7
23	B	615	CLA	C3-C5-C6-C7
23	b	602	CLA	CBA-CGA-O2A-C1
26	D	408	SQD	C24-C23-O48-C46
28	d	402	LHG	C24-C23-O8-C6
34	d	411	LMG	C29-C28-O8-C9
26	L	102	SQD	C8-C7-O47-C45
28	E	101	LHG	C8-C7-O7-C5
23	b	613	CLA	C13-C15-C16-C17
34	m	102	LMG	C37-C38-C39-C40
34	C	501	LMG	C29-C28-O8-C9
36	d	407	DGD	C2A-C1A-O1G-C1G
30	B	623	LMT	O5B-C5B-C6B-O6B
30	T	103	LMT	O5'-C5'-C6'-O6'
23	b	617	CLA	O1D-CGD-O2D-CED
35	C	521	HTG	S1-C1'-C2'-C3'
35	v	204	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
30	a	418	LMT	O5B-C5B-C6B-O6B
30	m	103	LMT	O5B-C5B-C6B-O6B
28	E	101	LHG	O9-C7-O7-C5
34	C	501	LMG	O10-C28-O8-C9
28	E	101	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
36	d	407	DGD	O1A-C1A-O1G-C1G
30	F	101	LMT	O5'-C5'-C6'-O6'
35	B	631	HTG	O5-C5-C6-O6
23	b	616	CLA	C13-C15-C16-C17
36	C	517	DGD	C4A-C5A-C6A-C7A
35	B	626	HTG	O5-C5-C6-O6
30	T	103	LMT	C4'-C5'-C6'-O6'
28	d	410	LHG	C30-C31-C32-C33
34	a	413	LMG	C15-C16-C17-C18
28	a	415	LHG	C17-C18-C19-C20
35	B	630	HTG	S1-C1'-C2'-C3'
30	B	623	LMT	C4B-C5B-C6B-O6B
30	z	101	LMT	C4'-C5'-C6'-O6'
30	Z	101	LMT	C5-C6-C7-C8
34	D	412	LMG	O6-C5-C6-O5
35	v	204	HTG	O5-C5-C6-O6
30	a	418	LMT	C4B-C5B-C6B-O6B
26	A	415	SQD	O5-C1-O6-C44
30	Z	101	LMT	O5'-C1'-O1'-C1
30	m	103	LMT	O5'-C1'-O1'-C1
27	a	414	PL9	C19-C21-C22-C23
27	a	414	PL9	C24-C26-C27-C28
36	d	407	DGD	C2A-C3A-C4A-C5A
26	B	621	SQD	C31-C32-C33-C34
28	D	411	LHG	C30-C31-C32-C33
35	b	623	HTG	C4-C5-C6-O6
36	c	919	DGD	C2B-C3B-C4B-C5B
23	b	617	CLA	CBA-CGA-O2A-C1
23	c	914	CLA	CBA-CGA-O2A-C1
26	B	621	SQD	C24-C23-O48-C46
30	B	644	LMT	O5'-C5'-C6'-O6'
35	v	204	HTG	C4-C5-C6-O6
35	c	923	HTG	C1'-C2'-C3'-C4'
30	F	101	LMT	C4'-C5'-C6'-O6'
35	B	631	HTG	C4-C5-C6-O6
34	C	501	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C15-C16-C17-C18
23	b	615	CLA	C5-C6-C7-C8
28	D	410	LHG	O2-C2-C3-O3
28	d	409	LHG	O2-C2-C3-O3
28	E	101	LHG	C23-C24-C25-C26
34	D	412	LMG	C2-C1-O1-C7
23	c	914	CLA	O1A-CGA-O2A-C1
30	z	101	LMT	O5'-C5'-C6'-O6'
23	B	602	CLA	C11-C10-C8-C9
23	B	602	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C14
23	b	602	CLA	C11-C10-C8-C9
23	b	607	CLA	C14-C13-C15-C16
23	b	617	CLA	C6-C7-C8-C9
23	c	907	CLA	C6-C7-C8-C9
23	b	616	CLA	O1D-CGD-O2D-CED
25	d	405	BCR	C21-C22-C23-C24
28	e	101	LHG	C18-C19-C20-C21
28	D	409	LHG	C23-C24-C25-C26
23	C	507	CLA	C10-C11-C12-C13
23	C	513	CLA	C15-C16-C17-C18
23	a	410	CLA	C8-C10-C11-C12
30	Z	101	LMT	O5'-C5'-C6'-O6'
23	B	605	CLA	C13-C15-C16-C17
23	c	910	CLA	C13-C15-C16-C17
35	B	625	HTG	C1'-C2'-C3'-C4'
35	D	414	HTG	C1'-C2'-C3'-C4'
23	B	602	CLA	C10-C11-C12-C13
23	B	607	CLA	C10-C11-C12-C13
23	b	617	CLA	C5-C6-C7-C8
23	b	617	CLA	C15-C16-C17-C18
23	c	902	CLA	O1D-CGD-O2D-CED
26	A	415	SQD	C23-C24-C25-C26
28	K	101	LHG	C23-C24-C25-C26
28	a	415	LHG	C7-C8-C9-C10
28	e	101	LHG	C23-C24-C25-C26
34	C	520	LMG	C10-C11-C12-C13
34	C	531	LMG	C28-C29-C30-C31
34	c	920	LMG	C28-C29-C30-C31
34	c	930	LMG	C10-C11-C12-C13
30	e	103	LMT	O1'-C1-C2-C3
23	A	408	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C13-C15-C16-C17
23	D	403	CLA	C15-C16-C17-C18
23	c	910	CLA	C15-C16-C17-C18
28	A	412	LHG	C24-C23-O8-C6
28	d	402	LHG	C5-C6-O8-C23
30	F	101	LMT	O1'-C1-C2-C3
34	J	101	LMG	O6-C5-C6-O5
23	b	607	CLA	C10-C11-C12-C13
23	b	617	CLA	C13-C15-C16-C17
23	d	404	CLA	C15-C16-C17-C18
28	a	415	LHG	C23-C24-C25-C26
36	D	407	DGD	C1B-C2B-C3B-C4B
23	b	612	CLA	C13-C15-C16-C17
23	A	408	CLA	C6-C7-C8-C10
23	B	607	CLA	C6-C7-C8-C10
23	a	407	CLA	C6-C7-C8-C10
23	b	607	CLA	C6-C7-C8-C10
23	d	404	CLA	C11-C10-C8-C7
23	B	607	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA
24	D	402	PHO	C2C-C3C-CAC-CBC
30	B	644	LMT	C4'-C5'-C6'-O6'
30	B	644	LMT	O5'-C1'-O1'-C1
23	c	914	CLA	C10-C11-C12-C13
27	a	414	PL9	C9-C11-C12-C13
28	E	101	LHG	C7-C8-C9-C10
36	d	407	DGD	C1A-C2A-C3A-C4A
35	b	622	HTG	S1-C1'-C2'-C3'
35	b	623	HTG	S1-C1'-C2'-C3'
30	B	623	LMT	O1'-C1-C2-C3
23	b	602	CLA	C3-C5-C6-C7
23	A	408	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	b	617	CLA	O1A-CGA-O2A-C1
26	B	621	SQD	O10-C23-O48-C46
30	m	103	LMT	O1'-C1-C2-C3
23	B	612	CLA	C15-C16-C17-C18
34	D	412	LMG	C4-C5-C6-O5
26	D	408	SQD	C8-C7-O47-C45
23	B	616	CLA	C10-C11-C12-C13
23	B	617	CLA	C15-C16-C17-C18
23	b	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C10-C11-C12-C13
28	A	412	LHG	C4-O6-P-O3
28	E	101	LHG	C3-O3-P-O6
28	a	415	LHG	C3-O3-P-O6
28	d	402	LHG	C3-O3-P-O6
28	l	101	LHG	C4-O6-P-O3
26	B	621	SQD	C23-C24-C25-C26
35	b	623	HTG	C1'-C2'-C3'-C4'
23	B	615	CLA	C5-C6-C7-C8
28	D	410	LHG	C1-C2-C3-O3
26	D	408	SQD	O49-C7-O47-C45
23	B	615	CLA	C8-C10-C11-C12
23	C	514	CLA	C8-C10-C11-C12
23	c	914	CLA	C16-C17-C18-C19
35	b	623	HTG	O5-C5-C6-O6
30	I	101	LMT	O1'-C1-C2-C3
36	c	919	DGD	C8A-C9A-CAA-CBA
28	D	411	LHG	C11-C12-C13-C14
23	C	504	CLA	O1D-CGD-O2D-CED
25	T	101	BCR	C13-C14-C15-C16
25	t	101	BCR	C13-C14-C15-C16
36	C	518	DGD	C1A-C2A-C3A-C4A
26	a	412	SQD	C18-C19-C20-C21
26	a	417	SQD	C34-C35-C36-C37
28	D	411	LHG	C17-C18-C19-C20
35	C	523	HTG	C2'-C3'-C4'-C5'
34	C	501	LMG	C11-C10-O7-C8
35	c	922	HTG	O5-C5-C6-O6
23	C	510	CLA	C3-C5-C6-C7
28	D	411	LHG	C28-C29-C30-C31
28	E	101	LHG	C25-C26-C27-C28
28	E	101	LHG	C29-C30-C31-C32
28	E	101	LHG	C31-C32-C33-C34
28	e	101	LHG	C14-C15-C16-C17
30	a	418	LMT	O1'-C1-C2-C3
34	B	622	LMG	C11-C12-C13-C14
34	C	501	LMG	C13-C14-C15-C16
34	C	501	LMG	C39-C40-C41-C42
34	a	413	LMG	C11-C12-C13-C14
34	c	920	LMG	C39-C40-C41-C42
26	A	415	SQD	C17-C18-C19-C20
26	D	408	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	a	412	SQD	C9-C10-C11-C12
26	a	412	SQD	C13-C14-C15-C16
28	A	412	LHG	C12-C13-C14-C15
28	D	409	LHG	C31-C32-C33-C34
28	a	415	LHG	C15-C16-C17-C18
28	d	408	LHG	C30-C31-C32-C33
28	d	410	LHG	C14-C15-C16-C17
30	a	418	LMT	C3-C4-C5-C6
34	C	501	LMG	C18-C19-C20-C21
34	C	501	LMG	C21-C22-C23-C24
34	C	531	LMG	C29-C30-C31-C32
34	C	531	LMG	C30-C31-C32-C33
34	J	101	LMG	C17-C18-C19-C20
36	C	519	DGD	C7A-C8A-C9A-CAA
36	C	519	DGD	C9B-CAB-CBB-CCB
36	c	919	DGD	CAA-CBA-CCA-CDA
34	C	501	LMG	O9-C10-O7-C8
28	K	101	LHG	C31-C32-C33-C34
28	a	415	LHG	C9-C10-C11-C12
28	e	101	LHG	C24-C25-C26-C27
30	a	418	LMT	C7-C8-C9-C10
34	C	501	LMG	C11-C12-C13-C14
34	C	501	LMG	C37-C38-C39-C40
36	C	518	DGD	CAA-CBA-CCA-CDA
23	A	408	CLA	O1D-CGD-O2D-CED
23	D	401	CLA	O1D-CGD-O2D-CED
26	A	410	SQD	C29-C30-C31-C32
26	B	621	SQD	C9-C10-C11-C12
26	B	621	SQD	C29-C30-C31-C32
28	D	411	LHG	C14-C15-C16-C17
28	D	411	LHG	C29-C30-C31-C32
28	K	101	LHG	C25-C26-C27-C28
28	L	101	LHG	C11-C12-C13-C14
30	m	103	LMT	C7-C8-C9-C10
34	a	413	LMG	C18-C19-C20-C21
34	c	920	LMG	C21-C22-C23-C24
36	C	518	DGD	C8A-C9A-CAA-CBA
26	A	410	SQD	C11-C12-C13-C14
34	C	520	LMG	C20-C21-C22-C23
34	C	531	LMG	C38-C39-C40-C41
34	c	920	LMG	C19-C20-C21-C22
34	m	102	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
36	C	518	DGD	C5A-C6A-C7A-C8A
36	D	407	DGD	C2B-C3B-C4B-C5B
36	D	407	DGD	C6B-C7B-C8B-C9B
36	c	919	DGD	C6A-C7A-C8A-C9A
34	D	412	LMG	C28-C29-C30-C31
26	L	102	SQD	C2-C1-O6-C44
30	B	644	LMT	C2'-C1'-O1'-C1
30	b	621	LMT	C2'-C1'-O1'-C1
26	L	102	SQD	C10-C11-C12-C13
28	D	411	LHG	C15-C16-C17-C18
28	e	101	LHG	C13-C14-C15-C16
28	e	101	LHG	C16-C17-C18-C19
34	D	412	LMG	C29-C30-C31-C32
34	c	930	LMG	C39-C40-C41-C42
36	C	517	DGD	C9A-CAA-CBA-CCA
36	C	519	DGD	CBA-CCA-CDA-CEA
36	h	102	DGD	C7A-C8A-C9A-CAA
23	D	404	CLA	C15-C16-C17-C18
23	C	507	CLA	C16-C17-C18-C20
23	c	903	CLA	C16-C17-C18-C19
23	c	914	CLA	C4-C3-C5-C6
26	L	102	SQD	C12-C13-C14-C15
26	a	412	SQD	C29-C30-C31-C32
26	x	101	SQD	C28-C29-C30-C31
28	A	412	LHG	C11-C10-C9-C8
28	E	101	LHG	C12-C13-C14-C15
30	I	101	LMT	C4-C5-C6-C7
34	B	622	LMG	C16-C17-C18-C19
34	C	501	LMG	C17-C18-C19-C20
34	c	920	LMG	C17-C18-C19-C20
34	c	920	LMG	C34-C35-C36-C37
34	m	102	LMG	C31-C32-C33-C34
35	B	626	HTG	C3'-C4'-C5'-C6'
36	C	517	DGD	C4B-C5B-C6B-C7B
36	D	407	DGD	C8A-C9A-CAA-CBA
23	A	406	CLA	C6-C7-C8-C9
23	A	408	CLA	C11-C12-C13-C14
23	C	513	CLA	C14-C13-C15-C16
23	a	407	CLA	C11-C12-C13-C14
34	a	413	LMG	C10-C11-C12-C13
26	A	410	SQD	C17-C18-C19-C20
26	A	410	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	L	102	SQD	C11-C10-C9-C8
26	L	102	SQD	C17-C18-C19-C20
28	A	412	LHG	C16-C17-C18-C19
28	L	101	LHG	C27-C28-C29-C30
28	a	415	LHG	C13-C14-C15-C16
28	d	410	LHG	C28-C29-C30-C31
34	c	920	LMG	C11-C12-C13-C14
34	c	920	LMG	C13-C14-C15-C16
36	C	518	DGD	CCA-CDA-CEA-CFA
36	c	918	DGD	C7A-C8A-C9A-CAA
36	c	918	DGD	C9A-CAA-CBA-CCA
23	c	907	CLA	C10-C11-C12-C13
28	A	412	LHG	O10-C23-O8-C6
28	a	415	LHG	C11-C12-C13-C14
30	T	103	LMT	C7-C8-C9-C10
30	a	422	LMT	C7-C8-C9-C10
34	D	412	LMG	C36-C37-C38-C39
34	c	920	LMG	C29-C30-C31-C32
28	d	408	LHG	O1-C1-C2-C3
28	d	410	LHG	O1-C1-C2-C3
35	B	630	HTG	C1'-C2'-C3'-C4'
23	B	617	CLA	C3-C5-C6-C7
26	x	101	SQD	O49-C7-O47-C45
23	C	507	CLA	C5-C6-C7-C8
26	x	101	SQD	C8-C7-O47-C45
28	A	412	LHG	C32-C33-C34-C35
34	C	520	LMG	C19-C20-C21-C22
34	C	520	LMG	C39-C40-C41-C42
35	B	625	HTG	C3'-C4'-C5'-C6'
36	c	918	DGD	C1A-C2A-C3A-C4A
26	a	417	SQD	C29-C30-C31-C32
28	A	412	LHG	C13-C14-C15-C16
28	A	412	LHG	C14-C15-C16-C17
28	D	409	LHG	C29-C30-C31-C32
28	D	410	LHG	C32-C33-C34-C35
30	a	418	LMT	C11-C10-C9-C8
34	a	413	LMG	C13-C14-C15-C16
34	a	413	LMG	C33-C34-C35-C36
34	c	920	LMG	C14-C15-C16-C17
35	b	628	HTG	C3'-C4'-C5'-C6'
35	c	923	HTG	C2'-C3'-C4'-C5'
23	A	406	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C16-C17-C18-C20
23	C	503	CLA	C16-C17-C18-C20
23	C	507	CLA	C16-C17-C18-C19
23	C	509	CLA	C16-C17-C18-C20
23	a	406	CLA	C16-C17-C18-C19
23	b	617	CLA	C16-C17-C18-C19
23	c	907	CLA	C16-C17-C18-C19
23	c	907	CLA	C16-C17-C18-C20
23	c	914	CLA	C16-C17-C18-C20
36	D	407	DGD	O6D-C1D-O3G-C3G
30	B	644	LMT	C11-C10-C9-C8
34	B	622	LMG	C38-C39-C40-C41
34	C	520	LMG	C31-C32-C33-C34
34	J	101	LMG	C18-C19-C20-C21
34	J	101	LMG	C36-C37-C38-C39
35	b	623	HTG	C3'-C4'-C5'-C6'
36	C	519	DGD	C8A-C9A-CAA-CBA
30	Z	101	LMT	O5B-C5B-C6B-O6B
23	a	406	CLA	C2C-C3C-CAC-CBC
26	A	415	SQD	C9-C10-C11-C12
26	A	415	SQD	C25-C26-C27-C28
26	A	415	SQD	C27-C28-C29-C30
26	a	412	SQD	C31-C32-C33-C34
26	x	101	SQD	C30-C31-C32-C33
28	A	412	LHG	C27-C28-C29-C30
28	A	412	LHG	C29-C30-C31-C32
28	d	402	LHG	C25-C26-C27-C28
30	F	101	LMT	C11-C10-C9-C8
34	C	531	LMG	C16-C17-C18-C19
34	c	920	LMG	C18-C19-C20-C21
34	c	930	LMG	C35-C36-C37-C38
36	c	919	DGD	C4A-C5A-C6A-C7A
34	C	501	LMG	C10-C11-C12-C13
26	B	621	SQD	C16-C17-C18-C19
26	a	412	SQD	C16-C17-C18-C19
28	L	101	LHG	C29-C30-C31-C32
34	B	622	LMG	C39-C40-C41-C42
34	j	101	LMG	C31-C32-C33-C34
36	d	407	DGD	C7A-C8A-C9A-CAA
26	a	412	SQD	C34-C35-C36-C37
28	E	101	LHG	C27-C28-C29-C30
30	z	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
34	d	411	LMG	C11-C12-C13-C14
36	C	517	DGD	C2B-C3B-C4B-C5B
36	d	407	DGD	C7B-C8B-C9B-CAB
23	c	907	CLA	C15-C16-C17-C18
30	e	103	LMT	C2-C1-O1'-C1'
26	a	412	SQD	C27-C28-C29-C30
26	a	417	SQD	C25-C26-C27-C28
28	E	101	LHG	C17-C18-C19-C20
28	d	408	LHG	C29-C30-C31-C32
28	l	101	LHG	C30-C31-C32-C33
34	C	520	LMG	C17-C18-C19-C20
36	C	519	DGD	C2A-C3A-C4A-C5A
36	H	103	DGD	C7A-C8A-C9A-CAA
36	c	918	DGD	C3A-C4A-C5A-C6A
36	c	918	DGD	C5A-C6A-C7A-C8A
36	d	407	DGD	C6A-C7A-C8A-C9A
36	d	407	DGD	C6B-C7B-C8B-C9B
23	B	615	CLA	O1D-CGD-O2D-CED
23	A	406	CLA	C16-C17-C18-C20
30	B	644	LMT	C7-C8-C9-C10
34	a	413	LMG	C21-C22-C23-C24
34	d	411	LMG	C38-C39-C40-C41
36	C	518	DGD	C9A-CAA-CBA-CCA
36	c	917	DGD	C2B-C3B-C4B-C5B
36	D	407	DGD	O1G-C1G-C2G-C3G
30	B	643	LMT	C1-C2-C3-C4
35	C	523	HTG	C1'-C2'-C3'-C4'
28	E	101	LHG	C33-C34-C35-C36
30	B	623	LMT	C3-C4-C5-C6
30	B	623	LMT	C7-C8-C9-C10
36	C	517	DGD	C8A-C9A-CAA-CBA
36	h	102	DGD	CAA-CBA-CCA-CDA
23	b	615	CLA	C3-C5-C6-C7
26	B	621	SQD	C28-C29-C30-C31
34	J	101	LMG	C19-C20-C21-C22
27	a	414	PL9	C15-C14-C16-C17
34	C	520	LMG	C29-C28-O8-C9
35	B	626	HTG	C4-C5-C6-O6
27	D	406	PL9	C28-C29-C31-C32
27	a	414	PL9	C13-C14-C16-C17
28	d	402	LHG	O1-C1-C2-O2
26	A	410	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
28	d	402	LHG	C29-C30-C31-C32
28	d	408	LHG	C15-C16-C17-C18
30	a	422	LMT	C3-C4-C5-C6
34	C	520	LMG	C12-C13-C14-C15
36	C	518	DGD	C3A-C4A-C5A-C6A
23	C	513	CLA	C16-C17-C18-C19
23	b	616	CLA	C16-C17-C18-C19
30	A	416	LMT	C3-C4-C5-C6
34	c	920	LMG	C15-C16-C17-C18
34	c	920	LMG	C16-C17-C18-C19
28	E	101	LHG	C34-C35-C36-C37
34	c	920	LMG	C12-C13-C14-C15
34	j	101	LMG	C37-C38-C39-C40
26	D	408	SQD	C23-C24-C25-C26
28	d	409	LHG	C1-C2-C3-O3
26	B	621	SQD	C13-C14-C15-C16
26	D	408	SQD	C26-C27-C28-C29
26	x	101	SQD	C34-C35-C36-C37
36	c	917	DGD	C9A-CAA-CBA-CCA
36	c	919	DGD	CBB-CCB-CDB-CEB
30	A	416	LMT	C1-C2-C3-C4
23	B	617	CLA	C2-C1-O2A-CGA
35	B	626	HTG	C1'-C2'-C3'-C4'
34	B	622	LMG	C37-C38-C39-C40
35	b	622	HTG	C2'-C3'-C4'-C5'
35	d	413	HTG	C3'-C4'-C5'-C6'
23	b	604	CLA	C5-C6-C7-C8
23	b	605	CLA	C13-C15-C16-C17
30	F	101	LMT	C1-C2-C3-C4
30	b	621	LMT	C4'-C5'-C6'-O6'
26	A	410	SQD	C33-C34-C35-C36
26	x	101	SQD	C32-C33-C34-C35
28	K	101	LHG	C14-C15-C16-C17
34	C	520	LMG	C34-C35-C36-C37
36	D	407	DGD	C7B-C8B-C9B-CAB
36	c	917	DGD	C4B-C5B-C6B-C7B
36	d	407	DGD	C4B-C5B-C6B-C7B
25	B	618	BCR	C1-C6-C7-C8
25	B	618	BCR	C5-C6-C7-C8
25	C	515	BCR	C23-C24-C25-C26
25	C	515	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	Y	101	BCR	C5-C6-C7-C8
25	d	405	BCR	C23-C24-C25-C26
28	K	101	LHG	C32-C33-C34-C35
36	d	407	DGD	CCA-CDA-CEA-CFA
28	L	101	LHG	C10-C11-C12-C13
36	h	102	DGD	C6B-C7B-C8B-C9B
26	D	408	SQD	C28-C29-C30-C31
28	d	408	LHG	C25-C26-C27-C28
36	C	519	DGD	C9A-CAA-CBA-CCA
36	c	917	DGD	C7A-C8A-C9A-CAA
23	C	510	CLA	C10-C11-C12-C13
23	b	602	CLA	C15-C16-C17-C18
26	a	417	SQD	C26-C27-C28-C29
28	A	412	LHG	C17-C18-C19-C20
27	D	406	PL9	C30-C29-C31-C32
23	A	408	CLA	C12-C13-C15-C16
23	B	604	CLA	C6-C7-C8-C10
23	B	605	CLA	C6-C7-C8-C10
23	D	403	CLA	C12-C13-C15-C16
23	a	410	CLA	C12-C13-C15-C16
23	b	612	CLA	C12-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C15
23	c	903	CLA	C11-C12-C13-C15
23	c	914	CLA	C2-C3-C5-C6
34	C	520	LMG	O10-C28-O8-C9
28	A	412	LHG	C33-C34-C35-C36
34	B	622	LMG	C13-C14-C15-C16
34	C	501	LMG	C12-C13-C14-C15
36	H	103	DGD	C9B-CAB-CBB-CCB
36	c	919	DGD	C2A-C3A-C4A-C5A
23	B	607	CLA	C8-C10-C11-C12
23	c	905	CLA	C13-C15-C16-C17
23	b	617	CLA	C16-C17-C18-C20
23	B	607	CLA	O1D-CGD-O2D-CED
34	B	622	LMG	C10-C11-C12-C13
26	x	101	SQD	C24-C23-O48-C46
26	A	415	SQD	C26-C27-C28-C29
28	K	101	LHG	C18-C19-C20-C21
28	d	410	LHG	C29-C30-C31-C32
30	F	101	LMT	C3-C4-C5-C6
30	T	103	LMT	O1'-C1-C2-C3
30	Z	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
34	B	622	LMG	C29-C30-C31-C32
34	d	411	LMG	C18-C19-C20-C21
26	x	101	SQD	C27-C28-C29-C30
30	B	644	LMT	C4-C5-C6-C7
34	c	920	LMG	C35-C36-C37-C38
26	D	408	SQD	C30-C31-C32-C33
26	D	408	SQD	C7-C8-C9-C10
40	V	203	HEC	C2C-C3C-CAC-CBC
28	A	412	LHG	C25-C26-C27-C28
28	E	101	LHG	C18-C19-C20-C21
30	F	101	LMT	C6-C7-C8-C9
36	D	407	DGD	C7A-C8A-C9A-CAA
30	z	101	LMT	C4B-C5B-C6B-O6B
30	B	623	LMT	C1-C2-C3-C4
30	a	418	LMT	C1-C2-C3-C4
23	a	406	CLA	C4C-C3C-CAC-CBC
30	B	643	LMT	C7-C8-C9-C10
30	b	621	LMT	O5'-C1'-O1'-C1
23	b	607	CLA	C15-C16-C17-C18
26	a	412	SQD	C12-C13-C14-C15
34	B	622	LMG	C32-C33-C34-C35
34	D	412	LMG	C11-C12-C13-C14
24	a	409	PHO	C2C-C3C-CAC-CBC
26	A	410	SQD	C18-C19-C20-C21
26	a	417	SQD	C30-C31-C32-C33
28	K	101	LHG	C26-C27-C28-C29
28	K	101	LHG	C28-C29-C30-C31
30	b	621	LMT	C7-C8-C9-C10
36	D	407	DGD	CCA-CDA-CEA-CFA
36	c	918	DGD	CAA-CBA-CCA-CDA
40	v	203	HEC	C2B-C3B-CAB-CBB
35	c	921	HTG	C4-C5-C6-O6
35	c	922	HTG	C4-C5-C6-O6
35	C	522	HTG	S1-C1'-C2'-C3'
23	C	504	CLA	C8-C10-C11-C12
26	A	415	SQD	C15-C16-C17-C18
30	Z	101	LMT	C4-C5-C6-C7
34	C	531	LMG	C18-C19-C20-C21
26	a	417	SQD	C27-C28-C29-C30
28	K	101	LHG	C33-C34-C35-C36
28	a	415	LHG	C12-C13-C14-C15
28	d	402	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
34	C	531	LMG	C31-C32-C33-C34
36	c	917	DGD	C5B-C6B-C7B-C8B
26	A	410	SQD	O6-C44-C45-O47
26	a	412	SQD	O6-C44-C45-O47
28	E	101	LHG	C10-C11-C12-C13
23	b	616	CLA	C16-C17-C18-C20
36	c	917	DGD	O6D-C5D-C6D-O5D
34	C	520	LMG	C11-C12-C13-C14
36	C	519	DGD	CAA-CBA-CCA-CDA
34	C	531	LMG	O6-C5-C6-O5
36	C	517	DGD	O6E-C5E-C6E-O5E
23	B	617	CLA	C13-C15-C16-C17
23	b	606	CLA	C2-C3-C5-C6
27	A	411	PL9	C4-C3-C7-C8
30	F	101	LMT	C5-C6-C7-C8
23	A	408	CLA	C6-C7-C8-C9
23	B	604	CLA	C6-C7-C8-C9
23	B	605	CLA	C6-C7-C8-C9
23	B	612	CLA	C14-C13-C15-C16
23	a	407	CLA	C6-C7-C8-C9
23	a	410	CLA	C14-C13-C15-C16
23	b	617	CLA	C14-C13-C15-C16
23	d	404	CLA	C11-C10-C8-C9
23	d	404	CLA	C14-C13-C15-C16
23	b	615	CLA	O1D-CGD-O2D-CED
35	B	624	HTG	C3'-C4'-C5'-C6'
36	c	918	DGD	C2B-C3B-C4B-C5B
28	a	415	LHG	C10-C11-C12-C13
28	d	402	LHG	C16-C17-C18-C19
35	D	414	HTG	C3'-C4'-C5'-C6'
34	j	101	LMG	O6-C5-C6-O5
26	A	410	SQD	C14-C15-C16-C17
30	T	103	LMT	C4-C5-C6-C7
25	T	101	BCR	C11-C12-C13-C14
26	x	101	SQD	O10-C23-O48-C46
28	a	415	LHG	C8-C7-O7-C5
34	a	413	LMG	C11-C10-O7-C8
28	A	412	LHG	C26-C27-C28-C29
34	C	520	LMG	C37-C38-C39-C40
36	C	517	DGD	C6A-C7A-C8A-C9A
36	H	103	DGD	CCA-CDA-CEA-CFA
23	B	614	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	Z	101	LMT	C2-C3-C4-C5
35	b	622	HTG	C3'-C4'-C5'-C6'
36	c	919	DGD	CBA-CCA-CDA-CEA
30	e	103	LMT	C1-C2-C3-C4
23	A	408	CLA	C15-C16-C17-C18
23	b	616	CLA	C10-C11-C12-C13
23	c	911	CLA	C8-C10-C11-C12
28	E	101	LHG	O6-C4-C5-C6
23	C	513	CLA	O1D-CGD-O2D-CED
26	L	102	SQD	C23-C24-C25-C26
28	a	415	LHG	C14-C15-C16-C17
30	A	416	LMT	C11-C10-C9-C8
34	C	531	LMG	C17-C18-C19-C20
23	C	503	CLA	C16-C17-C18-C19
36	C	519	DGD	C6B-C7B-C8B-C9B
26	A	410	SQD	C15-C16-C17-C18
28	K	101	LHG	C11-C12-C13-C14
36	H	103	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	CCB-CDB-CEB-CFB
23	C	514	CLA	C3-C5-C6-C7
26	A	410	SQD	C32-C33-C34-C35
34	m	102	LMG	C15-C16-C17-C18
23	b	615	CLA	C4-C3-C5-C6
24	a	408	PHO	C4-C3-C5-C6
28	E	101	LHG	C32-C33-C34-C35
34	C	531	LMG	C15-C16-C17-C18
34	c	920	LMG	C20-C21-C22-C23
34	d	411	LMG	C36-C37-C38-C39
36	C	518	DGD	C2B-C3B-C4B-C5B
30	z	101	LMT	C2B-C1B-O1B-C4'
28	L	101	LHG	C25-C26-C27-C28
34	C	520	LMG	C21-C22-C23-C24
34	C	531	LMG	C19-C20-C21-C22
36	h	102	DGD	C9B-CAB-CBB-CCB
26	a	417	SQD	C35-C36-C37-C38
28	e	101	LHG	C15-C16-C17-C18
30	e	103	LMT	C2-C3-C4-C5
34	C	520	LMG	C38-C39-C40-C41
34	d	411	LMG	C19-C20-C21-C22
30	m	104	LMT	O5'-C5'-C6'-O6'
36	c	917	DGD	O6E-C5E-C6E-O5E
26	A	415	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
26	B	621	SQD	C44-C45-C46-O48
26	D	408	SQD	O6-C44-C45-C46
26	a	417	SQD	O6-C44-C45-C46
28	E	101	LHG	C4-C5-C6-O8
28	K	101	LHG	C16-C17-C18-C19
34	C	501	LMG	C7-C8-C9-O8
28	K	101	LHG	C35-C36-C37-C38
36	d	407	DGD	C3A-C4A-C5A-C6A
34	C	531	LMG	C8-C7-O1-C1
34	c	930	LMG	C8-C7-O1-C1
36	C	518	DGD	C2G-C3G-O3G-C1D
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	918	DGD	C2G-C3G-O3G-C1D
26	A	410	SQD	C30-C31-C32-C33
28	d	402	LHG	C24-C25-C26-C27
30	a	418	LMT	C6-C7-C8-C9
23	C	510	CLA	C13-C15-C16-C17
26	B	621	SQD	C14-C15-C16-C17
26	a	412	SQD	C11-C12-C13-C14
28	D	411	LHG	C19-C20-C21-C22
28	K	101	LHG	C30-C31-C32-C33
28	d	410	LHG	C13-C14-C15-C16
34	a	413	LMG	C35-C36-C37-C38
36	h	102	DGD	O2G-C1B-C2B-C3B
26	x	101	SQD	C31-C32-C33-C34
30	B	623	LMT	C9-C10-C11-C12
36	H	103	DGD	CDB-CEB-CFB-CGB
36	h	102	DGD	CDB-CEB-CFB-CGB
23	C	503	CLA	O1D-CGD-O2D-CED
26	B	621	SQD	C12-C13-C14-C15
28	e	101	LHG	C26-C27-C28-C29
34	C	520	LMG	C16-C17-C18-C19
35	D	414	HTG	C4'-C5'-C6'-C7'
36	c	919	DGD	CDB-CEB-CFB-CGB
28	d	408	LHG	O1-C1-C2-O2
30	z	101	LMT	C3-C4-C5-C6
34	a	413	LMG	C34-C35-C36-C37
34	D	412	LMG	O10-C28-O8-C9
26	B	621	SQD	C34-C35-C36-C37
28	K	101	LHG	C10-C11-C12-C13
30	B	623	LMT	C6-C7-C8-C9
36	C	519	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
30	I	101	LMT	O5B-C5B-C6B-O6B
30	m	103	LMT	O5'-C5'-C6'-O6'
27	A	411	PL9	C15-C14-C16-C17
27	A	411	PL9	C18-C19-C21-C22
23	B	602	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	c	903	CLA	C16-C17-C18-C20
34	D	412	LMG	C29-C28-O8-C9
30	a	422	LMT	C4-C5-C6-C7
35	b	622	HTG	C4'-C5'-C6'-C7'
23	b	609	CLA	C13-C15-C16-C17
26	A	415	SQD	C16-C17-C18-C19
26	A	415	SQD	C35-C36-C37-C38
26	a	412	SQD	C19-C20-C21-C22
34	a	413	LMG	C40-C41-C42-C43
36	H	103	DGD	CBB-CCB-CDB-CEB
36	c	917	DGD	CDA-CEA-CFA-CGA
35	C	522	HTG	O5-C5-C6-O6
23	C	510	CLA	C2-C1-O2A-CGA
23	c	910	CLA	C2-C1-O2A-CGA
26	D	408	SQD	C9-C10-C11-C12
26	x	101	SQD	C29-C30-C31-C32
28	D	411	LHG	C18-C19-C20-C21
28	e	101	LHG	C11-C10-C9-C8
30	B	643	LMT	O1'-C1-C2-C3
34	a	413	LMG	C17-C18-C19-C20
28	d	402	LHG	O7-C7-C8-C9
26	x	101	SQD	C26-C27-C28-C29
30	B	643	LMT	C3-C4-C5-C6
23	c	908	CLA	C5-C6-C7-C8
23	a	410	CLA	O1D-CGD-O2D-CED
28	d	402	LHG	C23-C24-C25-C26
36	C	518	DGD	C2E-C1E-O5D-C6D
28	d	402	LHG	C10-C11-C12-C13
34	J	101	LMG	C37-C38-C39-C40
36	H	103	DGD	O2G-C1B-C2B-C3B
26	D	408	SQD	O6-C44-C45-O47
34	d	411	LMG	O1-C7-C8-O7
30	A	416	LMT	C9-C10-C11-C12
30	b	621	LMT	C9-C10-C11-C12
28	a	415	LHG	O9-C7-O7-C5
26	B	621	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
34	J	101	LMG	C12-C13-C14-C15
36	c	919	DGD	C8B-C9B-CAB-CBB
36	h	102	DGD	CBB-CCB-CDB-CEB
27	A	411	PL9	C20-C19-C21-C22
30	b	621	LMT	C6-C7-C8-C9
34	D	412	LMG	C21-C22-C23-C24
23	B	602	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C12-C13-C15
23	B	602	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	C	507	CLA	C11-C12-C13-C15
23	C	509	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	b	617	CLA	C12-C13-C15-C16
23	c	913	CLA	C11-C10-C8-C7
23	d	404	CLA	C12-C13-C15-C16
27	A	411	PL9	C13-C14-C16-C17
30	b	621	LMT	C5-C6-C7-C8
36	h	102	DGD	C5B-C6B-C7B-C8B
23	B	602	CLA	C11-C12-C13-C14
23	C	507	CLA	C11-C12-C13-C14
23	C	508	CLA	C11-C12-C13-C14
23	C	509	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	b	611	CLA	C11-C12-C13-C14
23	c	905	CLA	C11-C12-C13-C14
30	b	621	LMT	C1-C2-C3-C4
30	A	416	LMT	C2-C3-C4-C5
25	T	101	BCR	C11-C12-C13-C35
28	d	402	LHG	C30-C31-C32-C33
34	a	413	LMG	C14-C15-C16-C17
35	b	627	HTG	C3'-C4'-C5'-C6'
30	I	101	LMT	C9-C10-C11-C12
35	C	521	HTG	C3'-C4'-C5'-C6'
35	c	921	HTG	C2'-C3'-C4'-C5'
36	C	517	DGD	C7B-C8B-C9B-CAB
36	D	407	DGD	CBA-CCA-CDA-CEA
36	d	407	DGD	C5A-C6A-C7A-C8A
36	C	517	DGD	O6D-C5D-C6D-O5D
28	E	101	LHG	C1-C2-C3-O3
23	c	904	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	L	102	SQD	C34-C35-C36-C37
30	B	623	LMT	C3'-C4'-O1B-C1B
28	d	408	LHG	C23-C24-C25-C26
36	C	517	DGD	C1A-C2A-C3A-C4A
23	B	616	CLA	C5-C6-C7-C8
26	D	408	SQD	C33-C34-C35-C36
28	d	402	LHG	C26-C27-C28-C29
23	C	508	CLA	C16-C17-C18-C20
24	a	408	PHO	C8-C10-C11-C12
23	a	410	CLA	C3-C5-C6-C7
28	D	409	LHG	C25-C26-C27-C28
34	a	413	LMG	C20-C21-C22-C23
34	d	411	LMG	C20-C21-C22-C23
34	a	413	LMG	C31-C32-C33-C34
28	d	410	LHG	C10-C11-C12-C13
23	b	602	CLA	C4-C3-C5-C6
23	b	602	CLA	C2-C3-C5-C6
26	B	621	SQD	C17-C18-C19-C20
26	a	412	SQD	C24-C25-C26-C27
36	D	407	DGD	CDB-CEB-CFB-CGB
23	a	406	CLA	C15-C16-C17-C18
30	B	623	LMT	C2-C3-C4-C5
30	a	418	LMT	C2-C3-C4-C5
23	D	404	CLA	C16-C17-C18-C20
26	B	621	SQD	C30-C31-C32-C33
26	a	412	SQD	C26-C27-C28-C29
26	L	102	SQD	C7-C8-C9-C10
36	c	918	DGD	CDA-CEA-CFA-CGA
28	a	415	LHG	C29-C30-C31-C32
30	a	422	LMT	C5-C6-C7-C8
35	B	625	HTG	C4'-C5'-C6'-C7'
30	B	623	LMT	C2-C1-O1'-C1'
30	T	103	LMT	C2-C1-O1'-C1'
30	Z	101	LMT	C2-C1-O1'-C1'
26	A	410	SQD	C35-C36-C37-C38
36	h	102	DGD	CDA-CEA-CFA-CGA
34	J	101	LMG	C10-C11-C12-C13
23	B	613	CLA	C13-C15-C16-C17
26	a	412	SQD	C17-C18-C19-C20
23	B	607	CLA	C13-C15-C16-C17
23	B	614	CLA	C15-C16-C17-C18
23	c	913	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	A	410	SQD	O6-C44-C45-C46
26	L	102	SQD	C44-C45-C46-O48
26	a	412	SQD	O6-C44-C45-C46
28	A	412	LHG	C4-C5-C6-O8
34	D	412	LMG	O1-C7-C8-C9
34	D	412	LMG	C7-C8-C9-O8
34	a	413	LMG	C7-C8-C9-O8
34	d	411	LMG	O1-C7-C8-C9
34	d	411	LMG	C7-C8-C9-O8
26	x	101	SQD	C25-C26-C27-C28
35	d	413	HTG	C2'-C3'-C4'-C5'
36	c	919	DGD	CCB-CDB-CEB-CFB
28	L	101	LHG	C9-C10-C11-C12
23	C	514	CLA	O2A-C1-C2-C3
23	a	410	CLA	C10-C11-C12-C13
30	B	623	LMT	C11-C10-C9-C8
40	V	203	HEC	C4C-C3C-CAC-CBC
26	a	412	SQD	C10-C11-C12-C13
23	c	905	CLA	C4-C3-C5-C6
23	b	602	CLA	C16-C17-C18-C20
27	d	406	PL9	C43-C44-C46-C47
30	a	422	LMT	O1'-C1-C2-C3
36	D	407	DGD	C2A-C3A-C4A-C5A
36	C	519	DGD	CDA-CEA-CFA-CGA
23	c	909	CLA	C15-C16-C17-C18
26	a	412	SQD	C25-C26-C27-C28
23	B	611	CLA	C8-C10-C11-C12
26	A	415	SQD	C11-C12-C13-C14
28	d	402	LHG	C9-C10-C11-C12
34	D	412	LMG	C37-C38-C39-C40
34	c	930	LMG	C40-C41-C42-C43
36	c	919	DGD	C3A-C4A-C5A-C6A
34	a	413	LMG	O9-C10-O7-C8
23	C	508	CLA	C16-C17-C18-C19
23	D	404	CLA	C16-C17-C18-C19
35	d	413	HTG	C4'-C5'-C6'-C7'
28	D	411	LHG	C16-C17-C18-C19
26	D	408	SQD	C10-C11-C12-C13
30	F	101	LMT	C2-C3-C4-C5
23	A	405	CLA	C2C-C3C-CAC-CBC
34	j	101	LMG	C36-C37-C38-C39
26	B	621	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
26	L	102	SQD	O47-C45-C46-O48
34	C	501	LMG	O1-C7-C8-O7
34	D	412	LMG	O7-C8-C9-O8
28	l	101	LHG	C31-C32-C33-C34
23	C	509	CLA	C16-C17-C18-C19
23	C	513	CLA	C16-C17-C18-C20
26	A	415	SQD	C34-C35-C36-C37
34	m	102	LMG	C33-C34-C35-C36
28	e	101	LHG	C19-C20-C21-C22
34	C	520	LMG	C15-C16-C17-C18
34	d	411	LMG	C35-C36-C37-C38
35	C	522	HTG	C2'-C3'-C4'-C5'
36	D	407	DGD	CBB-CCB-CDB-CEB
23	D	403	CLA	C2-C1-O2A-CGA
28	d	409	LHG	C11-C10-C9-C8
30	B	623	LMT	C5'-C4'-O1B-C1B
23	A	408	CLA	C11-C10-C8-C9
23	B	617	CLA	C11-C12-C13-C14
23	B	617	CLA	C14-C13-C15-C16
23	D	404	CLA	C14-C13-C15-C16
23	a	410	CLA	C11-C10-C8-C9
23	b	602	CLA	C14-C13-C15-C16
23	c	913	CLA	C11-C10-C8-C9
24	a	409	PHO	C6-C7-C8-C9
28	L	101	LHG	C24-C25-C26-C27
23	D	403	CLA	C2C-C3C-CAC-CBC
28	d	408	LHG	C32-C33-C34-C35
30	A	416	LMT	C4-C5-C6-C7
30	B	644	LMT	C3-C4-C5-C6
34	C	520	LMG	C36-C37-C38-C39
36	d	407	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	CBA-CCA-CDA-CEA
23	c	910	CLA	C16-C17-C18-C19
30	z	101	LMT	O5B-C5B-C6B-O6B
25	D	405	BCR	C23-C24-C25-C26
25	D	405	BCR	C23-C24-C25-C30
25	b	618	BCR	C5-C6-C7-C8
23	B	612	CLA	C13-C15-C16-C17
36	d	407	DGD	CCB-CDB-CEB-CFB
26	B	621	SQD	O49-C7-O47-C45
34	d	411	LMG	C12-C13-C14-C15
23	a	406	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
34	d	411	LMG	C32-C33-C34-C35
36	d	407	DGD	CDA-CEA-CFA-CGA
27	a	414	PL9	C30-C29-C31-C32
28	A	412	LHG	C28-C29-C30-C31
34	m	102	LMG	C36-C37-C38-C39
23	A	408	CLA	C11-C10-C8-C7
23	B	617	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C15
23	C	513	CLA	C11-C10-C8-C7
23	C	514	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C12-C13-C15
23	D	404	CLA	C12-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C7
23	a	410	CLA	C11-C10-C8-C7
23	b	602	CLA	C11-C12-C13-C15
23	c	905	CLA	C11-C12-C13-C15
23	c	907	CLA	C11-C10-C8-C7
23	d	404	CLA	C6-C7-C8-C10
27	a	414	PL9	C28-C29-C31-C32
28	E	101	LHG	C35-C36-C37-C38
34	m	102	LMG	C19-C20-C21-C22
35	b	627	HTG	C4'-C5'-C6'-C7'
23	C	507	CLA	C13-C15-C16-C17
23	b	617	CLA	C8-C10-C11-C12
30	Z	101	LMT	C1-C2-C3-C4
26	B	621	SQD	C10-C11-C12-C13
36	c	917	DGD	C4D-C5D-C6D-O5D
26	a	417	SQD	C11-C12-C13-C14
28	K	101	LHG	C19-C20-C21-C22
35	B	631	HTG	C2'-C1'-S1-C1
28	d	408	LHG	C18-C19-C20-C21
23	b	605	CLA	C16-C17-C18-C20
36	D	407	DGD	C9A-CAA-CBA-CCA
28	K	101	LHG	C15-C16-C17-C18
34	a	413	LMG	C16-C17-C18-C19
34	C	501	LMG	C22-C23-C24-C25
36	h	102	DGD	CCA-CDA-CEA-CFA
23	B	602	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	D	404	CLA	CAD-CBD-CGD-O2D
23	a	406	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	904	CLA	CAD-CBD-CGD-O2D
23	c	911	CLA	CAD-CBD-CGD-O2D
23	c	914	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
24	a	409	PHO	CAD-CBD-CGD-O2D
26	B	621	SQD	C46-C45-O47-C7
28	d	409	LHG	C32-C33-C34-C35
34	m	102	LMG	C35-C36-C37-C38
34	j	101	LMG	C34-C35-C36-C37
27	A	411	PL9	C25-C24-C26-C27
34	D	412	LMG	O6-C1-O1-C7
26	B	621	SQD	C18-C19-C20-C21
34	J	101	LMG	C35-C36-C37-C38
30	Z	101	LMT	C4'-C5'-C6'-O6'
28	L	101	LHG	O6-C4-C5-O7
26	a	412	SQD	C14-C15-C16-C17
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	608	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	c	903	CLA	CHA-CBD-CGD-O1D
23	c	903	CLA	CHA-CBD-CGD-O2D
23	c	905	CLA	CHA-CBD-CGD-O1D
23	c	908	CLA	CHA-CBD-CGD-O1D
23	c	908	CLA	CHA-CBD-CGD-O2D
23	c	909	CLA	CHA-CBD-CGD-O1D
23	d	401	CLA	CHA-CBD-CGD-O2D
36	H	103	DGD	C9A-CAA-CBA-CCA
26	D	408	SQD	O47-C45-C46-O48
34	D	412	LMG	O1-C7-C8-O7
34	a	413	LMG	O7-C8-C9-O8
23	C	507	CLA	CBD-CGD-O2D-CED
35	B	624	HTG	C2'-C3'-C4'-C5'
28	d	409	LHG	O1-C1-C2-O2
34	C	520	LMG	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
36	D	407	DGD	C3A-C4A-C5A-C6A
35	b	623	HTG	C2'-C3'-C4'-C5'
27	a	414	PL9	C4-C3-C7-C8
30	z	101	LMT	O5B-C1B-O1B-C4'
34	C	501	LMG	C19-C20-C21-C22
23	B	614	CLA	C11-C10-C8-C9
23	b	615	CLA	C6-C7-C8-C9
23	c	908	CLA	C11-C10-C8-C9
28	K	101	LHG	C9-C10-C11-C12
28	D	409	LHG	C30-C31-C32-C33
34	C	520	LMG	C33-C34-C35-C36
34	j	101	LMG	C33-C34-C35-C36
23	b	616	CLA	C5-C6-C7-C8
23	D	404	CLA	C13-C15-C16-C17
26	L	102	SQD	C31-C32-C33-C34
34	m	102	LMG	C30-C31-C32-C33
36	C	518	DGD	CDA-CEA-CFA-CGA
23	C	511	CLA	C8-C10-C11-C12
40	v	203	HEC	C4B-C3B-CAB-CBB
36	d	407	DGD	C9B-CAB-CBB-CCB
28	A	412	LHG	C3-O3-P-O6
28	D	410	LHG	C4-O6-P-O3
26	D	408	SQD	C25-C26-C27-C28
26	L	102	SQD	C28-C29-C30-C31
23	b	606	CLA	C4-C3-C5-C6
28	A	412	LHG	C5-C4-O6-P
28	D	411	LHG	C2-C3-O3-P
28	d	402	LHG	C5-C4-O6-P
28	A	412	LHG	C31-C32-C33-C34
28	d	408	LHG	C27-C28-C29-C30
34	D	412	LMG	C12-C13-C14-C15
36	d	407	DGD	C3B-C4B-C5B-C6B
23	B	602	CLA	C4B-C3B-CAB-CBB
27	A	411	PL9	C3-C7-C8-C9
28	a	415	LHG	C3-O3-P-O4
28	a	415	LHG	C3-O3-P-O5
28	a	415	LHG	C4-O6-P-O5
28	d	402	LHG	C3-O3-P-O5
28	e	101	LHG	C4-O6-P-O4
28	l	101	LHG	C4-O6-P-O5
23	b	605	CLA	C16-C17-C18-C19
23	c	908	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	L	101	LHG	O6-C4-C5-C6
28	L	101	LHG	C12-C13-C14-C15
28	l	101	LHG	C28-C29-C30-C31
26	B	621	SQD	C24-C25-C26-C27
34	D	412	LMG	C18-C19-C20-C21
28	d	410	LHG	C18-C19-C20-C21
23	B	606	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	C	513	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	c	902	CLA	CAD-CBD-CGD-O1D
23	c	903	CLA	CAD-CBD-CGD-O1D
23	c	905	CLA	CAD-CBD-CGD-O1D
26	B	621	SQD	O5-C5-C6-S
26	x	101	SQD	C5-C6-S-O7
35	v	204	HTG	C2'-C3'-C4'-C5'
34	B	622	LMG	C28-C29-C30-C31
28	l	101	LHG	C5-C6-O8-C23
26	L	102	SQD	C15-C16-C17-C18
30	a	418	LMT	C5-C6-C7-C8
23	B	606	CLA	C16-C17-C18-C19
23	c	913	CLA	C16-C17-C18-C20
23	A	406	CLA	C12-C13-C15-C16
23	B	612	CLA	C11-C12-C13-C15
23	B	617	CLA	C11-C12-C13-C15
23	C	505	CLA	C11-C10-C8-C7
23	C	508	CLA	C11-C10-C8-C7
23	C	510	CLA	C6-C7-C8-C10
23	C	510	CLA	C11-C12-C13-C15
23	D	404	CLA	C6-C7-C8-C10
23	b	602	CLA	C11-C10-C8-C7
23	b	615	CLA	C2-C3-C5-C6
23	b	616	CLA	C12-C13-C15-C16
23	b	617	CLA	C6-C7-C8-C10
23	c	905	CLA	C11-C10-C8-C7
23	c	908	CLA	C11-C10-C8-C7
23	d	404	CLA	C11-C12-C13-C15
35	B	626	HTG	C2-C1-S1-C1'
35	V	204	HTG	C2-C1-S1-C1'
28	D	409	LHG	C11-C10-C9-C8
30	I	101	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
34	m	102	LMG	C18-C19-C20-C21
35	v	204	HTG	C3'-C4'-C5'-C6'
34	C	531	LMG	C32-C33-C34-C35
26	B	621	SQD	C8-C7-O47-C45
34	m	102	LMG	C29-C30-C31-C32
34	j	101	LMG	C13-C14-C15-C16
23	A	408	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C19
30	m	103	LMT	C1-C2-C3-C4
34	C	531	LMG	C13-C14-C15-C16
36	C	517	DGD	C4D-C5D-C6D-O5D
26	L	102	SQD	O6-C44-C45-C46
34	C	501	LMG	O1-C7-C8-C9
28	A	412	LHG	O7-C5-C6-O8
36	D	407	DGD	O1G-C1G-C2G-O2G
26	L	102	SQD	C24-C25-C26-C27
34	j	101	LMG	C38-C39-C40-C41
34	d	411	LMG	C28-C29-C30-C31
36	C	519	DGD	CBB-CCB-CDB-CEB
36	c	918	DGD	C5D-C6D-O5D-C1E
34	c	930	LMG	C14-C15-C16-C17
28	d	410	LHG	C2-C3-O3-P
23	d	404	CLA	C8-C10-C11-C12
28	d	408	LHG	C17-C18-C19-C20
34	c	920	LMG	C30-C31-C32-C33
23	B	603	CLA	C11-C12-C13-C14
23	C	505	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	D	404	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	a	407	CLA	C11-C10-C8-C9
23	b	614	CLA	C11-C12-C13-C14
23	c	903	CLA	C11-C12-C13-C14
23	d	404	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C12-C13-C14
28	A	412	LHG	C9-C10-C11-C12
23	b	608	CLA	C3-C5-C6-C7
26	A	415	SQD	C31-C32-C33-C34
30	a	418	LMT	O5'-C1'-O1'-C1
28	l	101	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	I	101	LMT	C6-C7-C8-C9
36	d	407	DGD	C4A-C5A-C6A-C7A
23	b	607	CLA	C2B-C3B-CAB-CBB
23	d	403	CLA	C2B-C3B-CAB-CBB
30	I	101	LMT	C1-C2-C3-C4
34	j	101	LMG	C12-C13-C14-C15
23	d	401	CLA	C13-C15-C16-C17
35	O	302	HTG	C1'-C2'-C3'-C4'
28	D	411	LHG	C32-C33-C34-C35
28	e	101	LHG	C25-C26-C27-C28
34	D	412	LMG	C30-C31-C32-C33
35	B	625	HTG	C2'-C3'-C4'-C5'
23	c	905	CLA	C2-C3-C5-C6
24	a	408	PHO	C2-C3-C5-C6
23	c	908	CLA	C13-C15-C16-C17
34	J	101	LMG	C16-C17-C18-C19
23	d	401	CLA	C2C-C3C-CAC-CBC
26	L	102	SQD	C13-C14-C15-C16
30	b	621	LMT	C2-C3-C4-C5
23	d	404	CLA	O1D-CGD-O2D-CED
28	D	409	LHG	C28-C29-C30-C31
26	L	102	SQD	C46-C45-O47-C7
23	A	405	CLA	C4C-C3C-CAC-CBC
34	d	411	LMG	C17-C18-C19-C20
36	C	519	DGD	C5A-C6A-C7A-C8A
35	d	413	HTG	C1'-C2'-C3'-C4'
28	K	101	LHG	C12-C13-C14-C15
34	J	101	LMG	C20-C21-C22-C23
30	B	623	LMT	O5B-C1B-O1B-C4'
23	C	505	CLA	C5-C6-C7-C8
28	K	101	LHG	C4-O6-P-O5
26	a	412	SQD	C30-C31-C32-C33
28	d	408	LHG	C24-C25-C26-C27
34	a	413	LMG	C30-C31-C32-C33
36	d	407	DGD	C8B-C9B-CAB-CBB
27	d	406	PL9	C30-C29-C31-C32
36	c	918	DGD	CCB-CDB-CEB-CFB
25	b	618	BCR	C1-C6-C7-C8
23	c	909	CLA	C13-C15-C16-C17
34	B	622	LMG	O8-C28-C29-C30
26	B	621	SQD	C27-C28-C29-C30
23	B	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	c	922	HTG	C1'-C2'-C3'-C4'
36	C	518	DGD	O6E-C1E-O5D-C6D
23	B	602	CLA	C2A-CAA-CBA-CGA
28	E	101	LHG	O7-C5-C6-O8
34	C	501	LMG	O7-C8-C9-O8
34	d	411	LMG	O7-C8-C9-O8
34	m	102	LMG	O7-C8-C9-O8
30	B	643	LMT	C2-C3-C4-C5
34	B	622	LMG	C15-C16-C17-C18
36	C	519	DGD	CCB-CDB-CEB-CFB
28	D	410	LHG	C3-O3-P-O6
28	d	402	LHG	C4-O6-P-O3
28	d	409	LHG	C3-O3-P-O6
28	D	409	LHG	C27-C28-C29-C30
36	C	519	DGD	CCA-CDA-CEA-CFA
34	m	102	LMG	C7-C8-C9-O8
36	h	102	DGD	CAB-CBB-CCB-CDB
23	A	406	CLA	C6-C7-C8-C10
23	B	614	CLA	C11-C10-C8-C7
23	d	401	CLA	C11-C12-C13-C15
36	h	102	DGD	C2B-C3B-C4B-C5B
34	a	413	LMG	O8-C28-C29-C30
23	b	617	CLA	C3-C5-C6-C7
34	D	412	LMG	C38-C39-C40-C41
23	B	615	CLA	C14-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	b	616	CLA	C14-C13-C15-C16
23	c	905	CLA	C11-C10-C8-C9
23	c	907	CLA	C11-C10-C8-C9
25	t	101	BCR	C9-C10-C11-C12
23	A	408	CLA	C16-C17-C18-C20
23	c	908	CLA	C16-C17-C18-C20
28	L	101	LHG	C11-C10-C9-C8
36	C	517	DGD	CCA-CDA-CEA-CFA
34	a	413	LMG	C12-C13-C14-C15
28	d	409	LHG	C35-C36-C37-C38
23	B	616	CLA	O1D-CGD-O2D-CED
34	C	501	LMG	C29-C30-C31-C32
23	a	407	CLA	C10-C11-C12-C13
23	c	903	CLA	C15-C16-C17-C18
28	A	412	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
34	C	520	LMG	C14-C15-C16-C17
36	h	102	DGD	C9A-CAA-CBA-CCA
36	c	917	DGD	C6A-C7A-C8A-C9A
34	d	411	LMG	C10-C11-C12-C13
34	m	102	LMG	O8-C28-C29-C30
27	A	411	PL9	C23-C24-C26-C27
36	c	917	DGD	C8A-C9A-CAA-CBA
26	A	415	SQD	C12-C13-C14-C15
26	A	415	SQD	C14-C15-C16-C17
23	A	406	CLA	C13-C15-C16-C17
23	B	609	CLA	C13-C15-C16-C17
23	D	401	CLA	C15-C16-C17-C18
34	m	102	LMG	C29-C28-O8-C9
23	d	403	CLA	C4B-C3B-CAB-CBB
25	k	102	BCR	C19-C20-C21-C22
27	D	406	PL9	C39-C41-C42-C43
27	a	414	PL9	C14-C16-C17-C18
34	m	102	LMG	O10-C28-O8-C9
28	l	101	LHG	C7-C8-C9-C10
23	b	613	CLA	C10-C11-C12-C13
30	b	621	LMT	C4-C5-C6-C7
28	d	402	LHG	O9-C7-C8-C9
26	A	410	SQD	C34-C35-C36-C37
23	C	513	CLA	C3-C5-C6-C7
28	d	409	LHG	C26-C27-C28-C29
34	B	622	LMG	C40-C41-C42-C43
27	d	406	PL9	C28-C29-C31-C32
34	d	411	LMG	C22-C23-C24-C25
23	C	508	CLA	C5-C6-C7-C8
23	C	513	CLA	C13-C15-C16-C17
36	H	103	DGD	O1B-C1B-C2B-C3B
26	B	621	SQD	C35-C36-C37-C38
34	j	101	LMG	C20-C21-C22-C23
23	b	607	CLA	C16-C17-C18-C20
36	c	918	DGD	C8B-C9B-CAB-CBB
23	c	902	CLA	C2A-CAA-CBA-CGA
26	L	102	SQD	O6-C44-C45-O47
28	A	412	LHG	C2-C3-O3-P
28	e	101	LHG	C2-C3-O3-P
36	D	407	DGD	CDA-CEA-CFA-CGA
26	B	621	SQD	C26-C27-C28-C29
28	d	410	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
27	d	406	PL9	C45-C44-C46-C47
26	A	415	SQD	C24-C25-C26-C27
24	A	407	PHO	C2-C3-C5-C6
34	c	920	LMG	C37-C38-C39-C40
36	C	519	DGD	O6D-C5D-C6D-O5D
23	C	510	CLA	C11-C12-C13-C14
23	b	611	CLA	C14-C13-C15-C16
36	C	519	DGD	C8B-C9B-CAB-CBB
37	E	105	HEM	CAD-CBD-CGD-O1D
34	m	102	LMG	C17-C18-C19-C20
37	e	105	HEM	CAD-CBD-CGD-O1D
30	F	101	LMT	O5'-C1'-O1'-C1
28	l	101	LHG	C12-C13-C14-C15
34	j	101	LMG	C35-C36-C37-C38
26	a	412	SQD	C35-C36-C37-C38
23	A	406	CLA	C11-C10-C8-C7
23	A	408	CLA	C11-C12-C13-C15
23	B	603	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
23	c	908	CLA	C11-C12-C13-C15
35	B	624	HTG	C4'-C5'-C6'-C7'
36	D	407	DGD	CAB-CBB-CCB-CDB
35	C	523	HTG	C4-C5-C6-O6
34	J	101	LMG	C34-C35-C36-C37
35	B	630	HTG	C3'-C4'-C5'-C6'
36	d	407	DGD	C8A-C9A-CAA-CBA
23	B	611	CLA	C2A-CAA-CBA-CGA
23	b	611	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	CAA-CBA-CGA-O2A
37	E	105	HEM	CAD-CBD-CGD-O2D
26	A	415	SQD	C24-C23-O48-C46
36	D	407	DGD	C3B-C4B-C5B-C6B
36	H	103	DGD	C6B-C7B-C8B-C9B
26	L	102	SQD	C11-C12-C13-C14
28	L	101	LHG	C26-C27-C28-C29
26	L	102	SQD	C30-C31-C32-C33
28	A	412	LHG	C11-C12-C13-C14
34	C	531	LMG	C39-C40-C41-C42
23	b	604	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C2B-C3B-CAB-CBB
23	C	502	CLA	C2B-C3B-CAB-CBB
35	B	626	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
28	L	101	LHG	C5-C6-O8-C23
28	d	408	LHG	C14-C15-C16-C17
26	a	417	SQD	C17-C18-C19-C20
34	d	411	LMG	C29-C30-C31-C32
26	x	101	SQD	O6-C44-C45-O47
34	a	413	LMG	O1-C7-C8-O7
26	L	102	SQD	C35-C36-C37-C38
23	b	612	CLA	C8-C10-C11-C12
28	l	101	LHG	C14-C15-C16-C17
28	l	101	LHG	C17-C18-C19-C20
34	m	102	LMG	C38-C39-C40-C41
23	c	910	CLA	C16-C17-C18-C20
26	D	408	SQD	C31-C32-C33-C34
23	d	403	CLA	C2-C1-O2A-CGA
23	c	914	CLA	C13-C15-C16-C17
26	L	102	SQD	C32-C33-C34-C35
23	B	604	CLA	C16-C17-C18-C20
35	B	624	HTG	C1'-C2'-C3'-C4'
23	b	612	CLA	C14-C13-C15-C16
36	c	917	DGD	CCA-CDA-CEA-CFA
26	L	102	SQD	C9-C10-C11-C12
40	V	203	HEC	CAD-CBD-CGD-O2D
36	h	102	DGD	O1B-C1B-C2B-C3B
25	a	411	BCR	C1-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C30
25	c	915	BCR	C1-C6-C7-C8
37	E	105	HEM	CAA-CBA-CGA-O1A
28	L	101	LHG	C32-C33-C34-C35
37	E	105	HEM	C2A-CAA-CBA-CGA
26	B	621	SQD	C45-C44-O6-C1
36	c	917	DGD	C5D-C6D-O5D-C1E
40	V	203	HEC	C2B-C3B-CAB-CBB
26	A	410	SQD	C28-C29-C30-C31
28	D	410	LHG	C14-C15-C16-C17
30	T	103	LMT	C1-C2-C3-C4
23	b	607	CLA	C16-C17-C18-C19
26	A	410	SQD	C24-C25-C26-C27
30	m	103	LMT	C2-C3-C4-C5
23	D	403	CLA	C4C-C3C-CAC-CBC
34	B	622	LMG	C14-C15-C16-C17
34	C	531	LMG	C35-C36-C37-C38
28	a	415	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
35	O	302	HTG	C3'-C4'-C5'-C6'
27	A	411	PL9	C39-C41-C42-C43
36	c	919	DGD	C9B-CAB-CBB-CCB
23	b	611	CLA	C12-C13-C15-C16
23	B	606	CLA	C13-C15-C16-C17
35	c	923	HTG	S1-C1'-C2'-C3'
35	d	413	HTG	S1-C1'-C2'-C3'
36	c	918	DGD	C2E-C1E-O5D-C6D
35	B	630	HTG	C4'-C5'-C6'-C7'
26	B	621	SQD	O6-C44-C45-O47
30	B	643	LMT	O5'-C5'-C6'-O6'
35	b	627	HTG	C2'-C3'-C4'-C5'
34	c	930	LMG	C11-C12-C13-C14
23	B	611	CLA	C4C-C3C-CAC-CBC
40	V	203	HEC	CAD-CBD-CGD-O1D
23	b	612	CLA	O1D-CGD-O2D-CED
23	b	611	CLA	C16-C17-C18-C20
36	C	517	DGD	CDA-CEA-CFA-CGA
23	A	406	CLA	C14-C13-C15-C16
23	A	408	CLA	C14-C13-C15-C16
23	B	612	CLA	C11-C12-C13-C14
23	C	508	CLA	C11-C10-C8-C9
23	C	508	CLA	C14-C13-C15-C16
23	c	906	CLA	C14-C13-C15-C16
23	c	908	CLA	C11-C12-C13-C14
23	c	910	CLA	C11-C10-C8-C9
37	e	105	HEM	CAD-CBD-CGD-O2D
23	B	611	CLA	CAD-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	B	617	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	511	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	611	CLA	CAD-CBD-CGD-O2D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	c	902	CLA	CAD-CBD-CGD-O2D
23	d	404	CLA	CAD-CBD-CGD-O2D
26	a	412	SQD	C33-C34-C35-C36
28	e	101	LHG	C12-C13-C14-C15
40	v	203	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	D	410	LHG	C11-C12-C13-C14
34	J	101	LMG	C4-C5-C6-O5
23	c	911	CLA	C2-C3-C5-C6
25	k	102	BCR	C7-C8-C9-C10
28	d	402	LHG	C13-C14-C15-C16
36	c	918	DGD	C4A-C5A-C6A-C7A
30	m	103	LMT	C4-C5-C6-C7
35	c	921	HTG	O5-C5-C6-O6
27	a	414	PL9	C31-C32-C33-C34
23	c	904	CLA	C10-C11-C12-C13
23	C	513	CLA	CAA-CBA-CGA-O2A
28	e	101	LHG	O7-C7-C8-C9
23	d	401	CLA	C4C-C3C-CAC-CBC
23	B	605	CLA	O2A-C1-C2-C3
23	D	403	CLA	O2A-C1-C2-C3
23	c	910	CLA	O2A-C1-C2-C3
23	c	913	CLA	O2A-C1-C2-C3
24	a	408	PHO	O2A-C1-C2-C3
26	a	412	SQD	C15-C16-C17-C18
28	d	402	LHG	C11-C12-C13-C14
28	d	408	LHG	C26-C27-C28-C29
36	c	918	DGD	C8A-C9A-CAA-CBA
26	A	410	SQD	O47-C7-C8-C9
26	A	415	SQD	O49-C7-O47-C45
34	D	412	LMG	C8-C9-O8-C28
23	A	406	CLA	CHA-CBD-CGD-O1D
23	B	603	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	617	CLA	CHA-CBD-CGD-O1D
23	C	505	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	513	CLA	CHA-CBD-CGD-O1D
23	D	401	CLA	CHA-CBD-CGD-O2D
23	a	407	CLA	CHA-CBD-CGD-O1D
23	b	604	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	617	CLA	CHA-CBD-CGD-O1D
23	c	907	CLA	CHA-CBD-CGD-O2D
23	c	910	CLA	CHA-CBD-CGD-O1D
23	c	910	CLA	CHA-CBD-CGD-O2D
34	D	412	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
30	F	101	LMT	C2'-C1'-O1'-C1
23	a	407	CLA	C2C-C3C-CAC-CBC
26	A	410	SQD	C9-C10-C11-C12
30	A	416	LMT	C7-C8-C9-C10
23	B	605	CLA	C16-C17-C18-C19
26	A	415	SQD	O47-C45-C46-O48
34	c	920	LMG	O10-C28-O8-C9
28	D	411	LHG	C12-C13-C14-C15
40	V	203	HEC	C4B-C3B-CAB-CBB
26	A	415	SQD	O10-C23-O48-C46
23	c	913	CLA	CAA-CBA-CGA-O2A
28	K	101	LHG	O7-C7-C8-C9
24	D	402	PHO	CHA-CBD-CGD-O1D
24	a	408	PHO	CHA-CBD-CGD-O1D
24	a	409	PHO	CHA-CBD-CGD-O1D
30	b	621	LMT	O5'-C5'-C6'-O6'
36	c	919	DGD	C2A-C1A-O1G-C1G
23	c	912	CLA	O1D-CGD-O2D-CED
23	b	602	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	b	607	CLA	C12-C13-C15-C16
23	b	614	CLA	C16-C17-C18-C19
28	E	101	LHG	O7-C7-C8-C9
34	J	101	LMG	C14-C15-C16-C17
23	B	616	CLA	C14-C13-C15-C16
23	b	602	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
23	b	607	CLA	C6-C7-C8-C9
23	d	401	CLA	C11-C12-C13-C14
36	C	519	DGD	C5B-C6B-C7B-C8B
23	B	614	CLA	C2B-C3B-CAB-CBB
40	v	203	HEC	CAD-CBD-CGD-O1D
34	c	920	LMG	C29-C28-O8-C9
28	e	101	LHG	O9-C7-C8-C9
23	b	611	CLA	C16-C17-C18-C19
23	C	504	CLA	C5-C6-C7-C8
23	B	608	CLA	O1D-CGD-O2D-CED
37	E	105	HEM	CAA-CBA-CGA-O2A
23	B	605	CLA	C16-C17-C18-C20
28	D	411	LHG	C24-C25-C26-C27
25	C	515	BCR	C21-C22-C23-C24
30	a	418	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C15-C16-C17-C18
35	c	923	HTG	C3'-C4'-C5'-C6'
23	C	514	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CAA-CBA-CGA-O1A
26	D	408	SQD	C44-C45-C46-O48
26	x	101	SQD	O6-C44-C45-C46
23	b	605	CLA	C15-C16-C17-C18
23	c	907	CLA	C5-C6-C7-C8
28	e	101	LHG	C7-C8-C9-C10
34	C	501	LMG	C20-C21-C22-C23
23	b	613	CLA	C8-C10-C11-C12
36	h	102	DGD	C7B-C8B-C9B-CAB
26	A	410	SQD	O49-C7-C8-C9
23	C	514	CLA	O1A-CGA-O2A-C1
23	C	502	CLA	C4B-C3B-CAB-CBB
23	c	902	CLA	C4B-C3B-CAB-CBB
27	a	414	PL9	C3-C7-C8-C9
28	D	410	LHG	C3-O3-P-O5
28	d	409	LHG	C3-O3-P-O5
30	B	623	LMT	C2B-C1B-O1B-C4'
28	E	101	LHG	O9-C7-C8-C9
36	C	518	DGD	CBA-CCA-CDA-CEA
36	c	919	DGD	O6D-C5D-C6D-O5D
25	j	104	BCR	C1-C6-C7-C8
25	j	104	BCR	C5-C6-C7-C8
26	A	415	SQD	C28-C29-C30-C31
23	b	604	CLA	C2A-CAA-CBA-CGA
35	O	302	HTG	C2'-C3'-C4'-C5'
30	m	104	LMT	C5-C6-C7-C8
23	B	608	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	b	608	CLA	CAD-CBD-CGD-O1D
23	d	401	CLA	CAD-CBD-CGD-O1D
26	x	101	SQD	O5-C5-C6-S
23	c	913	CLA	CAA-CBA-CGA-O1A
23	A	406	CLA	C11-C10-C8-C9
23	A	406	CLA	C11-C12-C13-C14
23	c	906	CLA	C11-C12-C13-C14
23	B	602	CLA	CBD-CGD-O2D-CED
26	L	102	SQD	C29-C30-C31-C32
23	B	617	CLA	C8-C10-C11-C12
23	c	906	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	L	101	LHG	O7-C7-C8-C9
28	l	101	LHG	C26-C27-C28-C29
34	B	622	LMG	C36-C37-C38-C39
34	C	531	LMG	O10-C28-O8-C9
28	D	409	LHG	C26-C27-C28-C29
23	B	613	CLA	C8-C10-C11-C12
23	c	904	CLA	C15-C16-C17-C18
28	K	101	LHG	O9-C7-C8-C9
23	C	508	CLA	C4-C3-C5-C6
28	D	410	LHG	C28-C29-C30-C31
34	C	531	LMG	C12-C13-C14-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	507	CLA	C3A-C2A-CAA-CBA
23	C	514	CLA	C11-C12-C13-C15
23	a	407	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	906	CLA	C12-C13-C15-C16
23	c	907	CLA	C6-C7-C8-C10
35	c	922	HTG	C2-C1-S1-C1'
34	a	413	LMG	C36-C37-C38-C39
23	C	506	CLA	CAA-CBA-CGA-O2A
27	A	411	PL9	C2-C3-C7-C8
37	e	105	HEM	CAA-CBA-CGA-O1A
26	a	417	SQD	C32-C33-C34-C35
28	d	410	LHG	C32-C33-C34-C35
36	C	519	DGD	O1G-C1A-C2A-C3A
36	c	918	DGD	O6E-C1E-O5D-C6D
23	A	408	CLA	C5-C6-C7-C8
28	d	402	LHG	C19-C20-C21-C22
23	C	502	CLA	CAA-CBA-CGA-O2A
28	D	411	LHG	O8-C23-C24-C25
34	c	920	LMG	O8-C28-C29-C30
23	C	502	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C8-C10-C11-C12
24	A	407	PHO	C4-C3-C5-C6
34	J	101	LMG	O7-C10-C11-C12

There are no ring outliers.

219 monomers are involved in 526 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	402	LHG	2	0
31	V	207	DMS	6	0
28	d	410	LHG	2	0
31	v	205	DMS	1	0
23	b	603	CLA	2	0
31	B	645	DMS	1	0
25	D	405	BCR	5	0
31	V	202	DMS	1	0
31	B	639	DMS	8	0
26	B	621	SQD	4	0
31	a	420	DMS	9	0
24	a	409	PHO	3	0
31	b	639	DMS	2	0
23	C	506	CLA	1	0
30	e	103	LMT	1	0
26	A	415	SQD	2	0
28	L	101	LHG	1	0
23	C	503	CLA	2	0
23	B	614	CLA	4	0
37	E	105	HEM	1	0
23	b	607	CLA	2	0
31	B	640	DMS	1	0
31	v	202	DMS	1	0
23	C	505	CLA	1	0
35	O	302	HTG	2	0
23	a	407	CLA	2	0
30	m	104	LMT	1	0
35	C	521	HTG	1	0
23	b	610	CLA	1	0
25	b	620	BCR	8	0
30	M	101	LMT	1	0
31	d	414	DMS	2	0
31	H	101	DMS	2	0
36	c	917	DGD	2	0
31	b	644	DMS	1	0
35	b	627	HTG	1	0
24	D	402	PHO	2	0
31	B	641	DMS	1	0
26	a	412	SQD	2	0
34	J	101	LMG	3	0
34	c	920	LMG	3	0
36	D	407	DGD	4	0
23	C	507	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	406	CLA	5	0
25	B	618	BCR	1	0
31	B	646	DMS	4	0
35	b	623	HTG	1	0
25	c	915	BCR	3	0
31	v	210	DMS	1	0
26	D	408	SQD	2	0
28	a	415	LHG	1	0
31	b	646	DMS	2	0
31	A	424	DMS	4	0
31	u	206	DMS	3	0
31	O	308	DMS	5	0
35	c	922	HTG	1	0
26	a	417	SQD	3	0
31	O	303	DMS	2	0
31	U	202	DMS	1	0
31	b	645	DMS	6	0
30	z	101	LMT	1	0
31	c	932	DMS	2	0
38	x	102	RRX	4	0
23	c	909	CLA	6	0
25	C	515	BCR	3	0
25	T	101	BCR	6	0
35	B	625	HTG	1	0
27	a	414	PL9	14	0
23	b	602	CLA	6	0
31	c	927	DMS	2	0
31	d	416	DMS	5	0
23	b	611	CLA	5	0
23	c	908	CLA	3	0
31	A	421	DMS	2	0
23	b	613	CLA	1	0
31	o	303	DMS	1	0
23	b	608	CLA	1	0
25	A	409	BCR	3	0
23	D	404	CLA	1	0
31	c	934	DMS	1	0
25	d	405	BCR	2	0
23	B	615	CLA	1	0
23	b	606	CLA	1	0
31	l	102	DMS	5	0
31	F	102	DMS	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	903	CLA	1	0
25	B	619	BCR	4	0
30	A	416	LMT	2	0
31	v	209	DMS	7	0
23	b	614	CLA	2	0
23	A	408	CLA	1	0
25	Y	101	BCR	1	0
23	D	403	CLA	2	0
31	B	648	DMS	2	0
36	C	518	DGD	1	0
35	c	921	HTG	1	0
23	C	504	CLA	4	0
31	C	525	DMS	1	0
31	C	529	DMS	2	0
31	O	304	DMS	1	0
36	C	517	DGD	1	0
23	B	616	CLA	3	0
31	B	636	DMS	5	0
31	i	105	DMS	3	0
34	d	411	LMG	5	0
36	c	918	DGD	1	0
35	b	622	HTG	3	0
23	c	902	CLA	2	0
31	h	104	DMS	1	0
31	u	205	DMS	2	0
26	L	102	SQD	4	0
31	e	104	DMS	1	0
36	d	407	DGD	6	0
28	D	411	LHG	5	0
23	B	603	CLA	1	0
31	c	929	DMS	2	0
23	b	604	CLA	2	0
31	B	638	DMS	3	0
23	C	512	CLA	2	0
34	B	622	LMG	2	0
35	B	630	HTG	1	0
27	A	411	PL9	12	0
37	e	105	HEM	1	0
34	C	501	LMG	1	0
34	D	412	LMG	5	0
23	c	905	CLA	1	0
26	x	101	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	h	101	DMS	2	0
23	A	406	CLA	1	0
25	B	620	BCR	3	0
23	c	904	CLA	2	0
31	O	311	DMS	3	0
35	B	624	HTG	2	0
25	C	530	BCR	2	0
23	C	513	CLA	5	0
23	C	502	CLA	1	0
30	I	101	LMT	2	0
31	O	305	DMS	5	0
31	D	416	DMS	6	0
31	U	204	DMS	4	0
30	Z	101	LMT	6	0
28	e	101	LHG	5	0
31	b	638	DMS	1	0
23	D	401	CLA	2	0
23	c	906	CLA	2	0
34	a	413	LMG	8	0
31	v	206	DMS	2	0
28	d	408	LHG	2	0
23	C	511	CLA	1	0
23	d	404	CLA	5	0
23	B	605	CLA	1	0
28	E	101	LHG	3	0
30	B	623	LMT	2	0
31	b	636	DMS	15	0
34	c	930	LMG	1	0
34	m	102	LMG	3	0
23	A	405	CLA	5	0
23	C	509	CLA	2	0
24	A	407	PHO	1	0
31	v	207	DMS	1	0
24	a	408	PHO	1	0
23	d	401	CLA	3	0
23	B	617	CLA	3	0
30	B	644	LMT	1	0
25	t	101	BCR	7	0
23	d	403	CLA	1	0
31	v	201	DMS	1	0
35	D	414	HTG	3	0
32	a	424	BCT	1	0

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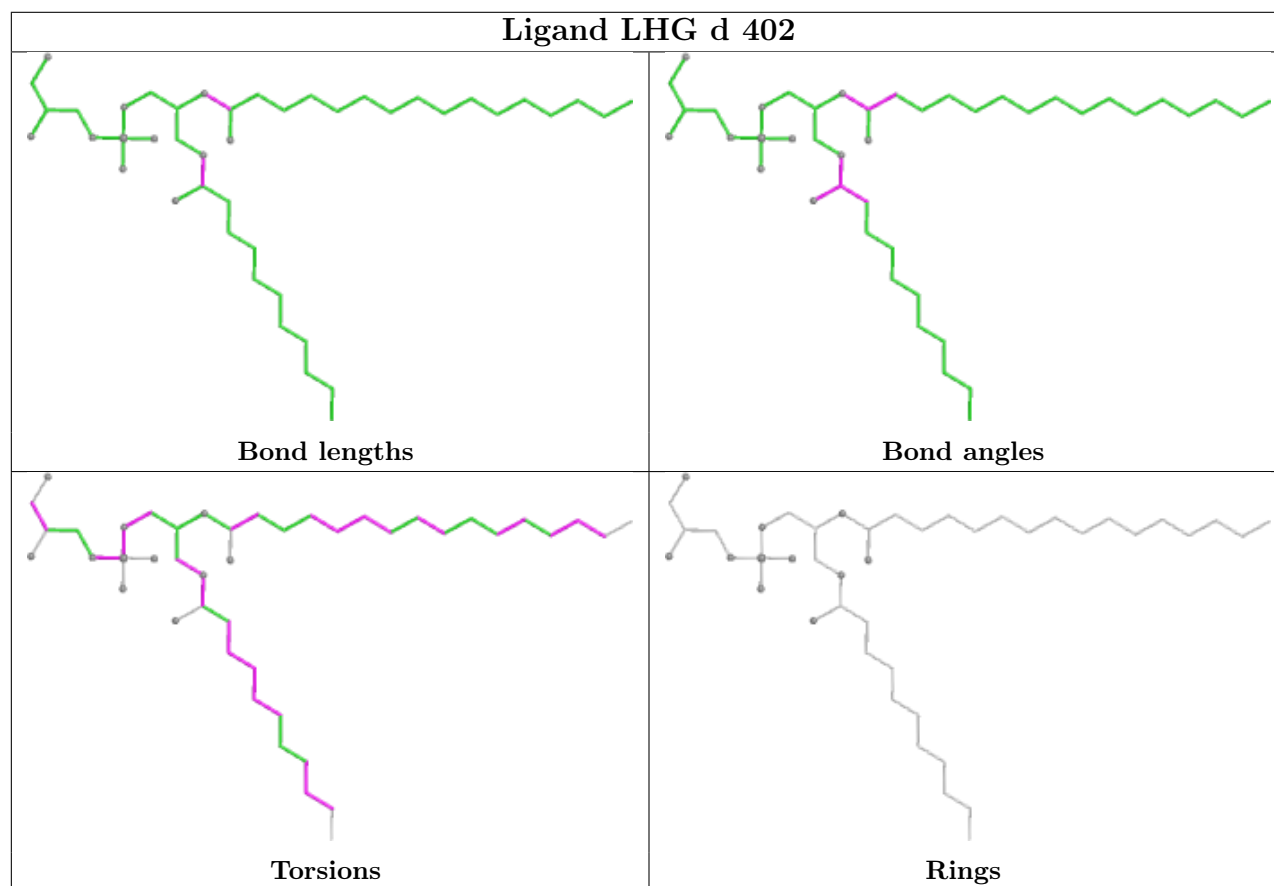
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	633	DMS	1	0
23	B	602	CLA	2	0
26	A	410	SQD	9	0
34	C	531	LMG	3	0
31	a	421	DMS	1	0
28	A	412	LHG	1	0
31	b	647	DMS	3	0
30	b	621	LMT	4	0
31	C	526	DMS	3	0
31	D	415	DMS	3	0
23	B	606	CLA	6	0
31	c	933	DMS	2	0
23	c	912	CLA	3	0
31	V	209	DMS	1	0
23	C	514	CLA	3	0
23	a	410	CLA	1	0
31	V	205	DMS	1	0
23	b	617	CLA	9	0
31	V	210	DMS	6	0
31	V	206	DMS	1	0
23	B	612	CLA	1	0
23	C	510	CLA	3	0
30	a	418	LMT	4	0
28	D	409	LHG	2	0
23	b	615	CLA	4	0
31	b	637	DMS	1	0
23	c	910	CLA	2	0
35	v	204	HTG	4	0
23	B	604	CLA	2	0
25	c	916	BCR	3	0
31	H	105	DMS	5	0
23	c	913	CLA	5	0
25	C	516	BCR	2	0
23	c	914	CLA	1	0
23	b	616	CLA	3	0
30	a	422	LMT	4	0
31	A	422	DMS	2	0
31	c	925	DMS	7	0
31	a	423	DMS	2	0
31	c	936	DMS	1	0
23	c	907	CLA	5	0
23	B	611	CLA	4	0

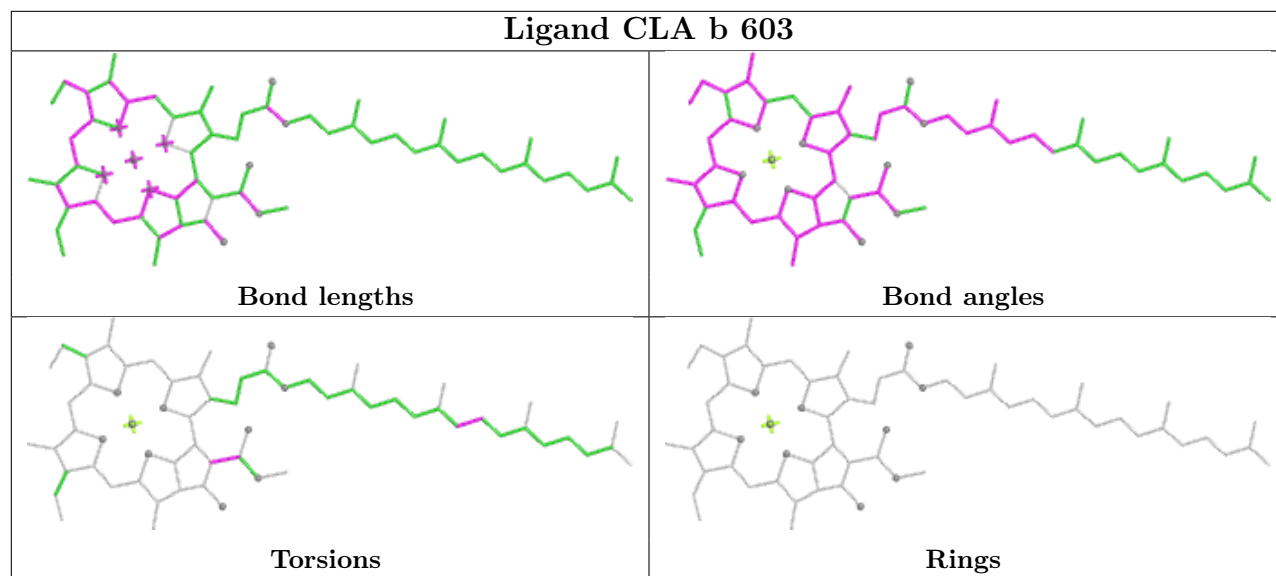
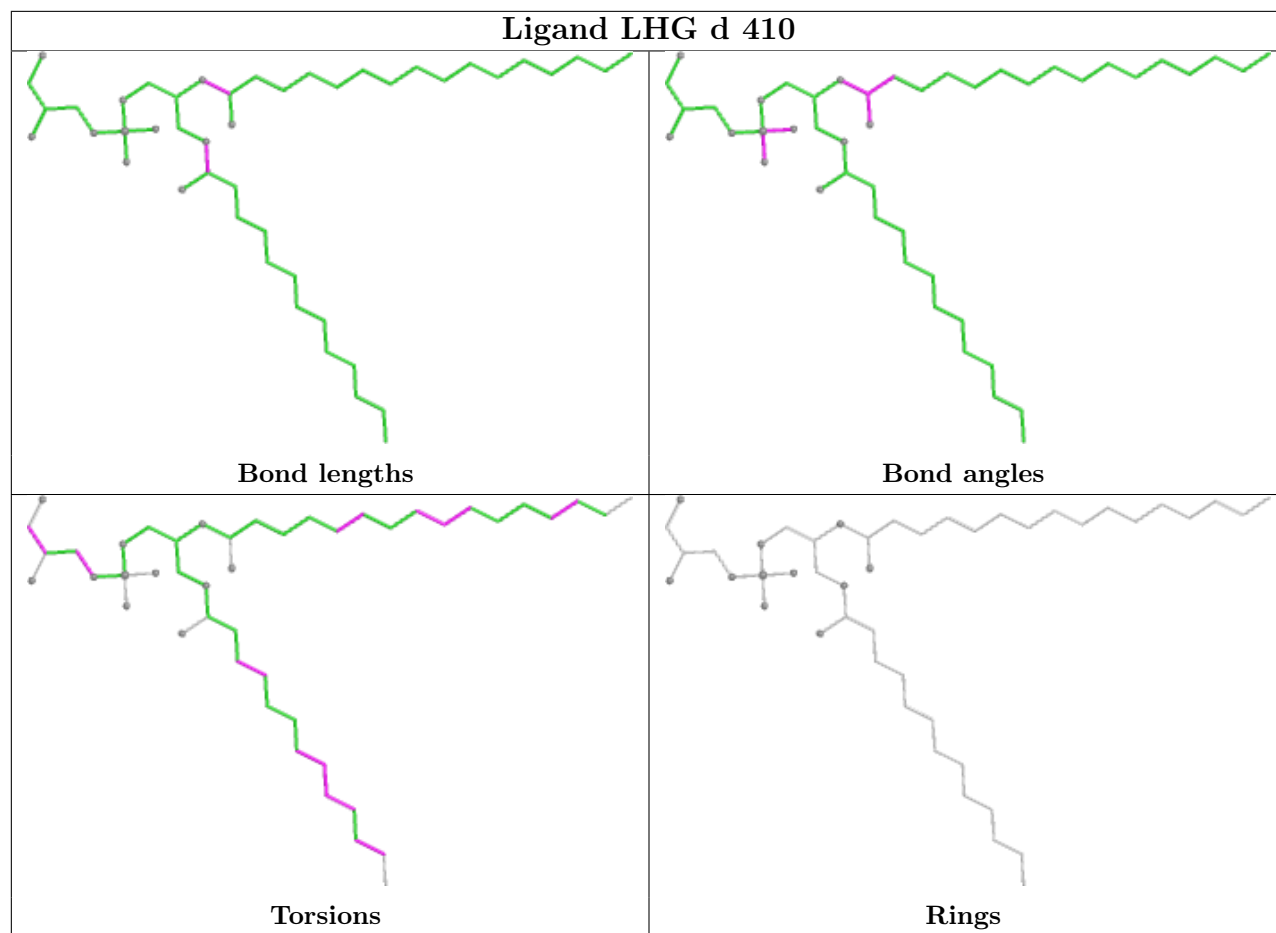
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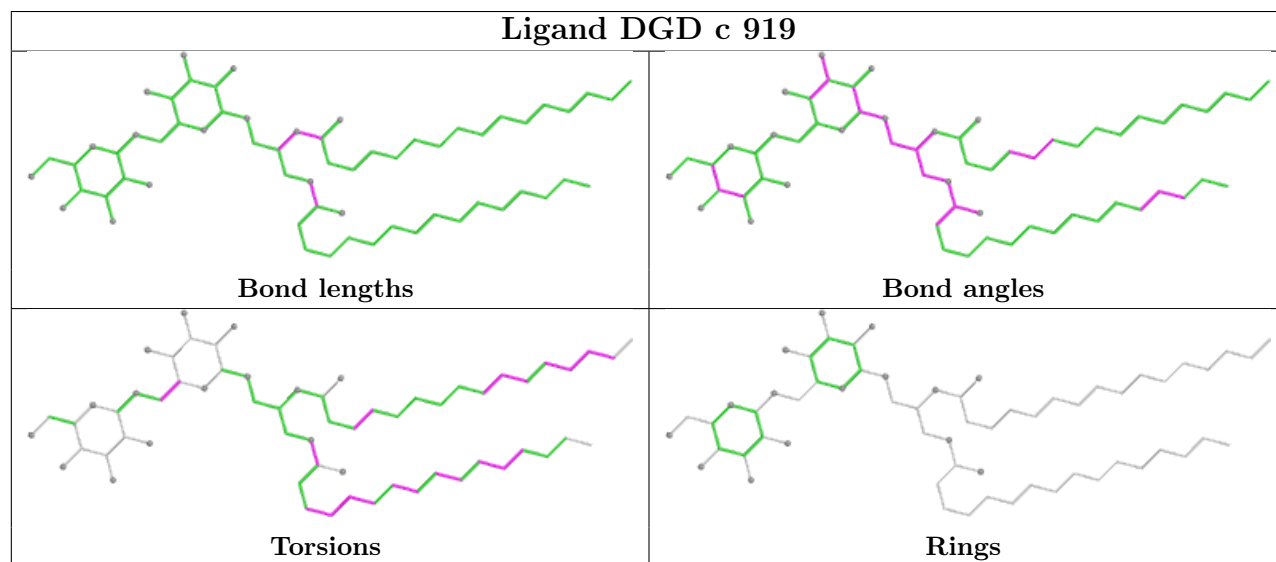
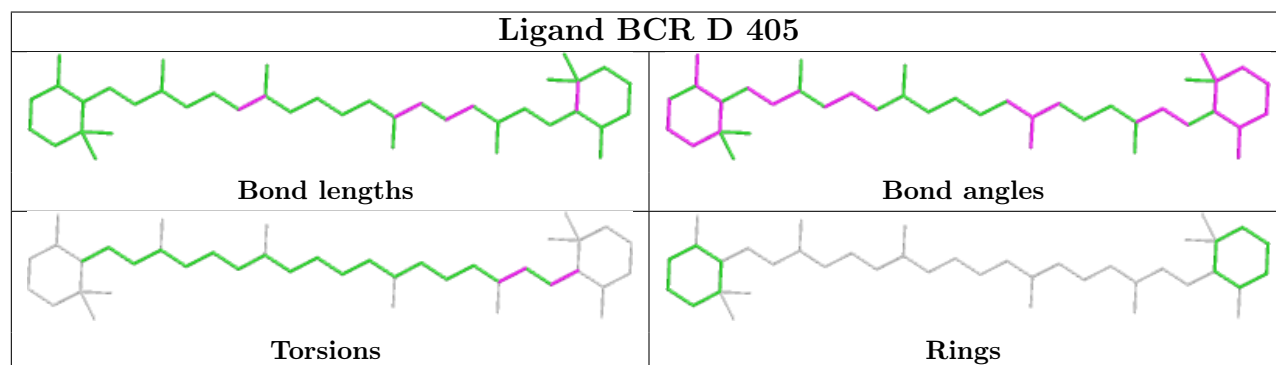
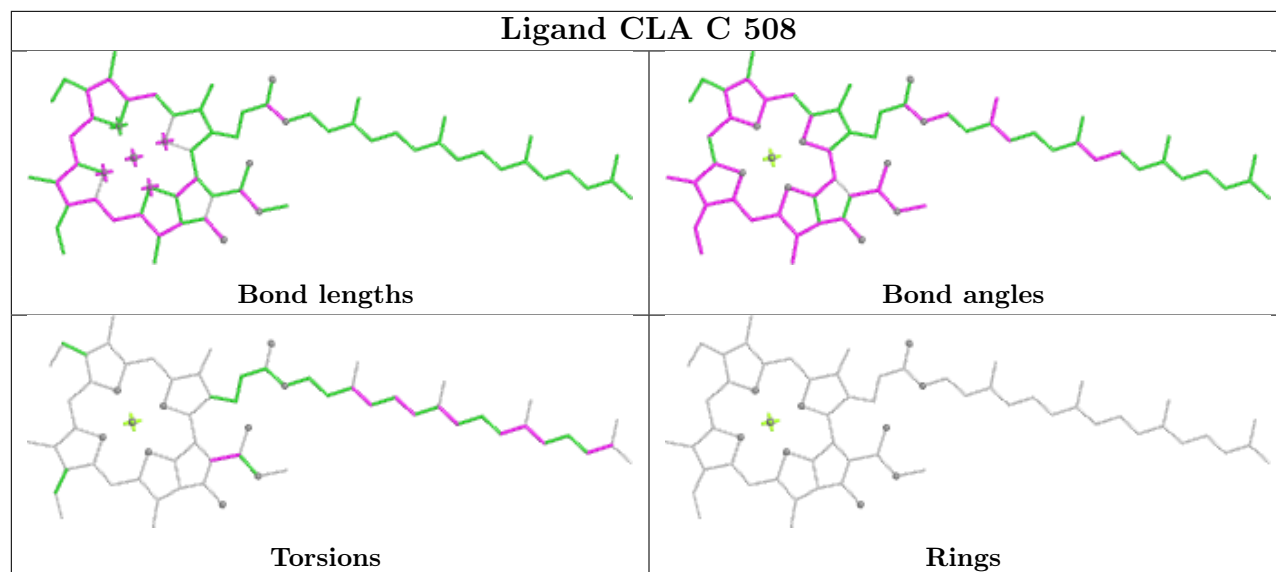
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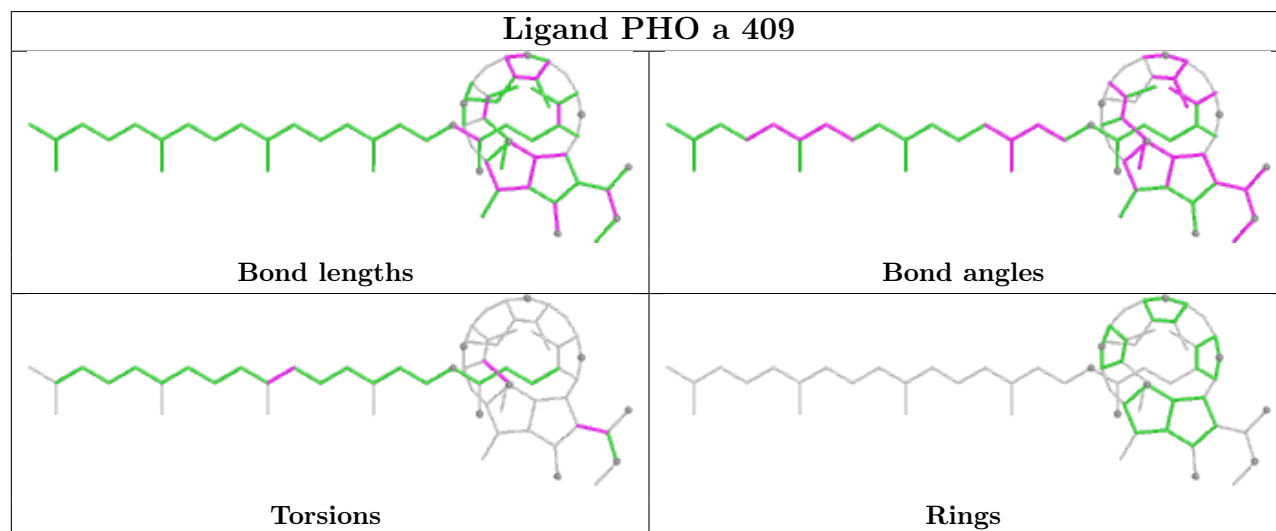
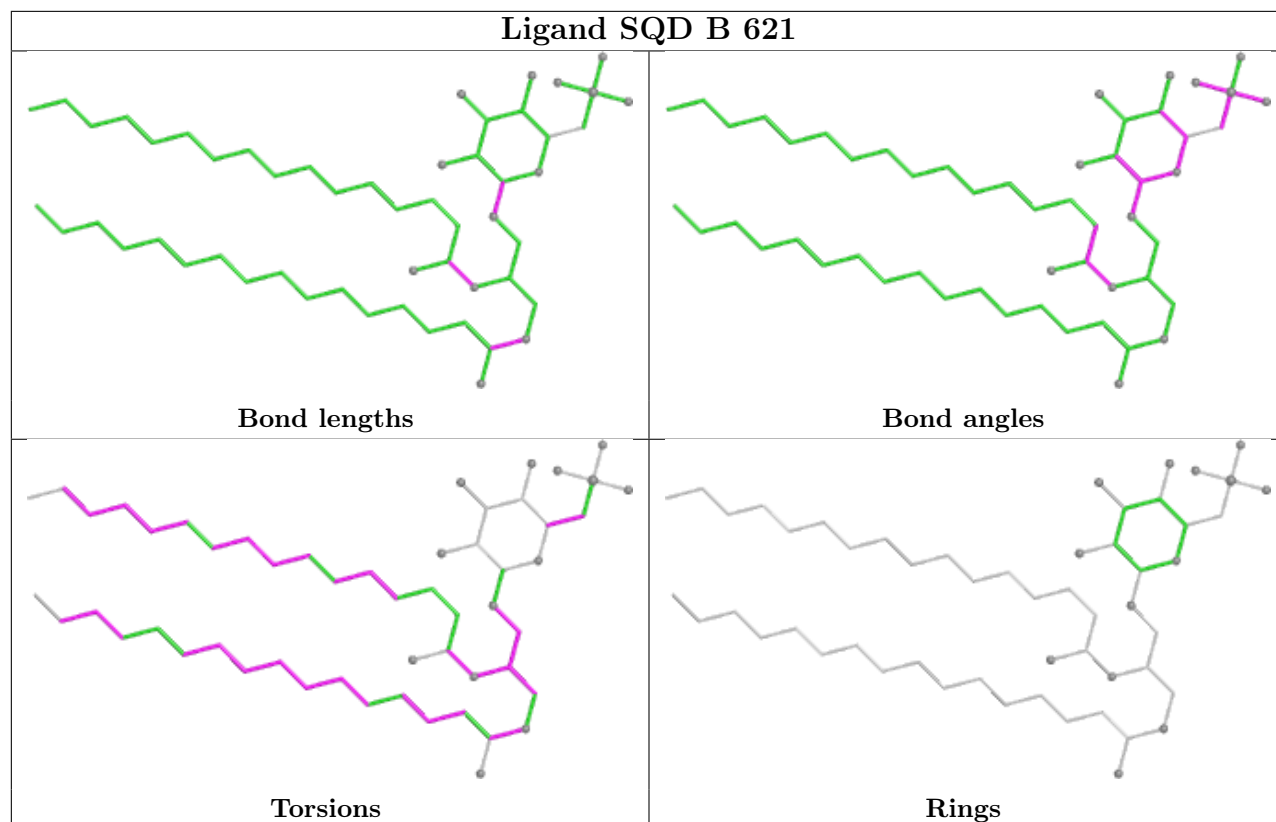
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	411	BCR	1	0
31	o	304	DMS	3	0
25	k	102	BCR	1	0
31	b	641	DMS	2	0
25	j	104	BCR	4	0
30	m	103	LMT	2	0
23	b	605	CLA	1	0
25	b	619	BCR	3	0

