Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2026 – 11:40 am BST

PDB ID	:	5E79 / pdb_00005e79
Title	:	Macromolecular diffractive imaging using imperfect crystals
Authors	:	Ayyer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on	:	2015-10-12
Resolution	:	3.50 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

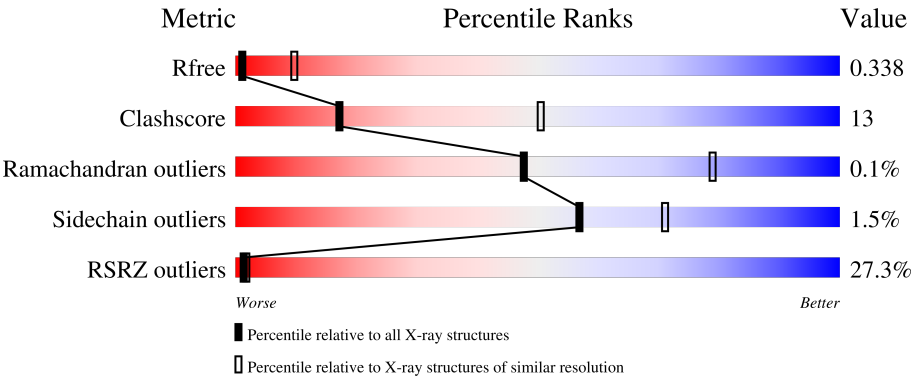
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 <=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	334	21% 77% 23%
1	a	334	33% 80% 20%
2	B	504	19% 77% 22%

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	b	504	32% 78% 21%
3	C	451	20% 80% 19%
3	c	451	34% 84% 16%
4	D	342	21% 75% 25%
4	d	342	32% 77% 23%
5	E	81	25% 77% 23%
5	e	81	46% 89% 11%
6	F	34	18% 50% 47%
6	f	34	32% 65% 35%
7	H	65	25% 74% 23%
7	h	65	38% 68% 31%
8	I	38	34% 74% 26%
8	i	38	42% 87% 13%
9	J	38	24% 95% 5%
9	j	38	37% 84% 16%
10	K	37	8% 70% 24% 5%
10	k	37	30% 57% 32% 8%
11	L	37	22% 68% 32%
11	l	37	32% 70% 27%
12	M	34	29% 74% 26%
12	m	34	35% 74% 21% 6%
13	O	243	23% 84% 16%
13	o	243	39% 84% 15%
14	T	30	13% 60% 40%
14	t	30	23% 70% 30%

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Mol	Chain	Length	Quality of chain
15	U	97	15% 88% 12%
15	u	97	31% 88% 12%
16	V	137	20% 88% 12%
16	v	137	26% 91% 9%
17	Y	29	24% 86% 14%
17	y	29	38% 86% 14%
18	X	39	15% 82% 18%
18	x	39	28% 77% 23%
19	Z	62	29% 94% 6%
19	z	62	47% 90% 10%

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
22	CL	U	201	-	-	-	X
22	CL	a	604	-	-	-	X
22	CL	u	201	-	-	-	X
26	BCR	A	610	-	X	-	-
26	BCR	B	618	-	X	X	-
26	BCR	B	619	-	X	-	-
26	BCR	B	620	-	X	-	-
26	BCR	C	514	-	X	-	-
26	BCR	F	101	-	X	-	-
26	BCR	H	101	-	X	-	-
26	BCR	I	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	K	102	-	X	-	-
26	BCR	T	101	-	X	X	-
26	BCR	a	610	-	X	-	-
26	BCR	b	619	-	X	X	-
26	BCR	b	620	-	X	-	-
26	BCR	b	621	-	X	-	-
26	BCR	c	514	-	X	-	-
26	BCR	c	515	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	BCR	c	521	-	X	-	-
26	BCR	f	101	-	X	X	-
26	BCR	h	101	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	t	101	-	X	X	-
27	PL9	D	405	-	X	-	-
27	PL9	a	611	-	-	-	X
27	PL9	d	404	-	X	-	-
29	LMG	Z	101	-	-	-	X
29	LMG	c	520	-	-	-	X
30	LHG	E	102	-	-	-	X
31	CA	b	602	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 50074 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			
1	a	334	Total	C	N	O	S	3	4	0
			2637	1730	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	13			
2	b	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	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	5	0
			3506	2296	584	613	13			
3	c	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			

- 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	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	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	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			668	436	107	125			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

- 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			

- 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	S	5	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

- 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
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			

- 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	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			

- 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	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total 774	C 491	N 129	O 154	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total 215	C 142	N 37	O 33	S 3	0	0	0
17	y	29	Total 215	C 142	N 37	O 33	S 3	0	0	0

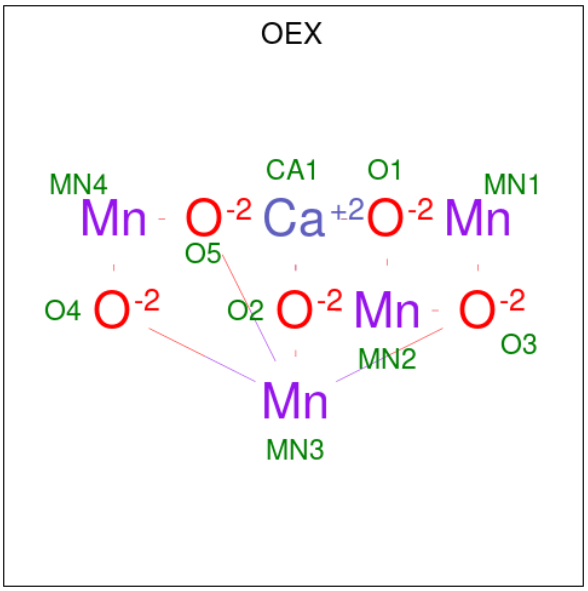
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total 292	C 196	N 46	O 50	0	1	0
18	x	39	Total 292	C 196	N 46	O 50	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total 479	C 328	N 72	O 77	S 2	0	0	0
19	z	62	Total 479	C 328	N 72	O 77	S 2	0	0	0

- 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		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

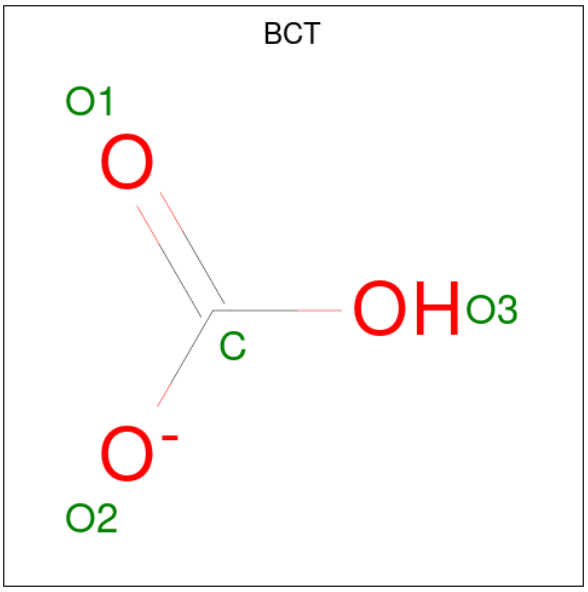
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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).

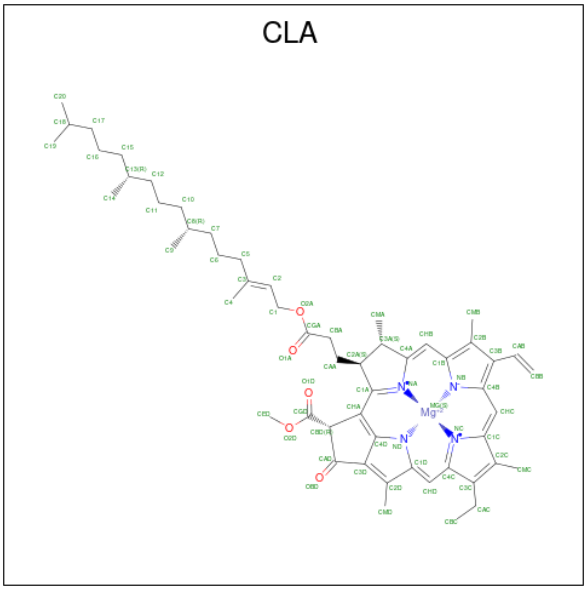
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	u	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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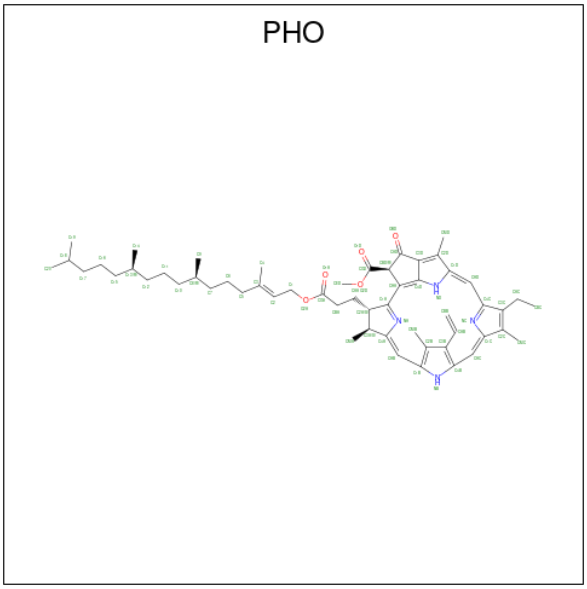
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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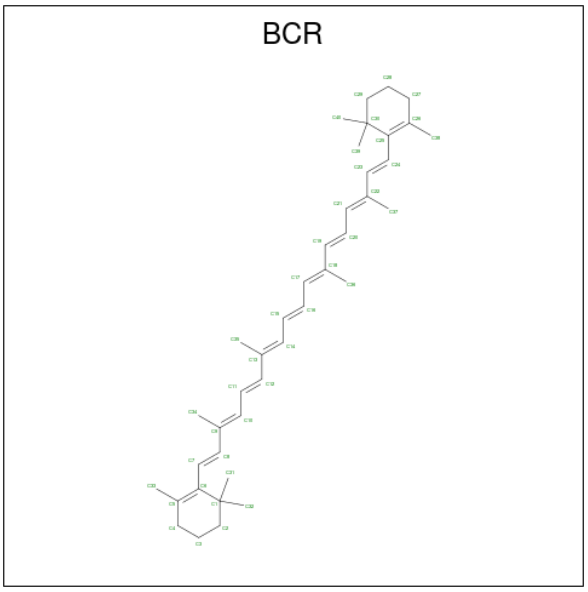
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



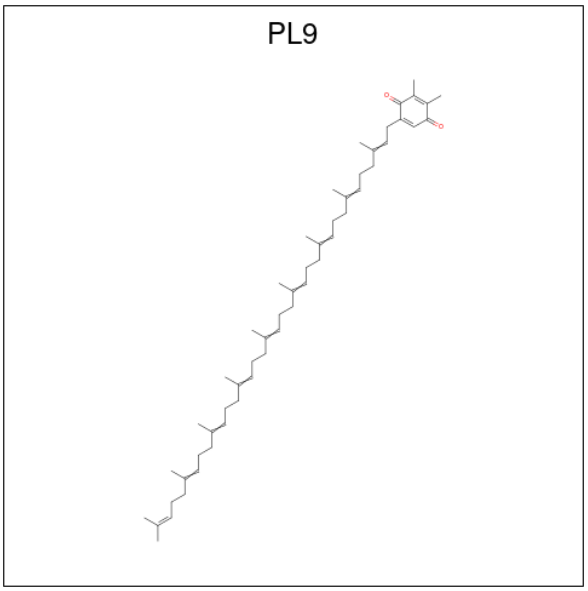
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	F	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	I	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	f	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

- 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: $C_{53}H_{80}O_2$).