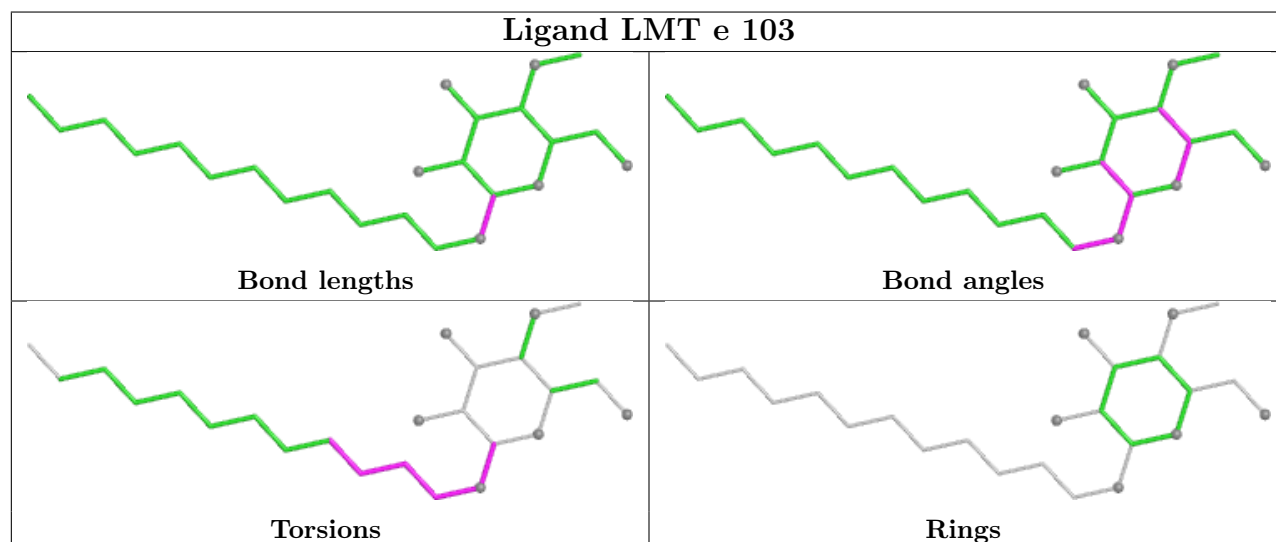
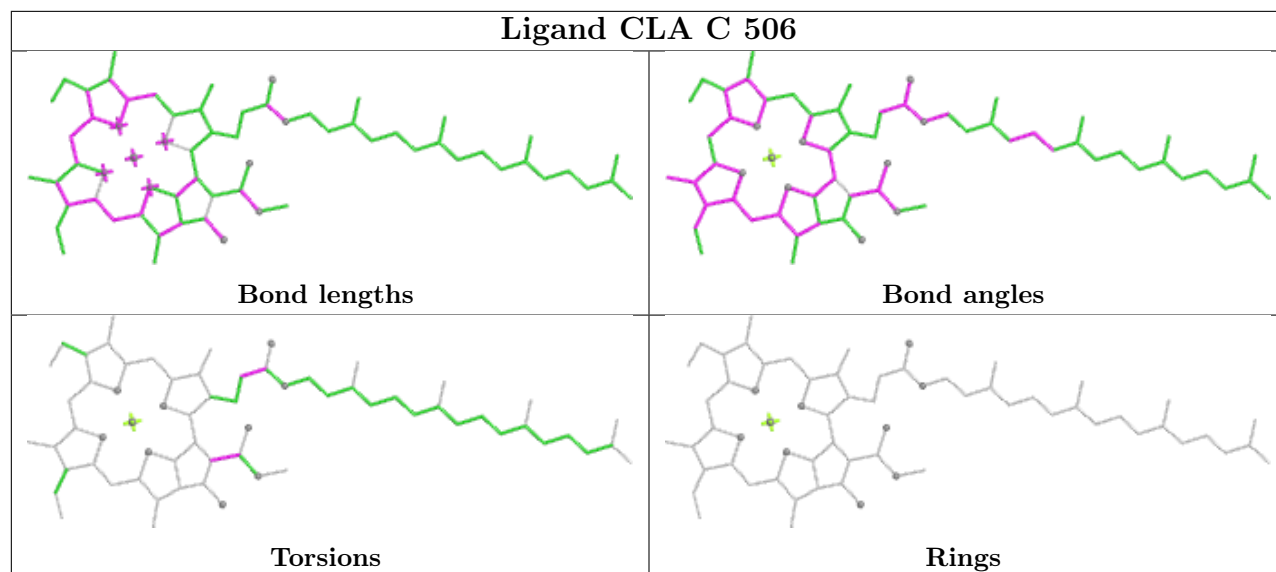
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

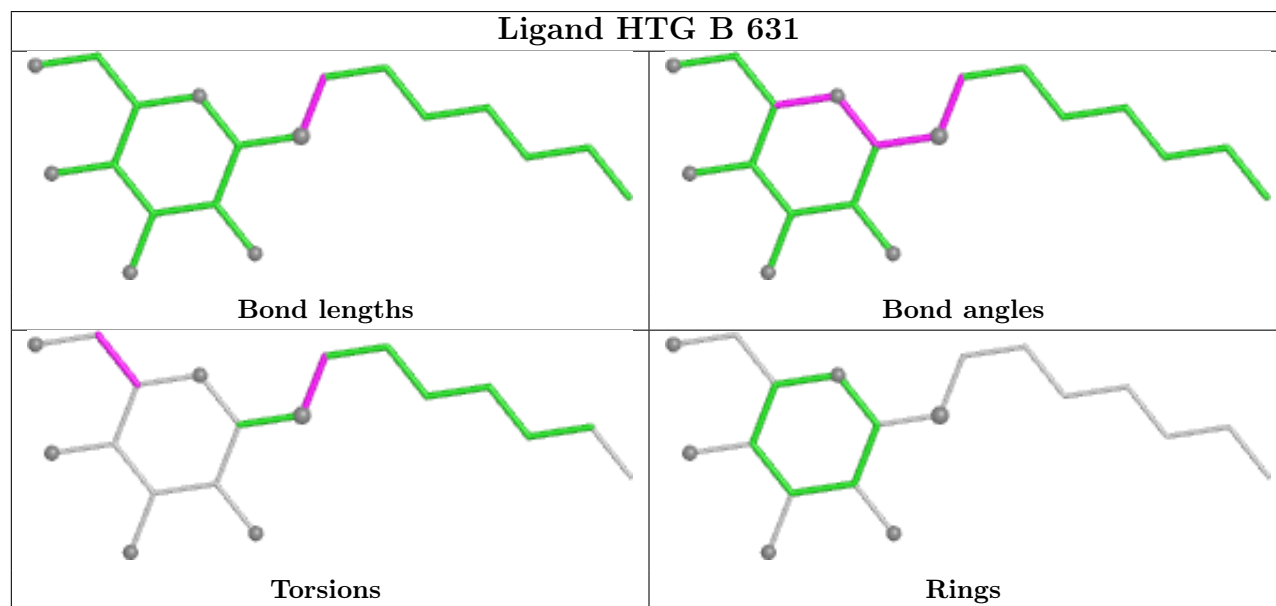
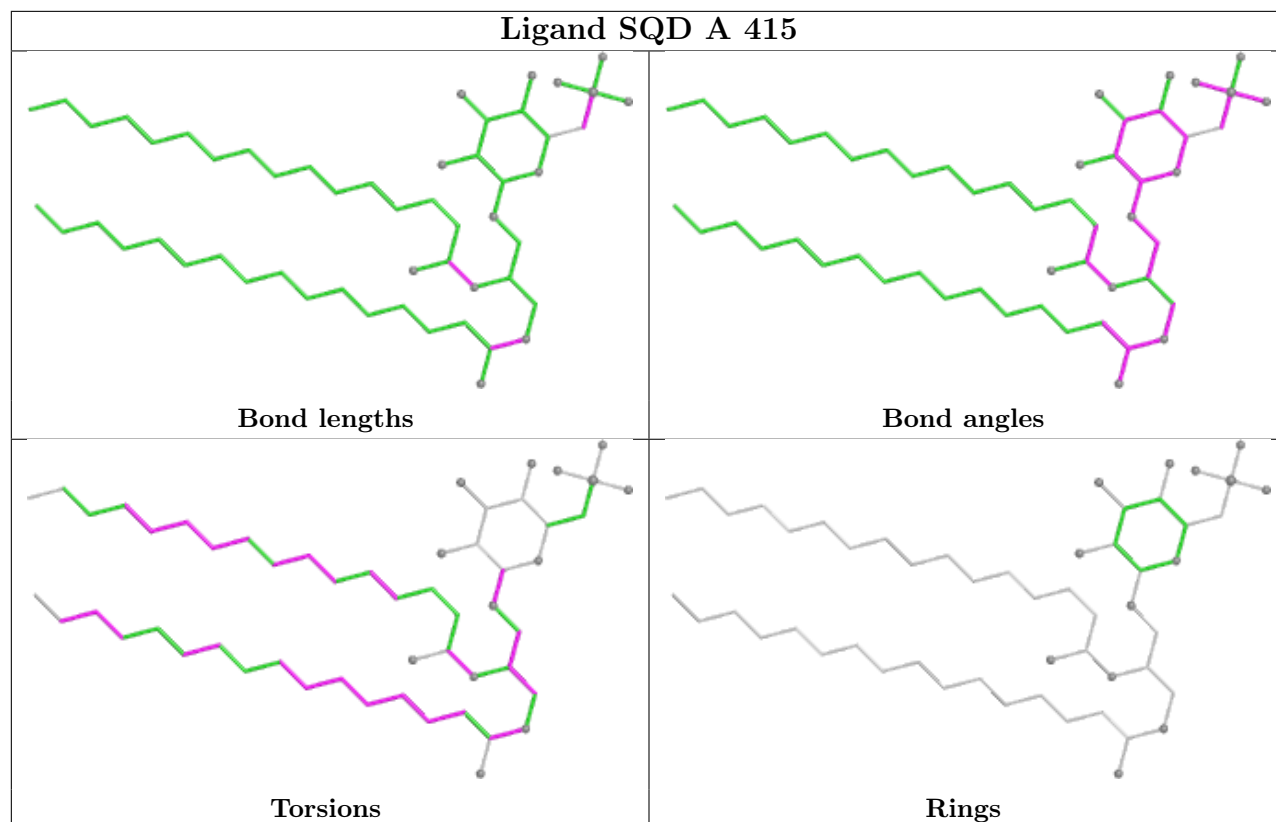


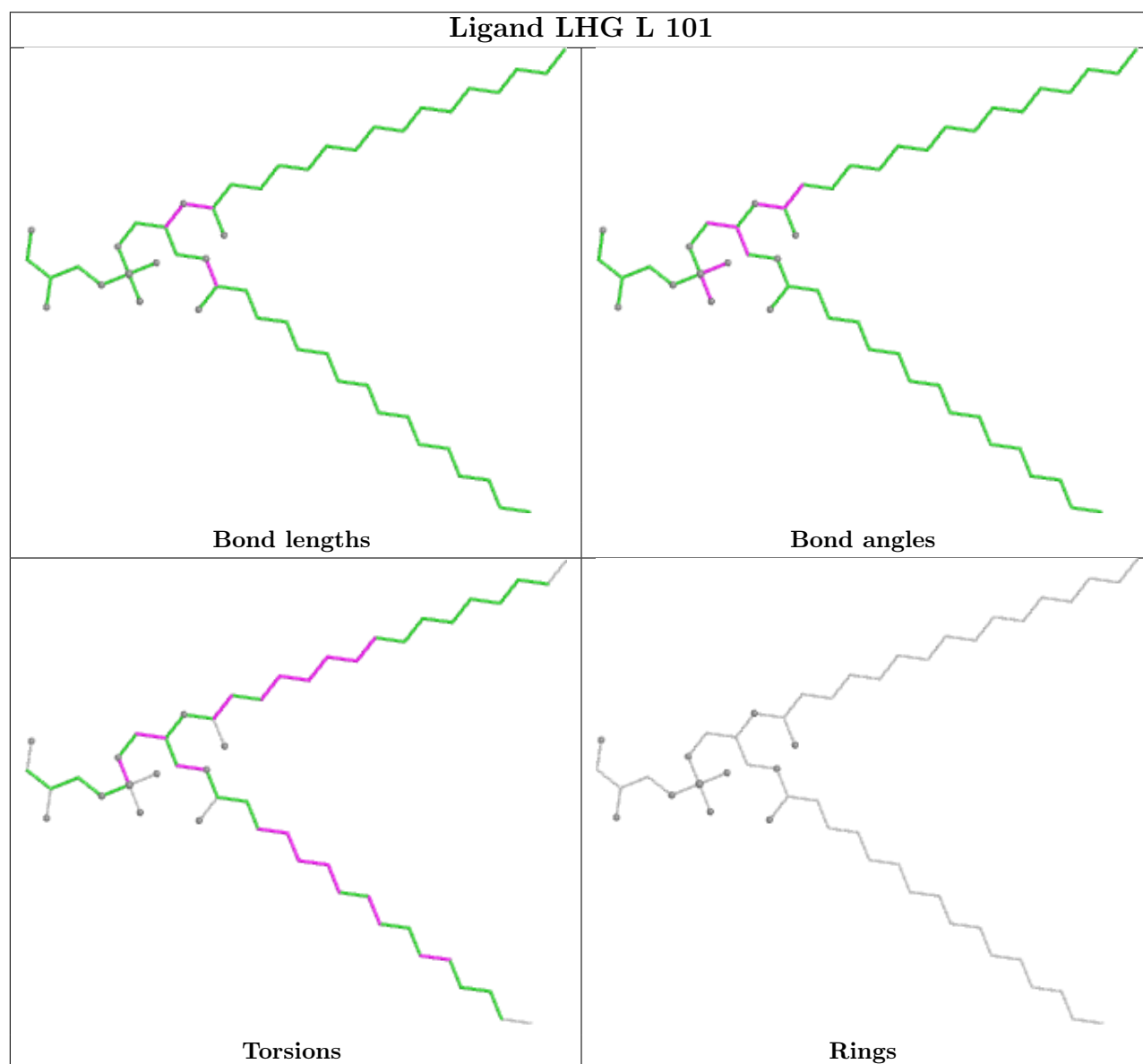
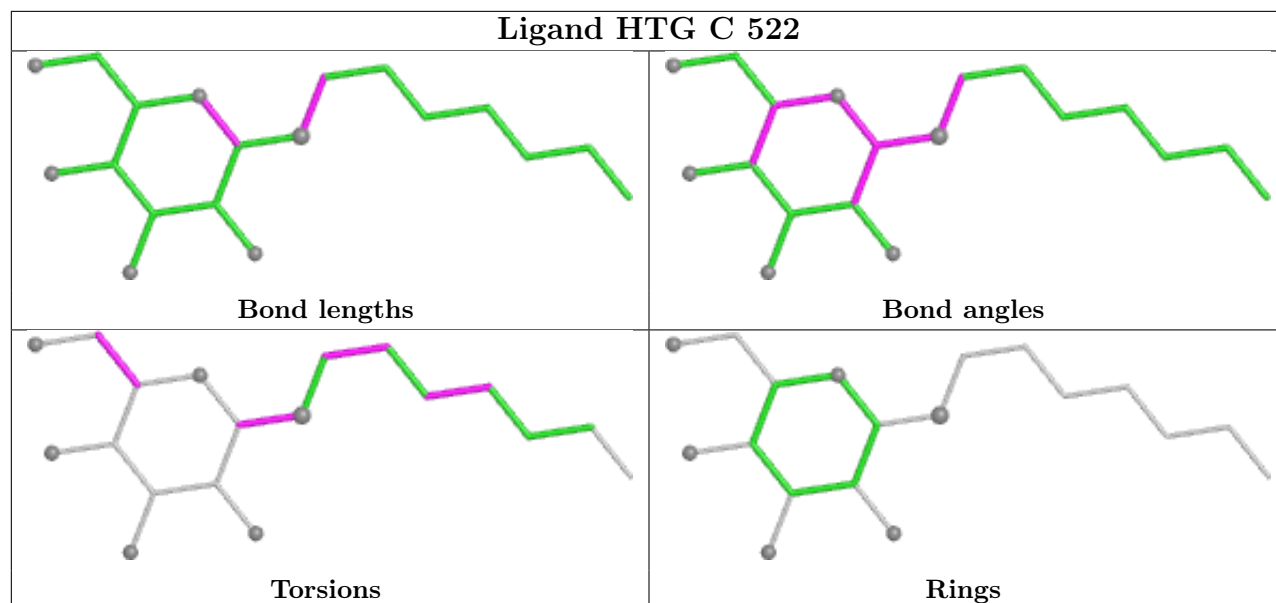


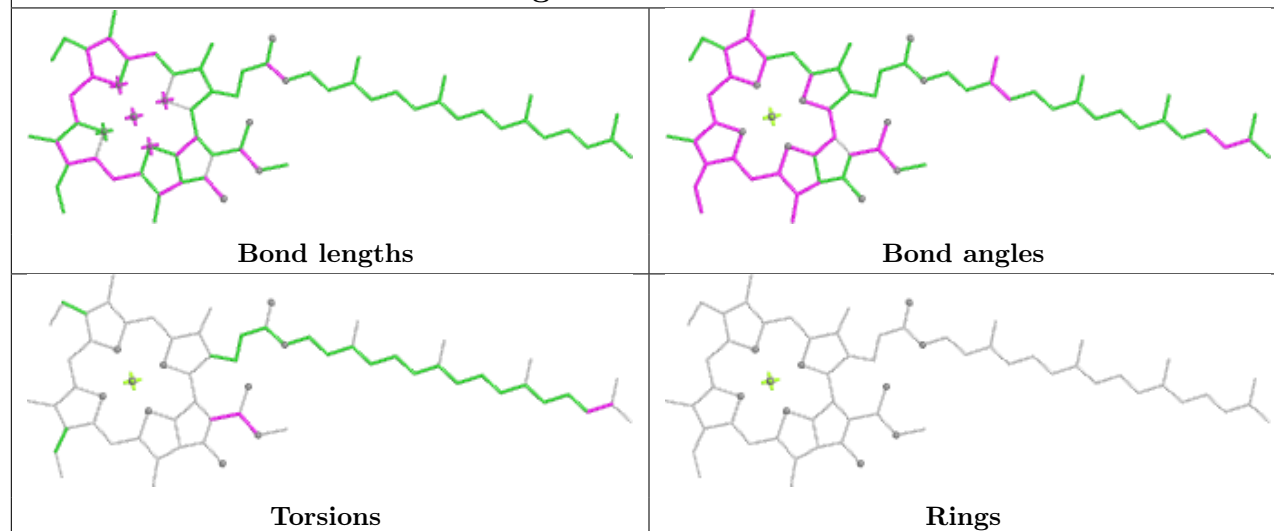
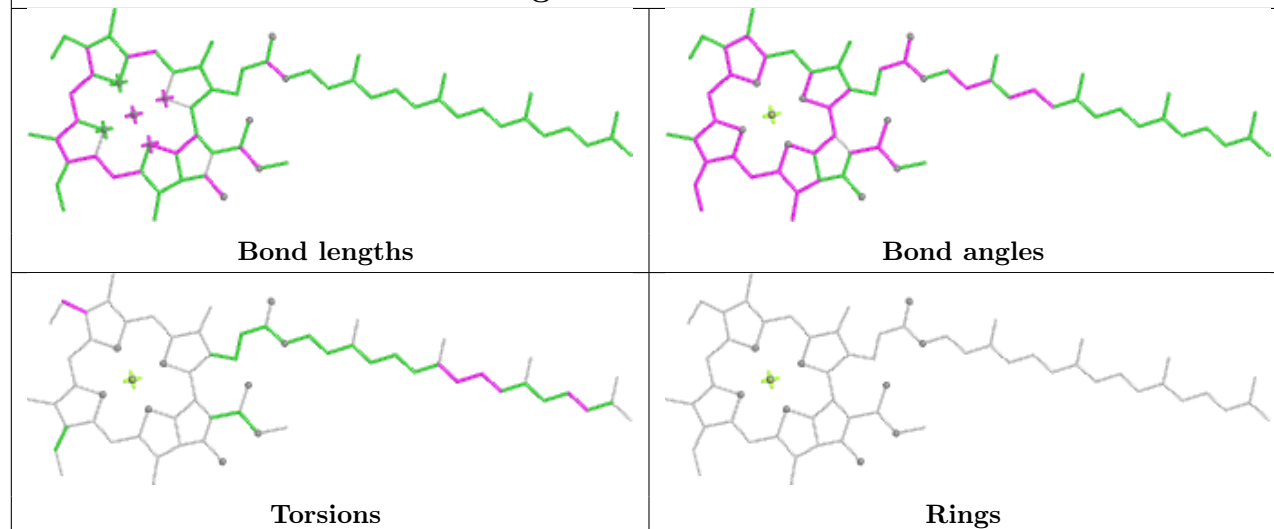


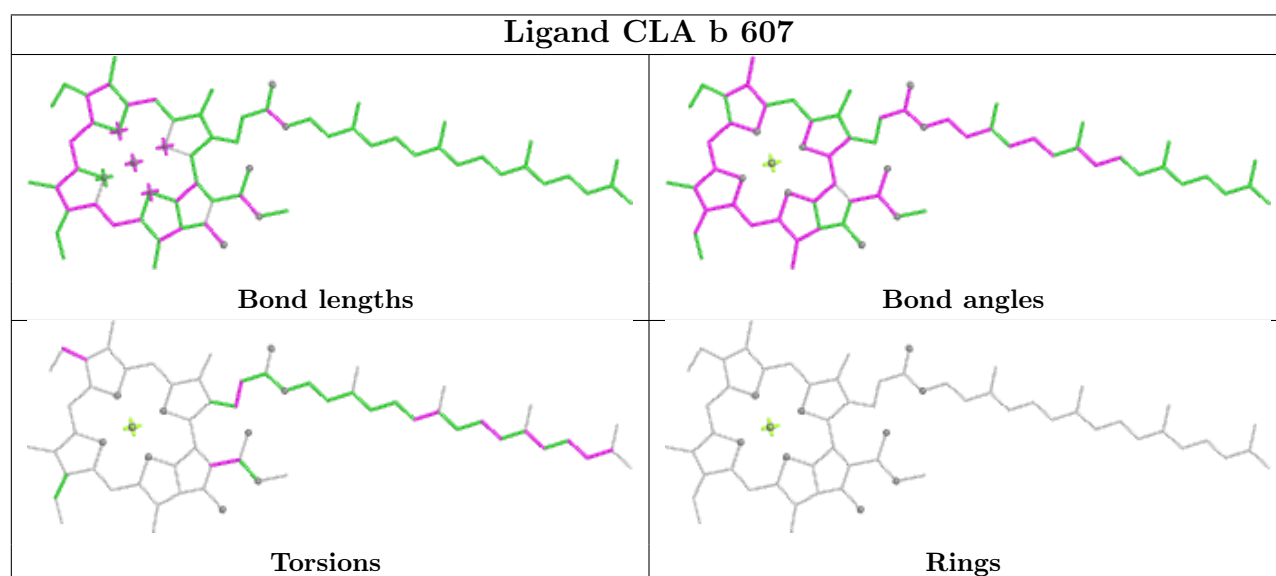
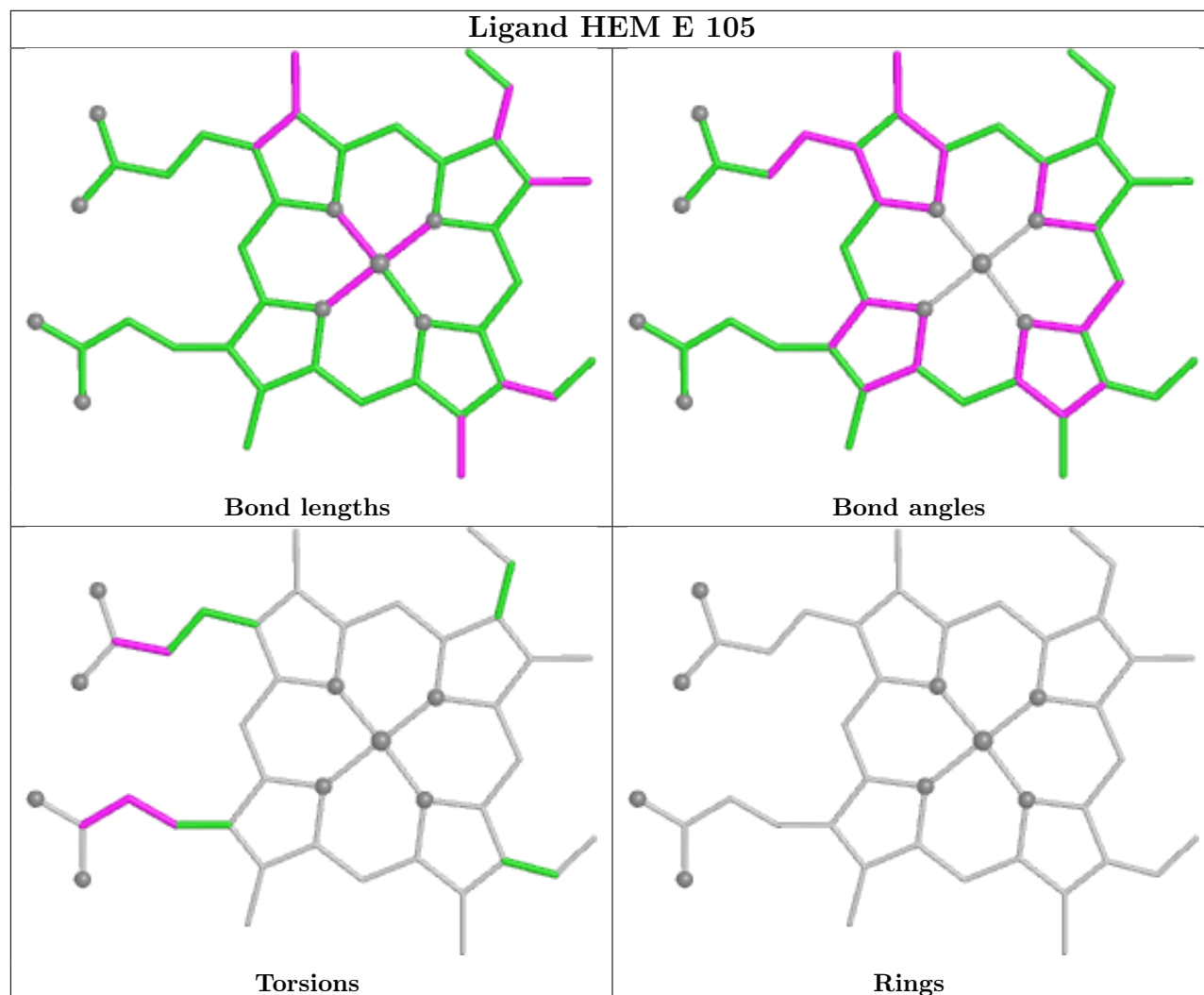




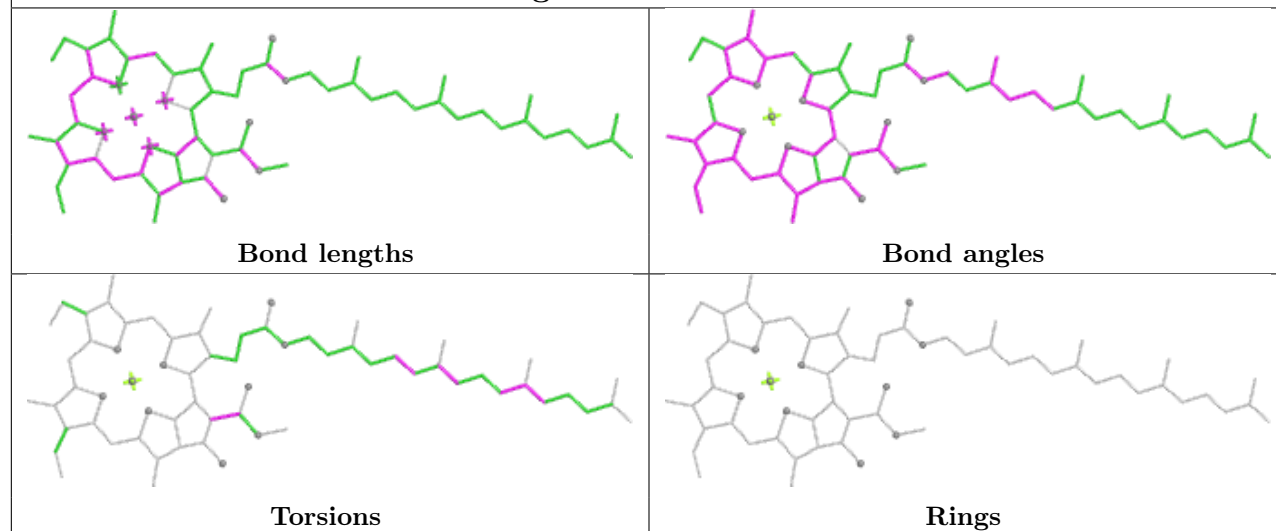




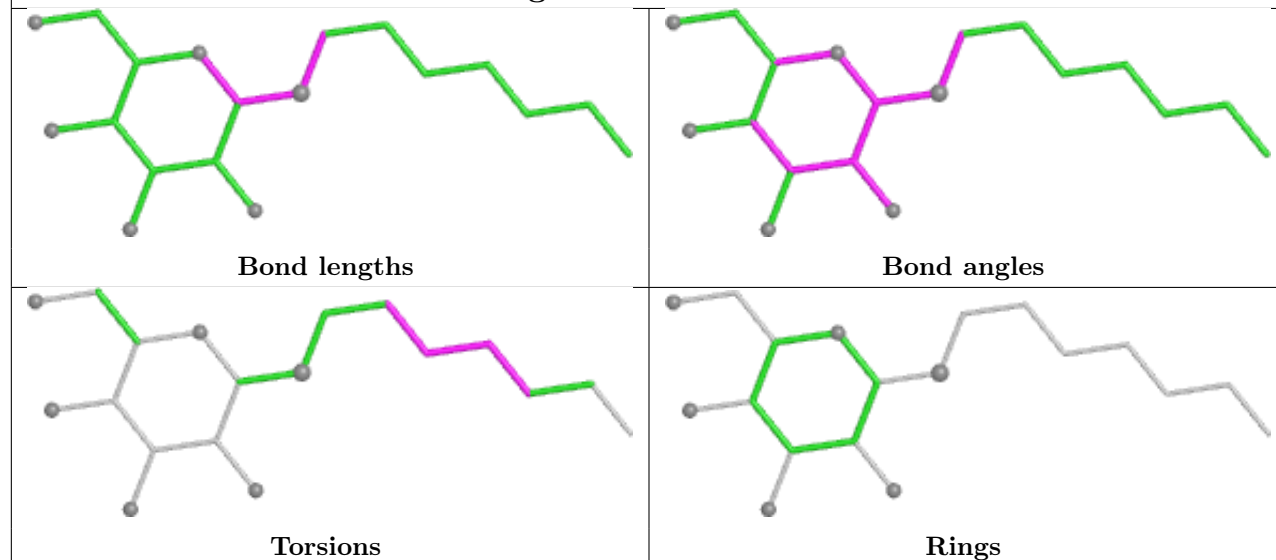
Ligand CLA C 503**Ligand CLA B 614**



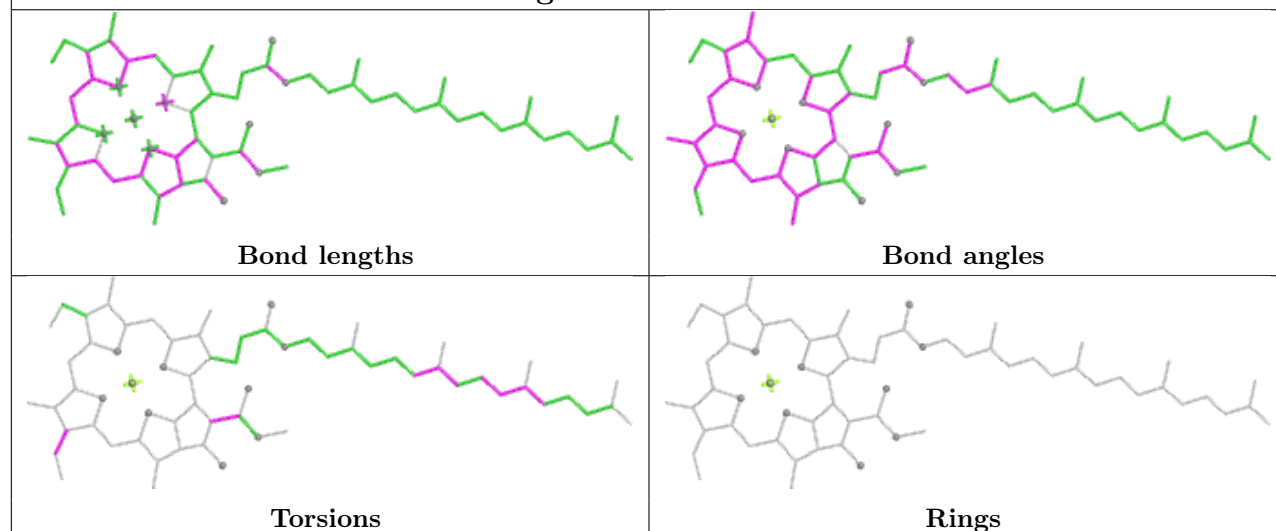
Ligand CLA C 505

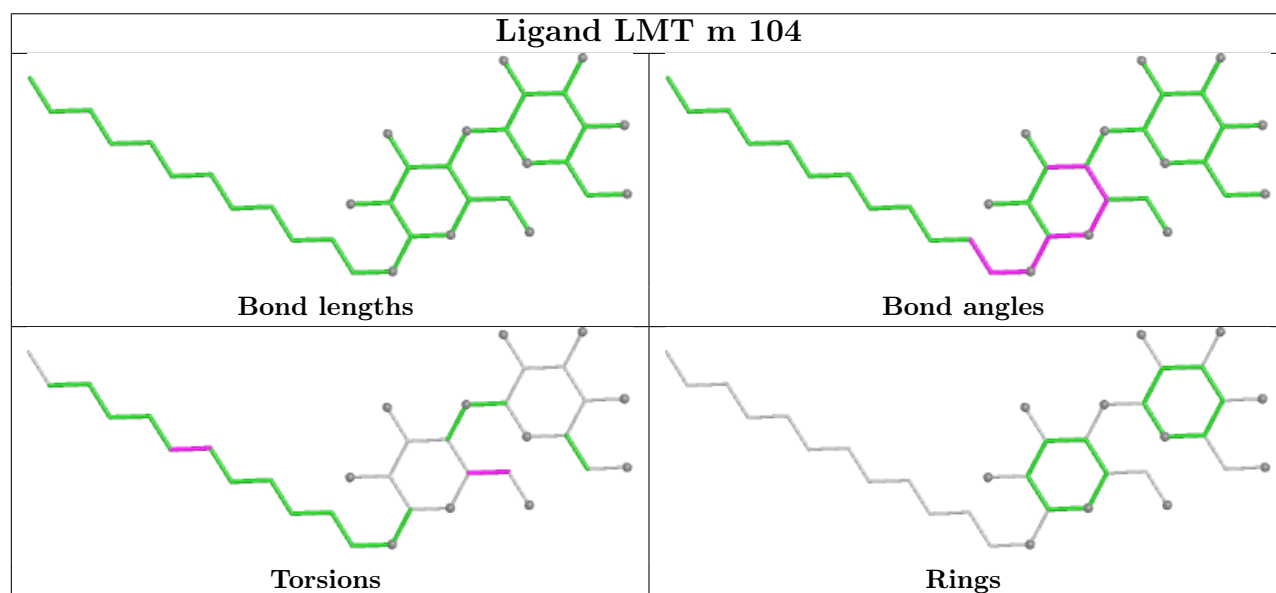
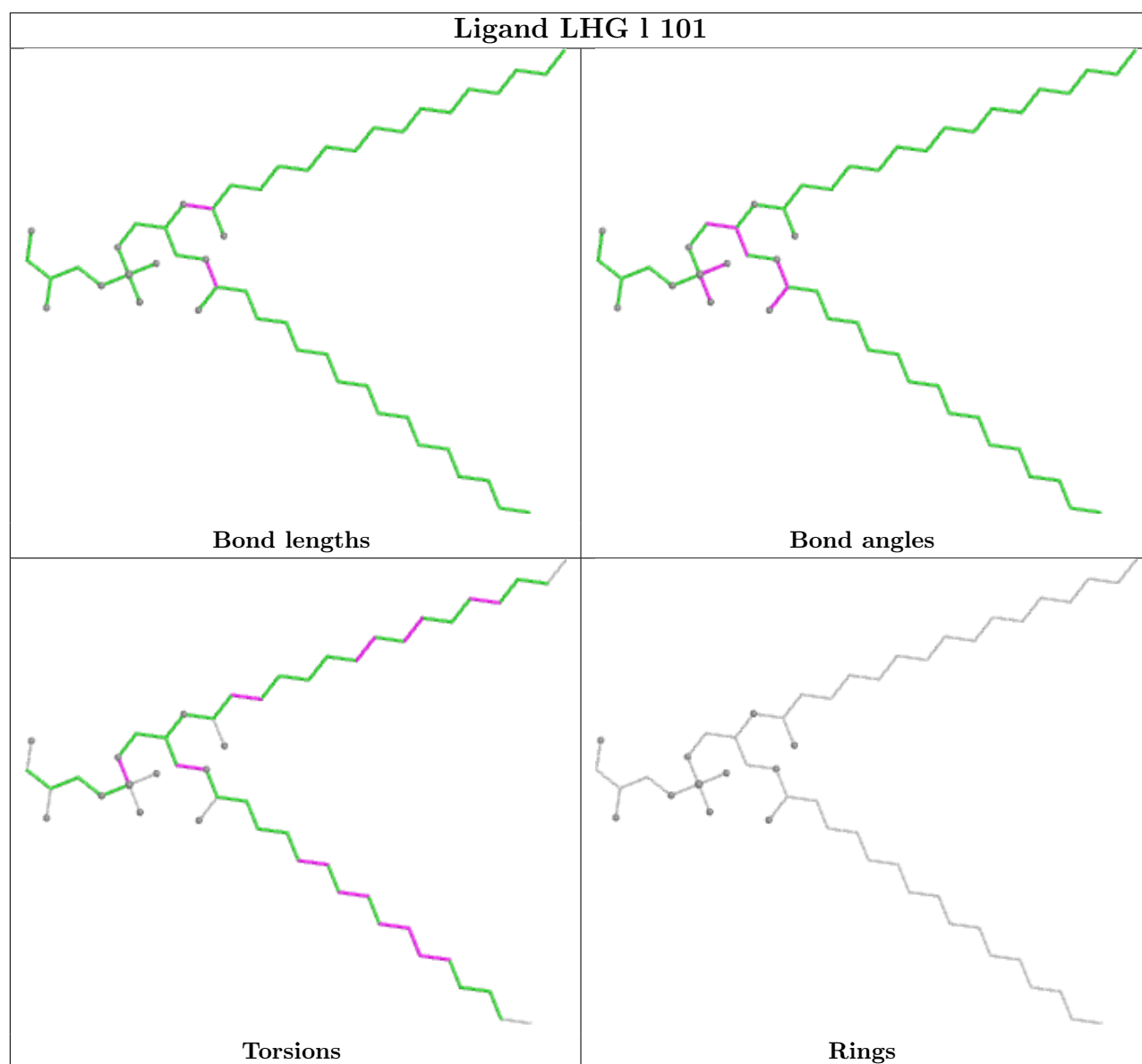


Ligand HTG O 302

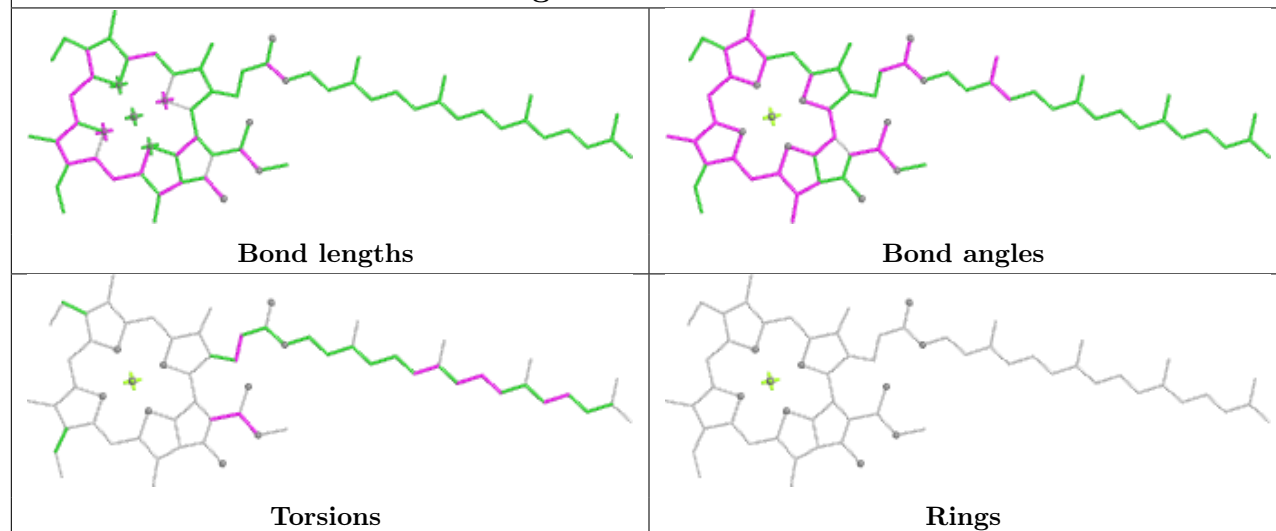


Ligand CLA a 407

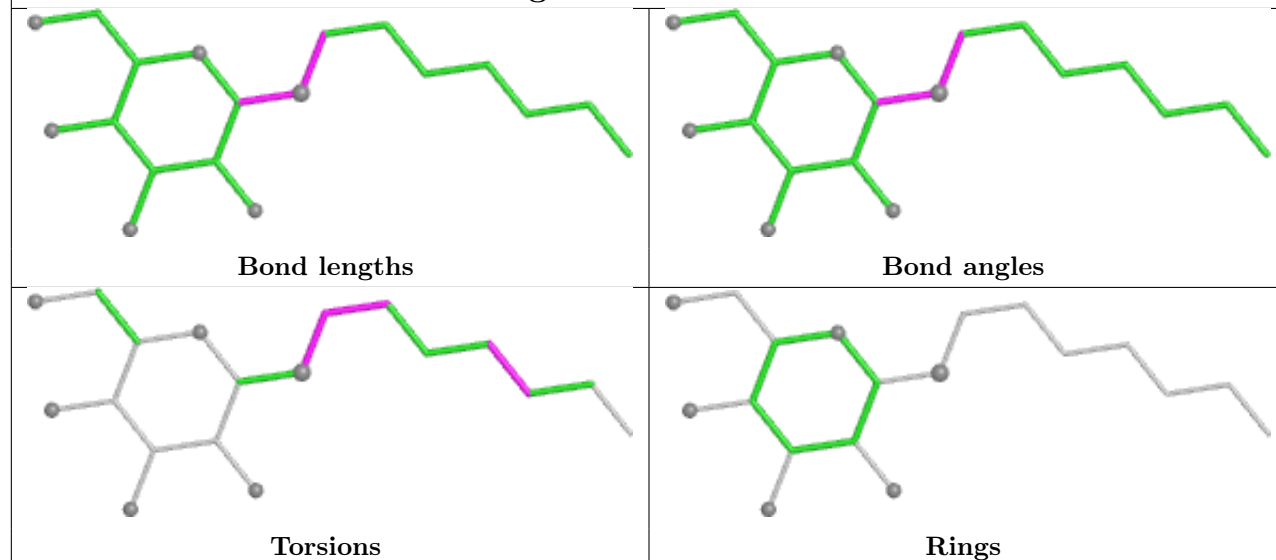




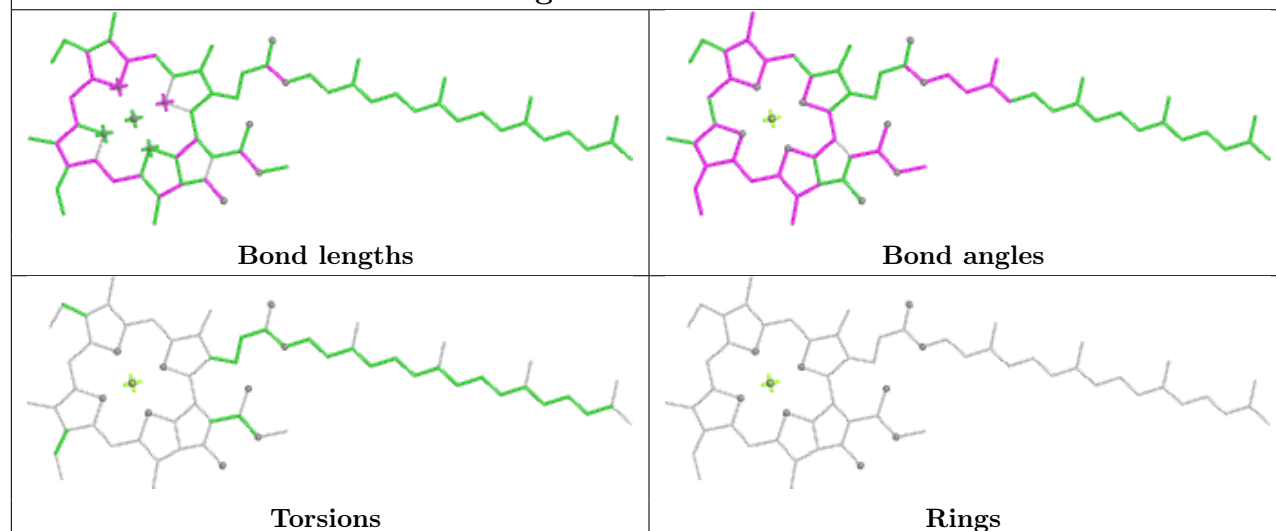
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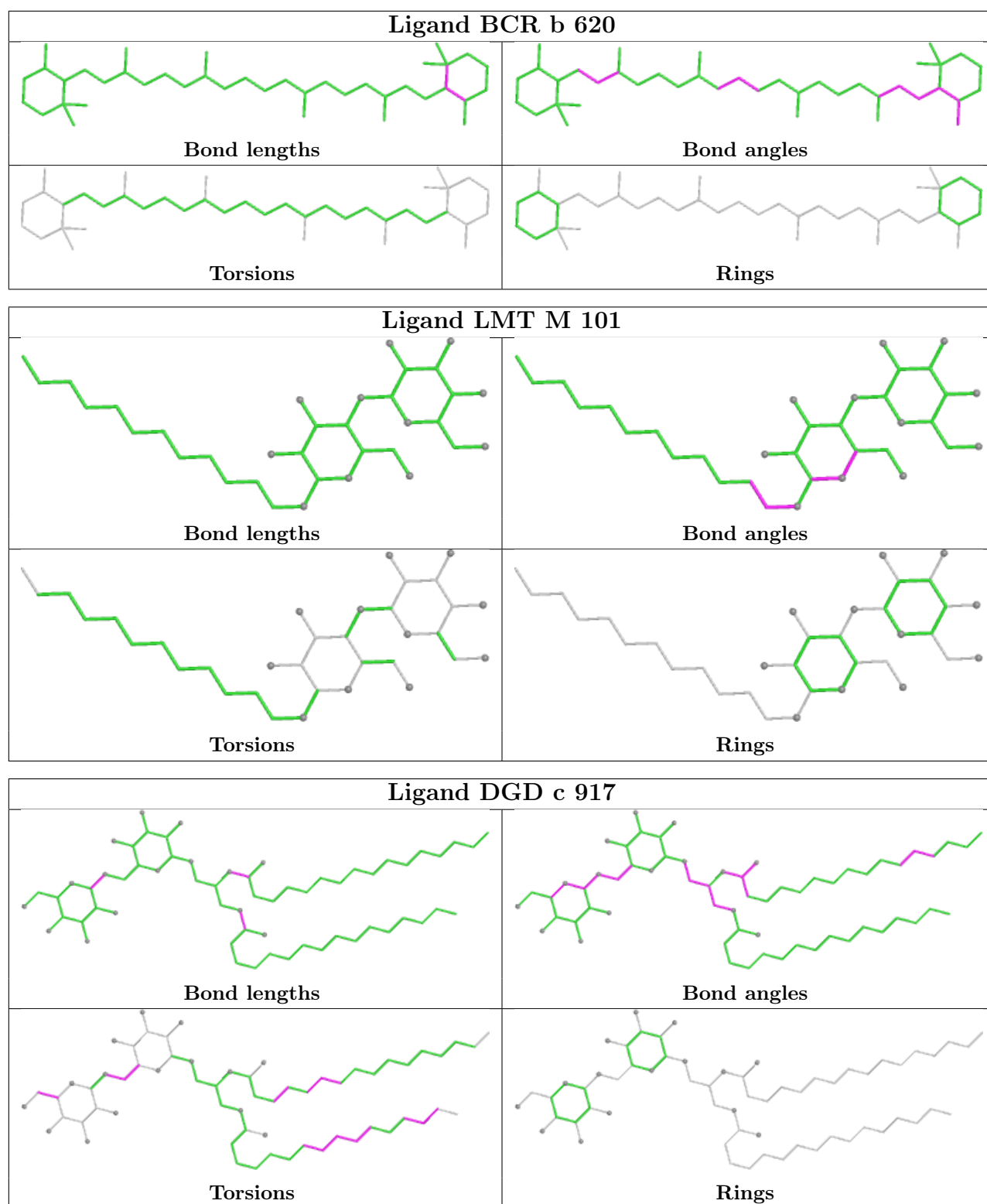


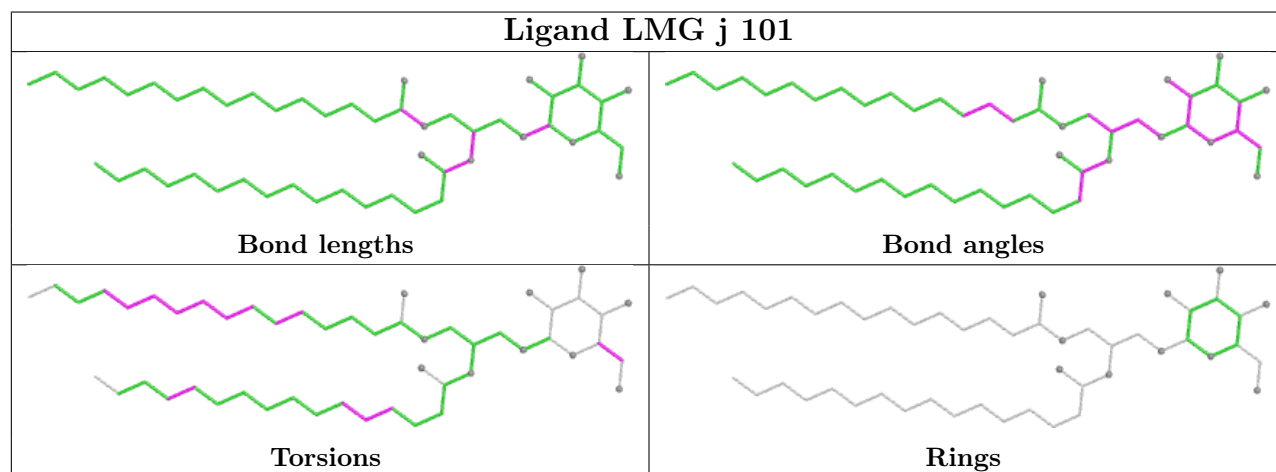
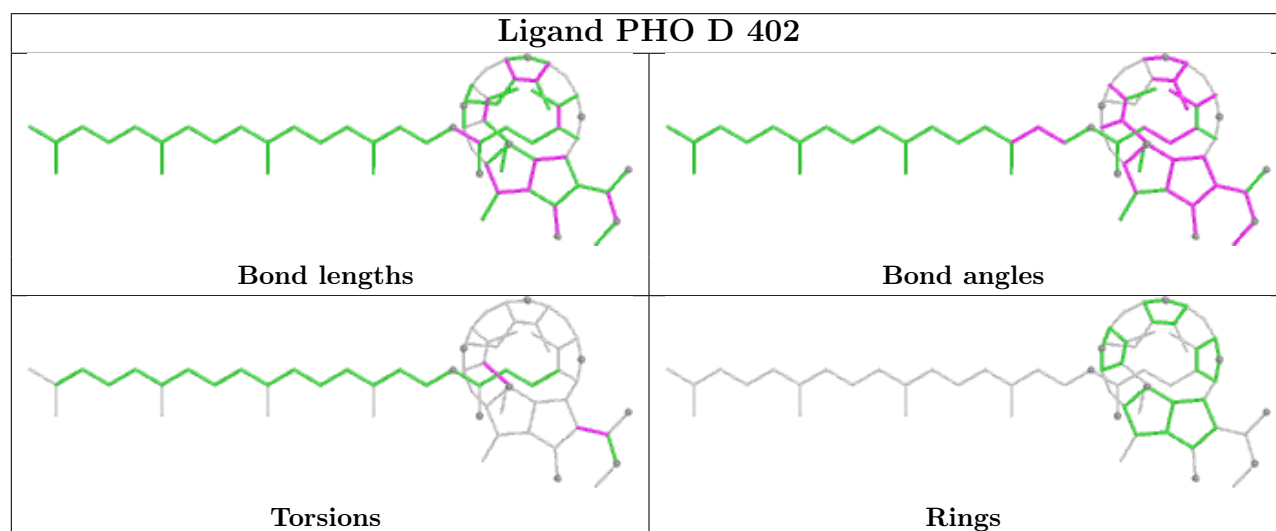
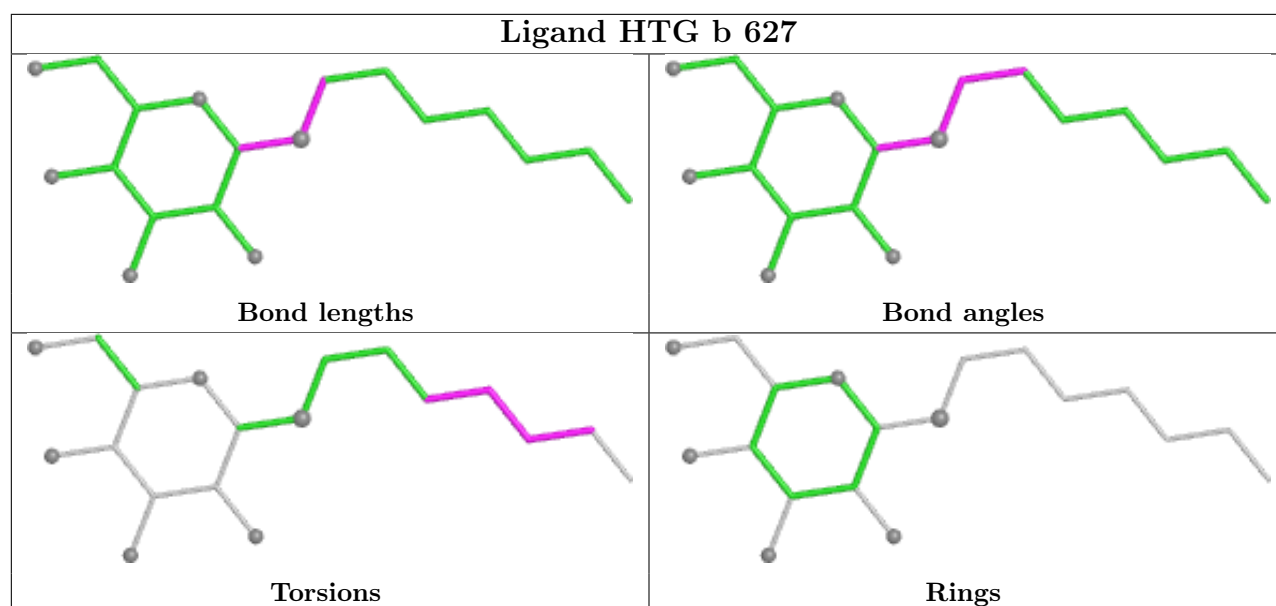
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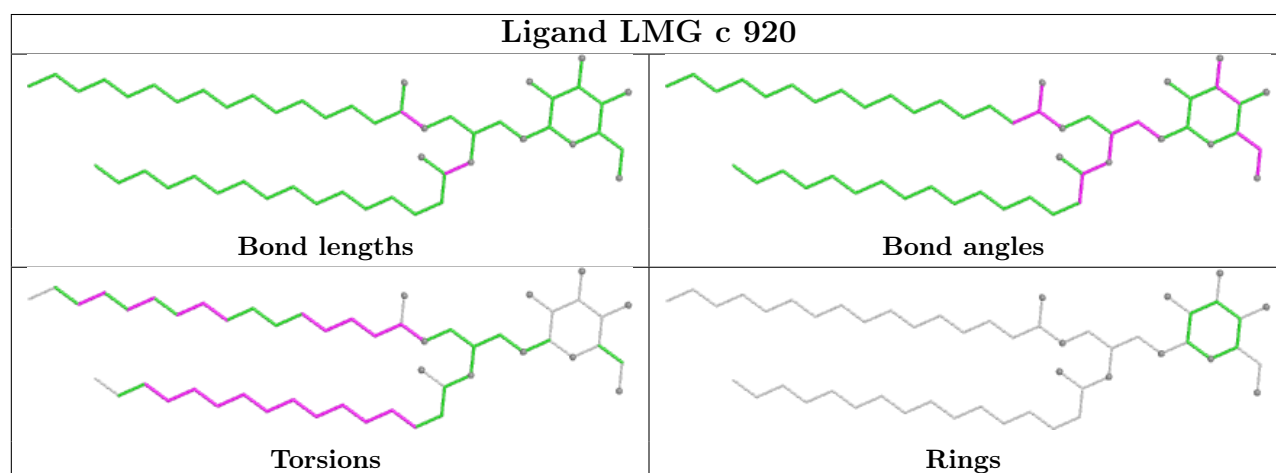
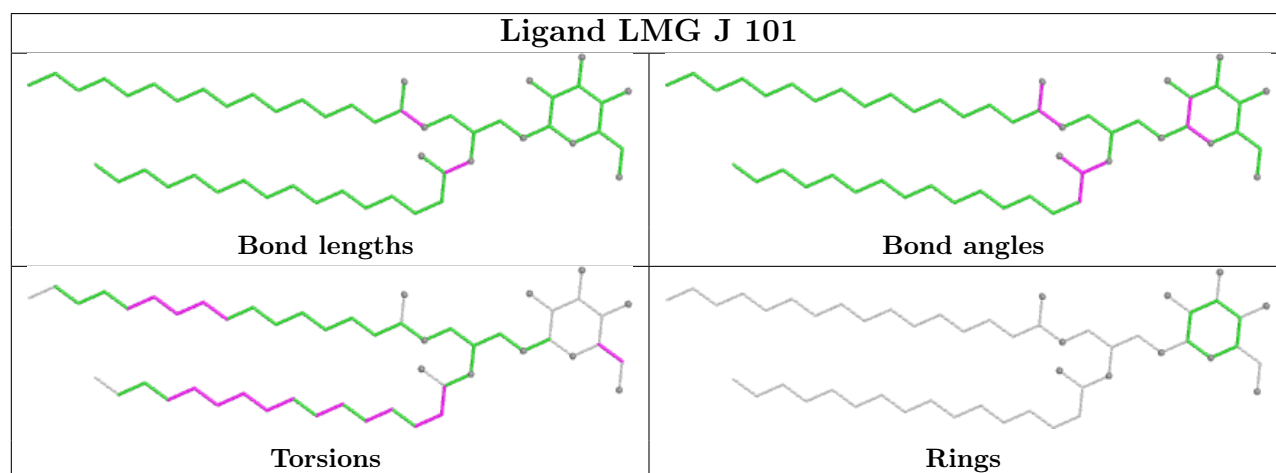
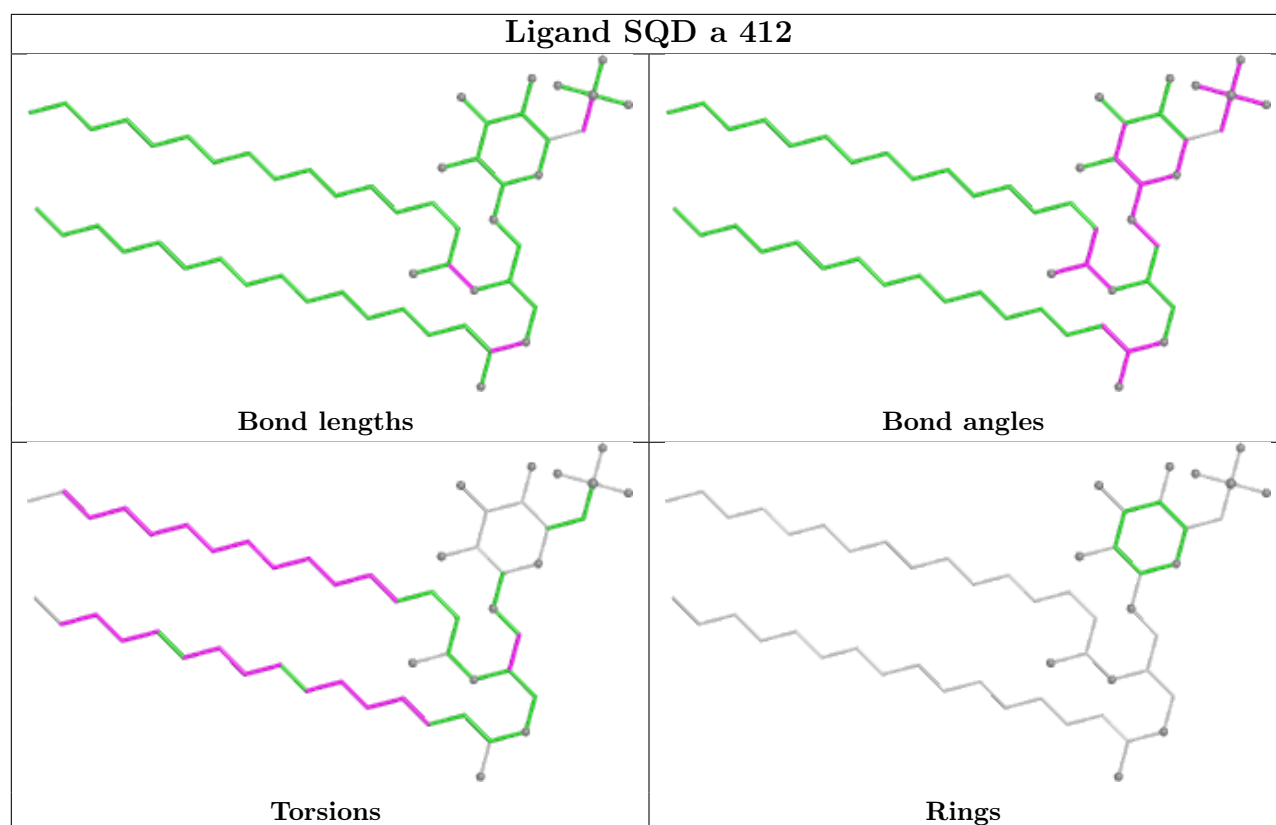


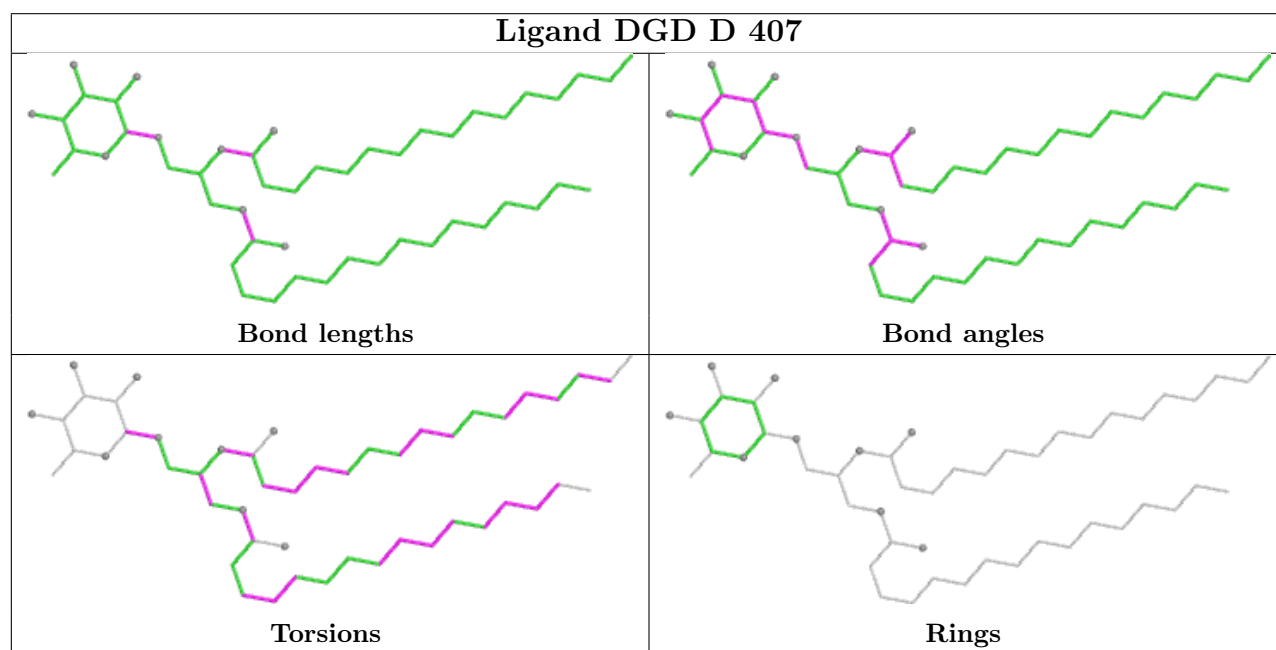
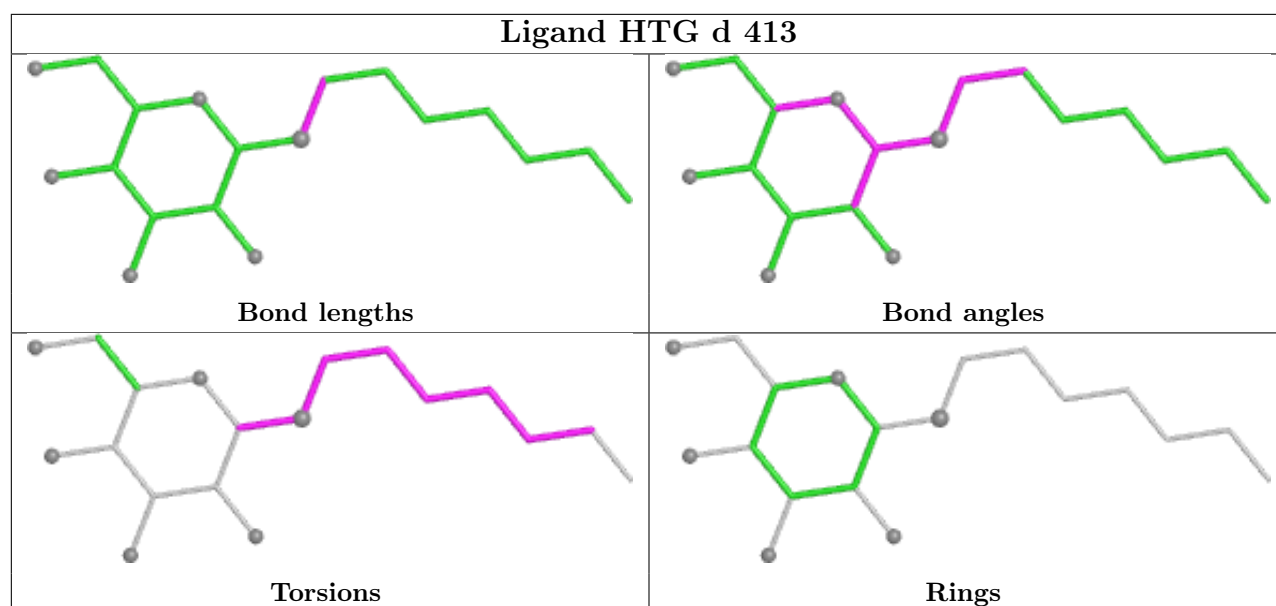
Ligand CLA b 610



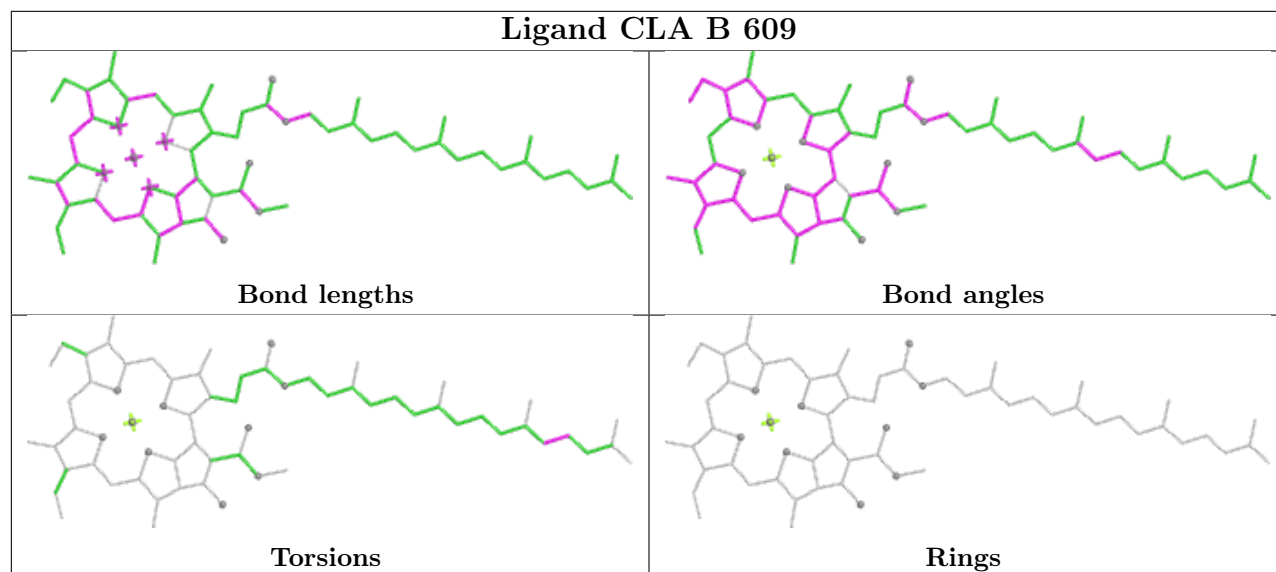




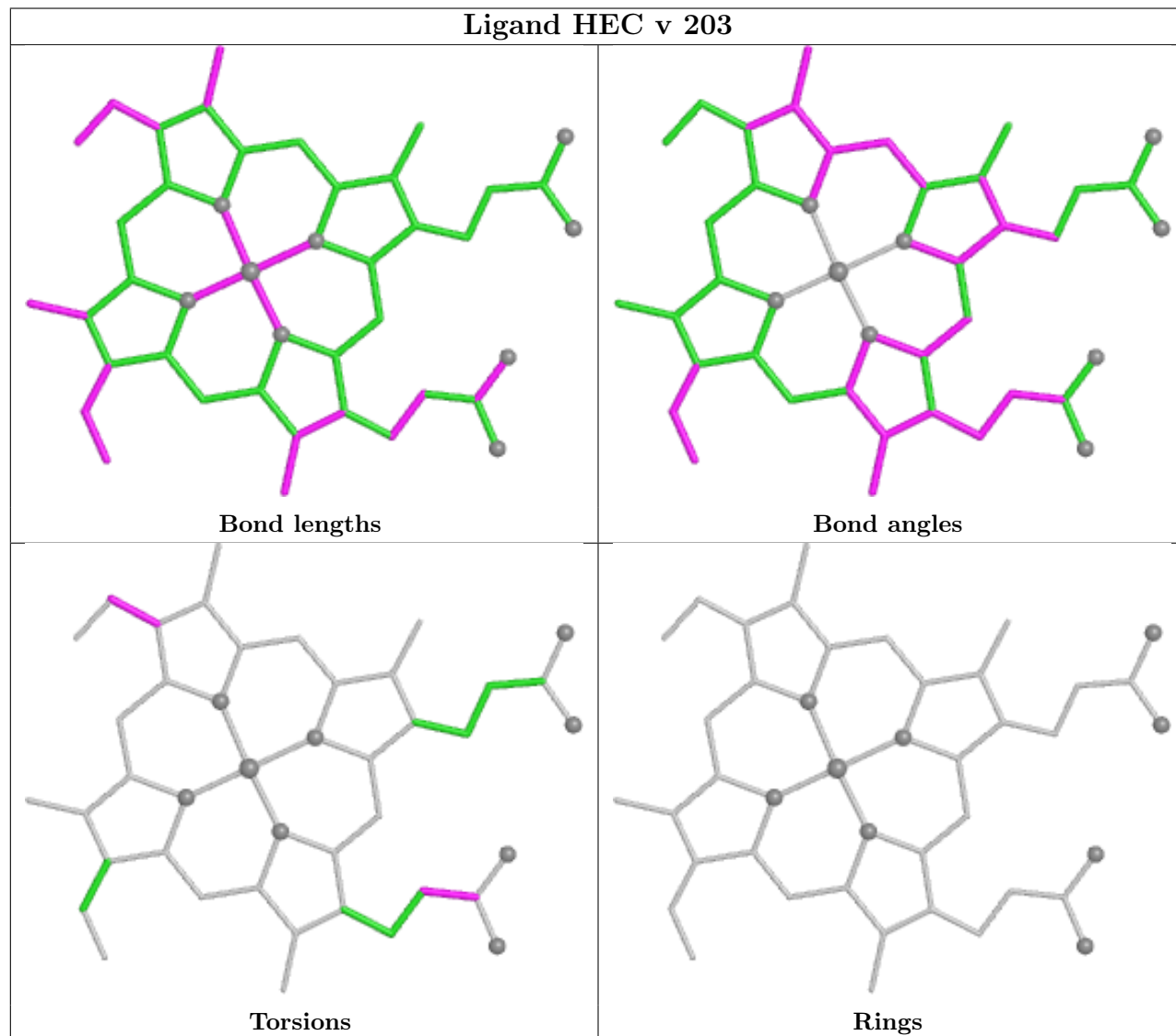


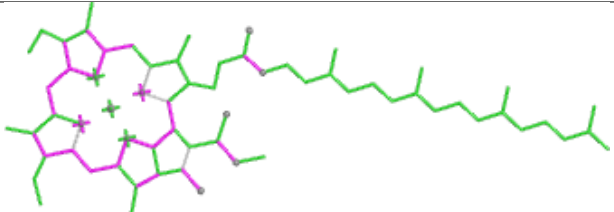
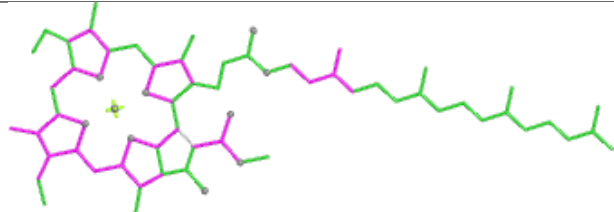
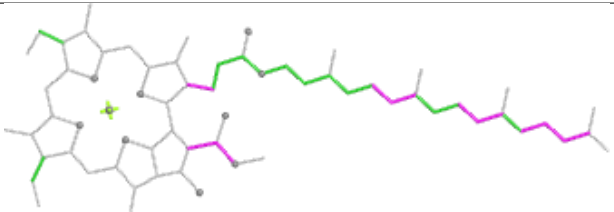
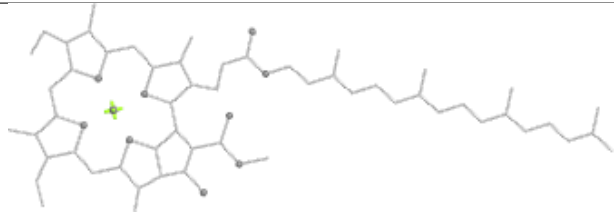


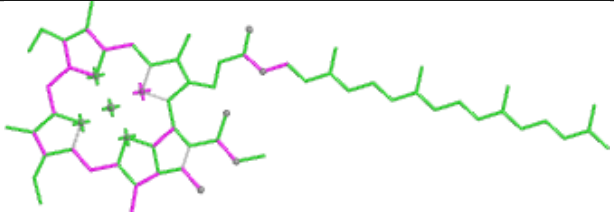
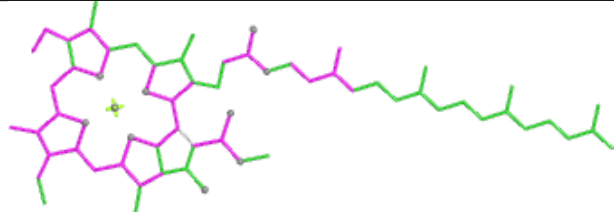
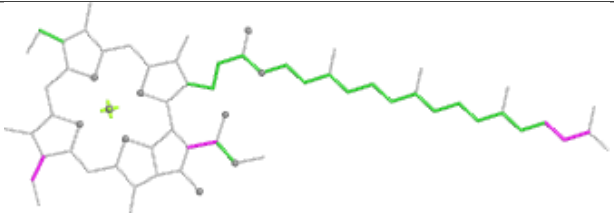
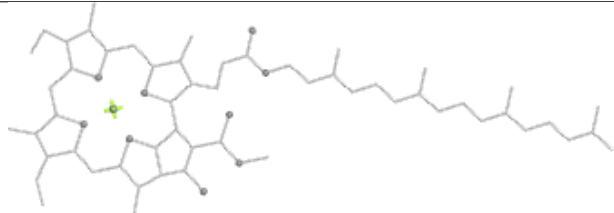
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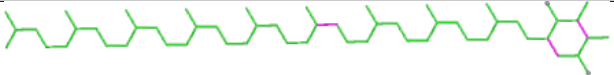
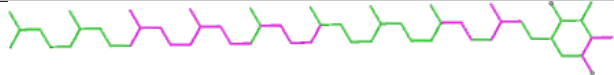
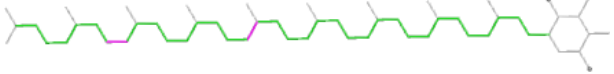
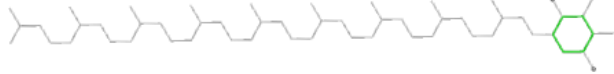


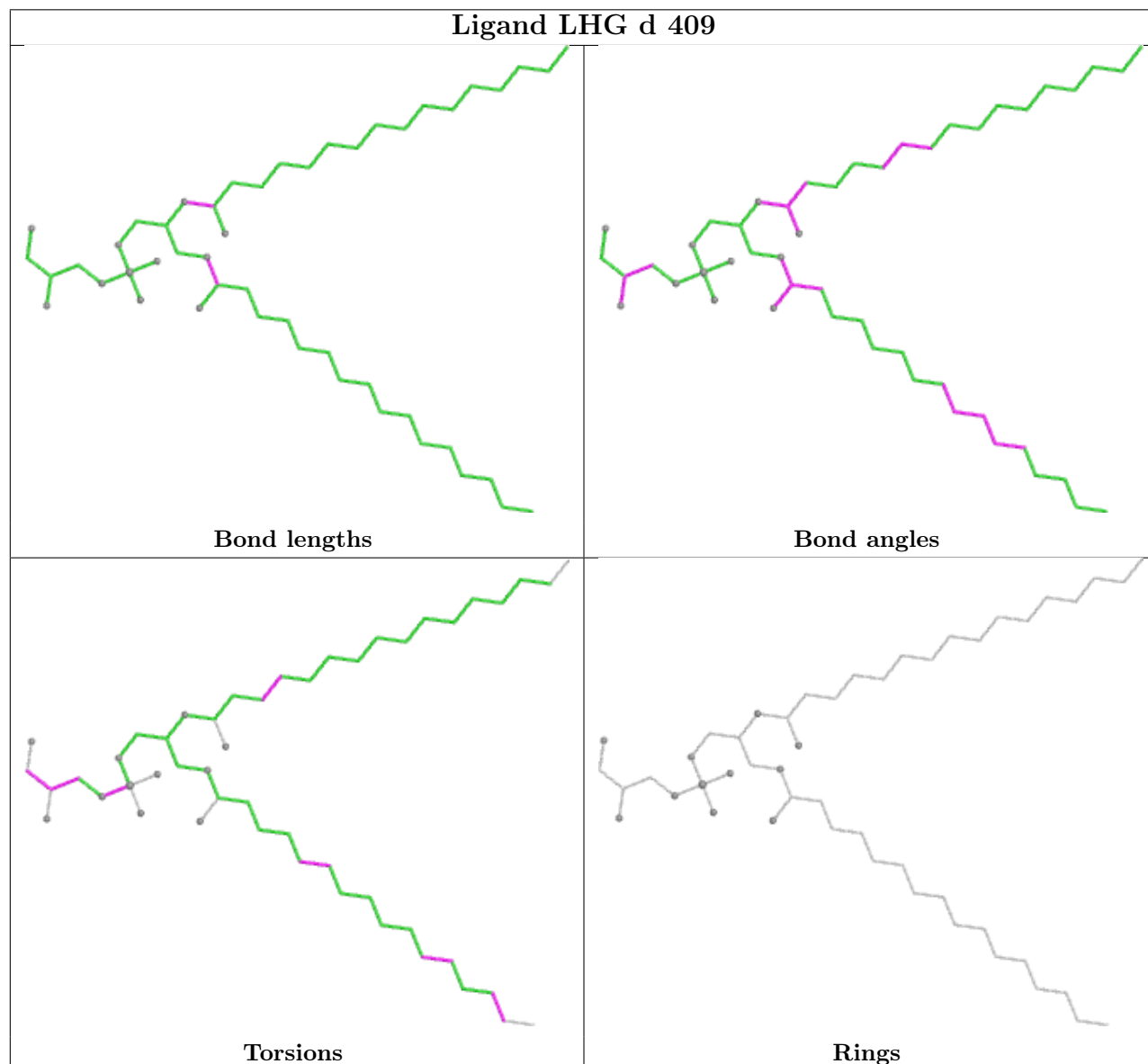
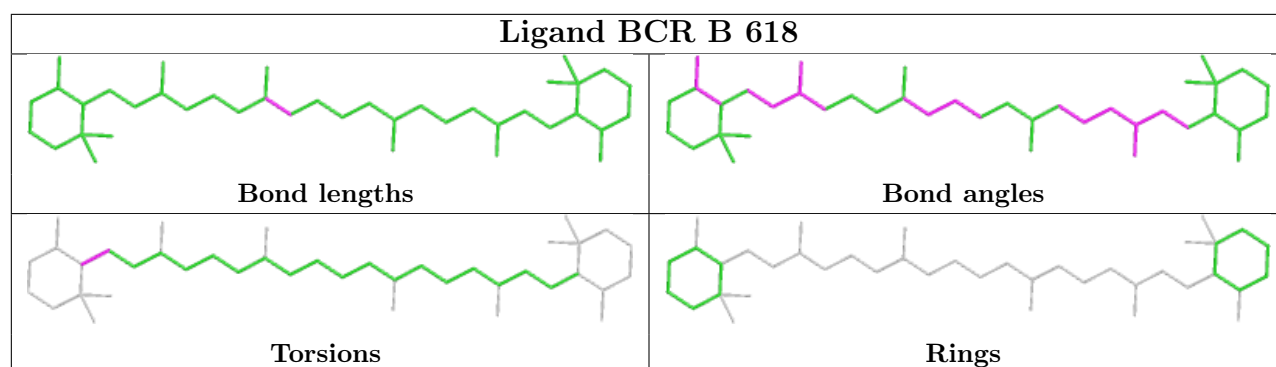
Ligand HEC v 203

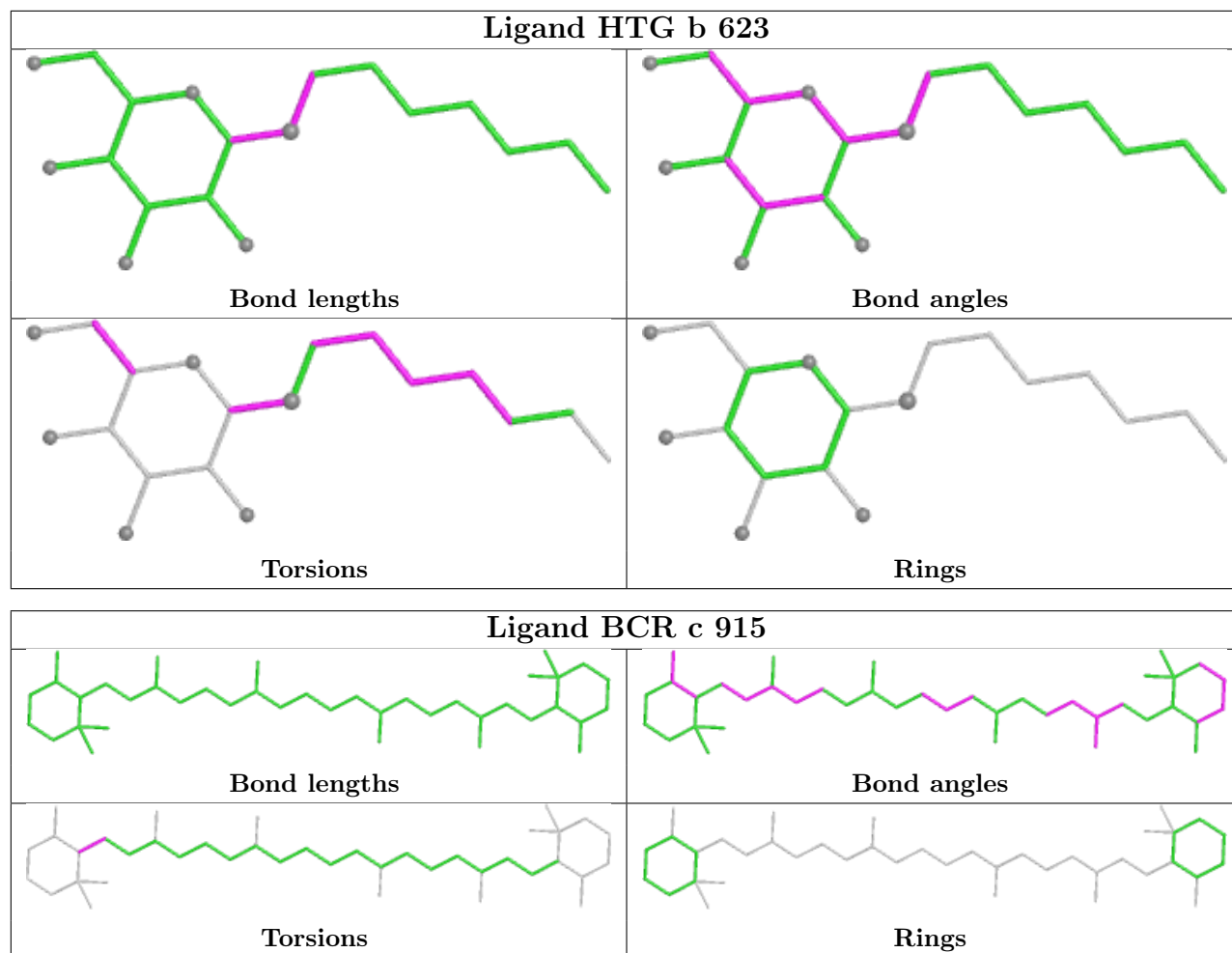


Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

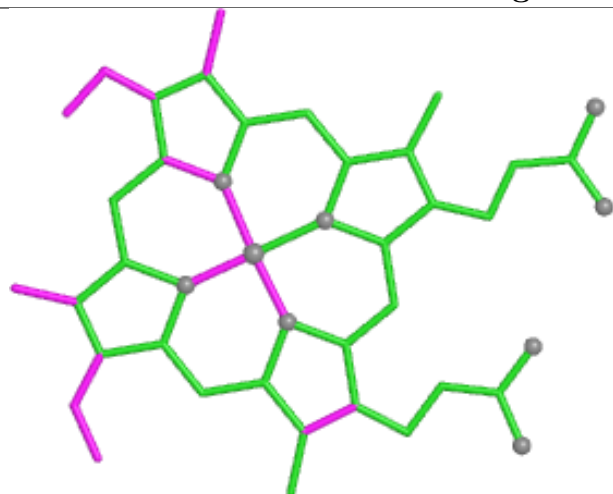
Ligand CLA a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