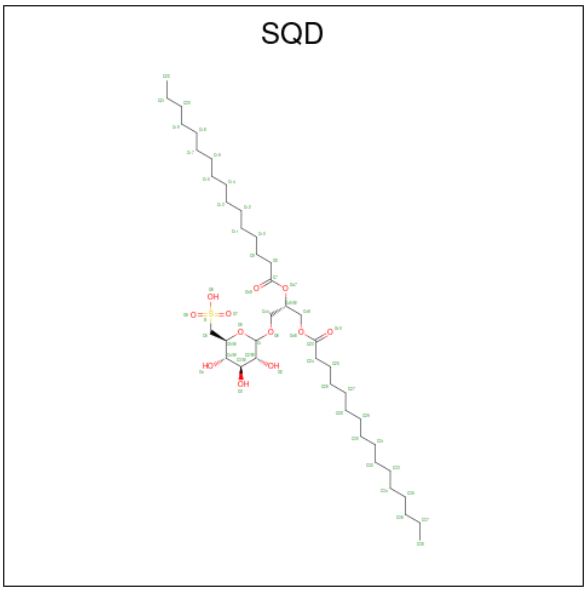
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



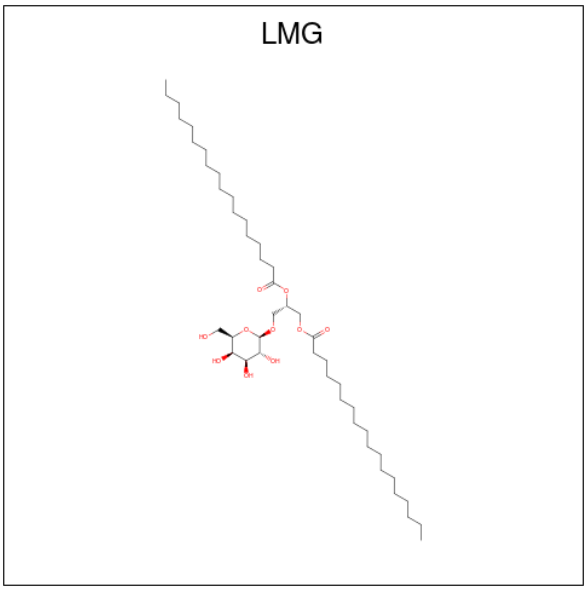
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O S 54 41 12 1	0	0
28	A	1	Total C O S 54 41 12 1	0	0
28	B	1	Total C O S 54 41 12 1	0	0
28	L	1	Total C O S 54 41 12 1	0	0
28	X	1	Total C O S 43 30 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	b	1	Total C O S 54 41 12 1	0	0
28	l	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	x	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



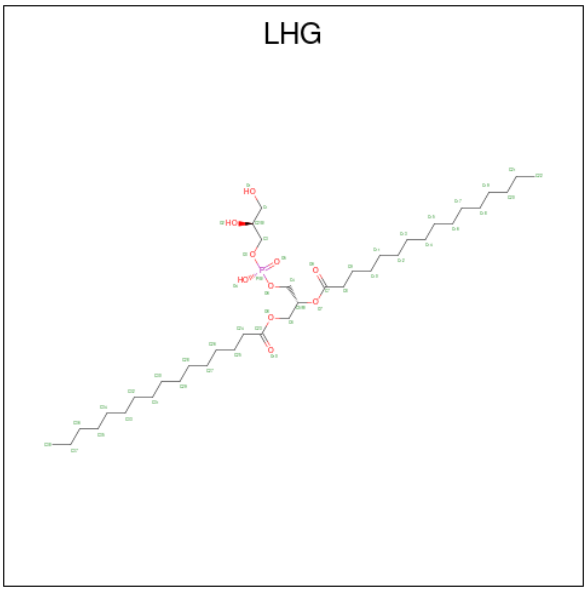
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	Z	1	Total	C	O	0	0
			37	27	10		
29	a	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	j	1	Total C O 51 41 10	0	0
29	z	1	Total C O 37 27 10	0	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O P 49 38 10 1	0	0
30	D	1	Total C O P 49 38 10 1	0	0
30	D	1	Total C O P 49 38 10 1	0	0
30	E	1	Total C O P 42 31 10 1	0	0
30	L	1	Total C O P 49 38 10 1	0	0
30	a	1	Total C O P 49 38 10 1	0	0
30	d	1	Total C O P 49 38 10 1	0	0
30	d	1	Total C O P 49 38 10 1	0	0
30	e	1	Total C O P 42 31 10 1	0	0

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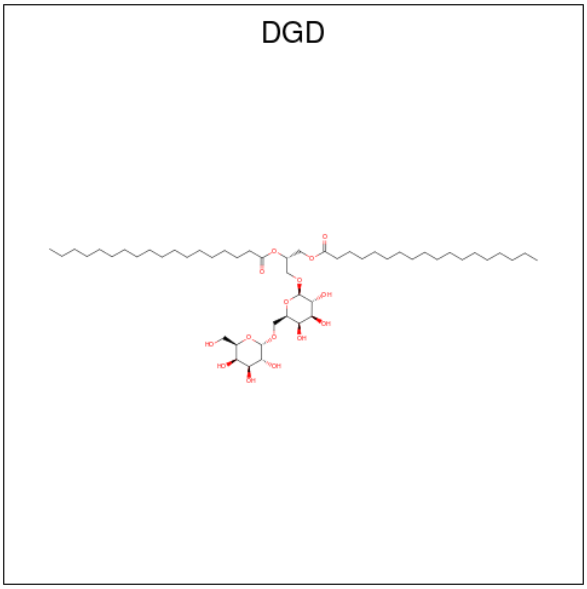
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	l	1	Total C O P 49 38 10 1	0	0

- Molecule 31 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total Ca 1 1	0	0
31	F	1	Total Ca 1 1	0	0
31	O	1	Total Ca 1 1	0	0
31	b	1	Total Ca 1 1	0	0
31	f	1	Total Ca 1 1	0	0
31	o	1	Total Ca 1 1	0	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



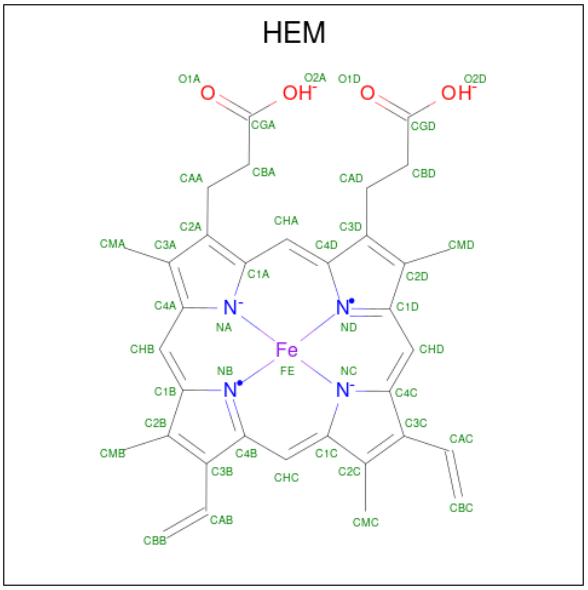
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	C	1	Total C O 62 47 15	0	0
32	C	1	Total C O 62 47 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	C	1	Total C O 62 47 15	0	0
32	E	1	Total C O 62 47 15	0	0
32	H	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	d	1	Total C O 62 47 15	0	0
32	h	1	Total C O 62 47 15	0	0

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

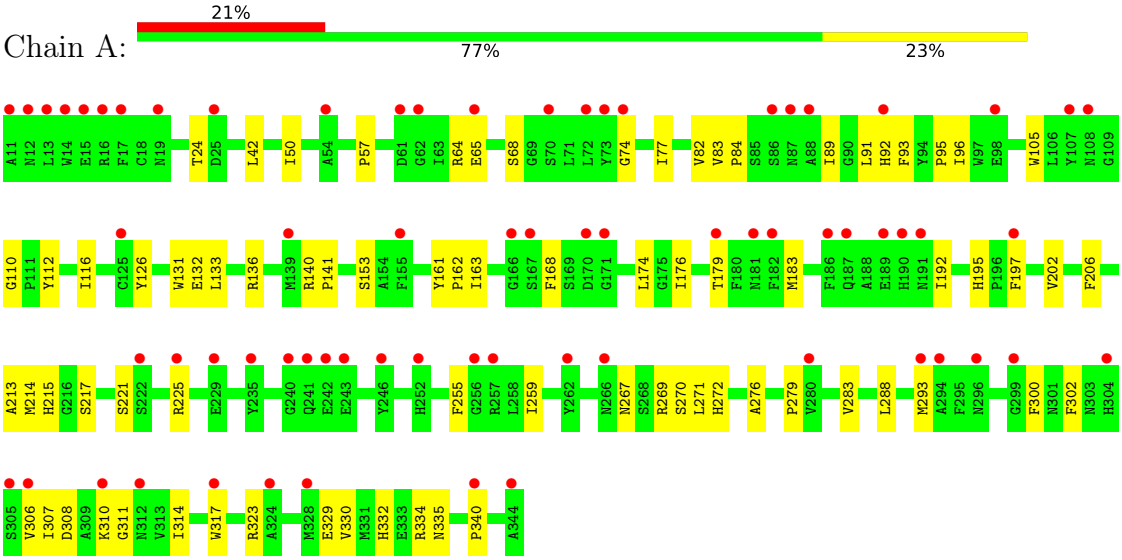
- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