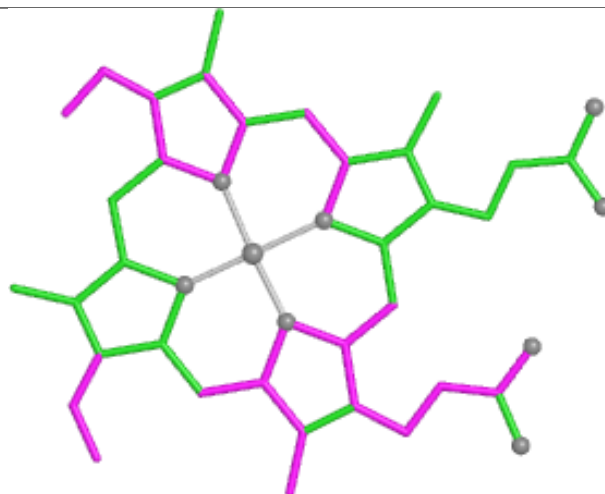




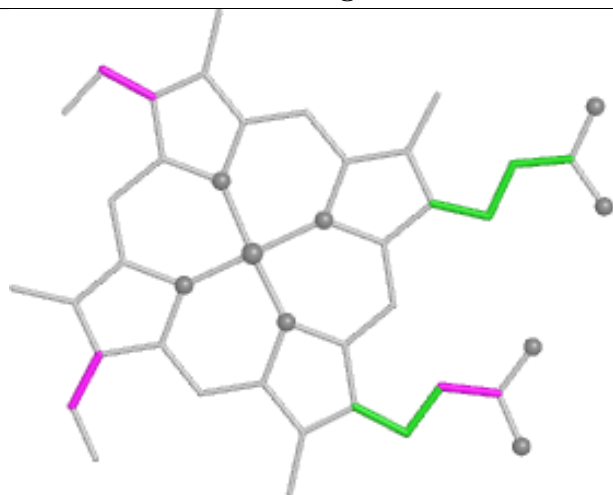
Ligand HEC V 203



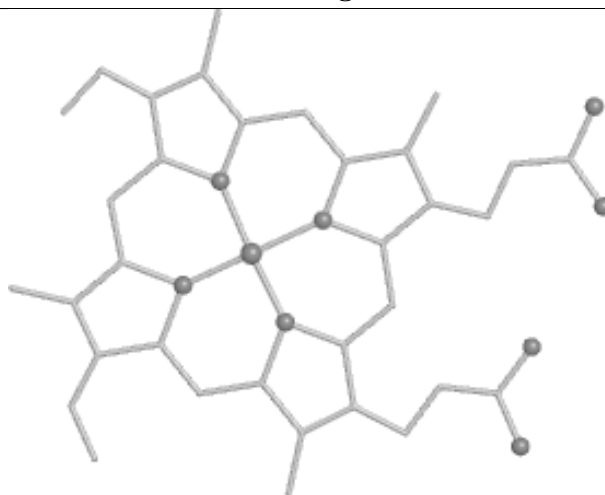
Bond lengths



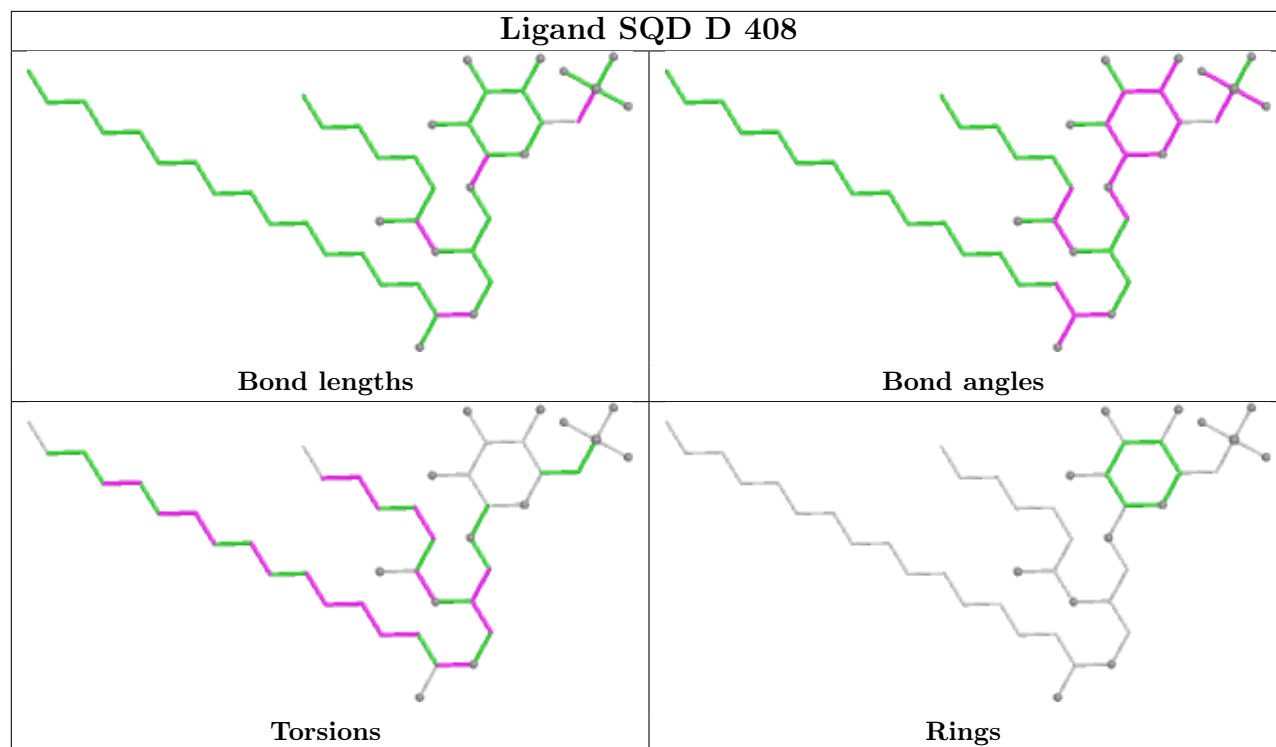
Bond angles



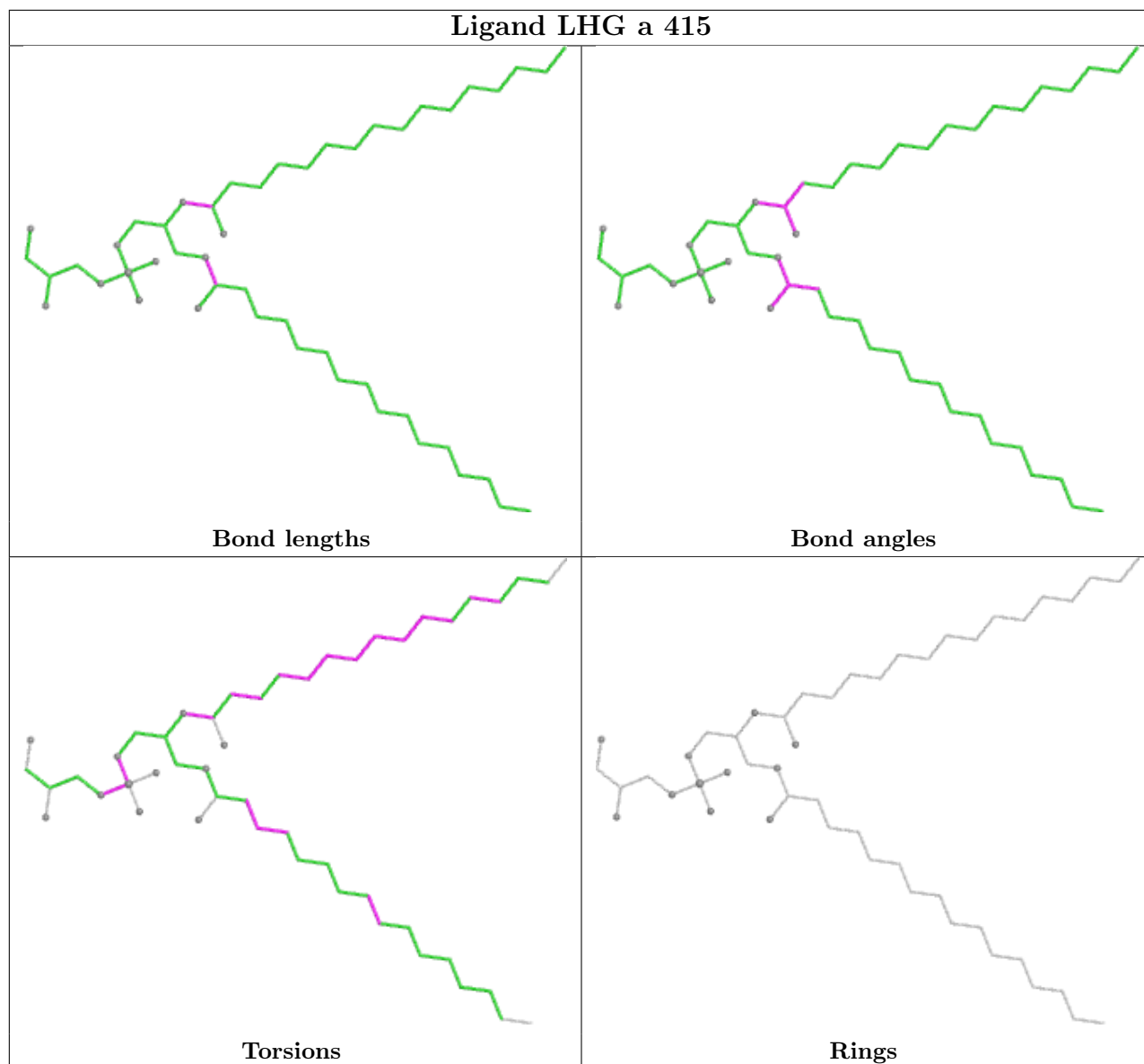
Torsions



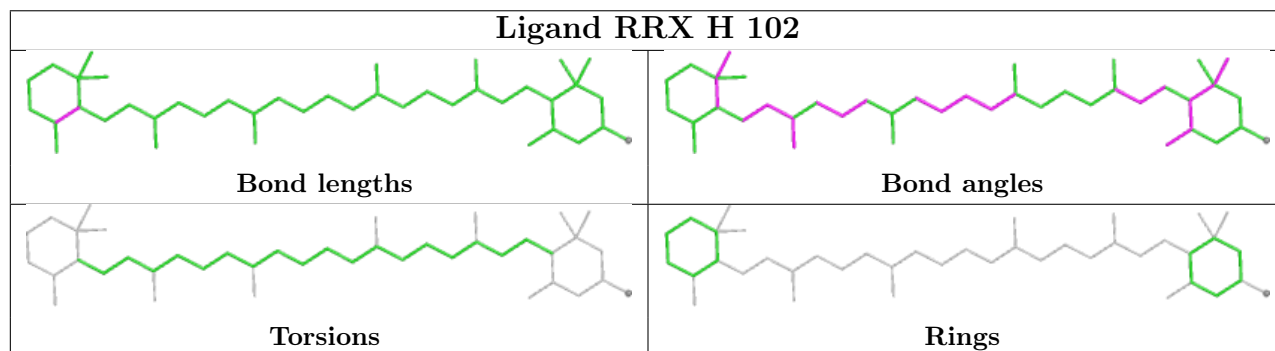
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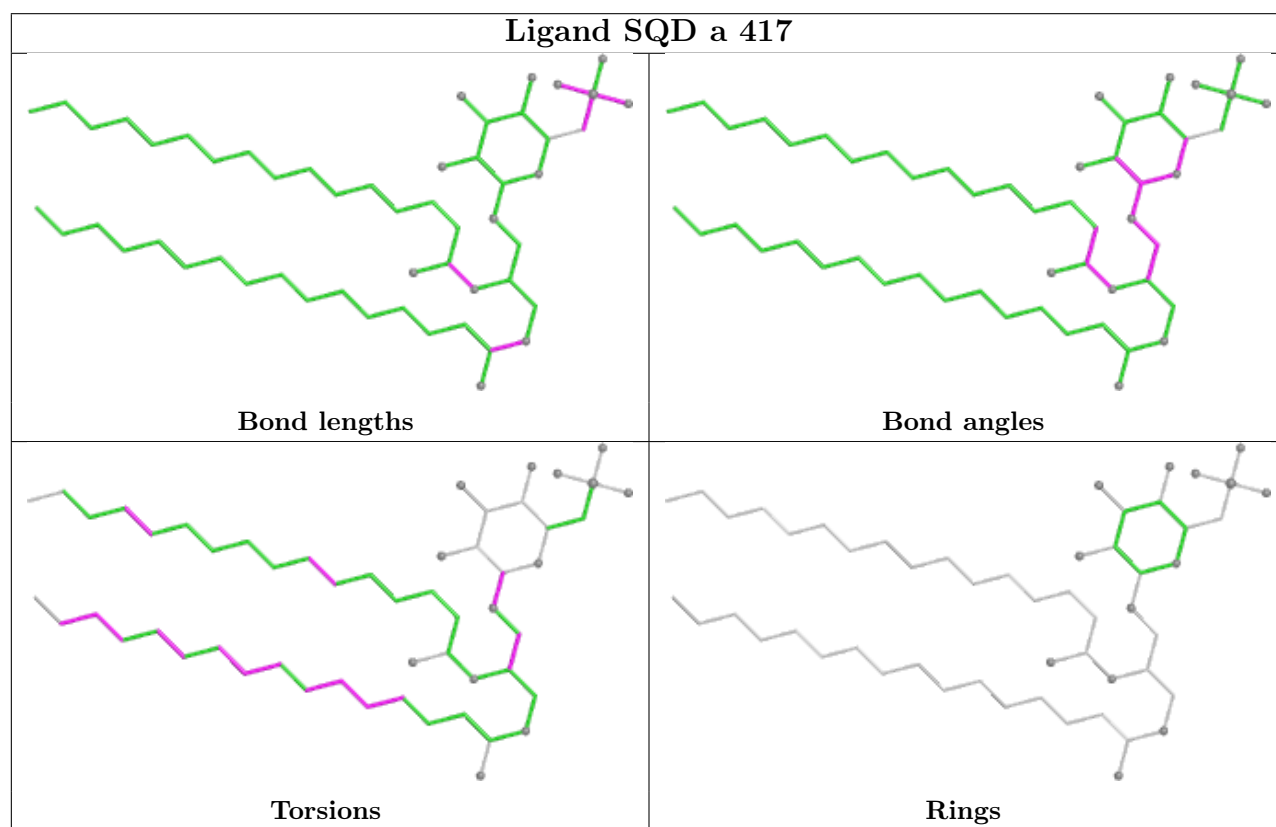
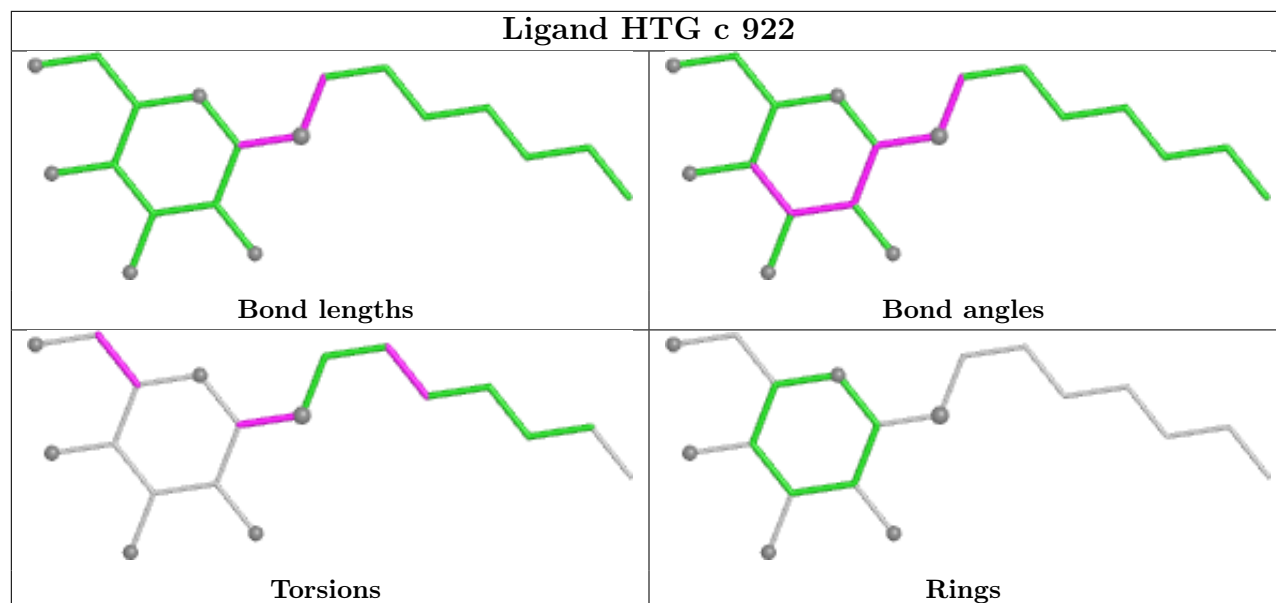


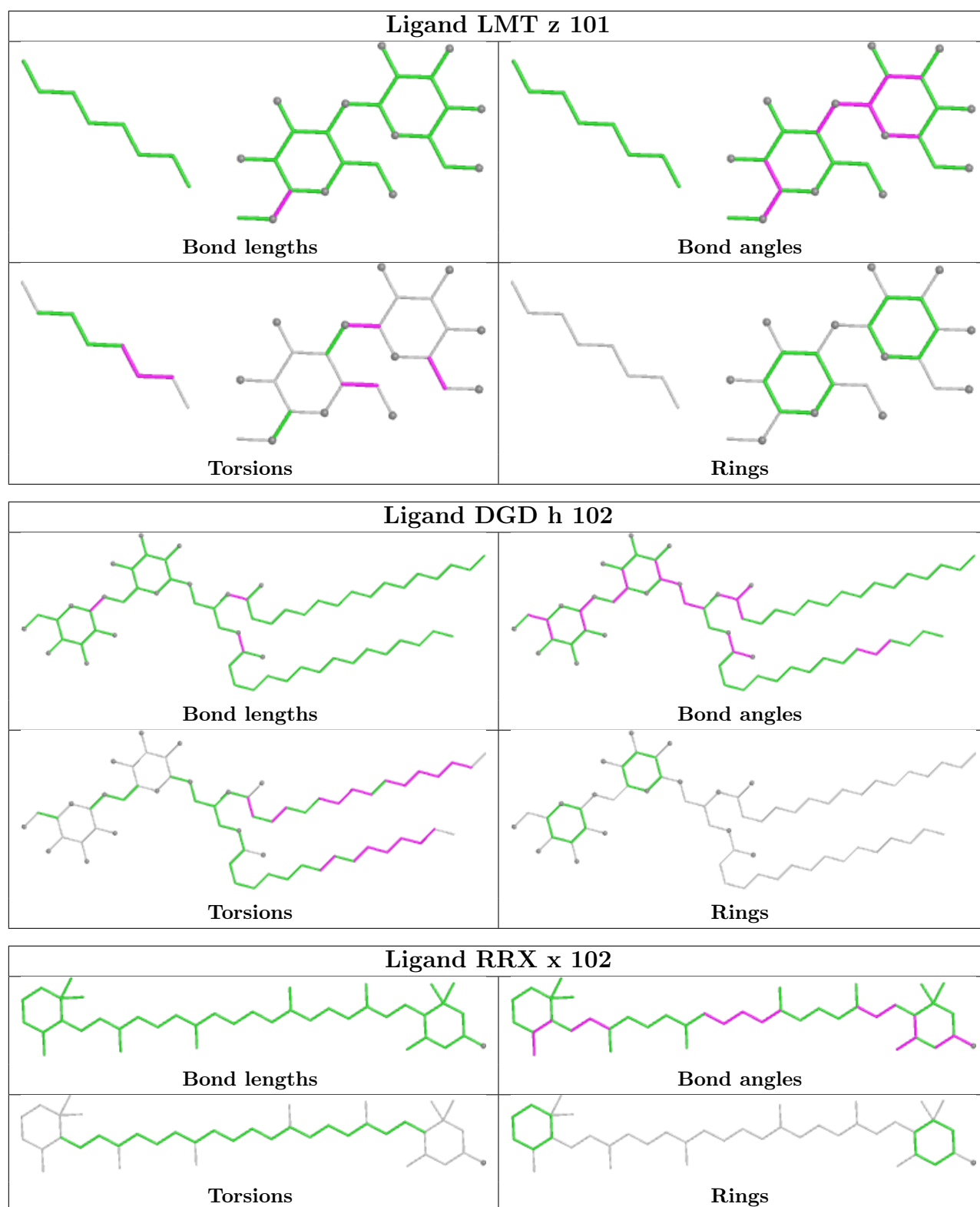
Ligand LHG a 415

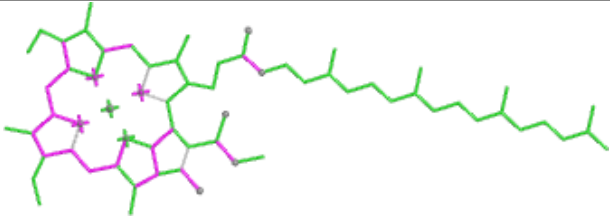
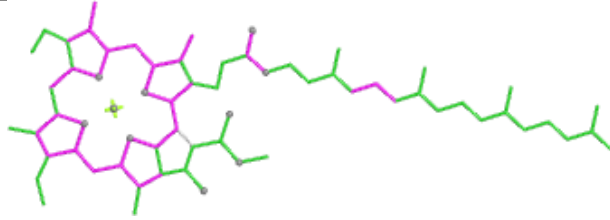
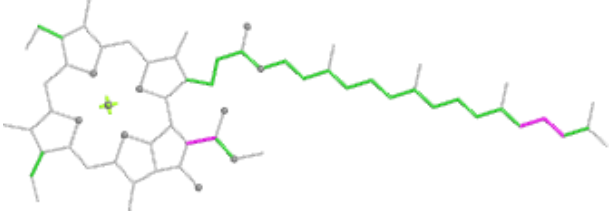
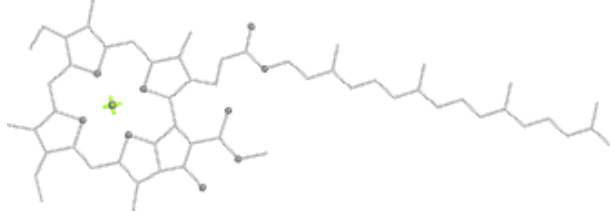
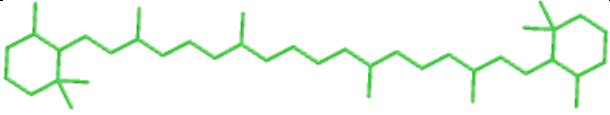
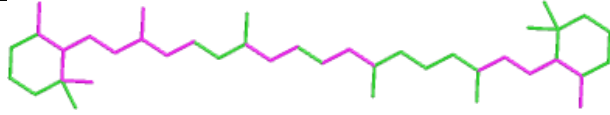
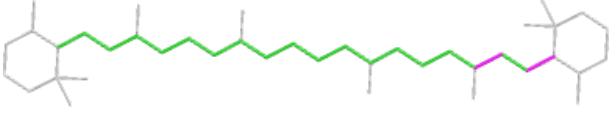
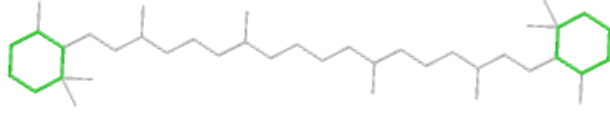
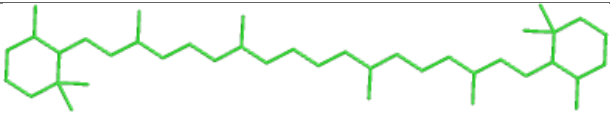
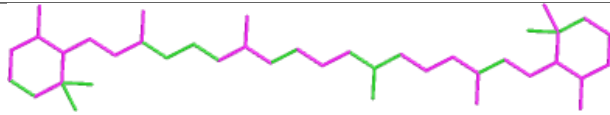
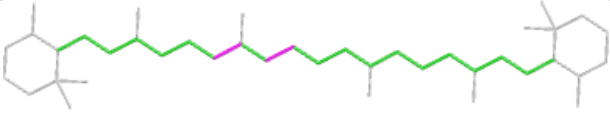
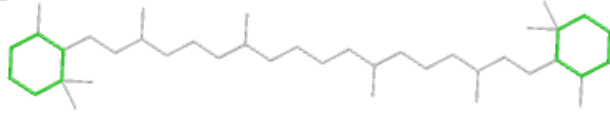


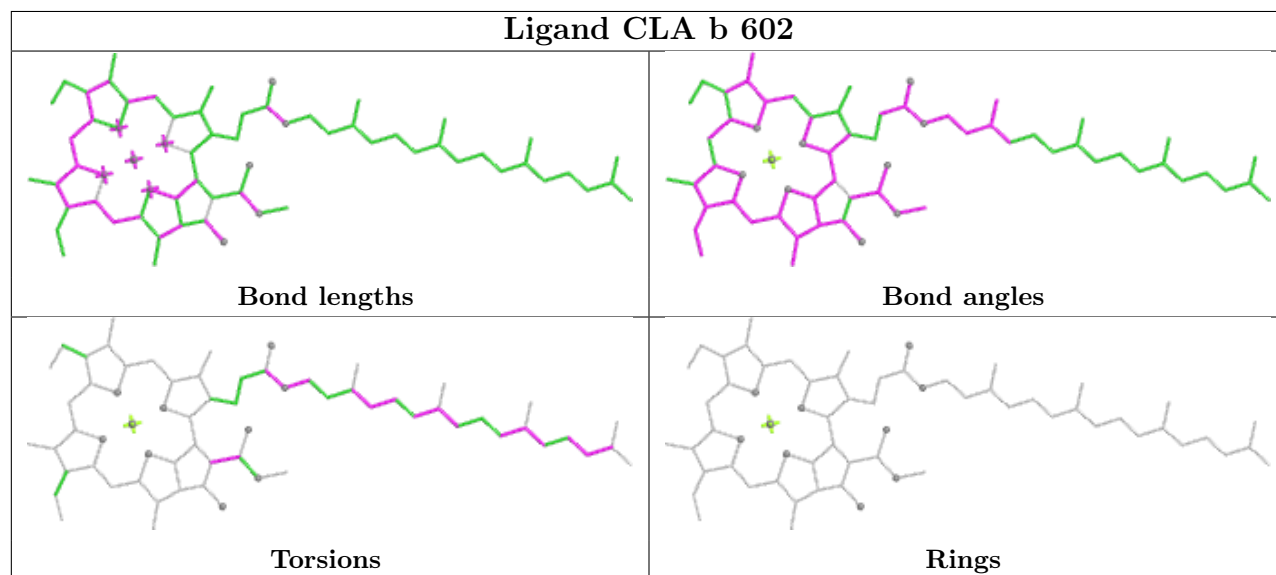
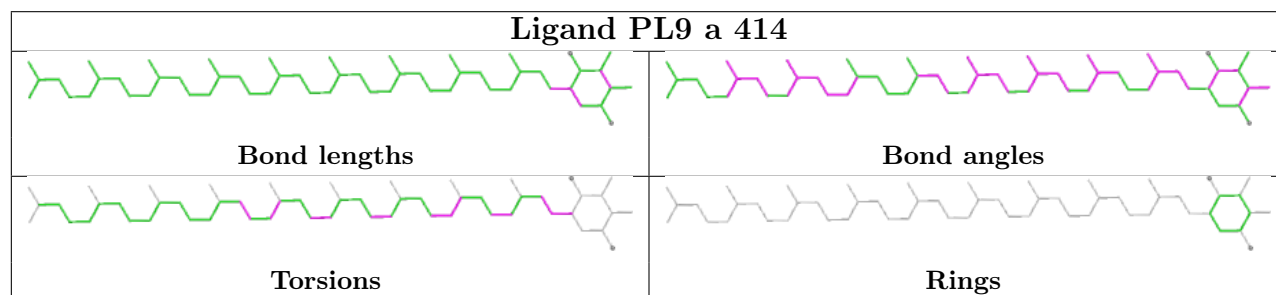
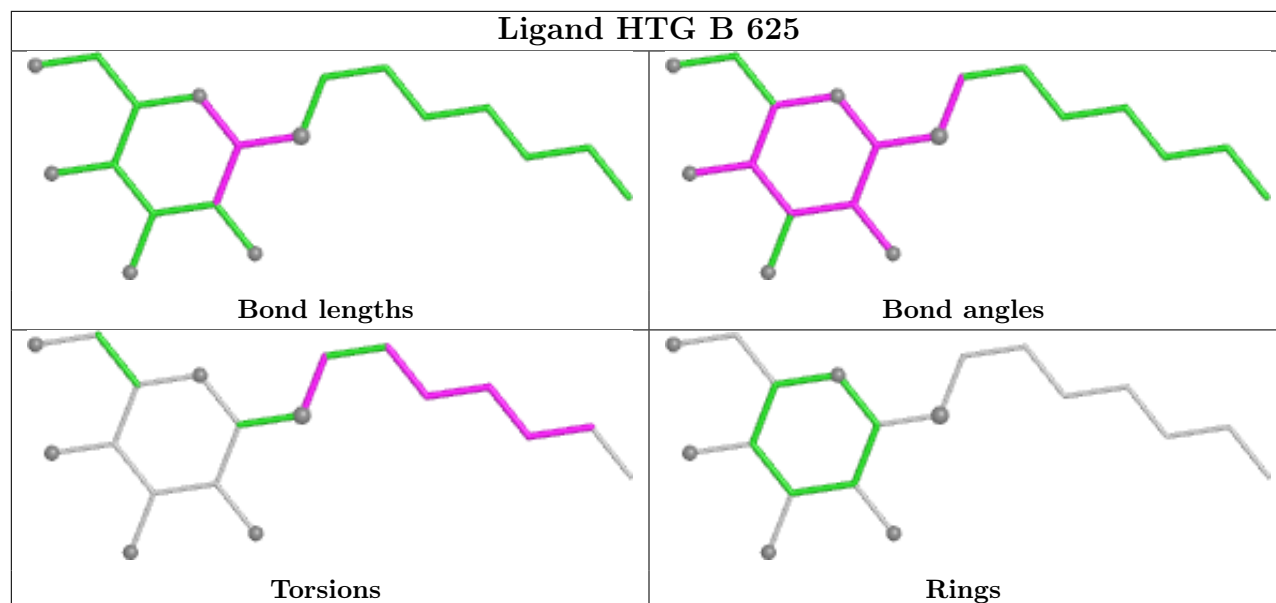
Ligand RRX H 102



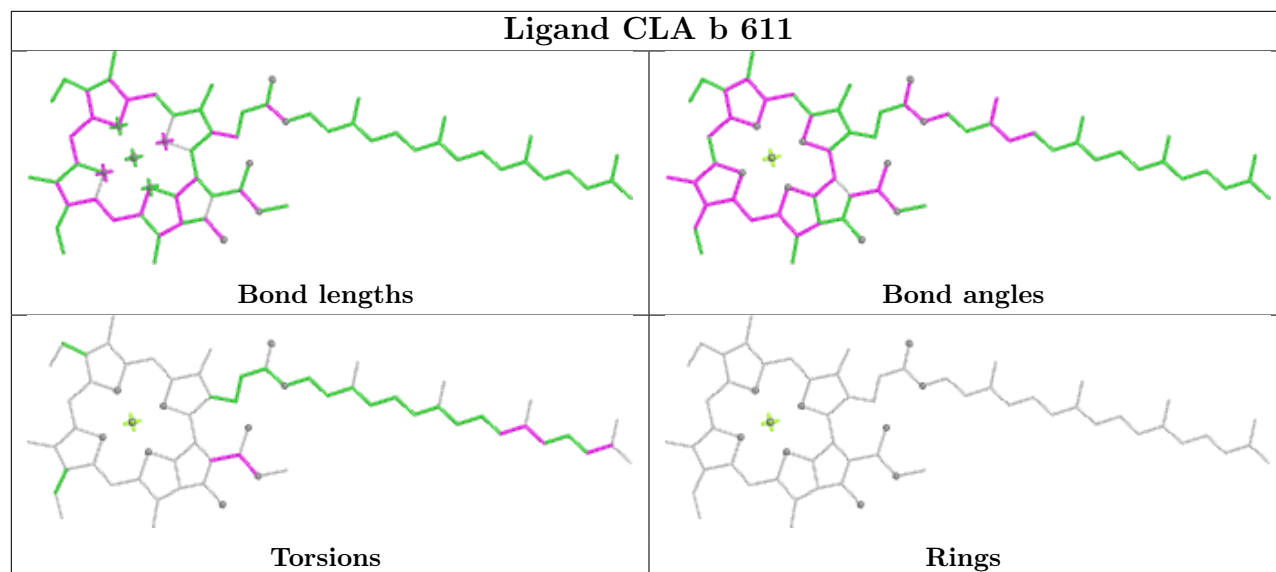




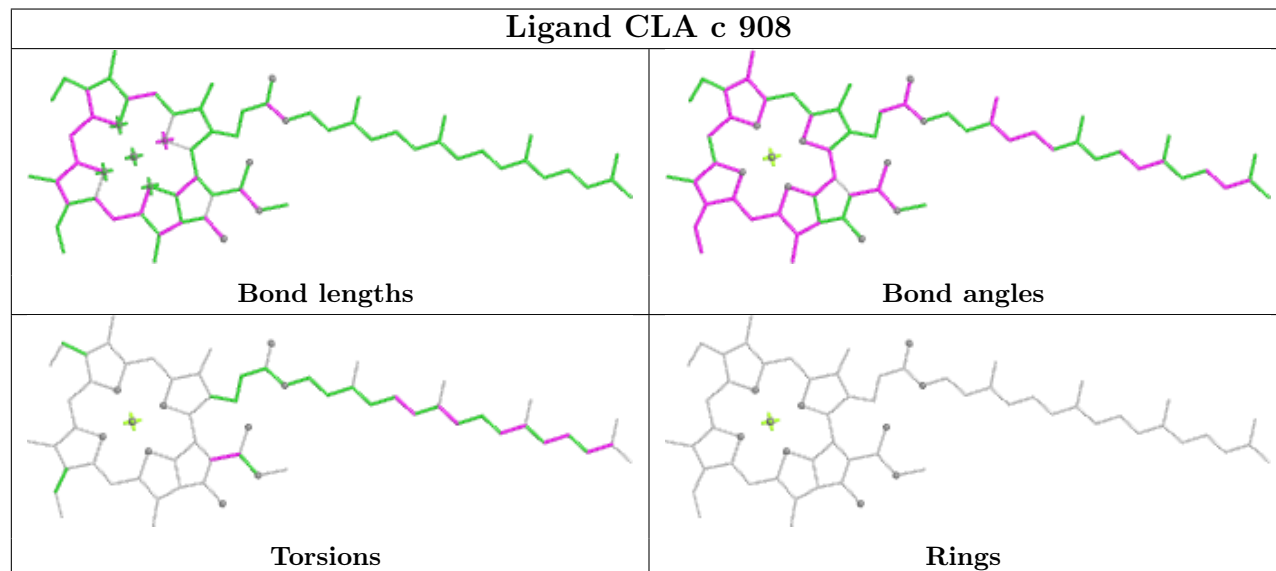
Ligand CLA c 909	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



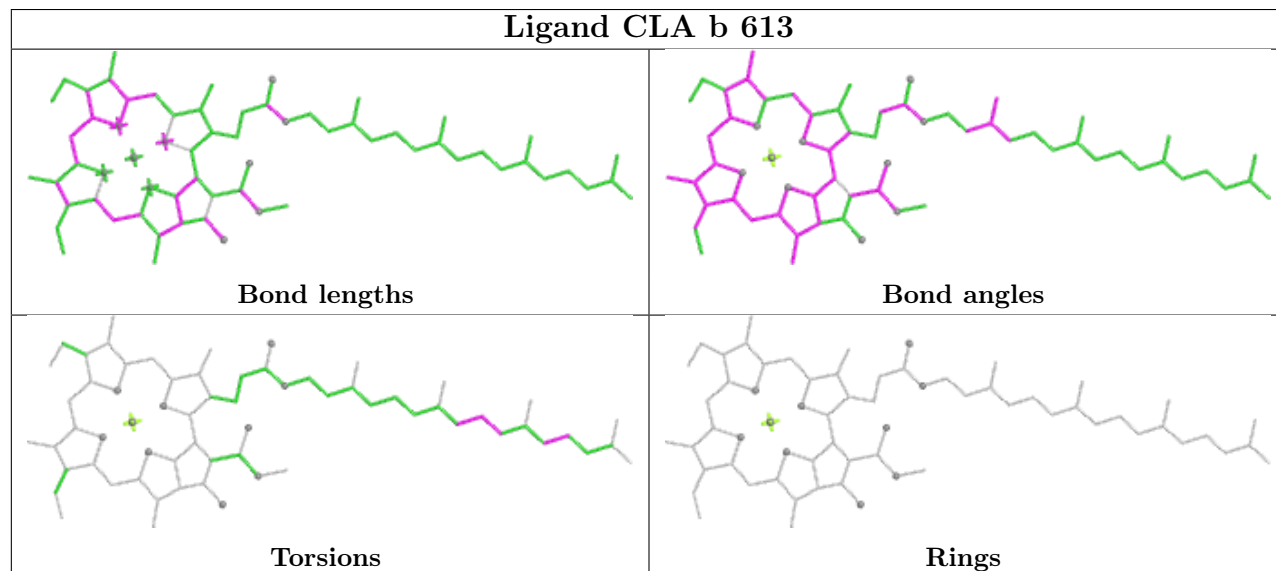
Ligand CLA b 611



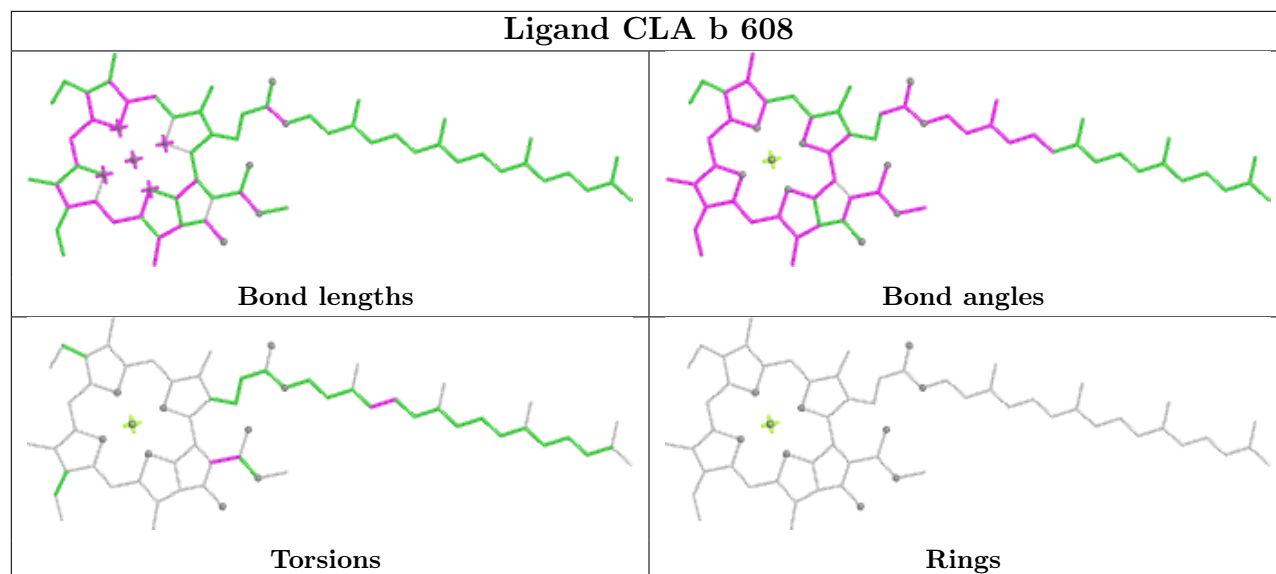
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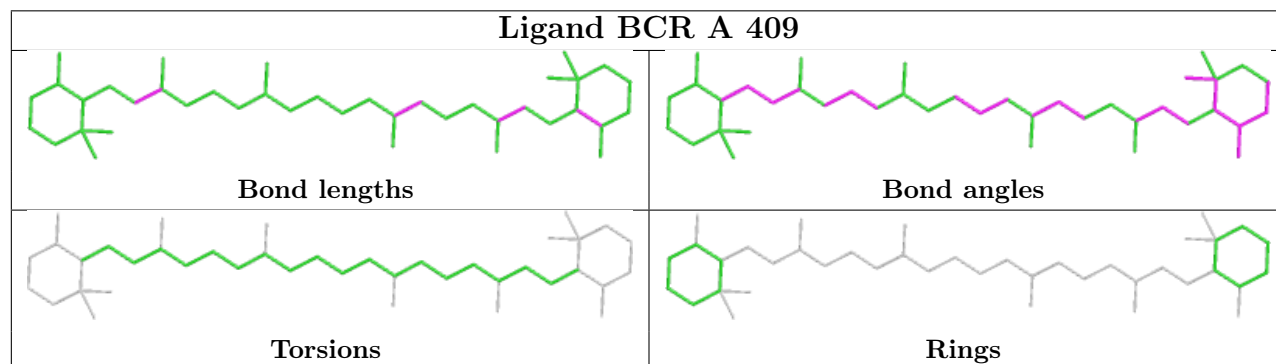
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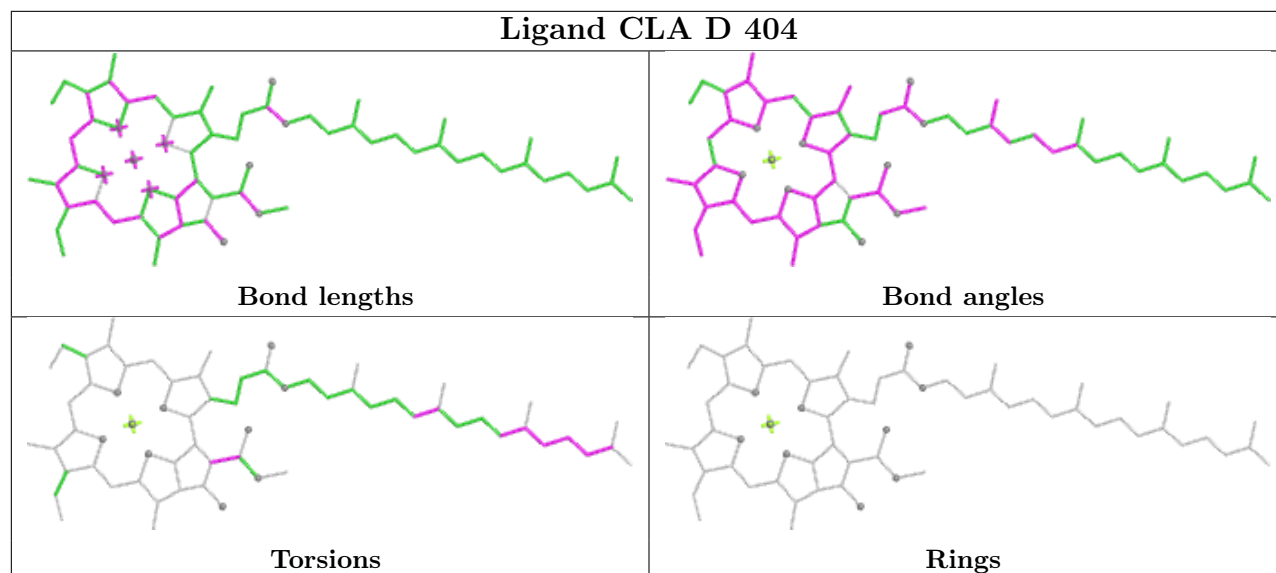
Ligand CLA b 608

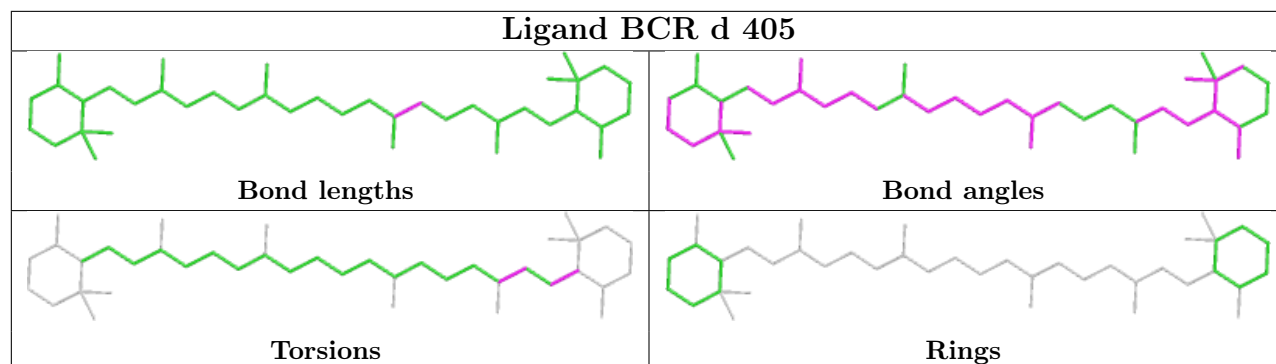
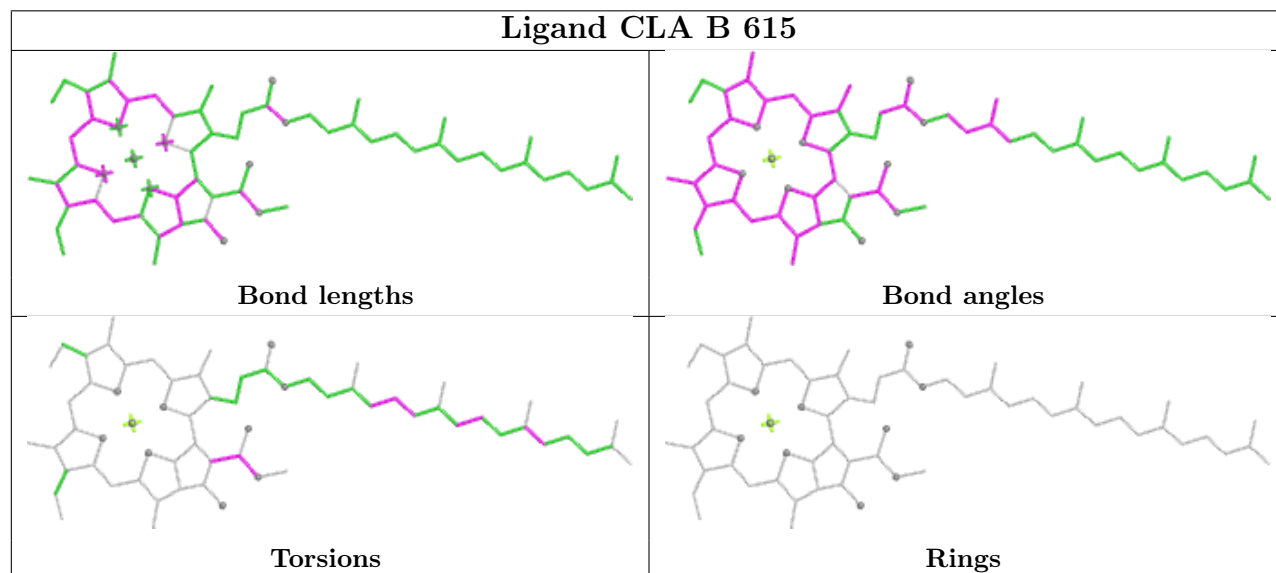
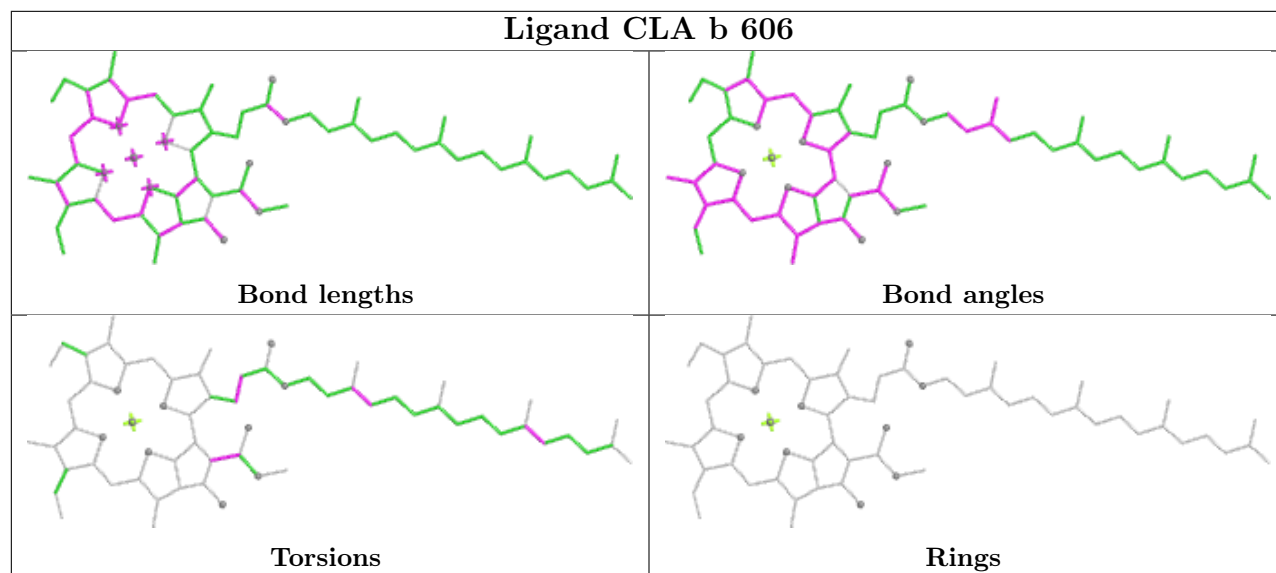


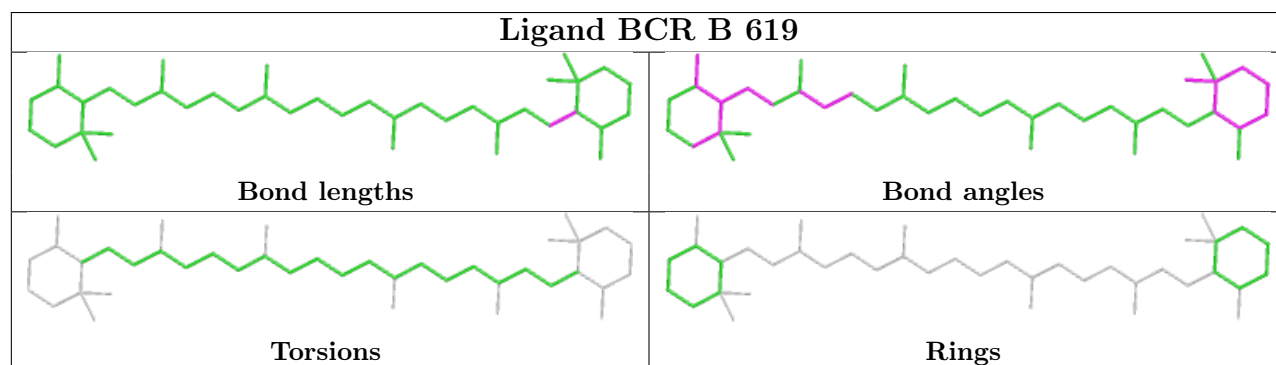
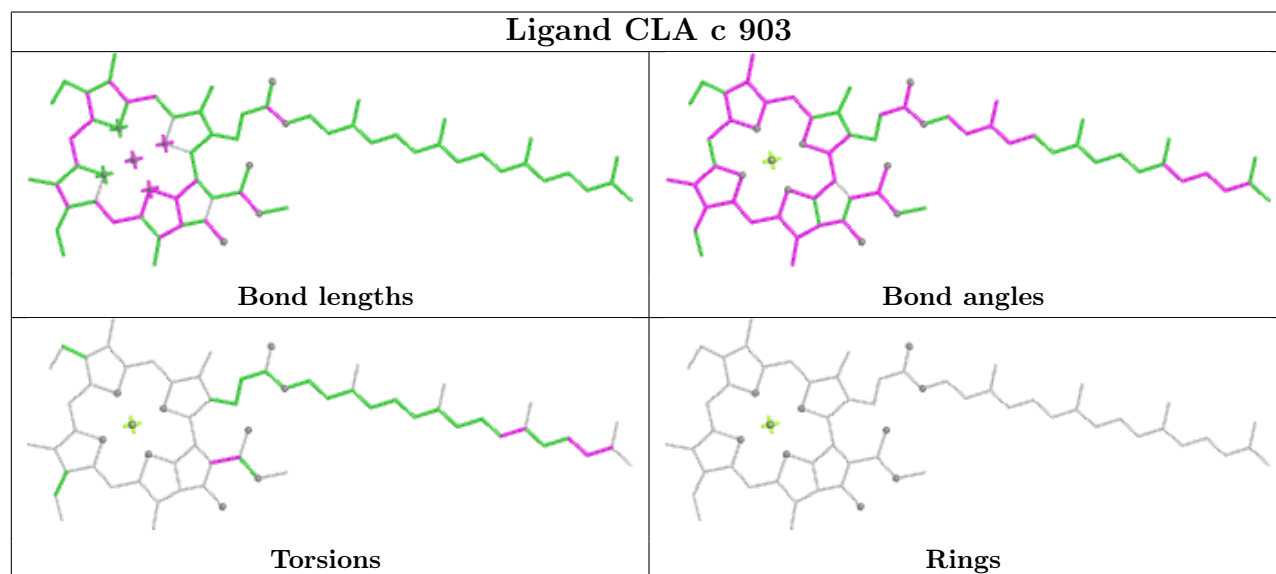
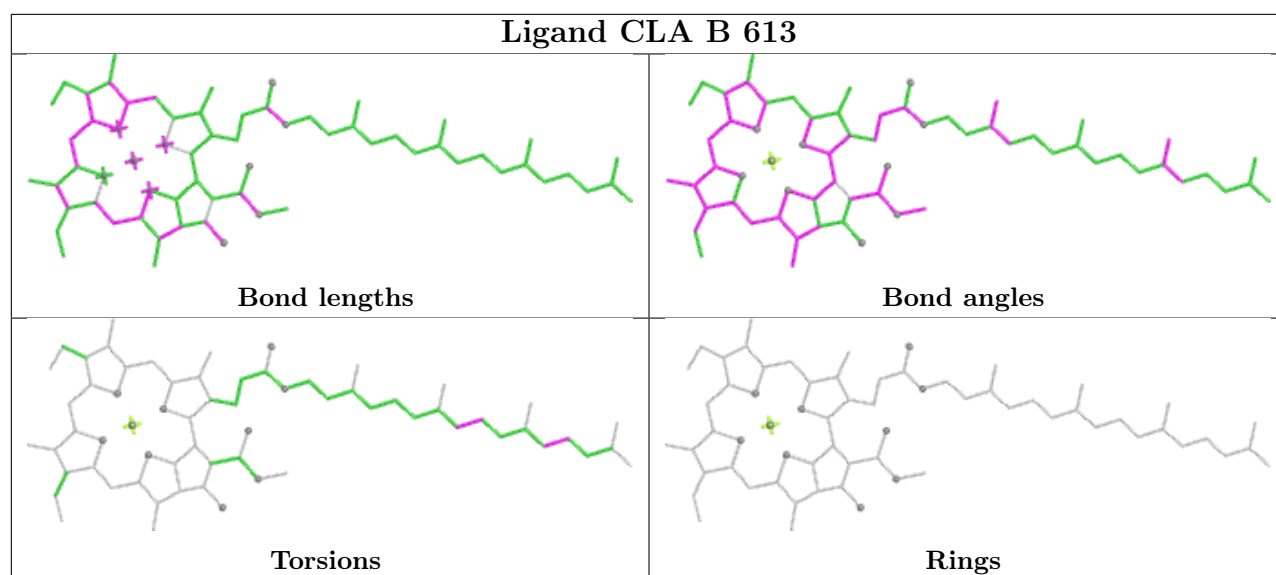
Ligand BCR A 409

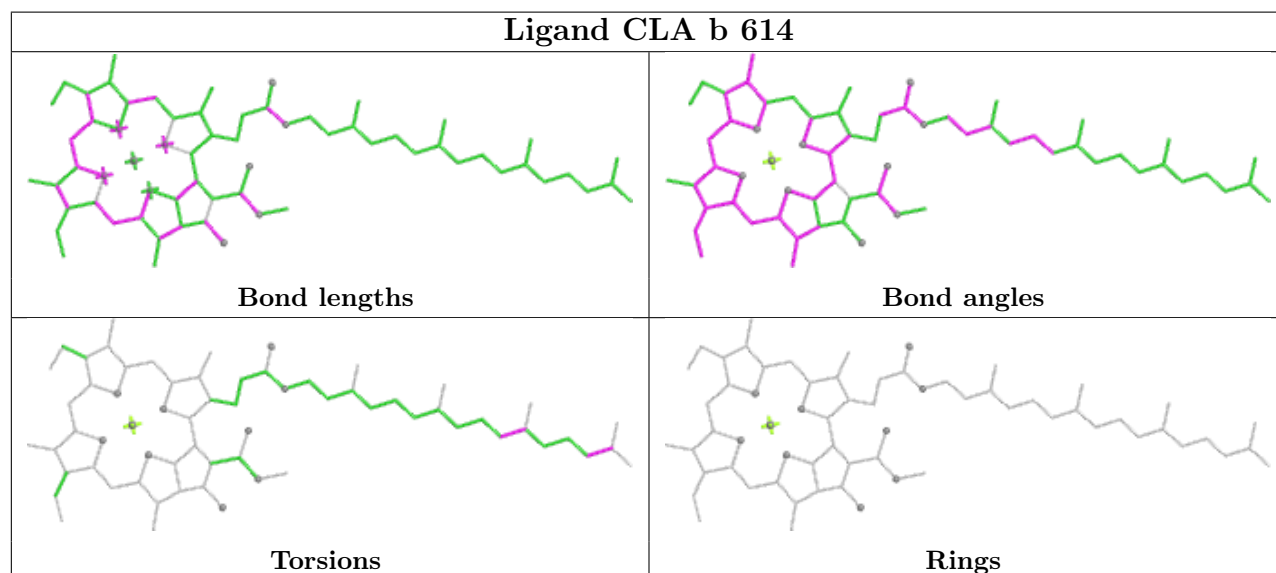
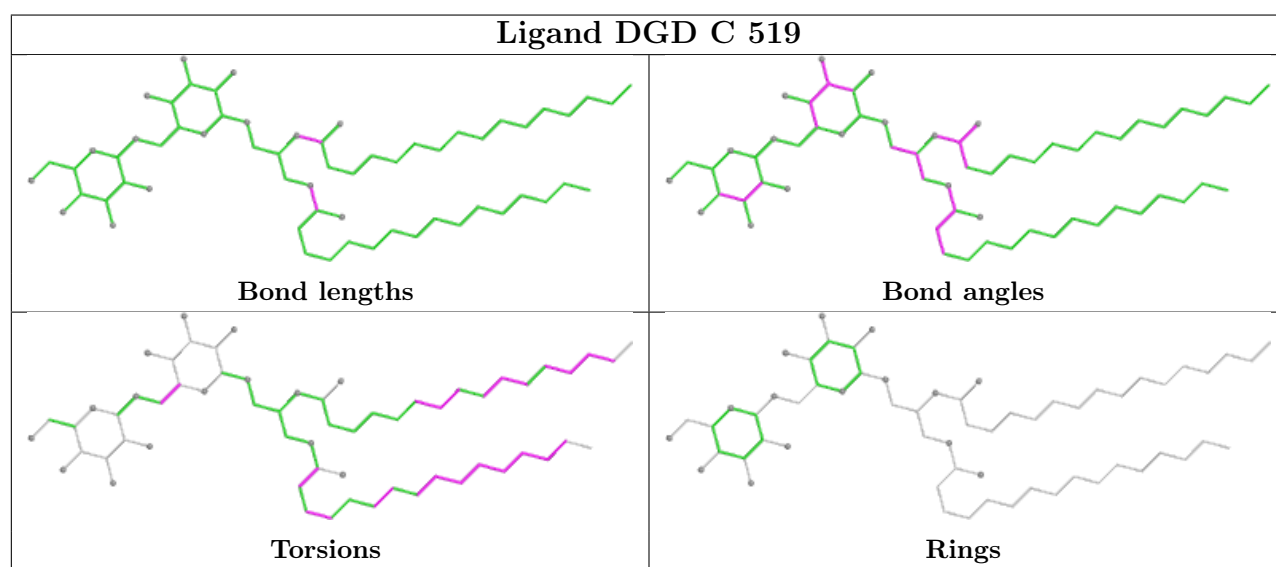
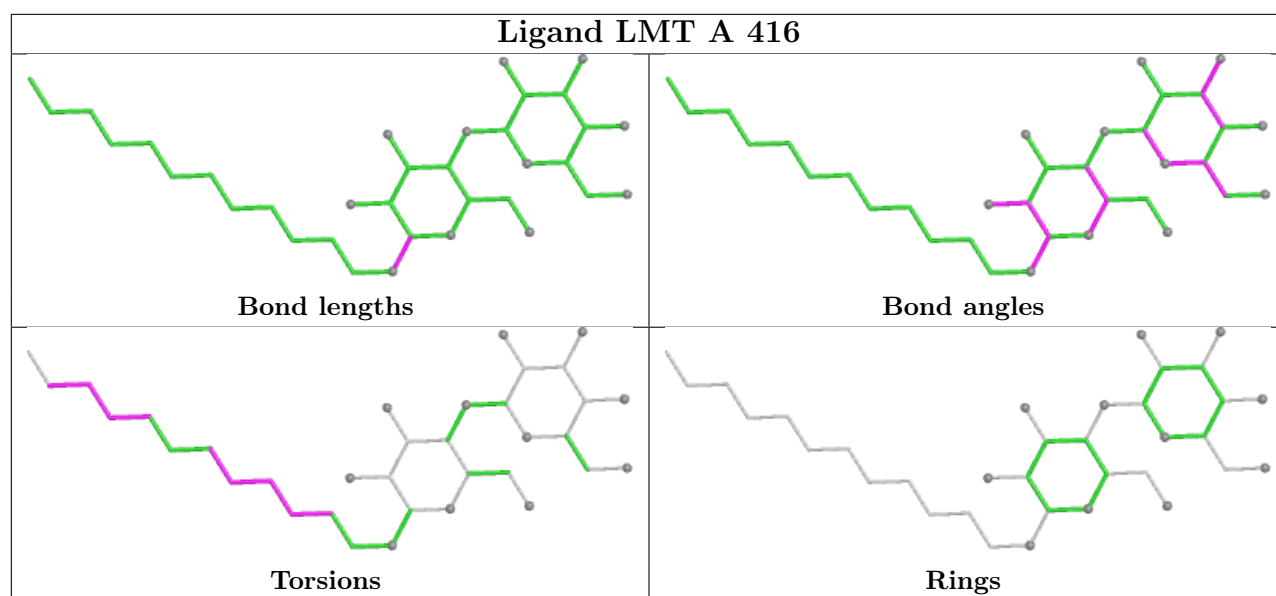


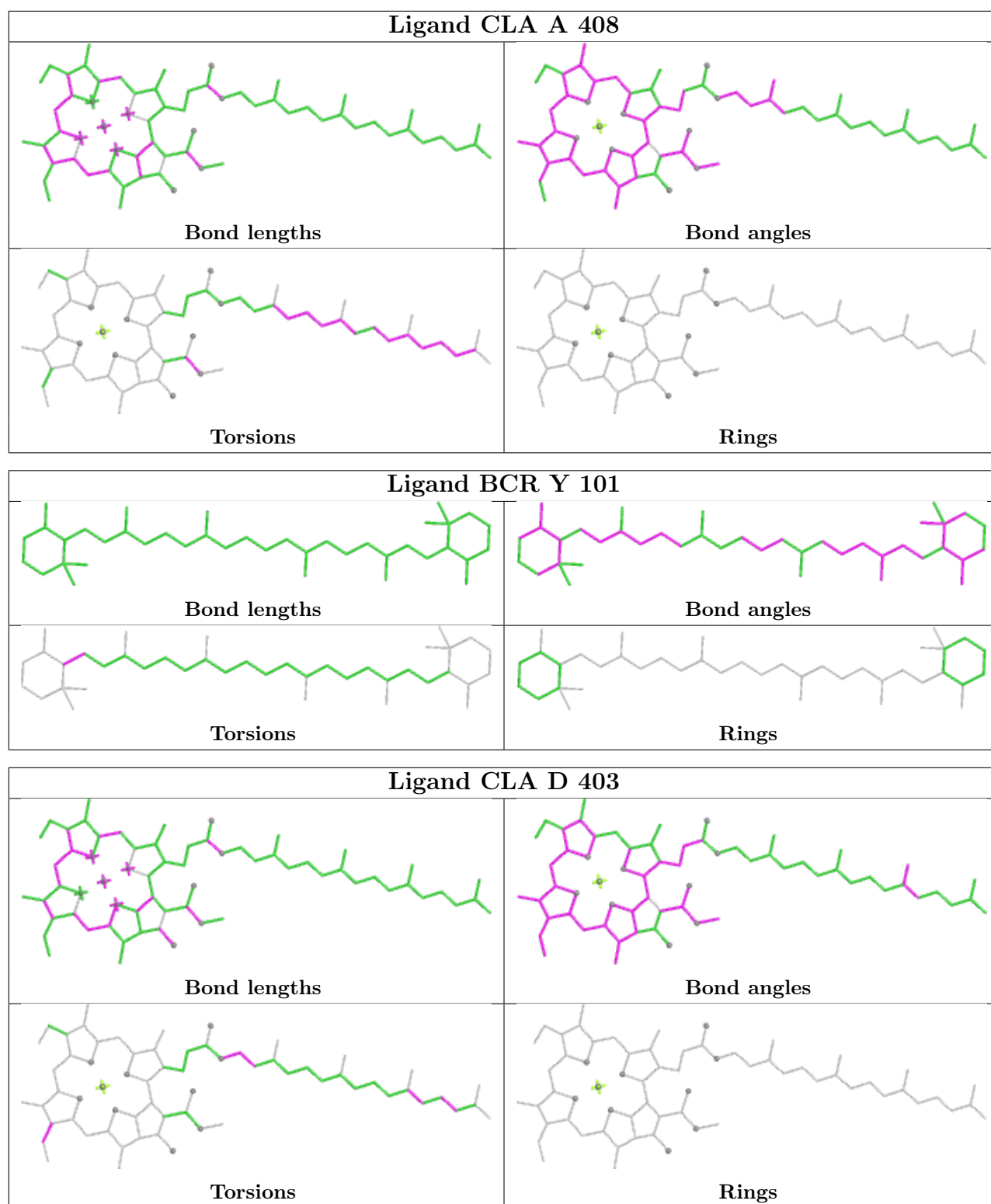
Ligand CLA D 404

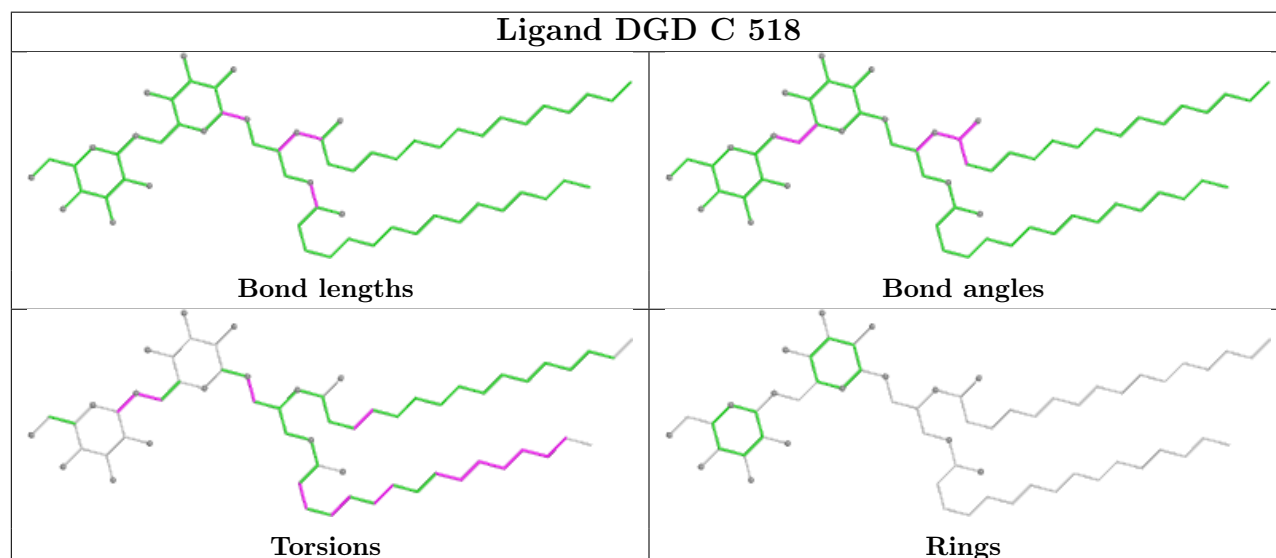
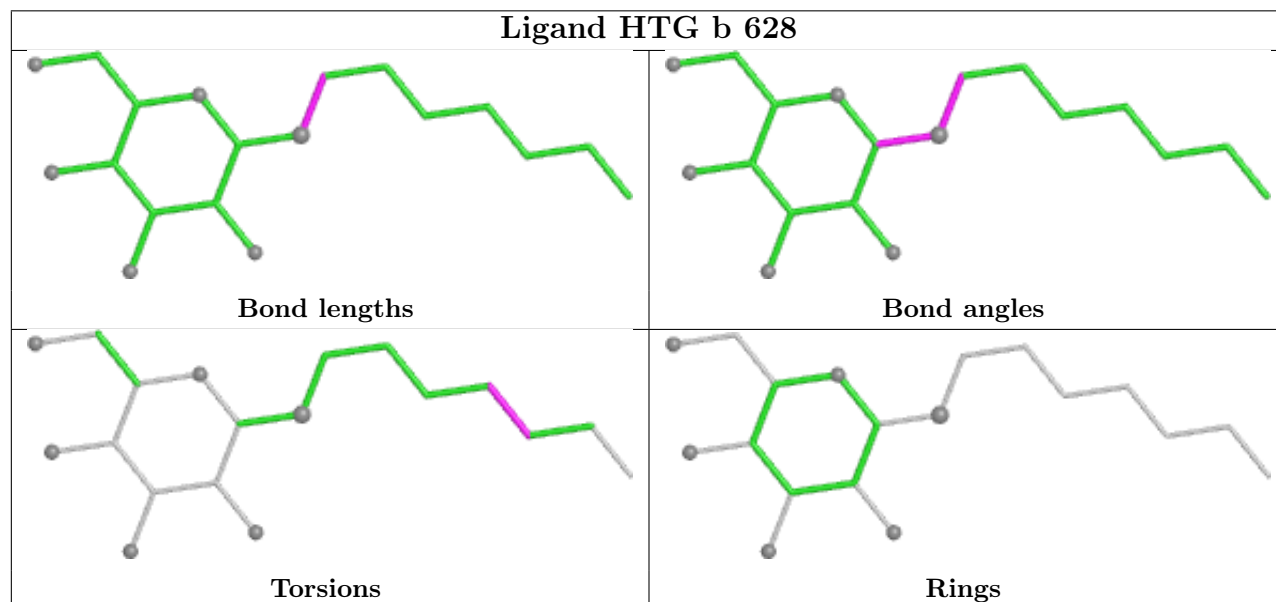
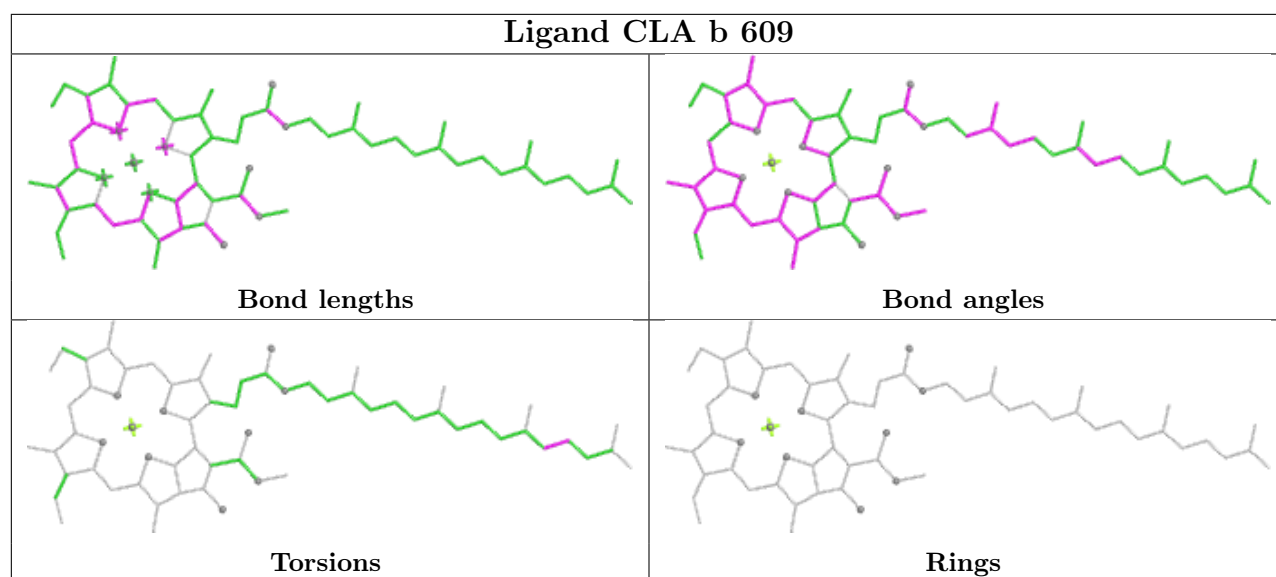


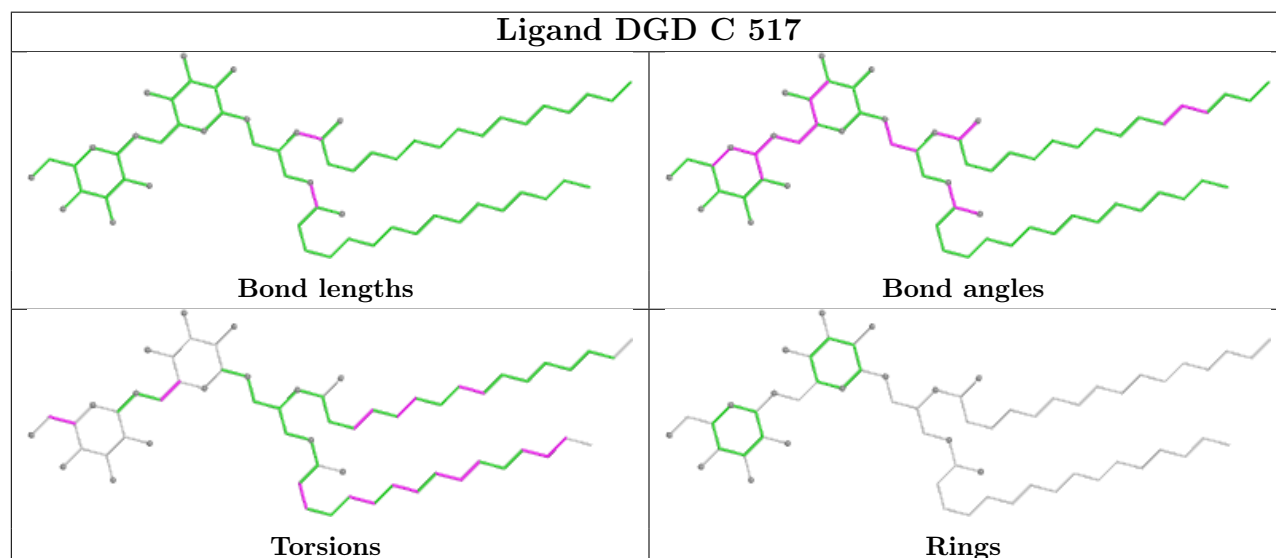
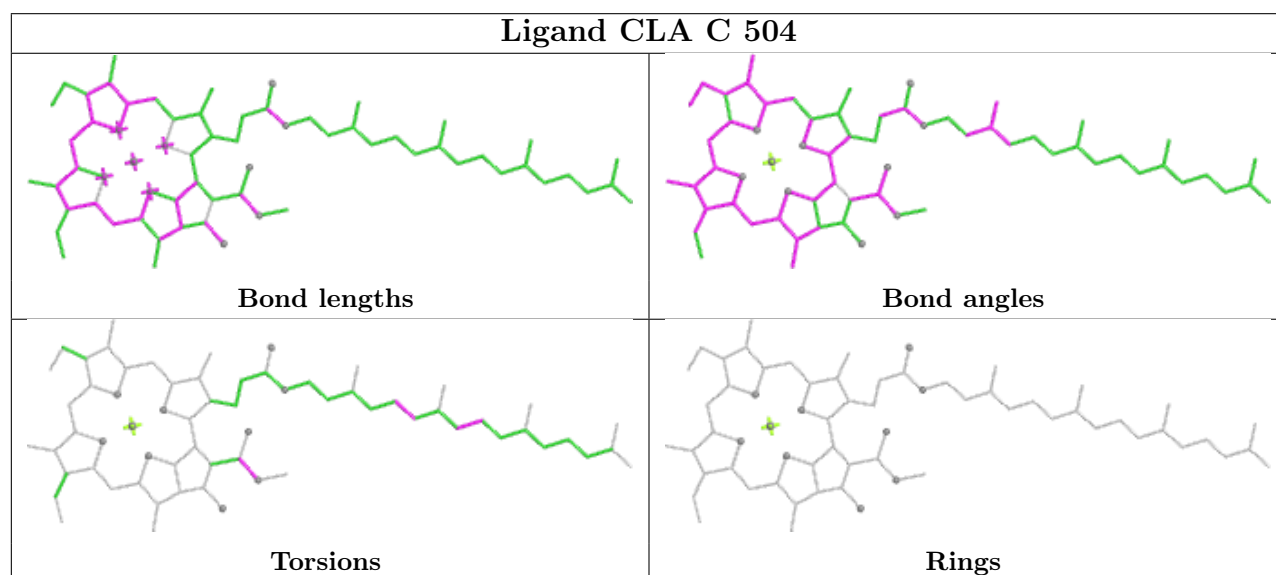
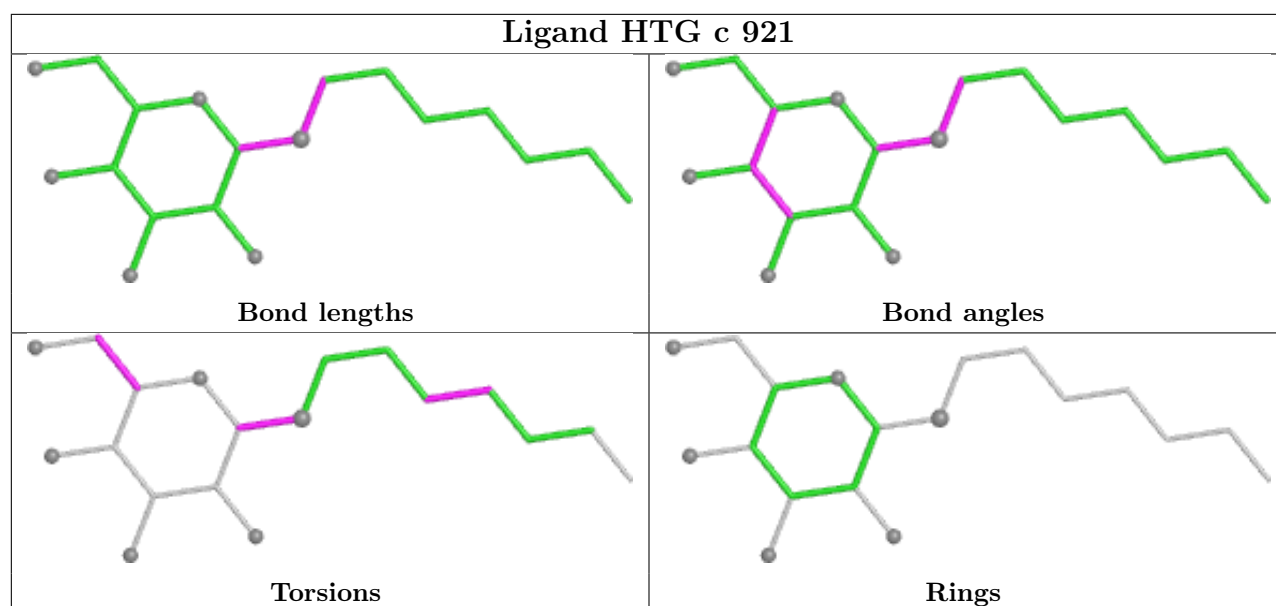
Ligand BCR d 405**Ligand CLA B 615****Ligand CLA b 606**

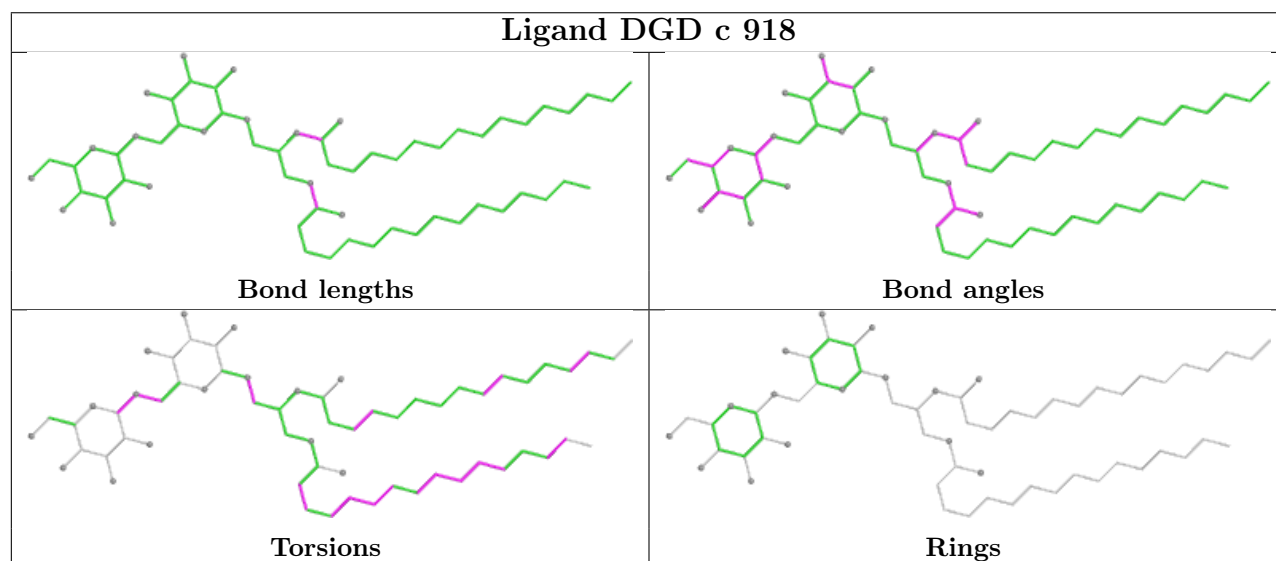
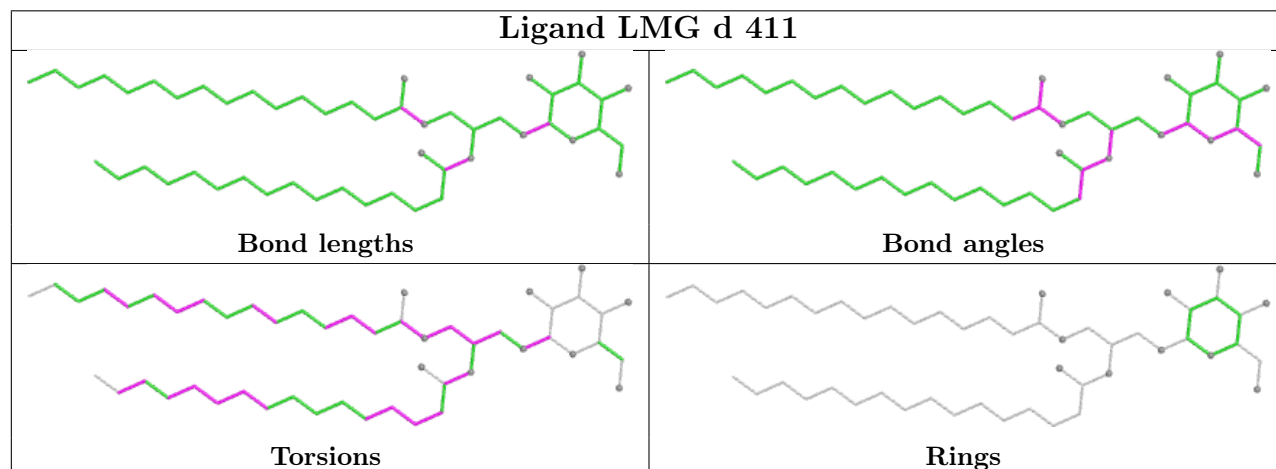
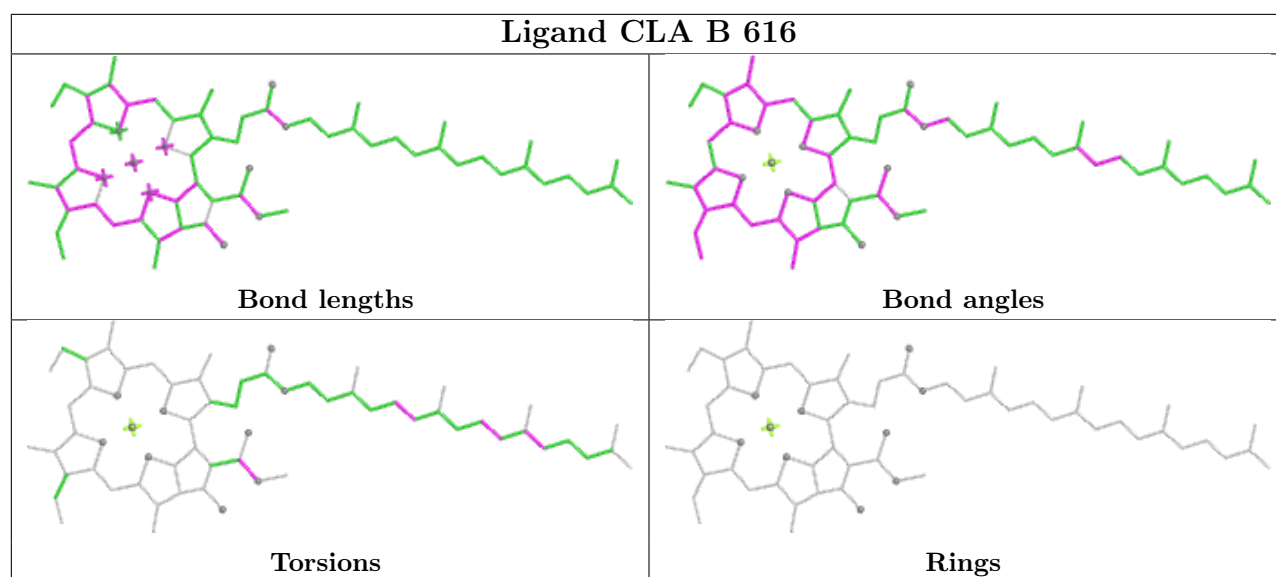




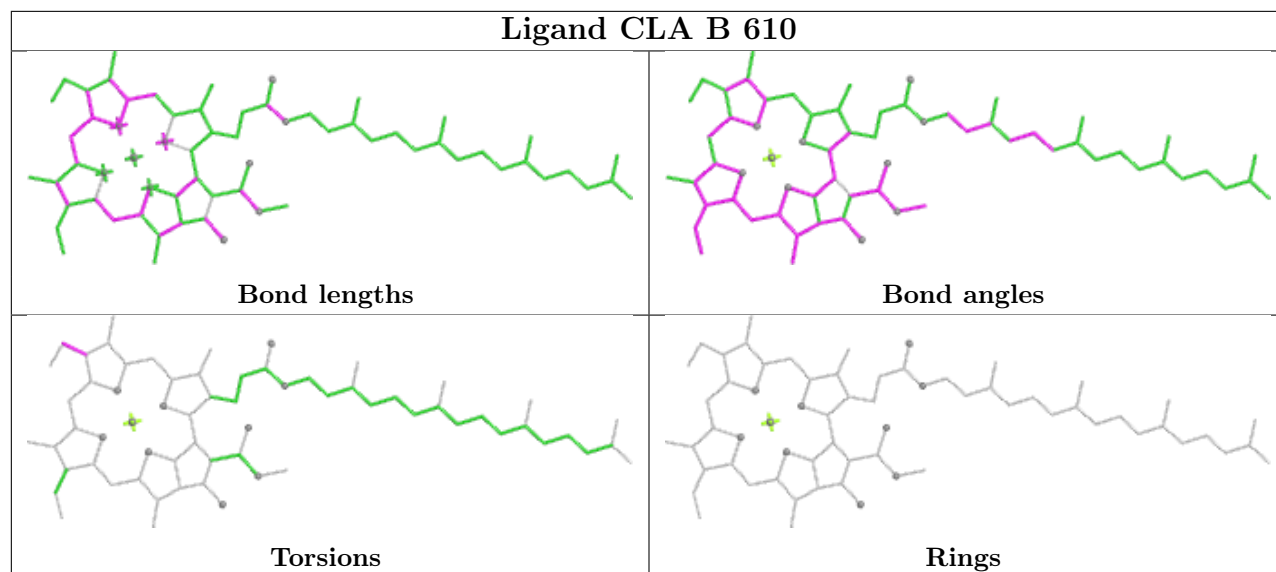




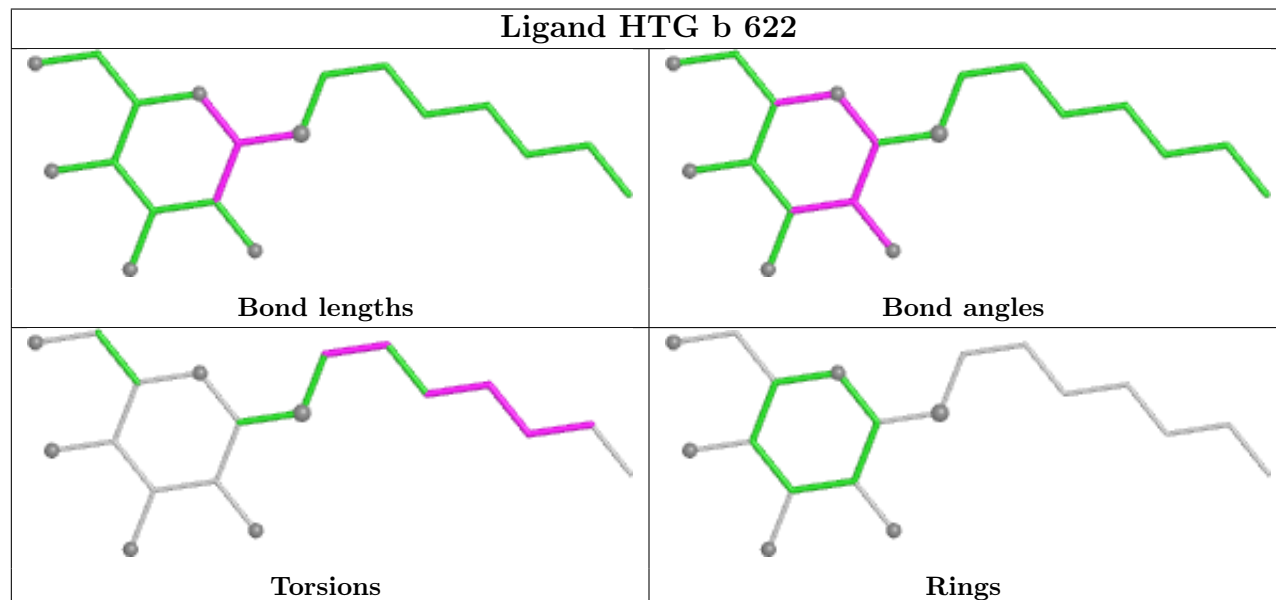




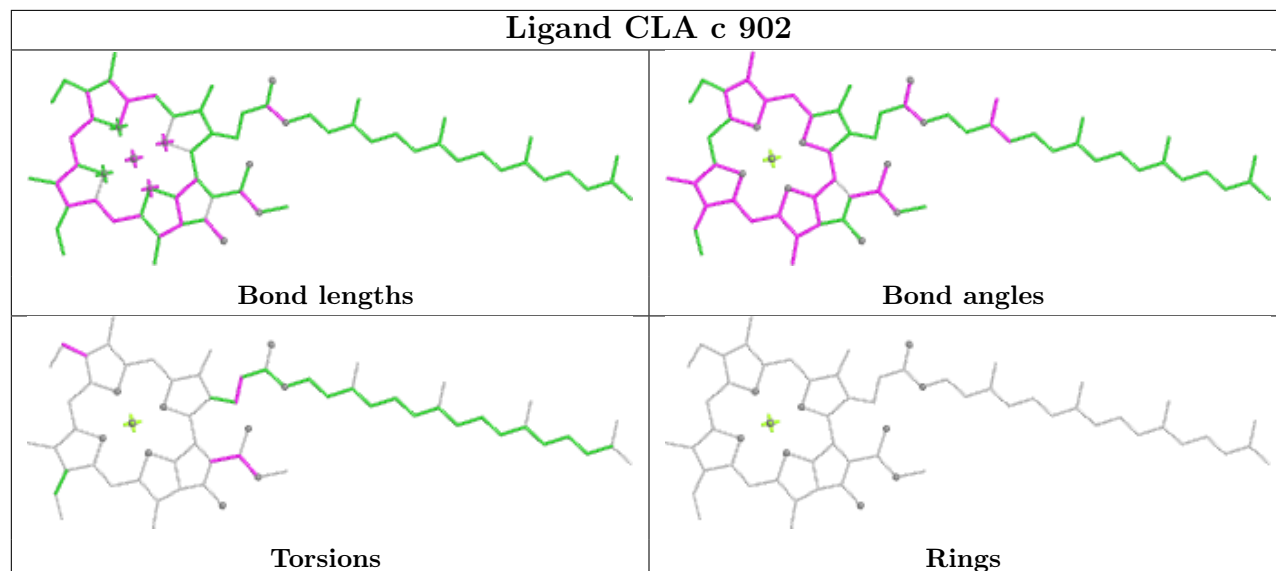
Ligand CLA B 610

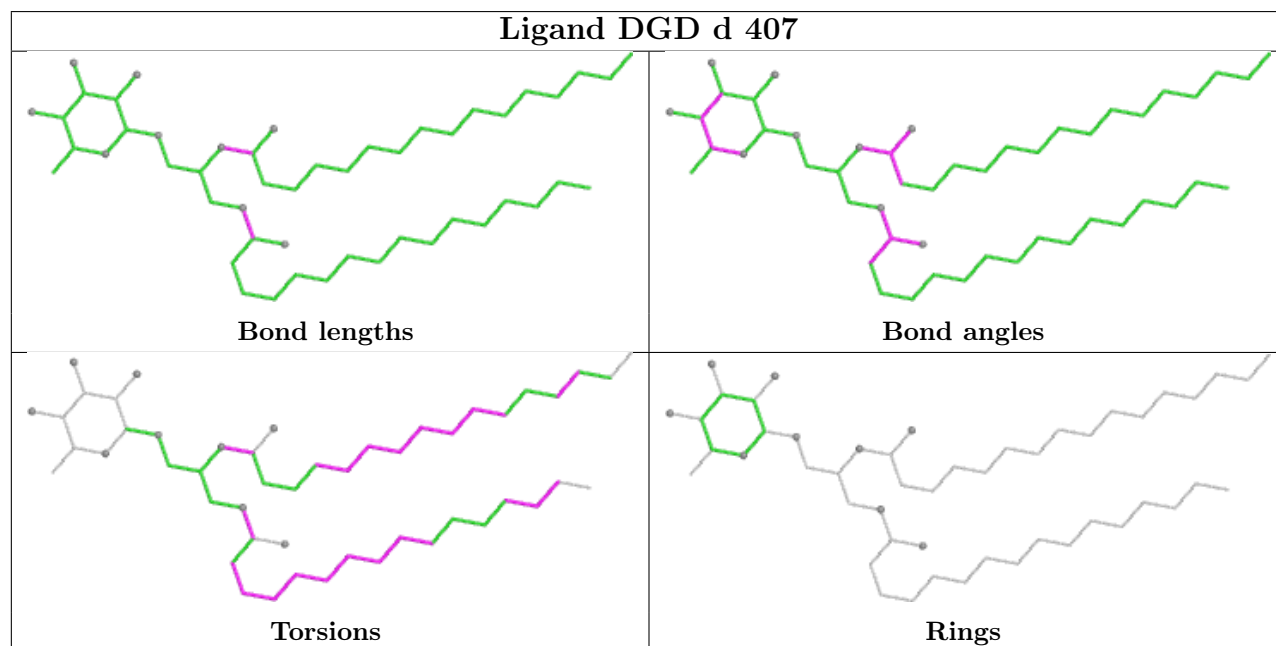
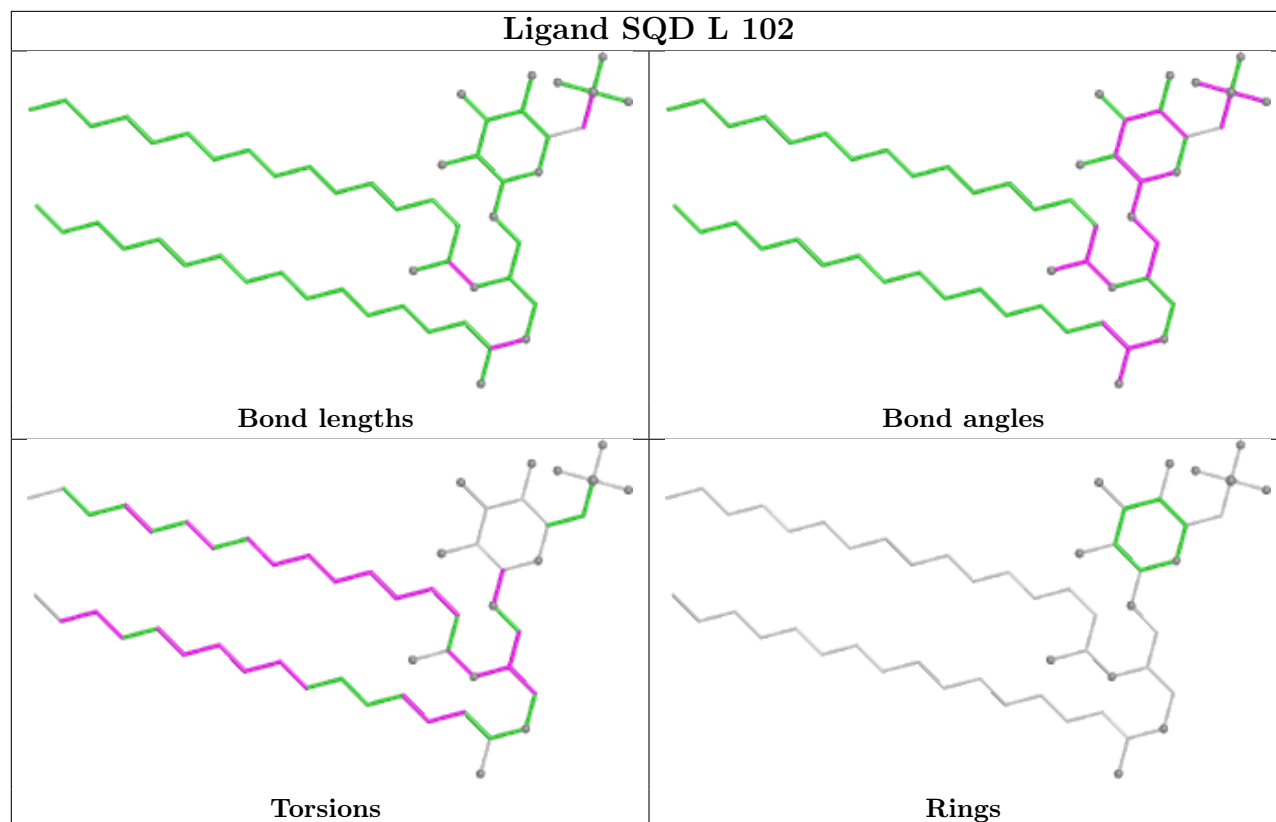


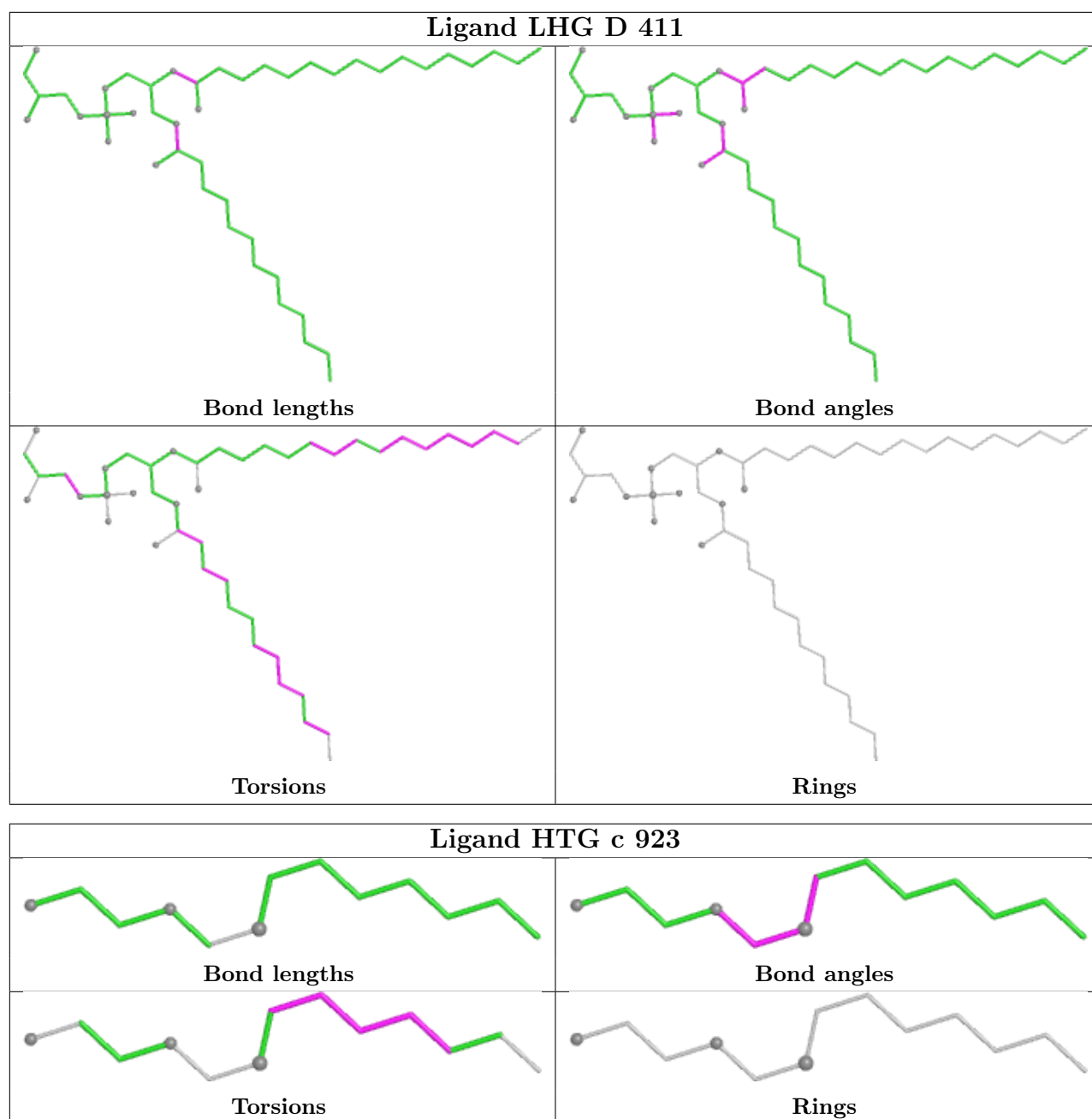
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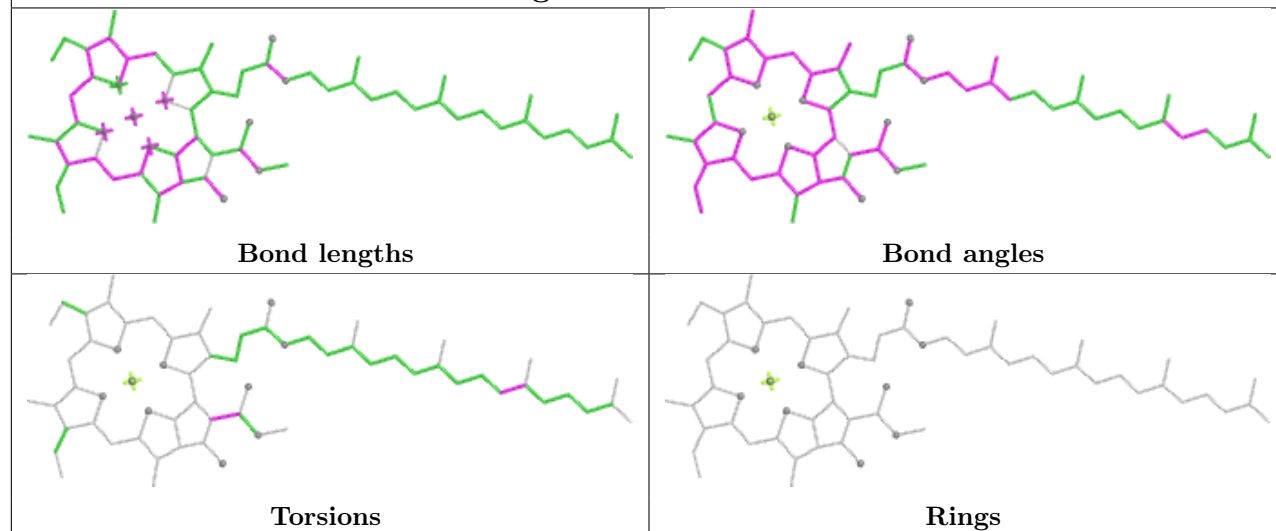
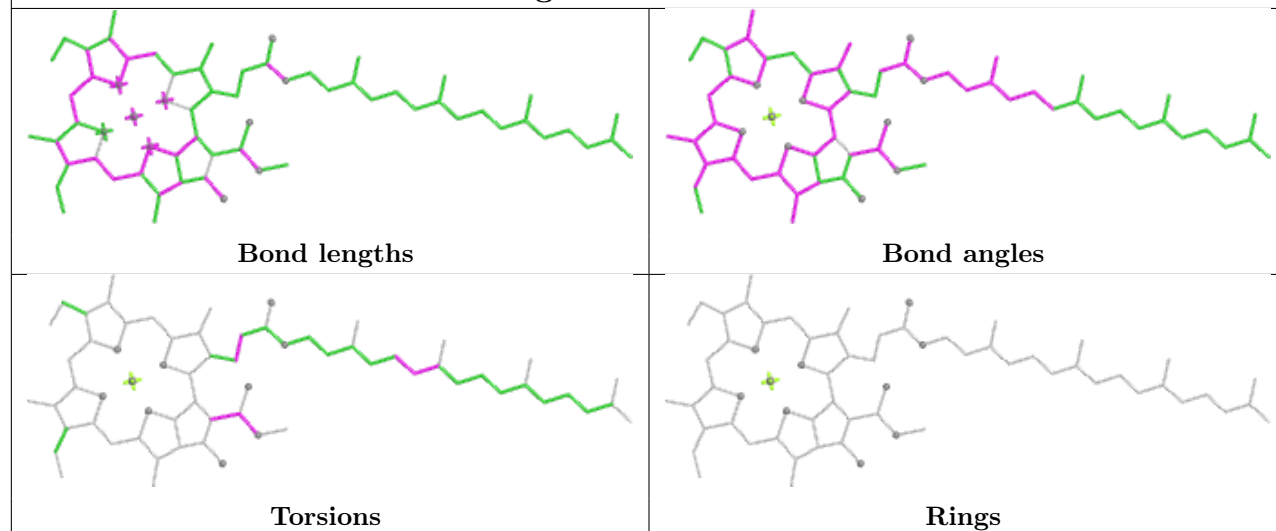
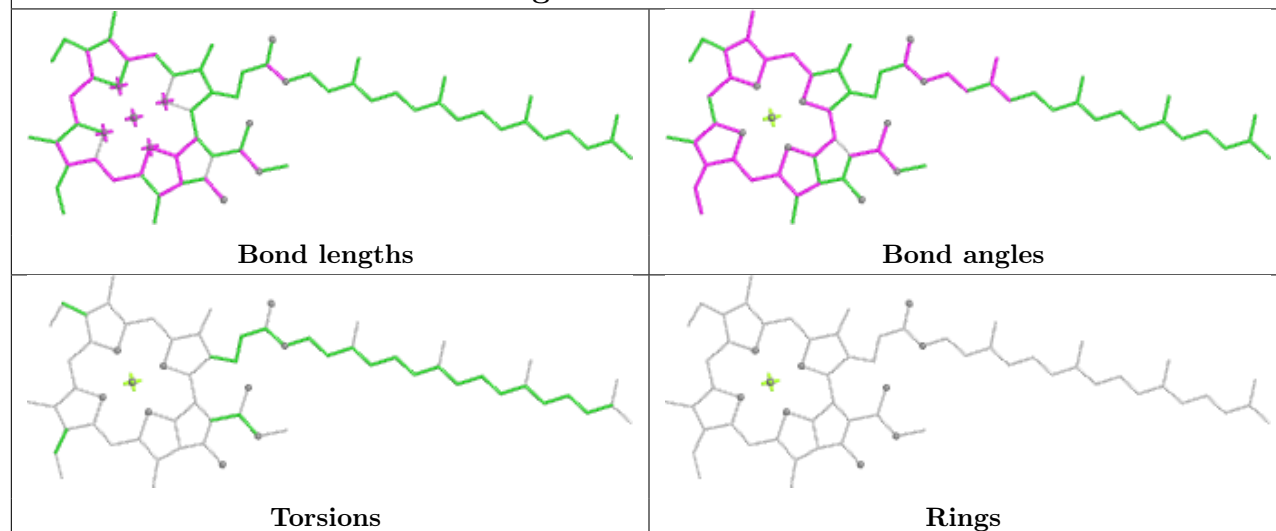


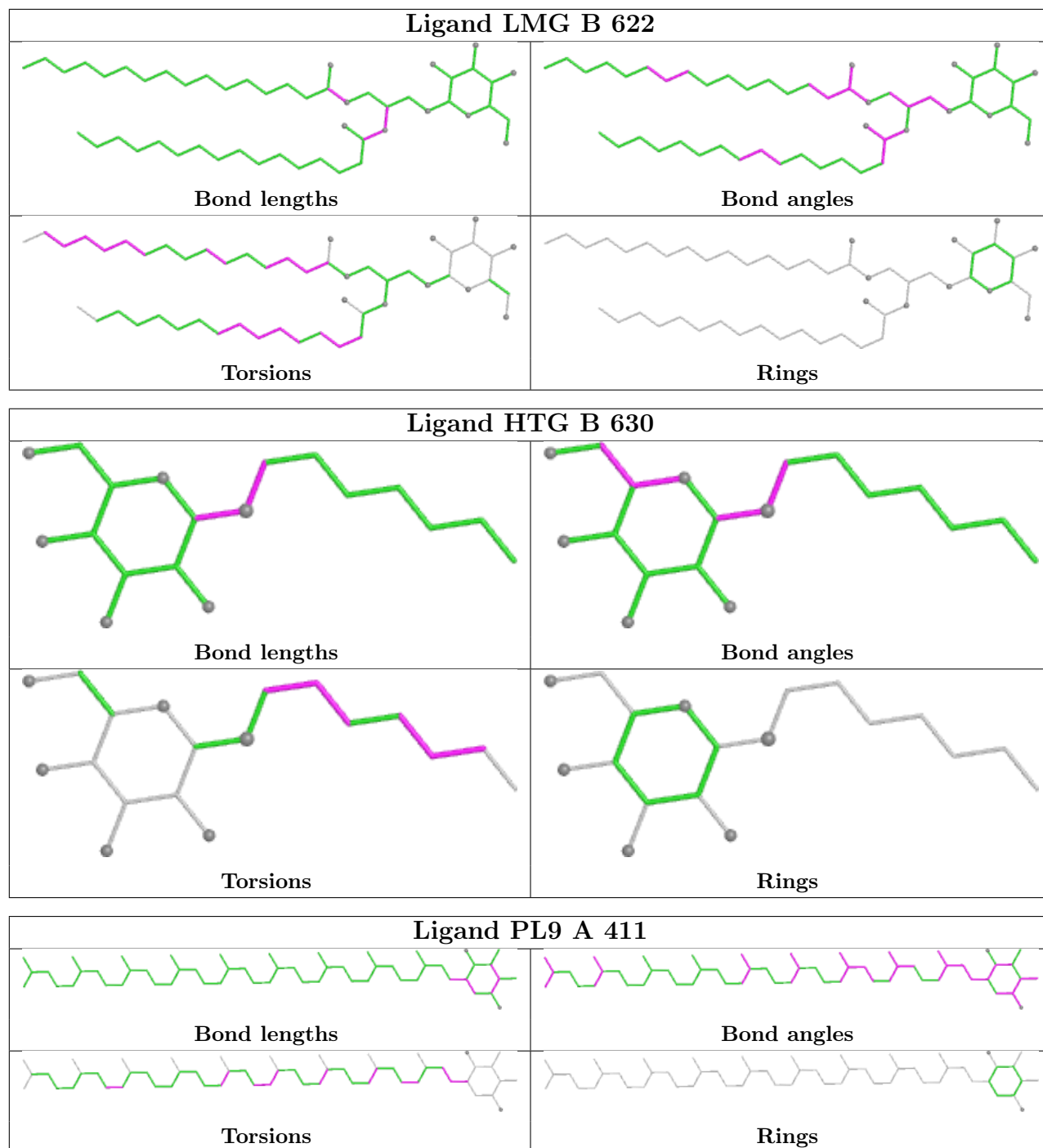
Ligand CLA c 902



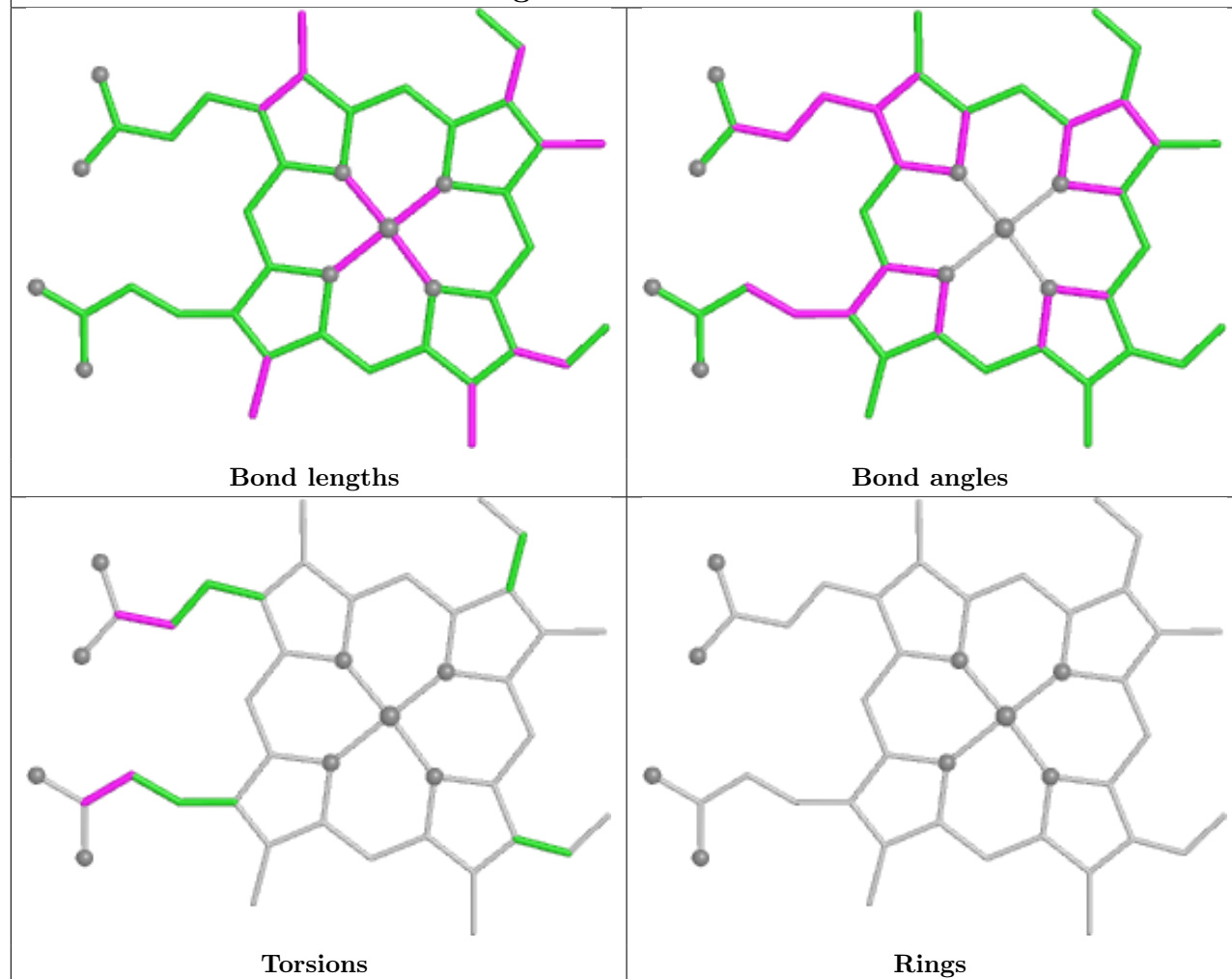




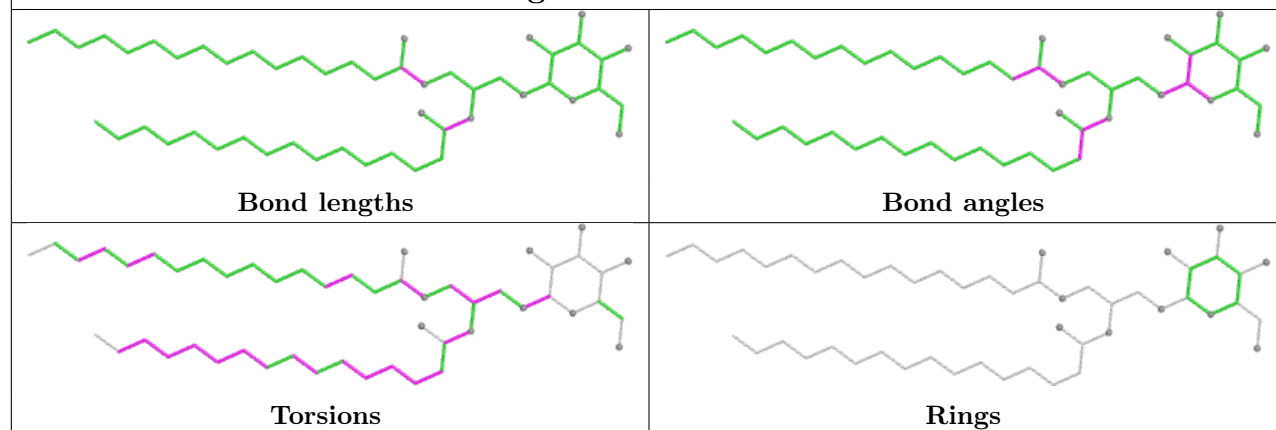
Ligand CLA B 603**Ligand CLA b 604****Ligand CLA C 512**

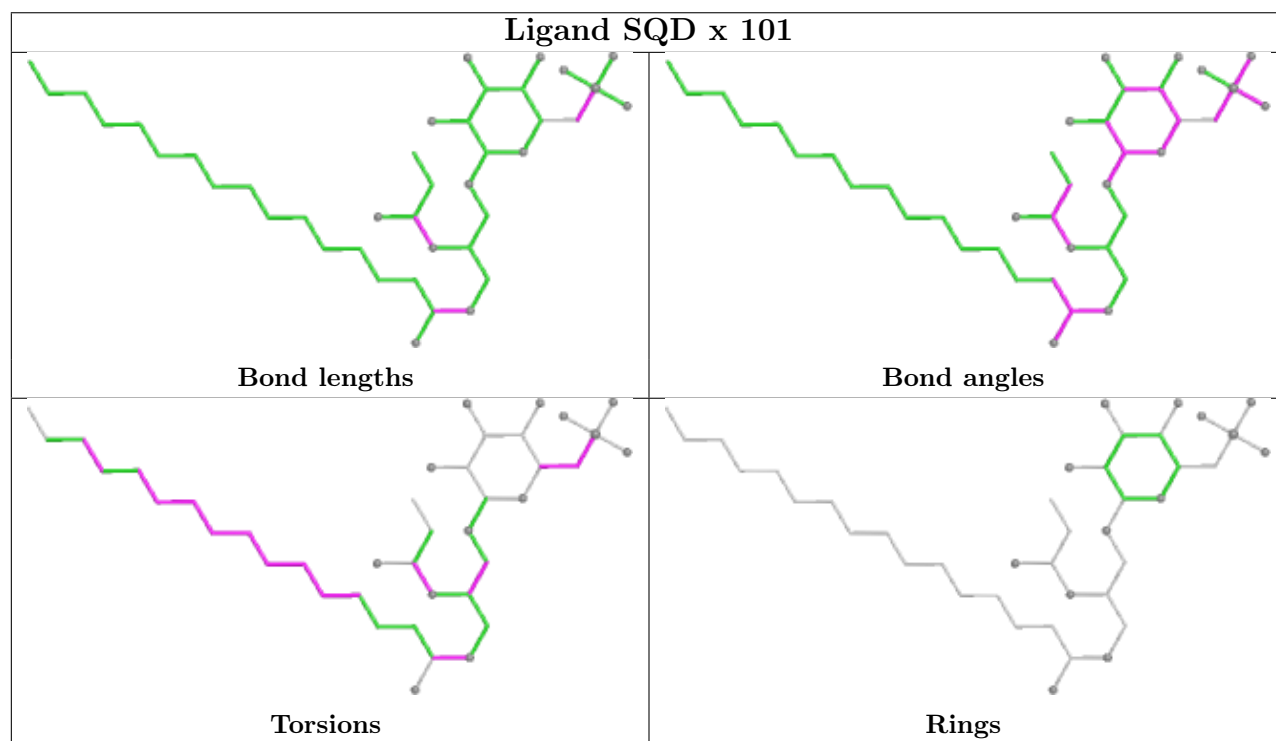
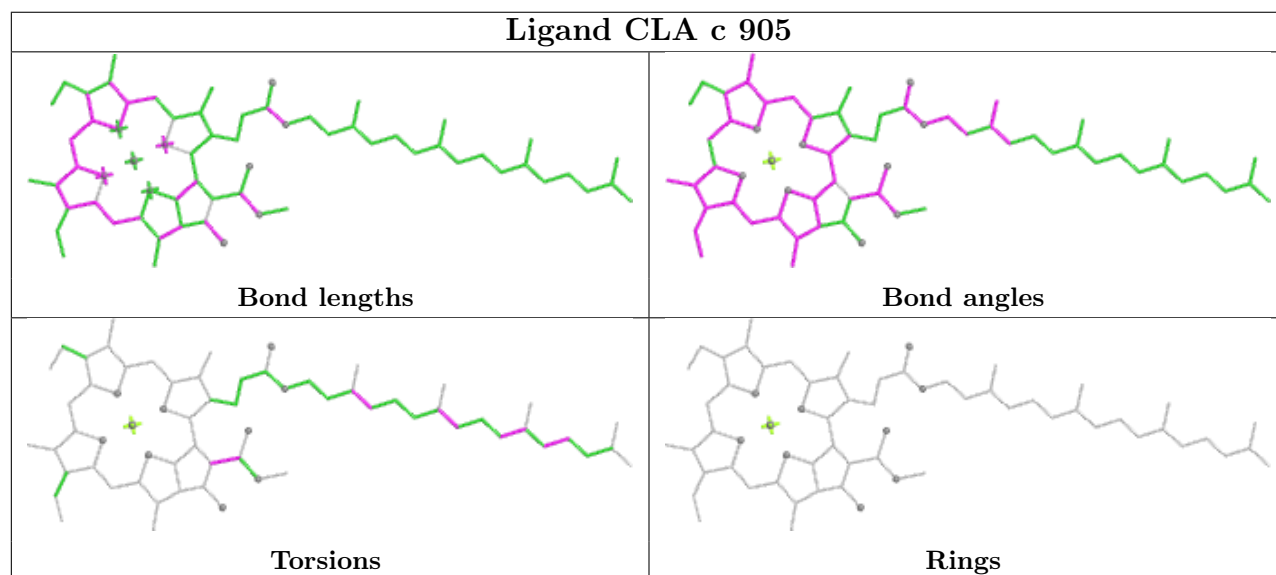
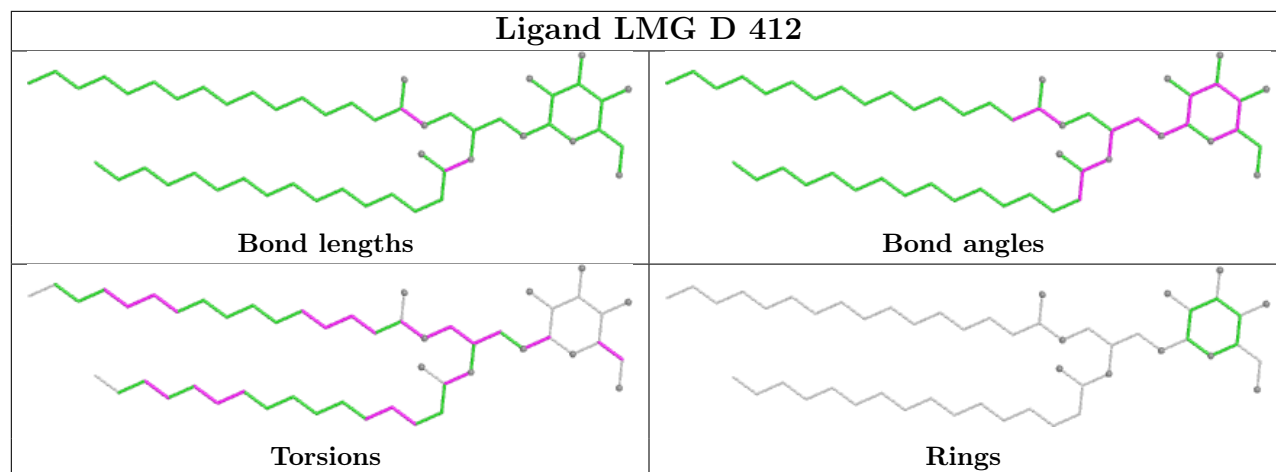


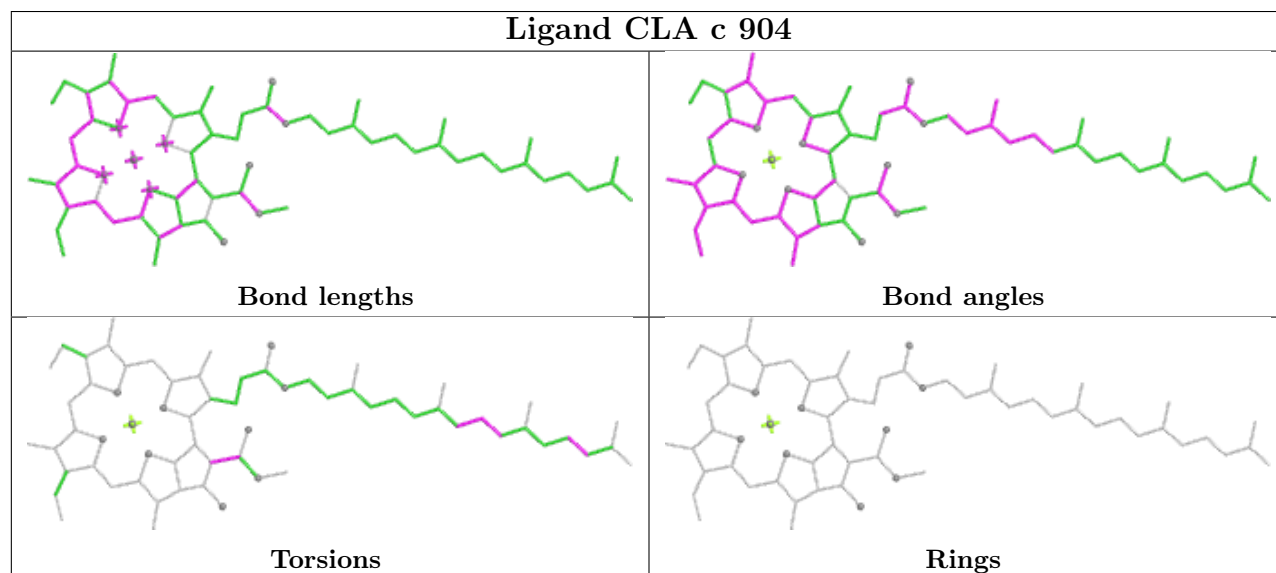
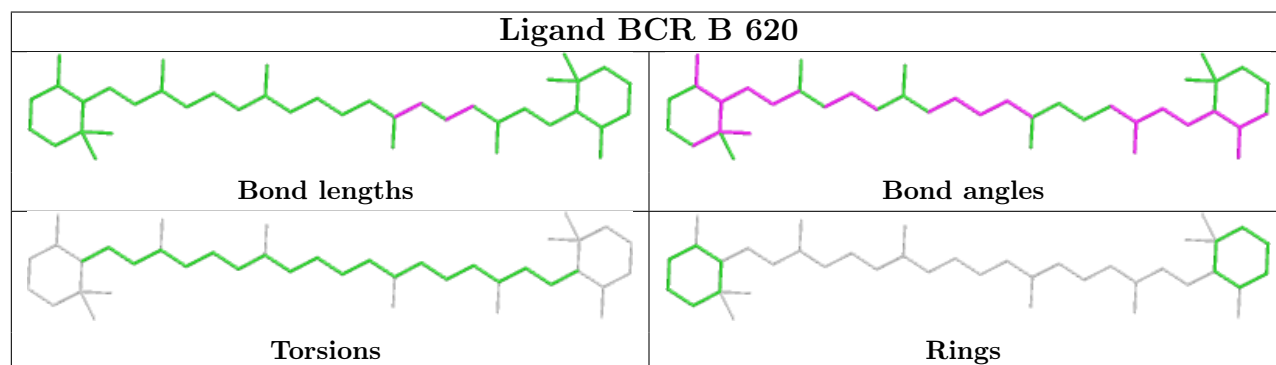
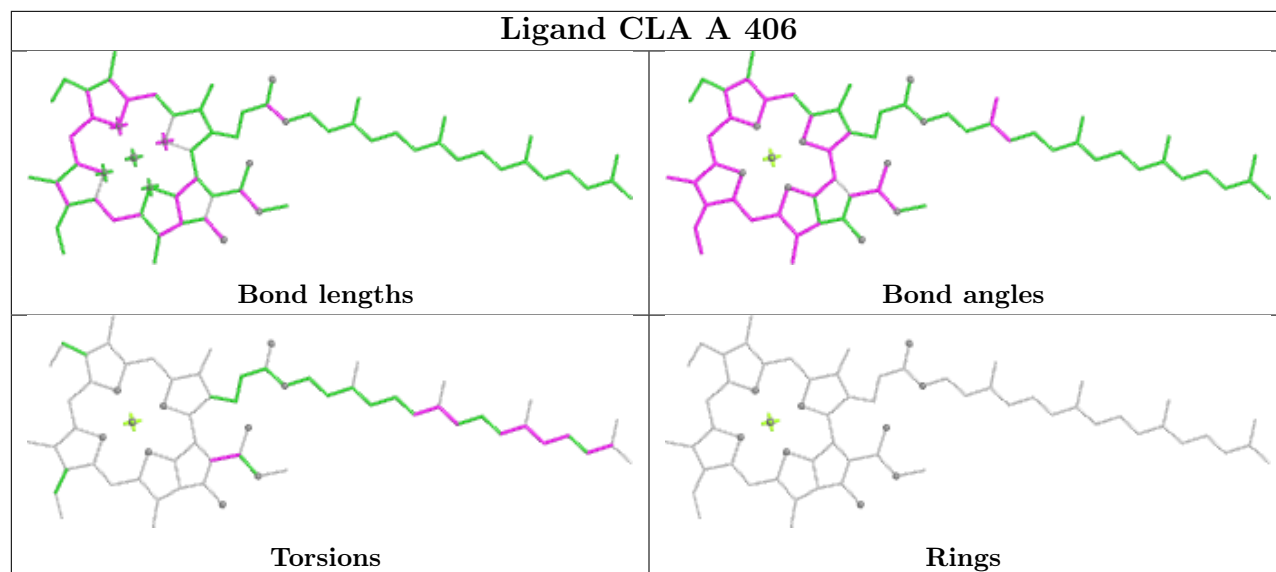
Ligand HEM e 105

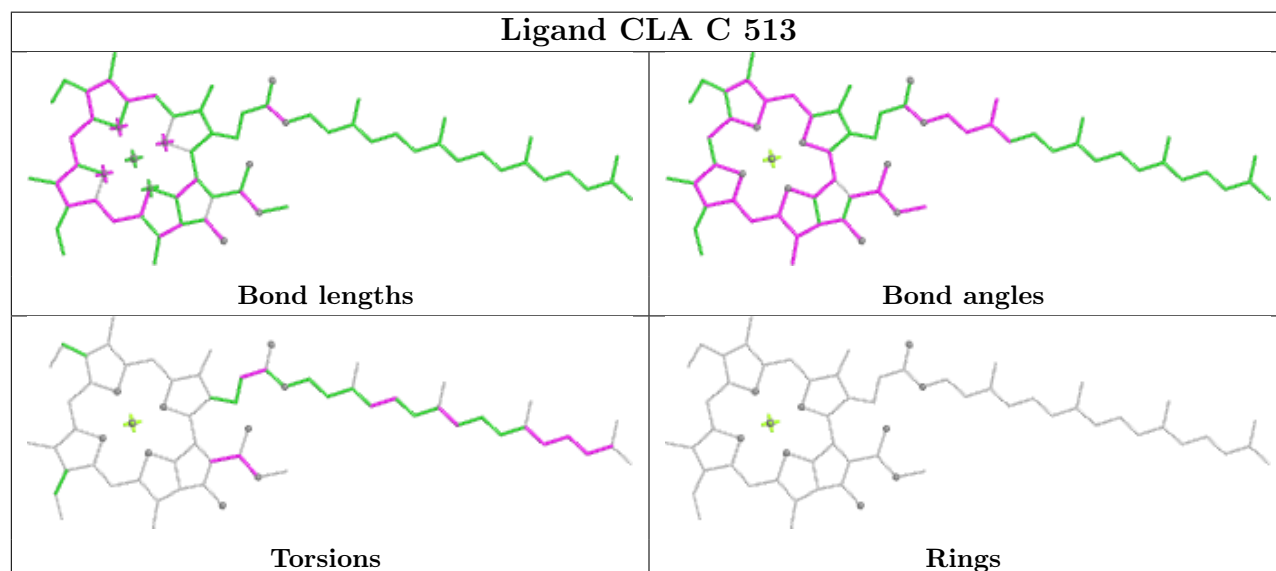
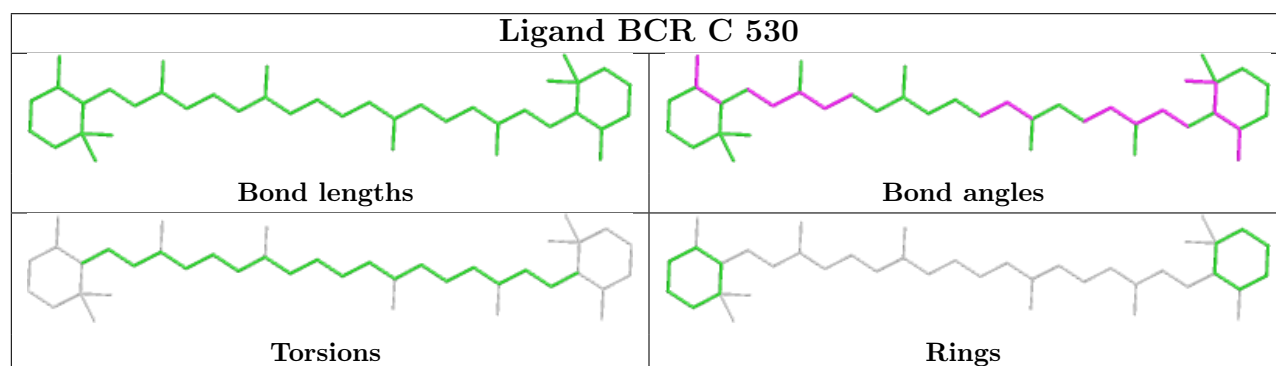
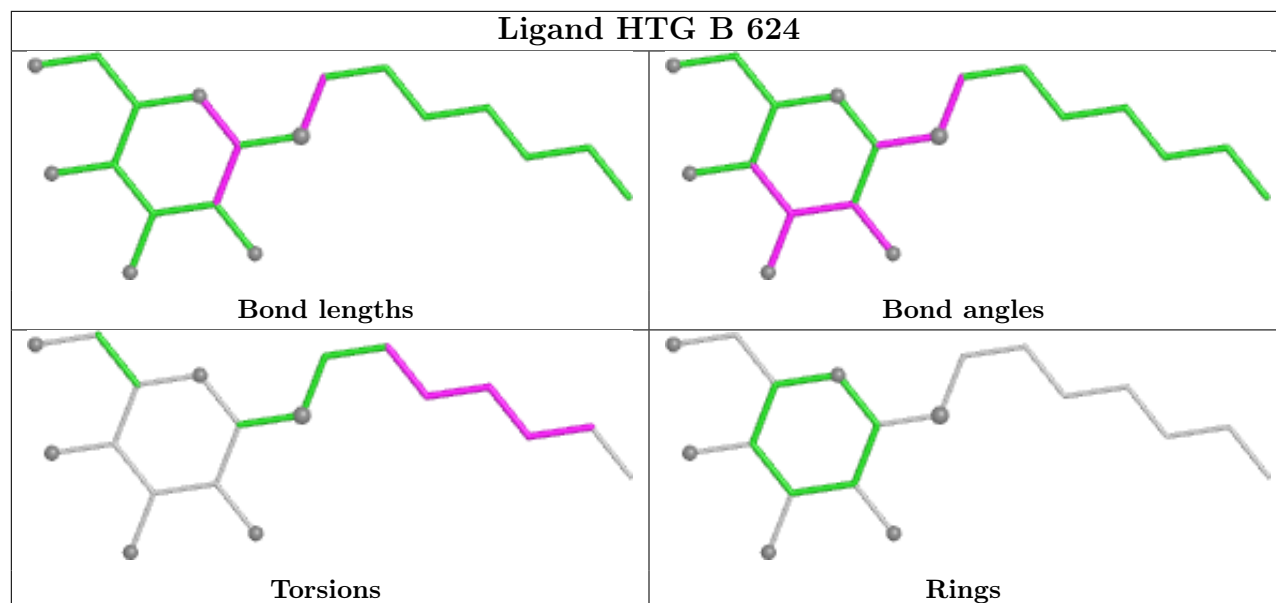


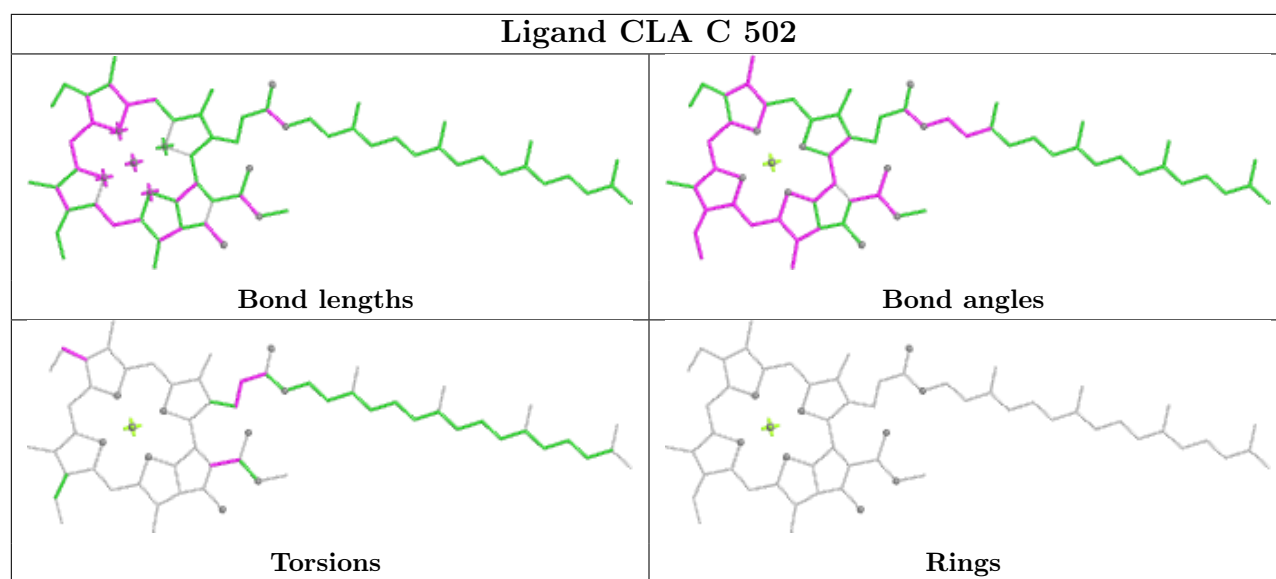
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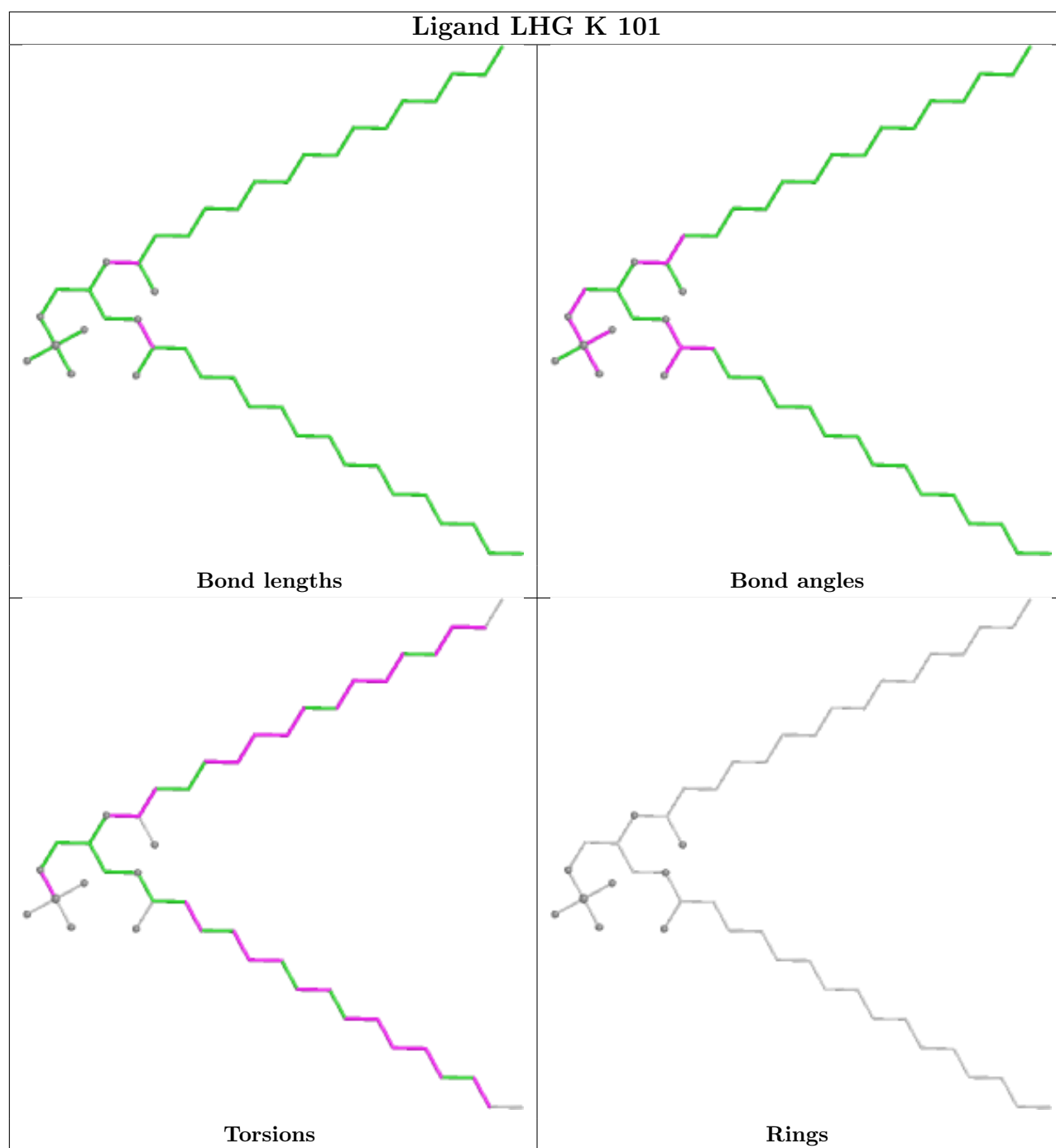


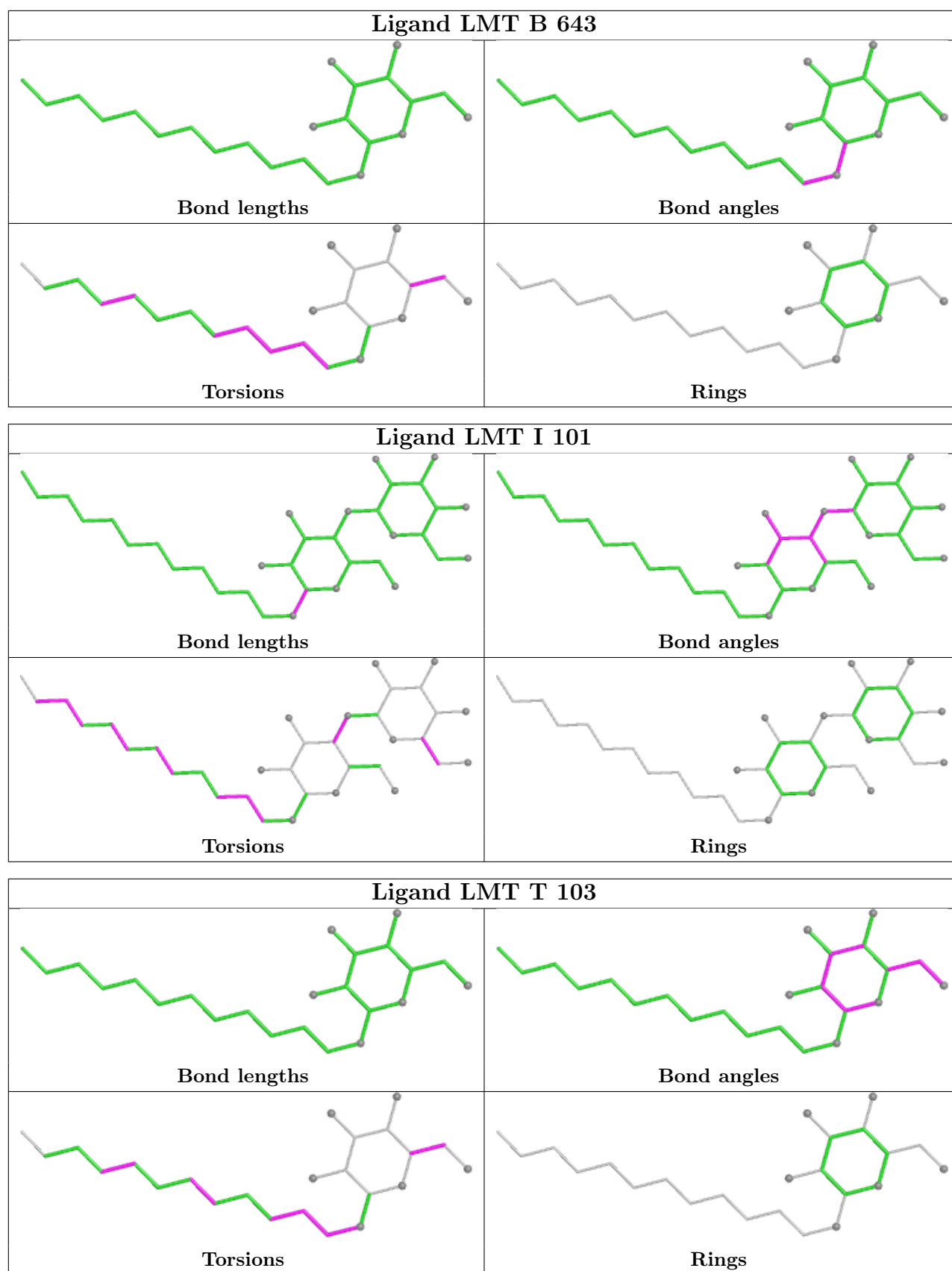


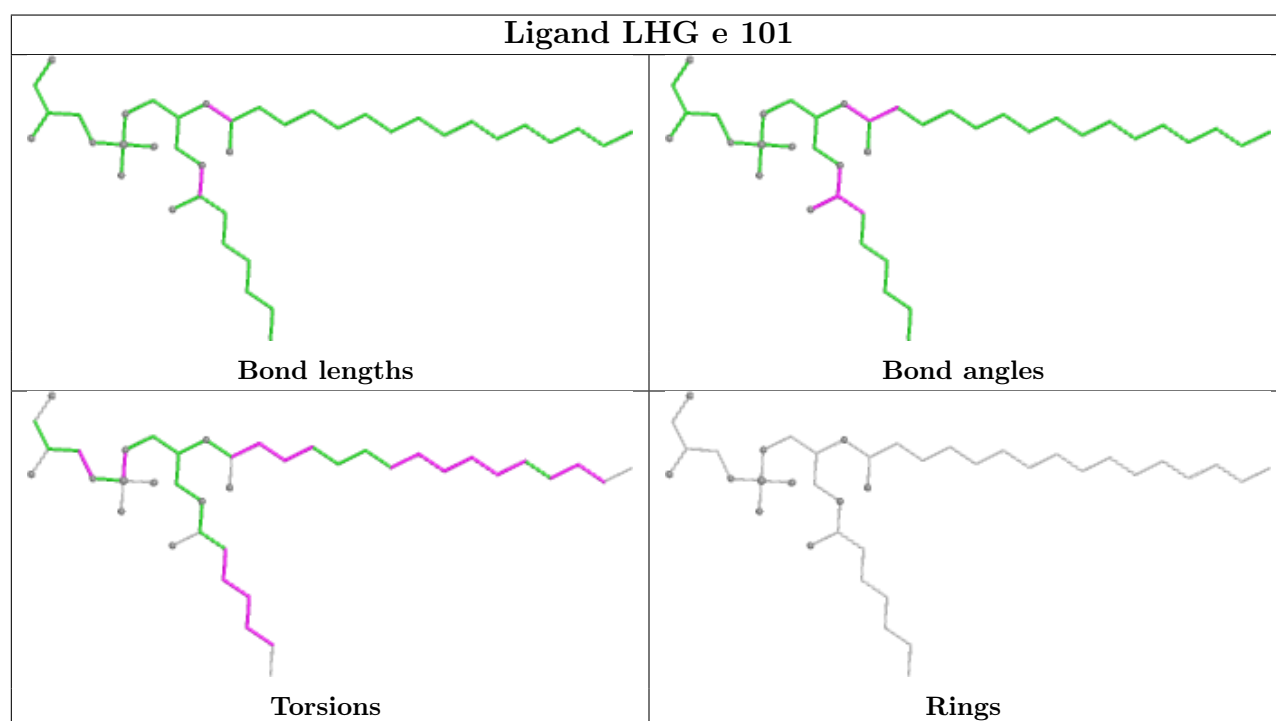
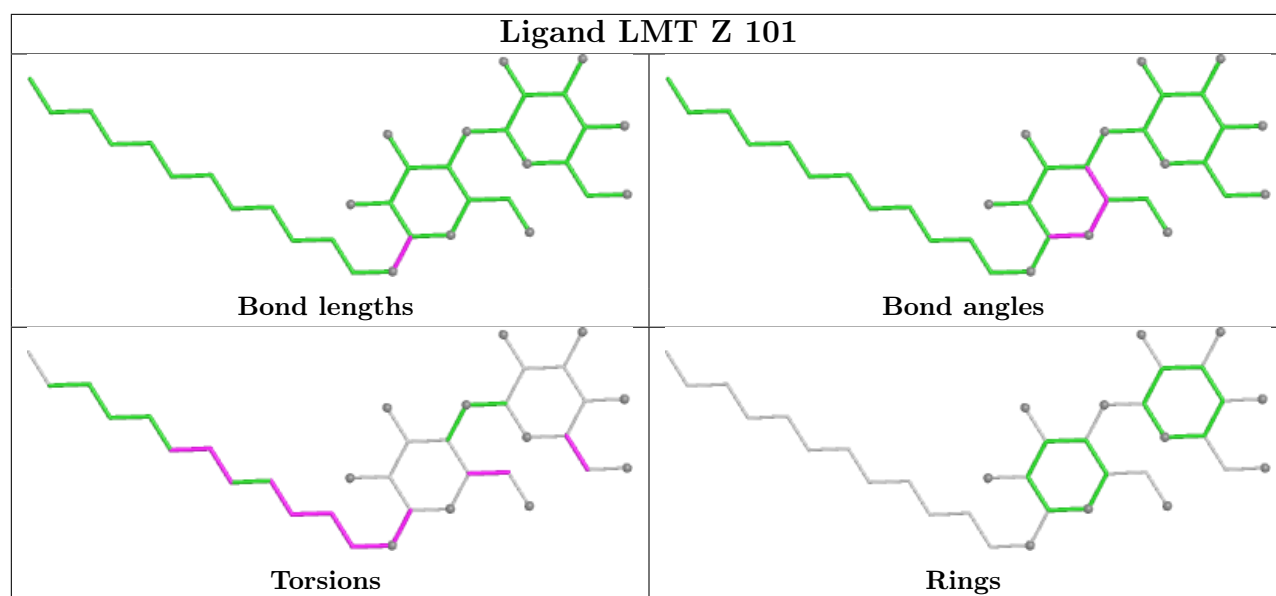




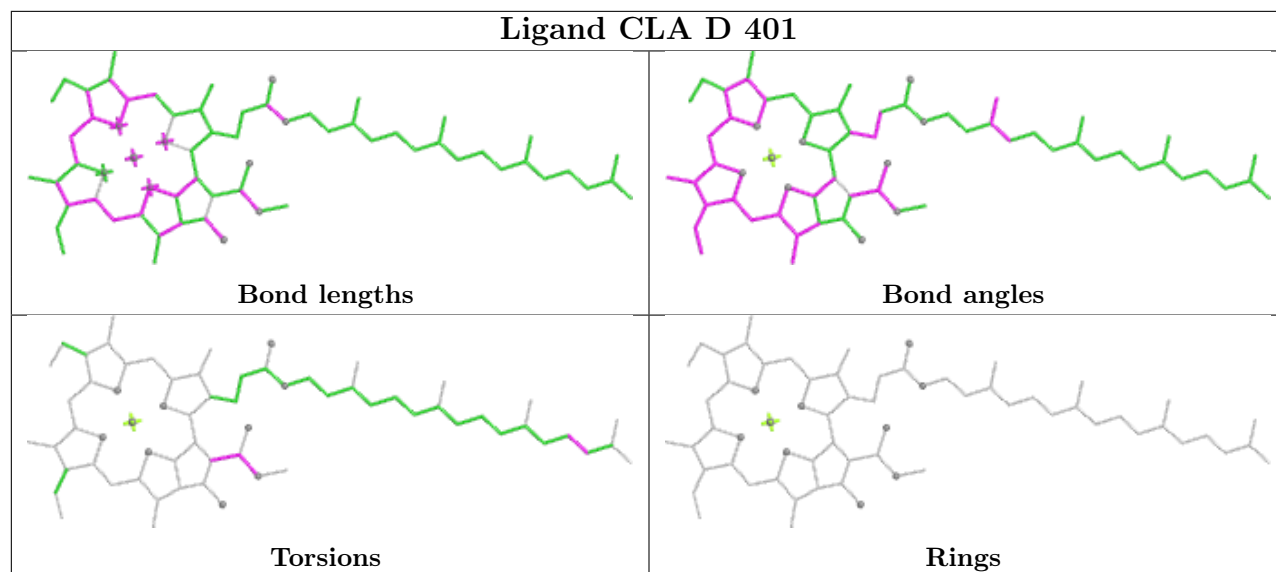




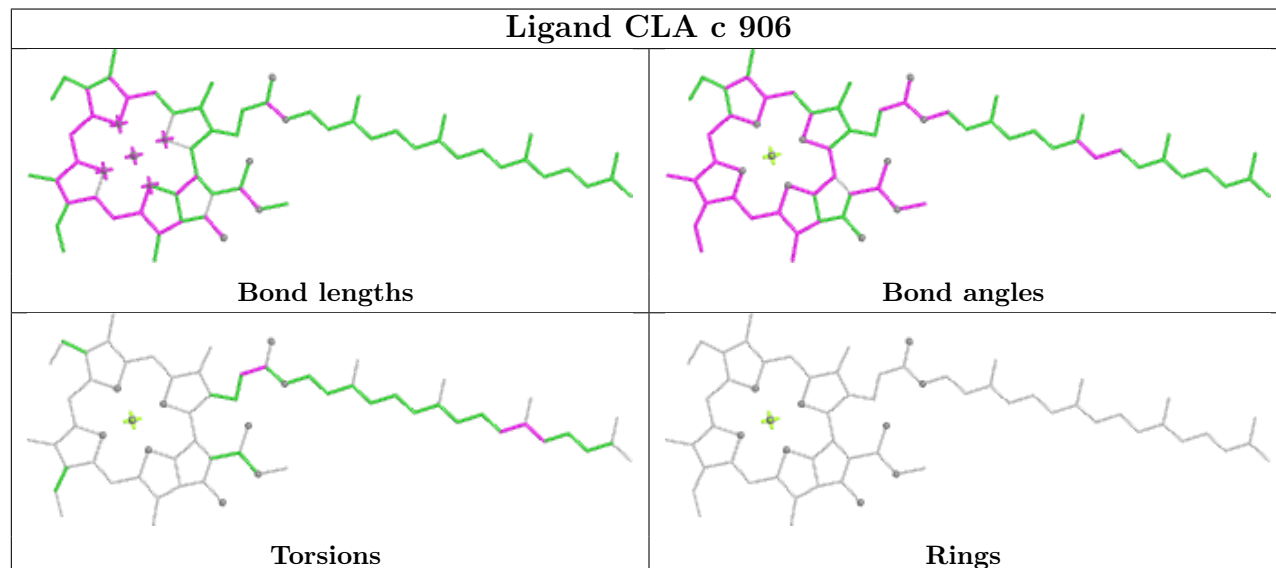




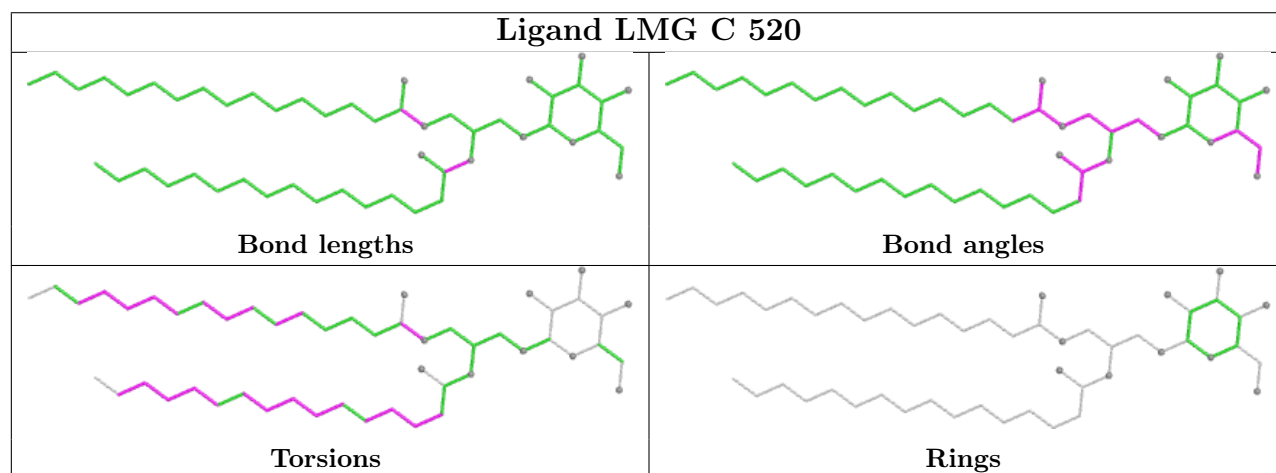
Ligand CLA D 401

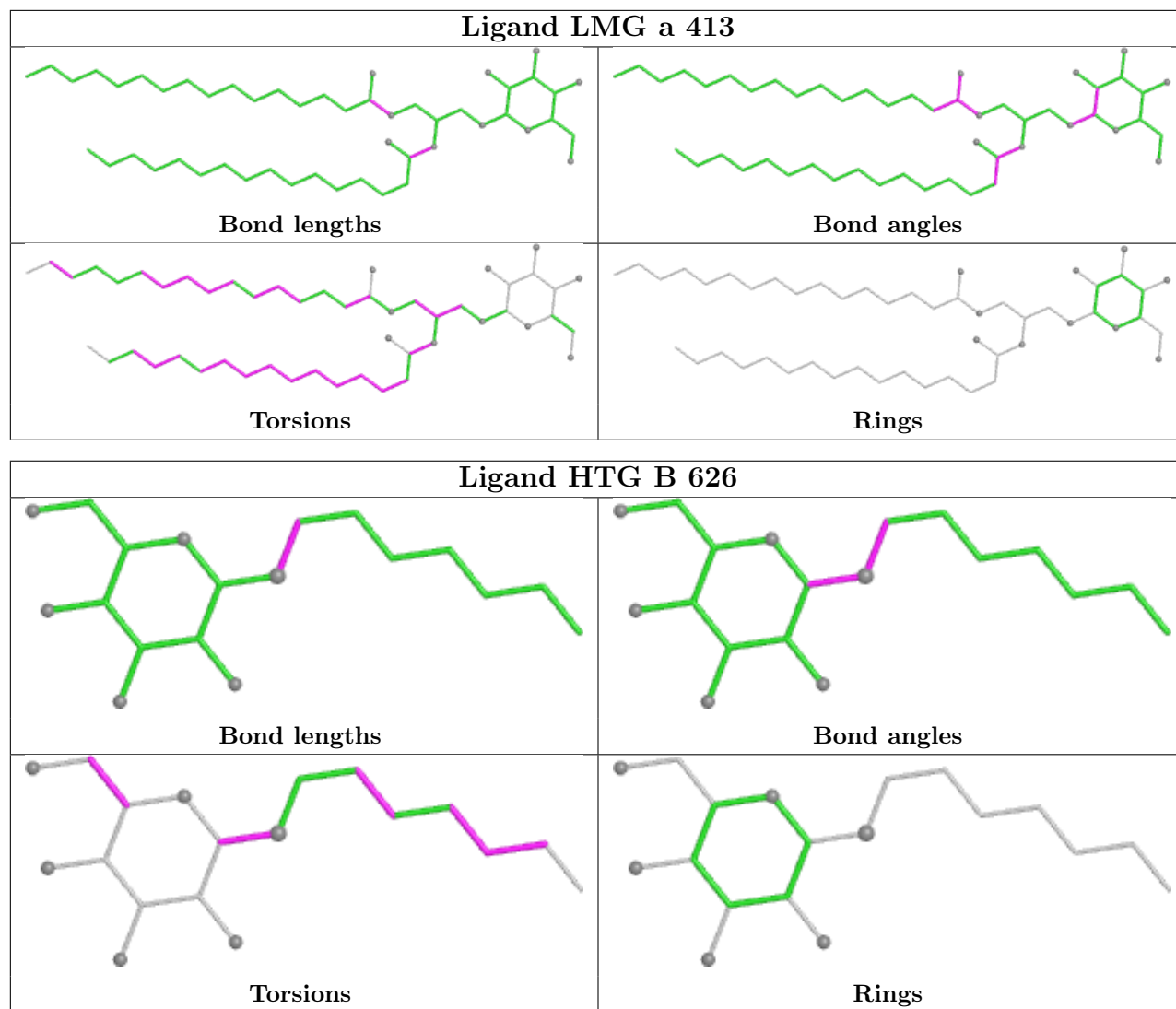


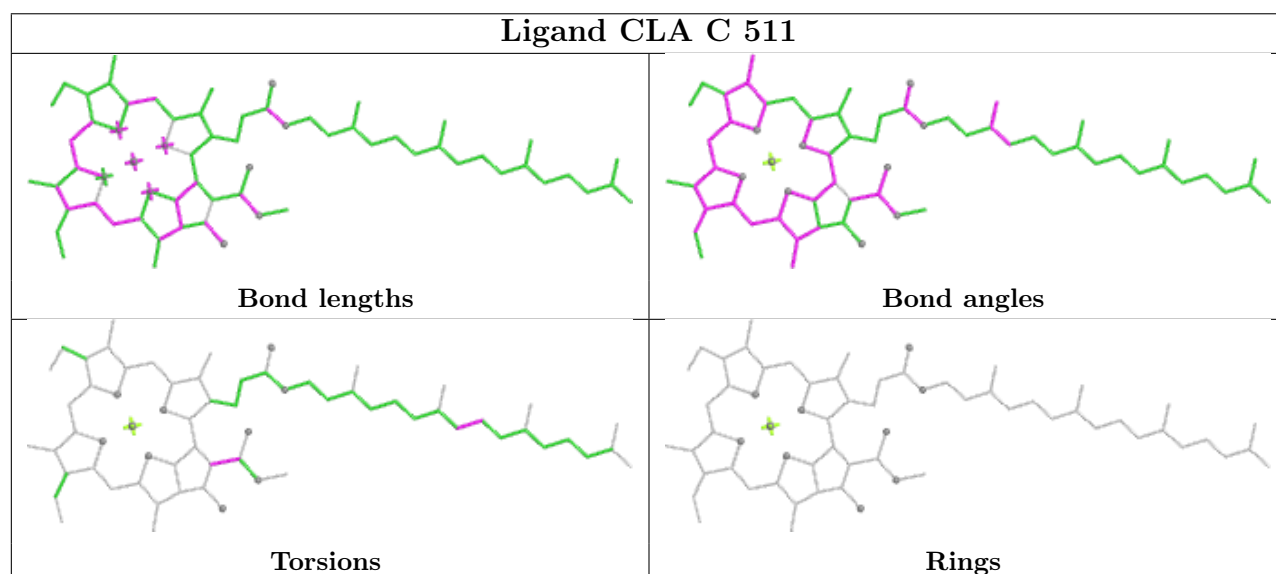
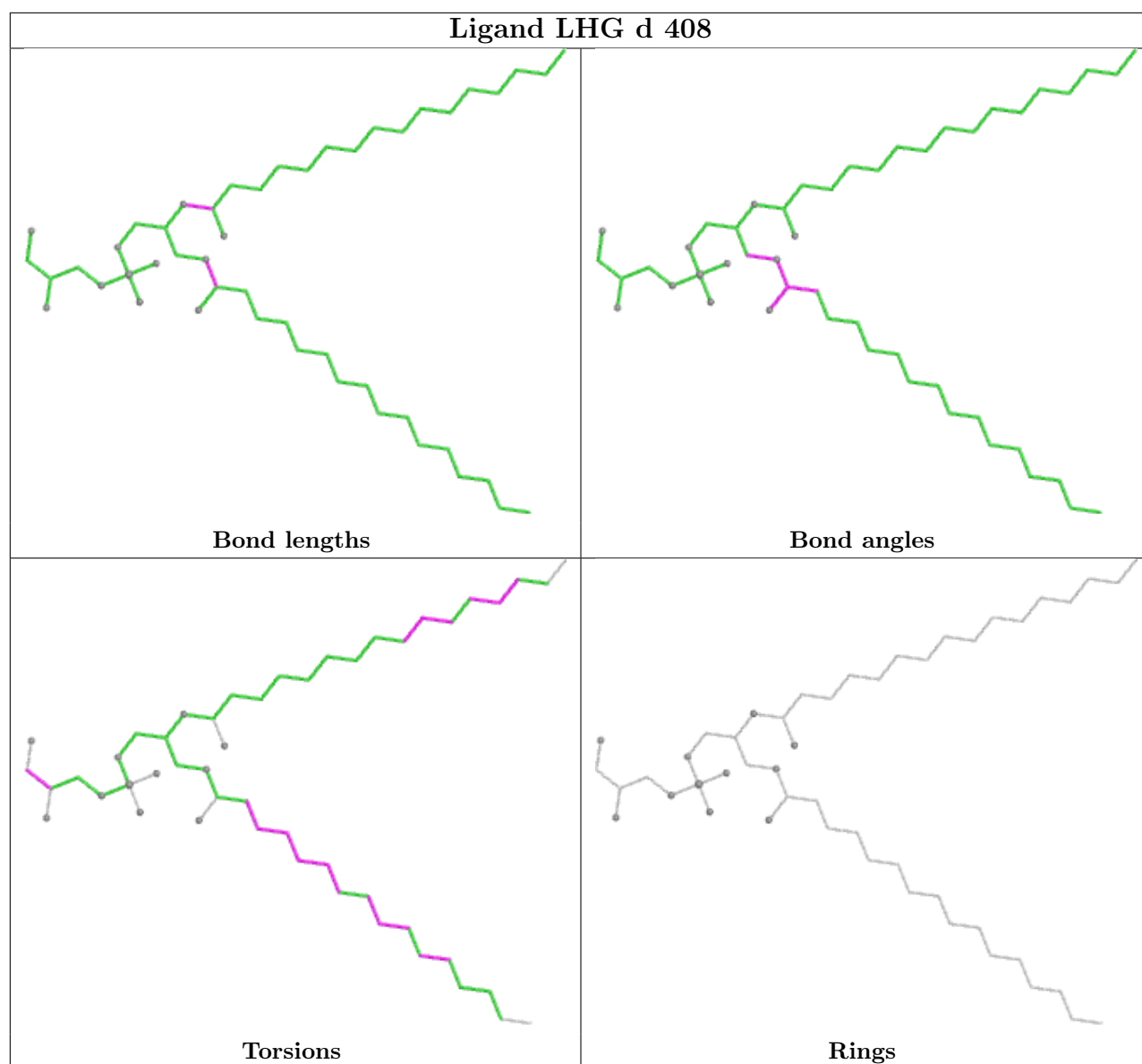
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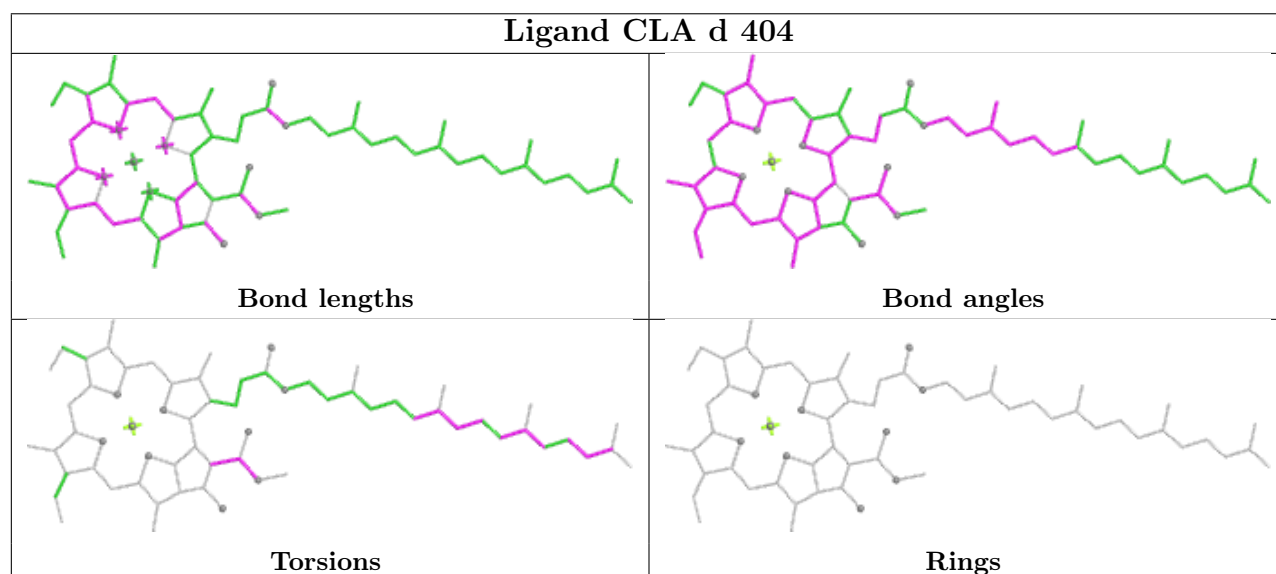
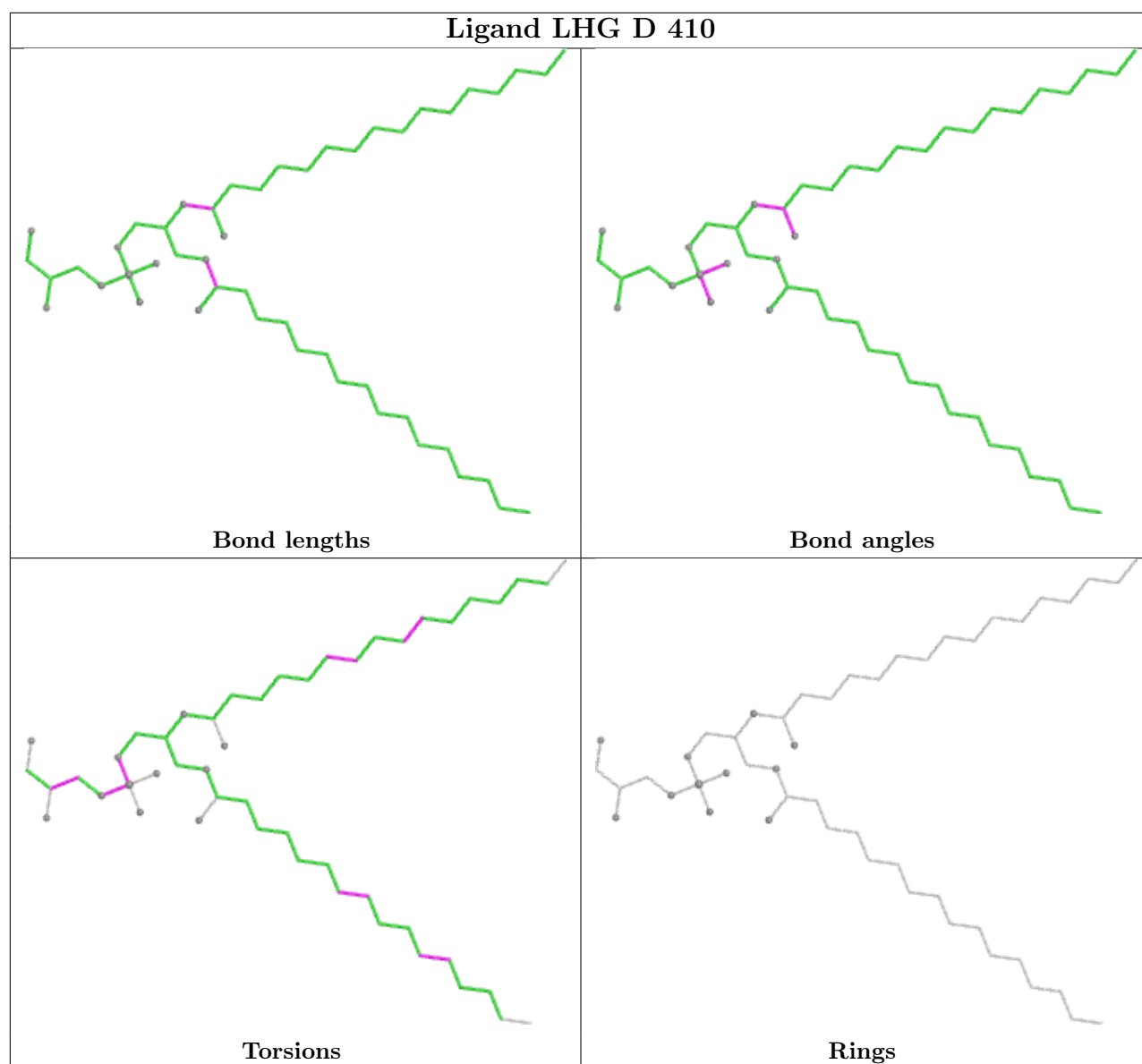


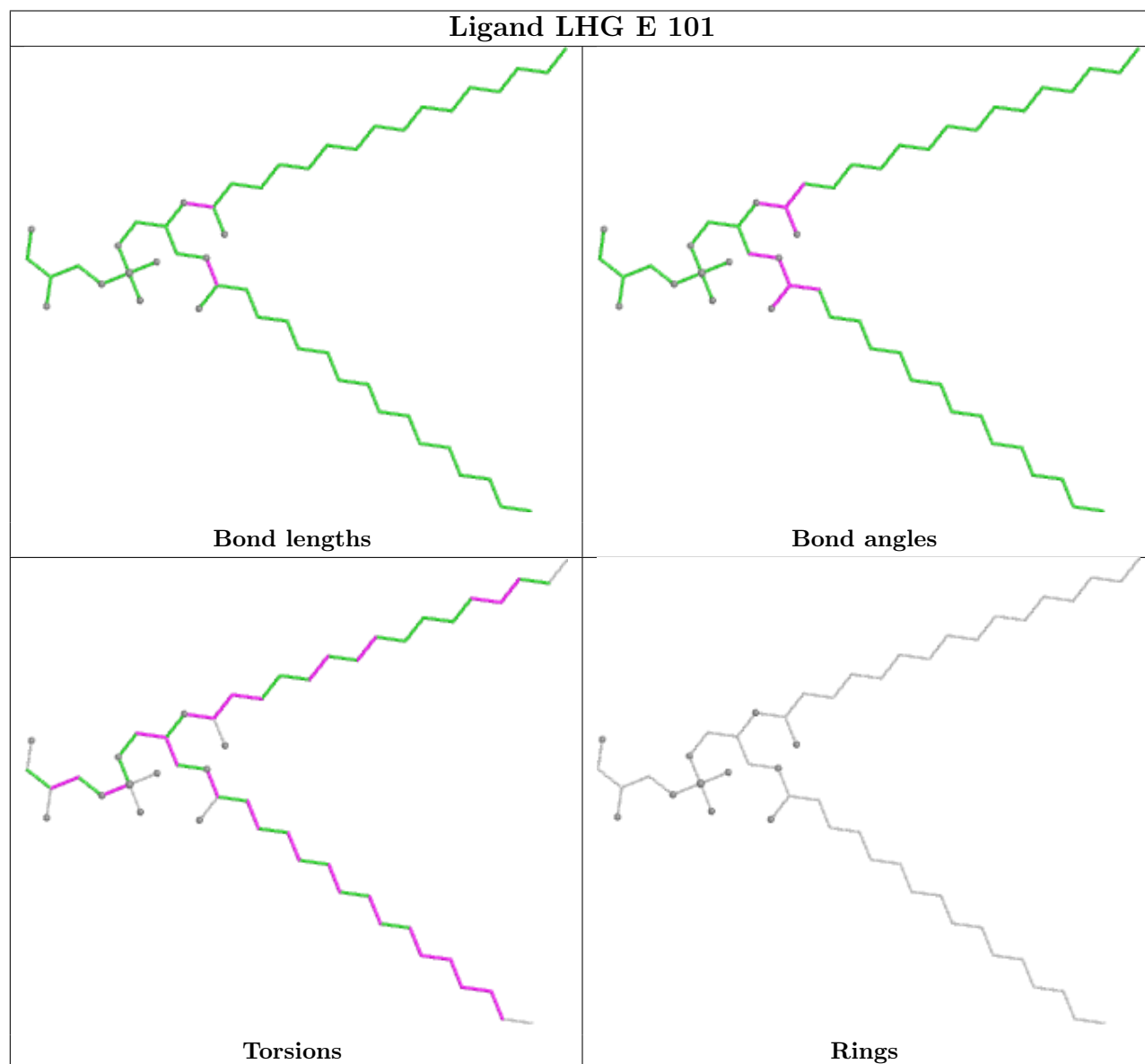
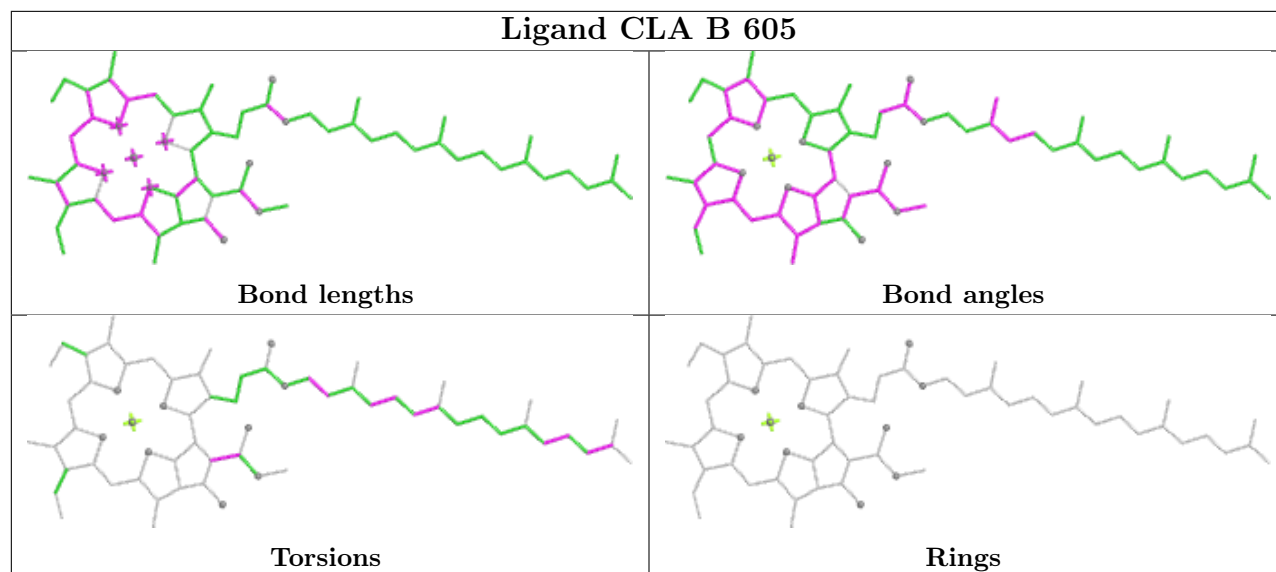
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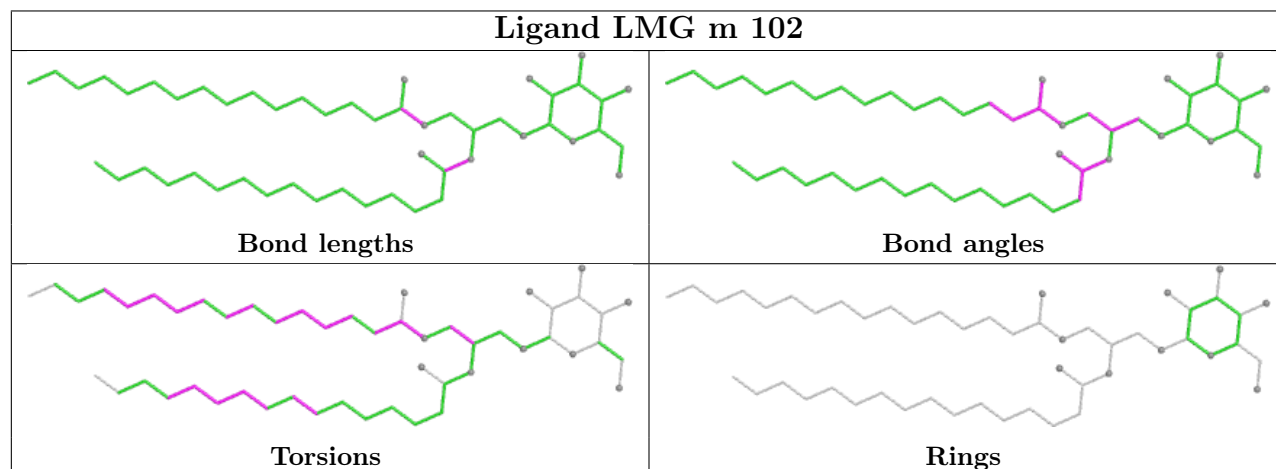
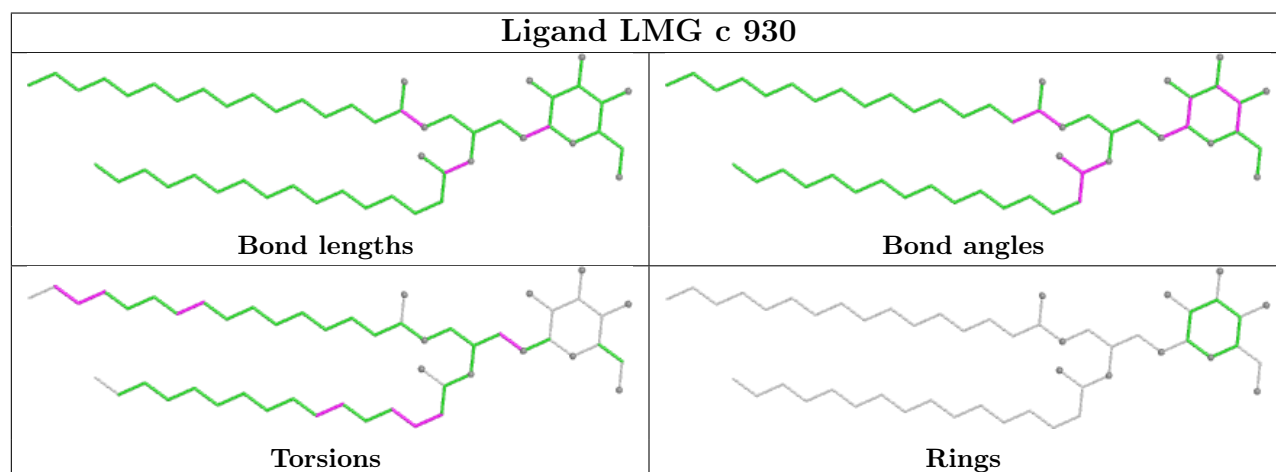
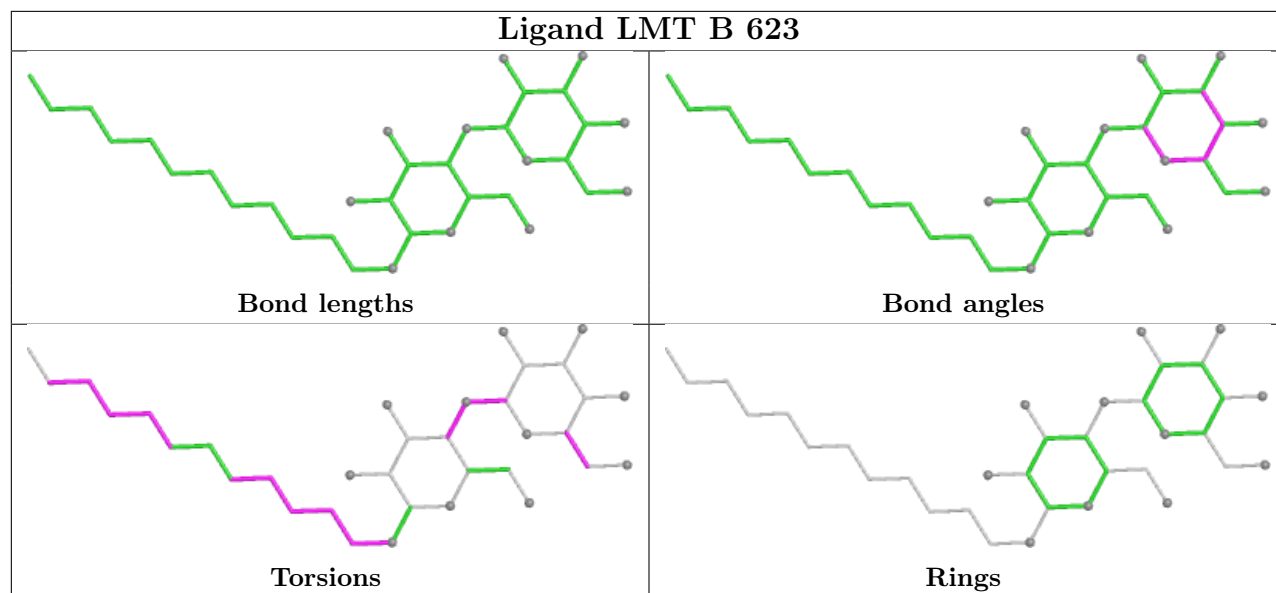


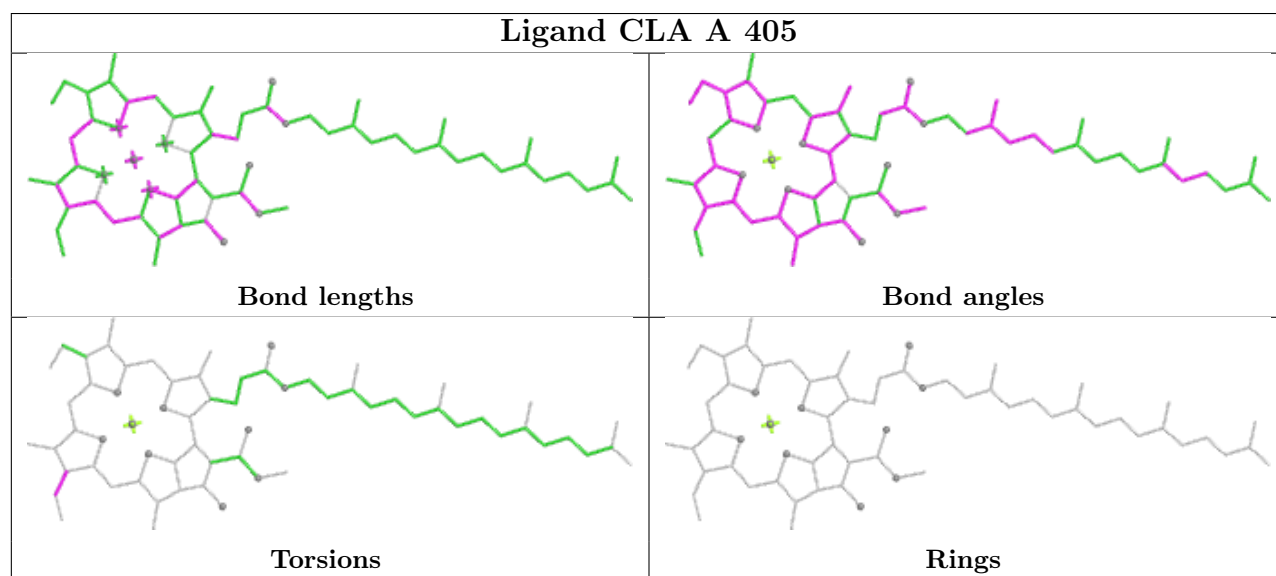
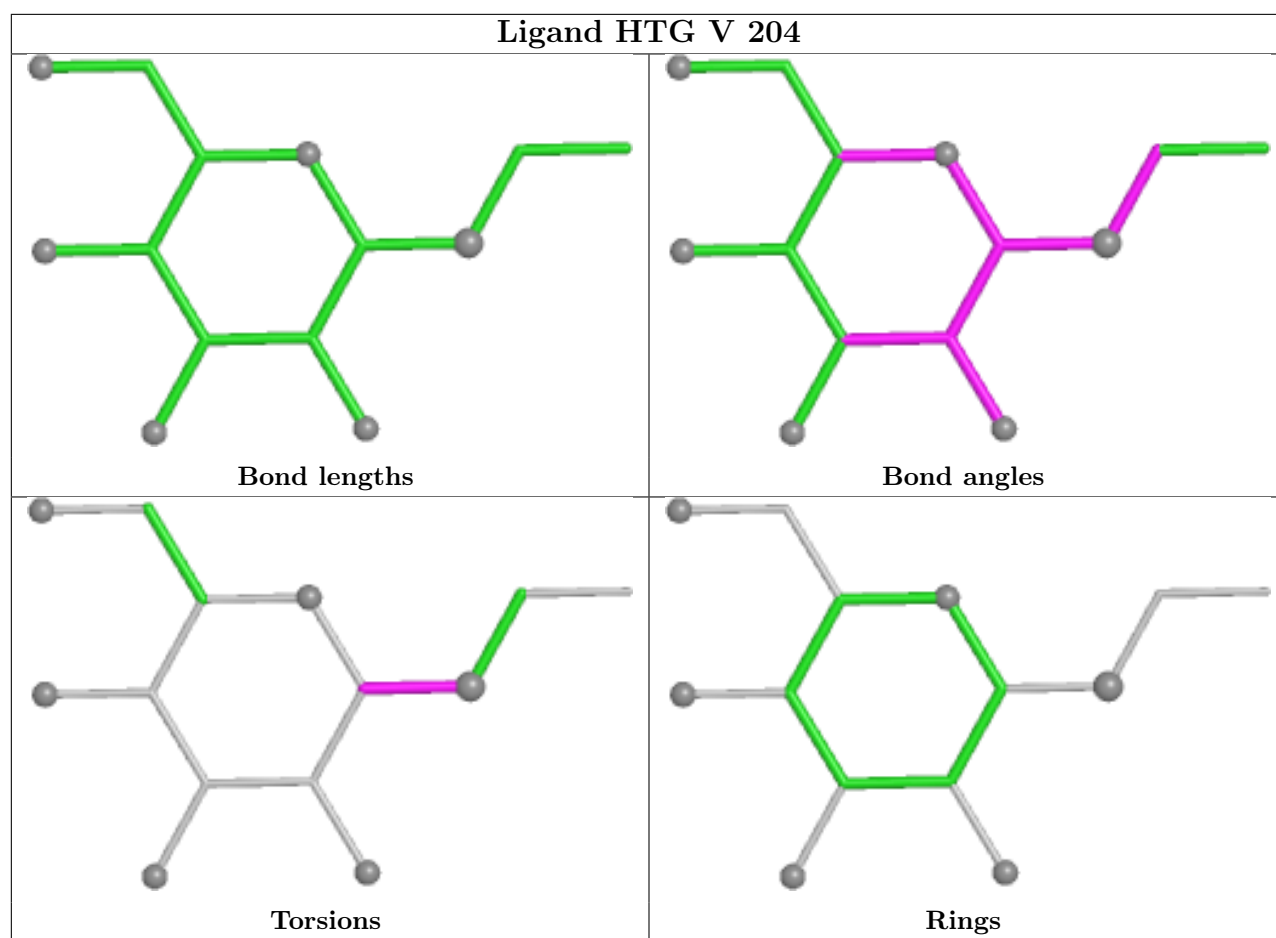


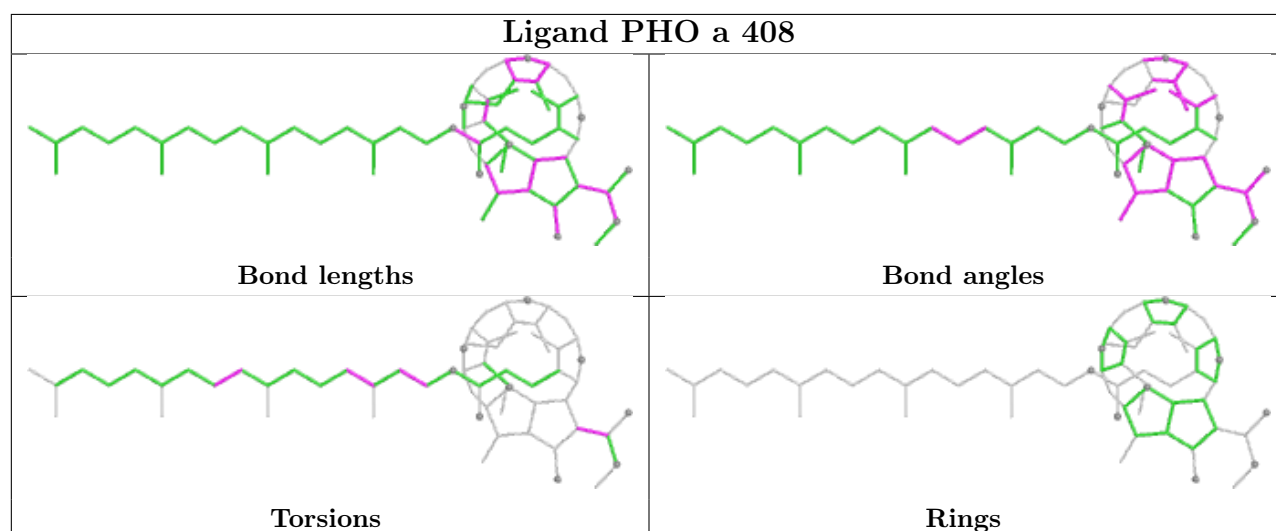
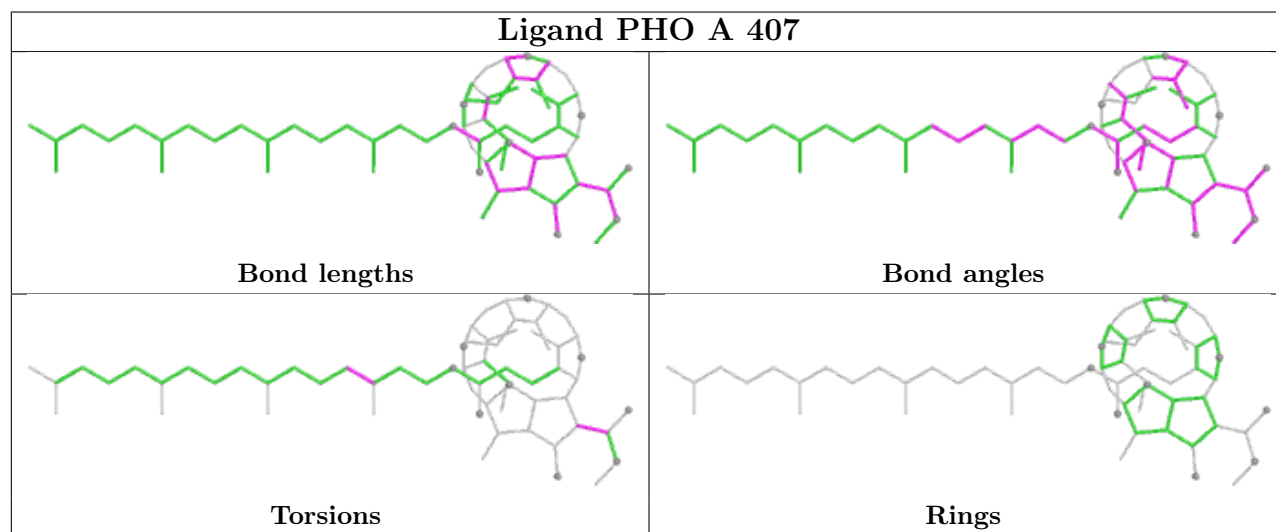
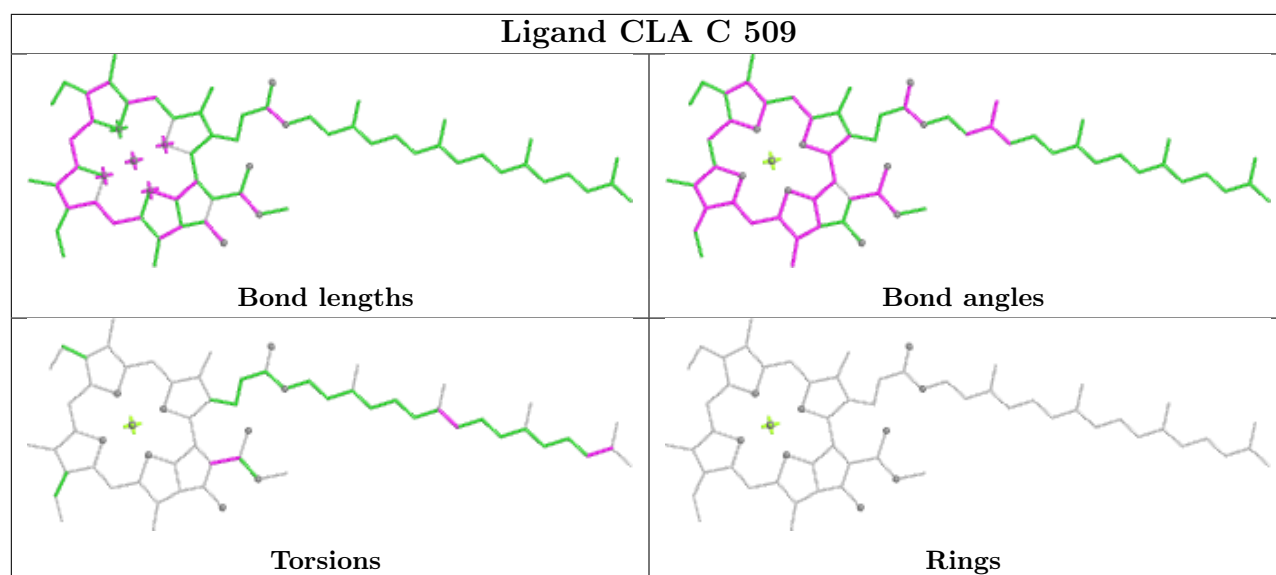