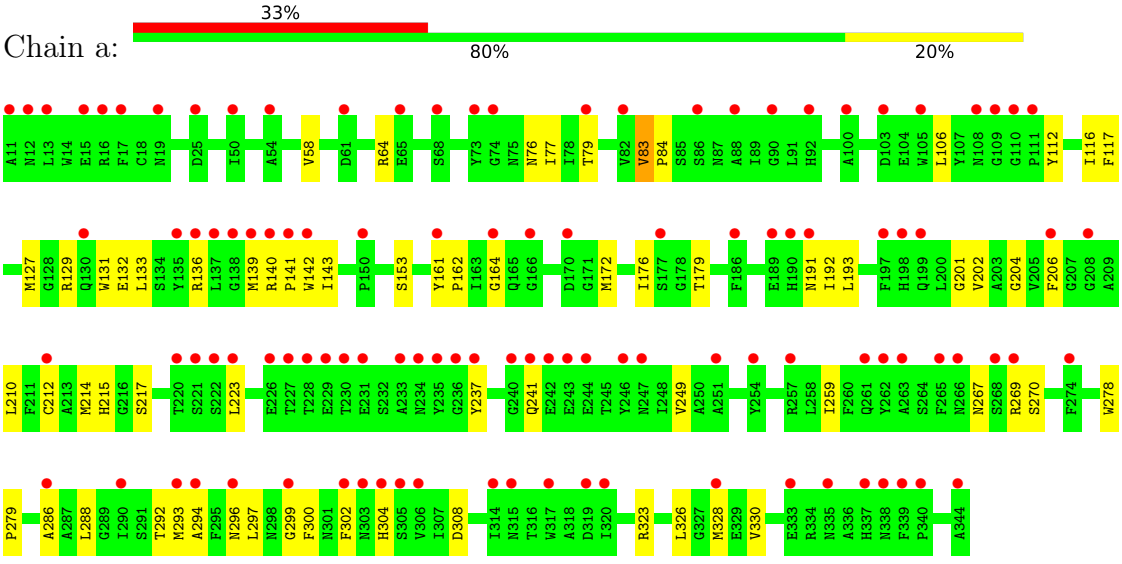
3 Residue-property plots (i)

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 1

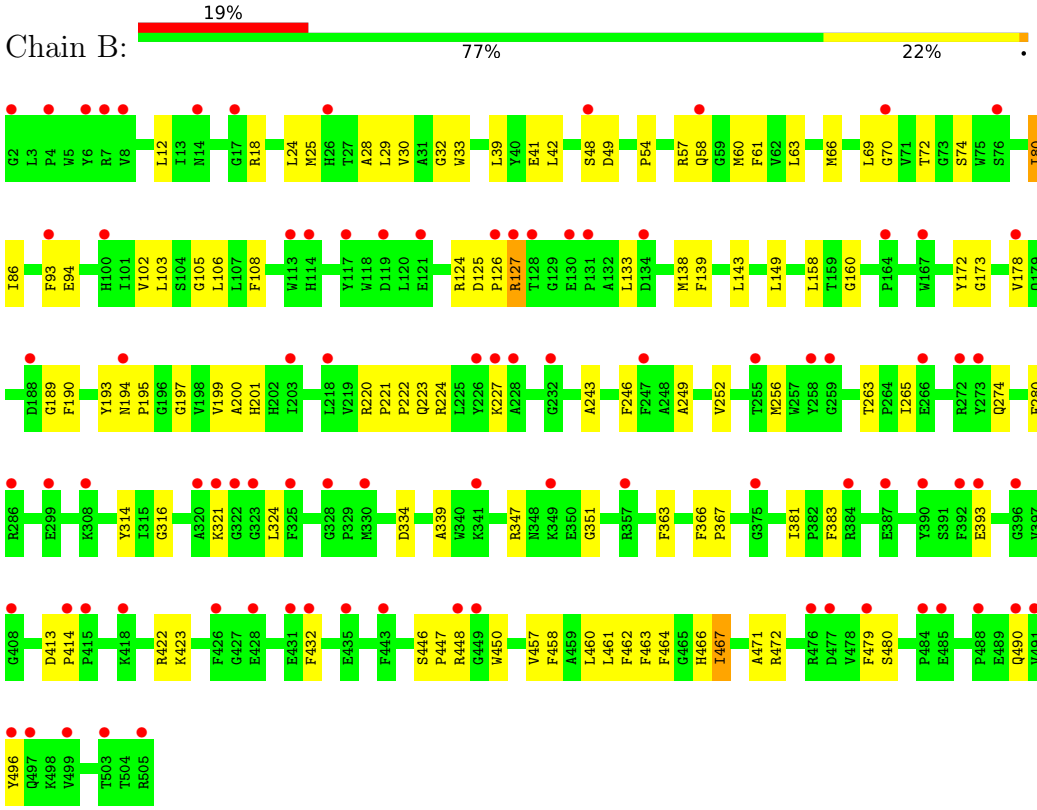


• Molecule 1: Photosystem II protein D1 1



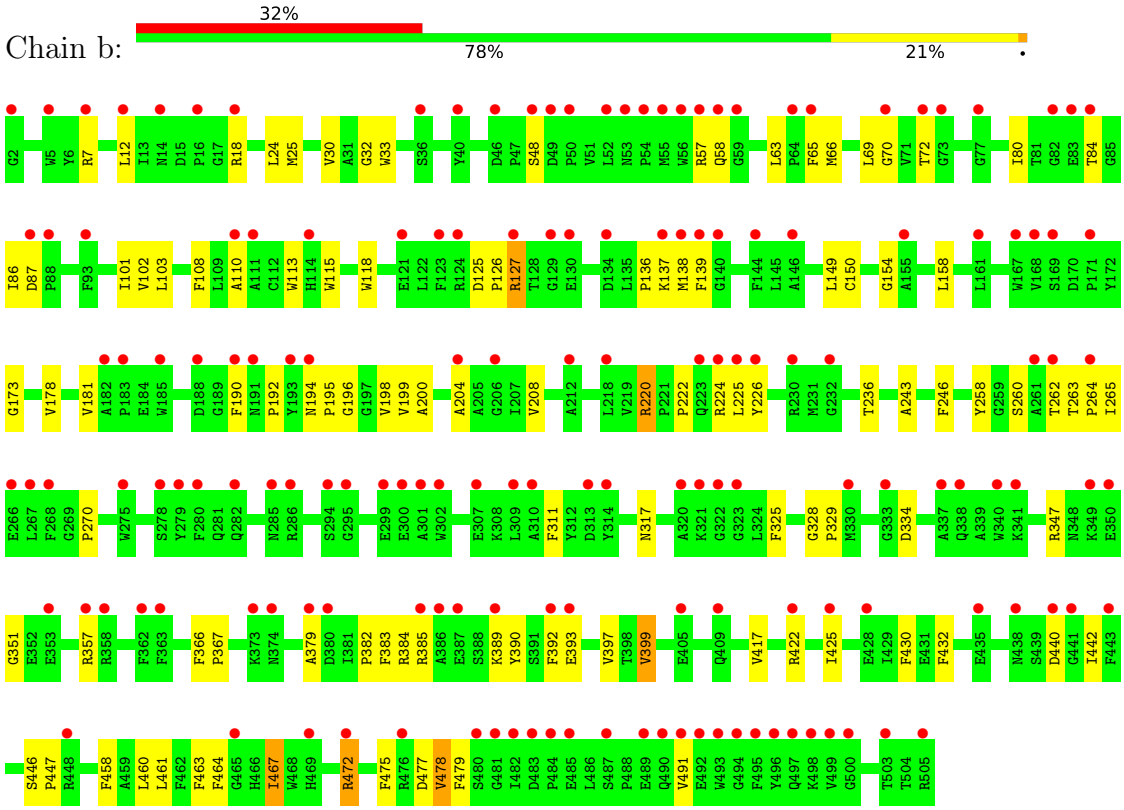
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



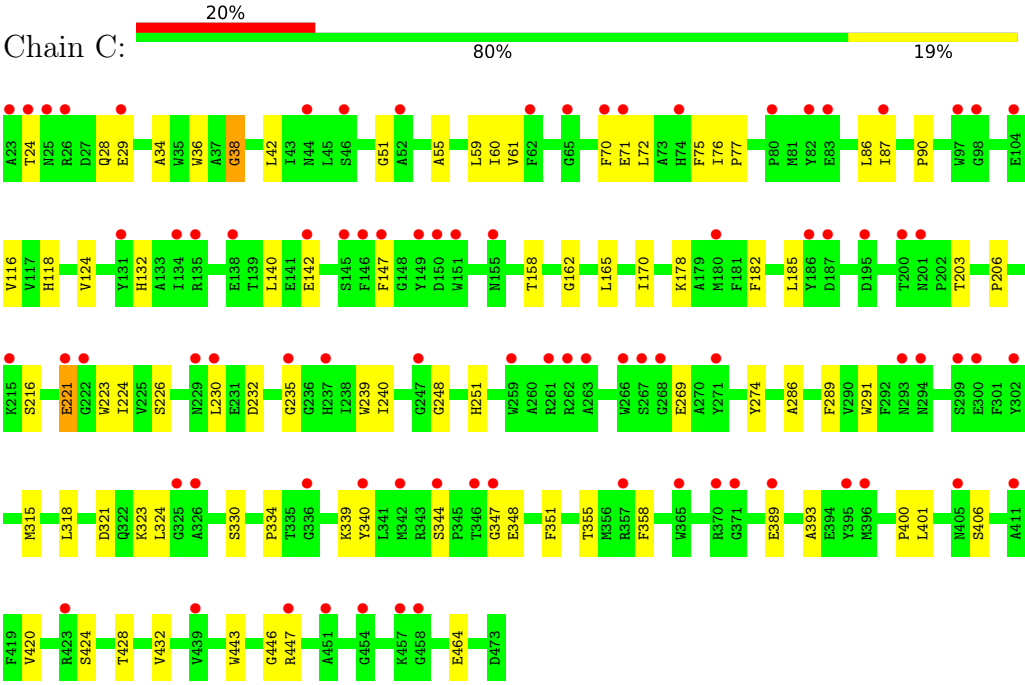
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