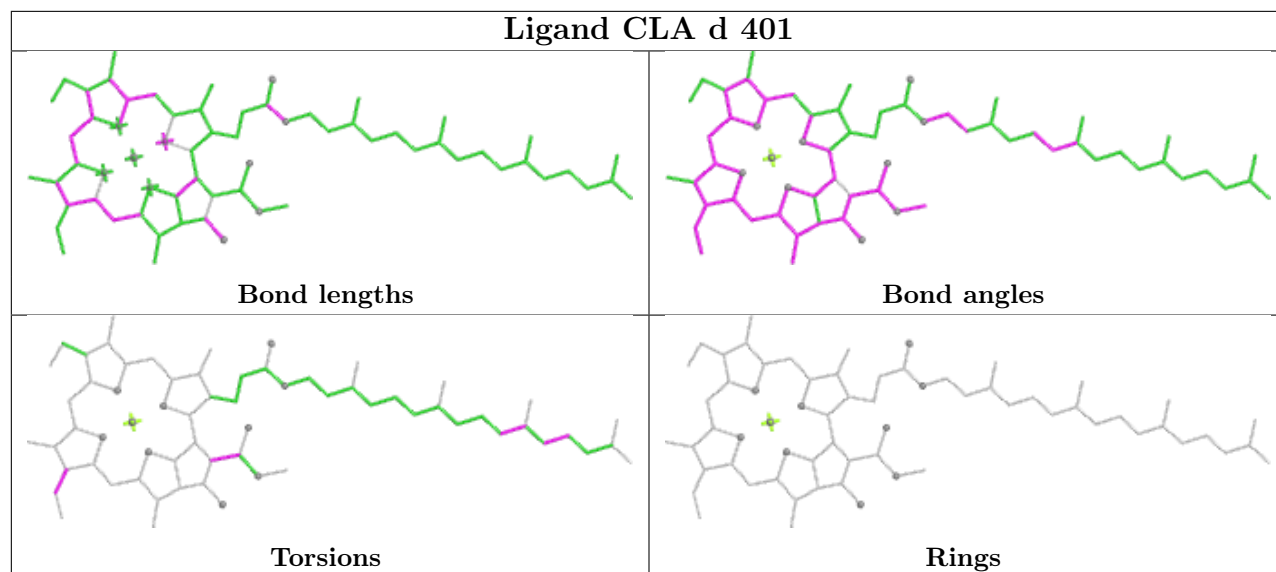




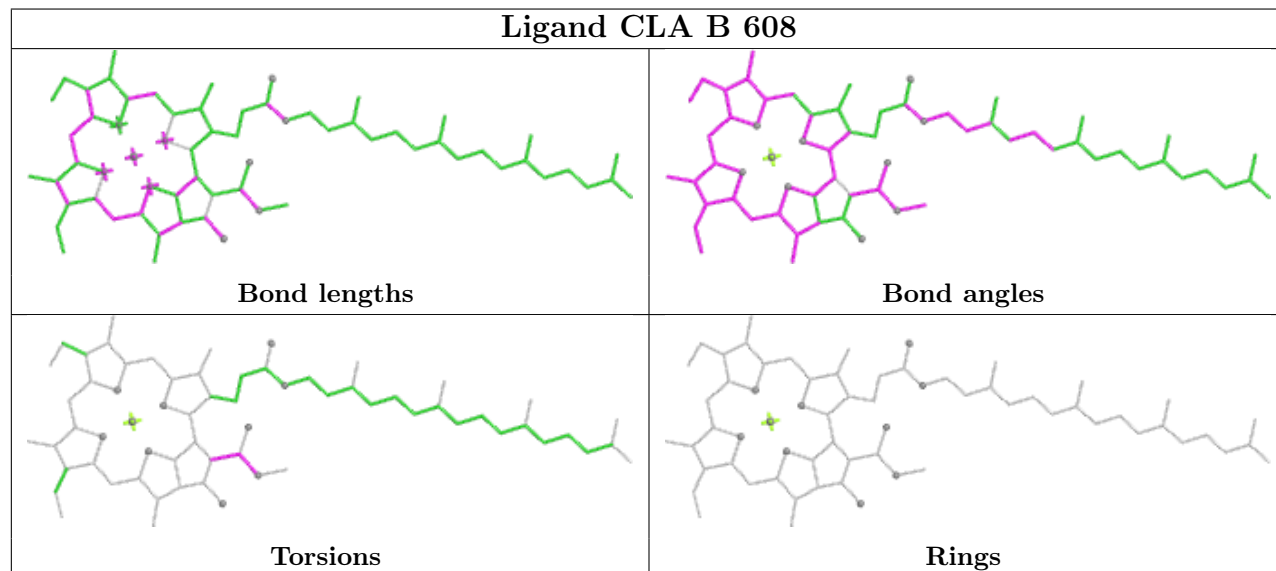




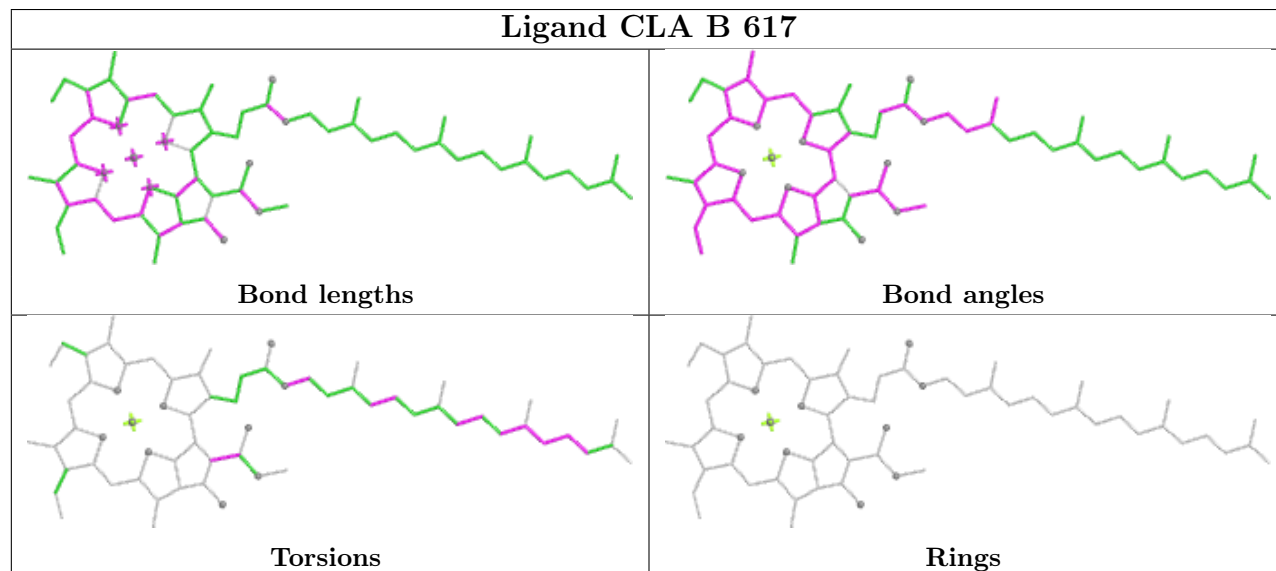
Ligand CLA d 401

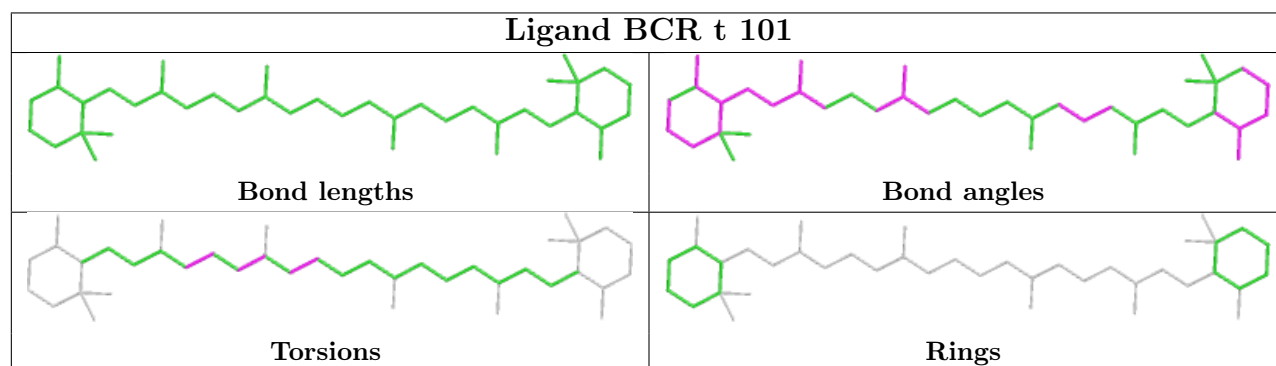
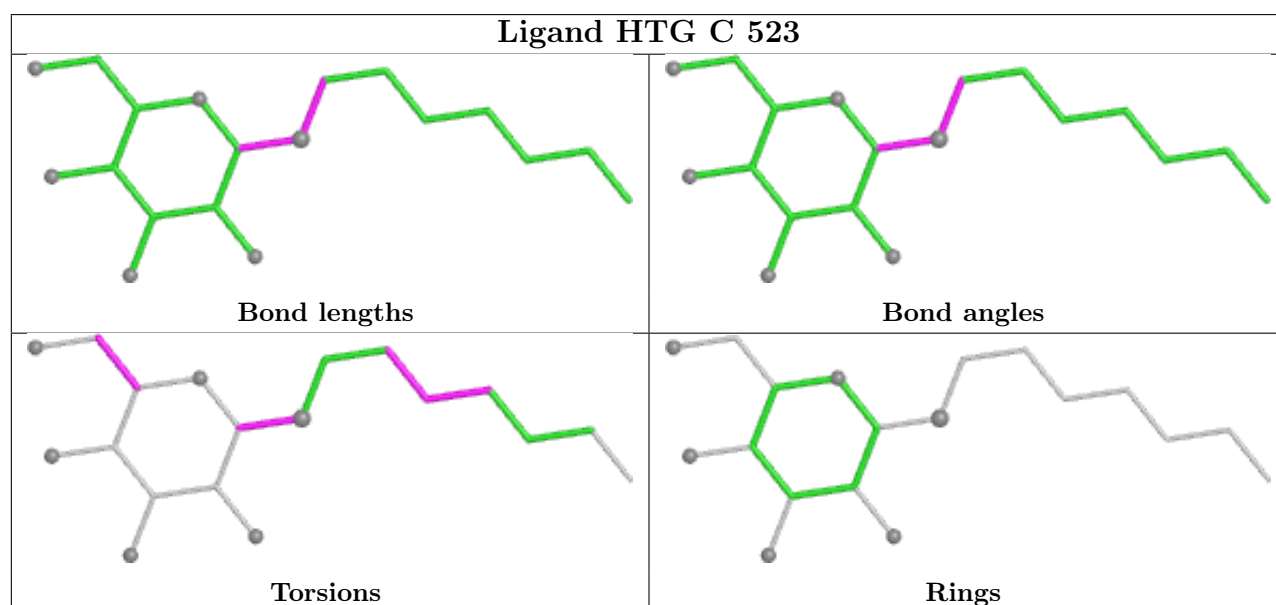
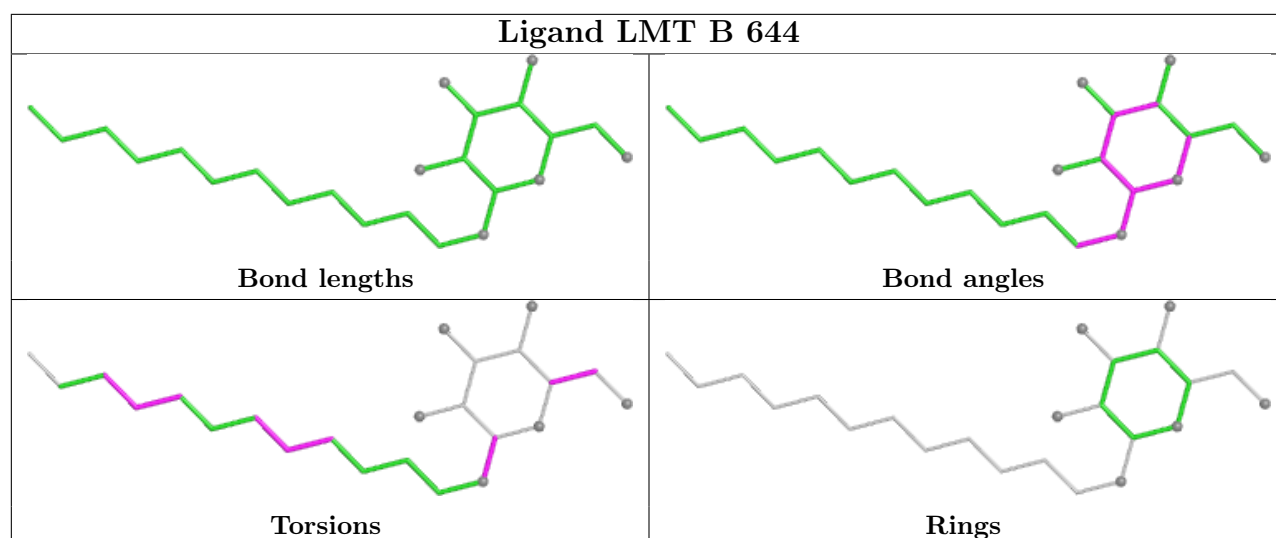


Ligand CLA B 608

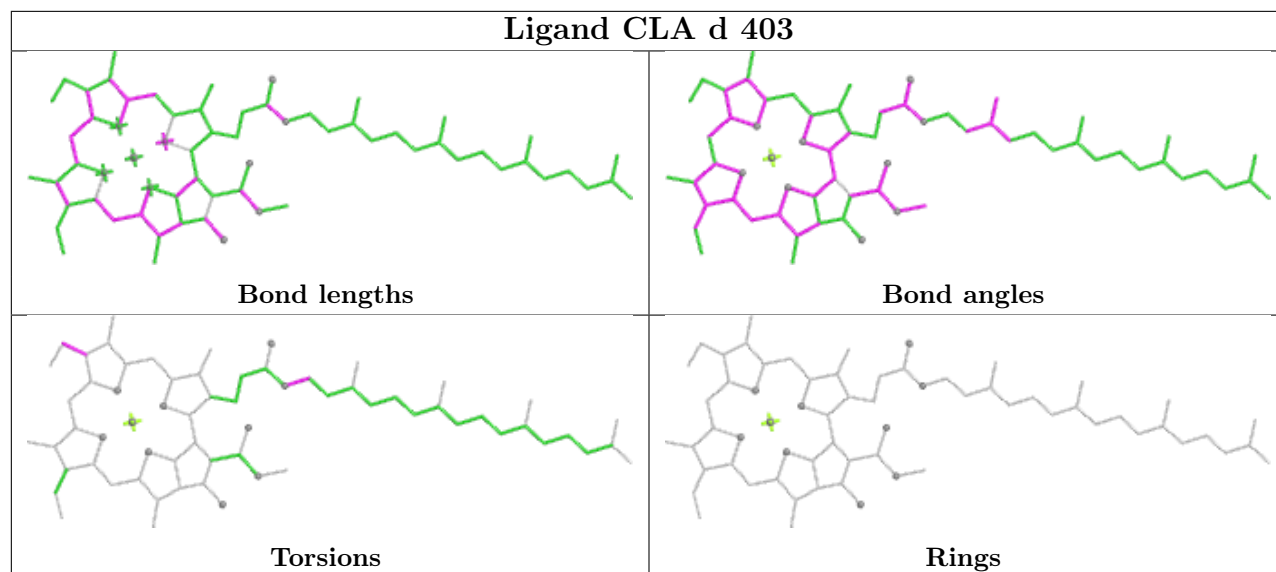


Ligand CLA B 617

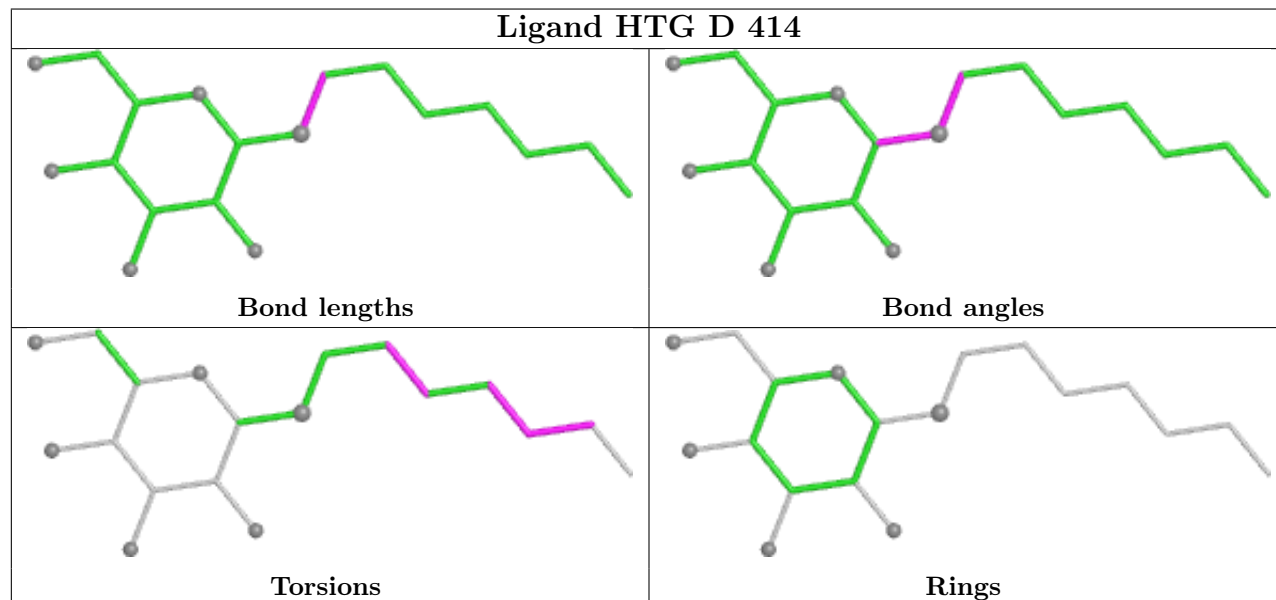




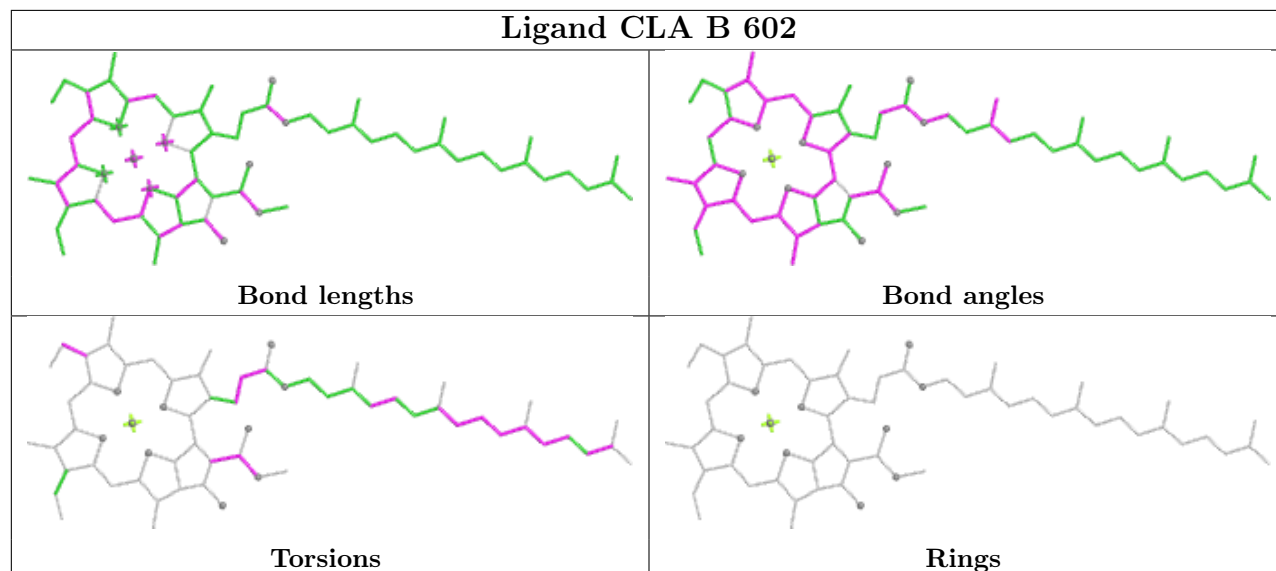
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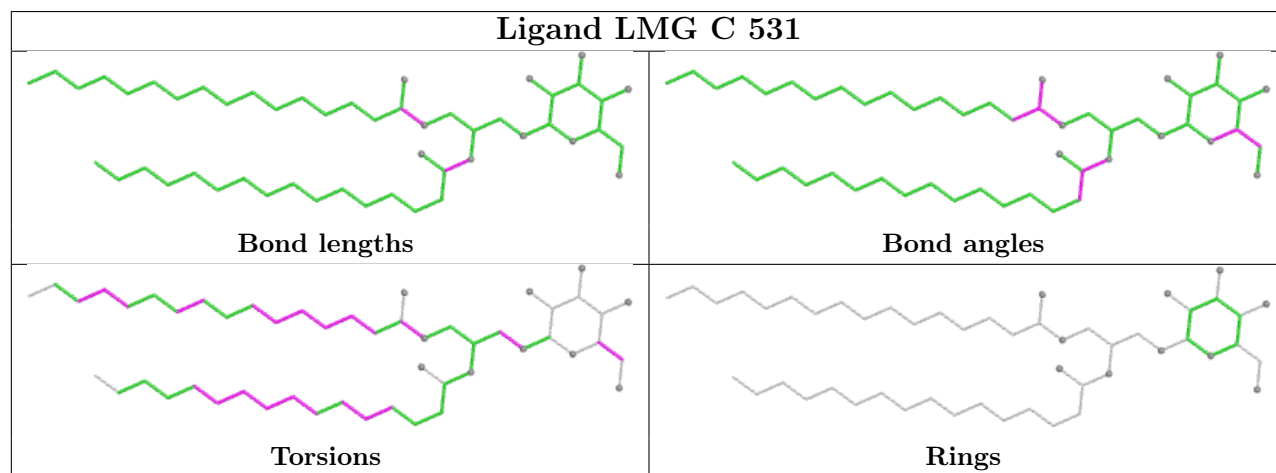
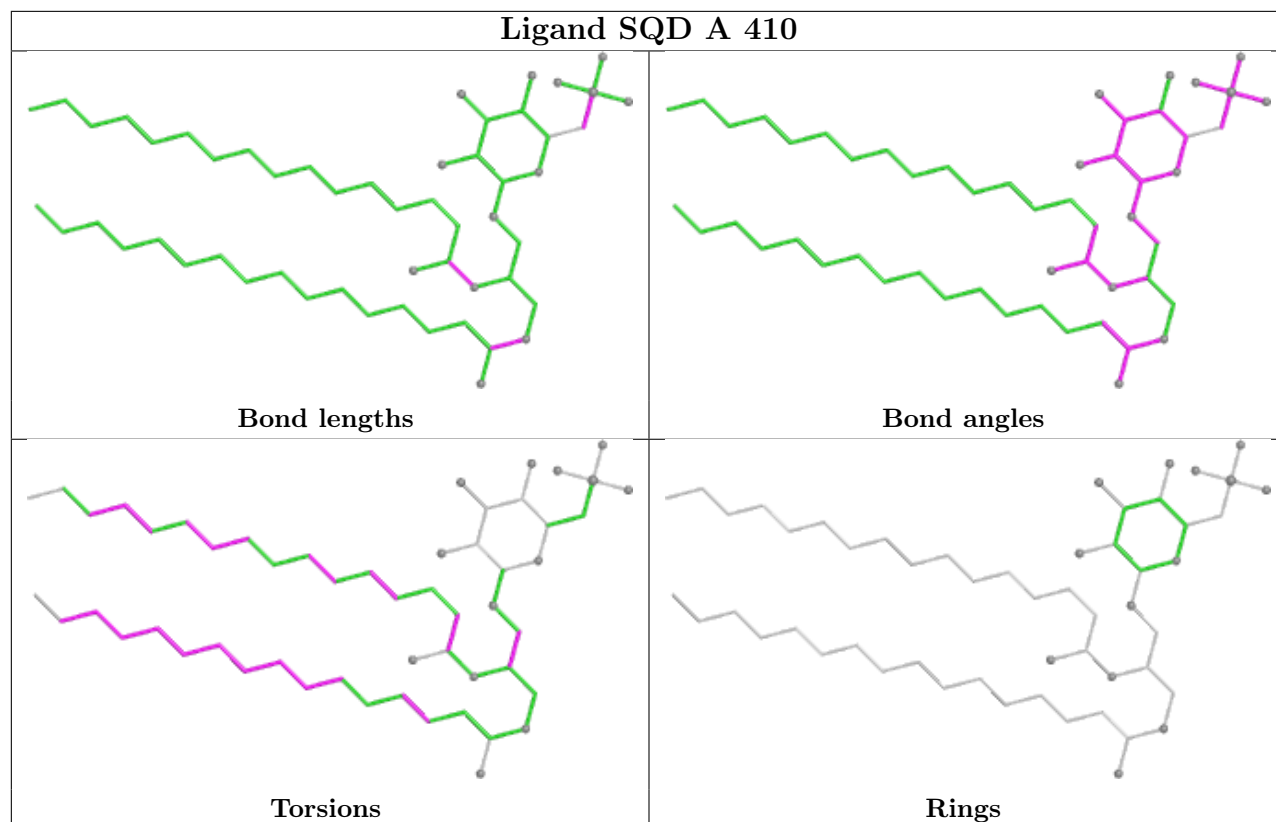


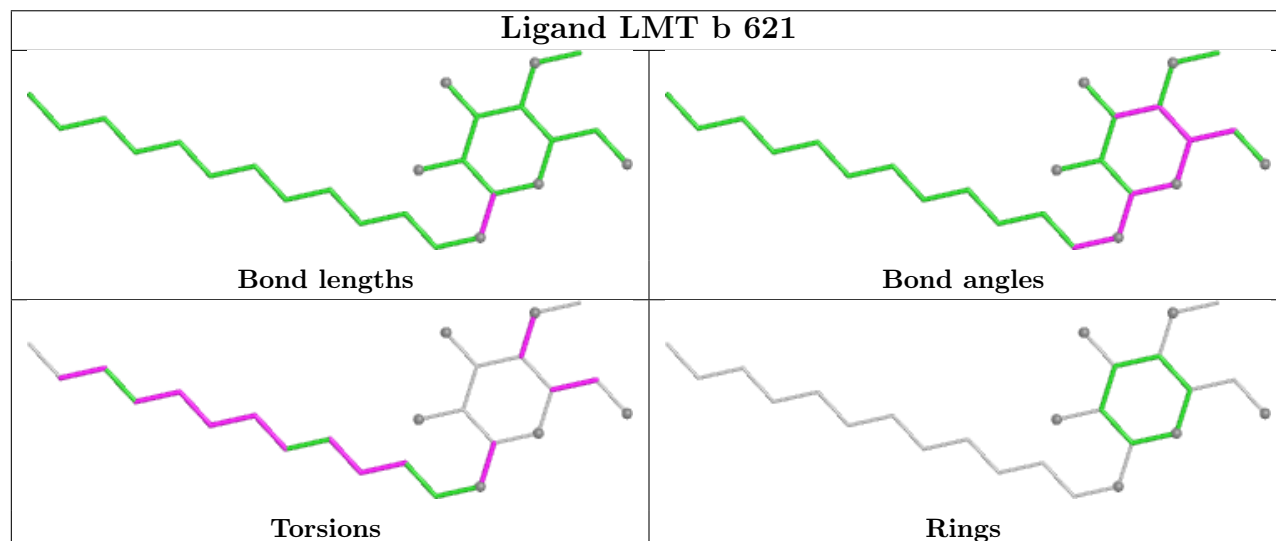
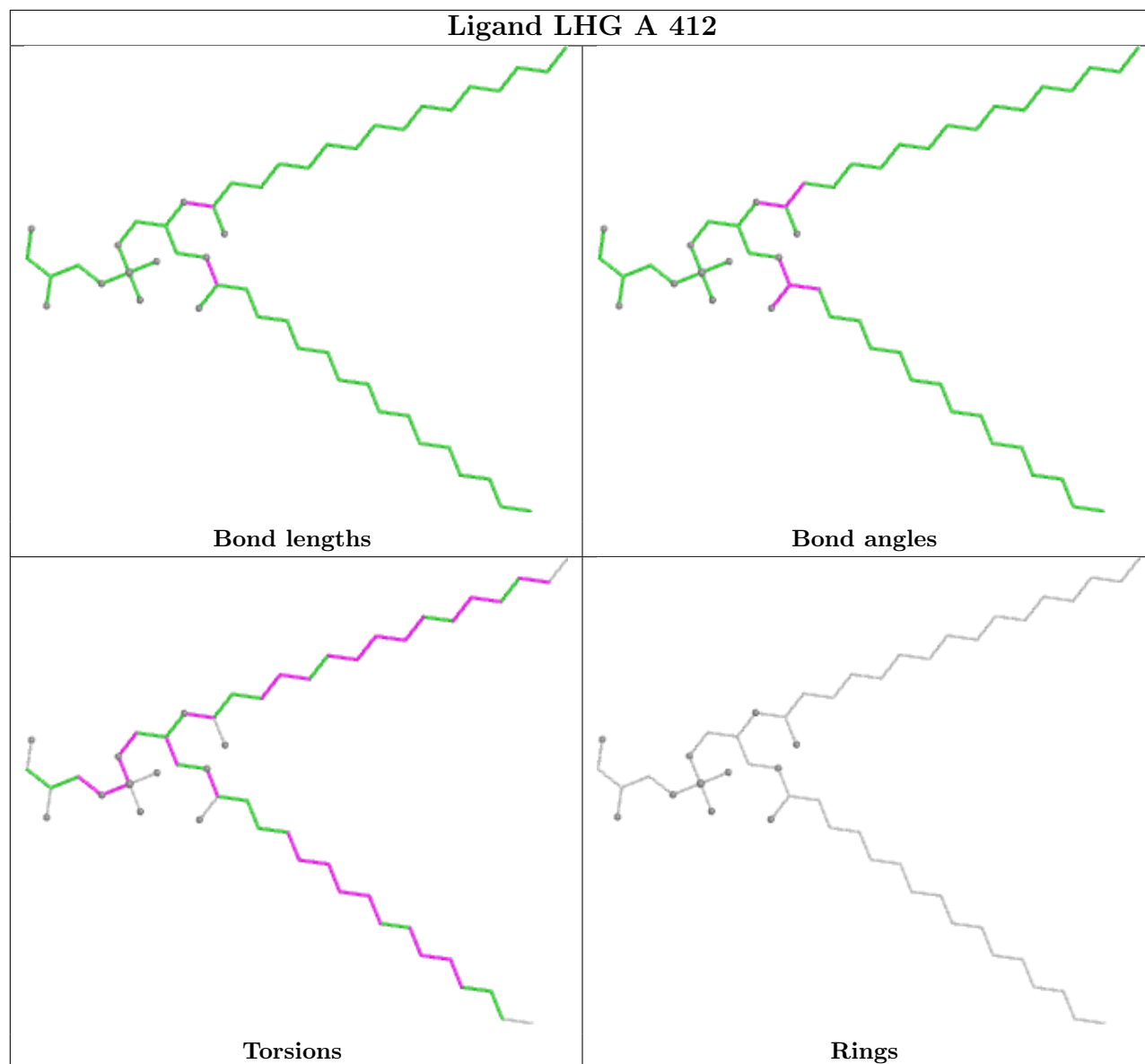
Ligand HTG D 414

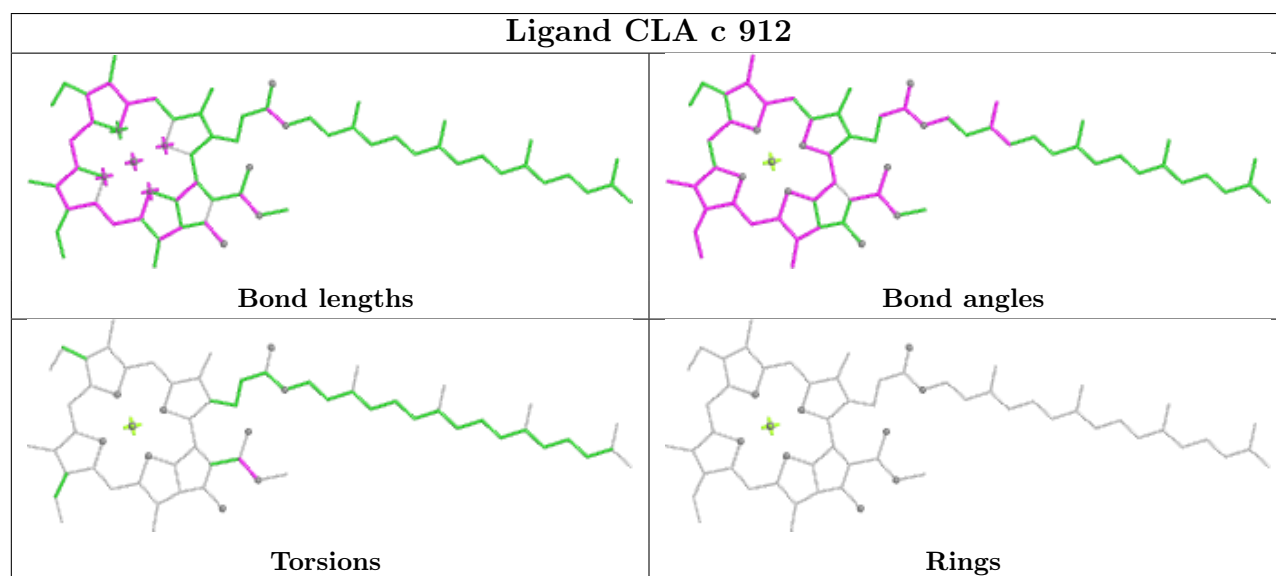
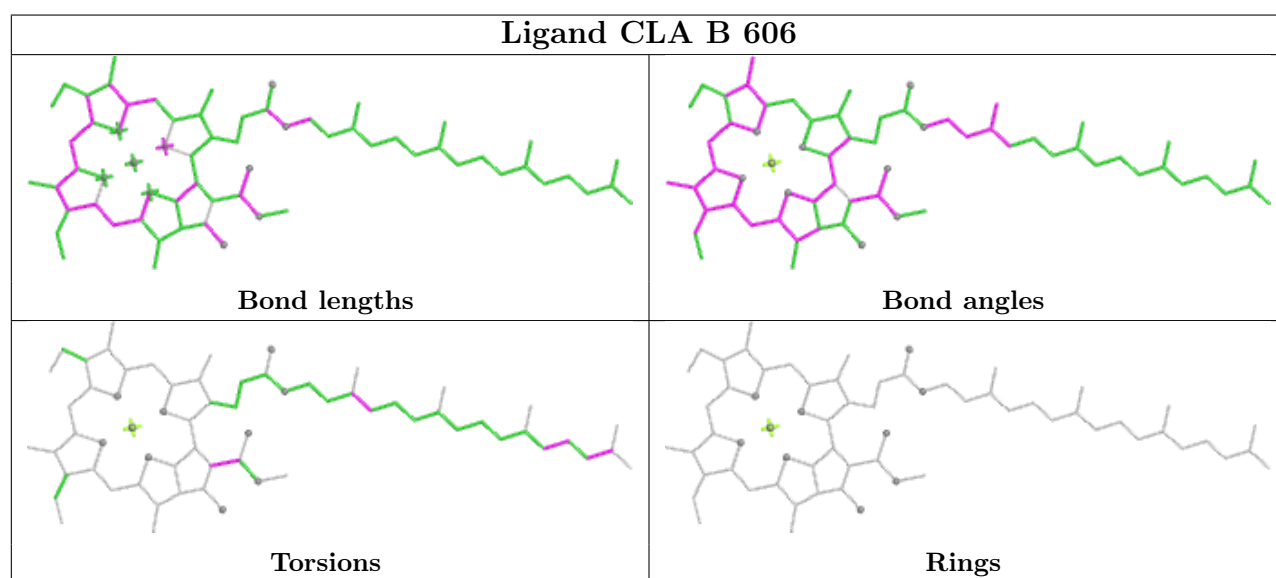
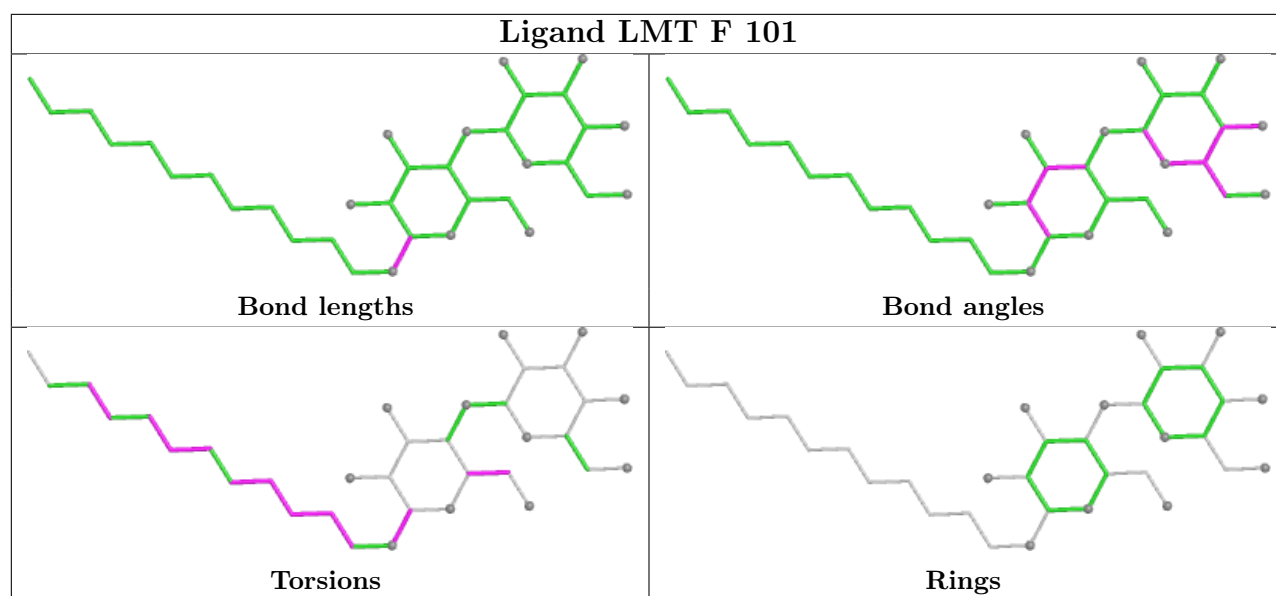


Ligand CLA B 602

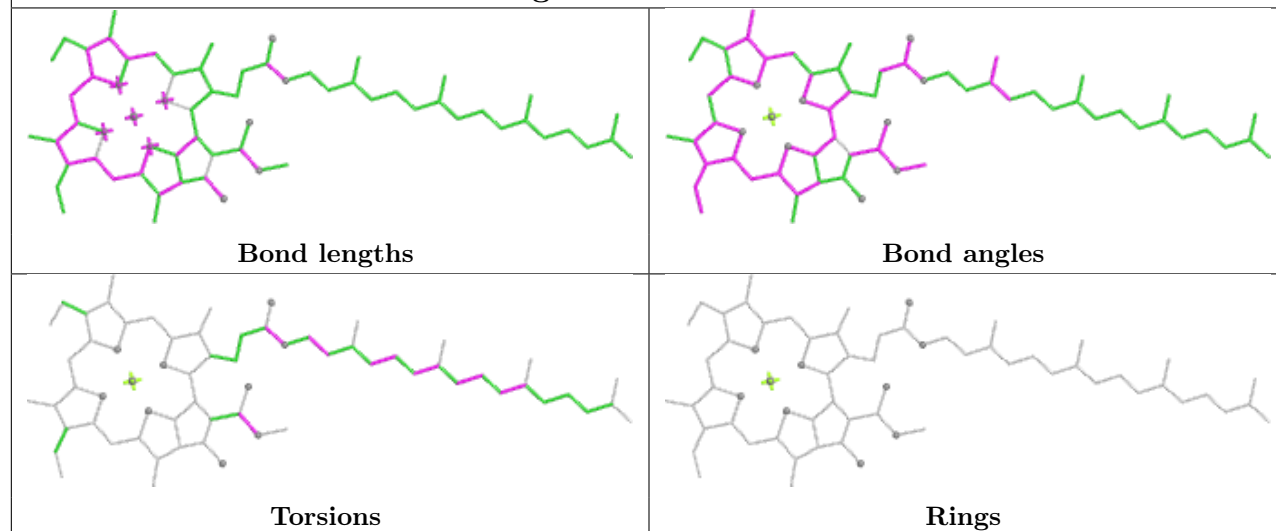




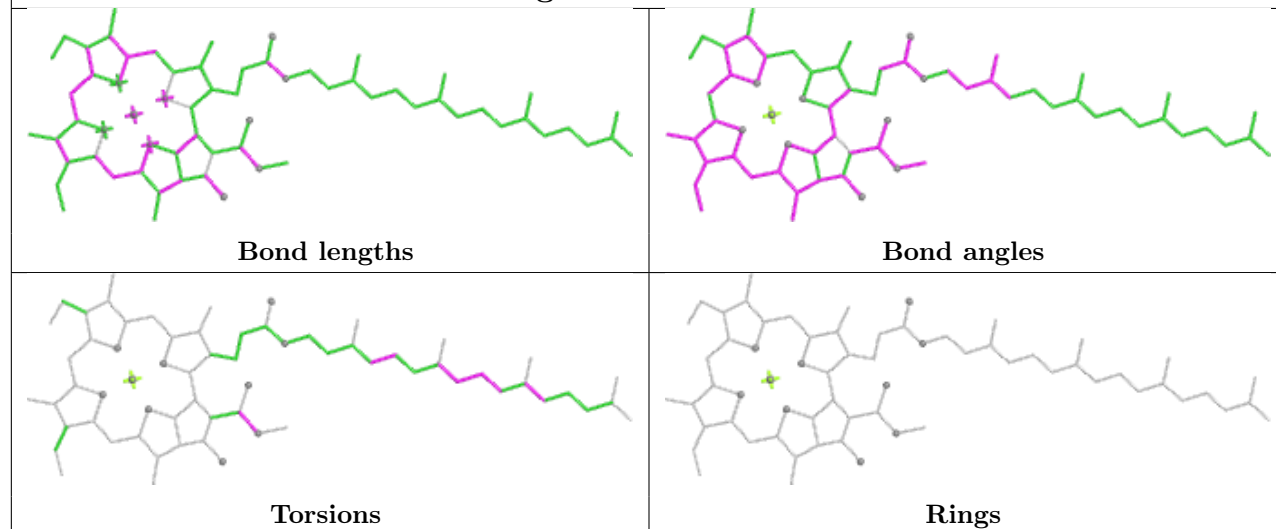




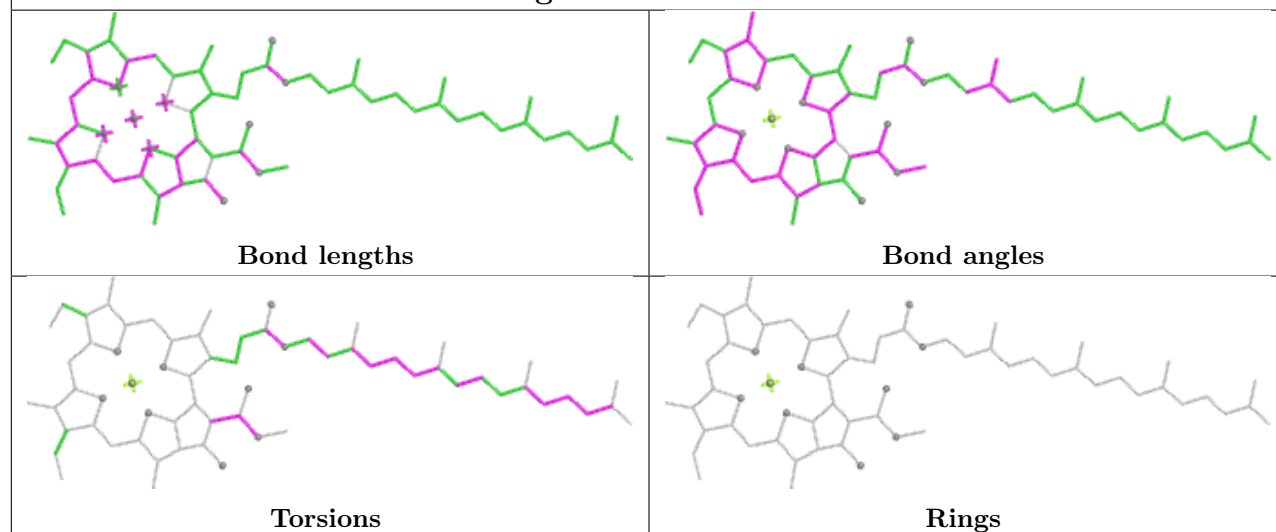
Ligand CLA C 514

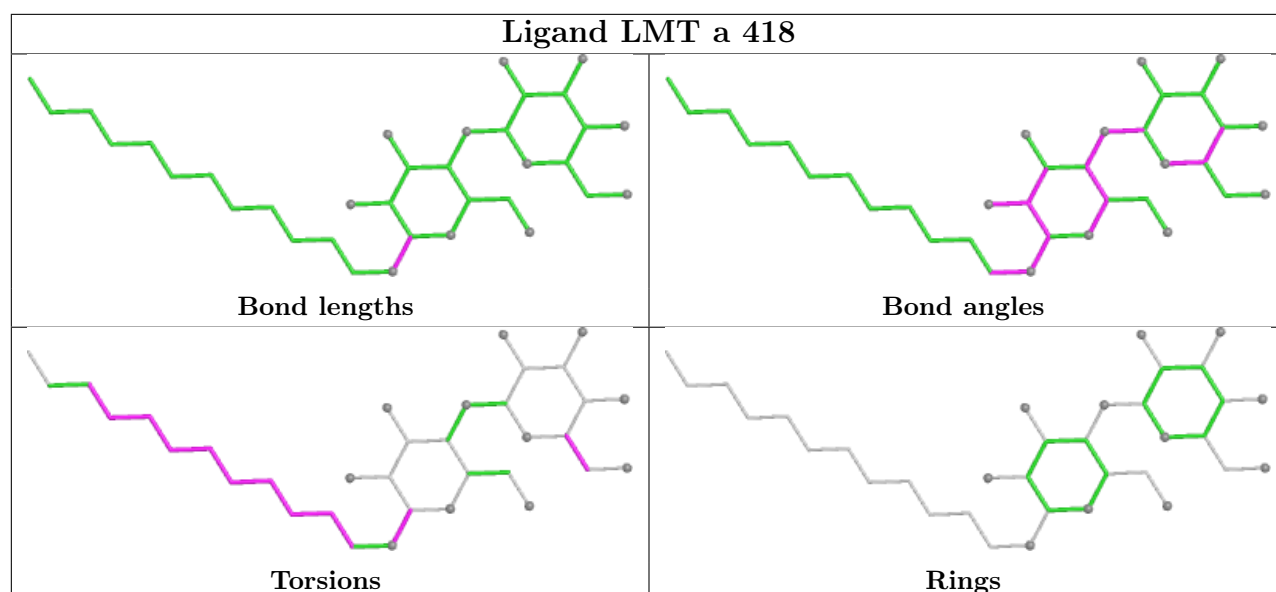
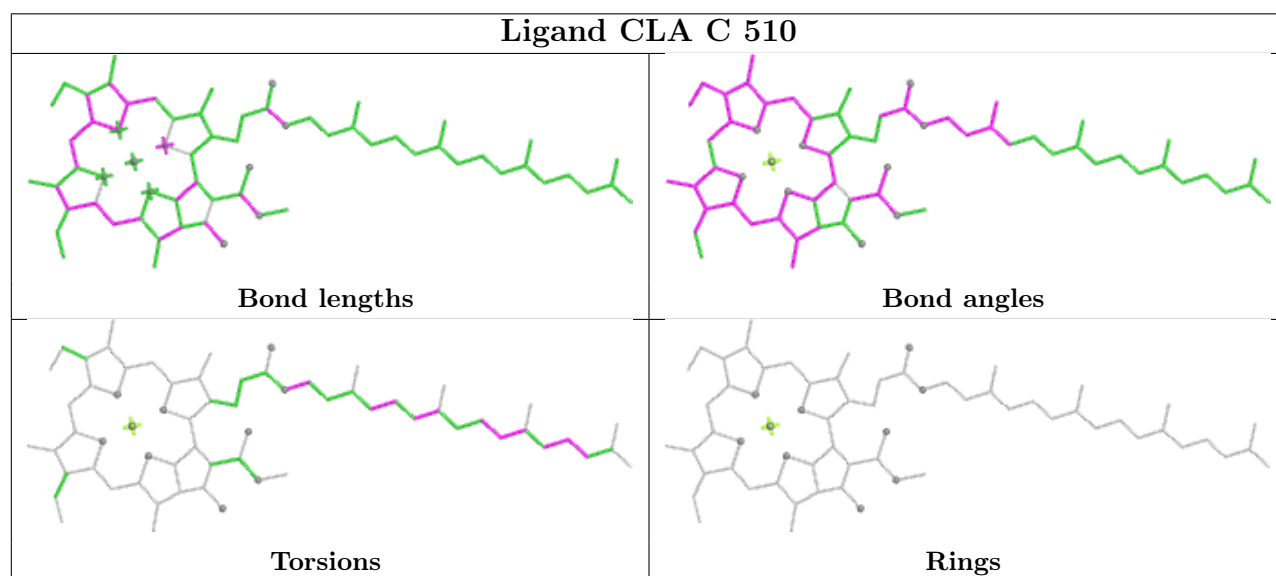
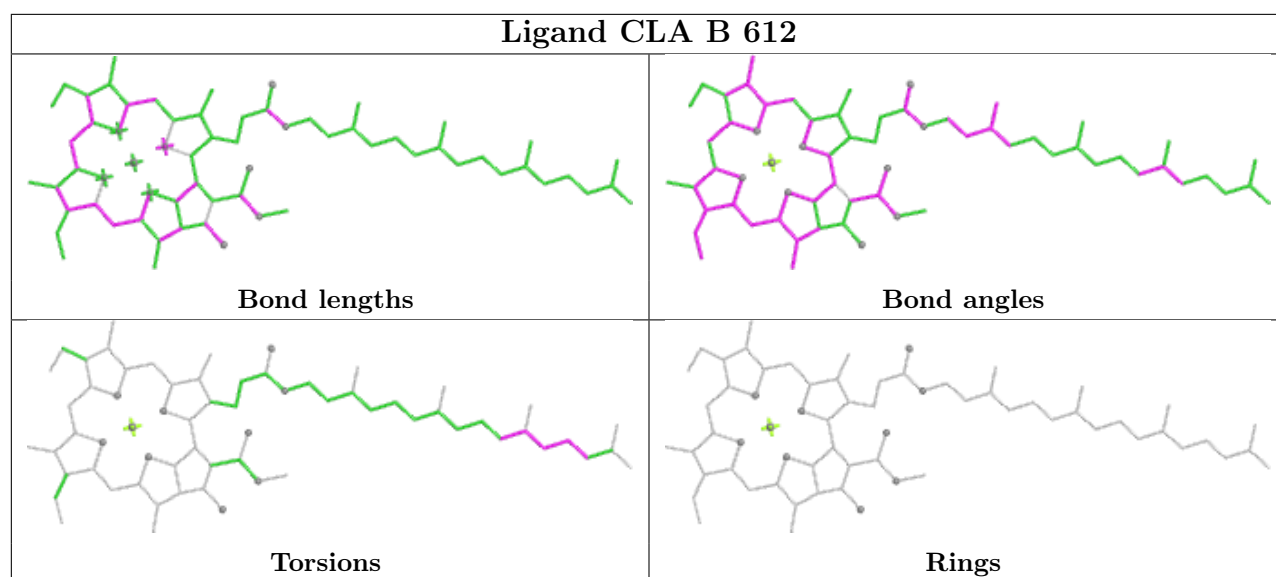


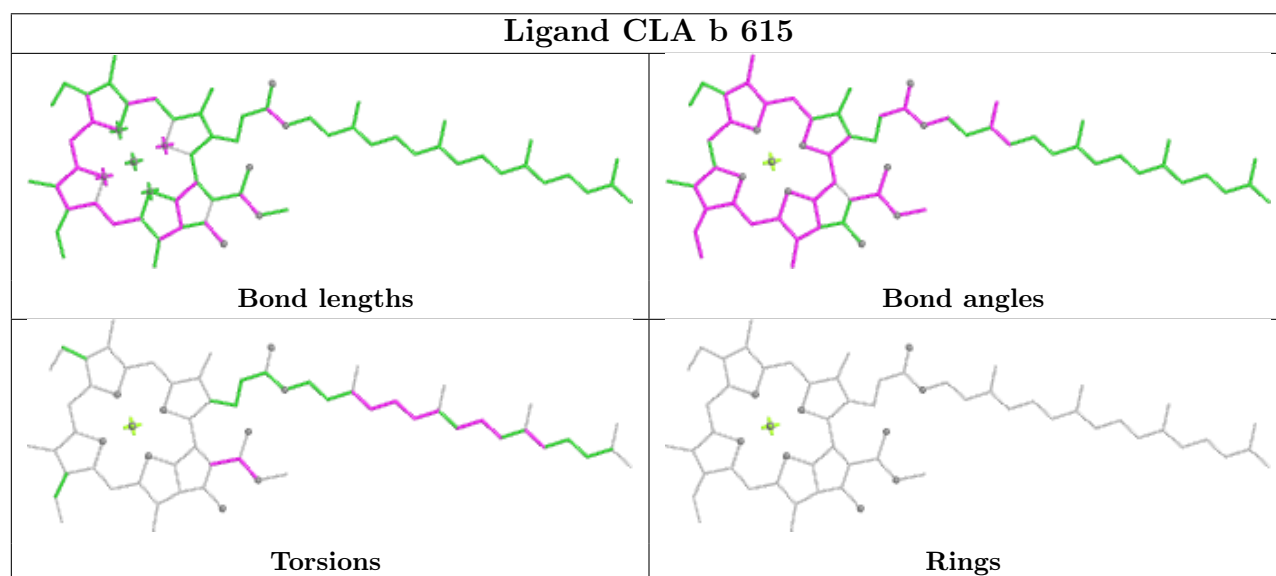
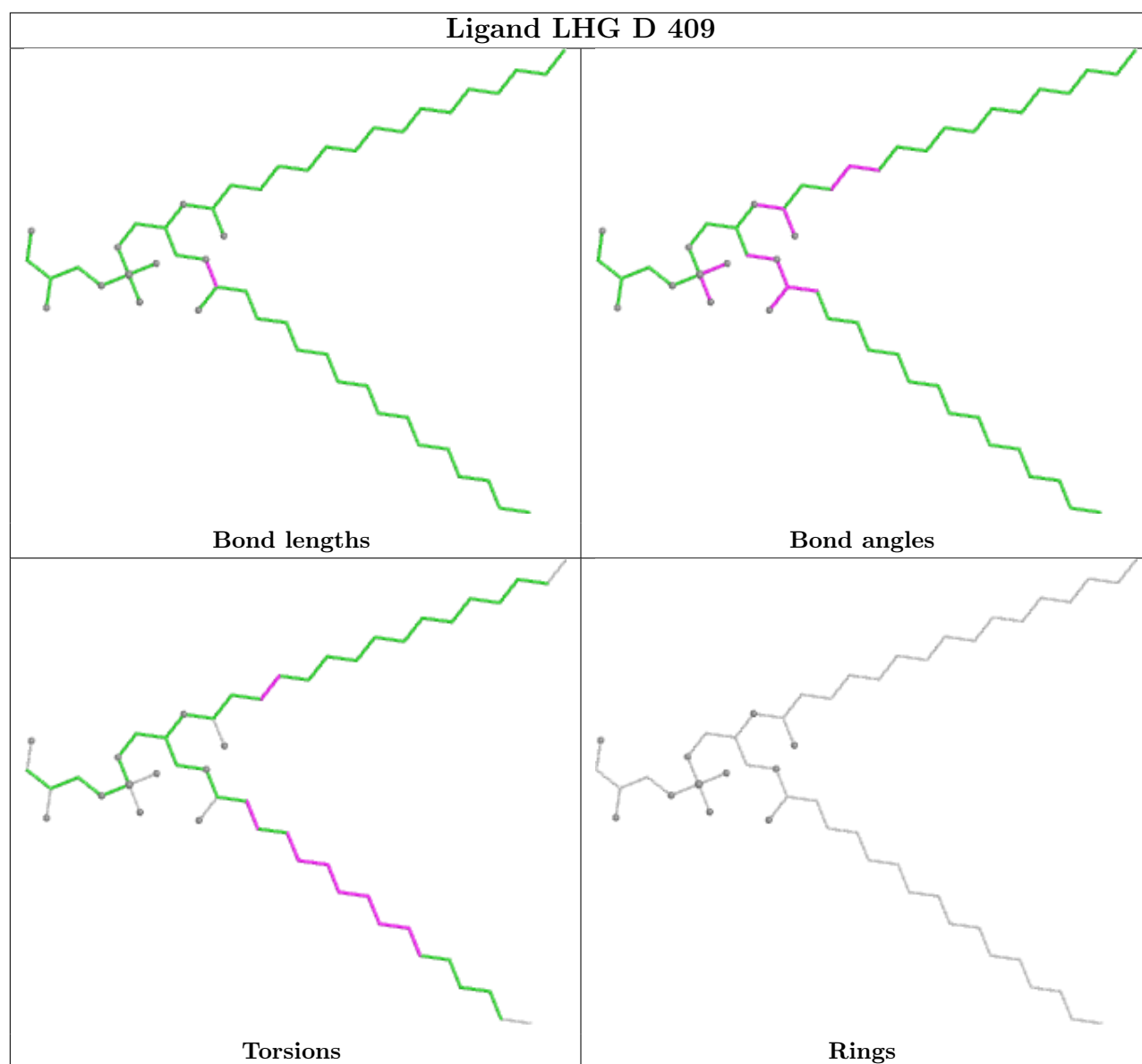
Ligand CLA a 410



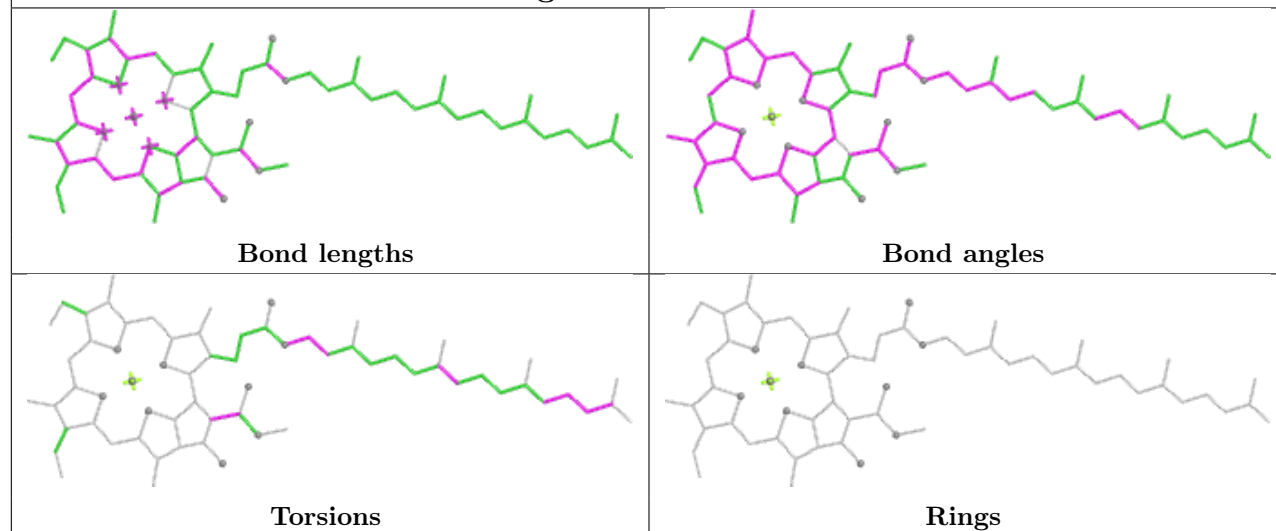
Ligand CLA b 617



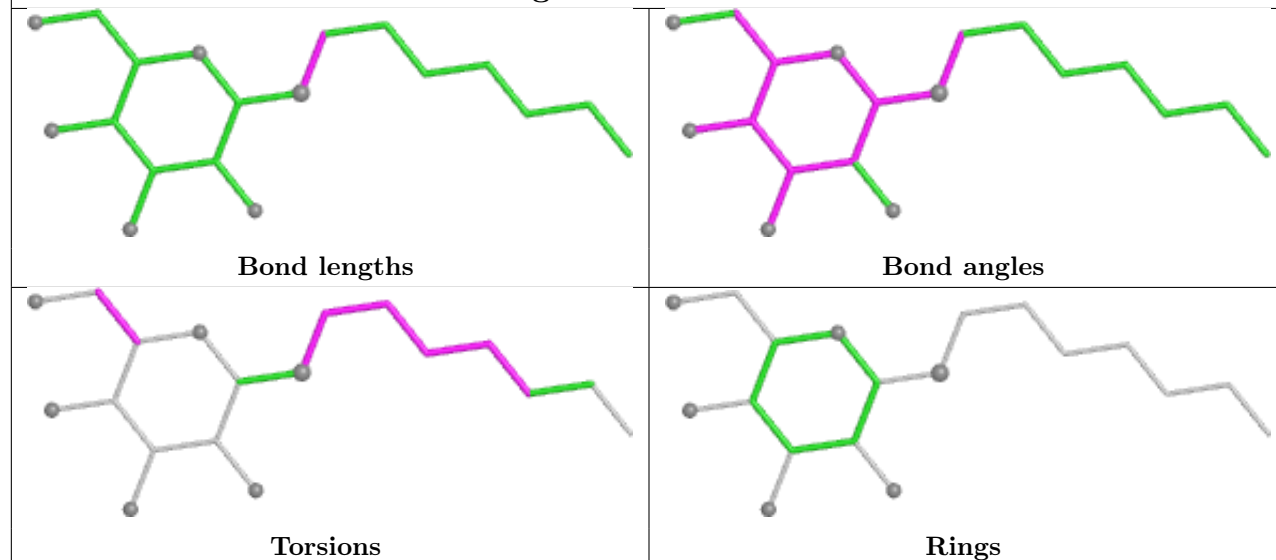




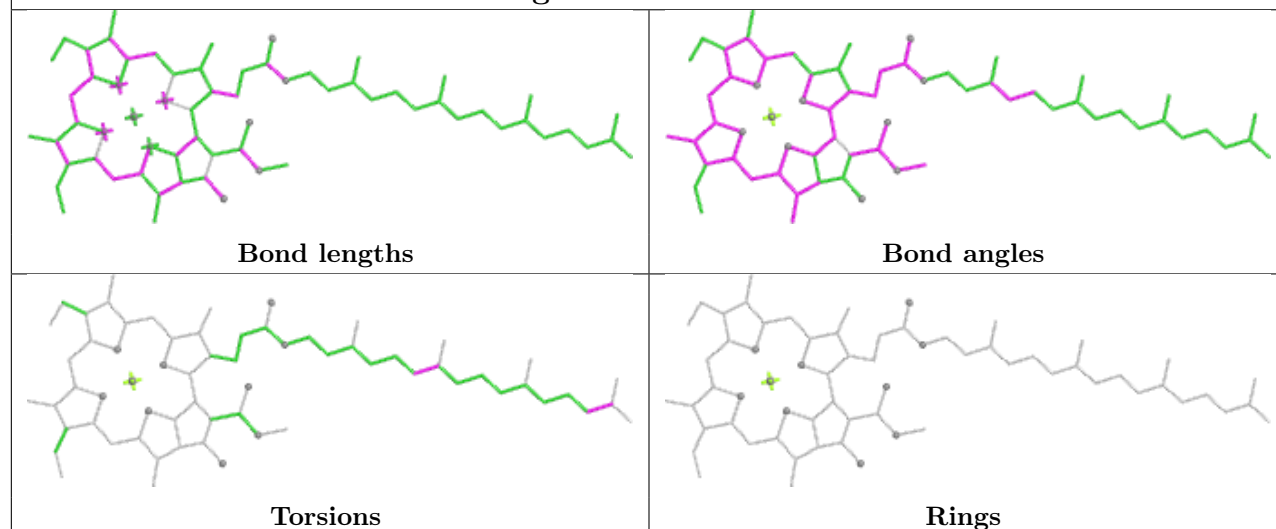
Ligand CLA c 910

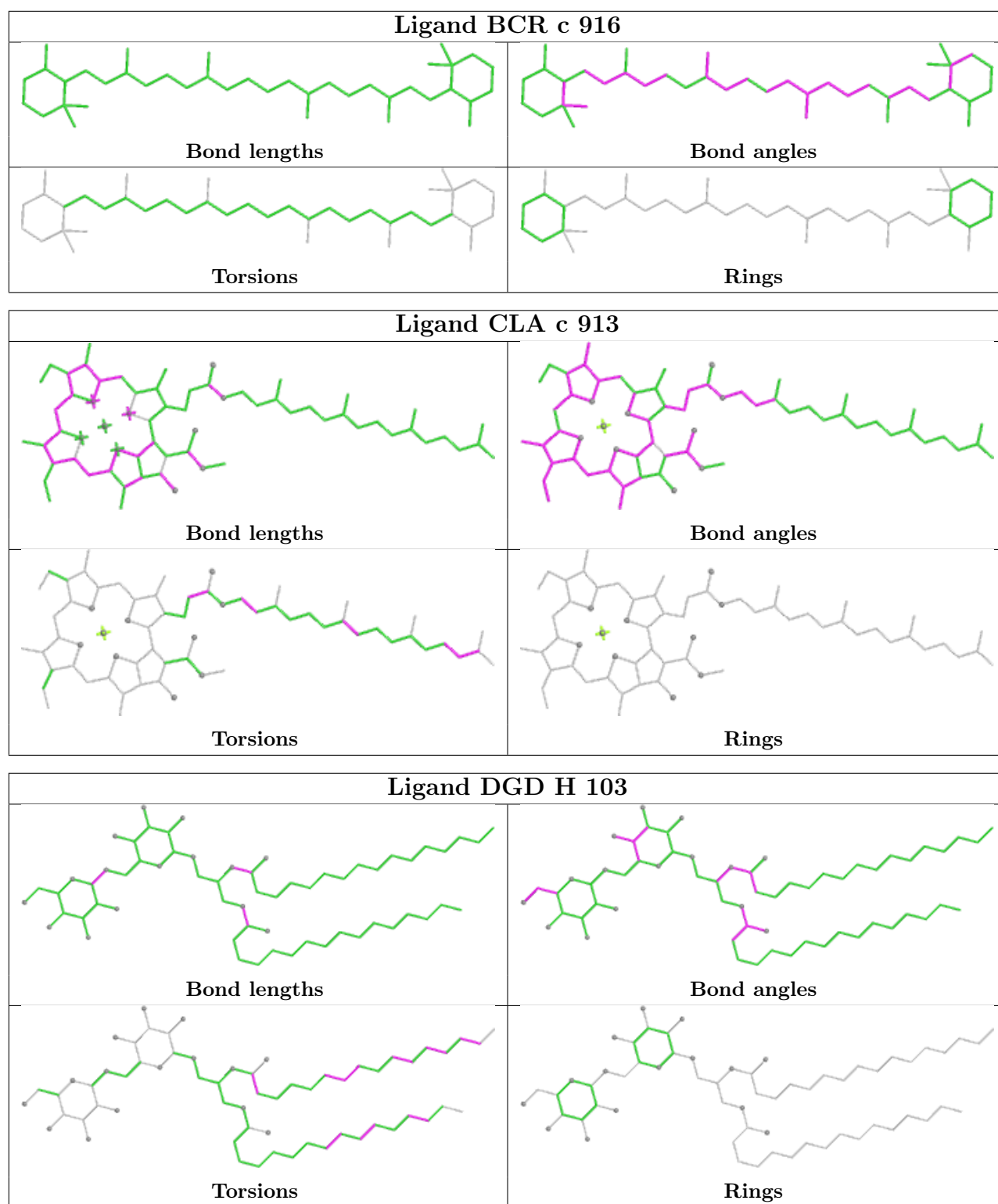


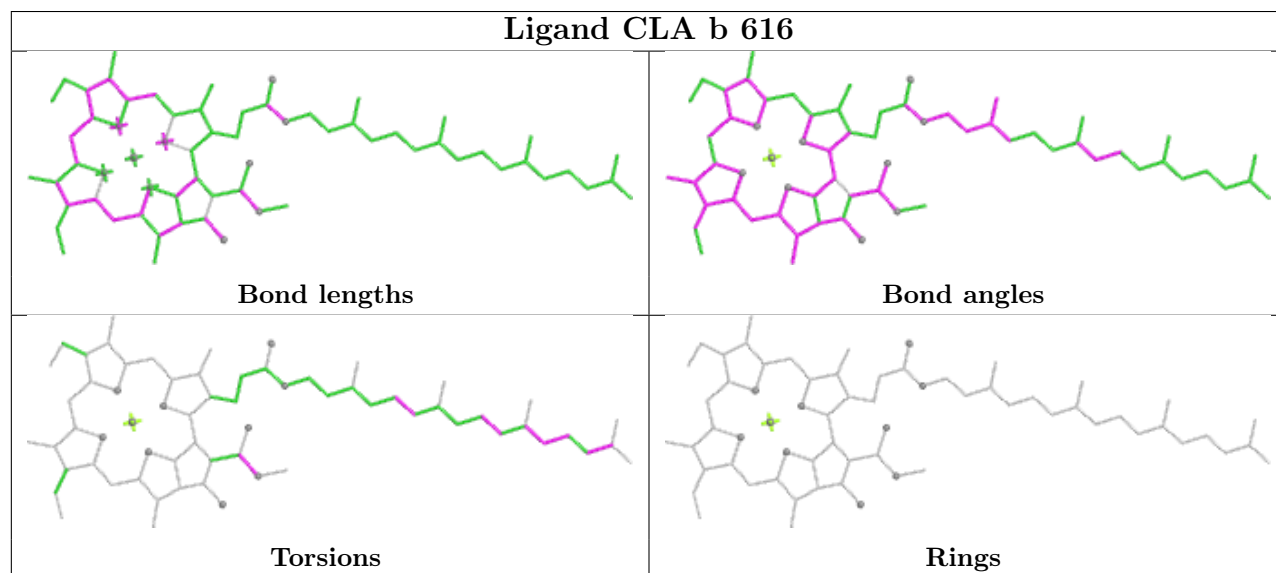
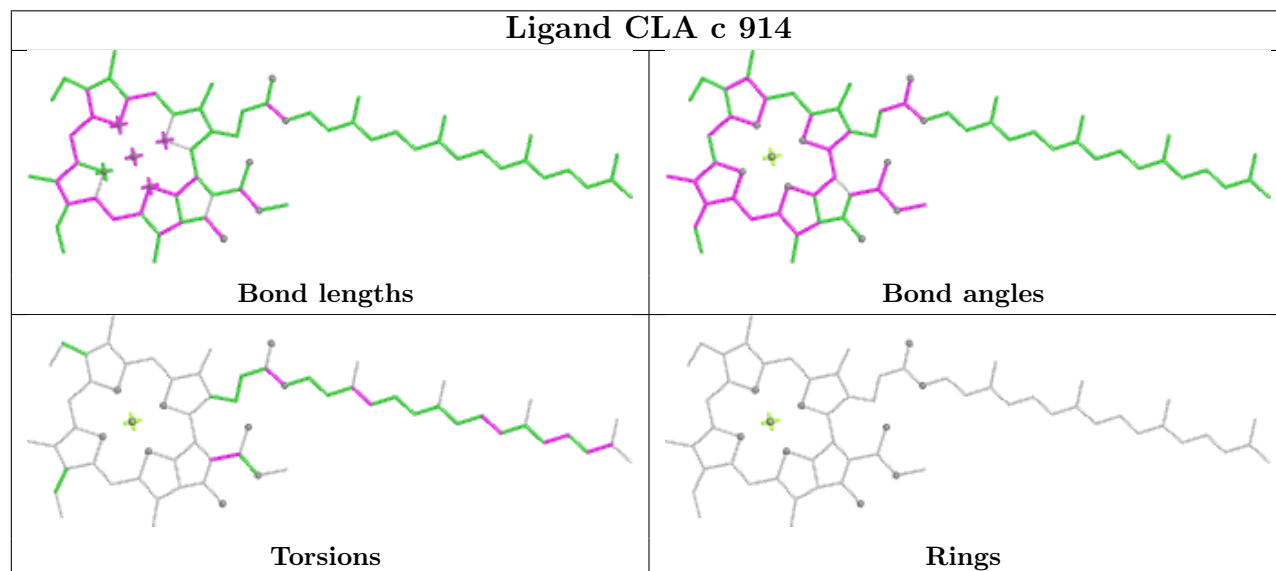
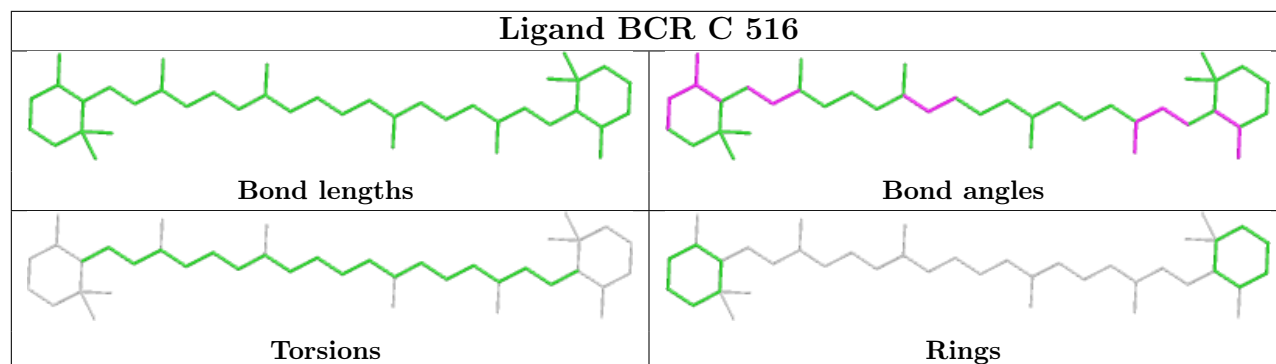
Ligand HTG v 204

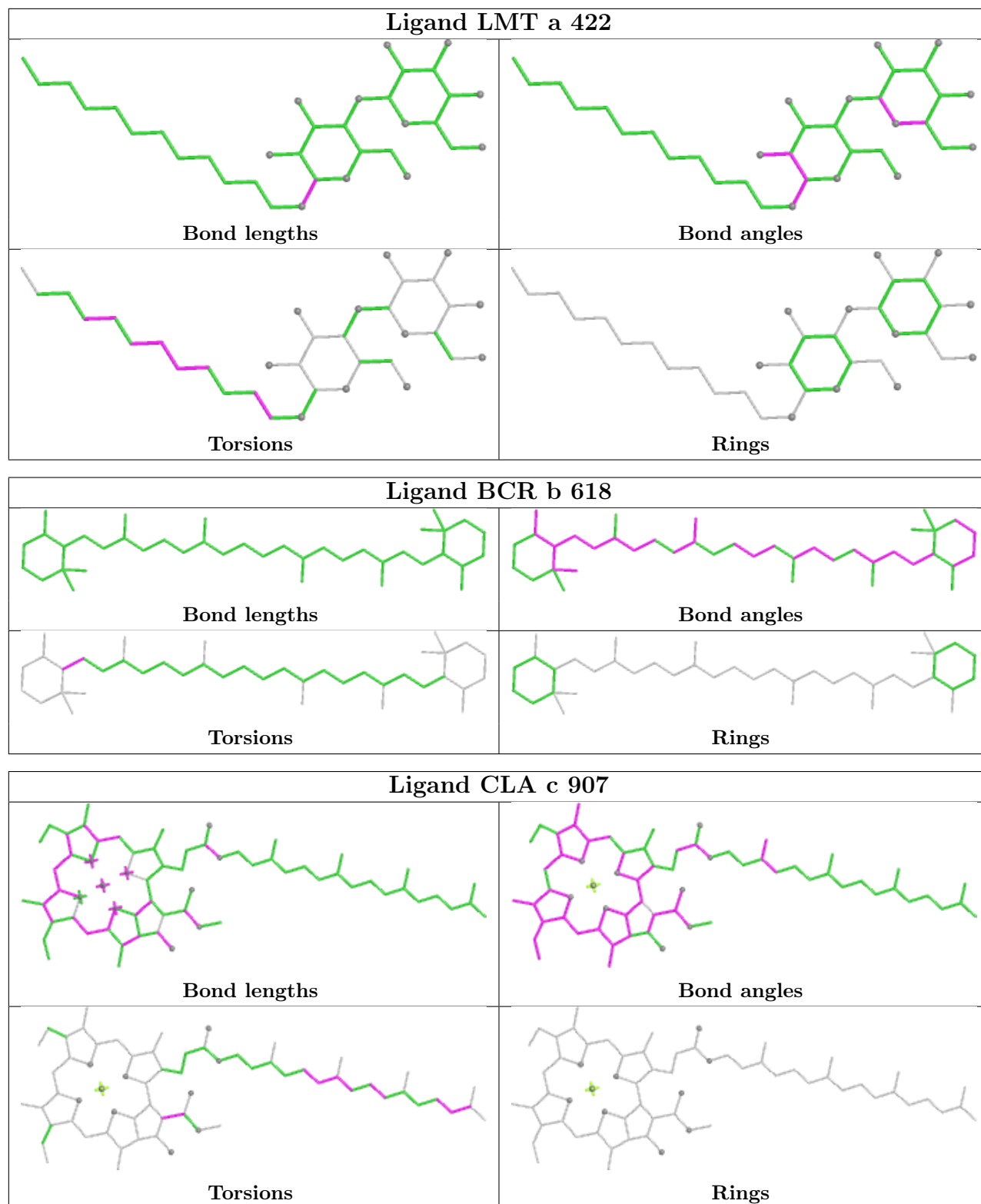


Ligand CLA B 604

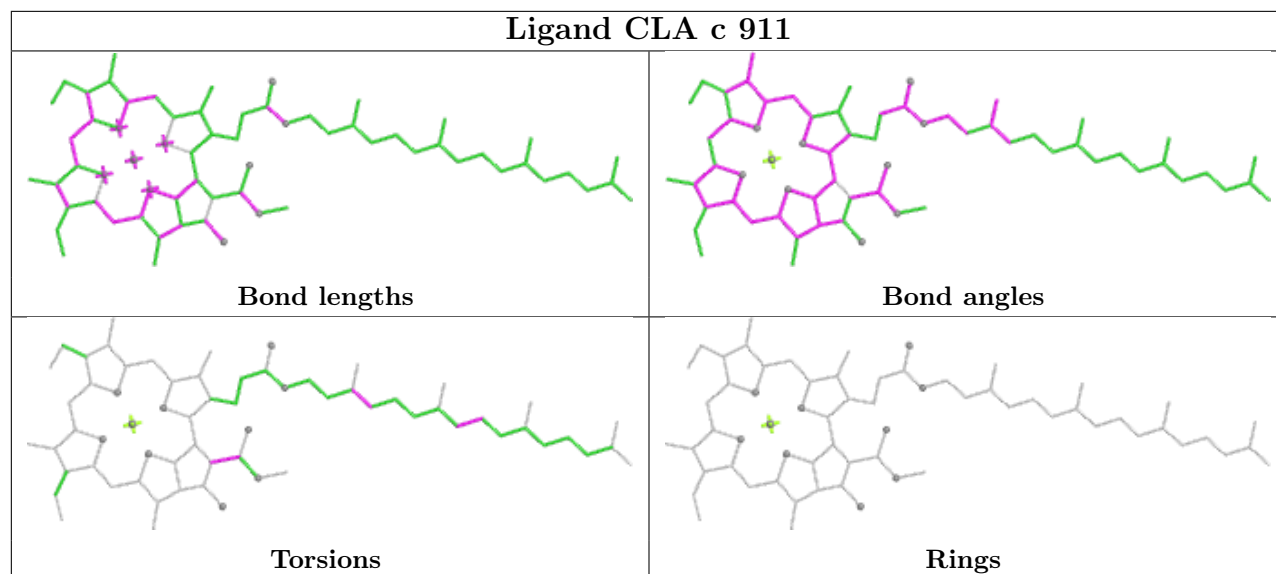




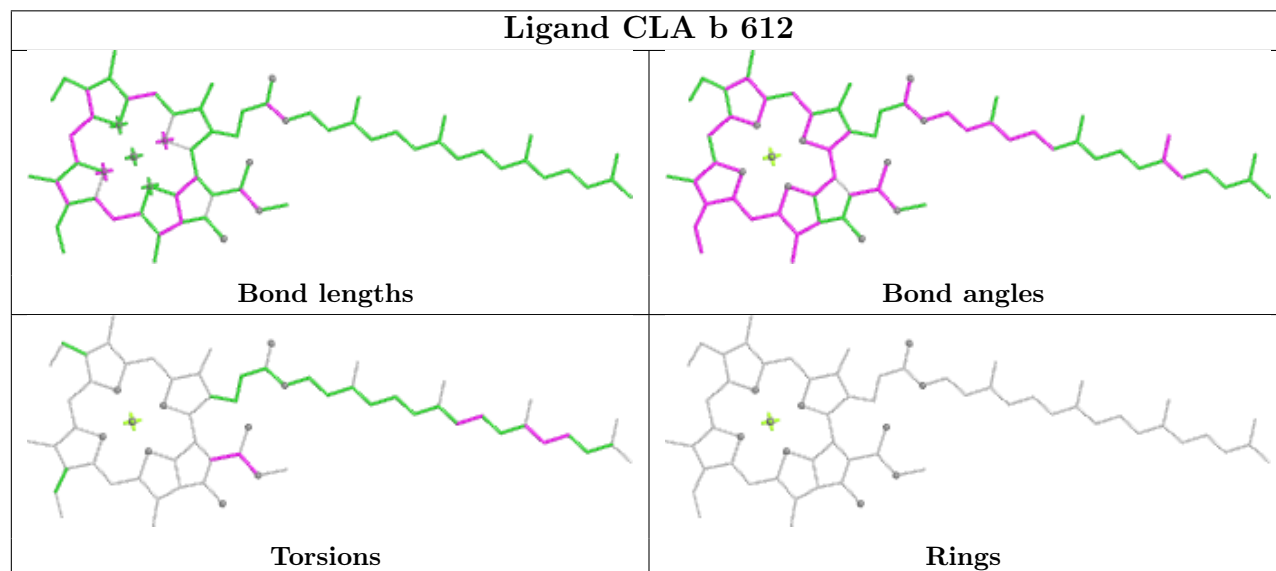




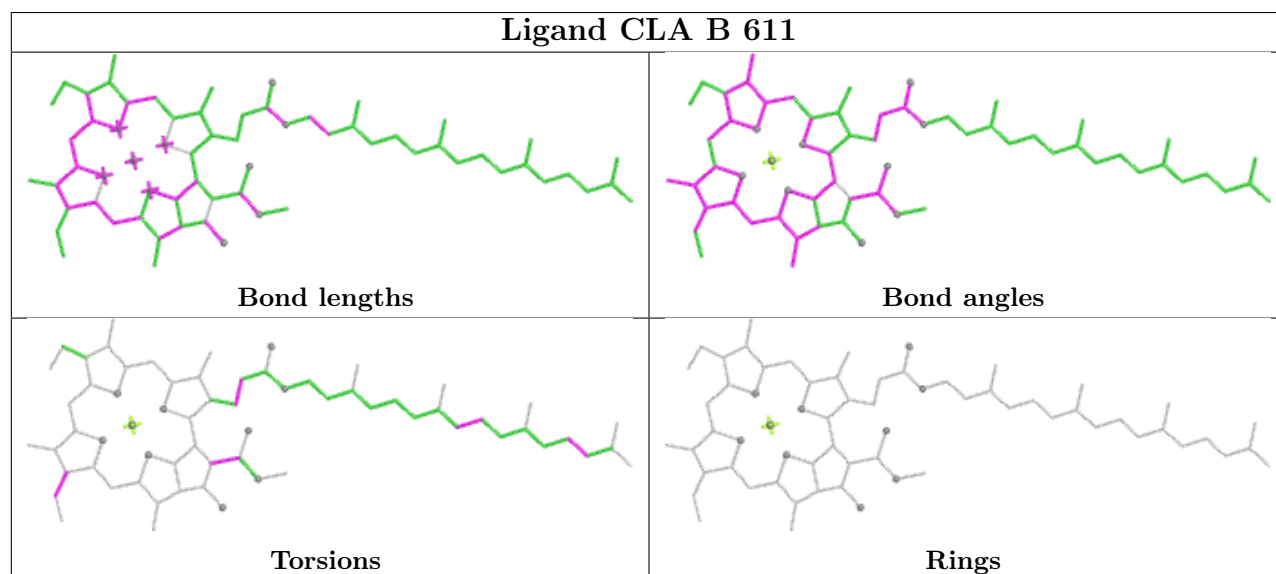
Ligand CLA c 911

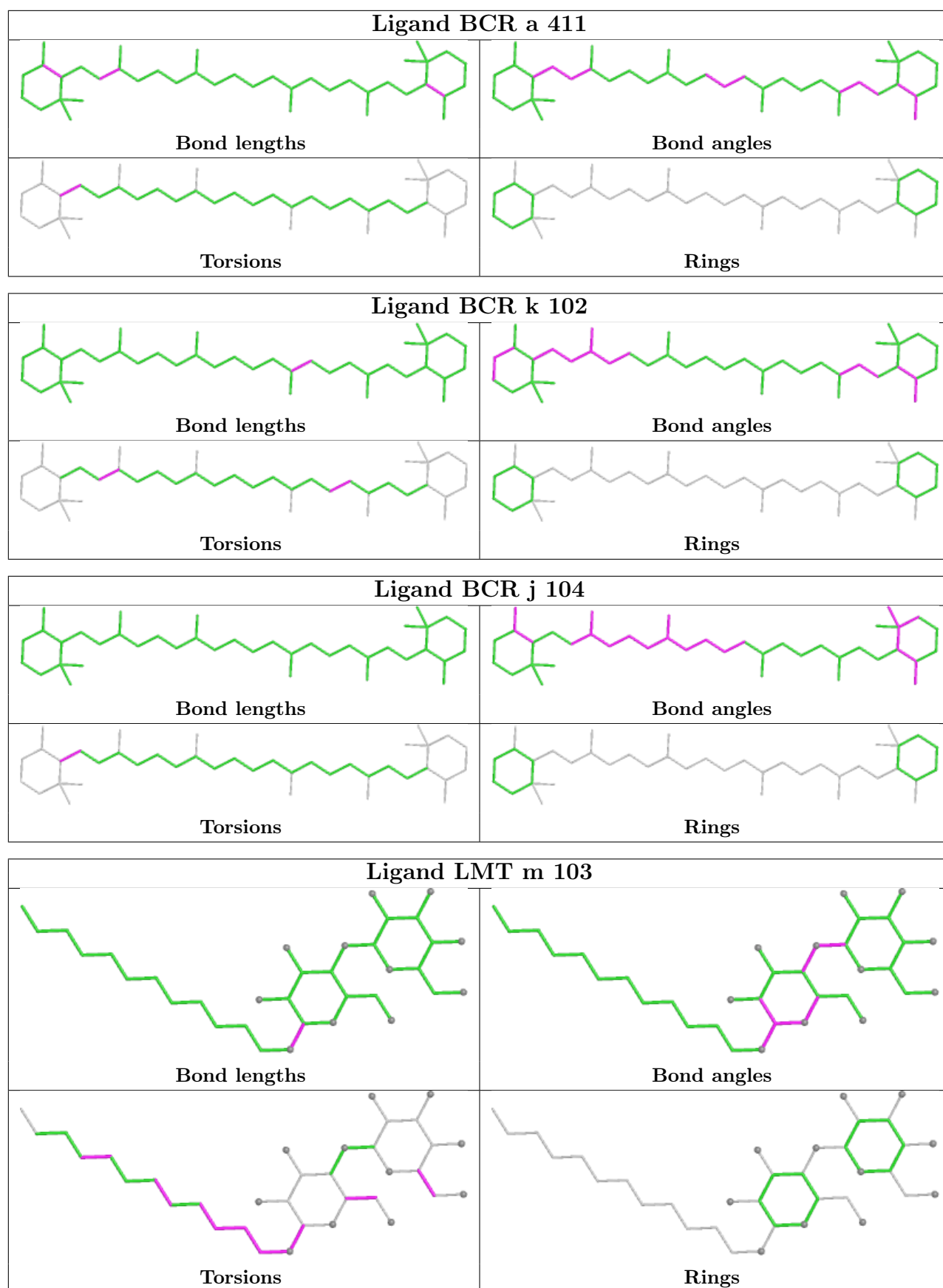


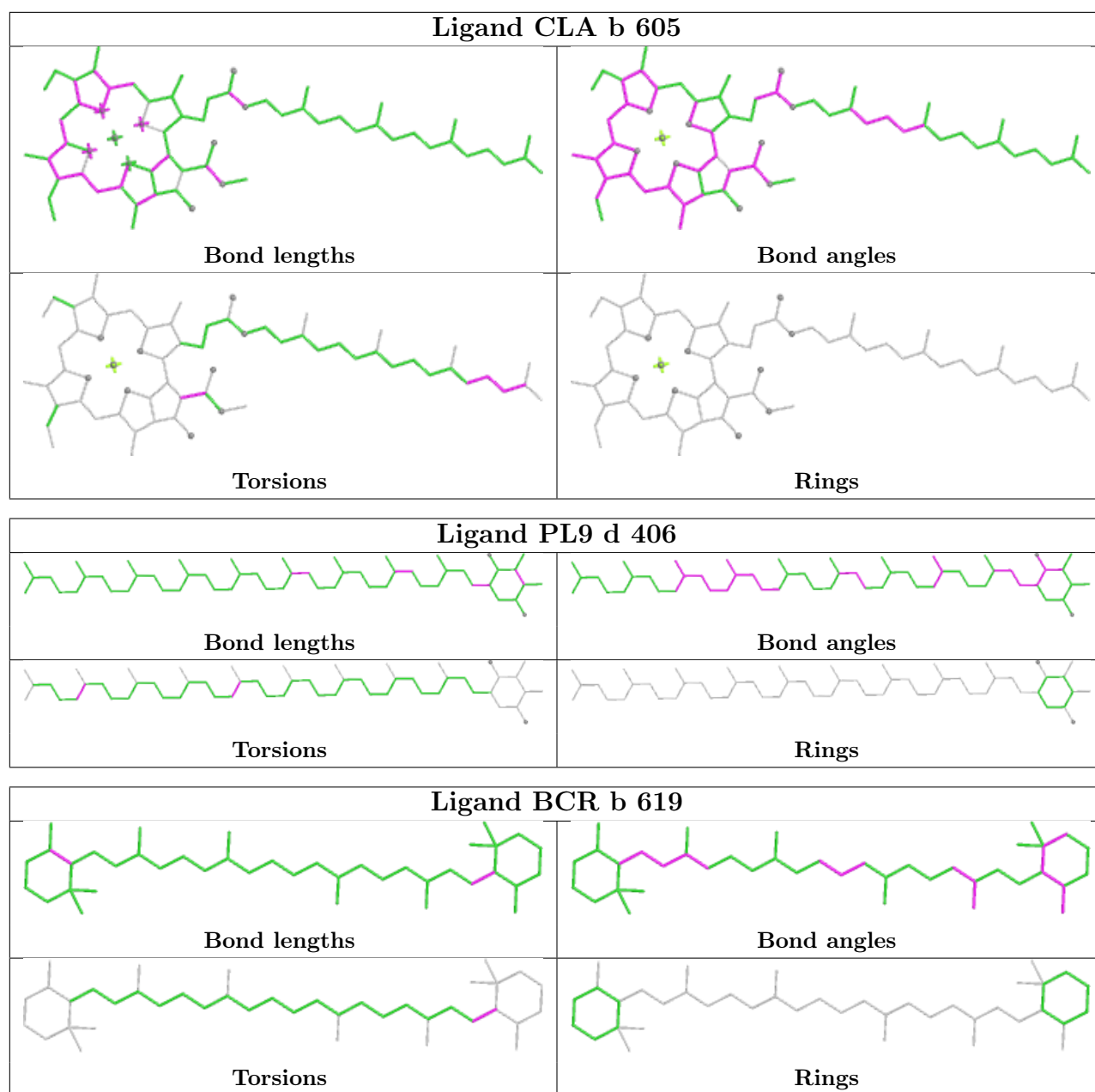
Ligand CLA b 612



Ligand CLA B 611







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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.44	3 (0%) 81 85	13, 21, 43, 67	1 (0%)
1	a	334/344 (97%)	-0.39	6 (1%) 67 73	13, 21, 44, 91	4 (1%)
2	B	505/505 (100%)	-0.19	13 (2%) 57 62	15, 25, 50, 81	4 (0%)
2	b	501/505 (99%)	-0.11	22 (4%) 39 42	15, 25, 53, 109	3 (0%)
3	C	451/455 (99%)	0.02	5 (1%) 78 82	16, 30, 46, 73	4 (0%)
3	c	455/455 (100%)	-0.02	4 (0%) 81 85	20, 31, 43, 68	1 (0%)
4	D	342/342 (100%)	-0.40	1 (0%) 90 93	12, 22, 41, 88	2 (0%)
4	d	342/342 (100%)	-0.49	1 (0%) 90 93	11, 22, 40, 73	2 (0%)
5	E	81/83 (97%)	0.87	11 (13%) 7 7	25, 45, 75, 97	0
5	e	79/83 (95%)	0.66	6 (7%) 20 22	28, 42, 67, 87	0
6	F	35/44 (79%)	0.35	2 (5%) 29 31	24, 35, 59, 96	0
6	f	32/44 (72%)	0.20	1 (3%) 51 56	26, 31, 70, 82	0
7	H	63/65 (96%)	0.30	1 (1%) 70 75	20, 33, 44, 77	2 (3%)
7	h	63/65 (96%)	0.44	2 (3%) 50 55	23, 34, 46, 72	1 (1%)
8	I	34/38 (89%)	0.31	0 100 100	27, 35, 58, 77	0
8	i	37/38 (97%)	0.37	2 (5%) 31 33	26, 32, 84, 89	0
9	J	36/40 (90%)	0.53	1 (2%) 55 59	24, 38, 65, 81	0
9	j	40/40 (100%)	0.42	2 (5%) 34 36	24, 36, 69, 76	0
10	K	37/37 (100%)	0.21	0 100 100	31, 37, 47, 56	0
10	k	37/37 (100%)	0.35	0 100 100	29, 37, 55, 66	0
11	L	37/37 (100%)	-0.34	2 (5%) 31 33	11, 20, 62, 80	1 (2%)
11	l	36/37 (97%)	-0.27	2 (5%) 30 32	12, 20, 68, 76	1 (2%)
12	M	34/36 (94%)	-0.26	2 (5%) 28 30	13, 23, 52, 75	1 (2%)
12	m	34/36 (94%)	-0.24	1 (2%) 53 58	15, 24, 53, 72	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.04	7 (2%) 53 58	16, 30, 55, 86	2 (0%)
13	o	243/244 (99%)	0.16	13 (5%) 32 34	16, 32, 65, 86	1 (0%)
14	T	29/32 (90%)	-0.21	1 (3%) 48 53	17, 21, 45, 81	0
14	t	30/32 (93%)	-0.13	2 (6%) 24 26	18, 22, 55, 85	0
15	U	97/104 (93%)	-0.07	1 (1%) 79 83	20, 28, 46, 59	0
15	u	97/104 (93%)	-0.14	1 (1%) 79 83	22, 27, 40, 63	1 (1%)
16	V	137/137 (100%)	-0.25	0 100 100	15, 26, 41, 59	1 (0%)
16	v	137/137 (100%)	0.15	1 (0%) 84 88	16, 33, 51, 71	1 (0%)
17	Y	29/30 (96%)	0.98	3 (10%) 12 14	38, 46, 69, 72	0
17	y	29/30 (96%)	0.77	2 (6%) 23 25	38, 47, 59, 69	0
18	X	38/40 (95%)	0.70	3 (7%) 18 20	21, 39, 58, 62	1 (2%)
18	x	38/40 (95%)	0.87	5 (13%) 7 8	30, 38, 83, 98	0
19	Z	62/62 (100%)	1.07	9 (14%) 6 6	36, 45, 83, 96	0
19	z	61/62 (98%)	1.36	9 (14%) 5 6	42, 52, 83, 103	0
All	All	5249/5350 (98%)	-0.05	147 (2%) 55 59	11, 27, 55, 109	35 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	5.5
18	x	37	VAL	5.3
2	b	487	SER	5.0
7	h	64	ALA	4.9
8	i	38	GLU	4.8
2	b	491	VAL	4.7
2	b	484	PRO	4.6
2	b	493	TRP	4.6
9	J	5	GLY	4.6
2	B	486	LEU	4.5
19	z	61	VAL	4.5
2	b	496	TYR	4.3
19	z	3	ILE	4.3
2	b	479	PHE	4.2
2	b	502	VAL	4.2
19	Z	33	TRP	4.1
14	T	30	THR	4.0
5	e	83	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
9	j	2	MET	3.9
5	E	79	PHE	3.9
5	E	83	LEU	3.8
5	E	80	LEU	3.8
2	B	494	GLY	3.8
19	z	2	THR	3.5
2	B	500	GLY	3.5
13	O	60	ARG	3.5
2	b	490	GLN	3.4
2	B	496	TYR	3.4
2	B	495	PHE	3.2
7	H	64	ALA	3.2
2	b	503	THR	3.2
14	t	31	LYS	3.1
2	B	479	PHE	3.1
5	e	61	ARG	3.1
17	y	18	VAL	3.1
3	C	143	TYR	3.0
6	F	11	VAL	3.0
9	j	1	MET	3.0
5	e	79	PHE	3.0
13	o	59	LYS	2.9
19	Z	41	PHE	2.9
19	z	33	TRP	2.9
2	b	504	THR	2.9
18	x	2	THR	2.9
2	b	489	GLU	2.9
17	Y	19	ILE	2.9
2	b	499	VAL	2.8
17	Y	18	VAL	2.8
5	E	61	ARG	2.8
3	c	19	ASN	2.8
2	b	492	GLU	2.8
6	f	14	PRO	2.8
13	o	38	TYR	2.8
1	A	11	ALA	2.8
5	E	73	LYS	2.8
2	B	504	THR	2.8
8	i	37	LEU	2.8
18	X	37	VAL	2.8
5	e	72	ALA	2.7
14	t	30	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	c	20	SER	2.7
5	E	76	VAL	2.7
19	Z	62	VAL	2.7
5	E	72	ALA	2.7
19	z	30	PRO	2.7
18	X	34	ILE	2.7
13	o	61	GLN	2.7
3	C	25	ASN	2.7
11	L	1	MET	2.6
2	b	497	GLN	2.6
19	Z	30	PRO	2.6
5	E	65	LEU	2.6
1	a	262	TYR	2.6
3	C	23	ALA	2.6
13	O	59	LYS	2.6
7	h	57	GLY	2.6
2	B	505	ARG	2.5
12	m	5	GLN	2.5
18	x	38	GLN	2.5
5	e	84	LYS	2.5
17	y	19	ILE	2.5
2	b	488	PRO	2.5
3	c	143	TYR	2.5
3	C	257	PHE	2.5
2	b	129	GLY	2.5
1	a	11	ALA	2.5
18	X	2	THR	2.5
5	E	84	LYS	2.5
19	z	4	LEU	2.5
2	B	499	VAL	2.5
13	o	29	ALA	2.4
13	O	58	ASN	2.4
15	u	8	GLU	2.4
18	x	36	LYS	2.4
3	c	21	ILE	2.4
13	o	36	GLN	2.4
2	b	295	GLY	2.4
6	F	16	PHE	2.4
19	Z	3	ILE	2.4
2	B	501	ASP	2.3
2	B	293	ALA	2.3
11	l	3	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
11	l	7	ARG	2.3
15	U	8	GLU	2.3
13	o	246	ALA	2.3
5	E	17	VAL	2.3
1	a	229	GLU	2.3
3	C	259	TRP	2.3
1	a	230	THR	2.3
4	D	11	GLU	2.3
12	M	34	LYS	2.3
2	b	494	GLY	2.2
11	L	3	PRO	2.2
5	e	60	GLN	2.2
19	Z	35	ARG	2.2
13	o	25	THR	2.2
19	Z	60	PHE	2.2
13	o	60	ARG	2.2
1	a	260	PHE	2.1
13	O	132	ASN	2.1
13	o	58	ASN	2.1
19	Z	7	LEU	2.1
17	Y	34	MET	2.1
1	A	262	TYR	2.1
2	B	503	THR	2.1
13	o	89	SER	2.1
12	M	33	GLN	2.1
13	o	32	ILE	2.1
18	x	34	ILE	2.1
2	b	128	THR	2.1
1	a	12	ASN	2.1
2	b	293	ALA	2.1
13	o	23	ASP	2.1
2	b	86	ILE	2.0
19	z	60	PHE	2.0
13	o	34	SER	2.0
5	E	4	THR	2.0
13	O	206	GLY	2.0
19	Z	39	LEU	2.0
13	O	29	ALA	2.0
4	d	11	GLU	2.0
13	O	181	GLU	2.0
19	z	1	MET	2.0
16	v	19	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	230	THR	2.0
19	z	38	GLN	2.0
2	B	488	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.97	0.07	27,32,36,36	0
14	FME	T	1	10/11	0.97	0.07	19,26,45,49	0
8	FME	i	1	10/11	0.97	0.06	28,29,33,33	0
14	FME	t	1	10/11	0.97	0.07	18,24,45,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	DMS	V	211	4/4	0.52	0.29	61,61,68,79	0
31	DMS	i	106	4/4	0.53	0.21	120,121,124,138	0
31	DMS	b	644	4/4	0.56	0.29	73,76,78,96	0
31	DMS	k	103	4/4	0.58	0.29	90,92,93,104	0
29	UNL	b	630	16/-	0.60	0.21	74,86,106,110	0
31	DMS	c	936	4/4	0.60	0.25	80,80,81,90	0
35	HTG	c	923	13/19	0.65	0.21	59,72,86,87	0
31	DMS	b	646	4/4	0.66	0.22	84,87,89,96	0
29	UNL	H	104	14/-	0.67	0.25	64,69,74,76	0
29	UNL	i	104	16/-	0.68	0.20	69,76,78,79	0
29	UNL	b	631	16/-	0.68	0.17	61,73,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	DGD	D	407	50/66	0.68	0.19	54,71,97,97	0
29	UNL	I	104	16/-	0.69	0.20	69,76,89,92	0
29	UNL	B	629	14/-	0.69	0.22	62,72,81,82	0
36	DGD	d	407	50/66	0.69	0.22	58,74,97,98	0
29	UNL	J	104	16/-	0.70	0.24	62,82,99,99	0
31	DMS	b	642	4/4	0.70	0.21	90,90,97,101	0
35	HTG	D	414	19/19	0.70	0.19	76,92,111,112	0
29	UNL	B	634	16/-	0.70	0.20	73,80,95,97	0
30	LMT	F	101	35/35	0.70	0.19	64,88,93,96	0
31	DMS	U	204	4/4	0.70	0.20	53,62,62,80	0
35	HTG	v	204	19/19	0.71	0.20	62,70,81,91	0
29	UNL	B	633	16/-	0.71	0.17	61,80,87,88	0
31	DMS	o	304	4/4	0.71	0.22	63,68,70,84	0
30	LMT	e	103	25/35	0.72	0.18	60,77,93,95	0
31	DMS	O	304	4/4	0.72	0.28	69,71,78,87	0
29	UNL	u	202	16/-	0.73	0.19	41,54,60,62	0
35	HTG	c	922	19/19	0.73	0.15	53,84,96,100	0
29	UNL	c	931	10/-	0.73	0.25	55,60,62,64	0
35	HTG	d	413	19/19	0.73	0.17	62,86,104,106	0
29	UNL	J	105	11/-	0.73	0.21	61,67,75,78	0
31	DMS	c	935	4/4	0.73	0.20	71,72,75,83	0
31	DMS	u	206	4/4	0.73	0.22	70,71,76,93	0
31	DMS	O	307	4/4	0.74	0.22	64,69,69,84	0
31	DMS	U	203	4/4	0.74	0.22	70,74,80,89	0
31	DMS	A	419	4/4	0.74	0.27	75,76,91,97	0
28	LHG	e	101	40/49	0.74	0.17	55,93,121,126	0
29	UNL	B	628	10/-	0.75	0.18	62,67,70,71	0
31	DMS	b	638	4/4	0.75	0.21	54,60,67,74	0
30	LMT	I	101	35/35	0.75	0.16	63,75,85,91	0
35	HTG	b	628	19/19	0.75	0.17	52,96,109,112	0
35	HTG	c	921	19/19	0.75	0.16	68,82,88,91	0
28	LHG	K	101	44/49	0.75	0.16	63,93,124,137	0
29	UNL	b	632	16/-	0.75	0.18	58,83,101,101	0
29	UNL	Z	103	9/-	0.75	0.17	50,61,69,70	0
29	UNL	e	102	16/-	0.75	0.21	54,61,69,72	0
29	UNL	a	416	10/-	0.75	0.22	54,68,75,76	0
29	UNL	b	629	12/-	0.75	0.19	49,59,70,71	0
30	LMT	A	416	35/35	0.76	0.17	42,63,86,98	0
31	DMS	O	310	4/4	0.76	0.22	61,67,74,76	0
29	UNL	B	632	16/-	0.76	0.20	44,61,68,70	0
29	UNL	b	626	16/-	0.76	0.19	59,68,73,73	0
29	UNL	B	635	9/-	0.76	0.19	60,67,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	UNL	E	103	13/-	0.76	0.20	63,68,85,87	0
31	DMS	D	417	4/4	0.76	0.23	53,54,58,59	0
28	LHG	A	412	49/49	0.76	0.19	59,83,104,111	0
29	UNL	I	103	16/-	0.77	0.17	51,57,70,74	0
31	DMS	b	639	4/4	0.77	0.17	41,55,63,67	0
28	LHG	E	101	49/49	0.77	0.20	39,83,104,109	0
31	DMS	V	207	4/4	0.77	0.20	51,52,60,62	0
29	UNL	E	102	16/-	0.77	0.23	58,61,76,77	0
29	UNL	i	103	16/-	0.78	0.17	58,61,67,70	0
28	LHG	d	402	44/49	0.78	0.17	59,78,125,135	0
30	LMT	a	418	35/35	0.78	0.15	44,63,79,80	0
29	UNL	u	201	11/-	0.78	0.20	39,50,60,61	0
31	DMS	c	934	4/4	0.78	0.19	87,87,89,99	0
29	UNL	a	419	6/-	0.78	0.13	47,53,53,53	0
31	DMS	B	641	4/4	0.78	0.23	62,63,65,66	0
27	PL9	a	414	55/55	0.78	0.20	46,61,86,88	0
31	DMS	b	637	4/4	0.78	0.23	61,63,68,74	0
31	DMS	H	101	4/4	0.78	0.23	54,58,62,65	0
29	UNL	I	102	13/-	0.79	0.16	47,53,65,69	0
29	UNL	T	102	13/-	0.79	0.19	62,68,75,75	0
31	DMS	h	105	4/4	0.79	0.18	76,83,89,90	0
29	UNL	t	102	16/-	0.79	0.16	53,62,74,75	0
29	UNL	d	417	11/-	0.79	0.17	48,63,69,71	0
29	UNL	A	414	13/-	0.79	0.18	58,71,83,83	0
31	DMS	b	647	4/4	0.79	0.23	67,78,85,86	0
30	LMT	z	101	32/35	0.79	0.17	43,88,96,99	0
31	DMS	O	311	4/4	0.80	0.24	59,59,71,73	0
28	LHG	a	415	49/49	0.80	0.16	56,72,99,108	0
31	DMS	c	929	4/4	0.80	0.23	46,62,67,70	0
29	UNL	k	101	8/-	0.80	0.28	59,71,78,80	0
29	UNL	z	102	13/-	0.80	0.17	53,62,72,75	0
35	HTG	B	626	19/19	0.80	0.14	52,88,96,96	0
35	HTG	B	631	19/19	0.80	0.15	41,88,97,100	0
29	UNL	U	201	14/-	0.80	0.18	38,50,58,61	0
30	LMT	m	103	35/35	0.81	0.15	48,92,102,103	0
31	DMS	b	643	4/4	0.81	0.19	81,82,85,85	0
31	DMS	d	418	4/4	0.81	0.19	68,69,71,71	0
35	HTG	b	623	19/19	0.81	0.15	47,76,83,84	0
31	DMS	d	419	4/4	0.81	0.21	63,70,76,82	0
31	DMS	B	647	4/4	0.81	0.16	81,85,85,89	0
31	DMS	O	309	4/4	0.81	0.21	53,63,64,70	0
31	DMS	B	649	4/4	0.81	0.18	70,71,73,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	PL9	A	411	55/55	0.81	0.18	45,59,80,84	0
29	UNL	b	625	10/-	0.81	0.17	44,59,68,68	0
34	LMG	C	531	51/55	0.81	0.16	38,78,93,98	0
34	LMG	D	412	51/55	0.81	0.17	37,65,106,119	0
26	SQD	x	101	41/54	0.82	0.16	54,76,95,101	0
35	HTG	V	204	14/19	0.82	0.15	42,45,71,82	0
31	DMS	B	640	4/4	0.82	0.21	50,56,60,61	0
30	LMT	Z	101	35/35	0.82	0.16	41,88,100,102	0
31	DMS	B	645	4/4	0.82	0.21	50,61,64,69	0
26	SQD	D	408	45/54	0.82	0.16	45,67,86,93	0
29	UNL	Z	102	14/-	0.82	0.16	63,67,74,76	0
34	LMG	c	930	51/55	0.82	0.14	33,69,81,84	0
34	LMG	d	411	51/55	0.82	0.17	39,70,101,108	0
30	LMT	B	623	35/35	0.82	0.15	48,72,89,93	0
29	UNL	E	104	16/-	0.82	0.20	67,71,74,76	0
29	UNL	A	417	4/-	0.83	0.15	58,61,63,67	0
31	DMS	A	421	4/4	0.83	0.23	57,63,74,78	0
31	DMS	a	421	4/4	0.83	0.21	81,84,85,92	0
31	DMS	h	104	4/4	0.83	0.14	97,99,103,103	0
30	LMT	B	643	24/35	0.83	0.18	50,77,114,118	0
30	LMT	a	422	35/35	0.83	0.14	61,74,82,85	0
31	DMS	H	105	4/4	0.83	0.15	60,74,74,84	0
35	HTG	C	522	19/19	0.83	0.14	41,78,86,87	0
35	HTG	C	523	19/19	0.83	0.15	60,78,95,97	0
31	DMS	A	418	4/4	0.83	0.21	70,79,79,85	0
29	UNL	j	103	16/-	0.84	0.17	45,56,61,62	0
31	DMS	b	635	4/4	0.84	0.18	53,63,69,71	0
31	DMS	c	937	4/4	0.84	0.16	76,80,84,84	0
30	LMT	B	644	24/35	0.84	0.13	34,52,81,87	0
31	DMS	c	933	4/4	0.84	0.18	61,64,65,77	0
29	UNL	C	532	11/-	0.84	0.16	54,59,66,66	0
31	DMS	l	102	4/4	0.85	0.17	64,65,70,84	0
29	UNL	b	624	16/-	0.85	0.15	42,51,58,60	0
31	DMS	b	645	4/4	0.85	0.20	70,77,83,84	0
31	DMS	v	206	4/4	0.85	0.16	66,68,76,78	0
26	SQD	B	621	54/54	0.85	0.14	43,63,88,93	0
29	UNL	B	627	16/-	0.85	0.15	38,45,55,60	0
31	DMS	h	103	4/4	0.85	0.17	82,84,97,101	0
26	SQD	L	102	54/54	0.85	0.15	42,58,87,90	0
35	HTG	B	625	19/19	0.85	0.16	28,42,49,51	0
29	UNL	d	412	16/-	0.85	0.14	31,40,54,57	0
31	DMS	V	210	4/4	0.85	0.16	64,65,67,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	C	533	4/4	0.85	0.17	67,67,68,71	0
30	LMT	T	103	24/35	0.86	0.14	34,56,76,83	0
31	DMS	U	202	4/4	0.86	0.21	33,45,50,55	0
29	UNL	i	101	16/-	0.86	0.14	37,43,60,60	0
35	HTG	b	622	19/19	0.86	0.15	28,41,57,64	0
31	DMS	v	208	4/4	0.86	0.15	54,67,71,87	0
29	UNL	m	101	11/-	0.86	0.14	47,51,56,58	0
29	UNL	i	102	16/-	0.86	0.15	52,62,75,76	0
30	LMT	b	621	25/35	0.86	0.13	45,70,90,91	0
29	UNL	M	102	11/-	0.86	0.14	45,50,63,69	0
31	DMS	a	401	4/4	0.86	0.17	75,81,85,96	0
31	DMS	O	308	4/4	0.86	0.20	54,64,77,81	0
29	UNL	A	413	16/-	0.86	0.14	38,43,70,76	0
26	SQD	a	417	54/54	0.86	0.12	38,53,72,73	0
35	HTG	C	521	19/19	0.87	0.13	61,66,74,77	0
31	DMS	b	641	4/4	0.87	0.15	52,59,66,66	0
30	LMT	m	104	35/35	0.87	0.11	34,51,56,58	0
31	DMS	u	204	4/4	0.87	0.17	62,68,68,73	0
29	UNL	X	101	16/-	0.87	0.14	33,37,60,61	0
31	DMS	v	202	4/4	0.87	0.19	68,74,76,81	0
31	DMS	B	646	4/4	0.87	0.17	76,77,77,84	0
31	DMS	A	422	4/4	0.87	0.15	65,68,68,71	0
31	DMS	h	101	4/4	0.87	0.16	47,51,52,53	0
26	SQD	A	415	54/54	0.87	0.13	39,54,72,76	0
31	DMS	C	527	4/4	0.87	0.18	58,68,73,83	0
31	DMS	C	529	4/4	0.87	0.19	54,66,72,74	0
31	DMS	i	105	4/4	0.87	0.20	61,64,71,73	0
31	DMS	V	209	4/4	0.87	0.18	58,59,62,65	0
31	DMS	b	640	4/4	0.87	0.19	67,70,78,83	0
34	LMG	C	520	51/55	0.88	0.14	31,61,74,79	0
31	DMS	V	208	4/4	0.88	0.17	69,70,71,72	0
31	DMS	A	424	4/4	0.88	0.19	53,54,58,69	0
34	LMG	a	413	51/55	0.88	0.12	41,53,68,74	0
31	DMS	o	303	4/4	0.88	0.16	51,55,67,70	0
31	DMS	C	528	4/4	0.88	0.14	60,63,65,66	0
31	DMS	B	642	4/4	0.88	0.14	46,54,59,67	0
31	DMS	u	205	4/4	0.88	0.16	41,50,54,58	0
31	DMS	O	305	4/4	0.88	0.17	65,70,70,77	0
31	DMS	O	306	4/4	0.88	0.17	68,68,73,76	0
31	DMS	B	648	4/4	0.88	0.23	43,45,47,48	0
29	UNL	J	103	16/-	0.88	0.15	46,54,60,63	0
31	DMS	C	525	4/4	0.89	0.23	39,39,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	e	104	4/4	0.89	0.16	72,73,78,83	0
31	DMS	B	639	4/4	0.89	0.15	44,48,51,54	0
23	CLA	b	602	65/65	0.89	0.12	29,42,66,71	0
31	DMS	V	202	4/4	0.89	0.18	31,32,38,48	0
31	DMS	V	205	4/4	0.89	0.15	49,60,60,63	0
31	DMS	V	206	4/4	0.89	0.15	55,55,55,61	0
31	DMS	a	423	4/4	0.89	0.17	53,56,63,73	0
31	DMS	v	209	4/4	0.89	0.17	49,50,58,64	0
31	DMS	B	638	4/4	0.89	0.15	55,60,62,71	0
31	DMS	b	636	4/4	0.89	0.16	44,48,50,52	0
34	LMG	B	622	51/55	0.90	0.11	31,41,52,67	0
34	LMG	C	501	51/55	0.90	0.12	37,51,63,70	0
30	LMT	M	101	35/35	0.90	0.11	31,50,59,60	0
23	CLA	C	514	65/65	0.90	0.11	37,47,67,72	0
31	DMS	d	414	4/4	0.90	0.18	62,66,71,78	0
31	DMS	d	415	4/4	0.90	0.18	45,53,57,73	0
29	UNL	D	413	16/-	0.90	0.12	36,42,57,58	0
23	CLA	C	507	65/65	0.90	0.12	25,42,79,81	0
34	LMG	m	102	51/55	0.90	0.12	33,41,54,61	0
31	DMS	c	932	4/4	0.91	0.13	54,57,63,64	0
25	BCR	C	515	40/40	0.91	0.09	35,43,46,48	0
31	DMS	v	205	4/4	0.91	0.13	63,66,68,69	0
29	UNL	x	103	15/-	0.91	0.13	31,40,57,58	0
26	SQD	A	410	54/54	0.91	0.12	31,55,74,80	0
31	DMS	d	416	4/4	0.91	0.18	47,52,59,64	0
34	LMG	c	920	51/55	0.91	0.13	27,55,81,84	0
31	DMS	u	203	4/4	0.92	0.18	38,50,51,52	0
26	SQD	a	412	54/54	0.92	0.12	31,53,72,76	0
31	DMS	a	420	4/4	0.92	0.12	48,61,64,66	0
31	DMS	O	303	4/4	0.92	0.12	59,66,69,73	0
31	DMS	v	210	4/4	0.92	0.12	62,65,68,72	0
35	HTG	B	630	19/19	0.92	0.10	41,55,62,66	0
23	CLA	B	602	65/65	0.92	0.10	28,39,75,85	0
35	HTG	b	627	19/19	0.92	0.10	39,59,72,82	0
31	DMS	D	415	4/4	0.93	0.13	50,53,56,59	0
31	DMS	v	207	4/4	0.93	0.13	53,54,54,60	0
23	CLA	c	913	65/65	0.93	0.09	30,39,65,68	0
31	DMS	C	526	4/4	0.93	0.14	49,56,57,62	0
23	CLA	c	914	65/65	0.93	0.10	36,44,76,80	0
23	CLA	C	513	65/65	0.93	0.10	34,42,73,76	0
25	BCR	Y	101	40/40	0.93	0.08	29,33,40,41	0
35	HTG	O	302	19/19	0.93	0.10	36,39,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	HTG	B	624	19/19	0.93	0.11	35,39,46,47	0
25	BCR	d	405	40/40	0.93	0.09	21,27,50,54	0
38	RRX	H	102	41/41	0.93	0.09	25,29,38,44	0
28	LHG	D	409	49/49	0.94	0.09	27,34,41,47	0
31	DMS	v	201	4/4	0.94	0.13	46,48,51,51	0
25	BCR	j	104	40/40	0.94	0.07	27,32,39,43	0
25	BCR	t	101	40/40	0.94	0.07	19,26,38,40	0
23	CLA	C	512	65/65	0.94	0.08	26,34,39,40	0
23	CLA	C	508	65/65	0.94	0.09	28,35,49,55	0
23	CLA	b	617	65/65	0.94	0.10	20,30,81,89	0
25	BCR	C	516	40/40	0.94	0.08	28,34,40,43	0
25	BCR	C	530	40/40	0.94	0.07	27,32,36,37	0
32	BCT	A	420	4/4	0.94	0.08	31,32,35,40	0
25	BCR	D	405	40/40	0.94	0.09	22,28,54,57	0
31	DMS	c	925	4/4	0.94	0.18	35,37,42,49	0
31	DMS	c	926	4/4	0.94	0.17	66,68,69,77	0
31	DMS	c	927	4/4	0.94	0.20	30,37,37,44	0
25	BCR	T	101	40/40	0.94	0.07	22,29,40,41	0
34	LMG	J	101	51/55	0.94	0.11	25,31,85,93	0
23	CLA	c	904	65/65	0.94	0.08	25,32,37,40	0
31	DMS	b	634	4/4	0.94	0.12	42,45,48,48	0
25	BCR	c	915	40/40	0.94	0.09	36,44,48,50	0
36	DGD	C	518	62/66	0.94	0.10	24,33,70,80	0
25	BCR	c	916	40/40	0.94	0.08	25,32,38,38	0
36	DGD	H	103	62/66	0.94	0.09	23,32,38,39	0
23	CLA	c	907	65/65	0.94	0.10	23,36,73,76	0
36	DGD	h	102	62/66	0.94	0.09	24,31,41,47	0
31	DMS	F	102	4/4	0.94	0.12	48,48,50,64	0
38	RRX	x	102	41/41	0.94	0.08	23,29,46,52	0
23	CLA	C	510	65/65	0.95	0.09	25,31,52,55	0
23	CLA	C	502	65/65	0.95	0.07	25,31,41,51	0
25	BCR	B	619	40/40	0.95	0.07	20,25,41,45	0
25	BCR	B	620	40/40	0.95	0.07	21,29,41,42	0
23	CLA	C	503	65/65	0.95	0.07	23,27,37,42	0
23	CLA	C	504	65/65	0.95	0.07	24,31,36,41	0
23	CLA	C	506	65/65	0.95	0.08	25,31,40,44	0
23	CLA	b	607	65/65	0.95	0.08	22,27,54,63	0
32	BCT	a	424	4/4	0.95	0.07	32,35,37,41	0
23	CLA	b	615	65/65	0.95	0.09	19,24,71,76	0
23	CLA	B	607	65/65	0.95	0.08	20,26,53,60	0
27	PL9	D	406	55/55	0.95	0.06	17,22,28,30	0
25	BCR	a	411	40/40	0.95	0.06	20,23,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	b	619	40/40	0.95	0.07	20,27,41,43	0
23	CLA	B	610	65/65	0.95	0.07	21,28,32,34	0
28	LHG	D	411	46/49	0.95	0.10	25,30,82,85	0
31	DMS	c	928	4/4	0.95	0.10	57,59,61,61	0
31	DMS	B	637	4/4	0.95	0.12	35,38,40,42	0
23	CLA	c	906	65/65	0.95	0.07	25,29,44,47	0
34	LMG	j	101	51/55	0.95	0.10	22,33,80,85	0
23	CLA	C	509	65/65	0.95	0.08	24,29,76,85	0
23	CLA	c	908	65/65	0.95	0.08	23,28,46,54	0
25	BCR	k	102	40/40	0.95	0.07	27,32,38,40	0
28	LHG	d	408	49/49	0.95	0.09	25,33,43,44	0
23	CLA	b	604	65/65	0.96	0.06	19,23,29,32	0
23	CLA	B	617	65/65	0.96	0.10	20,27,93,106	0
23	CLA	b	610	65/65	0.96	0.07	22,27,31,39	0
23	CLA	b	611	65/65	0.96	0.07	19,24,32,37	0
23	CLA	B	603	65/65	0.96	0.06	20,26,33,36	0
23	CLA	b	616	65/65	0.96	0.07	21,26,42,44	0
23	CLA	B	604	65/65	0.96	0.07	18,21,30,36	0
23	CLA	c	902	65/65	0.96	0.07	24,27,38,46	0
23	CLA	C	511	65/65	0.96	0.06	24,30,35,40	0
25	BCR	b	618	40/40	0.96	0.06	20,25,32,33	0
28	LHG	L	101	49/49	0.96	0.08	22,31,42,48	0
23	CLA	c	905	65/65	0.96	0.07	21,27,51,54	0
25	BCR	b	620	40/40	0.96	0.07	25,29,40,44	0
23	CLA	B	611	65/65	0.96	0.07	20,24,33,39	0
31	DMS	V	201	4/4	0.96	0.11	41,46,47,47	0
28	LHG	d	409	49/49	0.96	0.07	18,24,44,47	0
28	LHG	d	410	46/49	0.96	0.10	24,27,73,84	0
23	CLA	C	505	65/65	0.96	0.07	25,28,58,60	0
28	LHG	l	101	49/49	0.96	0.08	20,28,48,52	0
23	CLA	B	615	65/65	0.96	0.08	18,23,66,71	0
23	CLA	c	909	65/65	0.96	0.08	22,26,79,92	0
23	CLA	c	910	65/65	0.96	0.07	23,27,49,60	0
33	CA	o	302	1/1	0.96	0.06	43,43,43,43	0
23	CLA	c	911	65/65	0.96	0.06	20,26,36,40	0
36	DGD	C	517	62/66	0.96	0.09	21,29,69,71	0
23	CLA	c	912	65/65	0.96	0.07	26,31,37,41	0
36	DGD	C	519	62/66	0.96	0.09	21,28,68,83	0
23	CLA	B	616	65/65	0.96	0.07	23,27,43,49	0
23	CLA	b	603	65/65	0.96	0.07	21,24,33,41	0
36	DGD	c	917	62/66	0.96	0.09	20,30,74,77	0
36	DGD	c	918	62/66	0.96	0.08	24,30,75,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	DGD	c	919	62/66	0.96	0.08	22,29,50,56	0
23	CLA	d	404	65/65	0.96	0.08	22,27,66,72	0
31	DMS	D	416	4/4	0.96	0.12	56,57,58,62	0
25	BCR	A	409	40/40	0.96	0.06	19,23,29,32	0
25	BCR	B	618	40/40	0.96	0.06	19,24,30,33	0
23	CLA	A	408	65/65	0.97	0.09	18,22,89,96	0
23	CLA	b	608	65/65	0.97	0.05	16,20,28,36	0
23	CLA	d	401	65/65	0.97	0.05	15,17,26,31	0
23	CLA	d	403	65/65	0.97	0.06	13,18,36,42	0
23	CLA	b	609	65/65	0.97	0.06	19,23,31,32	0
24	PHO	A	407	64/64	0.97	0.05	17,19,22,22	0
24	PHO	D	402	64/64	0.97	0.05	16,21,25,29	0
24	PHO	a	408	64/64	0.97	0.05	15,18,20,22	0
24	PHO	a	409	64/64	0.97	0.05	17,22,27,30	0
23	CLA	B	608	65/65	0.97	0.05	16,19,32,35	0
23	CLA	B	609	65/65	0.97	0.06	19,23,28,29	0
31	DMS	B	636	4/4	0.97	0.09	18,20,22,28	0
23	CLA	b	612	65/65	0.97	0.06	18,21,36,42	0
27	PL9	d	406	55/55	0.97	0.05	16,21,27,34	0
23	CLA	b	613	65/65	0.97	0.06	18,24,29,34	0
23	CLA	b	614	65/65	0.97	0.06	17,21,47,54	0
28	LHG	D	410	49/49	0.97	0.07	20,27,42,46	0
23	CLA	A	406	65/65	0.97	0.07	18,20,90,96	0
23	CLA	B	605	65/65	0.97	0.07	18,21,52,53	0
23	CLA	B	612	65/65	0.97	0.06	17,20,36,52	0
23	CLA	D	403	65/65	0.97	0.05	13,17,33,41	0
33	CA	B	601	1/1	0.97	0.10	41,41,41,41	0
33	CA	O	301	1/1	0.97	0.06	42,42,42,42	0
23	CLA	c	903	65/65	0.97	0.06	20,24,37,43	0
23	CLA	D	404	65/65	0.97	0.08	23,27,67,73	0
23	CLA	a	406	65/65	0.97	0.05	14,17,25,37	0
23	CLA	a	407	65/65	0.97	0.08	17,20,95,102	0
23	CLA	a	410	65/65	0.97	0.10	17,22,91,94	0
23	CLA	B	613	65/65	0.97	0.06	18,23,28,31	0
23	CLA	B	614	65/65	0.97	0.05	18,20,44,51	0
23	CLA	B	606	65/65	0.97	0.06	18,22,32,34	0
31	DMS	b	633	4/4	0.97	0.07	21,23,24,25	0
37	HEM	E	105	43/43	0.97	0.08	36,42,46,47	0
37	HEM	e	105	43/43	0.97	0.08	35,39,51,63	0
23	CLA	b	605	65/65	0.97	0.07	17,22,53,55	0
23	CLA	b	606	65/65	0.97	0.06	18,22,29,33	0
33	CA	c	901	1/1	0.98	0.06	39,39,39,39	0

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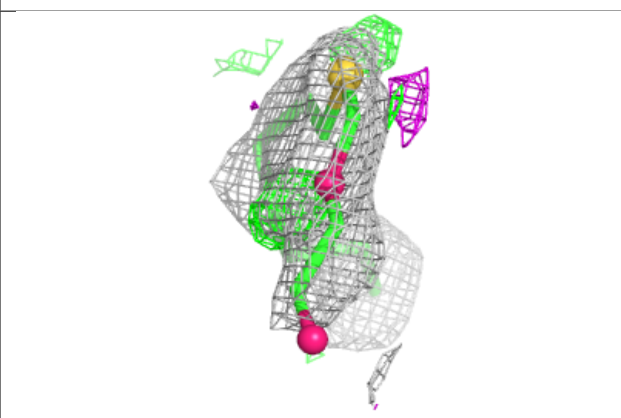
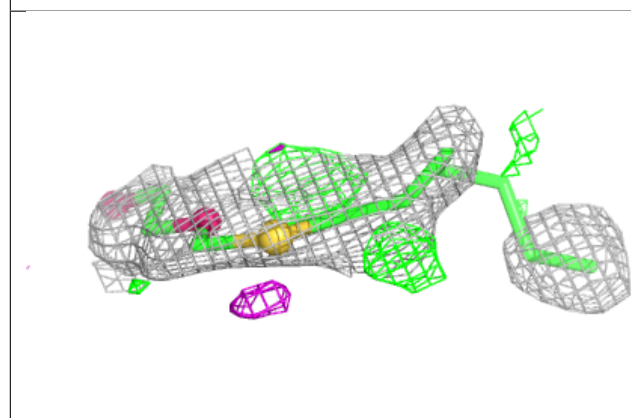
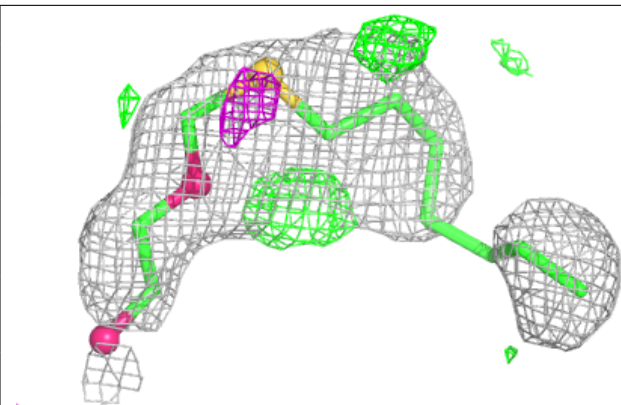
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	c	924	4/4	0.98	0.07	31,33,36,36	0
23	CLA	A	405	65/65	0.98	0.05	14,17,26,34	0
31	DMS	C	524	4/4	0.98	0.07	32,33,36,36	0
23	CLA	D	401	65/65	0.98	0.05	13,17,27,35	0
33	CA	b	601	1/1	0.98	0.07	41,41,41,41	0
40	HEC	v	203	43/43	0.98	0.07	22,27,29,32	0
31	DMS	A	423	4/4	0.99	0.05	23,27,27,28	0
21	FE2	a	403	1/1	0.99	0.02	25,25,25,25	0
22	CL	a	404	1/1	0.99	0.02	19,19,19,19	0
31	DMS	o	301	4/4	0.99	0.07	22,27,28,31	0
22	CL	a	405	1/1	0.99	0.02	21,21,21,21	0
39	MG	J	102	1/1	0.99	0.07	30,30,30,30	0
39	MG	j	102	1/1	0.99	0.07	28,28,28,28	0
40	HEC	V	203	43/43	0.99	0.05	19,22,26,29	0
21	FE2	A	402	1/1	0.99	0.03	28,28,28,28	0
20	OEX	A	401	10/10	1.00	0.03	19,21,23,24	0
20	OEX	a	402	10/10	1.00	0.02	21,23,24,24	0
22	CL	A	403	1/1	1.00	0.02	19,19,19,19	0
22	CL	A	404	1/1	1.00	0.02	20,20,20,20	0

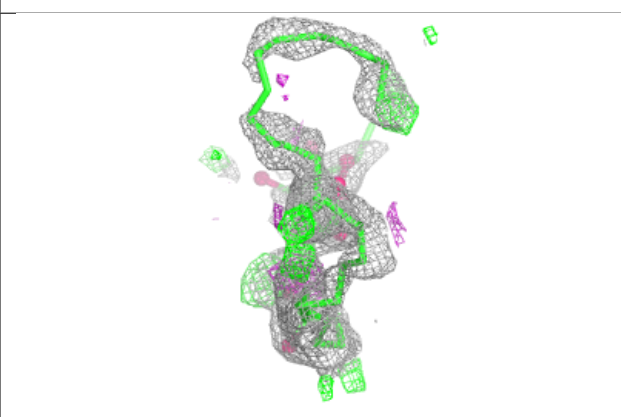
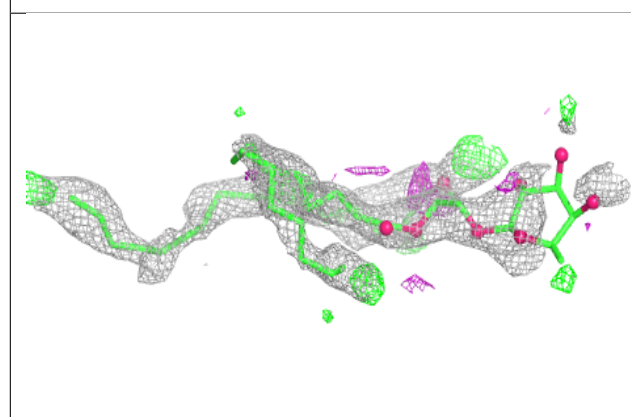
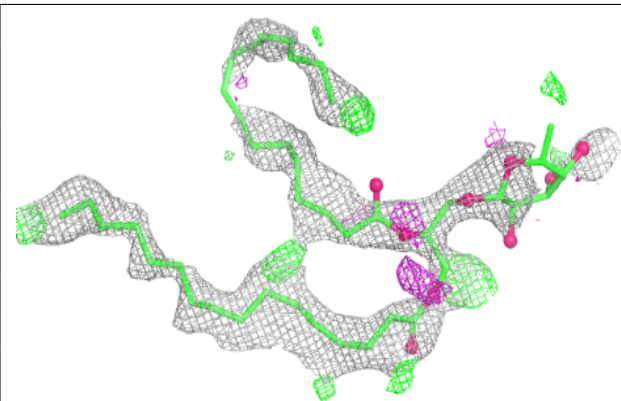
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HTG c 923:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

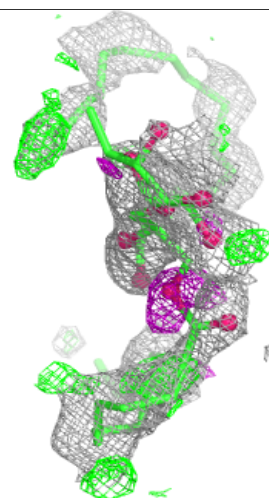
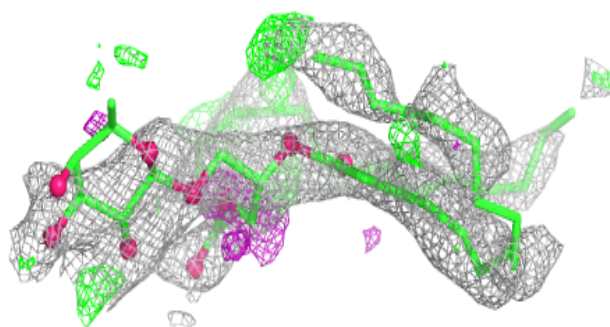
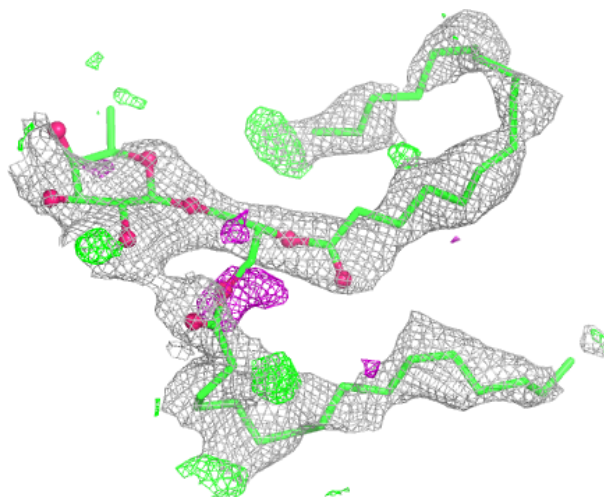
**Electron density around DGD D 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



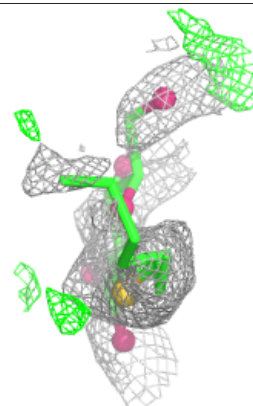
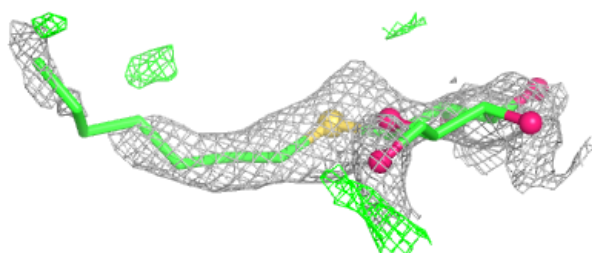
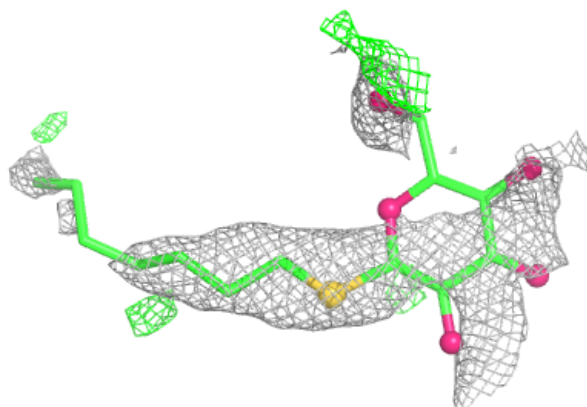
Electron density around DGD d 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

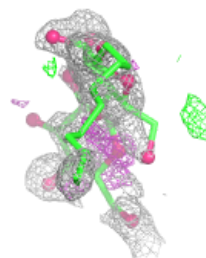
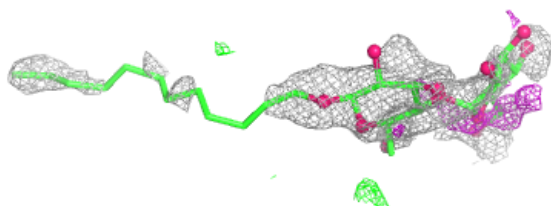
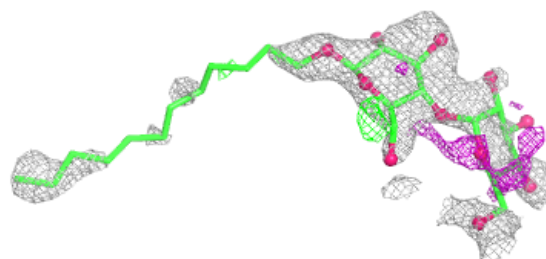


Electron density around HTG D 414:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

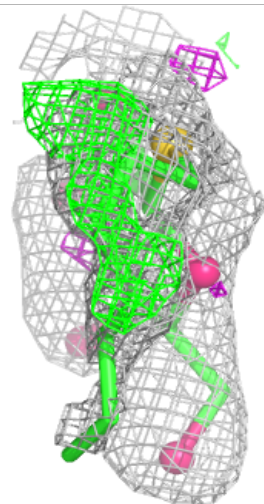
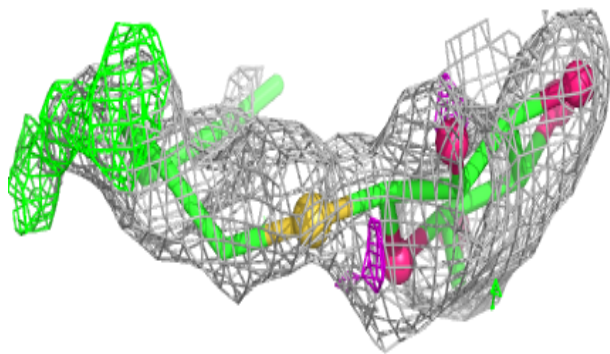
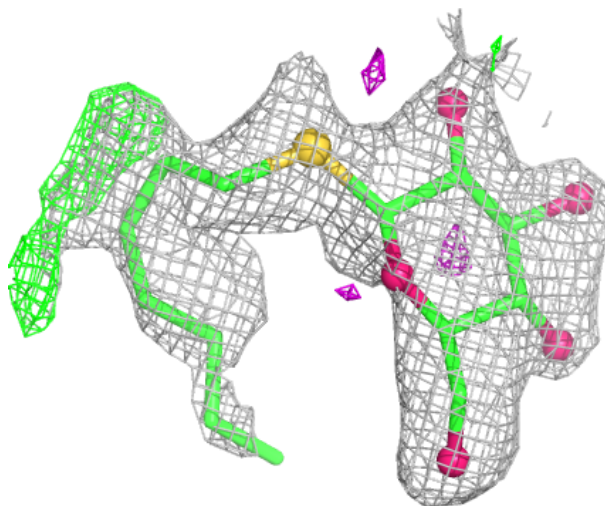
**Electron density around LMT F 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



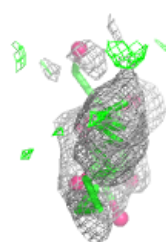
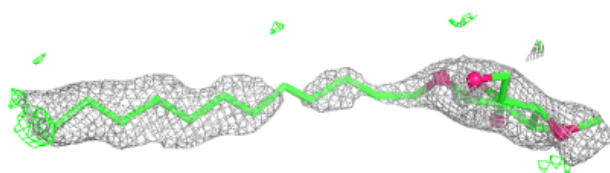
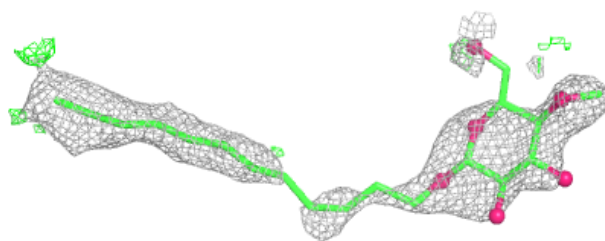
Electron density around HTG v 204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

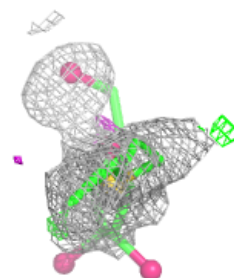
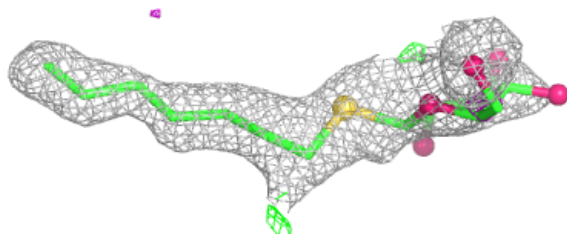
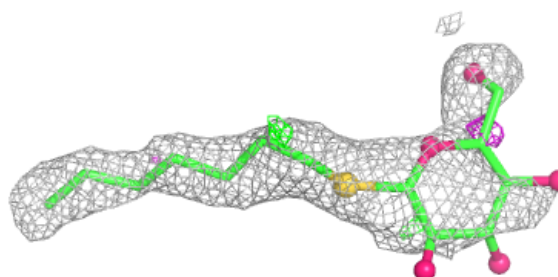


Electron density around LMT e 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

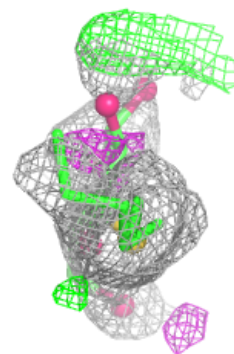
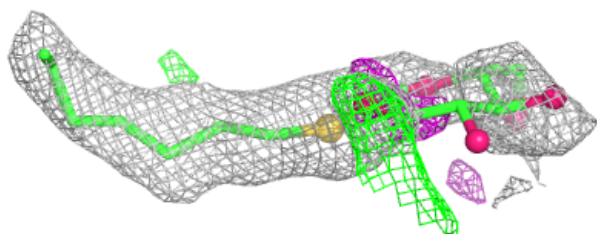
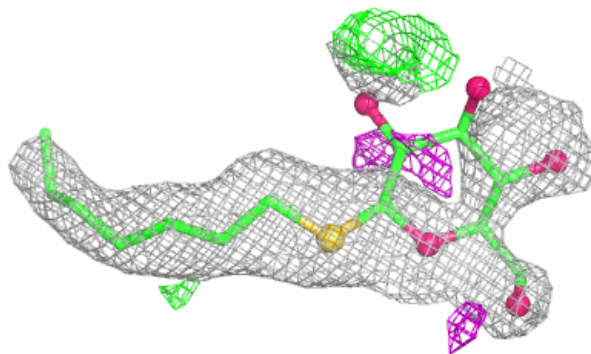
**Electron density around HTG c 922:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



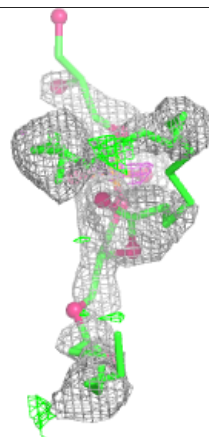
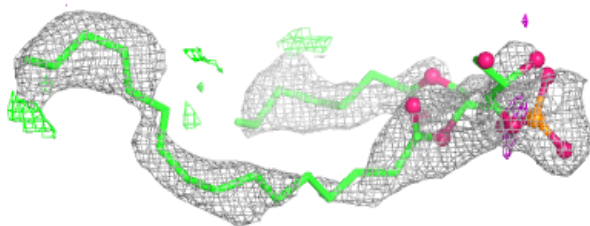
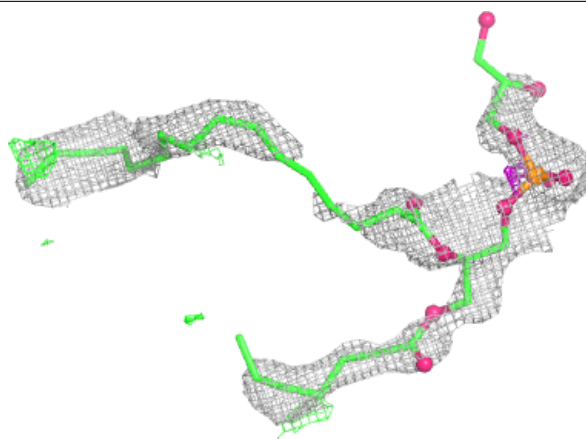
Electron density around HTG d 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



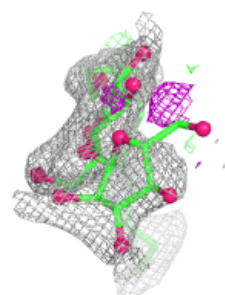
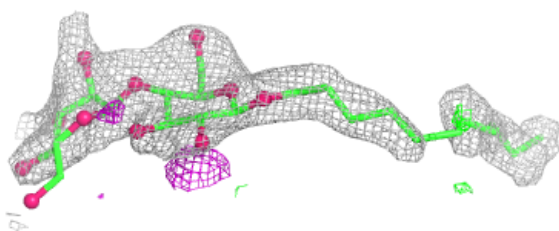
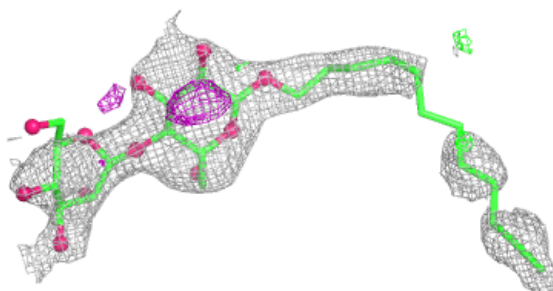
Electron density around LHG e 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

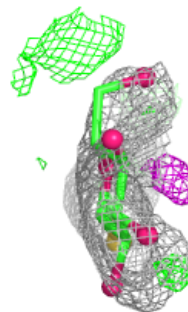
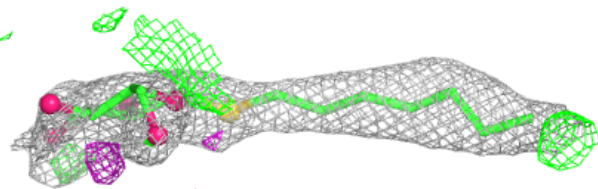
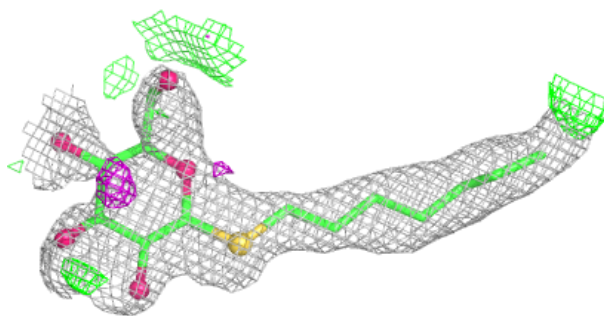


Electron density around LMT I 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

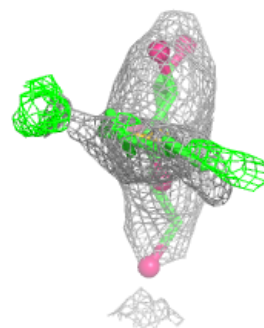
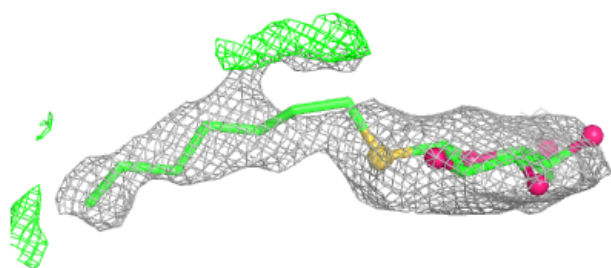
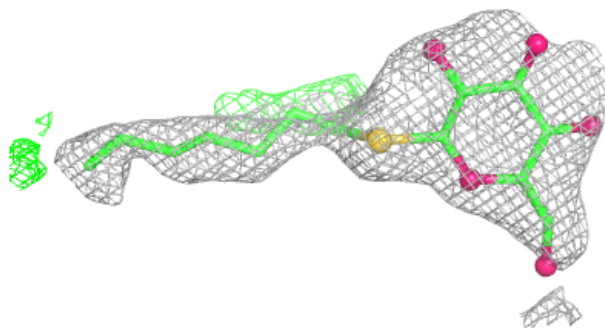
**Electron density around HTG b 628:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

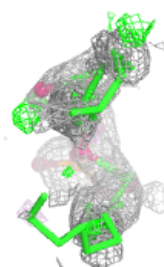
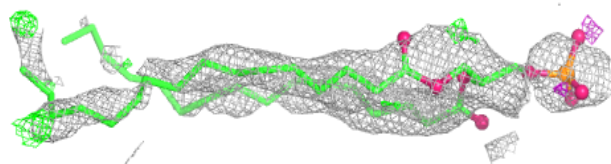
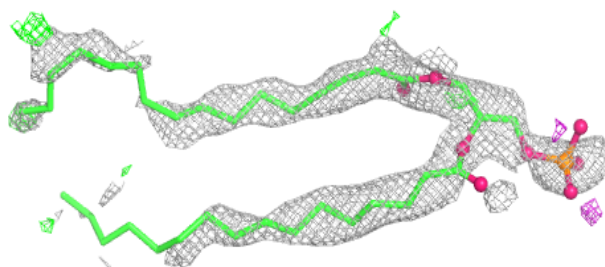


Electron density around HTG c 921:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

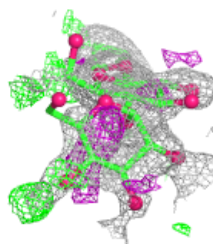
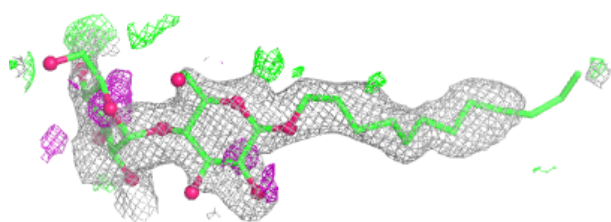
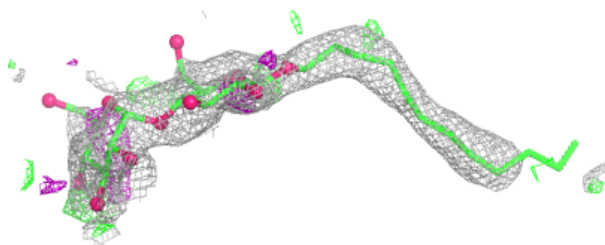
**Electron density around LHG K 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

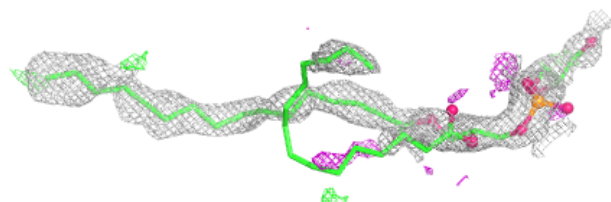
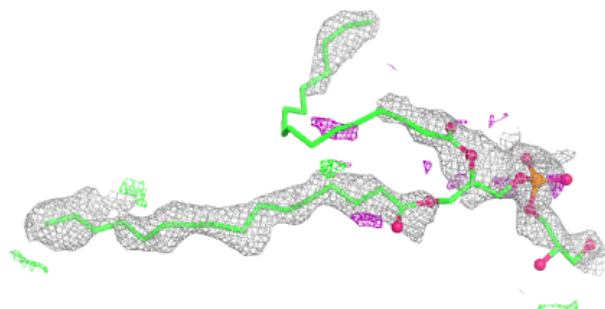


Electron density around LMT A 416:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

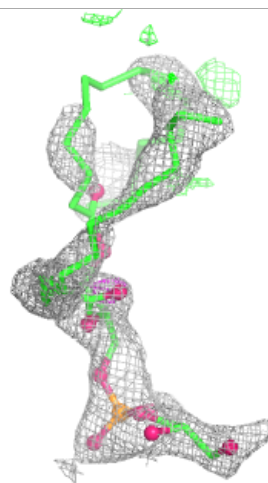
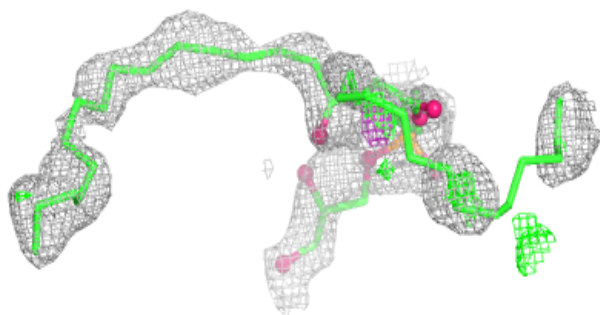
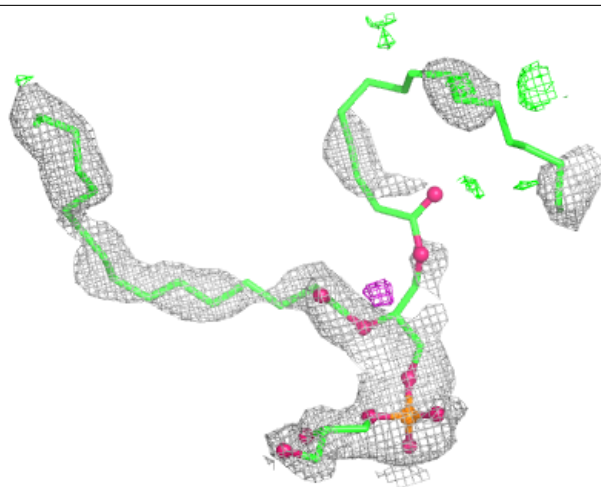
**Electron density around LHG A 412:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



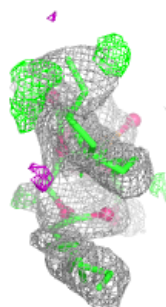
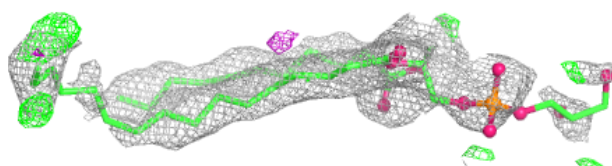
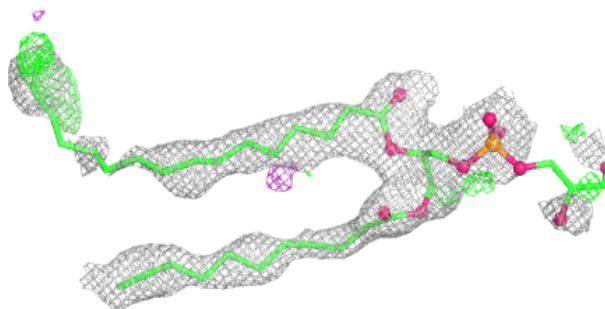
Electron density around LHG E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

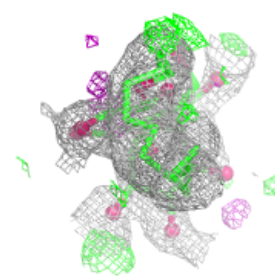
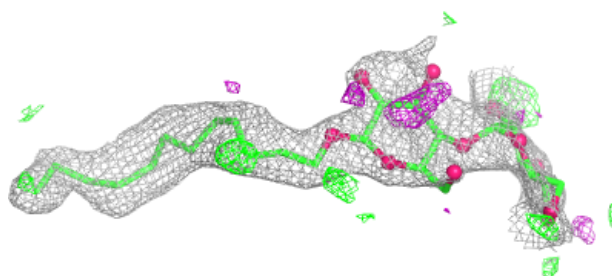
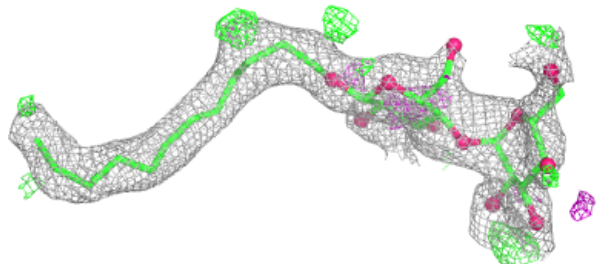


Electron density around LHG d 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

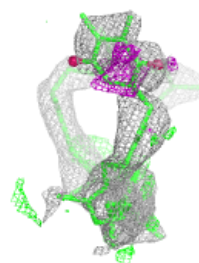
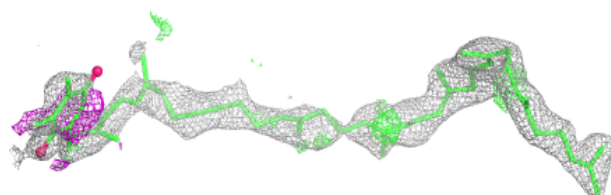
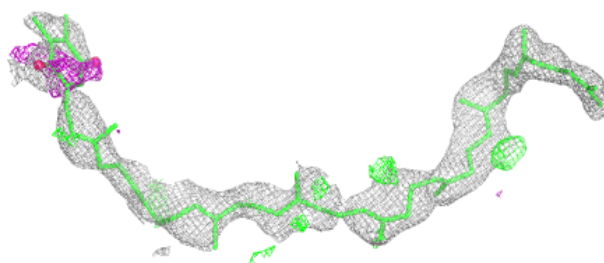
**Electron density around LMT a 418:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

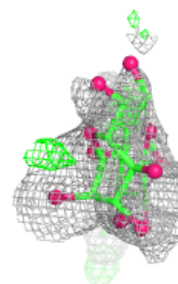
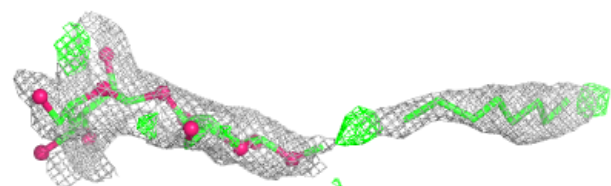
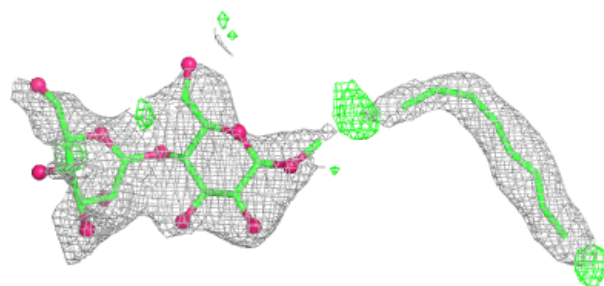


Electron density around PL9 a 414:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

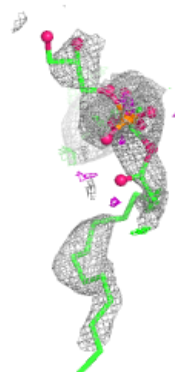
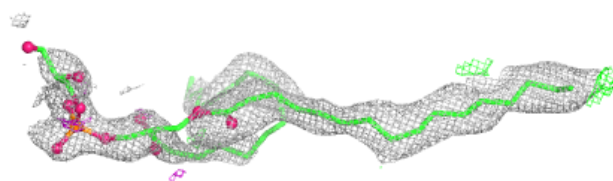
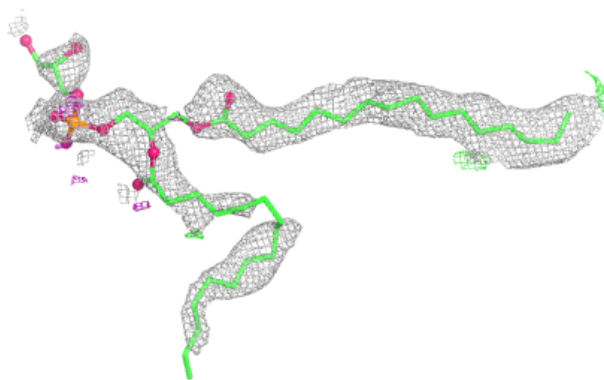
**Electron density around LMT z 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

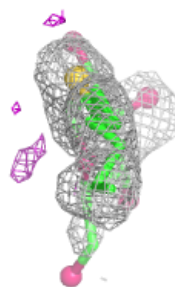
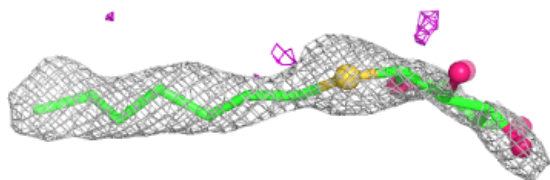
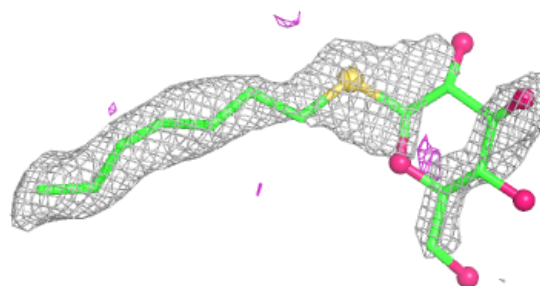


Electron density around LHG a 415:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

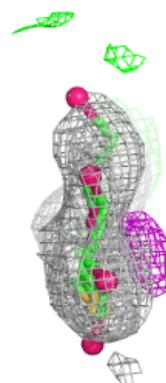
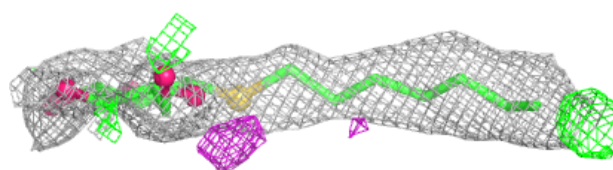
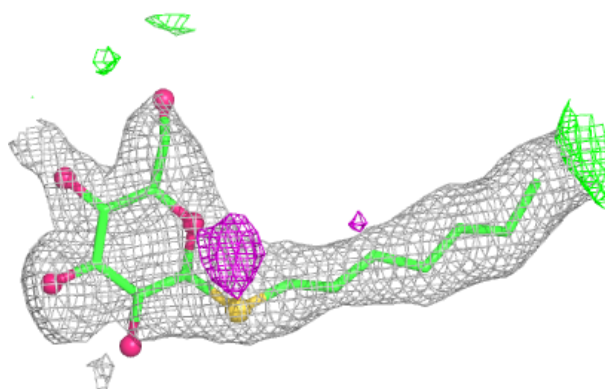
**Electron density around HTG B 626:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

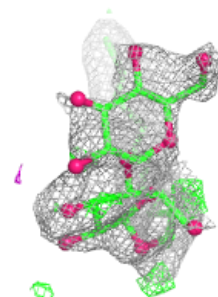
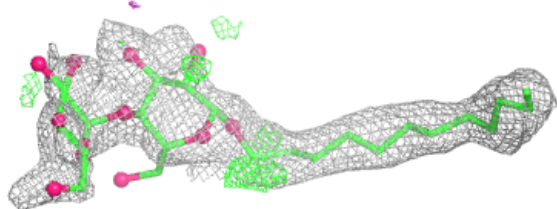
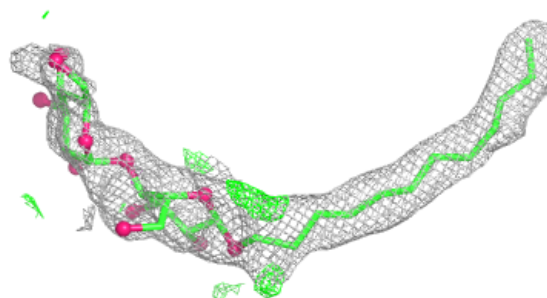


Electron density around HTG B 631:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

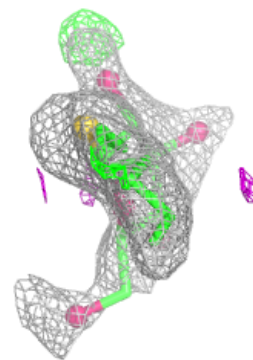
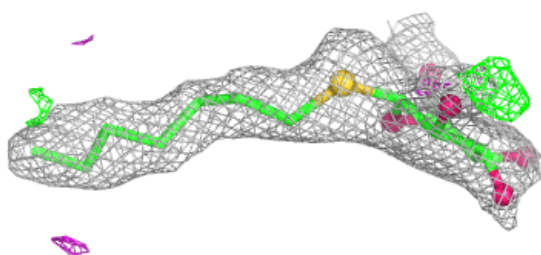
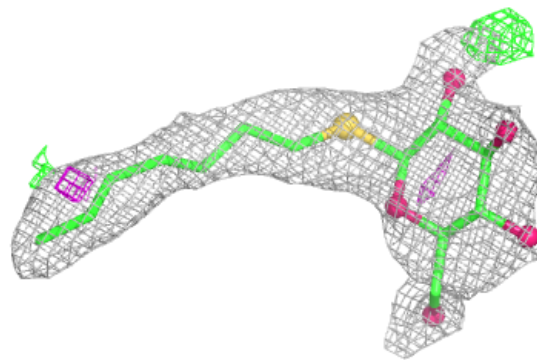
**Electron density around LMT m 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

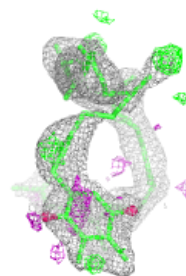
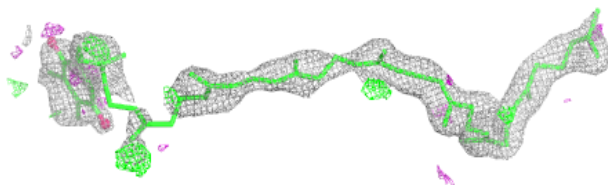
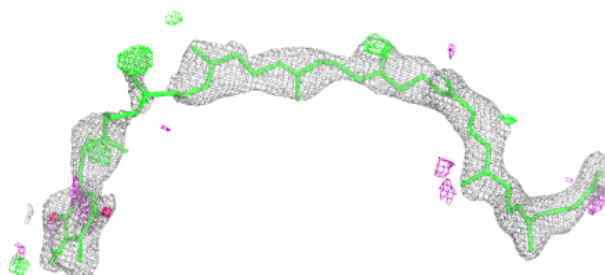


Electron density around HTG b 623:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

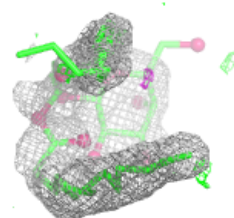
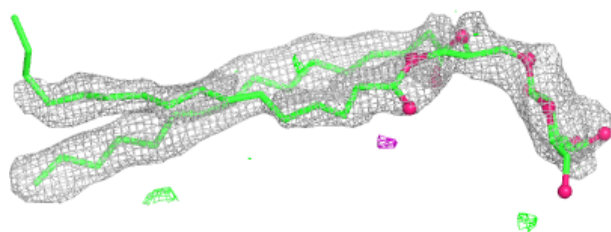
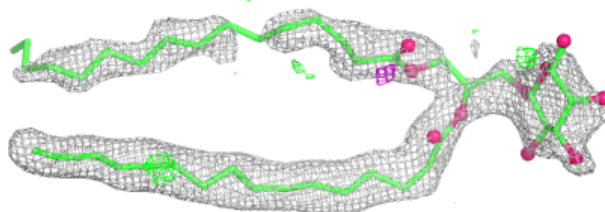
**Electron density around PL9 A 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

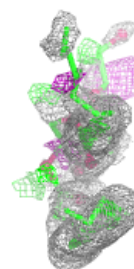
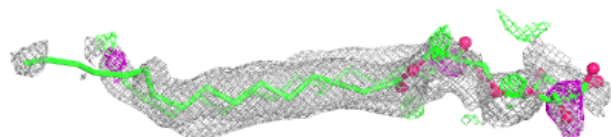
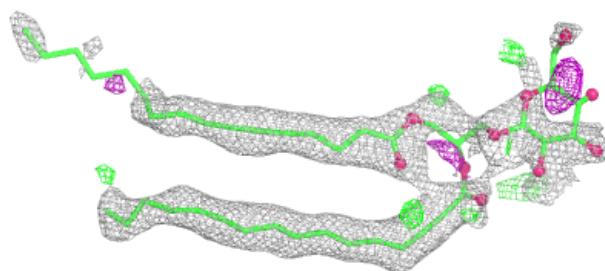


Electron density around LMG C 531:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

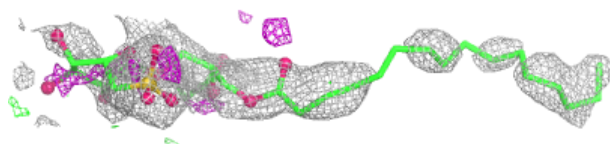
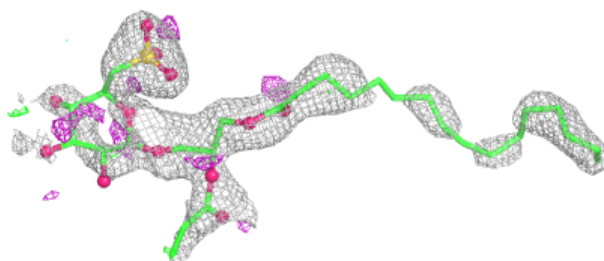
**Electron density around LMG D 412:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

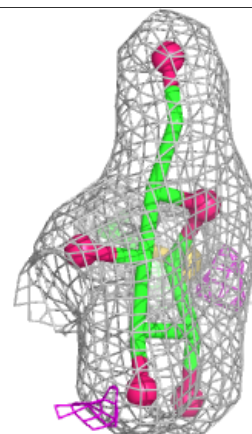
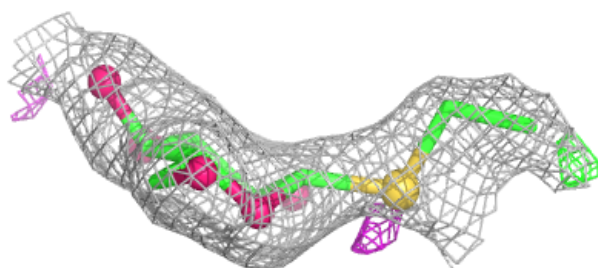
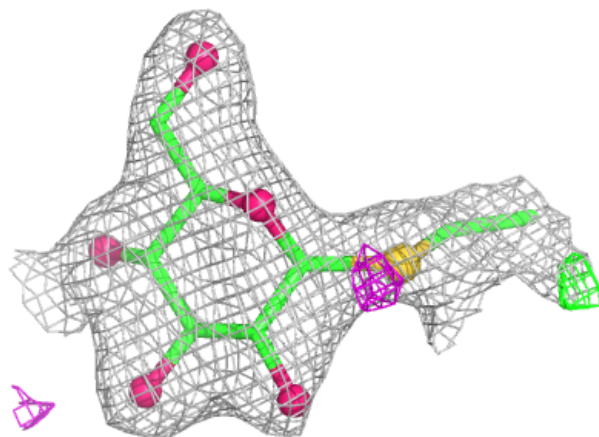


Electron density around SQD x 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

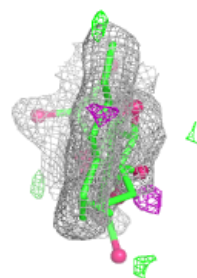
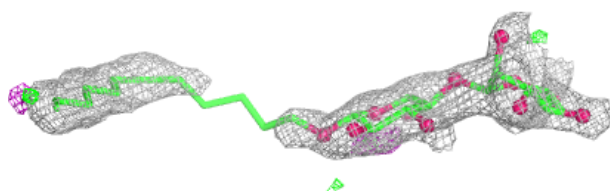
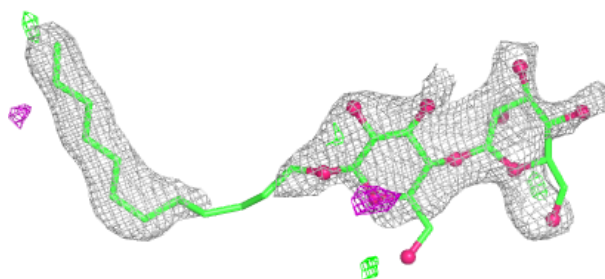
**Electron density around HTG V 204:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

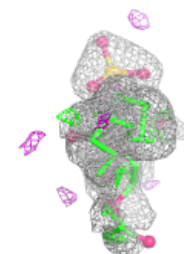
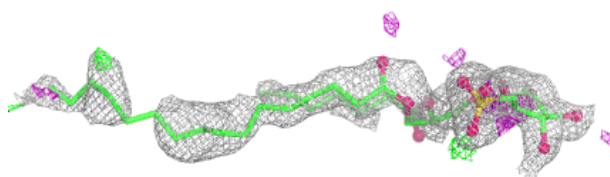
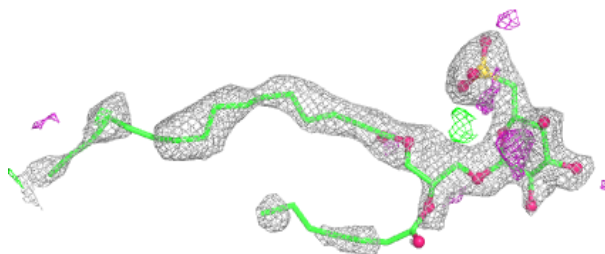


Electron density around LMT Z 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

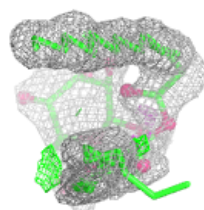
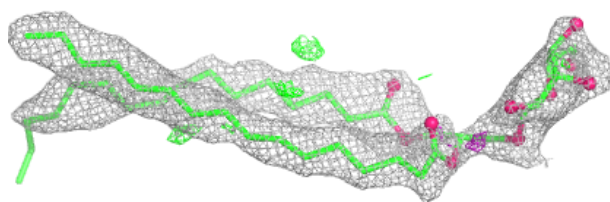
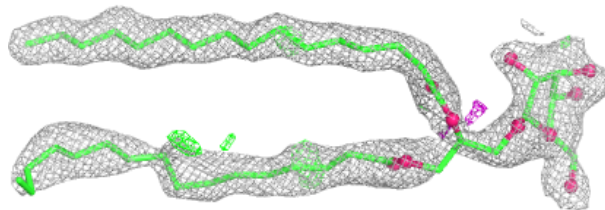
**Electron density around SQD D 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

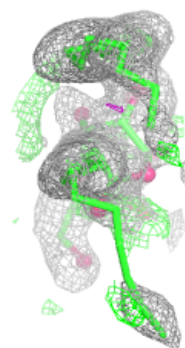
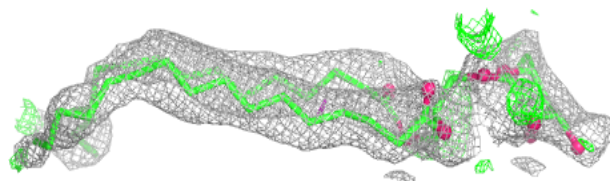
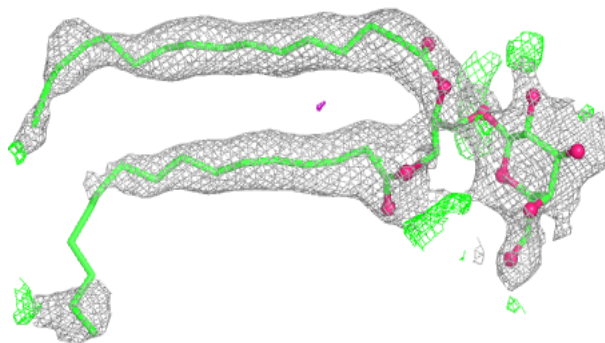


Electron density around LMG c 930:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

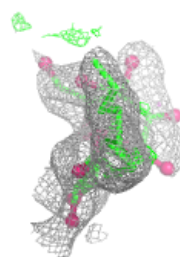
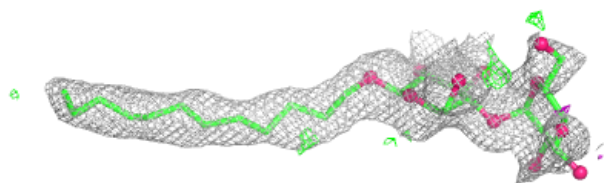
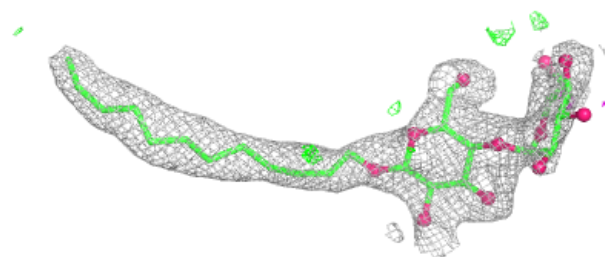
**Electron density around LMG d 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

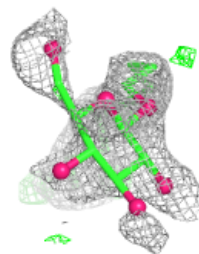
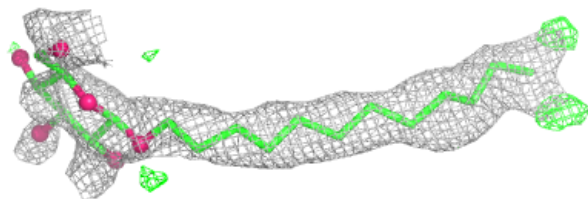
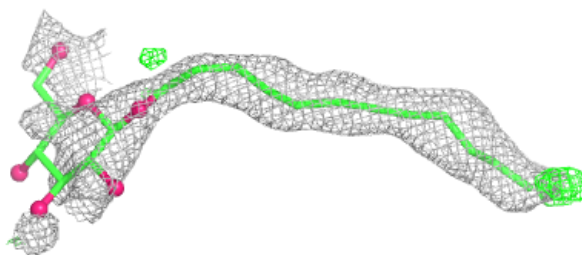


Electron density around LMT B 623:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

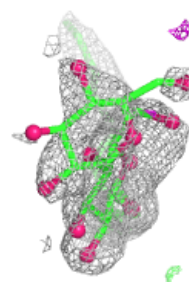
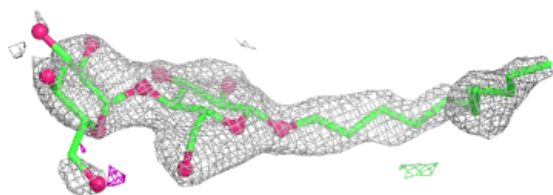
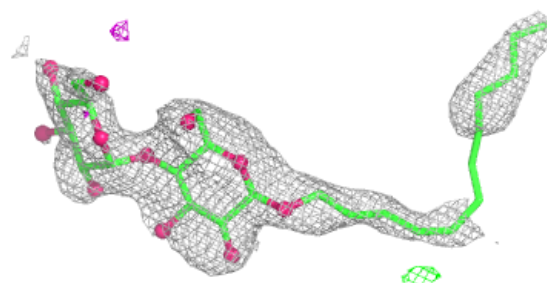
**Electron density around LMT B 643:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

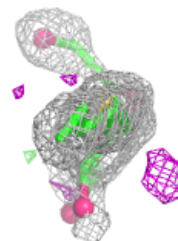
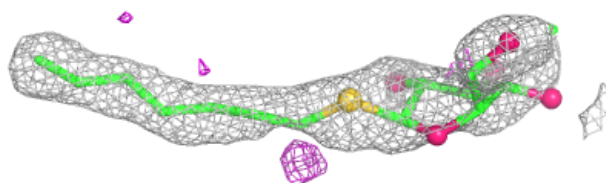
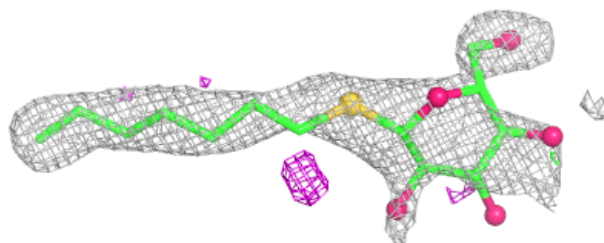


Electron density around LMT a 422:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

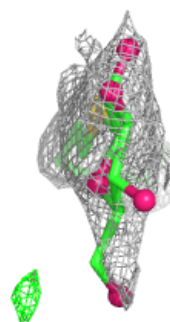
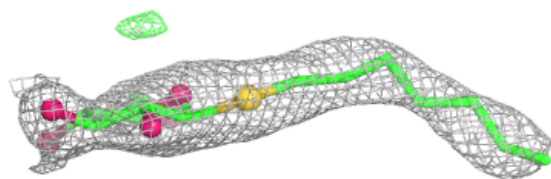
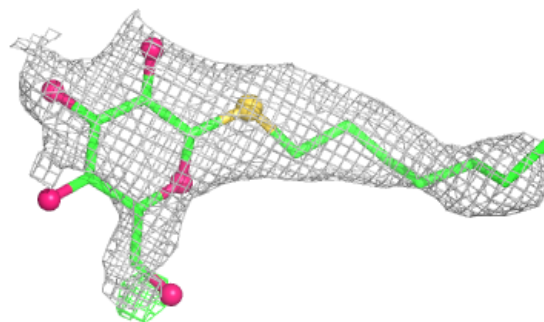
**Electron density around HTG C 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

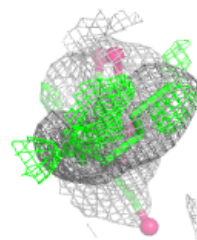
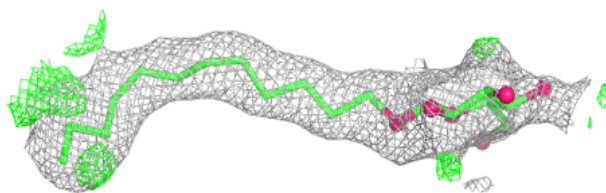
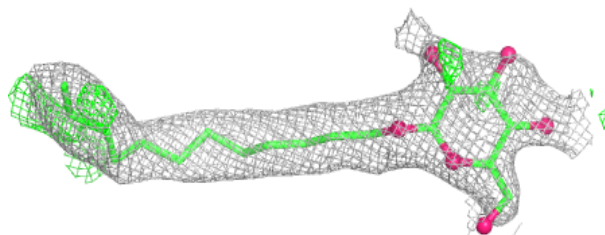


Electron density around HTG C 523:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

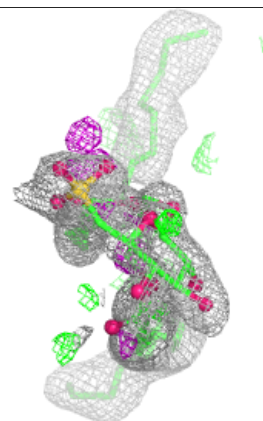
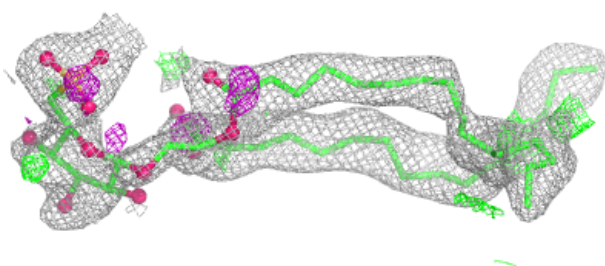
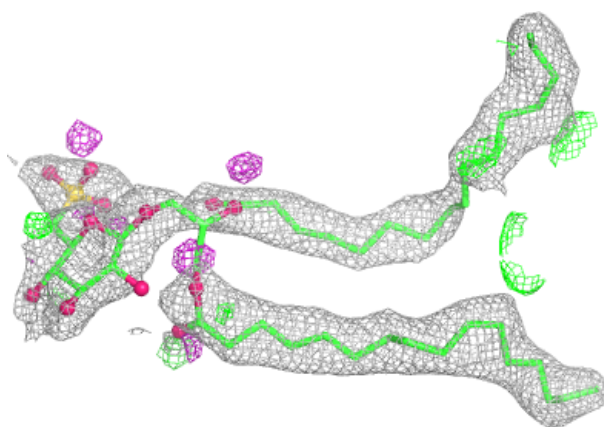
**Electron density around LMT B 644:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

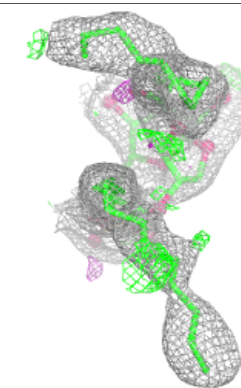
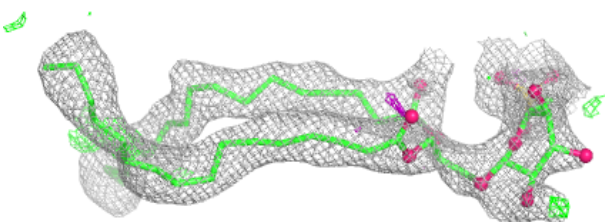
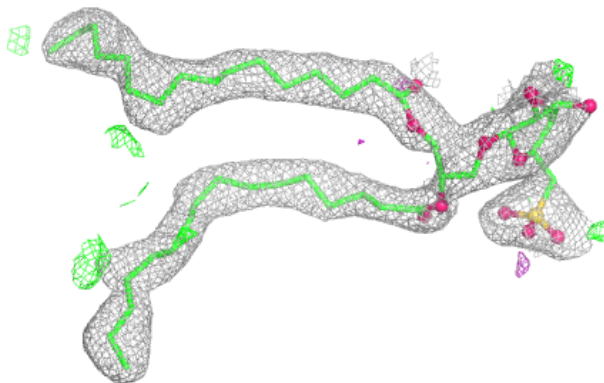


Electron density around SQD B 621:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

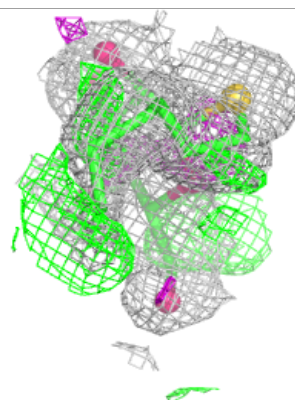
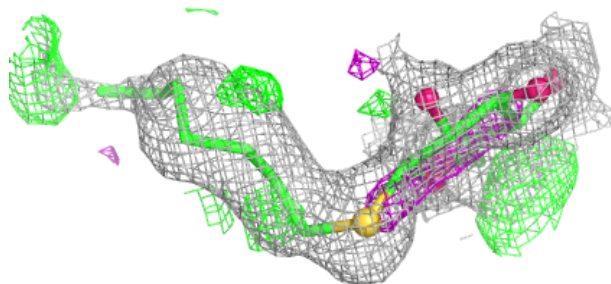
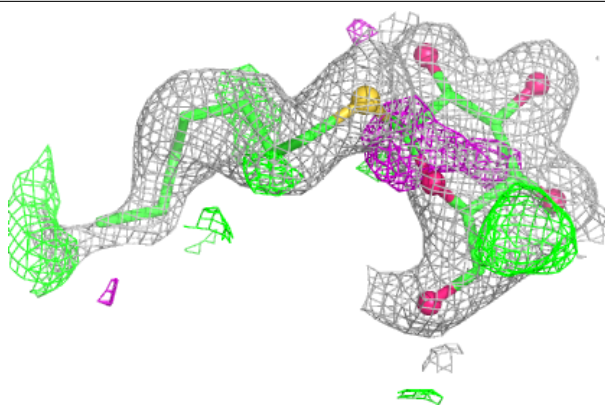
**Electron density around SQD L 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

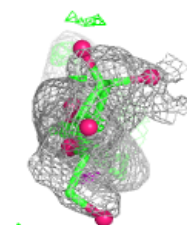
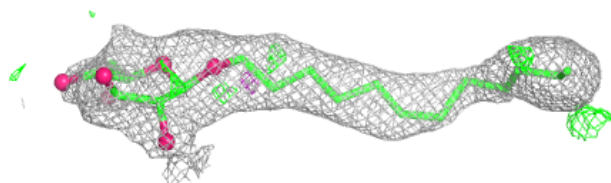
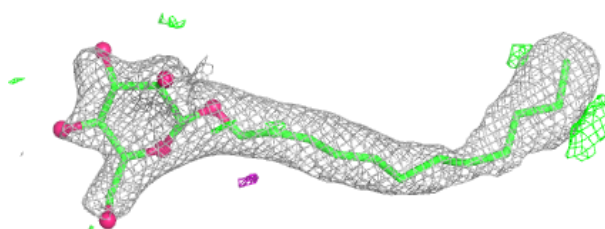


Electron density around HTG B 625:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

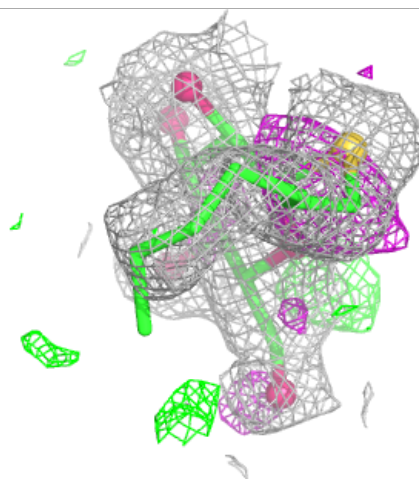
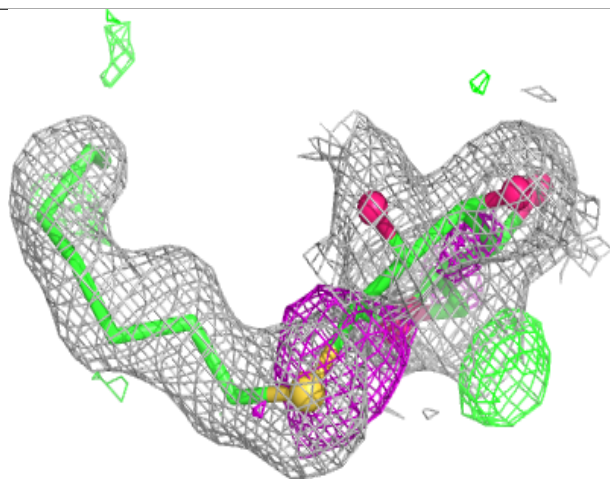
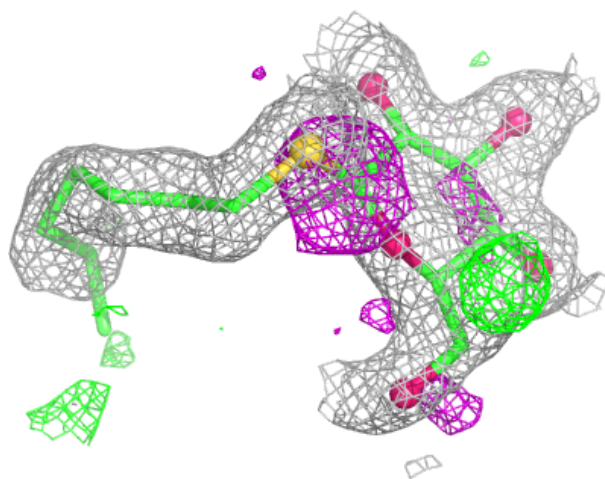
**Electron density around LMT T 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



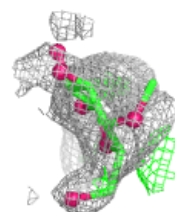
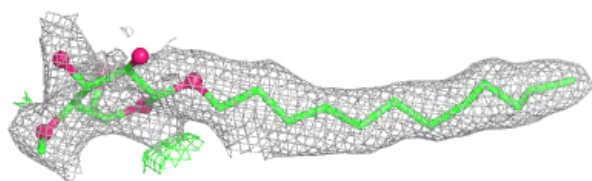
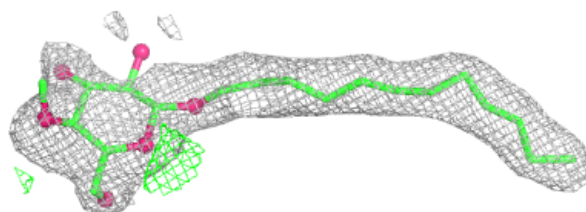
Electron density around HTG b 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

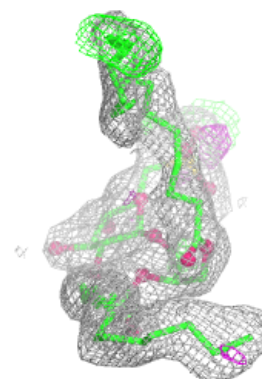
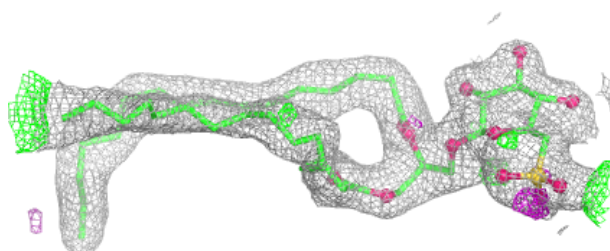
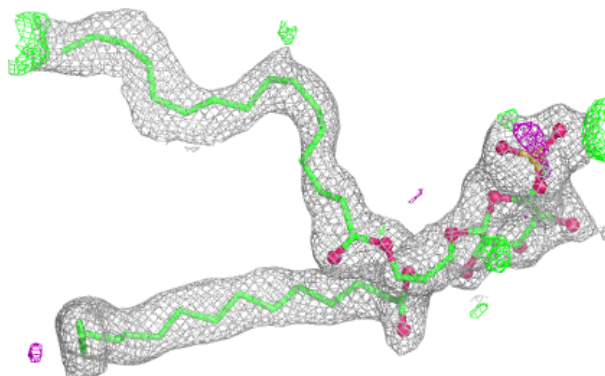


Electron density around LMT b 621:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

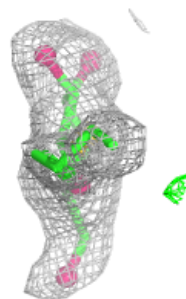
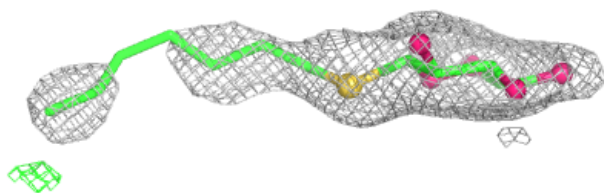
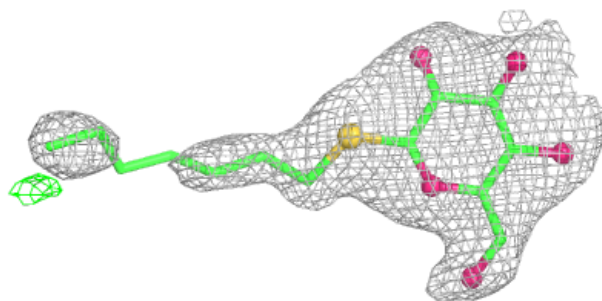
**Electron density around SQD a 417:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

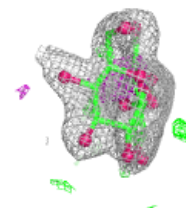
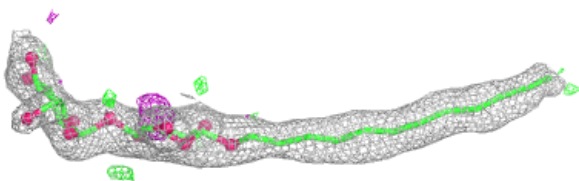
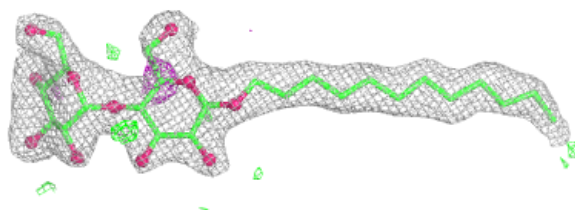


Electron density around HTG C 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

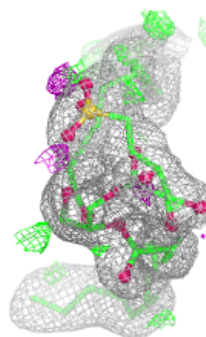
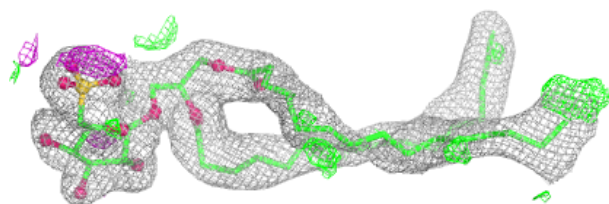
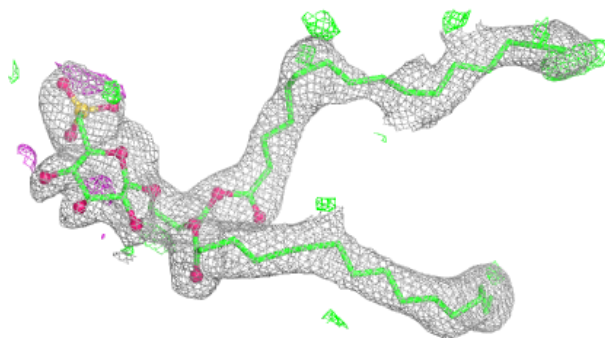
**Electron density around LMT m 104:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

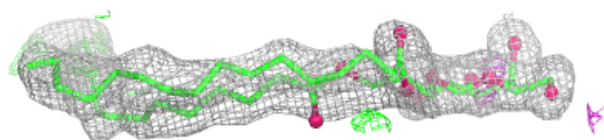


Electron density around SQD A 415:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

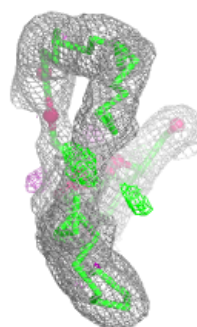
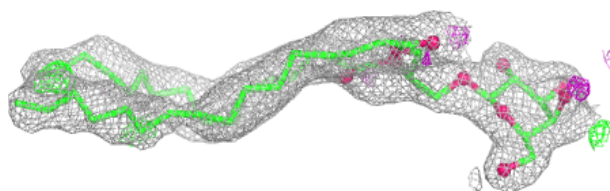
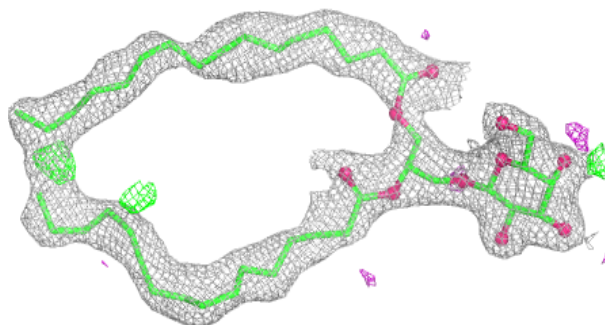
**Electron density around LMG C 520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

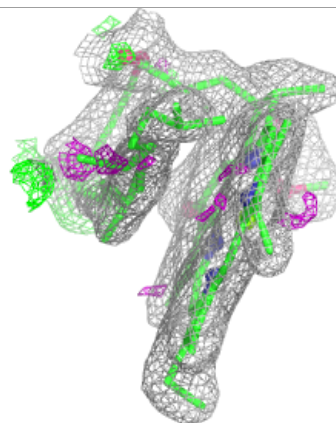
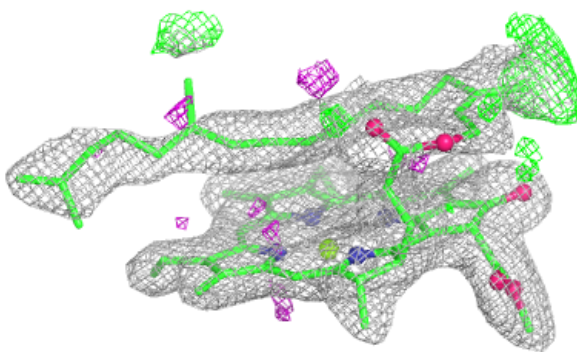
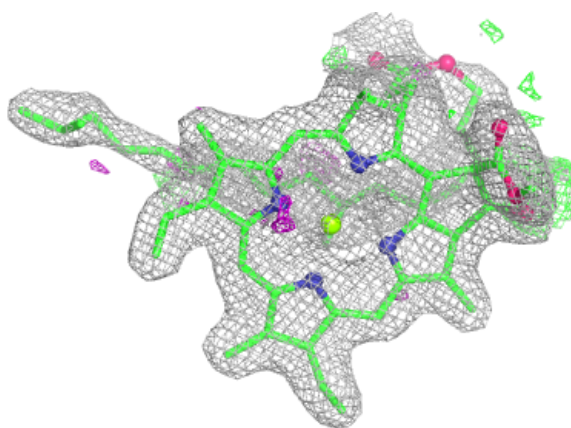


Electron density around LMG a 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

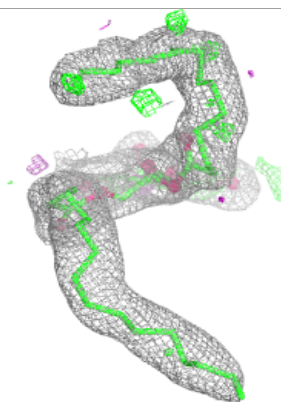
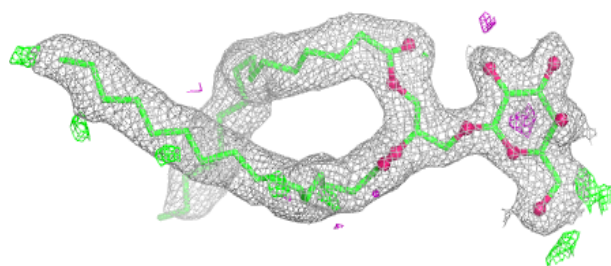
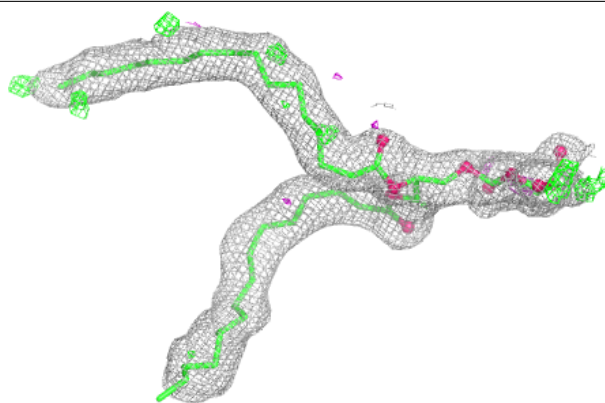
**Electron density around CLA b 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