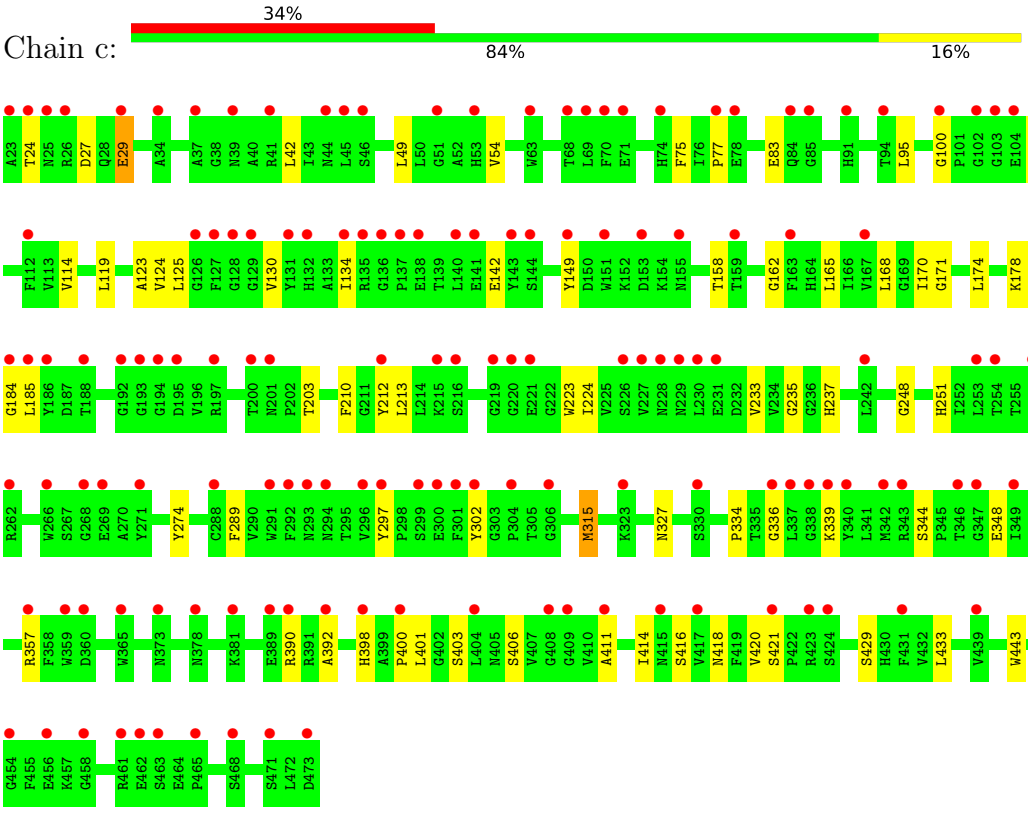
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



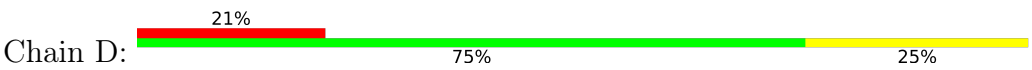
• Molecule 3: Photosystem II CP43 reaction center protein

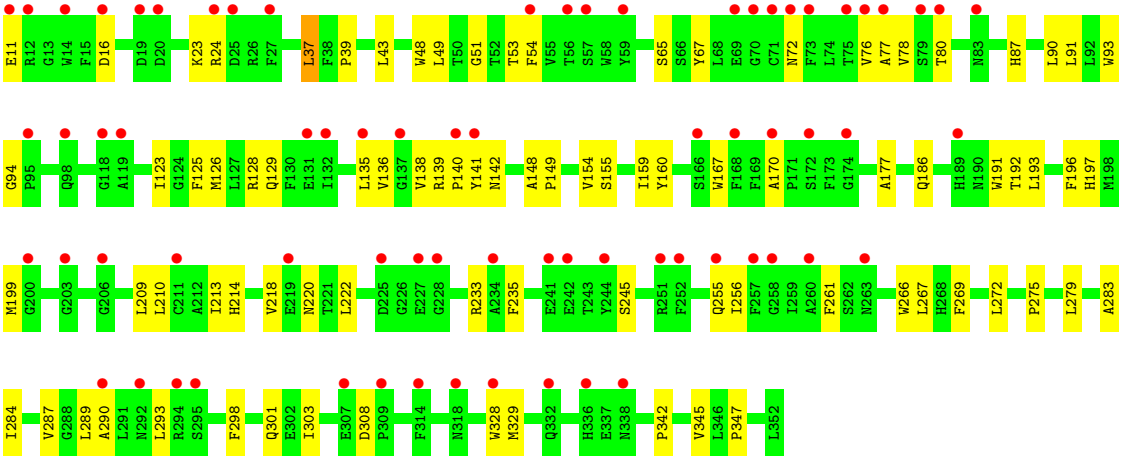
Chain c:



• Molecule 4: Photosystem II D2 protein

Chain D:

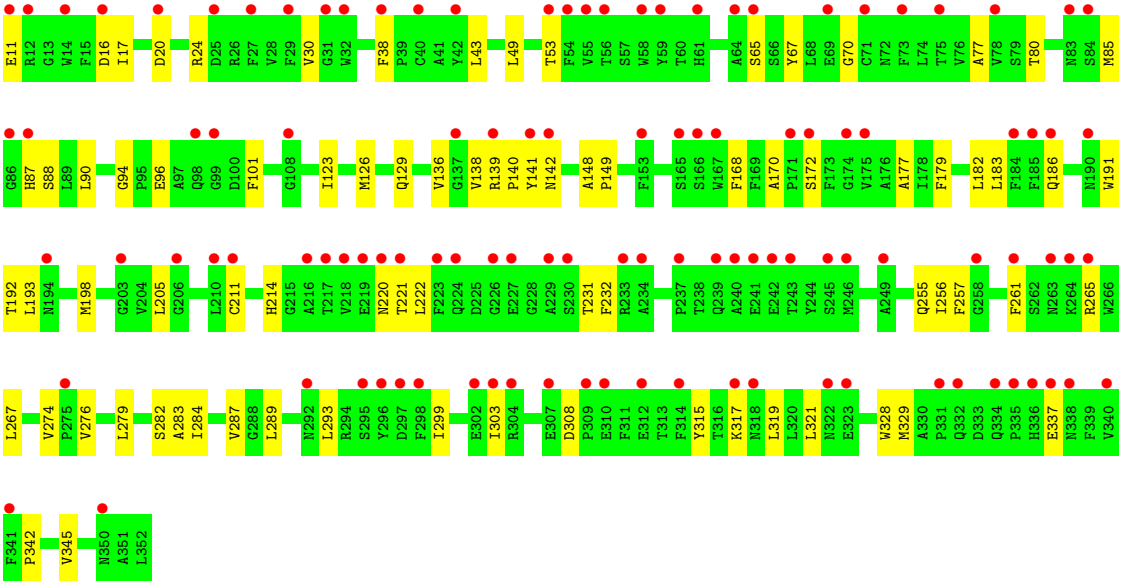




• Molecule 4: Photosystem II D2 protein

Chain d:

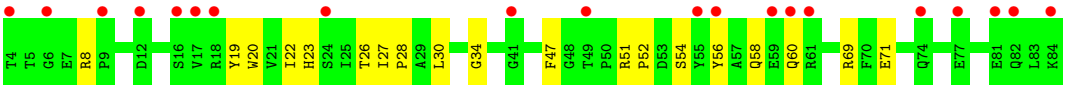




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

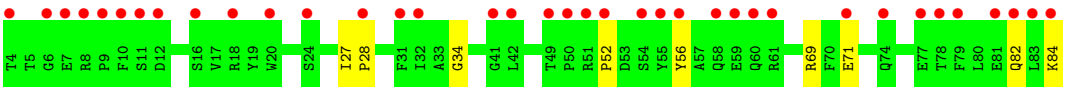




• Molecule 5: Cytochrome b559 subunit alpha

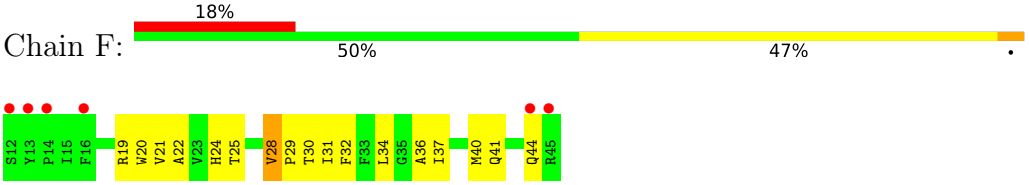
Chain e:





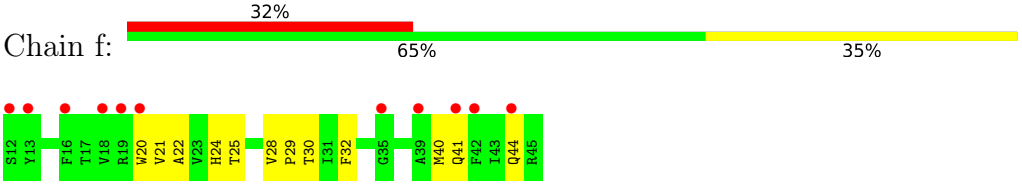
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



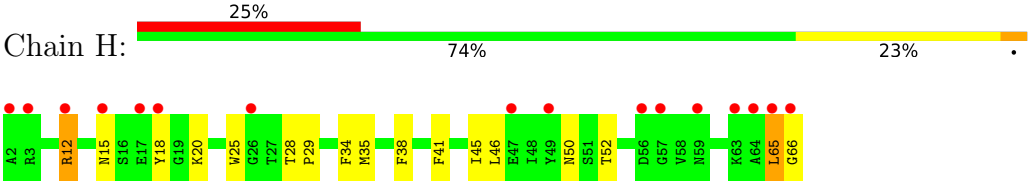
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



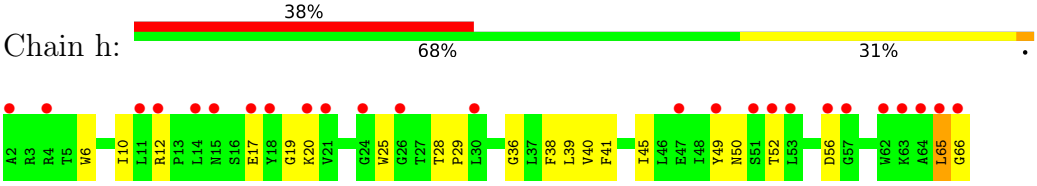
• Molecule 7: Photosystem II reaction center protein H

Chain H:



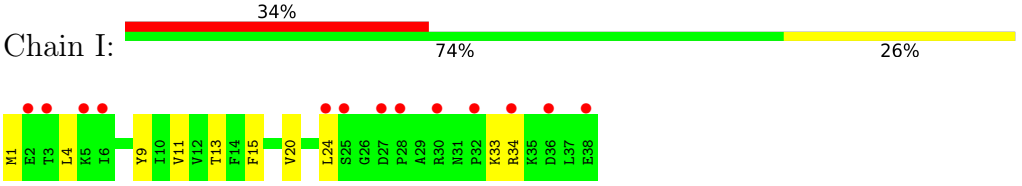
• Molecule 7: Photosystem II reaction center protein H

Chain h:



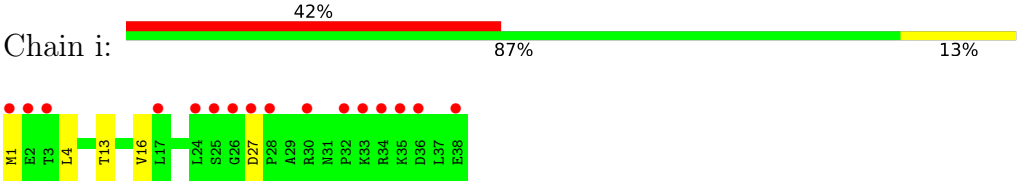
• Molecule 8: Photosystem II reaction center protein I

Chain I:



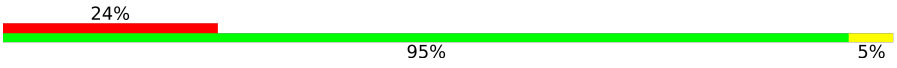
• Molecule 8: Photosystem II reaction center protein I

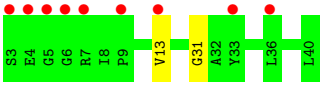
Chain i:



• Molecule 9: Photosystem II reaction center protein J

Chain J:

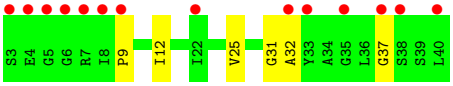




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

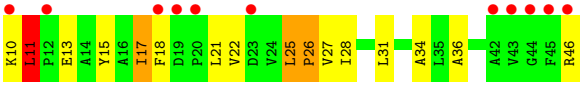




• Molecule 10: Photosystem II reaction center protein K

Chain k:

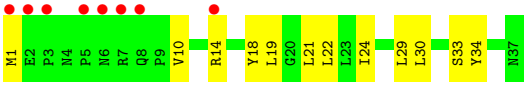




• Molecule 11: Photosystem II reaction center protein L

Chain L:

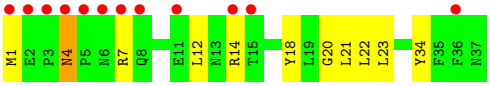




• Molecule 11: Photosystem II reaction center protein L

Chain l:

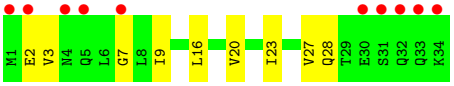




• Molecule 12: Photosystem II reaction center protein M

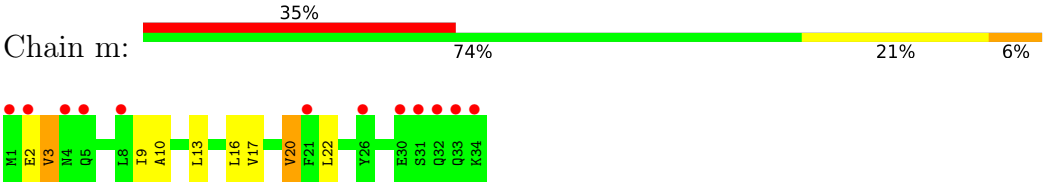
Chain M:





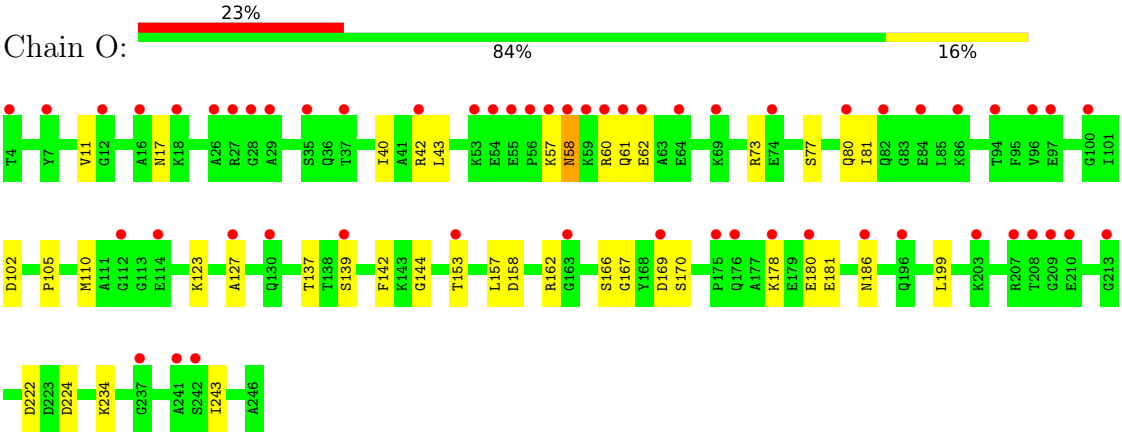
• Molecule 12: Photosystem II reaction center protein M

Chain m:



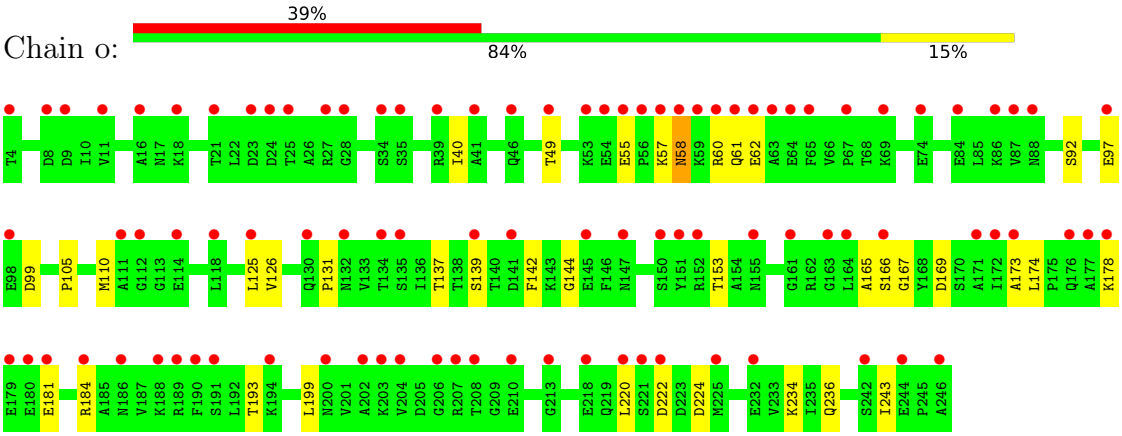
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



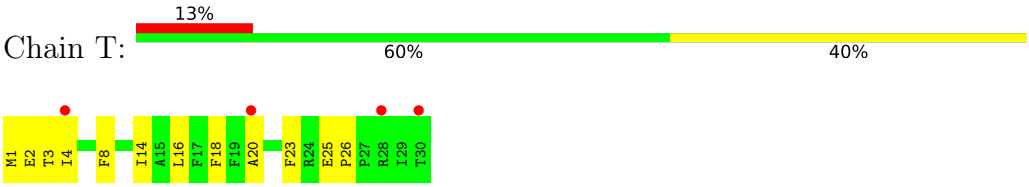
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



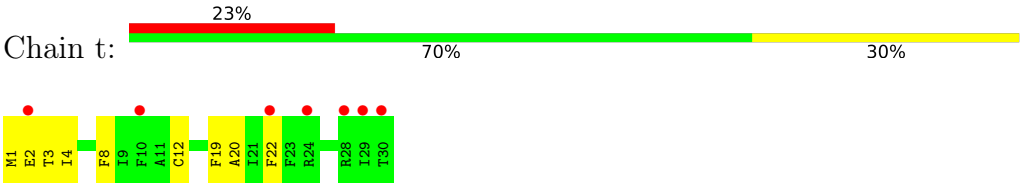
• Molecule 14: Photosystem II reaction center protein T

Chain T:



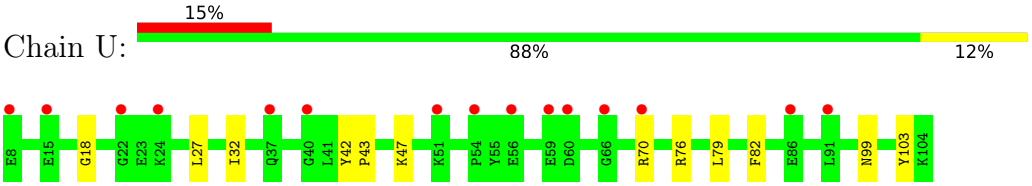
• Molecule 14: Photosystem II reaction center protein T

Chain t:



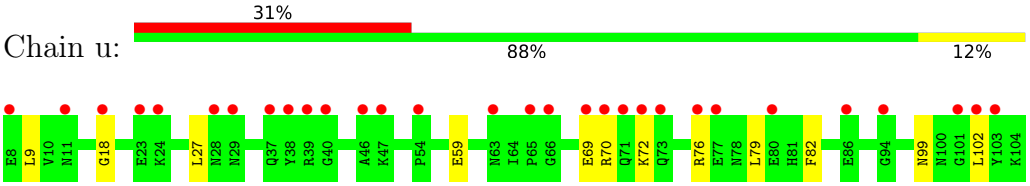
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



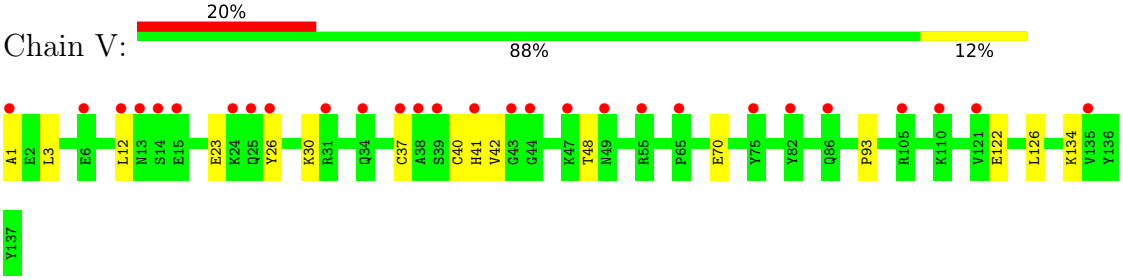
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



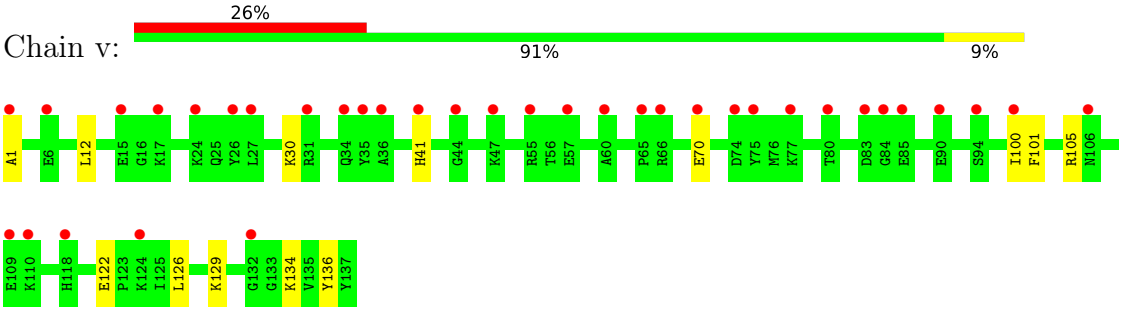
• Molecule 16: Cytochrome c-550

Chain V:



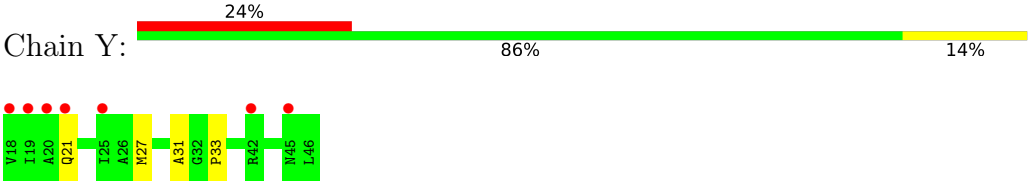
• Molecule 16: Cytochrome c-550

Chain v:



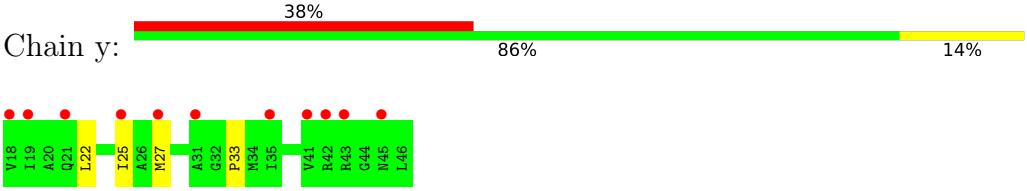
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



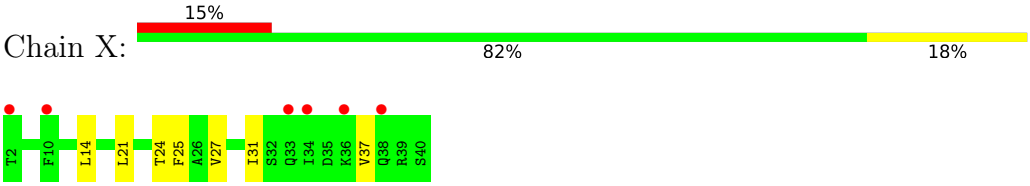
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



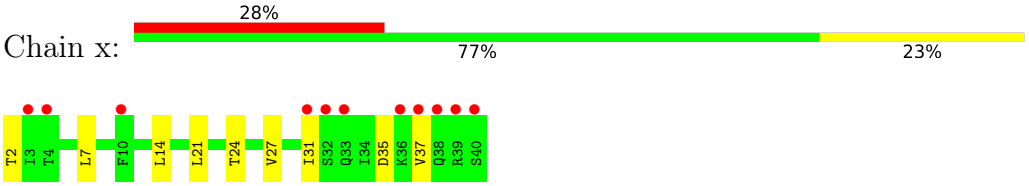
• Molecule 18: Photosystem II reaction center X protein

Chain X:



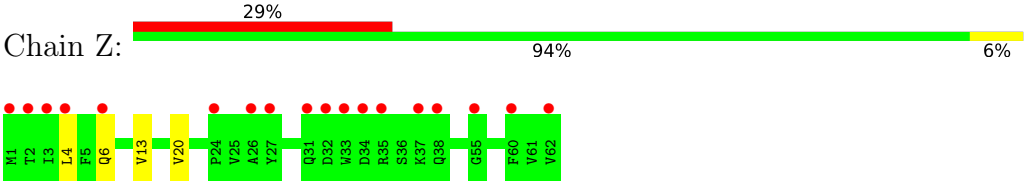
• Molecule 18: Photosystem II reaction center X protein

Chain x:



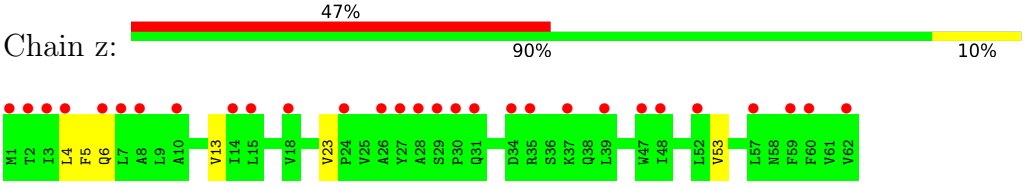
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	250.80Å 250.80Å 250.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 29.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.98-3.50) 99.8 (29.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.324 , 0.331 0.342 , 0.338	Depositor DCC
R_{free} test set	45921 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.7	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	50074	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.75	0/2734	0.99	1/3727 (0.0%)
1	a	0.64	0/2734	0.99	7/3727 (0.2%)
2	B	0.66	1/4194 (0.0%)	0.96	7/5713 (0.1%)
2	b	0.63	0/4194	0.96	13/5713 (0.2%)
3	C	0.64	0/3634	1.00	4/4947 (0.1%)
3	c	0.61	0/3634	0.95	5/4947 (0.1%)
4	D	0.67	0/2821	0.98	9/3844 (0.2%)
4	d	0.61	0/2821	0.93	6/3844 (0.2%)
5	E	0.62	0/693	0.94	0/944
5	e	0.60	0/693	0.93	0/944
6	F	0.76	1/284 (0.4%)	0.95	0/387
6	f	0.60	0/284	0.92	0/387
7	H	0.63	0/544	0.94	1/739 (0.1%)
7	h	0.64	0/544	0.91	1/739 (0.1%)
8	I	0.71	0/327	0.96	0/439
8	i	0.61	0/327	0.89	0/439
9	J	0.67	0/278	0.89	0/376
9	j	0.56	0/278	0.93	0/376
10	K	0.65	0/303	1.03	2/416 (0.5%)
10	k	0.77	0/303	1.41	4/416 (1.0%)
11	L	0.72	0/319	0.94	0/433
11	l	0.62	0/319	0.89	2/433 (0.5%)
12	M	0.69	0/278	1.18	1/378 (0.3%)
12	m	0.66	0/278	1.10	4/378 (1.1%)
13	O	0.59	0/1926	0.92	1/2611 (0.0%)
13	o	0.54	0/1926	0.88	2/2611 (0.1%)
14	T	0.81	0/282	0.90	0/382
14	t	0.65	0/282	0.92	0/382
15	U	0.63	0/785	0.87	0/1064
15	u	0.61	0/785	0.88	0/1064
16	V	0.64	0/1096	0.97	0/1487
16	v	0.56	0/1096	0.92	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Y	0.61	0/216	0.96	1/289 (0.3%)
17	y	0.62	0/216	0.97	0/289
18	X	0.64	0/298	0.91	0/403
18	x	0.65	0/298	0.96	0/403
19	Z	0.61	0/490	1.00	0/669
19	z	0.68	1/490 (0.2%)	1.01	1/669 (0.1%)
All	All	0.64	3/43004 (0.0%)	0.96	73/58496 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	z	23	VAL	CA-CB	6.75	1.57	1.54
6	F	28	VAL	CA-CB	5.67	1.57	1.54
2	B	381	ILE	CA-CB	-5.42	1.48	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	k	11	LEU	CA-C-N	-8.17	109.63	119.84
10	k	11	LEU	C-N-CA	-8.17	109.63	119.84
4	d	170	ALA	CA-C-N	-8.03	111.73	119.76
4	d	170	ALA	C-N-CA	-8.03	111.73	119.76
4	D	170	ALA	CA-C-N	-7.58	112.18	119.76
4	D	170	ALA	C-N-CA	-7.58	112.18	119.76
3	c	336	GLY	N-CA-C	-7.23	105.26	114.37
1	a	83	VAL	CA-C-N	7.22	127.26	119.89
1	a	83	VAL	C-N-CA	7.22	127.26	119.89
7	H	52	THR	N-CA-C	-6.91	103.85	112.90
2	b	478	VAL	N-CA-C	6.88	118.70	112.17
2	b	328	GLY	CA-C-N	6.63	126.54	119.85
2	b	328	GLY	C-N-CA	6.63	126.54	119.85
4	D	308	ASP	CA-C-N	6.57	127.41	120.12
4	D	308	ASP	C-N-CA	6.57	127.41	120.12
3	c	100	GLY	CA-C-N	6.45	126.48	119.90
3	c	100	GLY	C-N-CA	6.45	126.48	119.90
4	d	308	ASP	CA-C-N	6.31	127.12	120.12
4	d	308	ASP	C-N-CA	6.31	127.12	120.12
3	C	38	GLY	N-CA-C	6.28	120.49	112.83
2	b	87	ASP	CA-C-N	6.27	126.81	120.04
2	b	87	ASP	C-N-CA	6.27	126.81	120.04
13	O	11	VAL	N-CA-C	6.11	117.17	108.93
4	d	94	GLY	CA-C-N	6.08	126.19	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	94	GLY	C-N-CA	6.08	126.19	119.87
19	z	53	VAL	N-CA-C	6.07	116.25	110.42
2	b	48	SER	CA-C-N	-5.83	117.15	122.28
2	b	48	SER	C-N-CA	-5.83	117.15	122.28
2	b	220	ARG	CA-C-N	5.83	123.92	119.66
2	b	220	ARG	C-N-CA	5.83	123.92	119.66
17	Y	31	ALA	N-CA-C	5.75	118.02	111.11
12	m	17	VAL	CA-C-N	-5.67	113.18	119.19
12	m	17	VAL	C-N-CA	-5.67	113.18	119.19
12	m	3	VAL	N-CA-C	5.59	116.14	110.05
4	D	37	LEU	N-CA-C	5.57	117.04	110.97
1	a	202	VAL	N-CA-C	5.55	115.75	110.42
4	D	94	GLY	CA-C-N	5.51	125.60	119.87
4	D	94	GLY	C-N-CA	5.51	125.60	119.87
2	B	194	ASN	CA-C-N	5.50	125.16	119.05
2	B	194	ASN	C-N-CA	5.50	125.16	119.05
12	m	3	VAL	CB-CA-C	-5.50	105.54	111.59
7	h	52	THR	N-CA-C	-5.46	105.74	112.90
2	B	48	SER	CA-C-N	-5.46	117.48	122.28
2	B	48	SER	C-N-CA	-5.46	117.48	122.28
4	D	80	THR	CA-C-N	-5.45	114.63	120.03
4	D	80	THR	C-N-CA	-5.45	114.63	120.03
16	v	105	ARG	N-CA-C	5.43	117.96	111.71
10	K	25	LEU	CA-C-N	-5.41	114.05	119.56
10	K	25	LEU	C-N-CA	-5.41	114.05	119.56
2	b	399	VAL	N-CA-C	5.37	115.85	108.12
2	b	196	GLY	N-CA-C	-5.37	106.21	113.24
2	B	49	ASP	CA-C-N	5.36	125.03	119.56
2	B	49	ASP	C-N-CA	5.36	125.03	119.56
10	k	18	PHE	N-CA-C	5.34	122.17	110.80
10	k	25	LEU	N-CA-C	5.32	121.56	109.81
2	B	221	PRO	O-C-N	5.25	123.73	121.31
3	C	221	GLU	N-CA-C	-5.25	105.09	112.12
3	C	60	ILE	N-CA-C	5.23	115.44	110.42
3	C	291	TRP	N-CA-C	5.23	117.06	111.36
1	a	204	GLY	N-CA-C	5.16	118.49	112.50
1	a	83	VAL	N-CA-C	5.14	113.05	108.63
1	a	142	TRP	N-CA-C	5.12	119.22	112.92
13	o	55	GLU	CA-C-N	5.12	125.36	119.83
13	o	55	GLU	C-N-CA	5.12	125.36	119.83
3	c	421	SER	CA-C-N	5.11	125.40	119.47
3	c	421	SER	C-N-CA	5.11	125.40	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	l	4	ASN	CA-C-N	5.10	125.55	120.04
11	l	4	ASN	C-N-CA	5.10	125.55	120.04
1	A	83	VAL	N-CA-C	5.05	112.97	108.63
12	M	7	GLY	N-CA-C	-5.02	106.66	113.24
1	a	77	ILE	N-CA-C	5.02	115.74	110.62
2	b	194	ASN	CA-C-N	5.01	124.61	119.05
2	b	194	ASN	C-N-CA	5.01	124.61	119.05