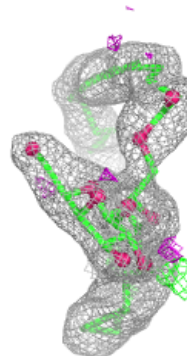
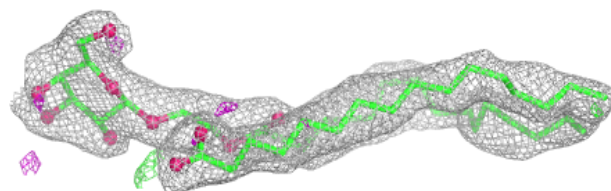
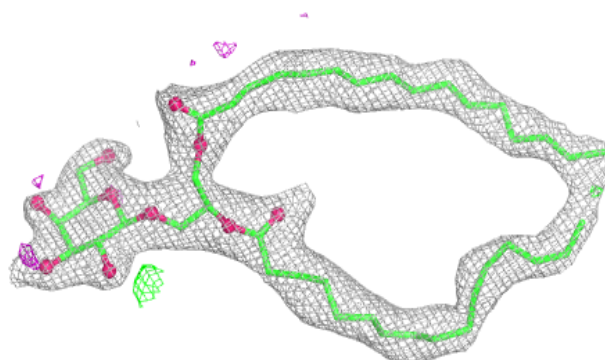


Electron density around LMG B 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

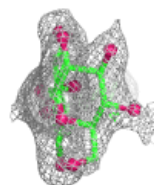
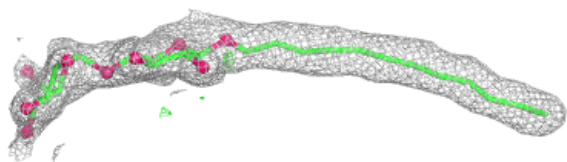
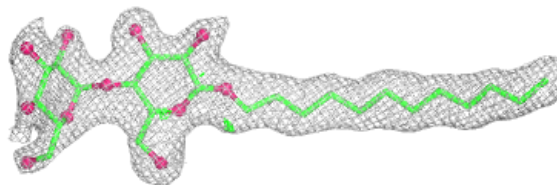
**Electron density around LMG C 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

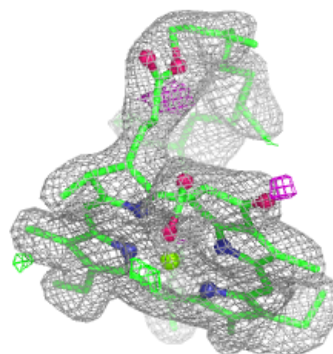
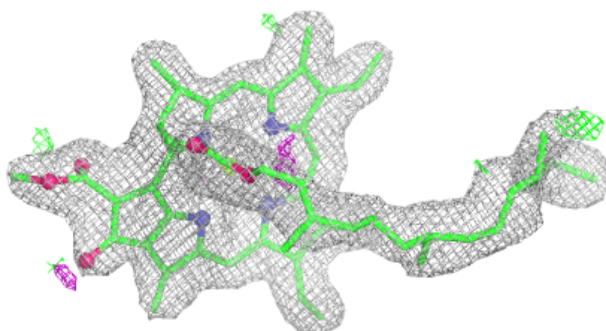
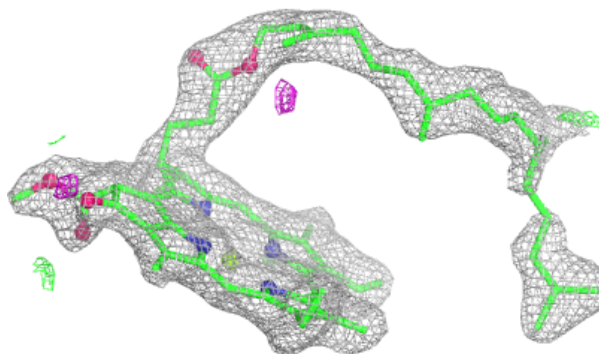


Electron density around LMT M 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

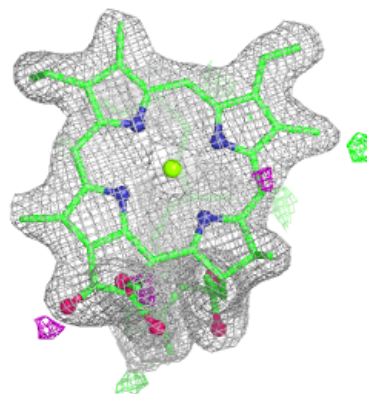
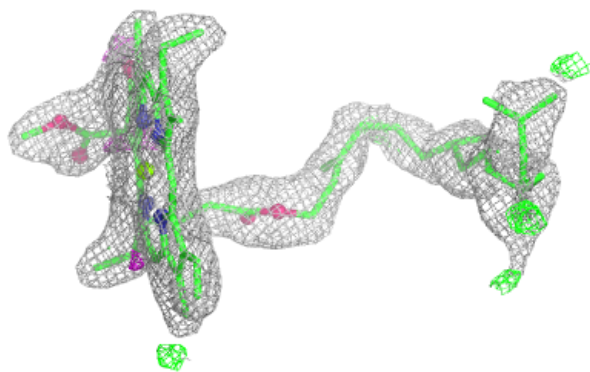
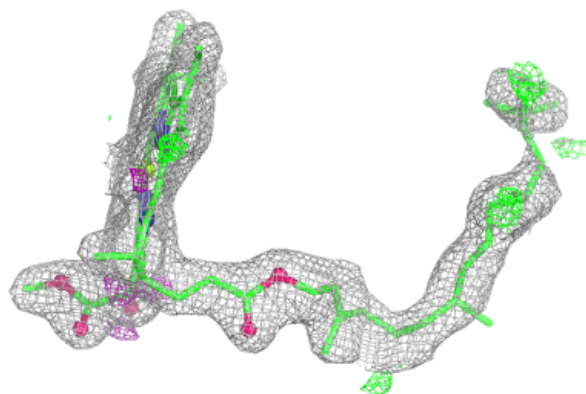
**Electron density around CLA C 514:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



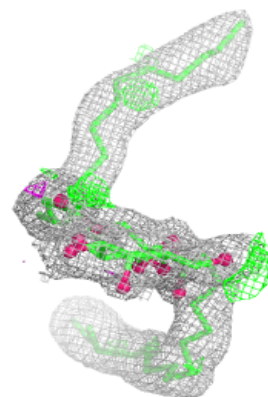
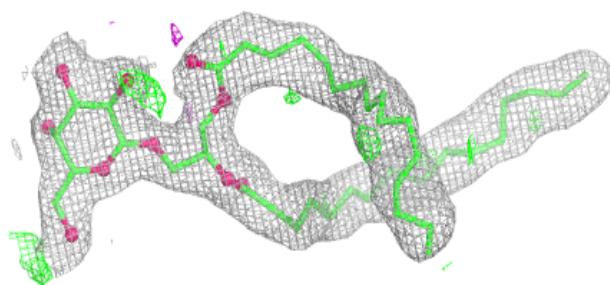
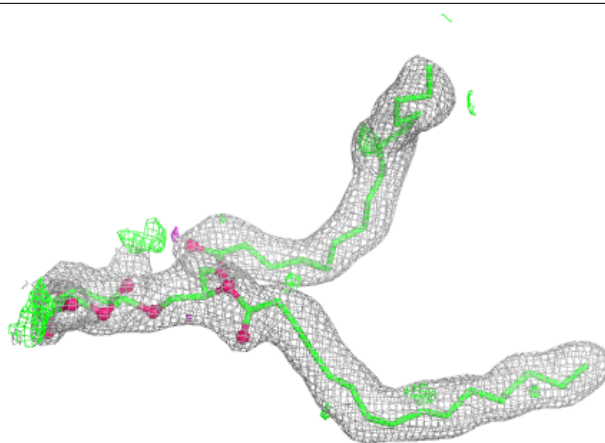
Electron density around CLA C 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

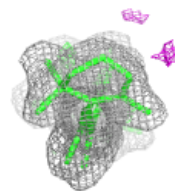
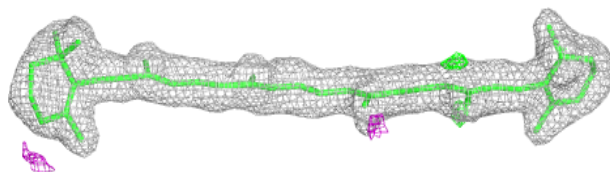
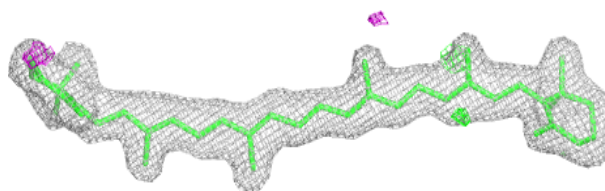


Electron density around LMG m 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

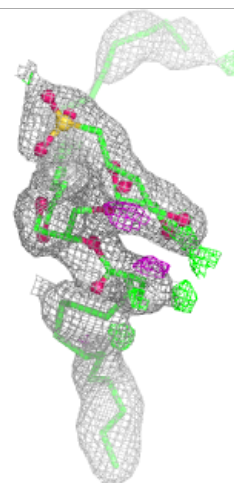
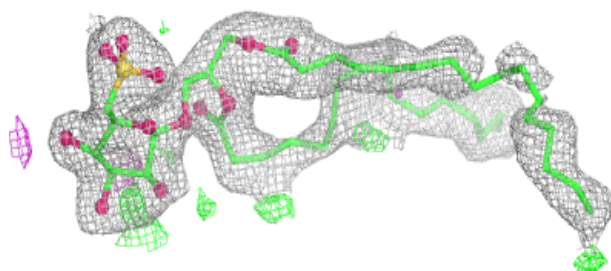
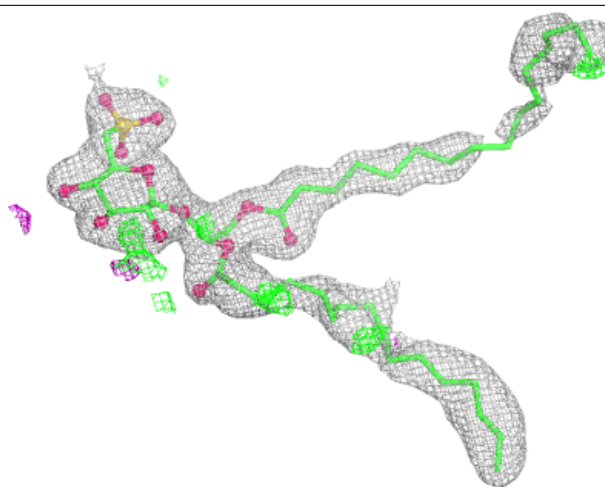
**Electron density around BCR C 515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



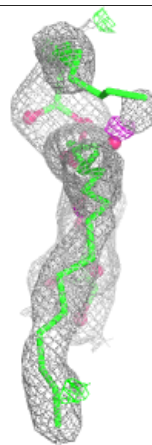
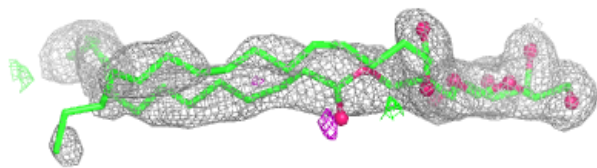
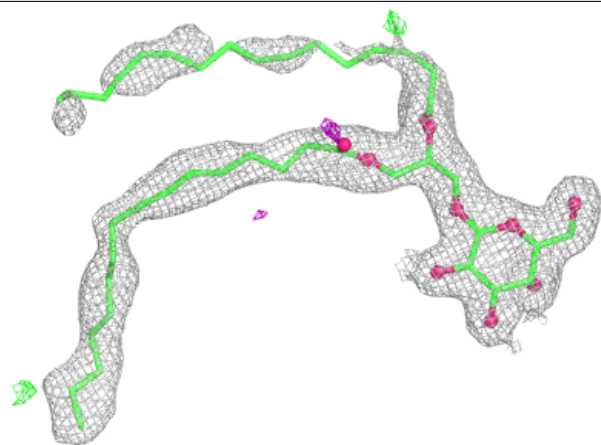
Electron density around SQD A 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



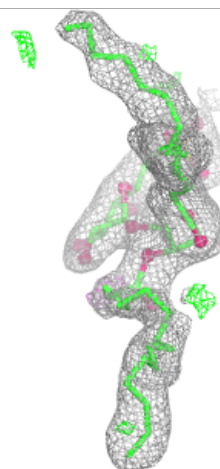
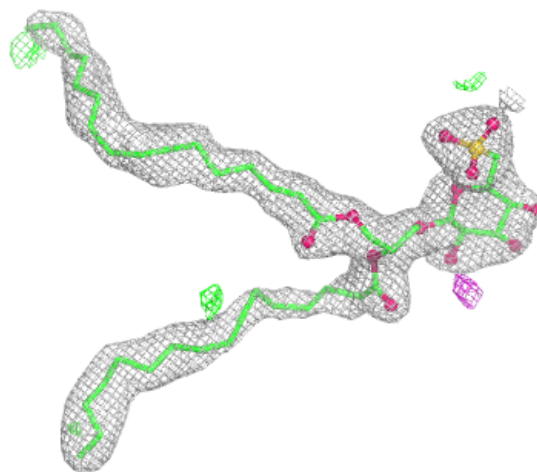
Electron density around LMG c 920:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



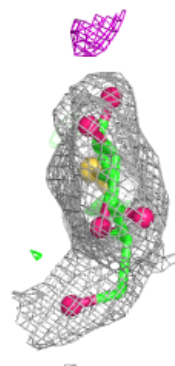
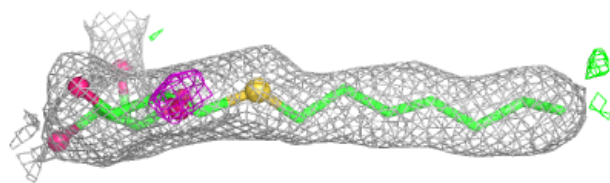
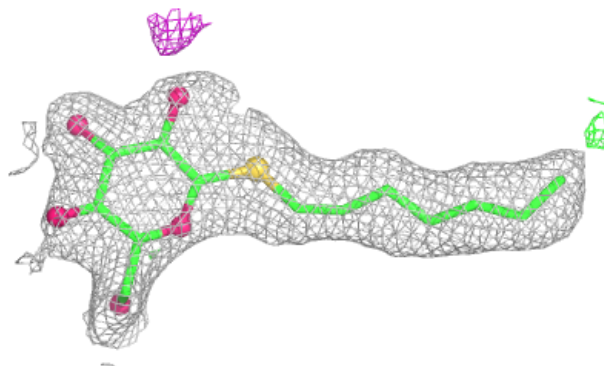
Electron density around SQD a 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

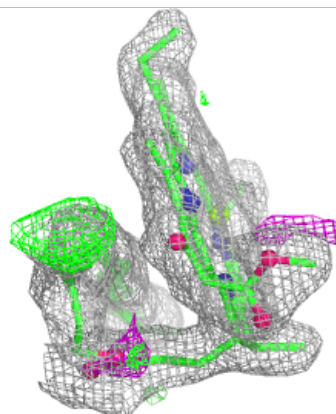
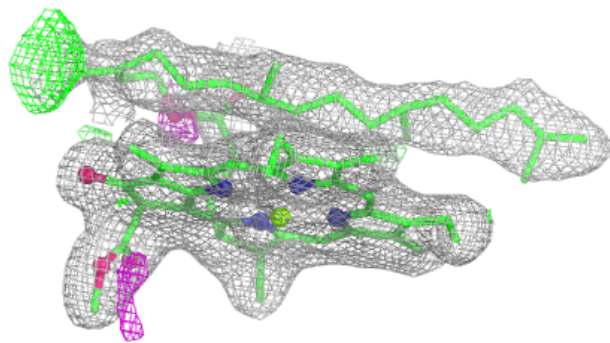
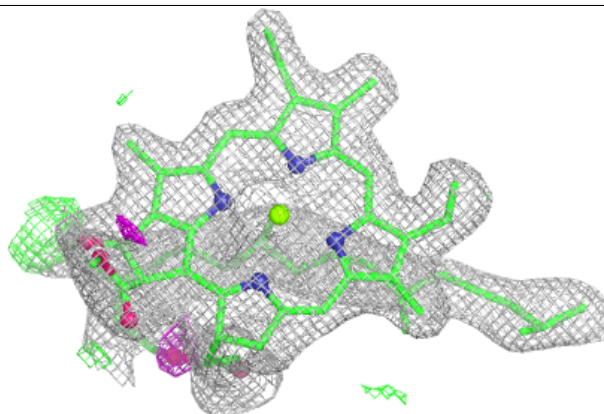


Electron density around HTG B 630:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

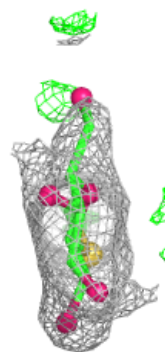
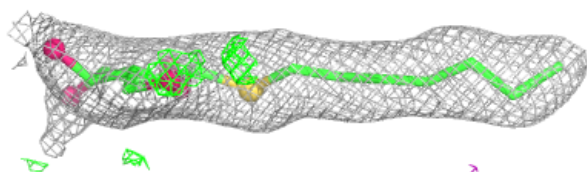
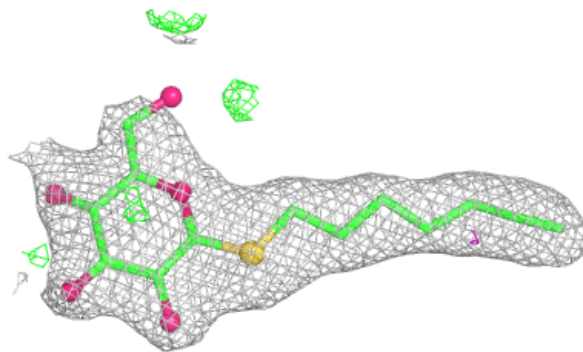
**Electron density around CLA B 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



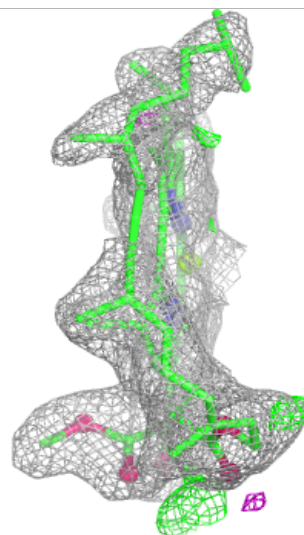
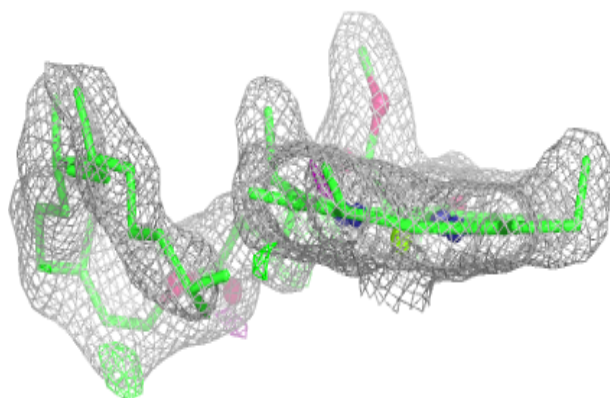
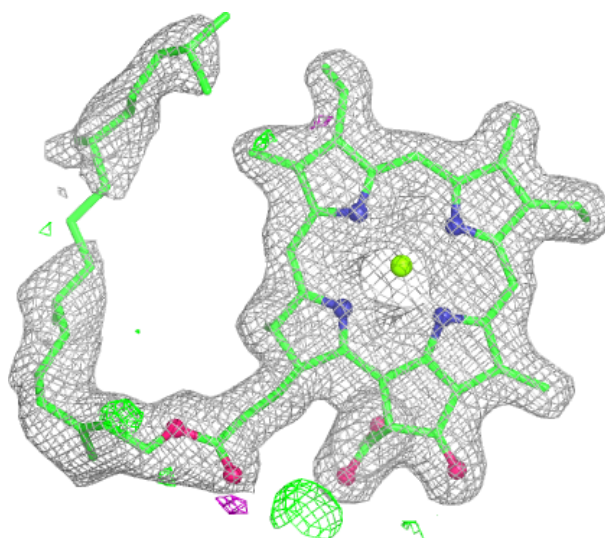
Electron density around HTG b 627:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



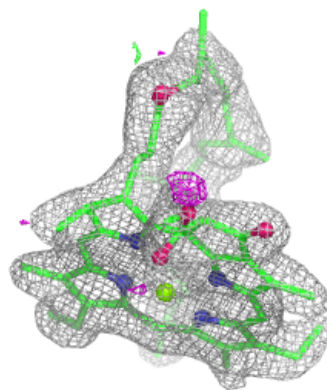
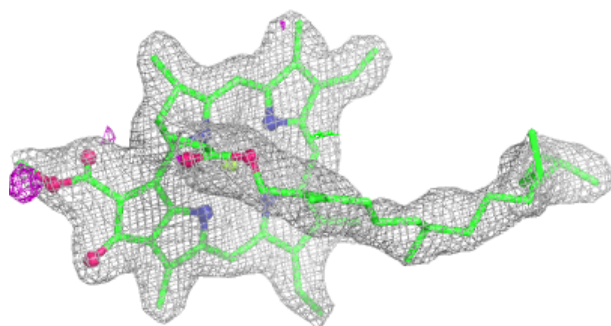
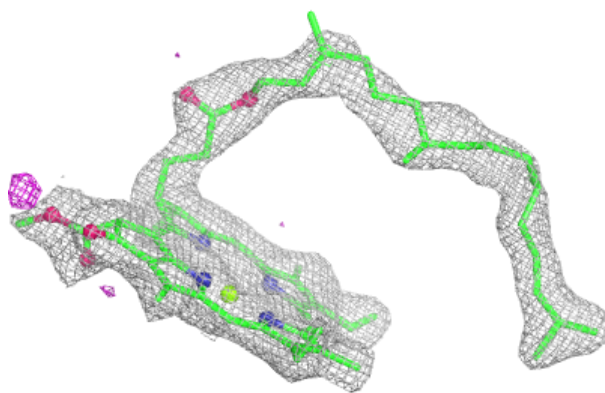
Electron density around CLA c 913:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



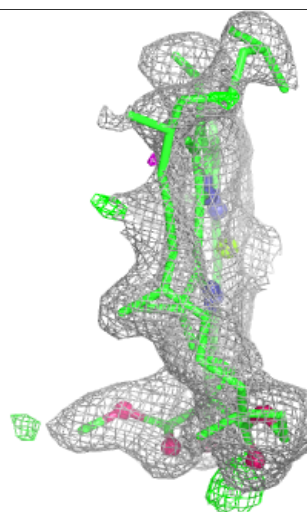
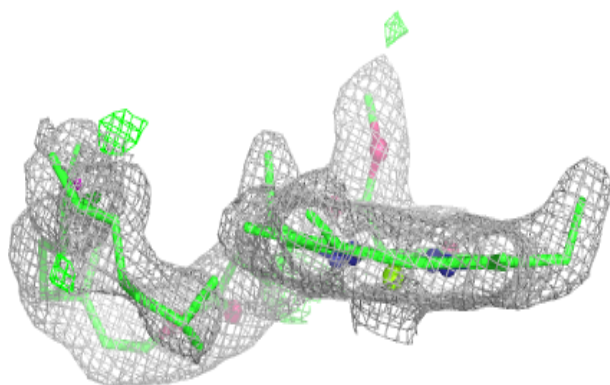
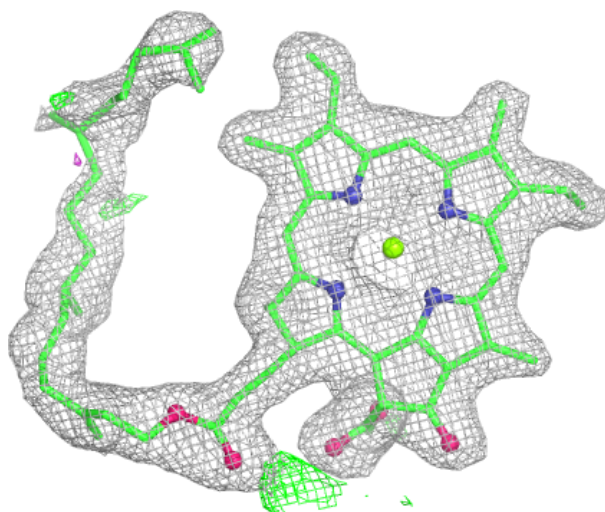
Electron density around CLA c 914:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



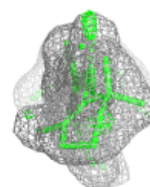
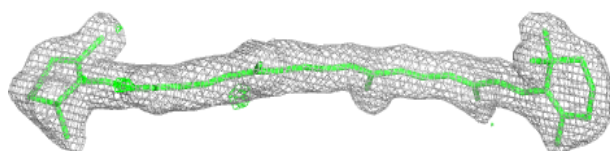
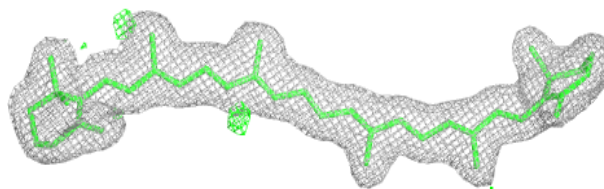
Electron density around CLA C 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

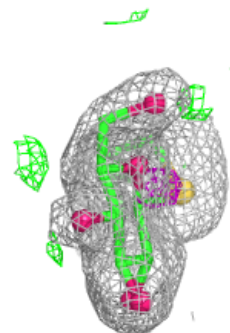
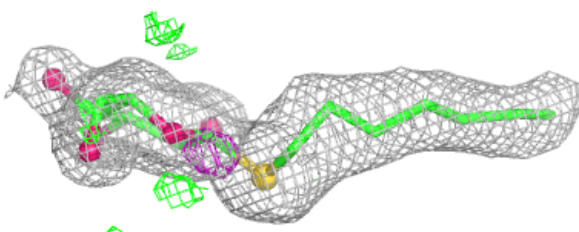
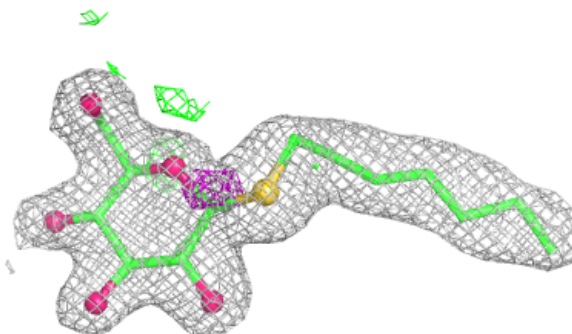


Electron density around BCR Y 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

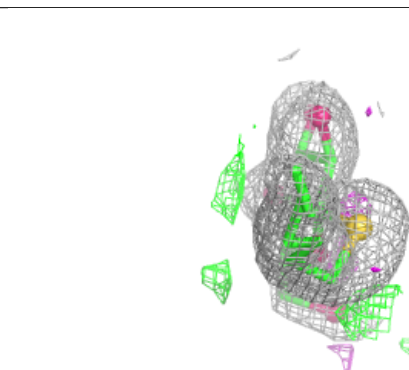
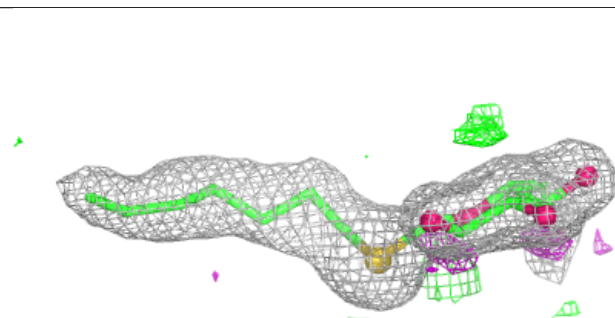
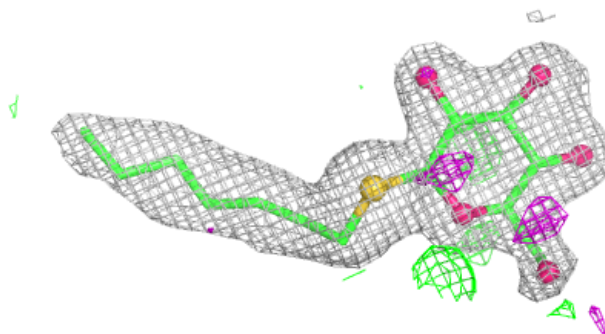
**Electron density around HTG O 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

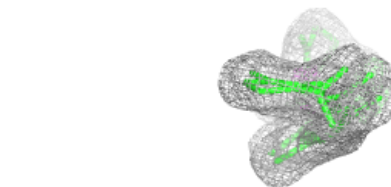
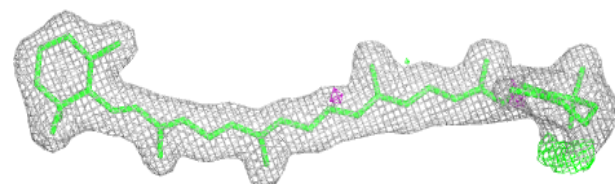
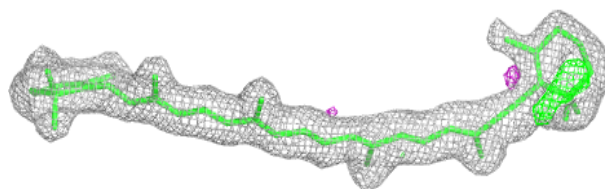


Electron density around HTG B 624:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

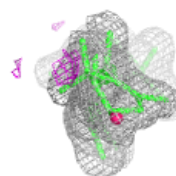
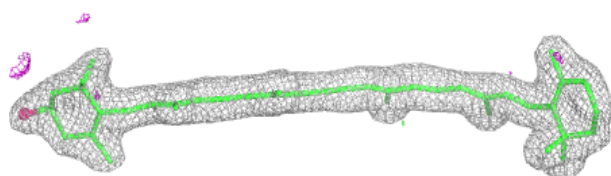
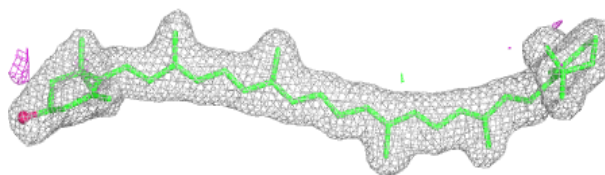
**Electron density around BCR d 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

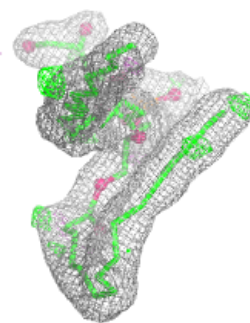
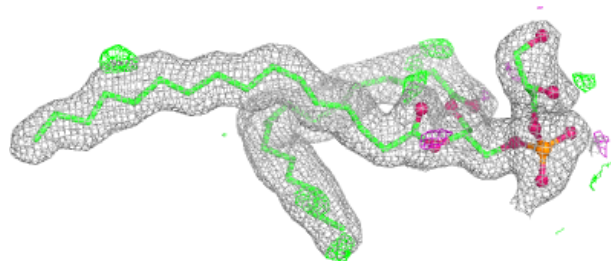
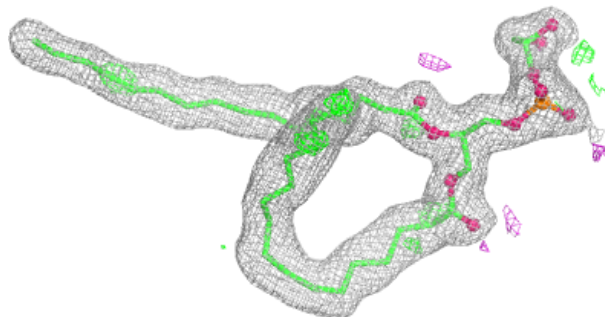


Electron density around RRX H 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

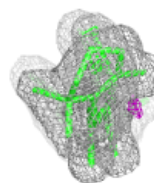
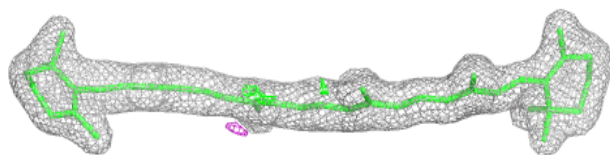
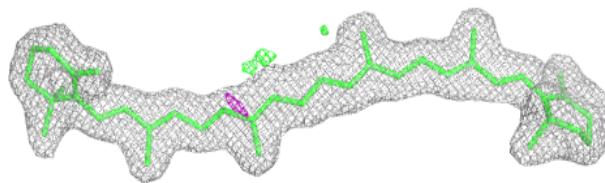
**Electron density around LHG D 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

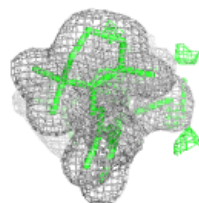
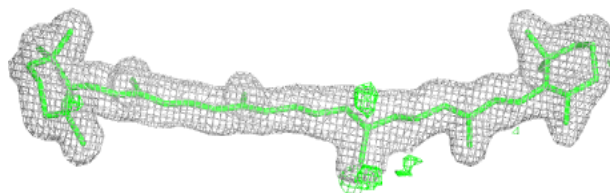
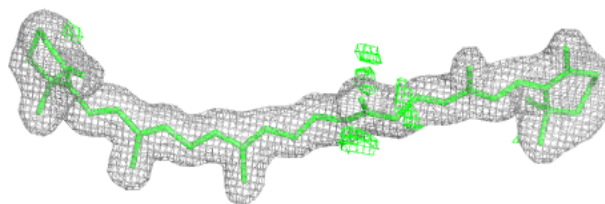


Electron density around BCR j 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

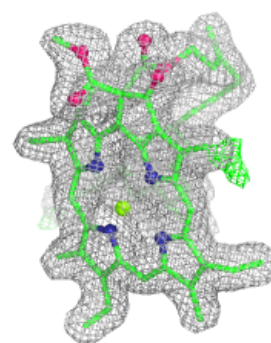
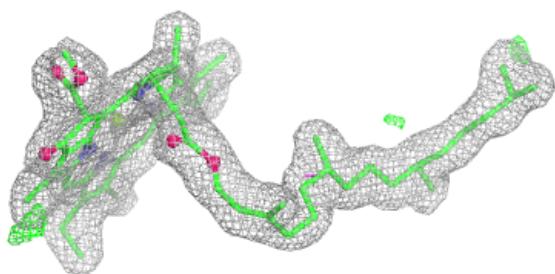
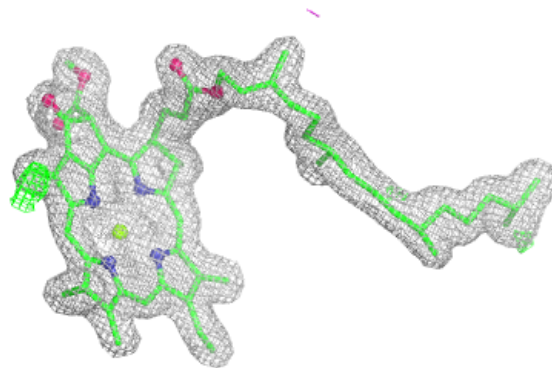
**Electron density around BCR t 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



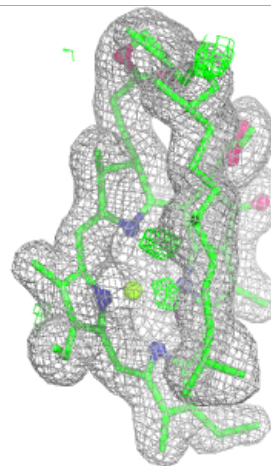
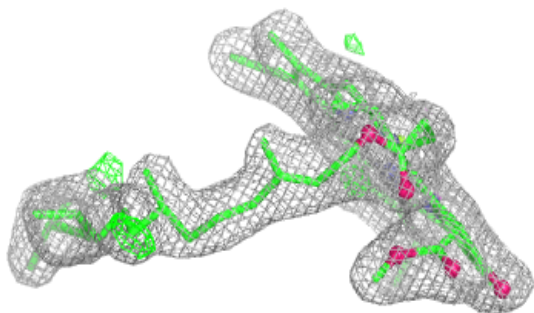
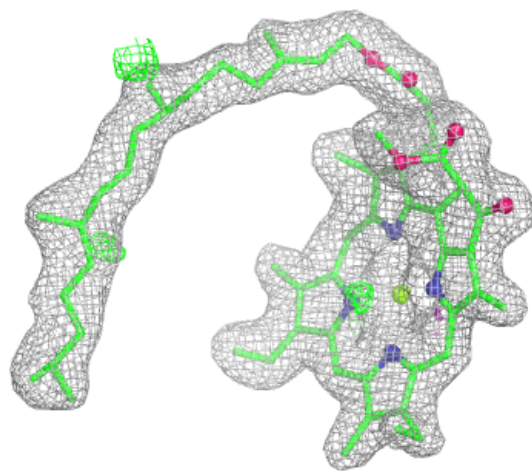
Electron density around CLA C 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



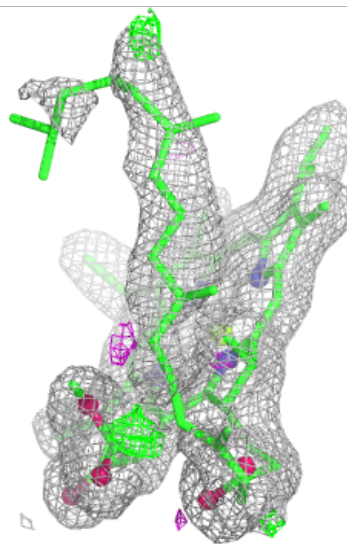
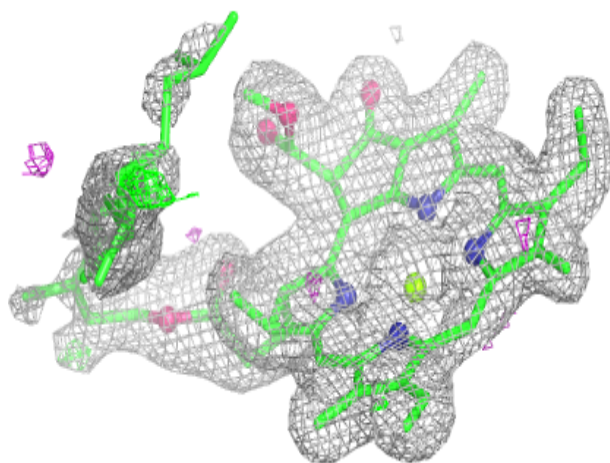
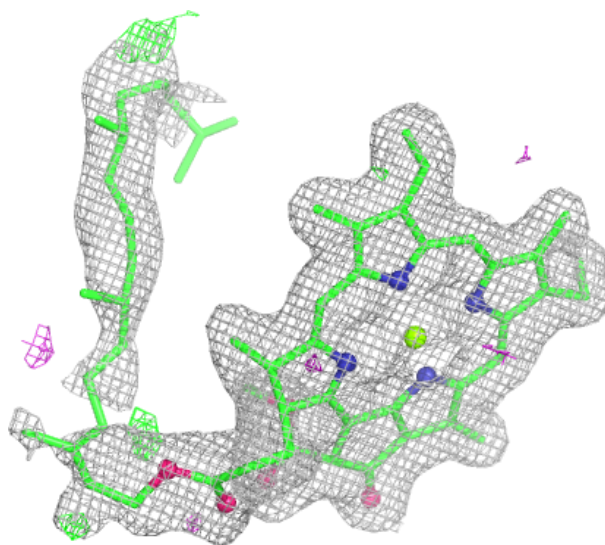
Electron density around CLA C 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



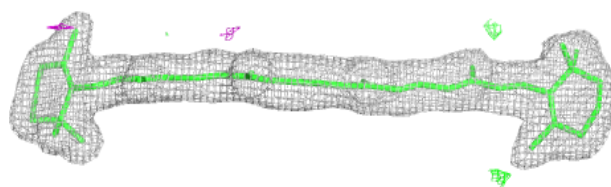
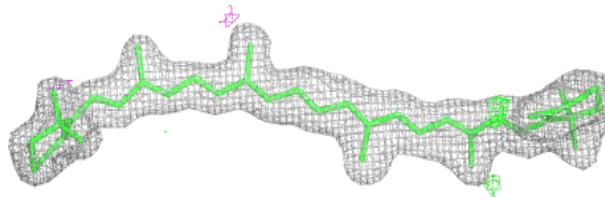
Electron density around CLA b 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

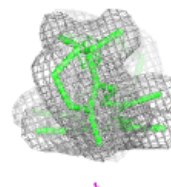
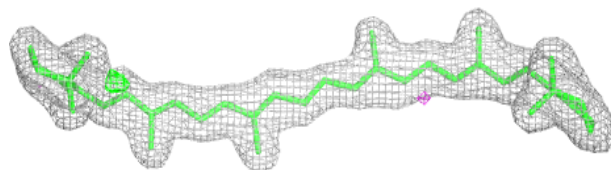
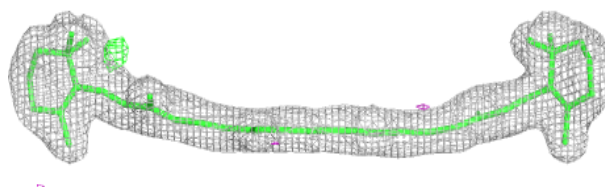


Electron density around BCR C 516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

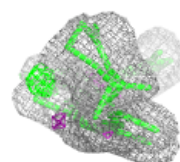
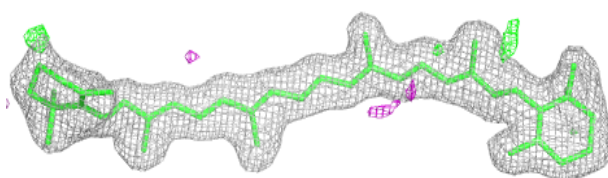
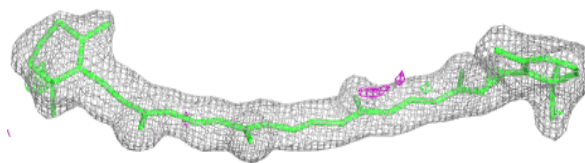
**Electron density around BCR C 530:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

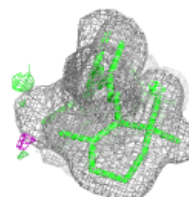
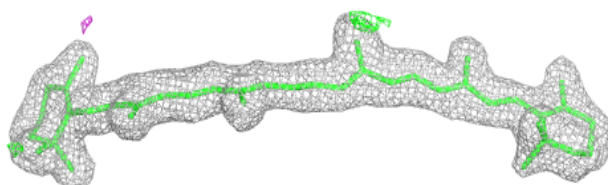
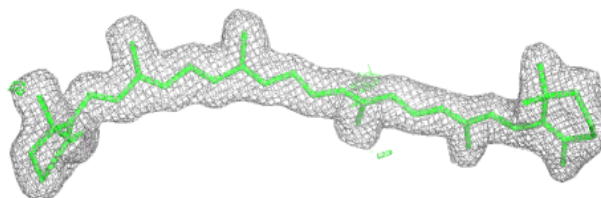


Electron density around BCR D 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

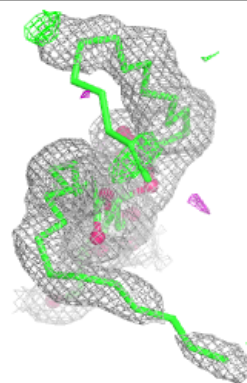
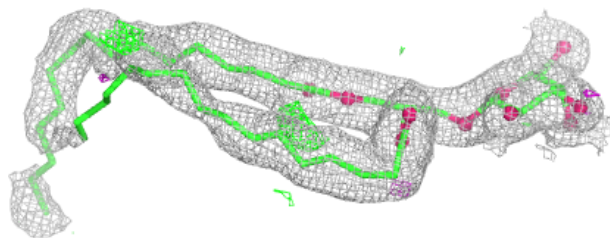
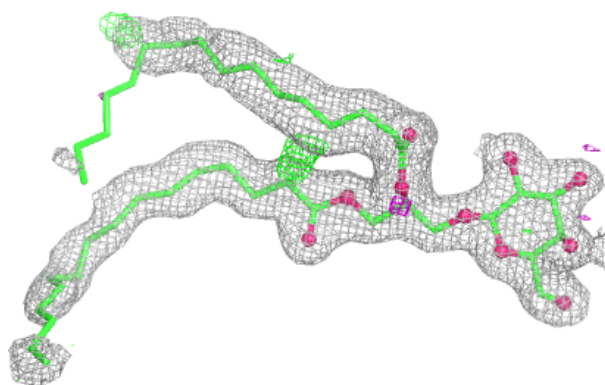
**Electron density around BCR T 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

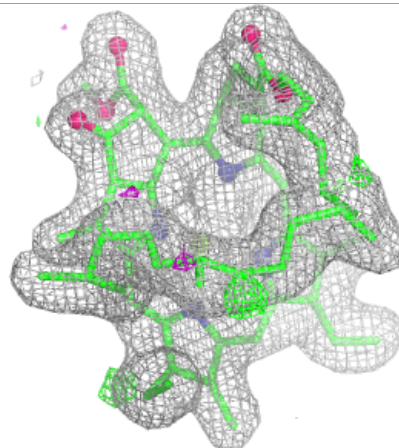
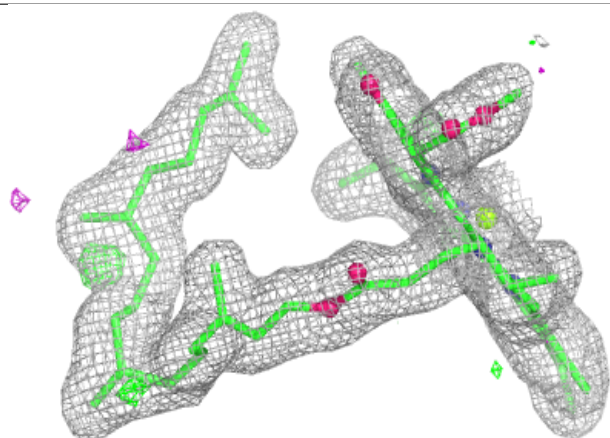
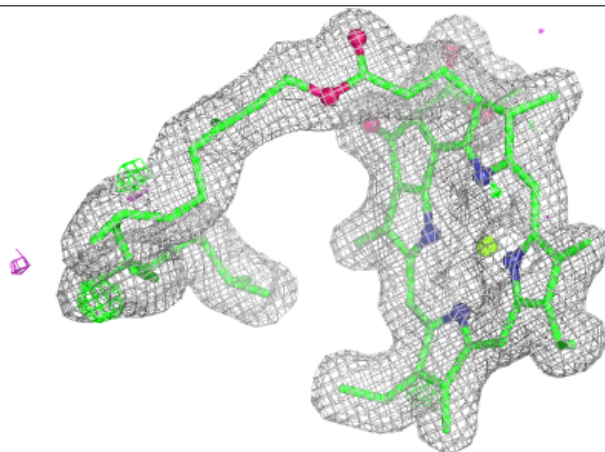


Electron density around LMG J 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

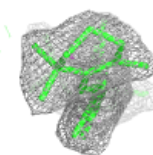
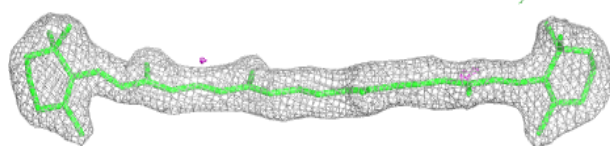
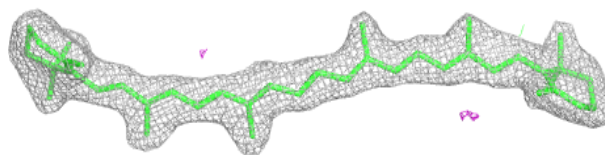
**Electron density around CLA c 904:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

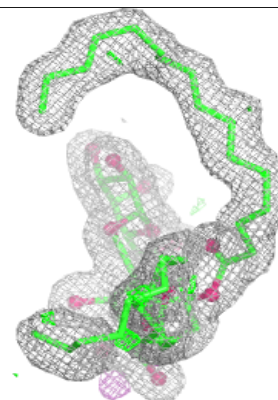
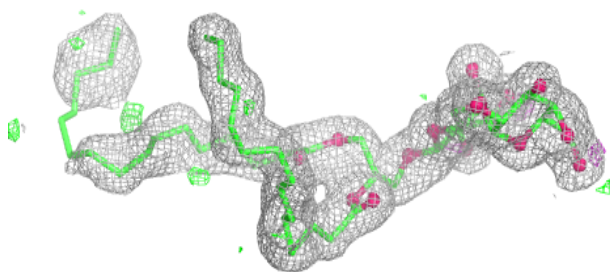
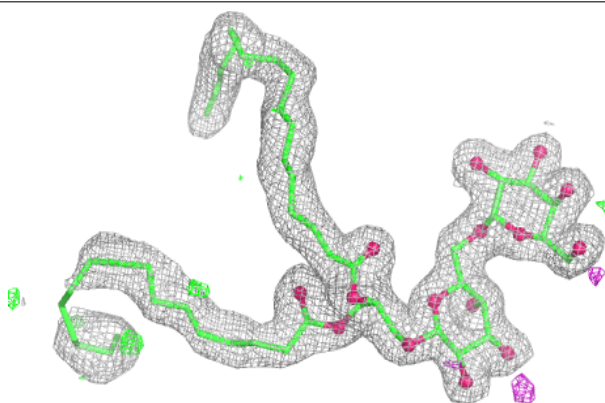


Electron density around BCR c 915:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

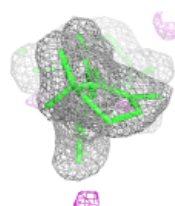
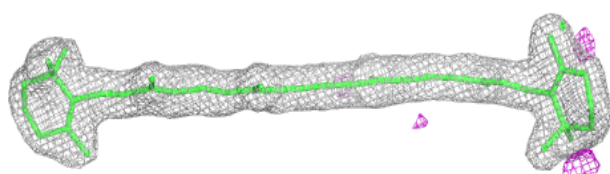
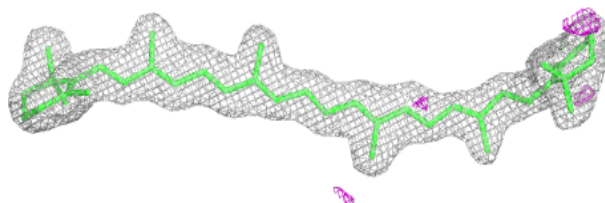
**Electron density around DGD C 518:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

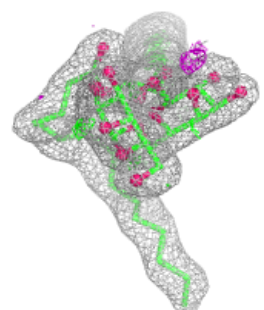
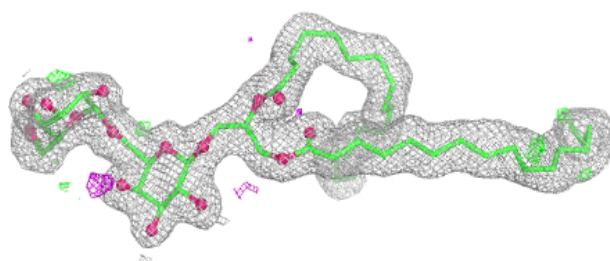
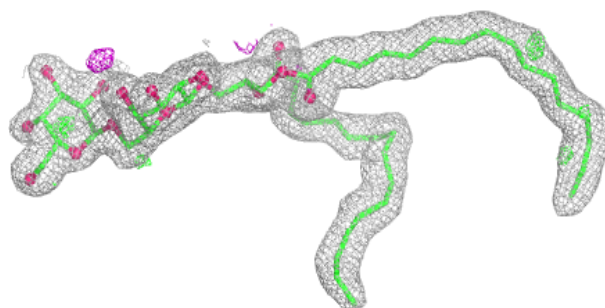


Electron density around BCR c 916:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

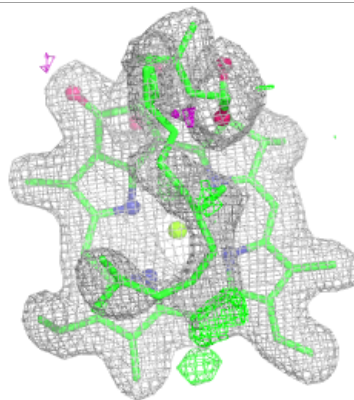
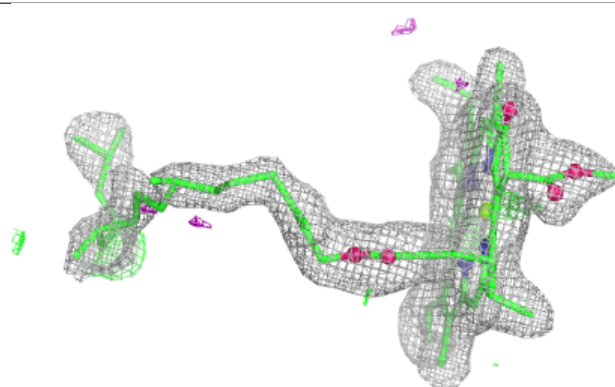
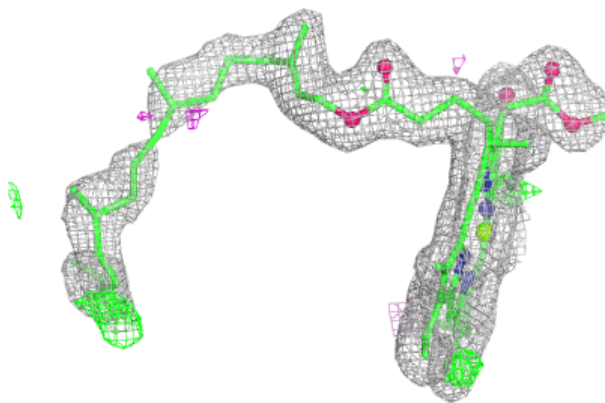
**Electron density around DGD H 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

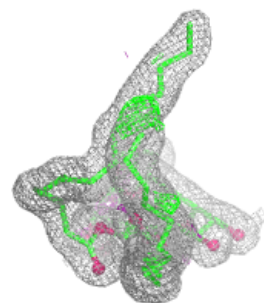
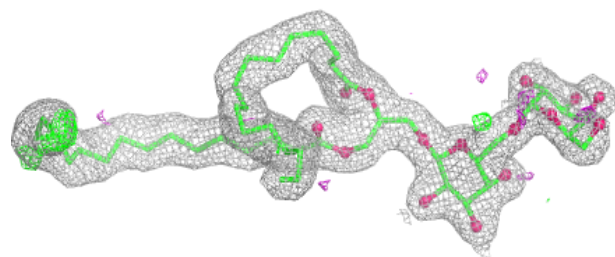
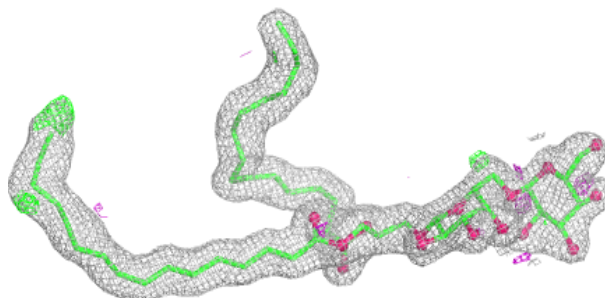


Electron density around CLA c 907:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

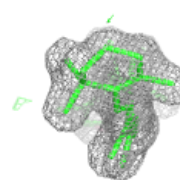
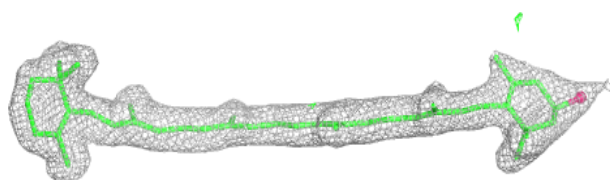
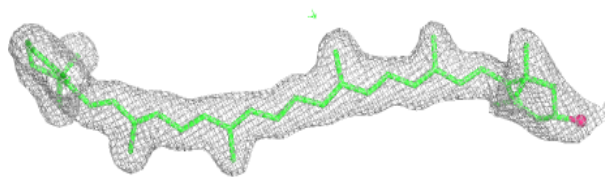
**Electron density around DGD h 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



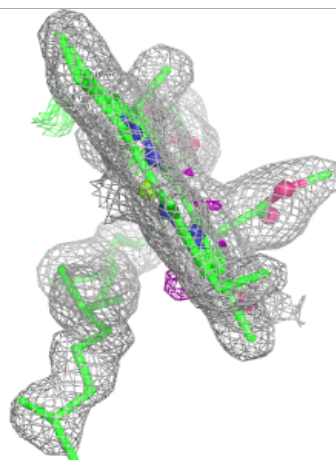
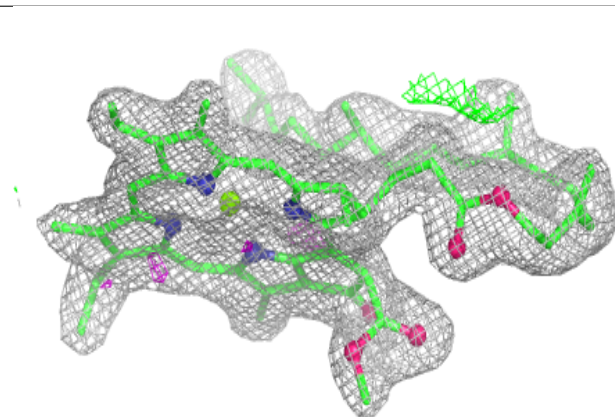
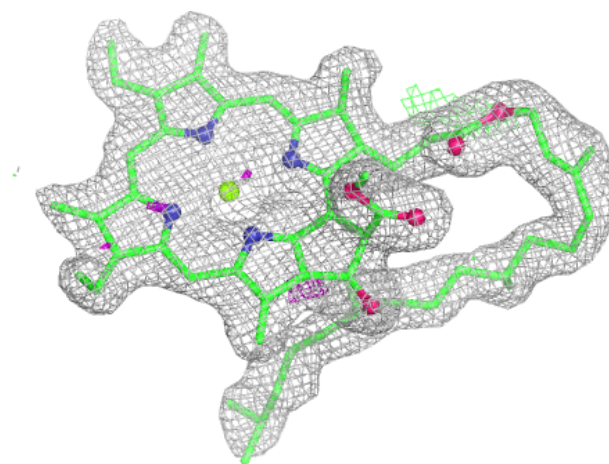
Electron density around RRX x 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



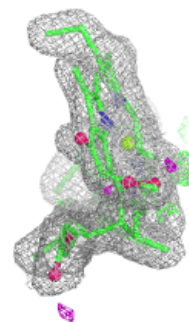
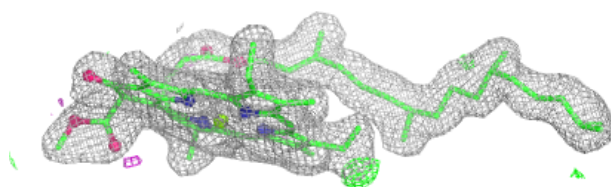
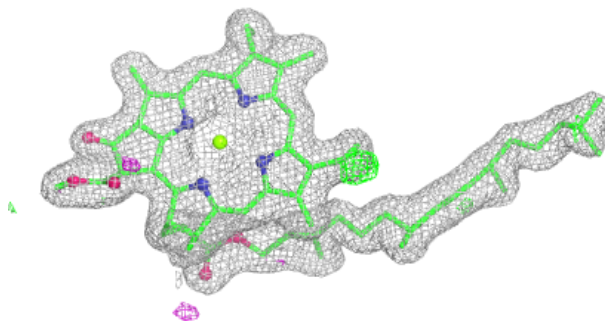
Electron density around CLA C 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

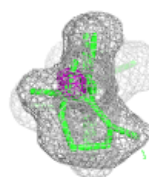
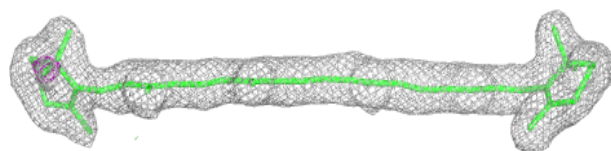
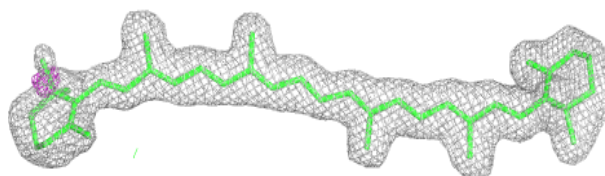


Electron density around CLA C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

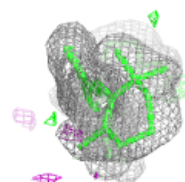
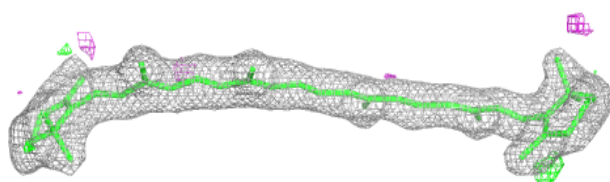
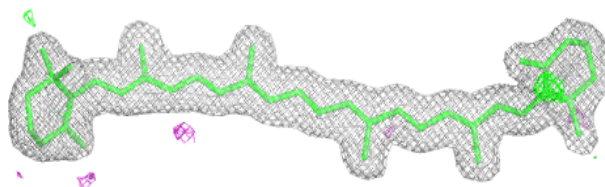
**Electron density around BCR B 619:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

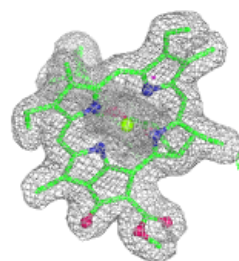
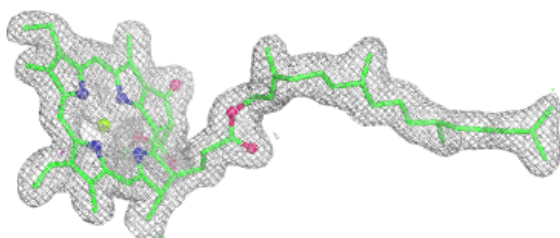
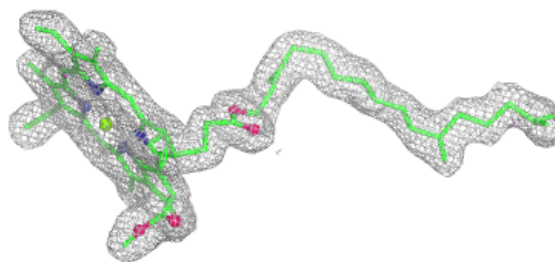


Electron density around BCR B 620:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

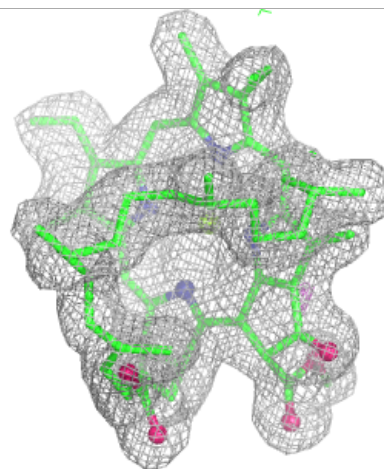
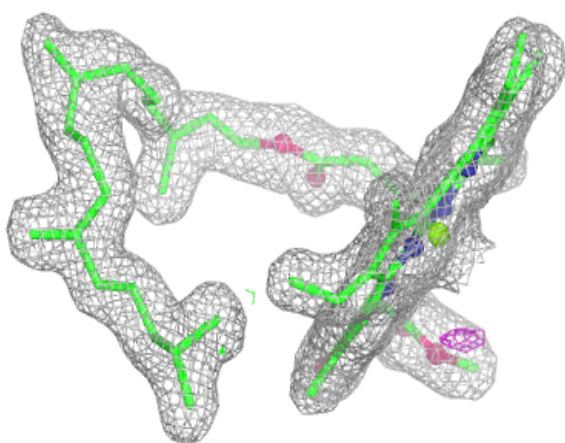
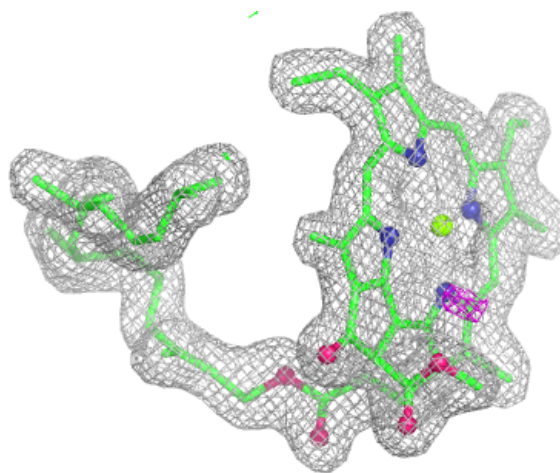
**Electron density around CLA C 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



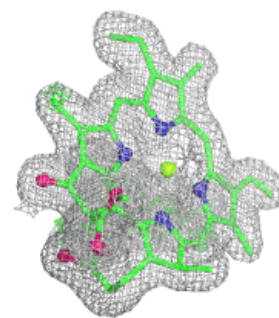
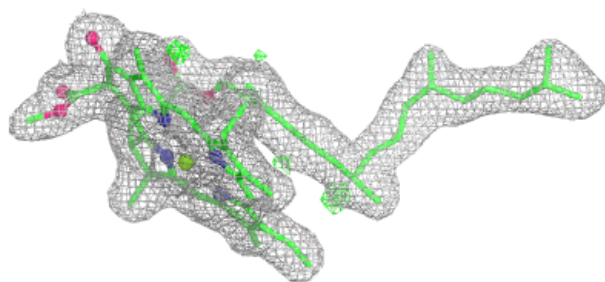
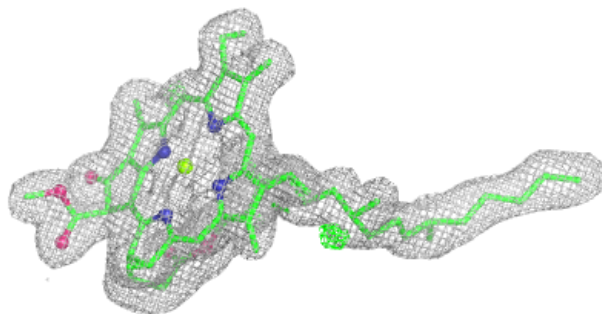
Electron density around CLA C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



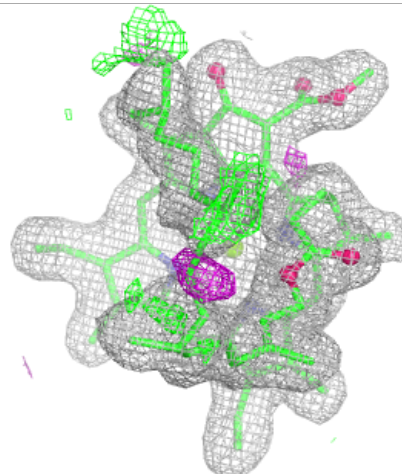
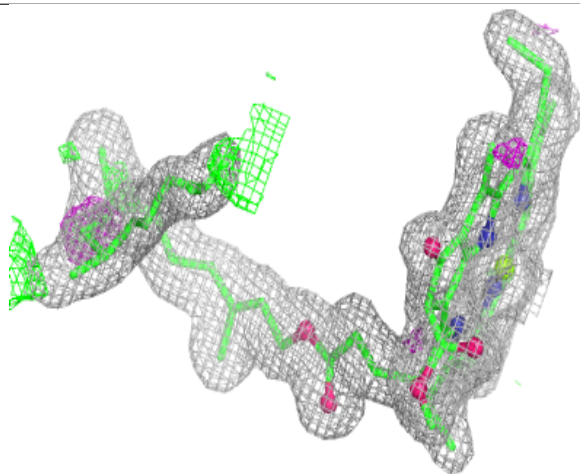
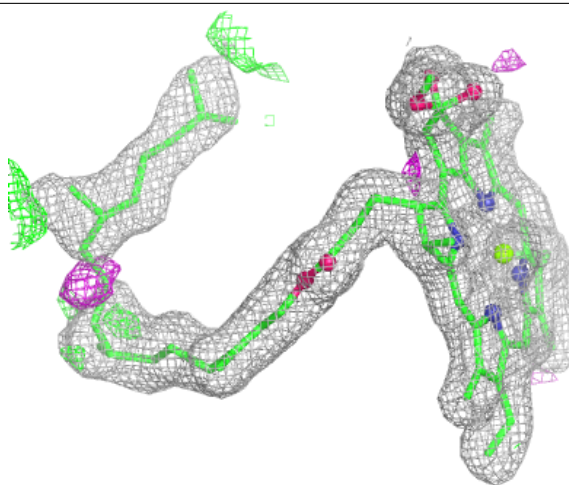
Electron density around CLA C 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



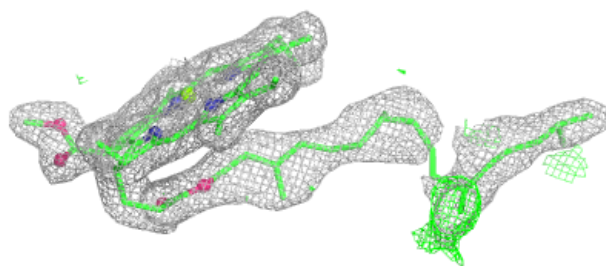
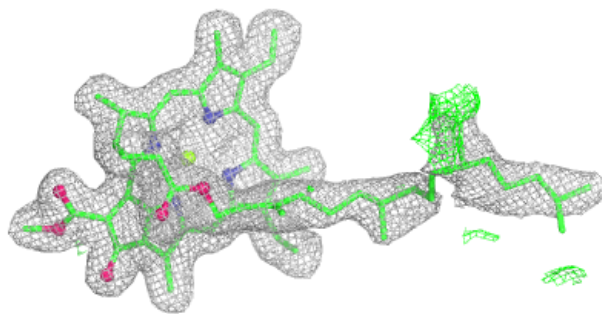
Electron density around CLA b 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



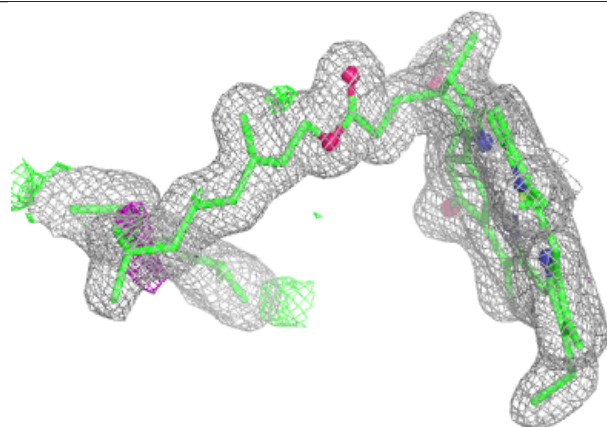
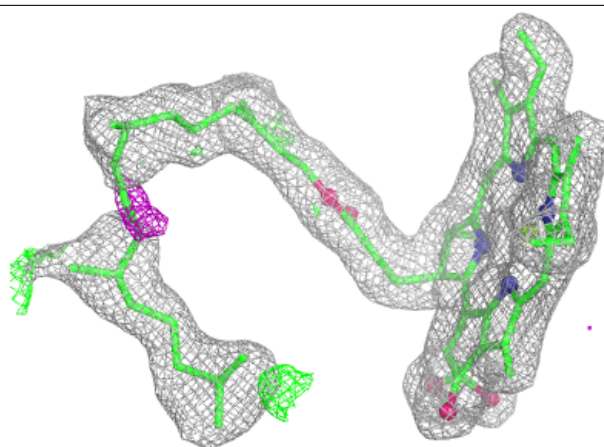
Electron density around CLA b 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

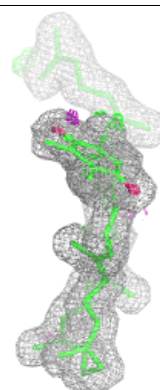
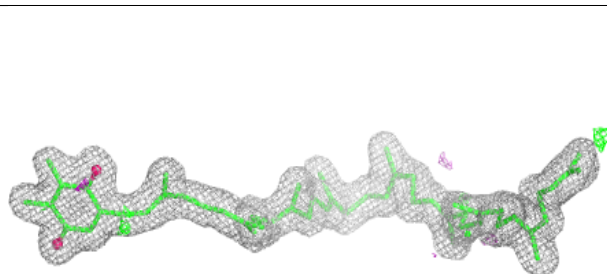
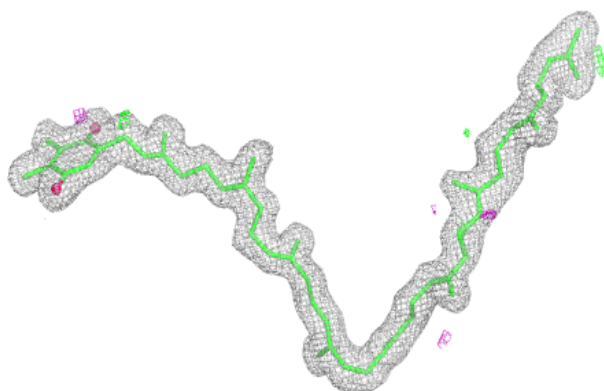


Electron density around CLA B 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

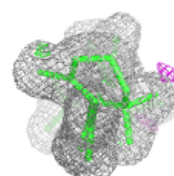
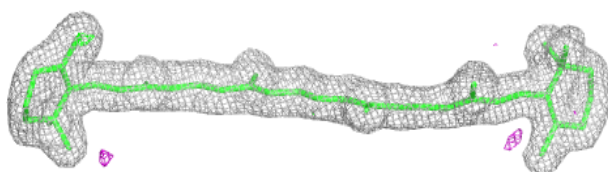
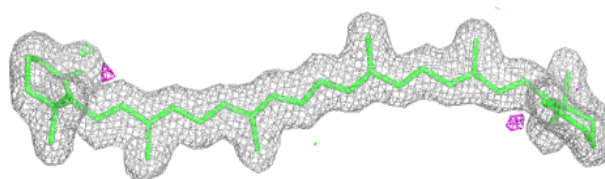
**Electron density around PL9 D 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

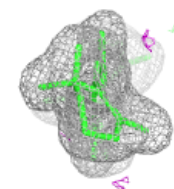
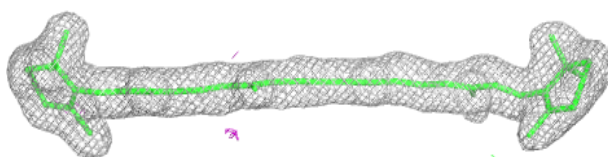
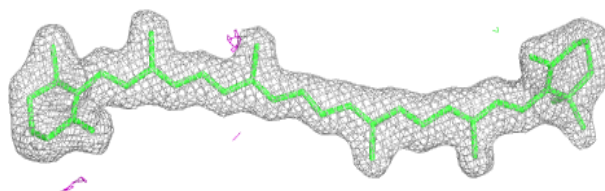


Electron density around BCR a 411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

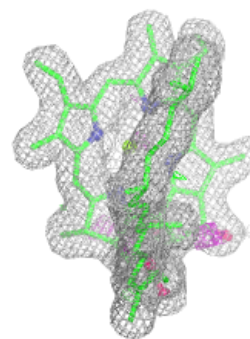
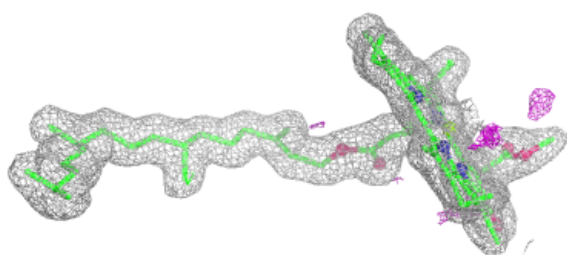
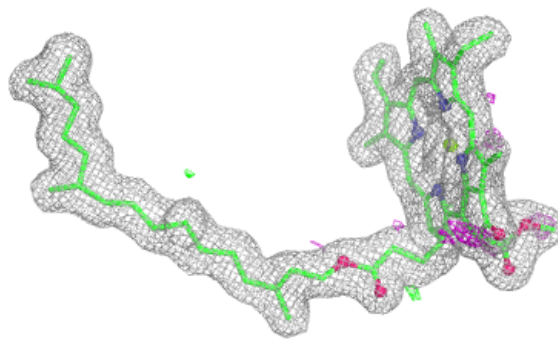
**Electron density around BCR b 619:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

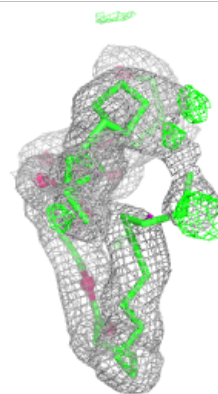
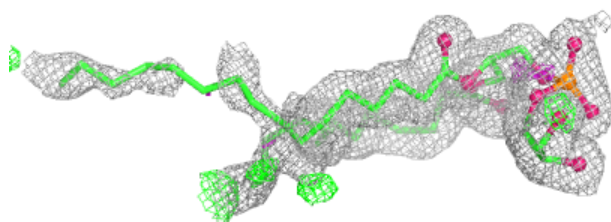
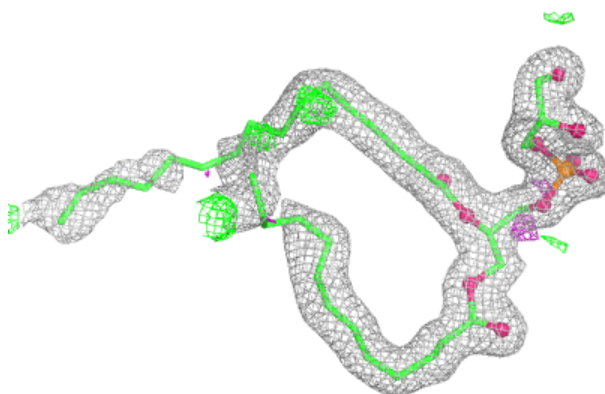


Electron density around CLA B 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

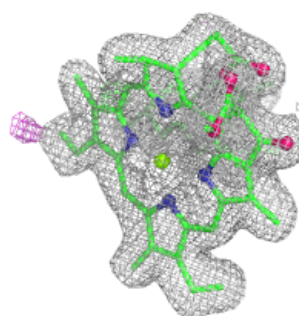
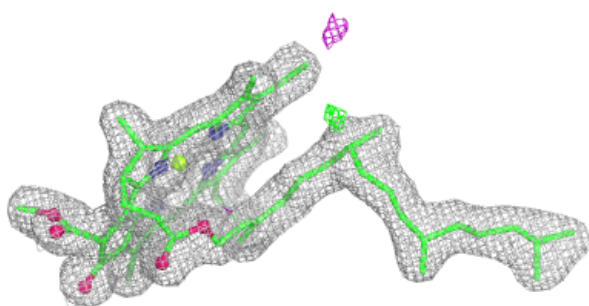
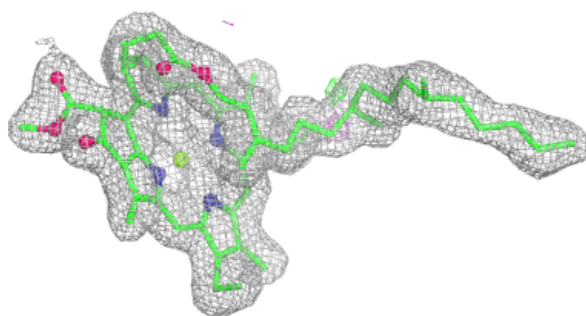
**Electron density around LHG D 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

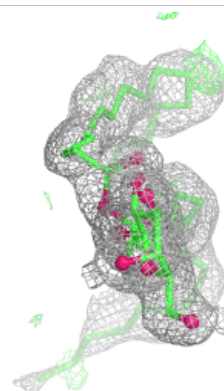
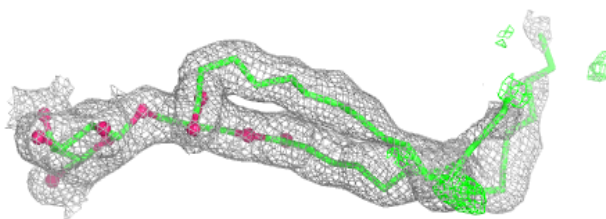
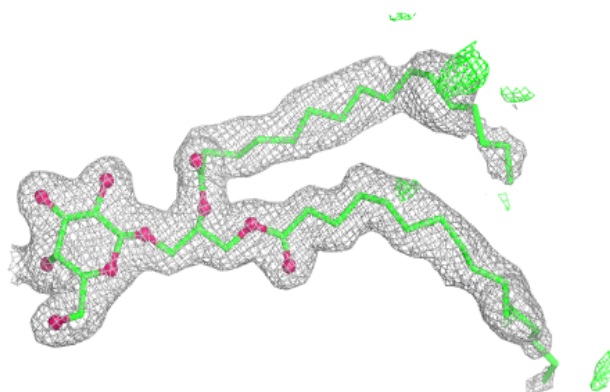


Electron density around CLA c 906:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

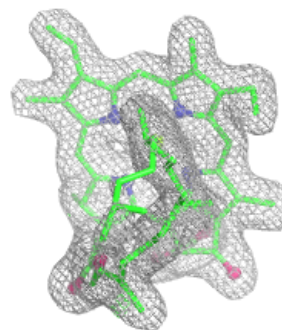
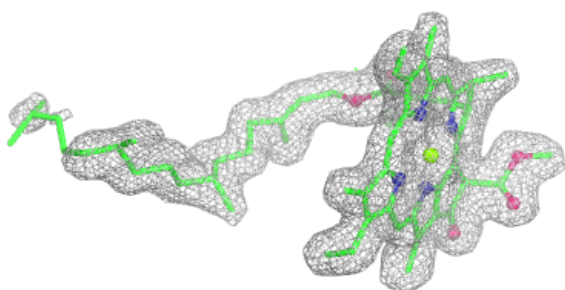
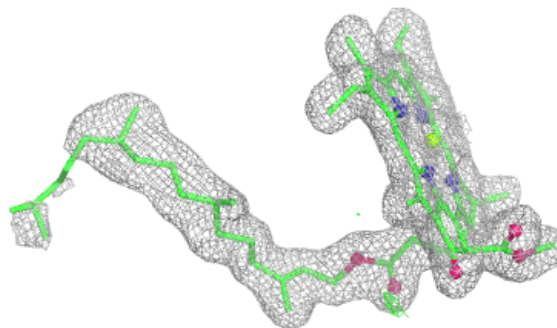
**Electron density around LMG j 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



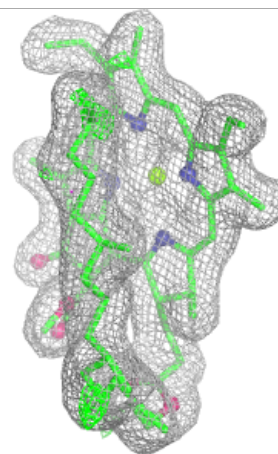
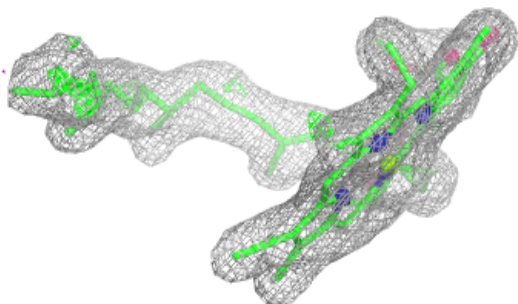
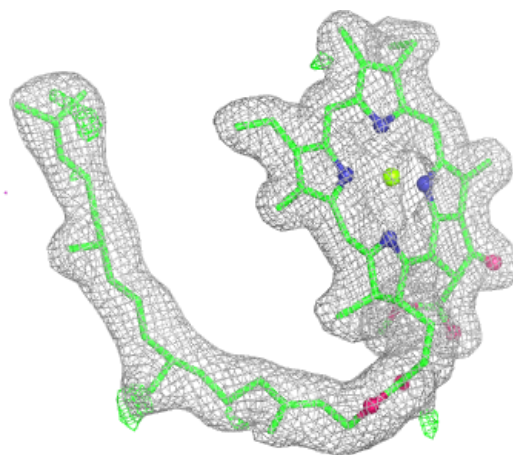
Electron density around CLA C 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



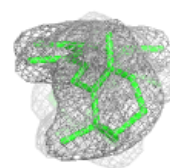
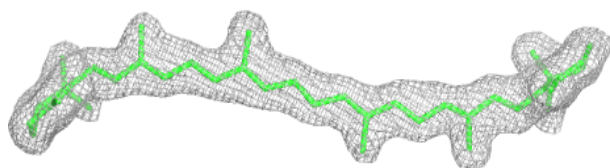
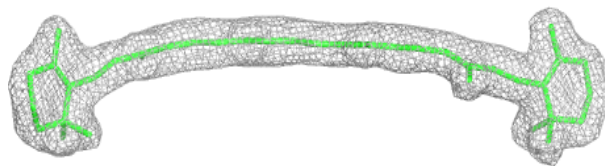
Electron density around CLA c 908:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

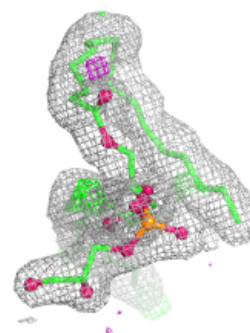
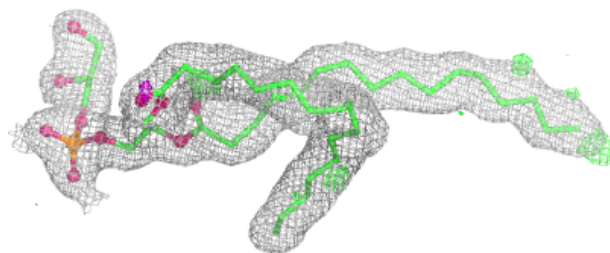
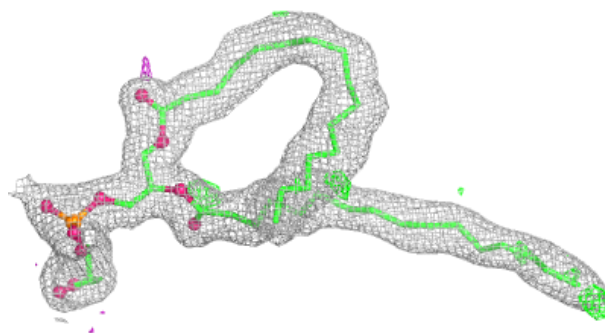


Electron density around BCR k 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

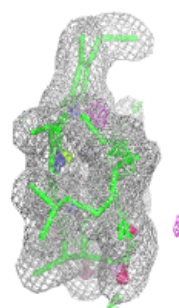
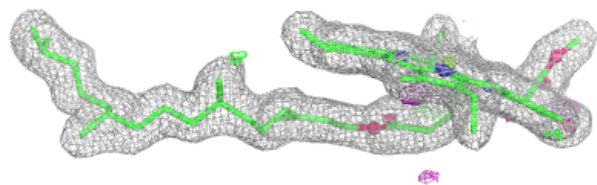
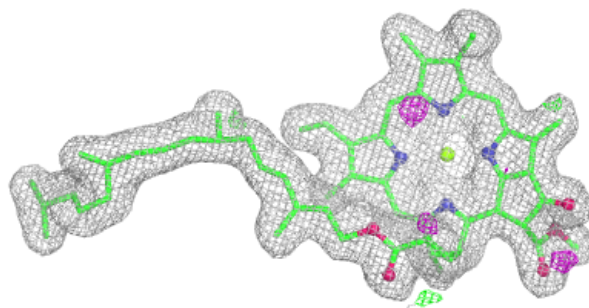
**Electron density around LHG d 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



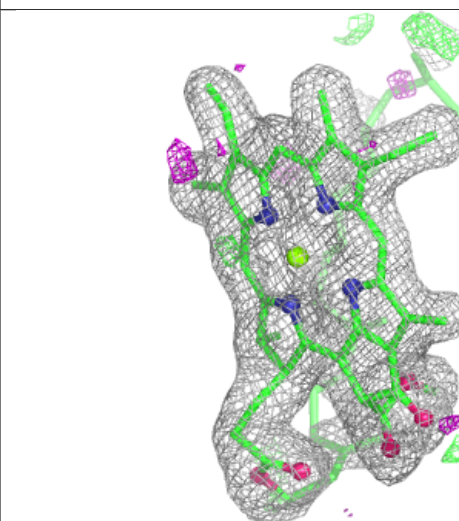
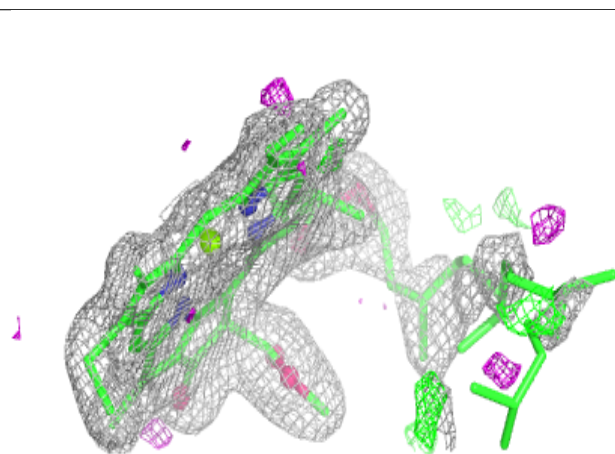
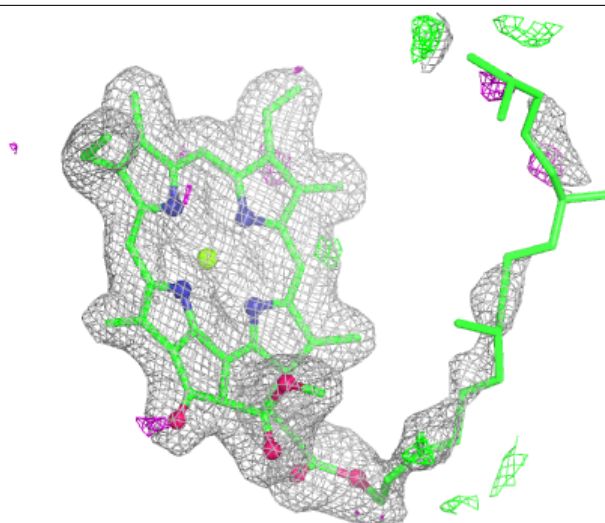
Electron density around CLA b 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



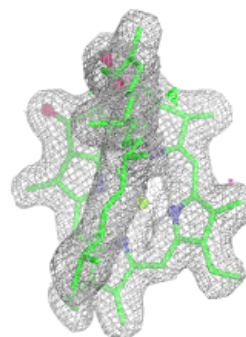
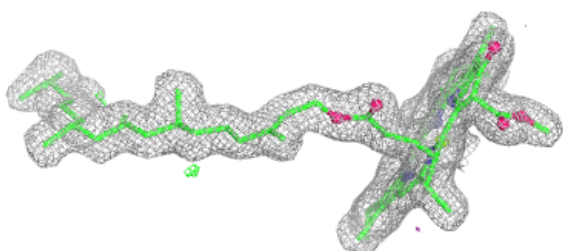
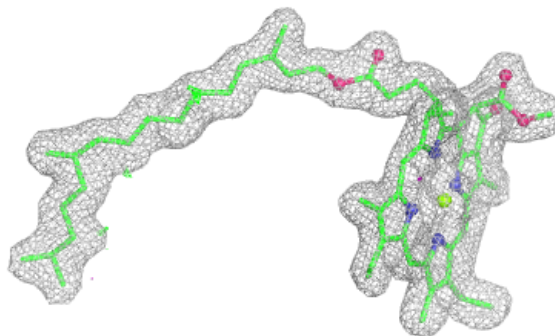
Electron density around CLA B 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

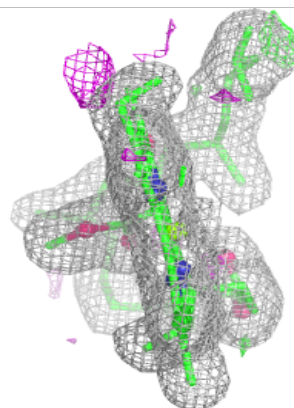
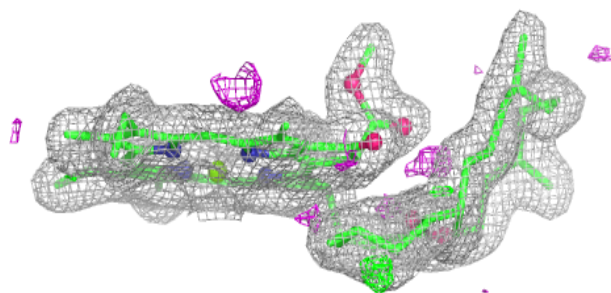
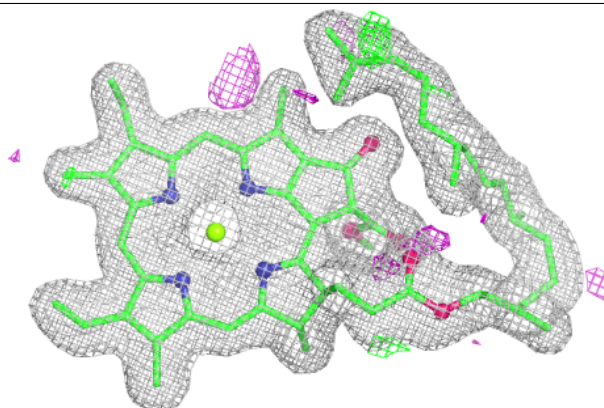


Electron density around CLA b 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

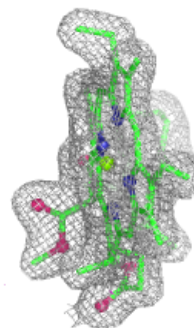
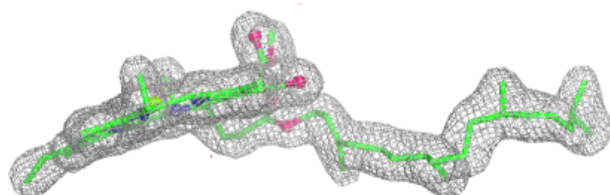
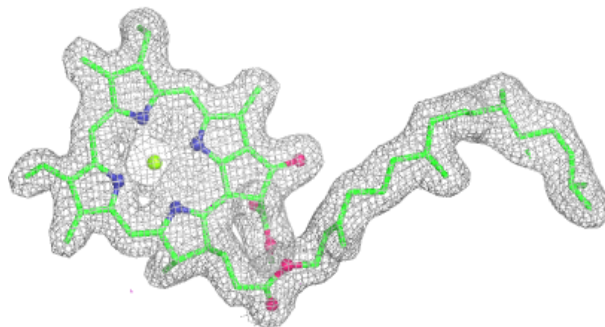
**Electron density around CLA b 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



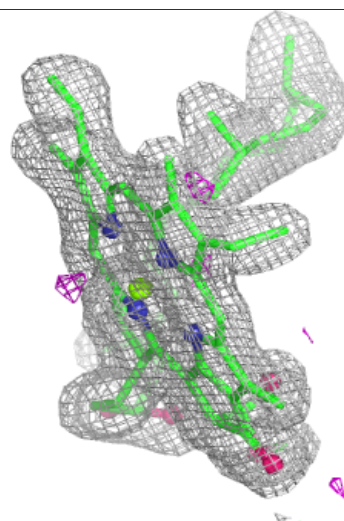
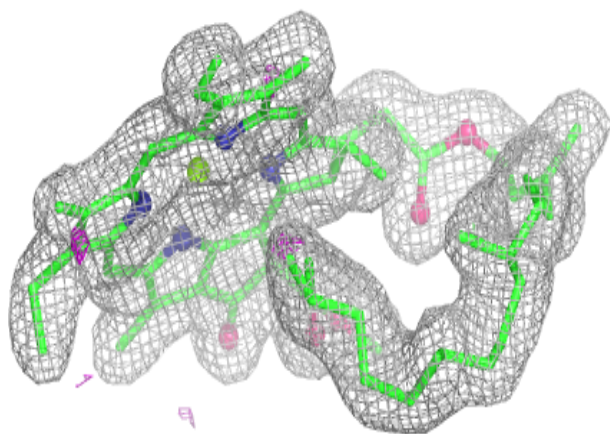
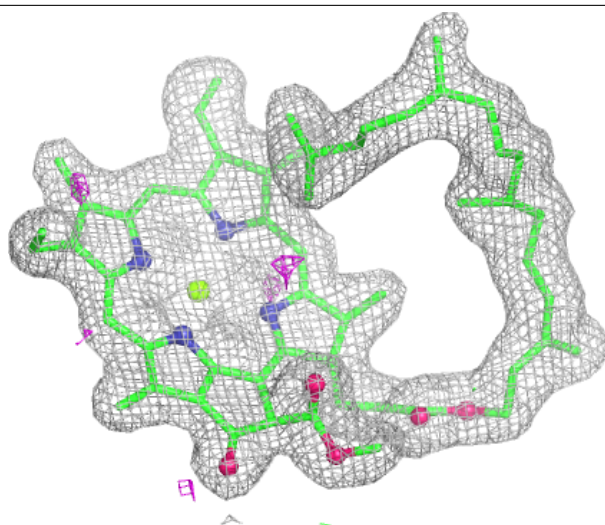
Electron density around CLA B 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



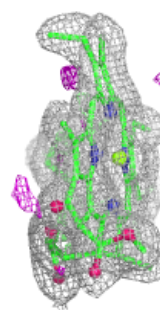
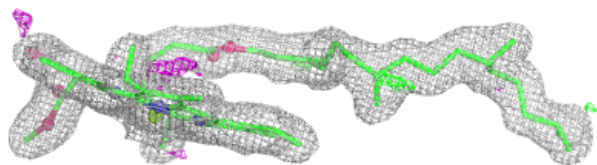
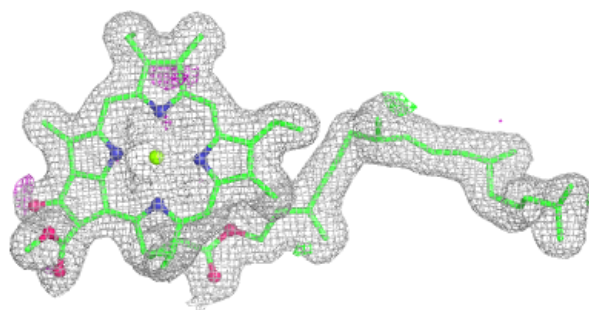
Electron density around CLA b 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

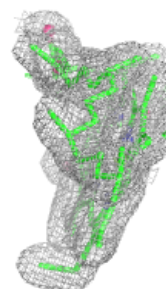
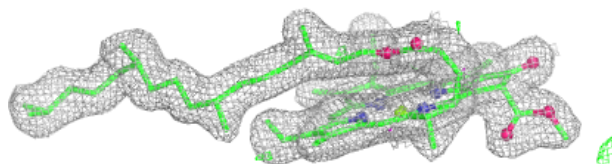
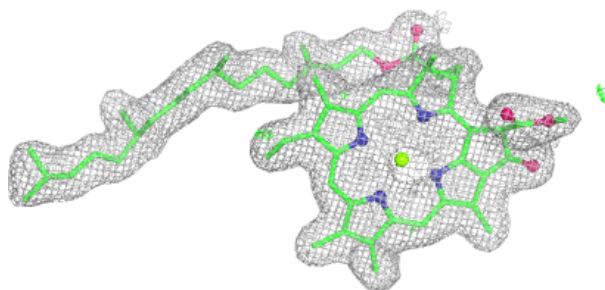


Electron density around CLA B 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

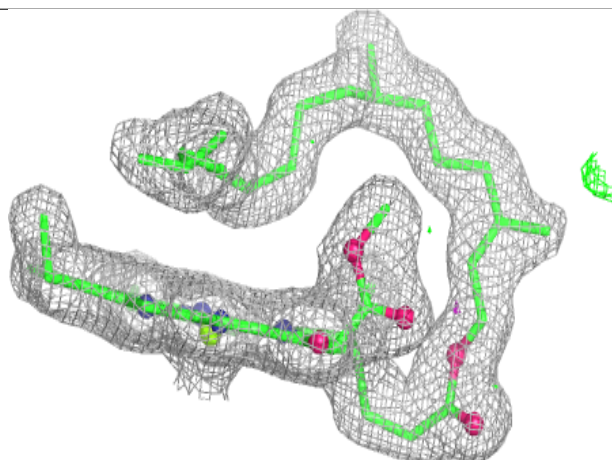
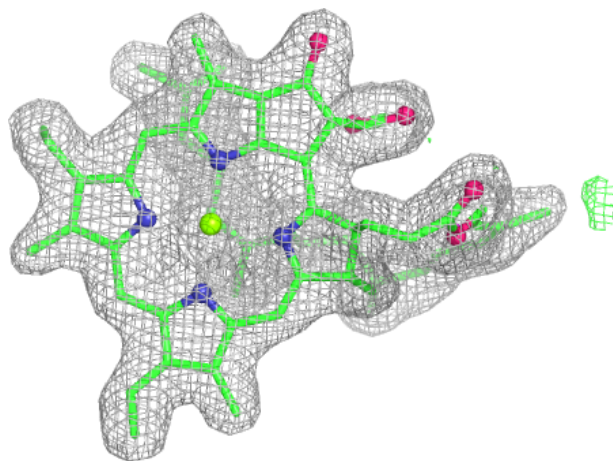
**Electron density around CLA c 902:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