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	2637	0	2551	68	0
1	a	2637	0	2551	59	0
2	B	4024	0	3901	100	0
2	b	4024	0	3901	99	0
3	C	3506	0	3439	67	0
3	c	3506	0	3439	61	0
4	D	2726	0	2627	76	0
4	d	2726	0	2627	65	0
5	E	668	0	658	16	0
5	e	668	0	658	7	0
6	F	275	0	282	17	0
6	f	275	0	282	11	0
7	H	525	0	558	20	0
7	h	525	0	558	18	0
8	I	320	0	339	7	0
8	i	320	0	339	4	0
9	J	272	0	279	2	0
9	j	272	0	279	5	0
10	K	293	0	305	10	0
10	k	293	0	305	15	0
11	L	309	0	327	14	0
11	l	309	0	327	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	272	0	300	10	0
12	m	272	0	300	11	0
13	O	1883	0	1865	28	0
13	o	1883	0	1865	26	0
14	T	270	0	278	15	0
14	t	270	0	278	13	0
15	U	774	0	773	9	0
15	u	774	0	773	8	0
16	V	1072	0	1088	13	0
16	v	1072	0	1088	9	0
17	Y	215	0	246	2	0
17	y	215	0	246	6	0
18	X	292	0	328	8	0
18	x	292	0	328	9	0
19	Z	479	0	516	2	0
19	z	479	0	516	2	0
20	A	10	0	0	0	0
20	a	10	0	0	1	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	1	0
22	U	1	0	0	0	0
22	a	2	0	0	0	0
22	u	1	0	0	0	0
23	A	4	0	1	0	0
23	a	4	0	1	0	0
24	A	195	0	216	19	0
24	B	1105	0	1224	67	0
24	C	845	0	936	53	0
24	D	195	0	216	13	0
24	a	260	0	288	16	0
24	b	1105	0	1224	59	0
24	c	845	0	936	40	0
24	d	130	0	144	7	0
25	A	64	0	74	3	0
25	D	64	0	74	10	0
25	a	64	0	74	2	0
25	d	64	0	74	4	0
26	A	40	0	55	14	0
26	B	120	0	165	58	0
26	C	40	0	55	14	0
26	F	40	0	55	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	H	40	0	55	16	0
26	I	40	0	55	18	0
26	K	80	0	110	29	0
26	T	40	0	55	22	0
26	a	40	0	55	13	0
26	b	120	0	166	59	0
26	c	120	0	165	53	0
26	f	40	0	55	21	0
26	h	40	0	55	17	0
26	k	40	0	55	18	0
26	t	40	0	55	23	0
27	A	55	0	80	11	0
27	D	55	0	80	13	0
27	a	55	0	80	12	0
27	d	55	0	80	7	0
28	A	108	0	156	7	0
28	B	54	0	30	8	0
28	L	54	0	26	12	0
28	X	43	0	53	3	0
28	a	108	0	156	3	0
28	b	54	0	30	12	0
28	l	54	0	29	5	0
28	x	43	0	53	4	0
29	A	51	0	72	2	0
29	B	51	0	72	2	0
29	C	102	0	144	4	0
29	D	51	0	72	7	0
29	Z	37	0	44	0	0
29	a	51	0	72	1	0
29	b	51	0	72	4	0
29	c	102	0	144	2	0
29	j	51	0	72	6	0
29	z	37	0	44	1	0
30	A	49	0	74	10	0
30	D	98	0	148	8	0
30	E	42	0	57	0	0
30	L	49	0	74	6	0
30	a	49	0	74	10	0
30	d	98	0	148	4	0
30	e	42	0	57	2	0
30	l	49	0	74	6	0
31	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	F	1	0	0	0	0
31	O	1	0	0	0	0
31	b	1	0	0	0	0
31	f	1	0	0	0	0
31	o	1	0	0	0	0
32	C	186	0	246	5	0
32	E	62	0	82	1	0
32	H	62	0	82	6	0
32	c	186	0	246	8	0
32	d	62	0	82	4	0
32	h	62	0	82	6	0
33	E	43	0	30	6	0
33	V	43	0	30	7	0
33	e	43	0	30	2	0
33	v	43	0	30	4	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	50074	0	51320	1280	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 13.