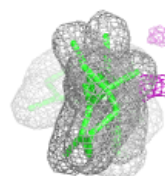
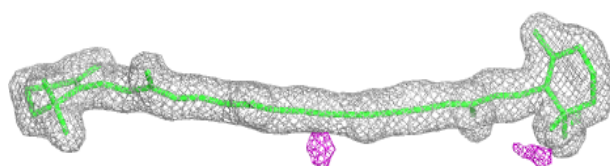
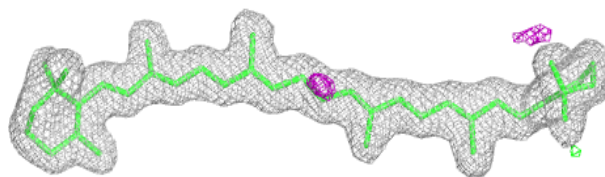
Electron density around CLA C 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



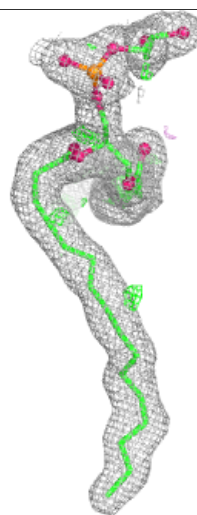
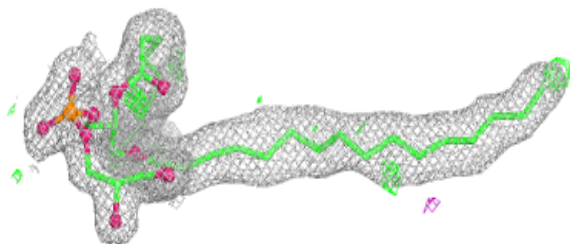
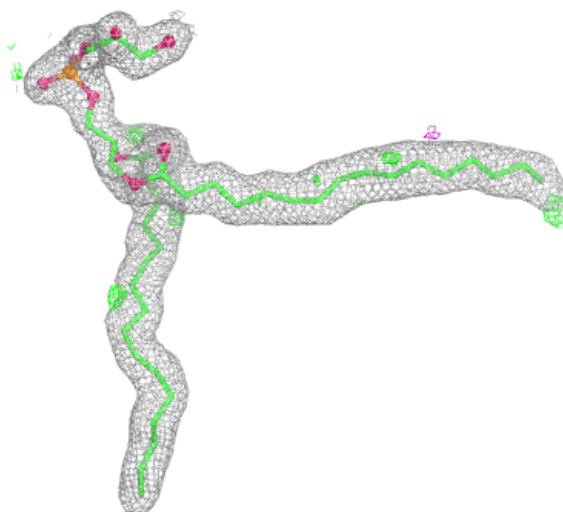
Electron density around BCR b 618:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



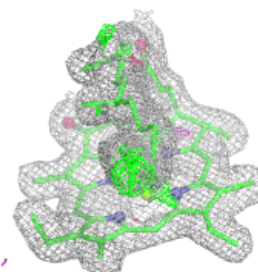
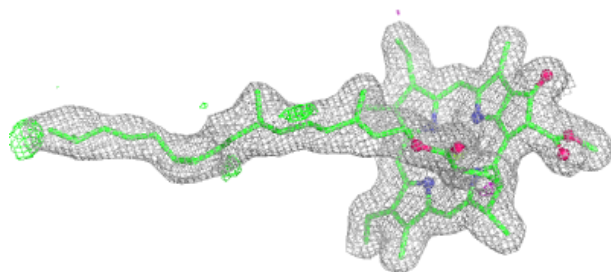
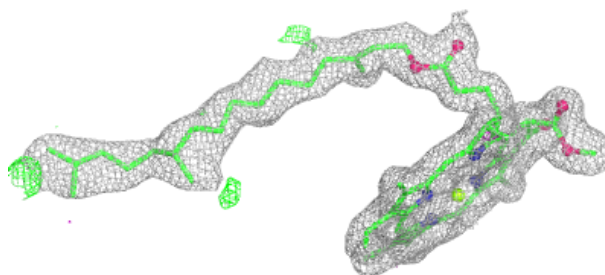
Electron density around LHG L 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

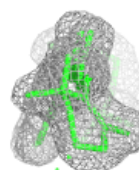
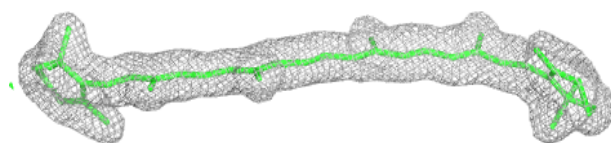
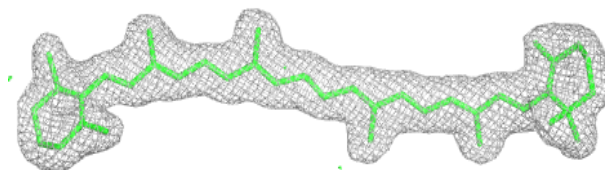


Electron density around CLA c 905:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

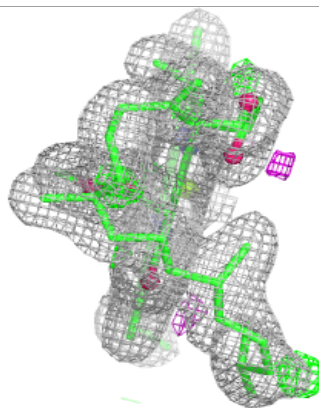
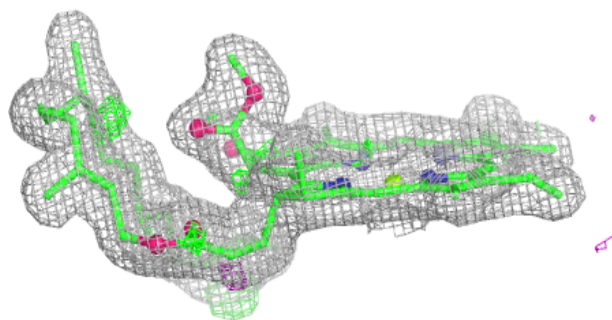
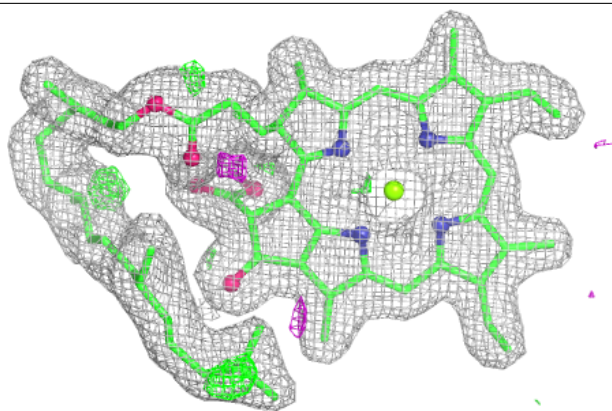
**Electron density around BCR b 620:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

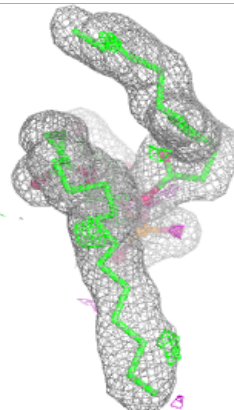
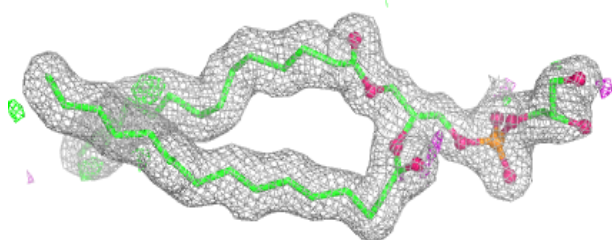
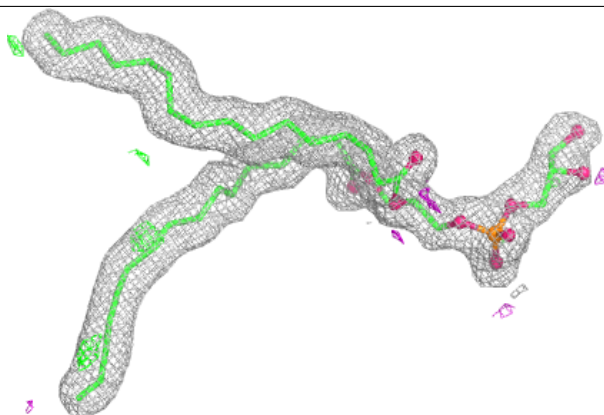


Electron density around CLA B 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

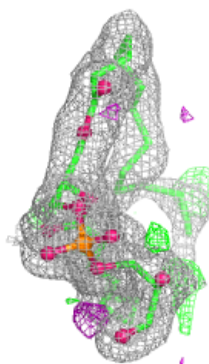
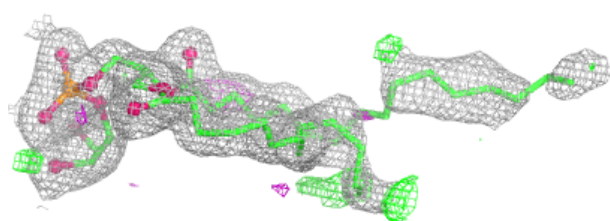
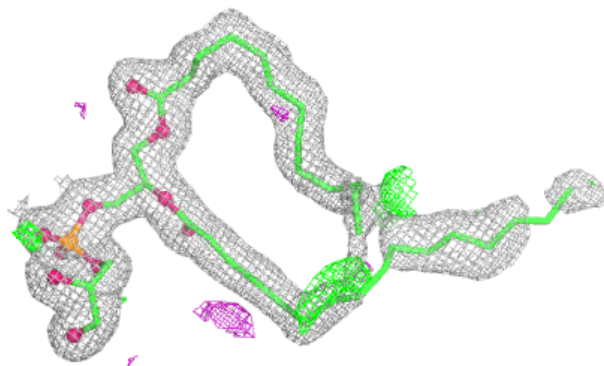
**Electron density around LHG d 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

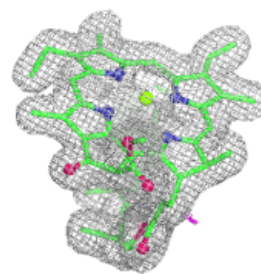
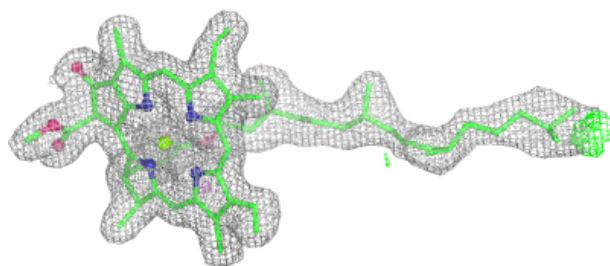
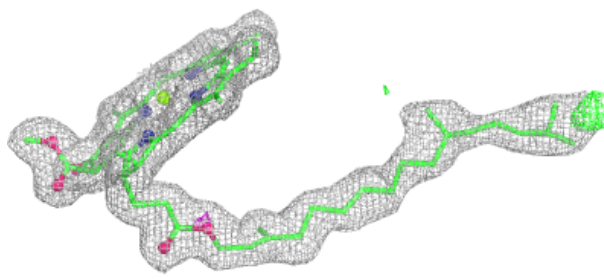


Electron density around LHG d 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

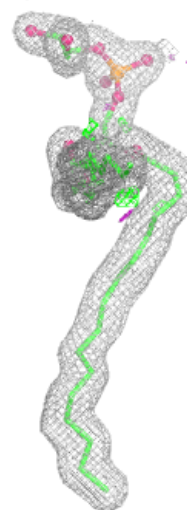
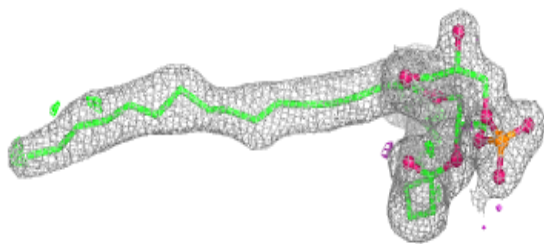
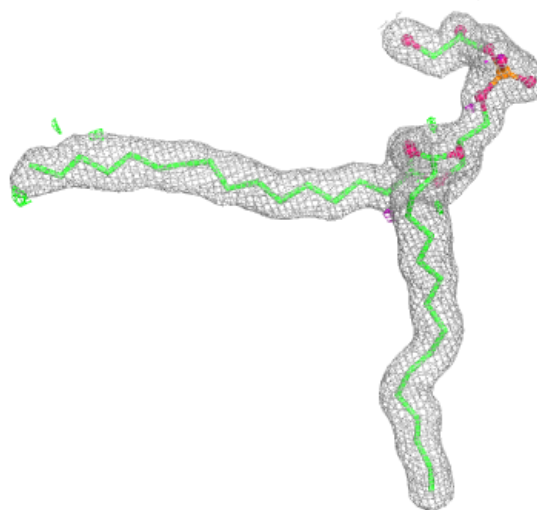
**Electron density around CLA C 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



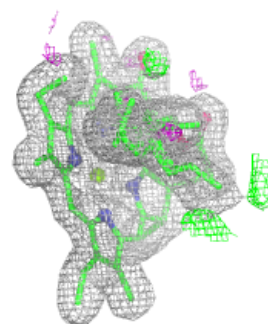
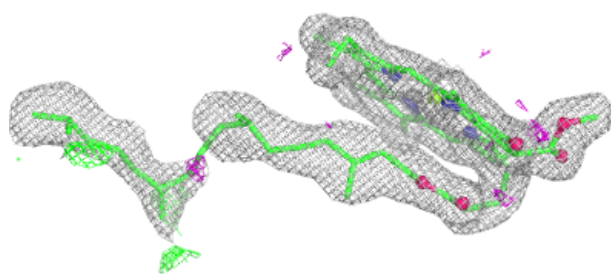
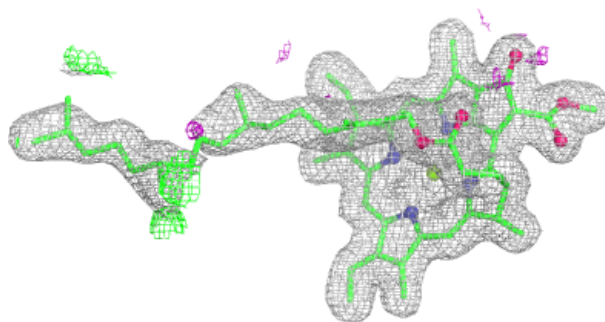
Electron density around LHG 1 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

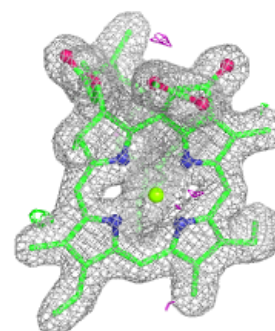
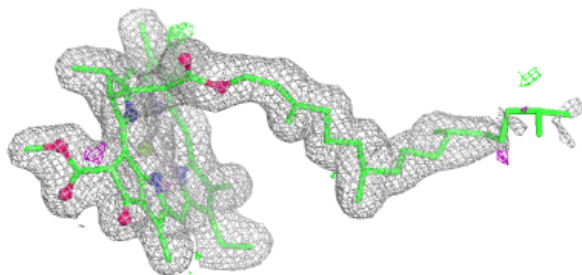
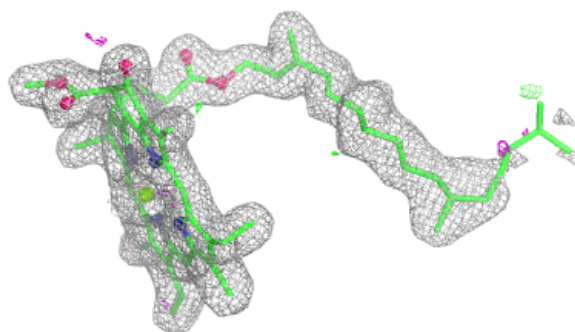


Electron density around CLA B 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

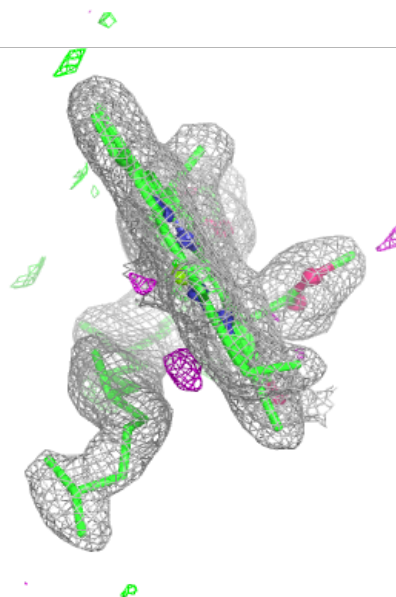
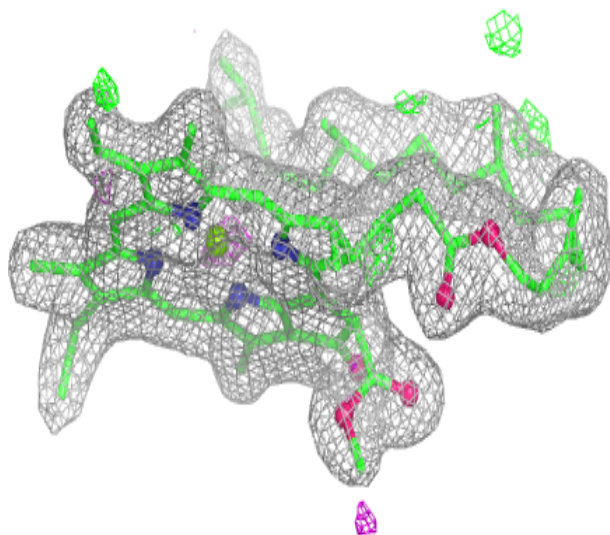
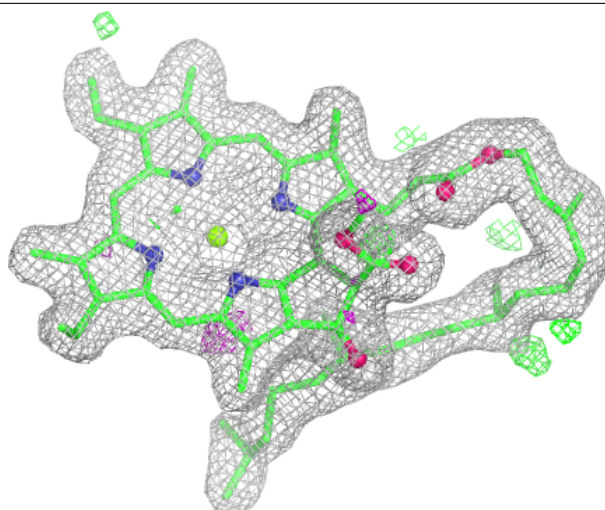
**Electron density around CLA c 909:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



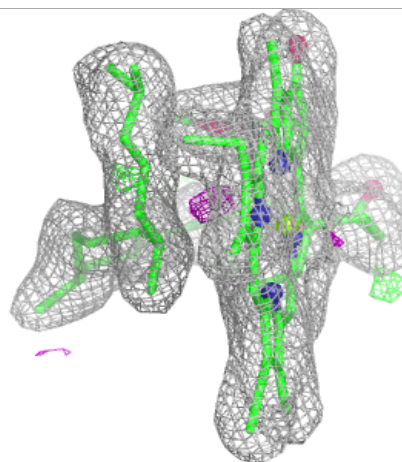
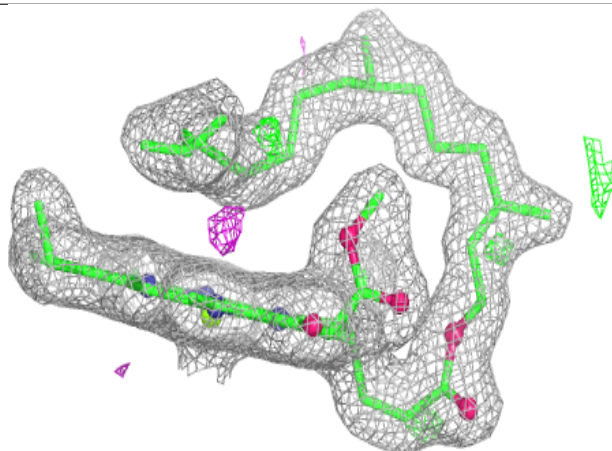
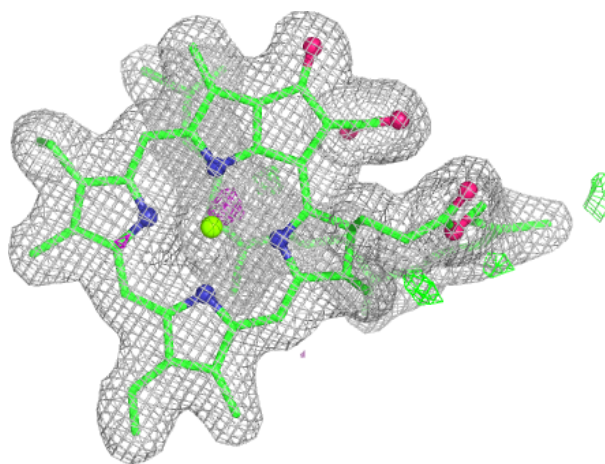
Electron density around CLA c 910:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



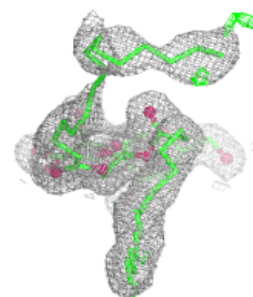
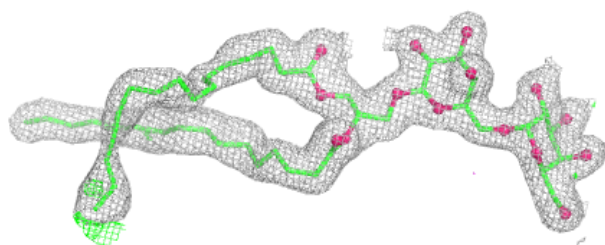
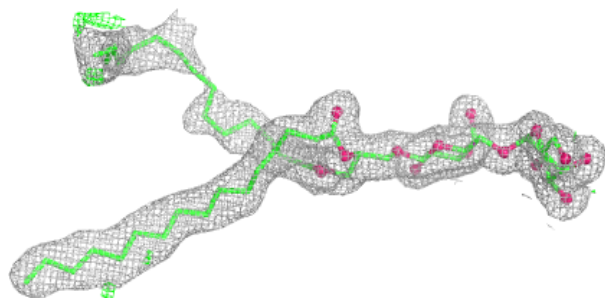
Electron density around CLA c 911:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

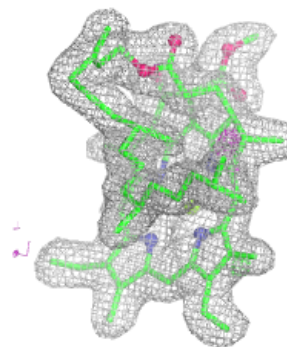
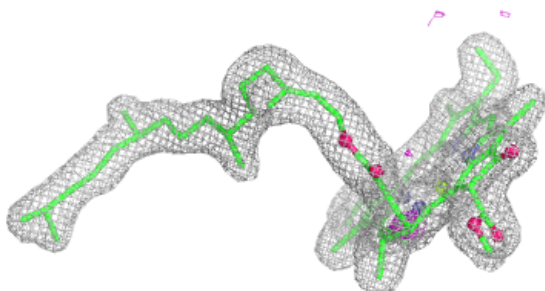
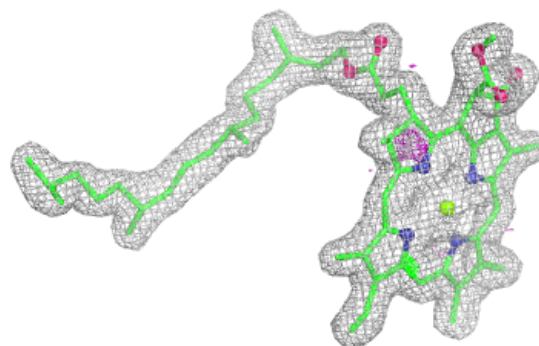


Electron density around DGD C 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

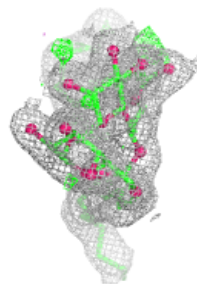
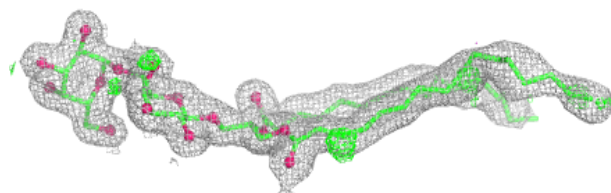
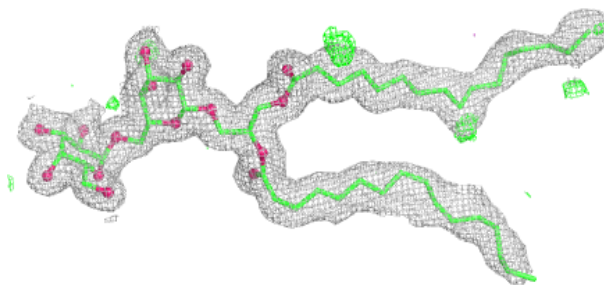
**Electron density around CLA c 912:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



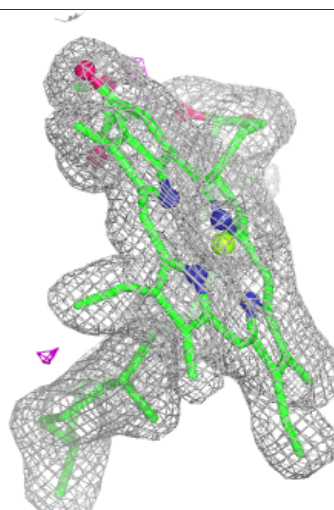
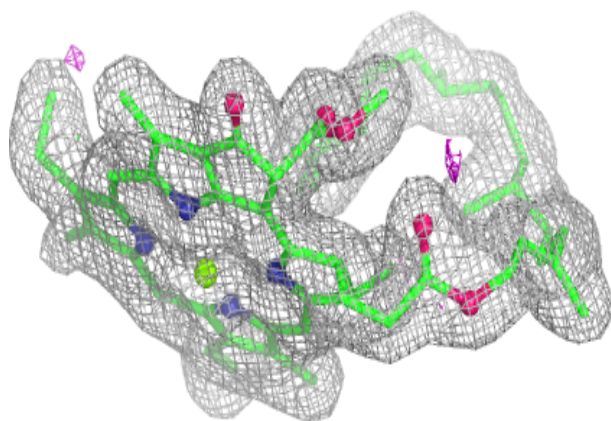
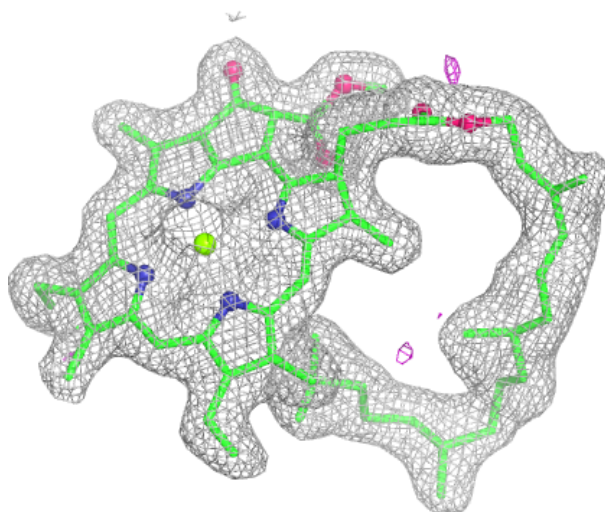
Electron density around DGD C 519:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



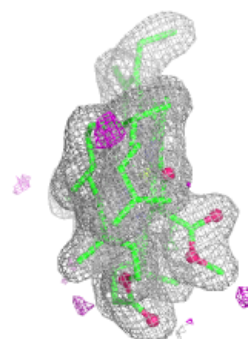
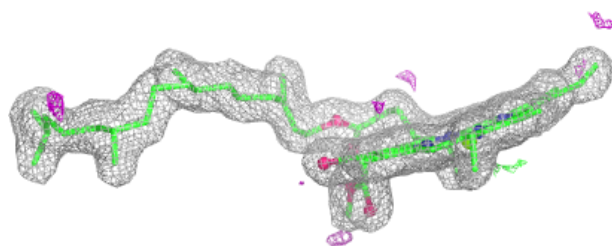
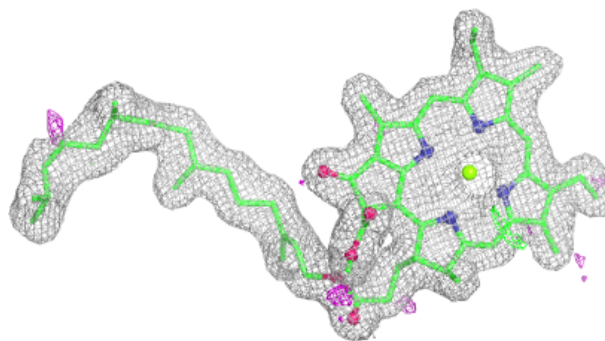
Electron density around CLA B 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

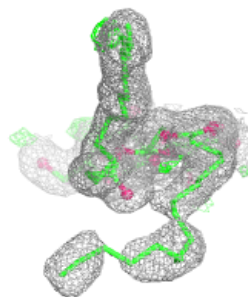
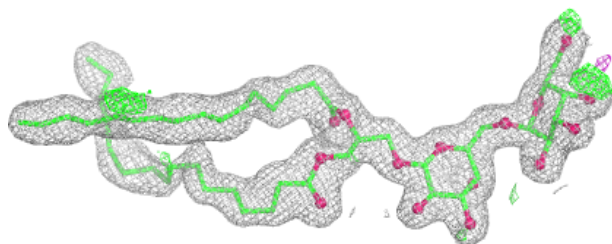
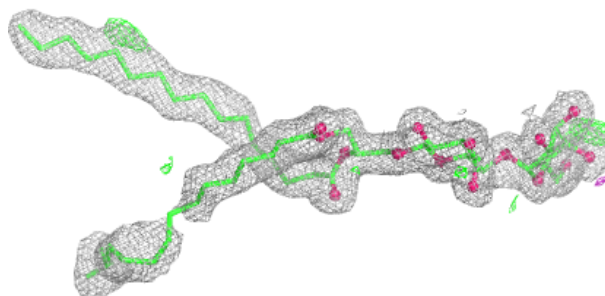


Electron density around CLA b 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

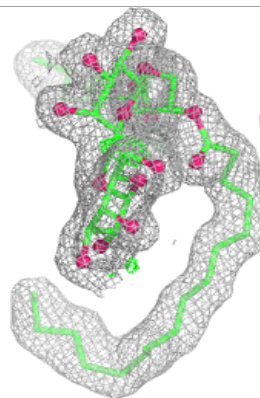
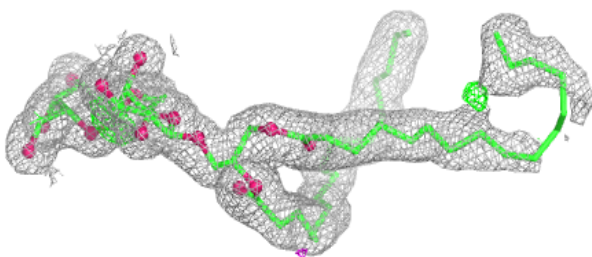
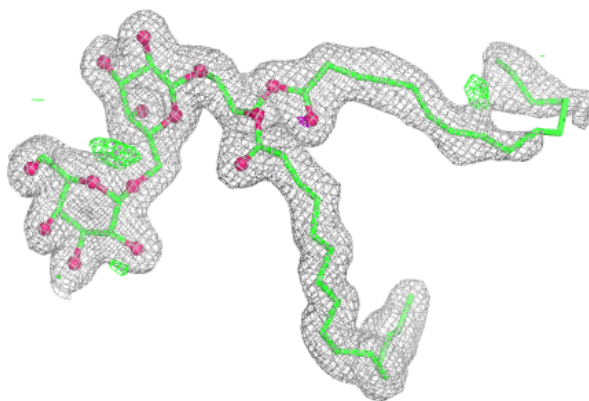
**Electron density around DGD c 917:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

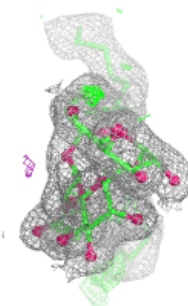
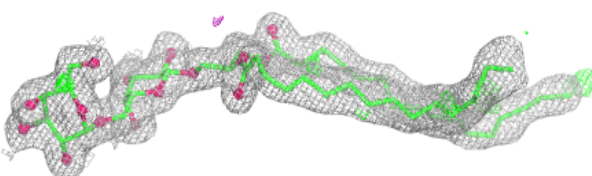
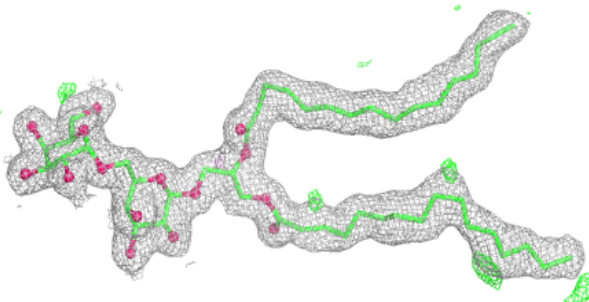


Electron density around DGD c 918:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

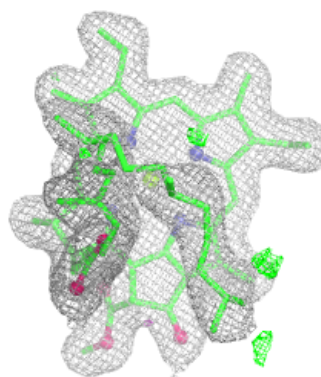
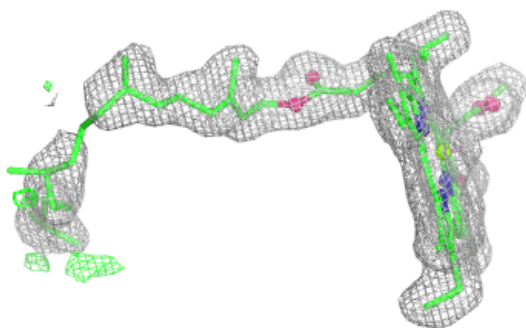
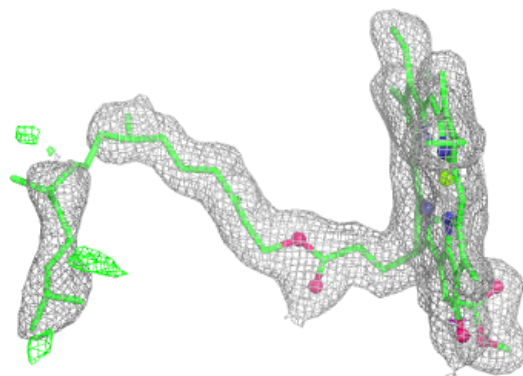
**Electron density around DGD c 919:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

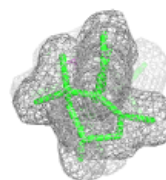
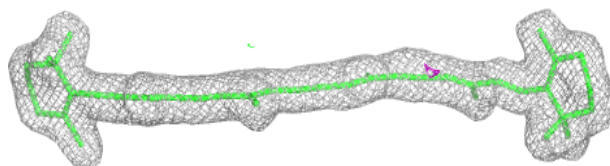
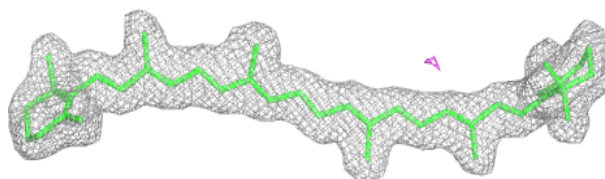


Electron density around CLA d 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

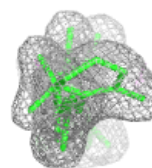
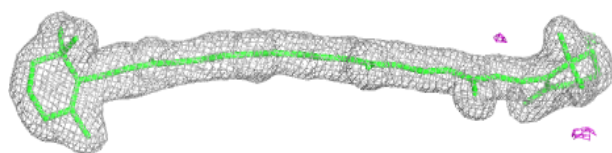
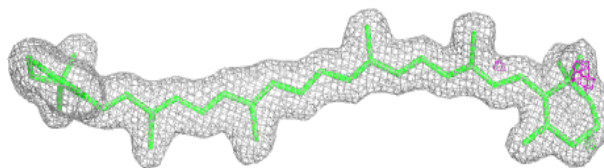
**Electron density around BCR A 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

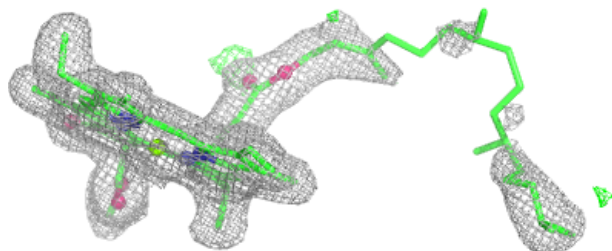
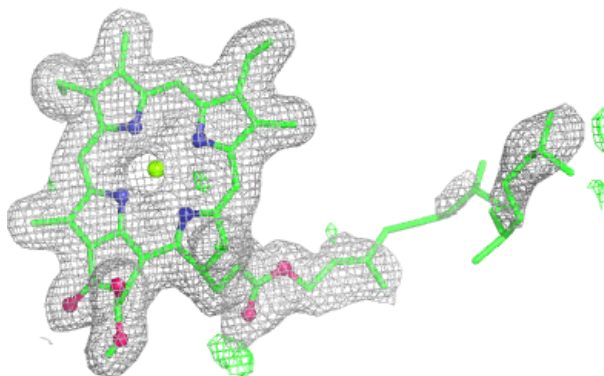


Electron density around BCR B 618:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

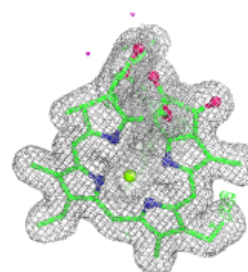
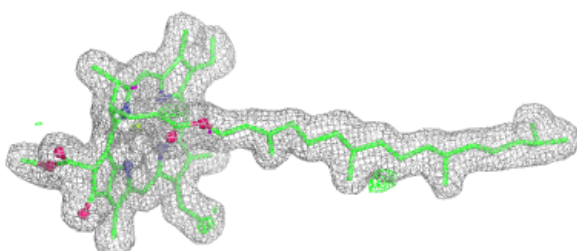
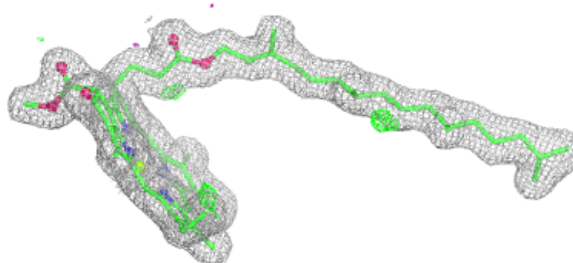
**Electron density around CLA A 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

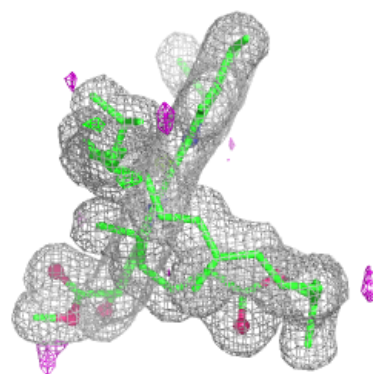
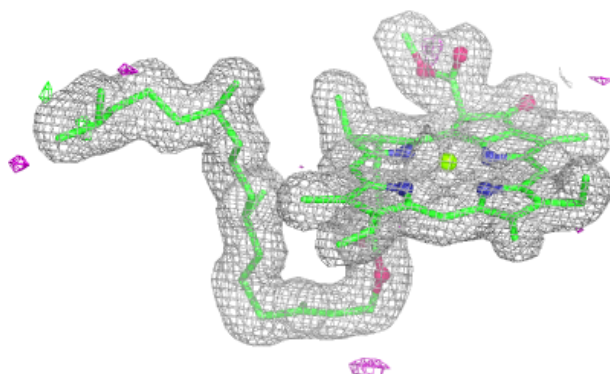
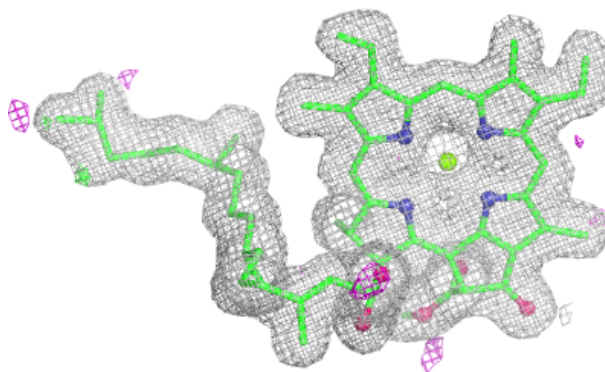


Electron density around CLA b 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

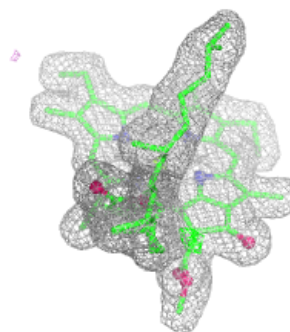
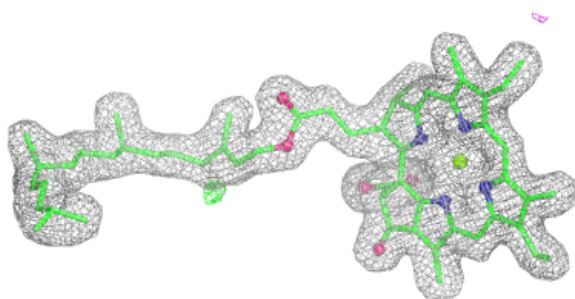
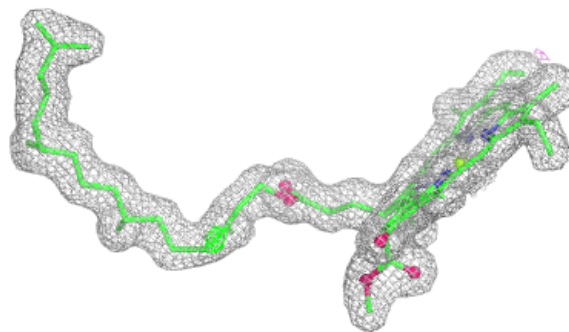
**Electron density around CLA d 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

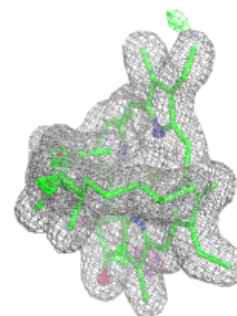
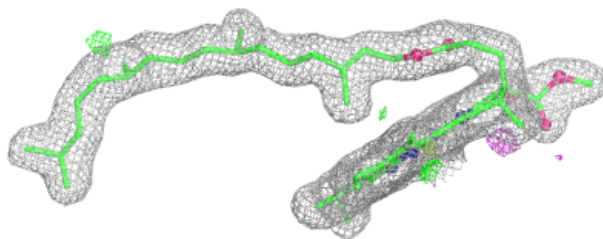
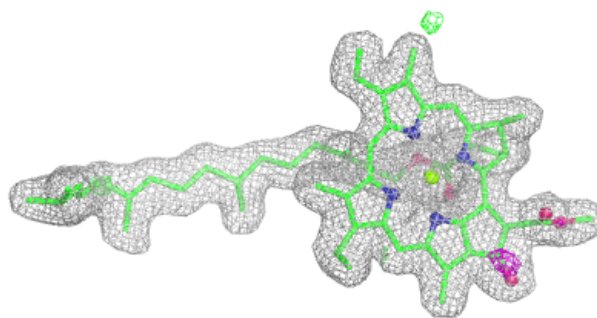


Electron density around CLA d 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

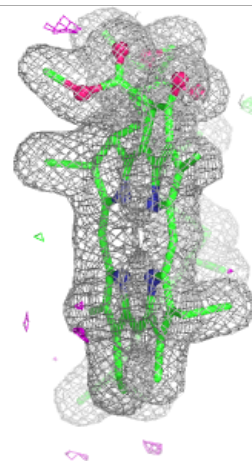
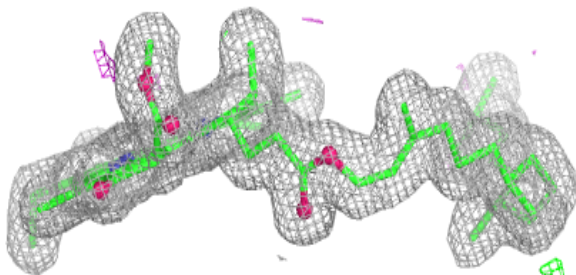
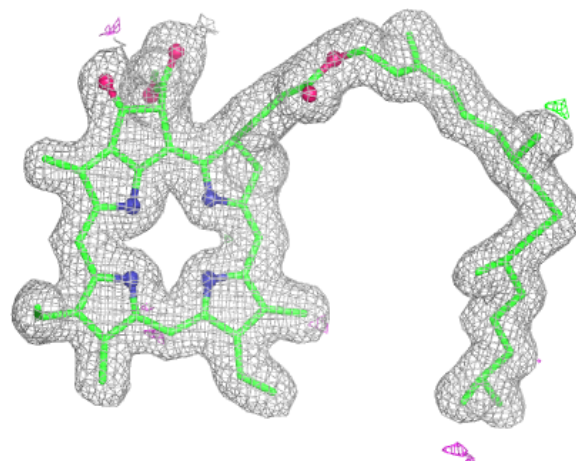
**Electron density around CLA b 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



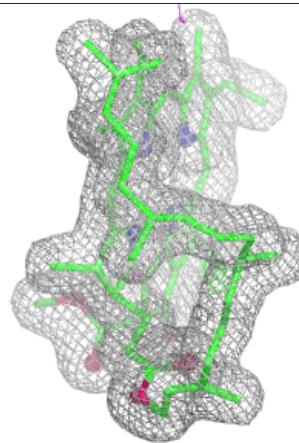
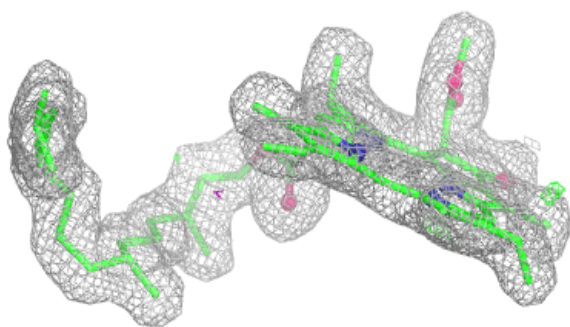
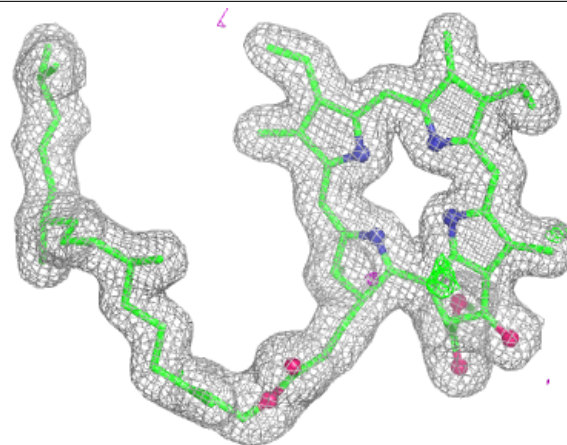
Electron density around PHO A 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



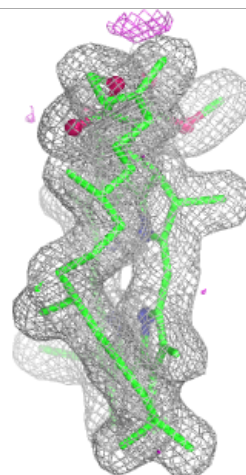
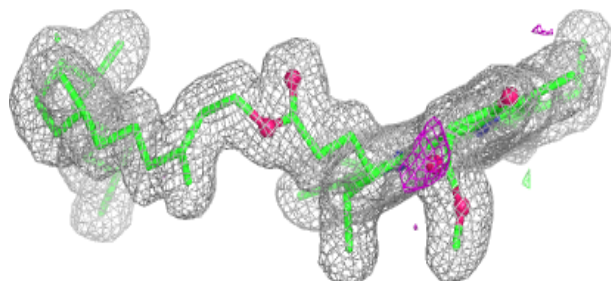
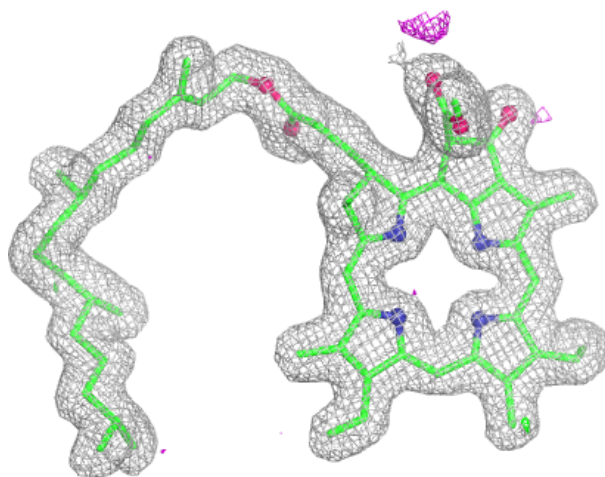
Electron density around PHO D 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



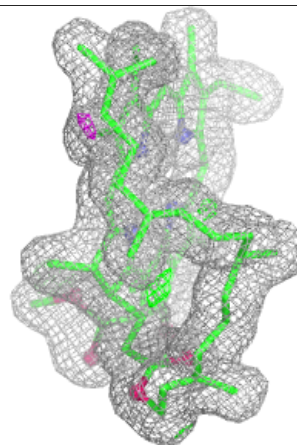
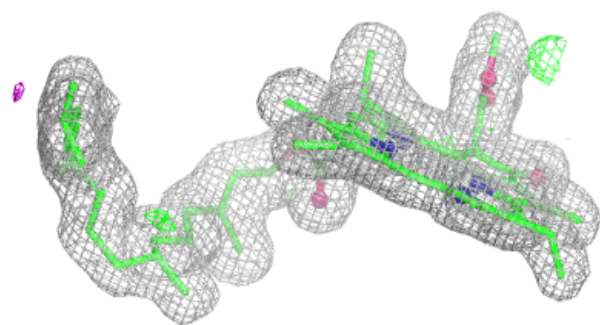
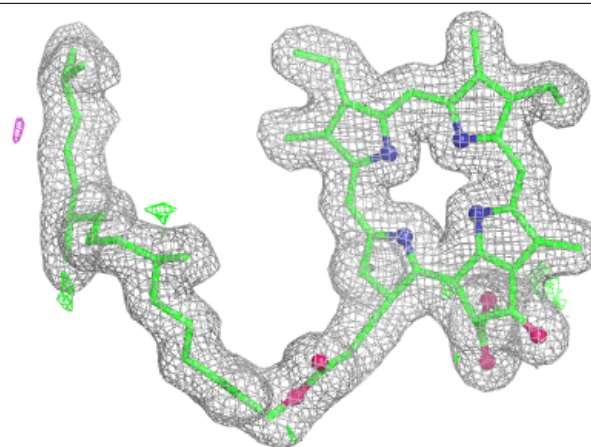
Electron density around PHO a 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



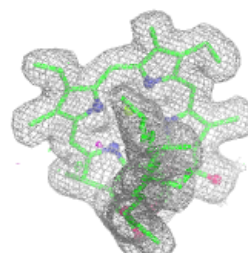
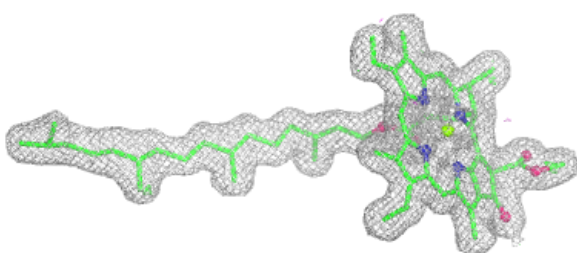
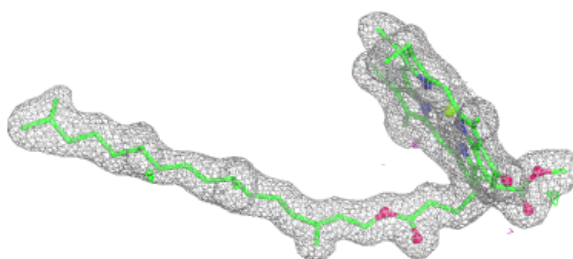
Electron density around PHO a 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

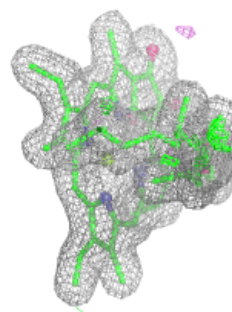
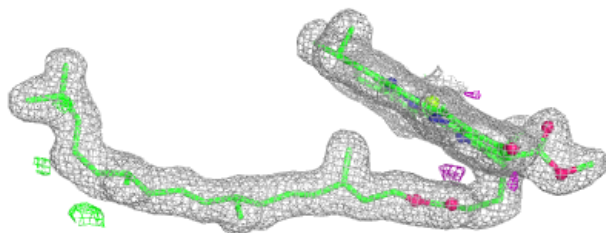
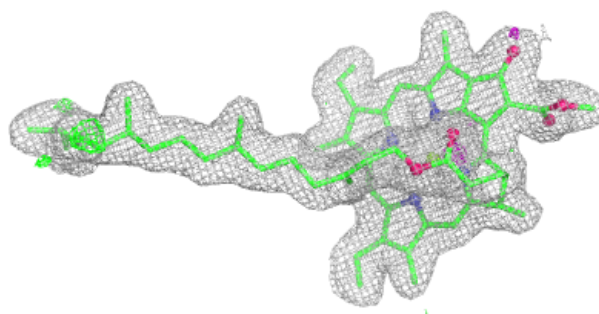


Electron density around CLA B 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

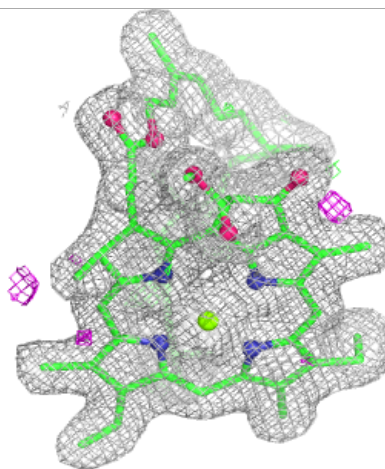
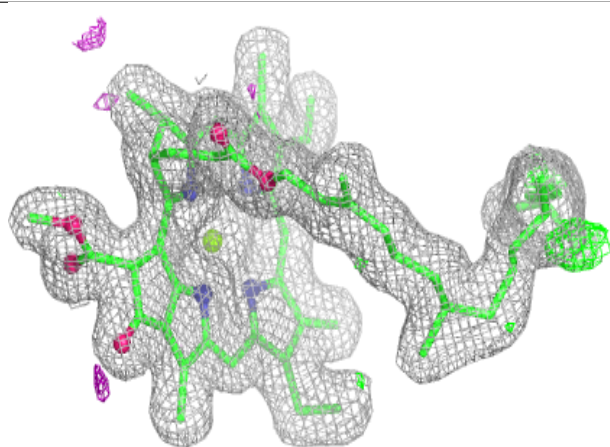
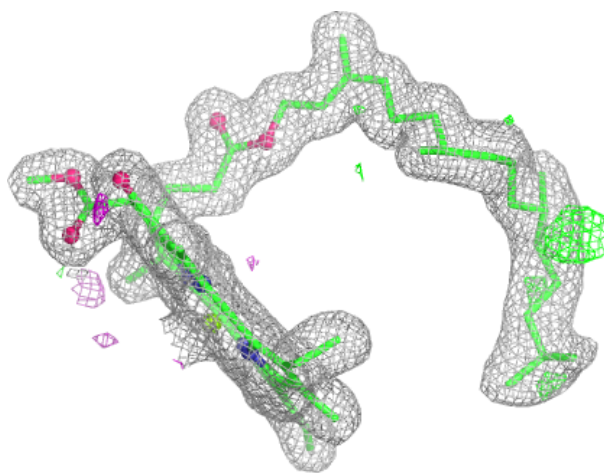
**Electron density around CLA B 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



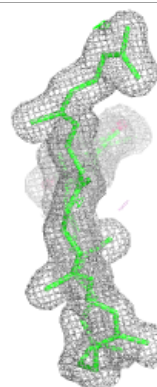
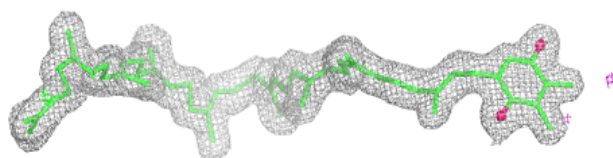
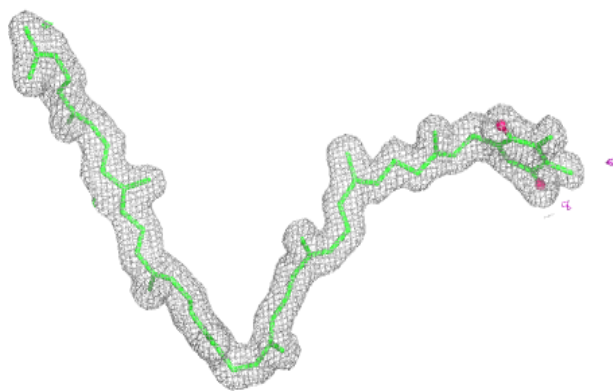
Electron density around CLA b 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

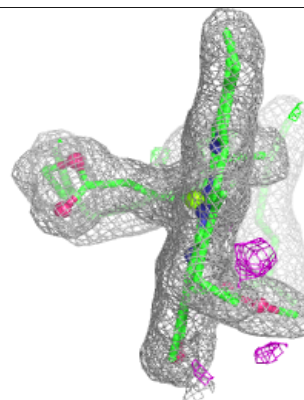
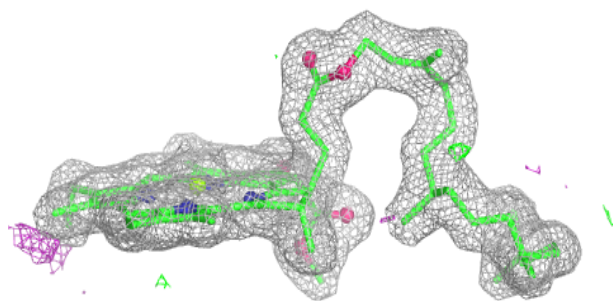
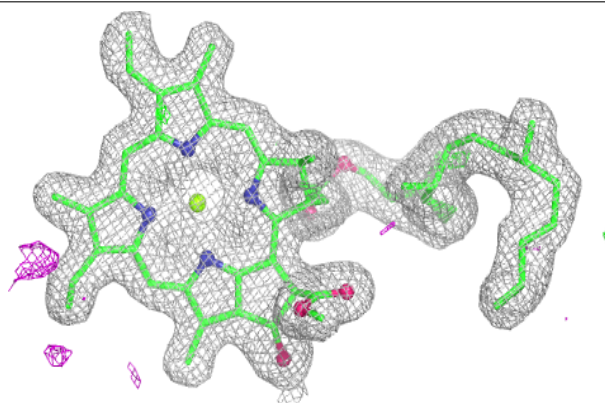


Electron density around PL9 d 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

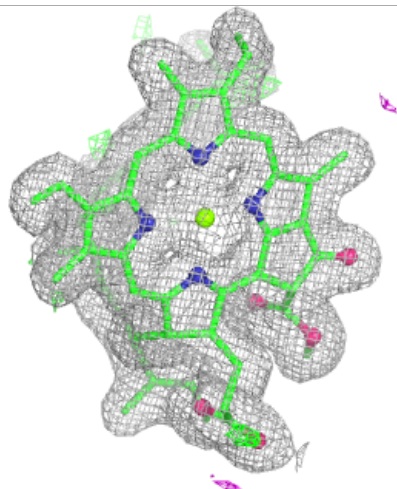
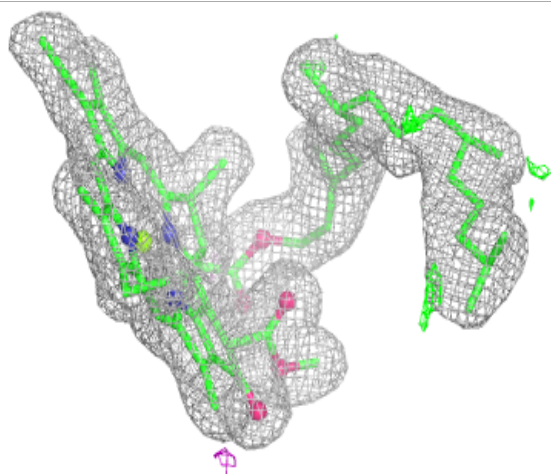
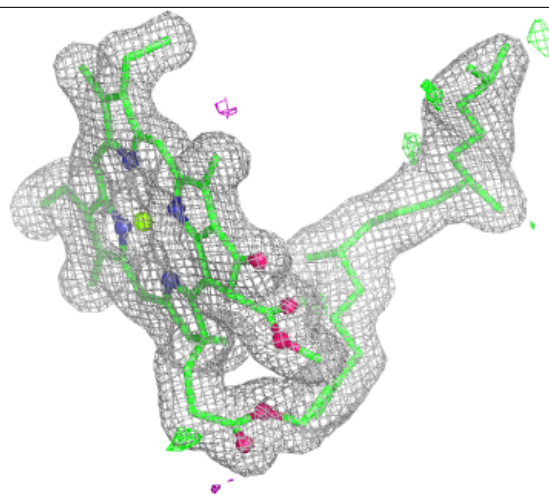
**Electron density around CLA b 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



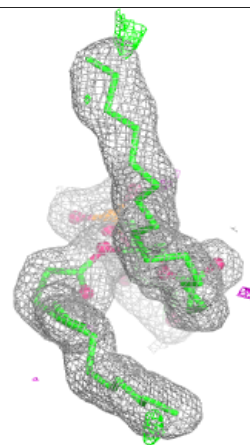
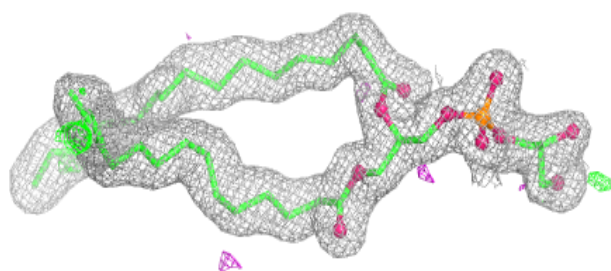
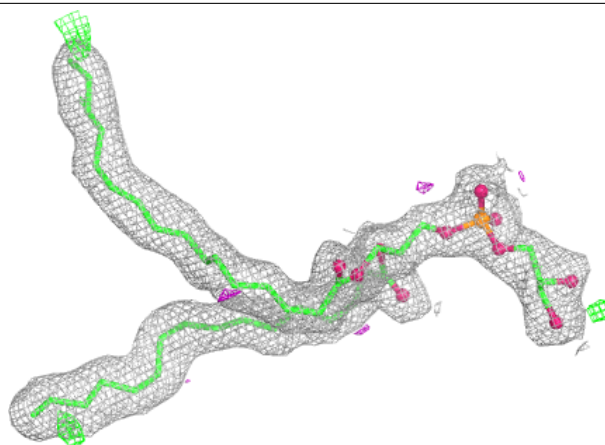
Electron density around CLA b 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



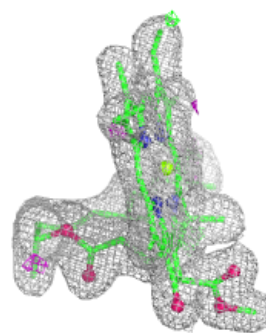
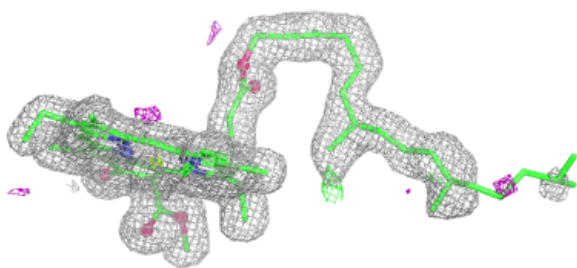
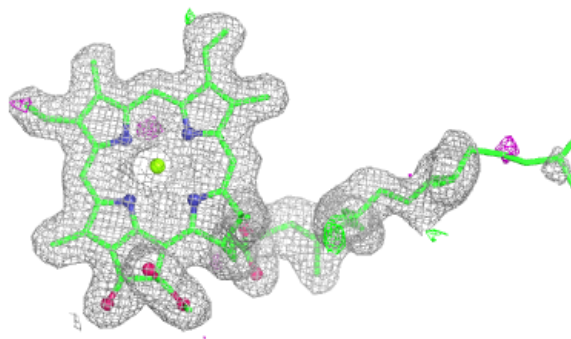
Electron density around LHG D 410:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

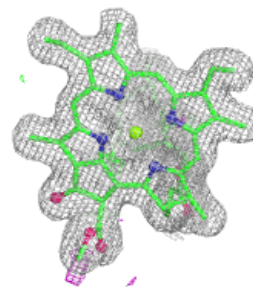
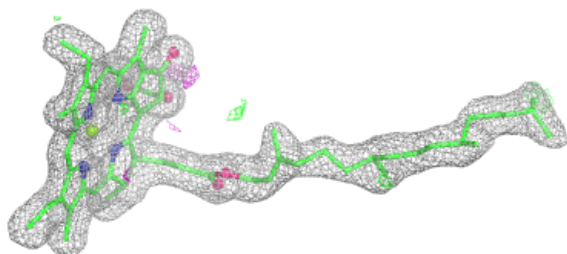
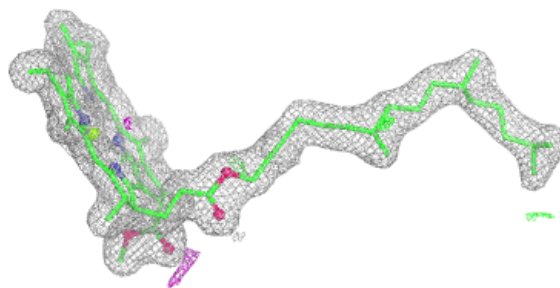


Electron density around CLA A 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

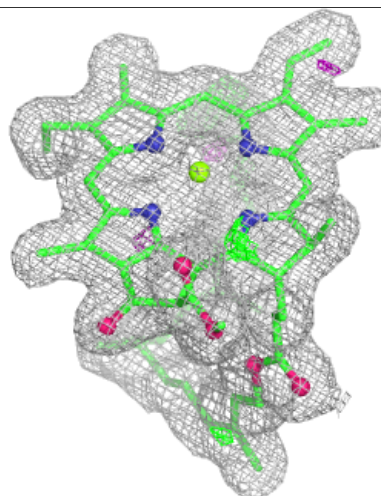
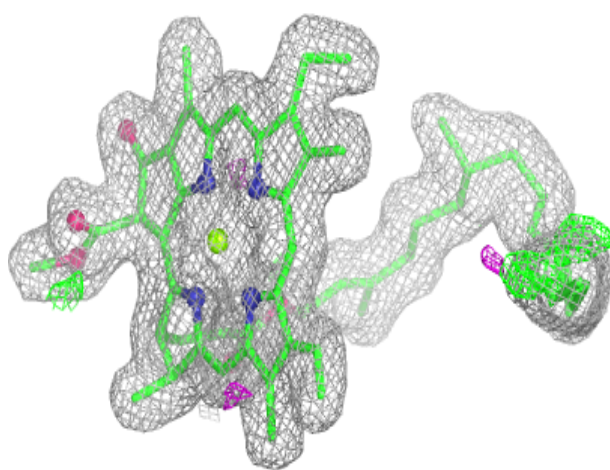
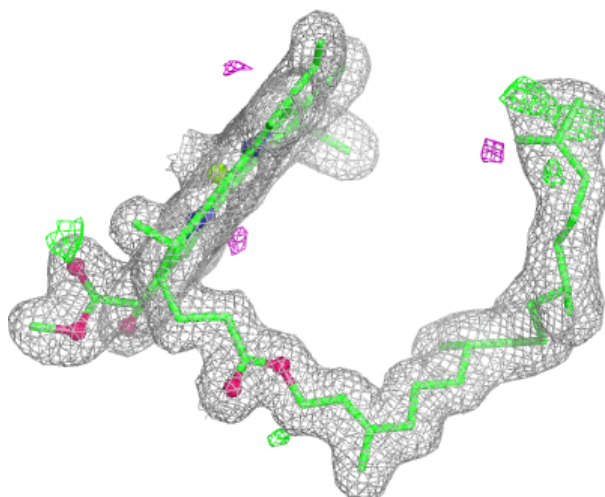
**Electron density around CLA B 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



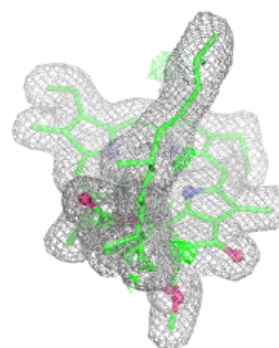
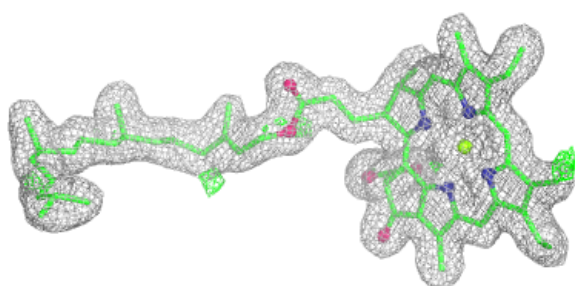
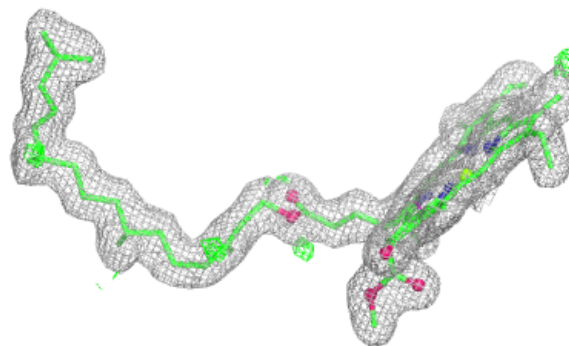
Electron density around CLA B 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

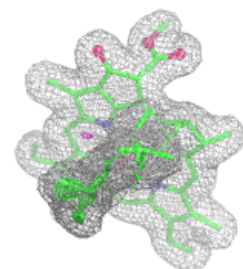
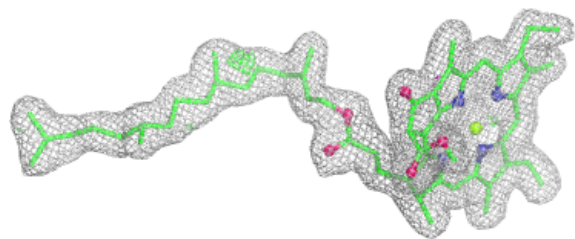
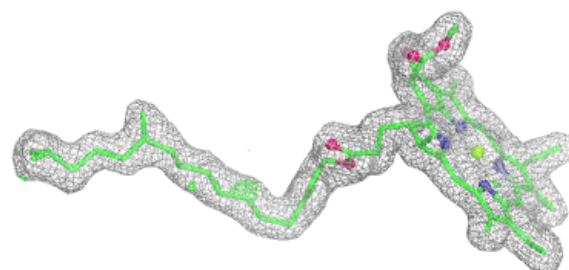


Electron density around CLA D 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

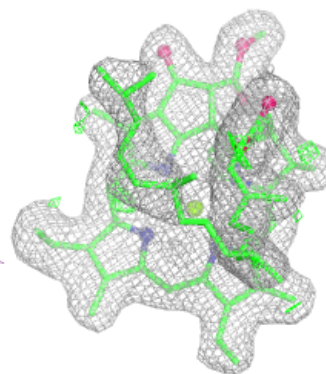
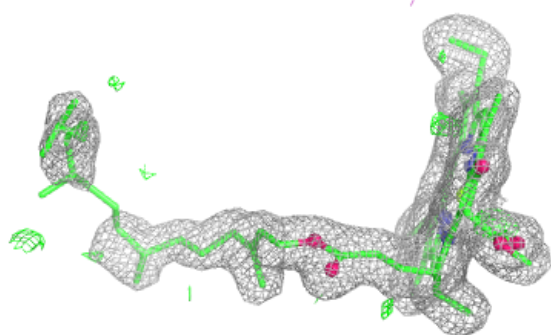
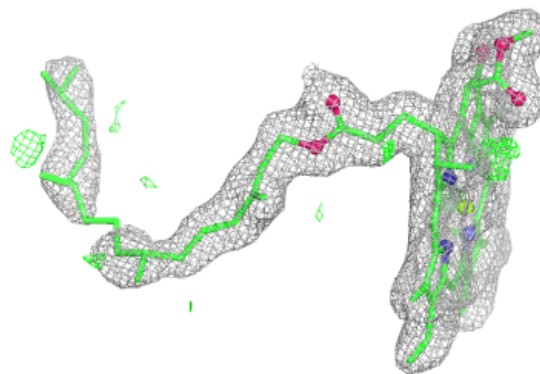
**Electron density around CLA c 903:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

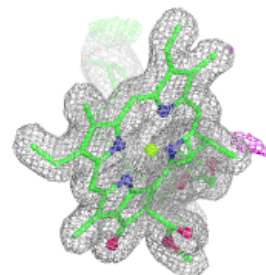
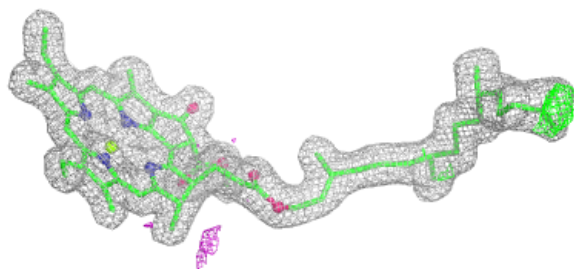
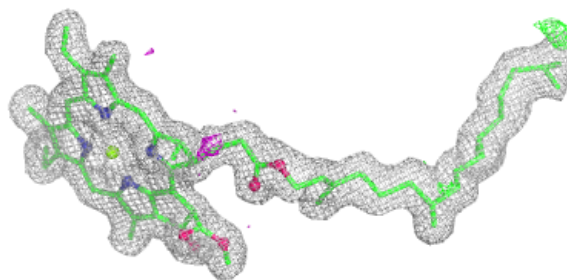


Electron density around CLA D 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

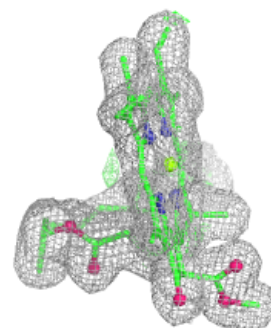
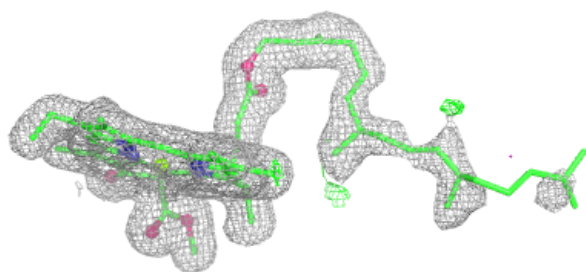
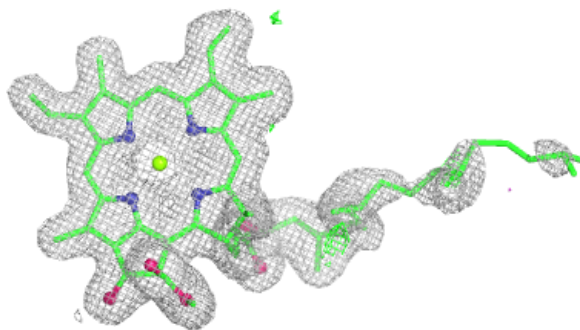
**Electron density around CLA a 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

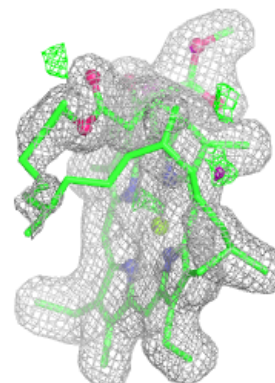
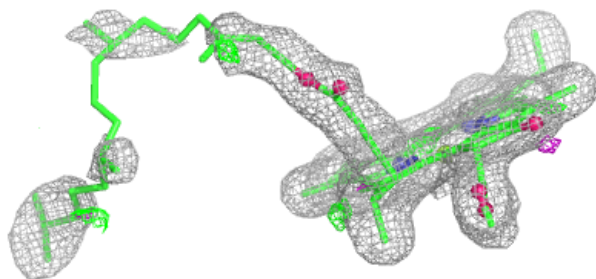
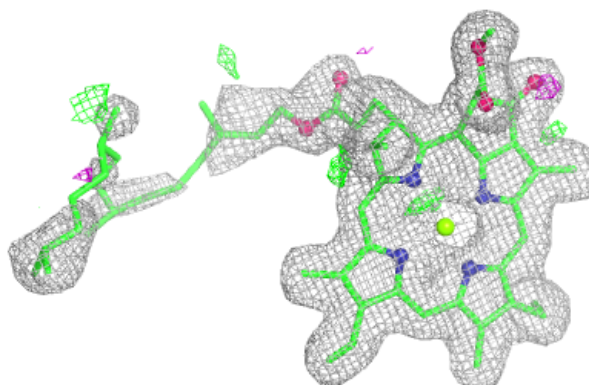


Electron density around CLA a 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

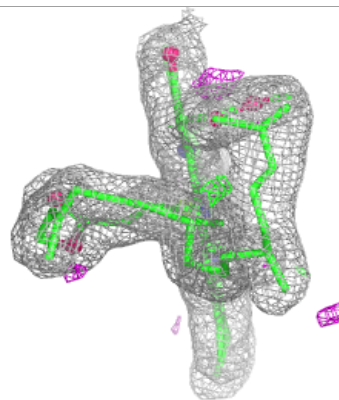
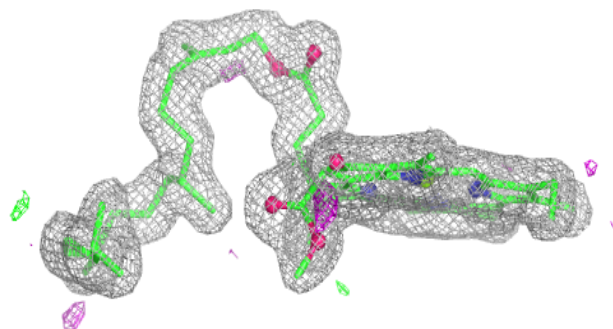
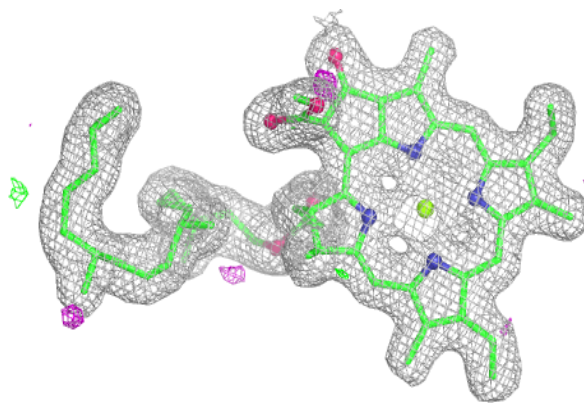
**Electron density around CLA a 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



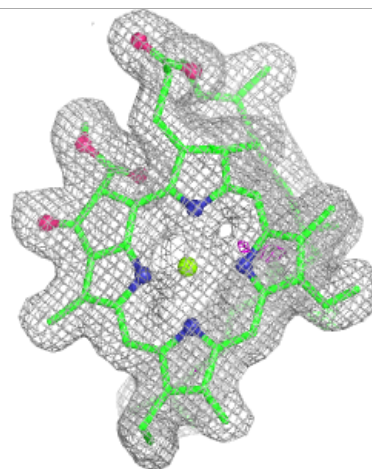
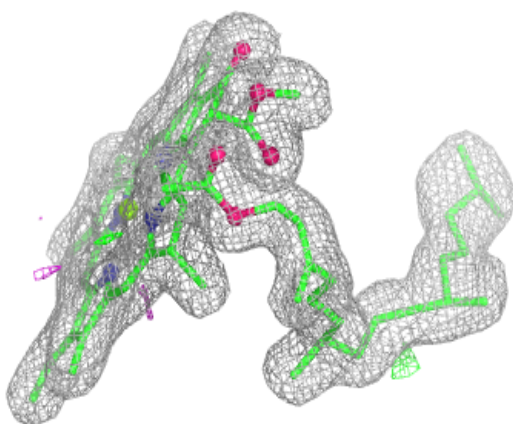
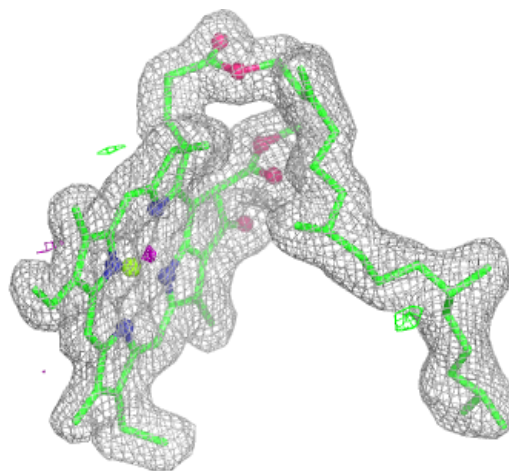
Electron density around CLA B 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



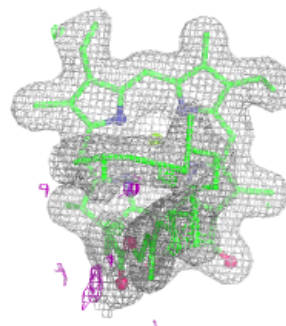
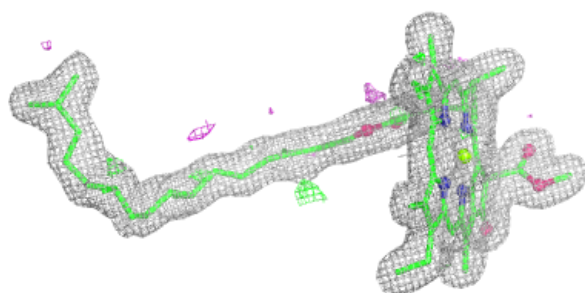
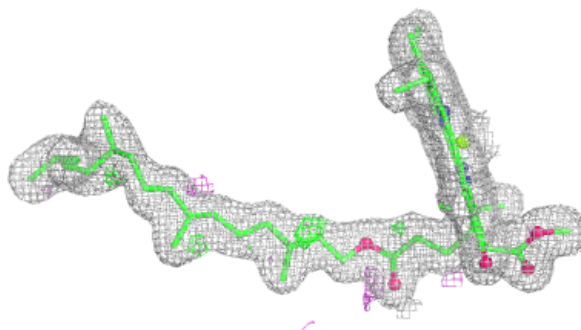
Electron density around CLA B 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



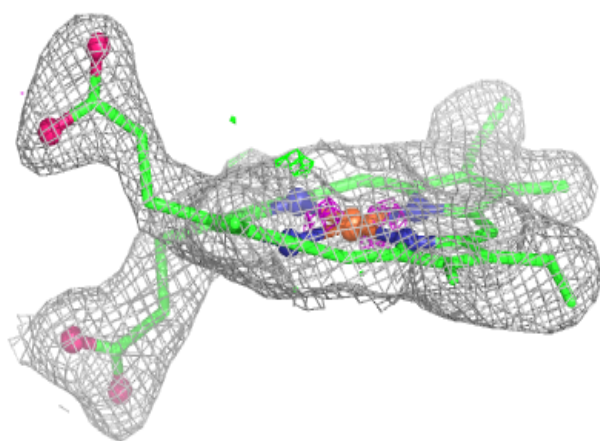
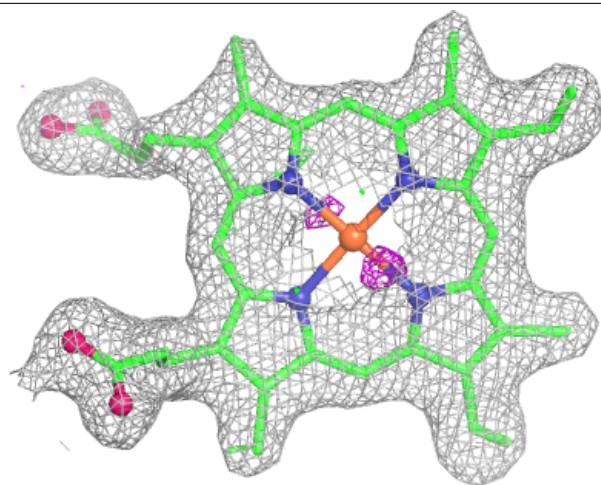
Electron density around CLA B 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



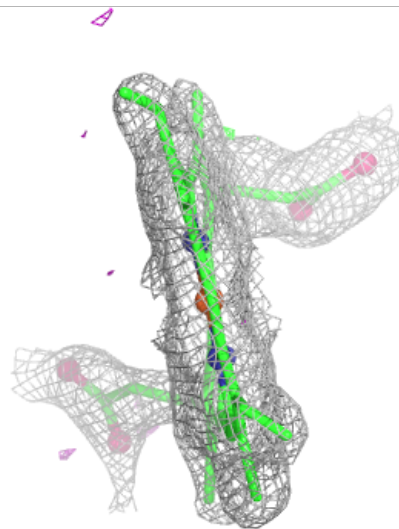
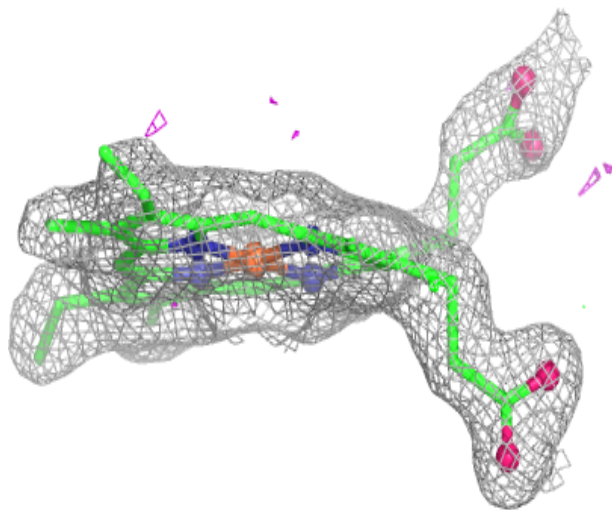
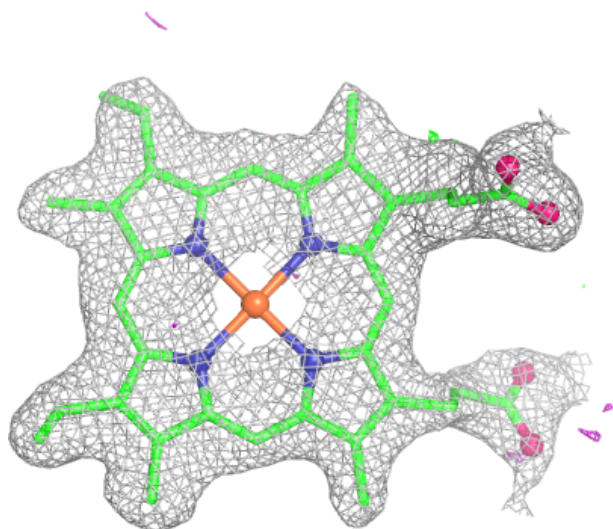
Electron density around HEM E 105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



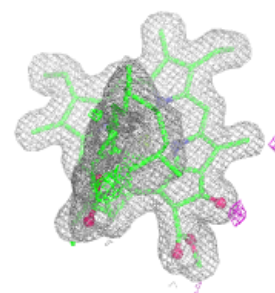
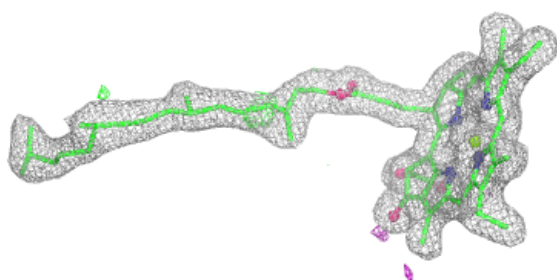
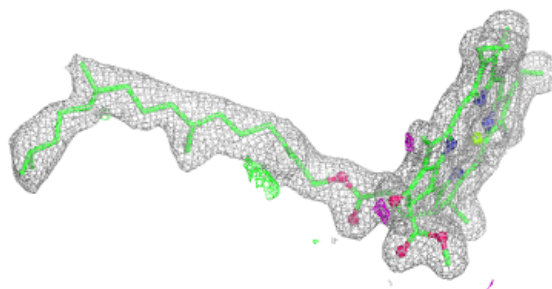
Electron density around HEM e 105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

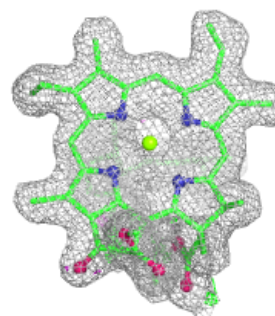
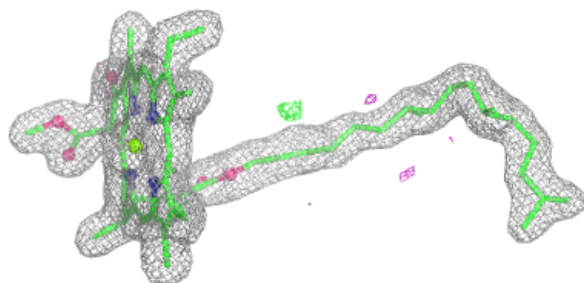
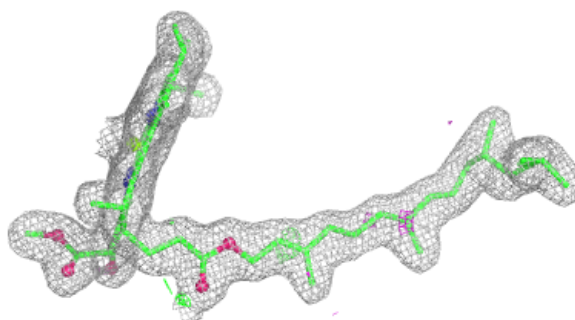


Electron density around CLA b 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

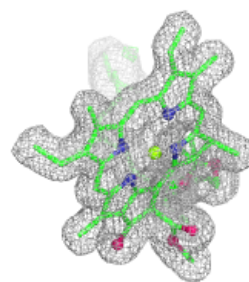
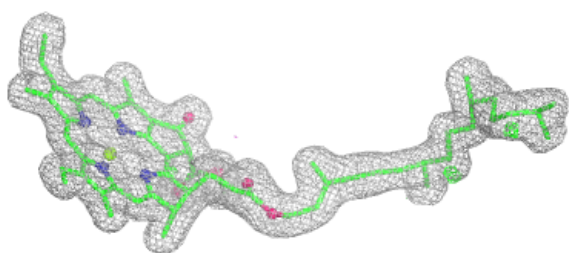
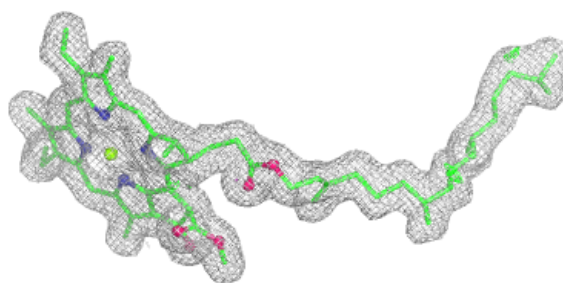
**Electron density around CLA b 606:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

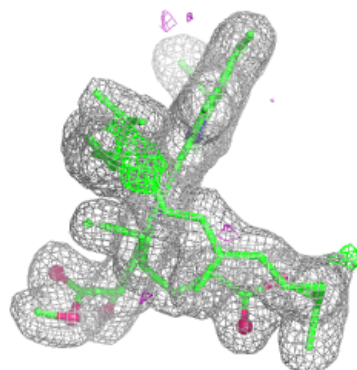
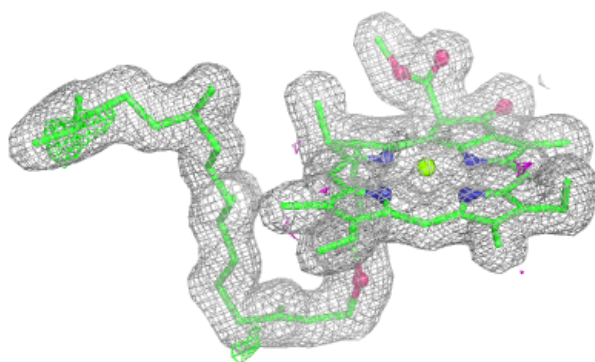
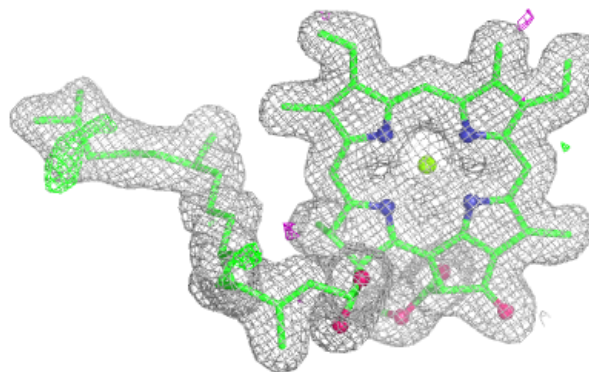


Electron density around CLA A 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

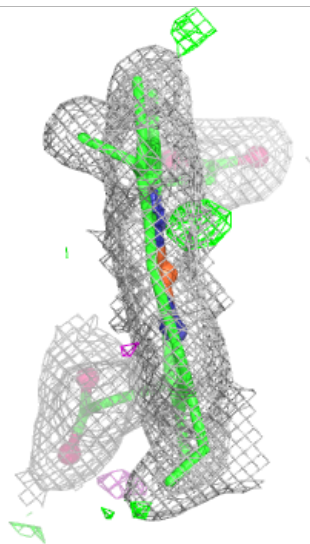
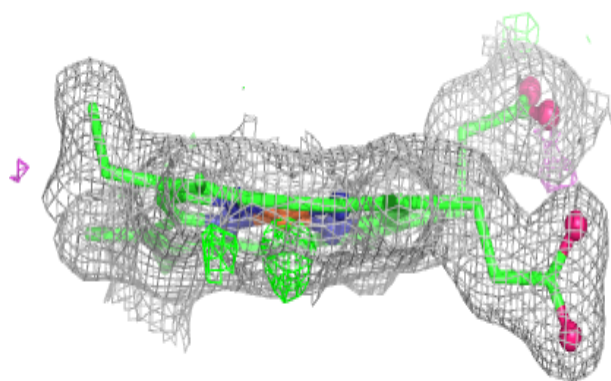
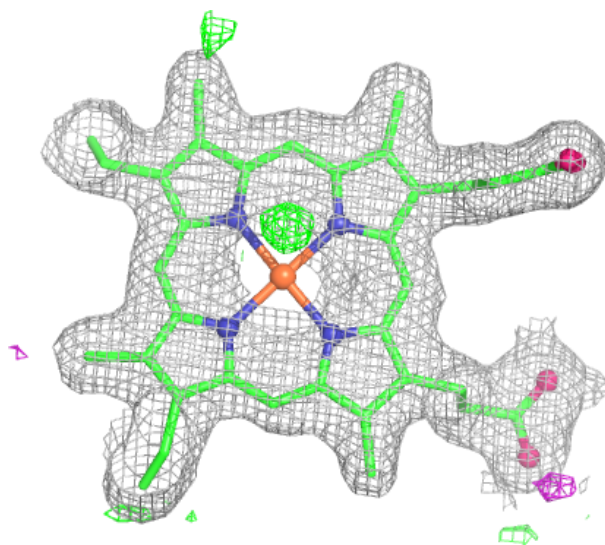
**Electron density around CLA D 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



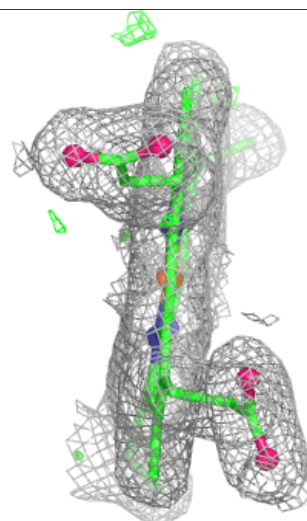
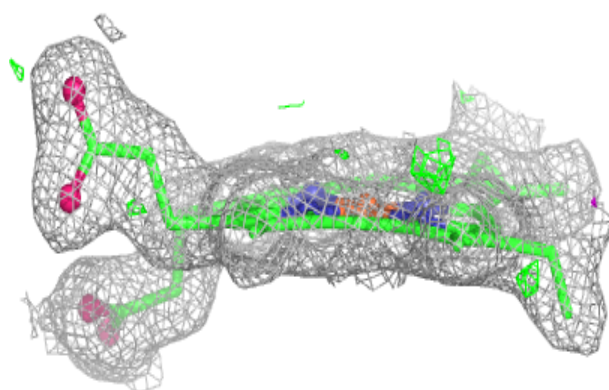
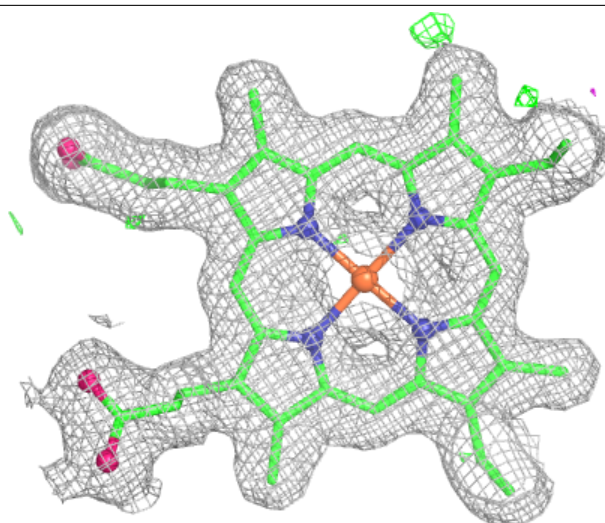
Electron density around HEC v 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC V 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.