All (1280) 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)
26:T:101:BCR:C22	26:T:101:BCR:C37	1.74	1.65
26:B:619:BCR:C19	26:B:619:BCR:C20	1.76	1.64
26:B:620:BCR:C37	26:B:620:BCR:C22	1.76	1.64
26:c:514:BCR:C20	26:c:514:BCR:C19	1.74	1.62
26:b:619:BCR:C22	26:b:619:BCR:C37	1.75	1.62
26:t:101:BCR:C20	26:t:101:BCR:C19	1.76	1.62
26:b:619:BCR:C19	26:b:619:BCR:C20	1.75	1.62
26:B:618:BCR:C18	26:B:618:BCR:C36	1.77	1.61
26:B:619:BCR:C18	26:B:619:BCR:C36	1.76	1.61
26:f:101:BCR:C37	26:f:101:BCR:C22	1.75	1.61
26:C:514:BCR:C20	26:C:514:BCR:C21	1.78	1.61
26:T:101:BCR:C20	26:T:101:BCR:C21	1.78	1.61
26:t:101:BCR:C18	26:t:101:BCR:C36	1.78	1.61
26:T:101:BCR:C20	26:T:101:BCR:C19	1.75	1.61
26:k:101:BCR:C37	26:k:101:BCR:C22	1.75	1.61
26:B:618:BCR:C20	26:B:618:BCR:C19	1.75	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:621:BCR:C18	26:b:621:BCR:C36	1.78	1.60
26:c:515:BCR:C20	26:c:515:BCR:C21	1.78	1.60
26:H:101:BCR:C18	26:H:101:BCR:C36	1.79	1.60
26:K:102:BCR:C20	26:K:102:BCR:C21	1.79	1.59
26:b:620:BCR:C36	26:b:620:BCR:C18	1.79	1.59
26:B:618:BCR:C37	26:B:618:BCR:C22	1.75	1.59
26:A:610:BCR:C18	26:A:610:BCR:C36	1.79	1.59
26:F:101:BCR:C20	26:F:101:BCR:C21	1.80	1.59
26:b:621:BCR:C37	26:b:621:BCR:C22	1.77	1.59
26:h:101:BCR:C18	26:h:101:BCR:C36	1.81	1.59
26:F:101:BCR:C18	26:F:101:BCR:C36	1.77	1.59
26:a:610:BCR:C18	26:a:610:BCR:C36	1.78	1.59
26:c:515:BCR:C20	26:c:515:BCR:C19	1.74	1.59
26:k:101:BCR:C21	26:k:101:BCR:C20	1.78	1.59
26:C:514:BCR:C18	26:C:514:BCR:C36	1.80	1.58
26:b:619:BCR:C20	26:b:619:BCR:C21	1.79	1.58
26:C:514:BCR:C37	26:C:514:BCR:C22	1.76	1.58
26:f:101:BCR:C18	26:f:101:BCR:C36	1.78	1.58
26:F:101:BCR:C20	26:F:101:BCR:C19	1.74	1.57
26:T:101:BCR:C18	26:T:101:BCR:C36	1.79	1.57
26:a:610:BCR:C21	26:a:610:BCR:C20	1.77	1.57
26:t:101:BCR:C37	26:t:101:BCR:C22	1.75	1.57
26:c:515:BCR:C18	26:c:515:BCR:C36	1.80	1.57
26:c:521:BCR:C19	26:c:521:BCR:C20	1.80	1.57
26:B:618:BCR:C20	26:B:618:BCR:C21	1.80	1.57
26:h:101:BCR:C20	26:h:101:BCR:C19	1.75	1.57
26:A:610:BCR:C21	26:A:610:BCR:C20	1.77	1.56
26:A:610:BCR:C37	26:A:610:BCR:C22	1.75	1.56
26:c:514:BCR:C20	26:c:514:BCR:C21	1.76	1.56
26:B:620:BCR:C18	26:B:620:BCR:C36	1.80	1.56
26:I:101:BCR:C21	26:I:101:BCR:C20	1.78	1.56
26:K:102:BCR:C22	26:K:102:BCR:C37	1.76	1.56
26:b:620:BCR:C20	26:b:620:BCR:C21	1.77	1.56
26:K:102:BCR:C18	26:K:102:BCR:C36	1.80	1.56
26:H:101:BCR:C20	26:H:101:BCR:C21	1.76	1.55
26:k:101:BCR:C18	26:k:101:BCR:C36	1.80	1.55
26:K:101:BCR:C37	26:K:101:BCR:C22	1.75	1.55
26:B:620:BCR:C20	26:B:620:BCR:C21	1.78	1.55
26:h:101:BCR:C20	26:h:101:BCR:C21	1.78	1.55
26:b:619:BCR:C18	26:b:619:BCR:C36	1.79	1.54
26:K:101:BCR:C21	26:K:101:BCR:C20	1.78	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:521:BCR:C22	26:c:521:BCR:C37	1.83	1.54
26:a:610:BCR:C37	26:a:610:BCR:C22	1.75	1.54
26:b:621:BCR:C20	26:b:621:BCR:C19	1.82	1.54
26:t:101:BCR:C20	26:t:101:BCR:C21	1.79	1.54
26:c:521:BCR:C18	26:c:521:BCR:C36	1.82	1.54
26:B:619:BCR:C20	26:B:619:BCR:C21	1.80	1.53
26:I:101:BCR:C18	26:I:101:BCR:C36	1.79	1.53
26:f:101:BCR:C21	26:f:101:BCR:C20	1.78	1.53
26:K:101:BCR:C18	26:K:101:BCR:C36	1.78	1.52
26:c:514:BCR:C18	26:c:514:BCR:C36	1.80	1.52
26:c:521:BCR:C20	26:c:521:BCR:C21	1.83	1.52
26:b:621:BCR:C20	26:b:621:BCR:C21	1.90	1.48
2:b:113:TRP:HB2	26:b:621:BCR:H21C	1.32	1.12
3:c:165:LEU:HD21	24:c:506:CLA:HAB	1.41	1.01
24:b:609:CLA:HMC2	26:b:620:BCR:HC8	1.44	1.00
26:B:618:BCR:C37	26:B:618:BCR:C21	2.42	0.97
26:T:101:BCR:C37	26:T:101:BCR:C21	2.43	0.96
26:b:621:BCR:C36	26:b:621:BCR:C19	2.44	0.96
28:b:601:SQD:H121	24:b:616:CLA:H43	1.44	0.95
26:B:618:BCR:H12C	26:B:619:BCR:H10C	1.48	0.94
2:B:106:LEU:HB3	26:B:620:BCR:H15C	1.49	0.94
26:k:101:BCR:C37	26:k:101:BCR:C21	2.45	0.93
26:c:521:BCR:C20	26:c:521:BCR:C22	2.45	0.93
26:B:619:BCR:C19	26:B:619:BCR:C36	2.47	0.93
26:c:514:BCR:C20	26:c:514:BCR:C22	2.45	0.93
26:K:102:BCR:C20	26:K:102:BCR:C22	2.46	0.92
26:b:619:BCR:C37	26:b:619:BCR:C21	2.43	0.92
3:C:124:VAL:HG11	26:C:514:BCR:H17C	1.48	0.92
26:b:619:BCR:C19	26:b:619:BCR:H20C	2.01	0.90
26:A:610:BCR:C21	26:A:610:BCR:C37	2.48	0.90
26:h:101:BCR:C19	26:h:101:BCR:H20C	2.02	0.89
24:B:615:CLA:H43	28:B:622:SQD:H121	1.54	0.89
26:K:101:BCR:C37	26:K:101:BCR:C21	2.45	0.89
26:K:102:BCR:C21	26:K:102:BCR:C37	2.49	0.89
26:c:514:BCR:C19	26:c:514:BCR:H20C	2.01	0.88
26:B:620:BCR:C37	26:B:620:BCR:C21	2.46	0.88
26:C:514:BCR:C20	26:C:514:BCR:C22	2.47	0.88
26:T:101:BCR:C19	26:T:101:BCR:H20C	2.01	0.87
26:b:620:BCR:C20	26:b:620:BCR:C22	2.46	0.87
26:c:515:BCR:C19	26:c:515:BCR:H20C	2.02	0.87
26:b:619:BCR:C21	26:b:619:BCR:H20C	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:101:BCR:C22	26:T:101:BCR:C20	2.50	0.87
26:c:514:BCR:C21	26:c:514:BCR:H20C	2.03	0.86
26:A:610:BCR:C21	26:A:610:BCR:H20C	2.05	0.86
26:B:618:BCR:C19	26:B:618:BCR:H20C	2.03	0.86
26:b:621:BCR:C37	26:b:621:BCR:C21	2.50	0.86
26:B:619:BCR:C20	26:B:619:BCR:C18	2.51	0.86
26:T:101:BCR:C21	26:T:101:BCR:H20C	2.04	0.86
26:a:610:BCR:C21	26:a:610:BCR:H20C	2.03	0.86
26:B:620:BCR:C22	26:B:620:BCR:C20	2.51	0.85
26:t:101:BCR:C21	26:t:101:BCR:H20C	2.06	0.85
26:h:101:BCR:C21	26:h:101:BCR:H20C	2.05	0.85
26:F:101:BCR:C19	26:F:101:BCR:H20C	2.03	0.85
26:a:610:BCR:C20	26:a:610:BCR:C22	2.48	0.85
26:h:101:BCR:C20	26:h:101:BCR:C22	2.48	0.84
18:x:24:THR:HA	28:x:101:SQD:H331	1.59	0.84
26:I:101:BCR:C21	26:I:101:BCR:H20C	2.04	0.84
26:b:621:BCR:C22	26:b:621:BCR:C20	2.55	0.84
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.39	0.84
26:t:101:BCR:C37	26:t:101:BCR:C21	2.49	0.84
26:b:619:BCR:C22	26:b:619:BCR:C20	2.50	0.83
26:k:101:BCR:C21	26:k:101:BCR:H20C	2.08	0.83
26:C:514:BCR:C21	26:C:514:BCR:C37	2.48	0.83
26:a:610:BCR:C21	26:a:610:BCR:C37	2.49	0.83
26:f:101:BCR:C37	26:f:101:BCR:C21	2.50	0.83
26:K:101:BCR:C36	26:K:101:BCR:C19	2.55	0.83
26:B:618:BCR:C20	26:B:618:BCR:C22	2.50	0.83
26:K:102:BCR:C21	26:K:102:BCR:H20C	2.06	0.83
26:c:515:BCR:C21	26:c:515:BCR:H20C	2.05	0.82
26:h:101:BCR:C18	26:h:101:BCR:C20	2.54	0.82
26:F:101:BCR:C36	26:F:101:BCR:C17	2.58	0.82
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.60	0.82
2:b:127:ARG:HH11	2:b:127:ARG:HG3	1.44	0.82
2:b:432:PHE:O	13:o:178:LYS:NZ	2.12	0.82
26:t:101:BCR:C19	26:t:101:BCR:H20C	2.03	0.82
26:B:620:BCR:C21	26:B:620:BCR:H20C	2.09	0.82
26:k:101:BCR:C22	26:k:101:BCR:C20	2.53	0.82
26:I:101:BCR:C20	26:I:101:BCR:C22	2.49	0.81
26:b:620:BCR:C21	26:b:620:BCR:H20C	2.05	0.81
26:B:619:BCR:C21	26:B:619:BCR:H20C	2.09	0.81
24:a:609:CLA:HAC1	26:a:610:BCR:H15C	1.63	0.81
26:c:514:BCR:C20	26:c:514:BCR:C18	2.51	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:514:BCR:C36	26:C:514:BCR:C19	2.57	0.81
26:f:101:BCR:C21	26:f:101:BCR:H20C	2.08	0.81
30:A:615:LHG:H382	30:A:615:LHG:H112	1.63	0.80
7:H:38:PHE:HB2	26:H:101:BCR:H10C	1.62	0.80
26:B:619:BCR:C19	26:B:619:BCR:H20C	2.05	0.80
3:c:124:VAL:HG11	26:c:514:BCR:H17C	1.64	0.80
26:b:621:BCR:C19	26:b:621:BCR:H20C	2.10	0.79
26:c:521:BCR:C19	26:c:521:BCR:H20C	2.08	0.79
4:d:24:ARG:HD3	18:x:37:VAL:HG22	1.63	0.79
26:c:521:BCR:C19	26:c:521:BCR:C36	2.58	0.79
26:B:618:BCR:C21	26:B:618:BCR:H20C	2.07	0.78
30:a:616:LHG:H151	30:a:616:LHG:H352	1.64	0.78
26:c:521:BCR:C21	26:c:521:BCR:H20C	2.11	0.78
24:c:501:CLA:H193	24:c:507:CLA:HBB1	1.64	0.78
26:C:514:BCR:C21	26:C:514:BCR:H20C	2.06	0.78
26:K:101:BCR:C21	26:K:101:BCR:H20C	2.08	0.77
26:A:610:BCR:C36	26:A:610:BCR:C19	2.57	0.77
26:F:101:BCR:C21	26:F:101:BCR:H20C	2.08	0.76
26:T:101:BCR:C19	26:T:101:BCR:C36	2.59	0.76
26:c:515:BCR:C19	26:c:515:BCR:C36	2.56	0.76
26:H:101:BCR:C20	26:H:101:BCR:C22	2.53	0.75
11:L:14:ARG:HD3	28:L:102:SQD:H241	1.68	0.75
3:C:339:LYS:NZ	15:U:99:ASN:O	2.18	0.75
26:A:610:BCR:C20	26:A:610:BCR:C22	2.54	0.75
26:b:620:BCR:C36	26:b:620:BCR:C19	2.58	0.75
4:D:193:LEU:O	11:L:34:TYR:OH	2.02	0.75
26:K:101:BCR:H16C	17:Y:33:PRO:HD3	1.68	0.75
24:b:603:CLA:H152	26:h:101:BCR:H17C	1.68	0.75
24:B:602:CLA:HHC	24:B:602:CLA:HBB1	1.68	0.74
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.68	0.74
5:e:56:TYR:O	16:v:1:ALA:N	2.16	0.74
24:c:510:CLA:HBC3	24:c:510:CLA:H192	1.70	0.74
32:d:405:DGD:HA91	26:f:101:BCR:H322	1.70	0.74
2:B:479:PHE:O	4:D:139:ARG:NH2	2.21	0.74
26:H:101:BCR:C21	26:H:101:BCR:H20C	2.10	0.73
4:D:87:HIS:ND1	32:H:102:DGD:O2D	2.15	0.73
26:a:610:BCR:C36	26:a:610:BCR:C19	2.59	0.73
26:c:515:BCR:C20	26:c:515:BCR:C22	2.53	0.73
26:t:101:BCR:C19	26:t:101:BCR:C36	2.59	0.73
28:L:102:SQD:O49	28:b:601:SQD:C46	2.29	0.73
24:a:607:CLA:H152	27:a:611:PL9:H262	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:33:TRP:N	26:b:620:BCR:H15C	2.04	0.73
26:c:515:BCR:C20	26:c:515:BCR:C18	2.58	0.73
26:I:101:BCR:C20	26:I:101:BCR:C37	2.67	0.72
1:A:214:MET:HG2	27:A:611:PL9:H102	1.71	0.72
3:C:213[B]:LEU:HD21	26:I:101:BCR:H20C	1.71	0.72
26:T:101:BCR:C20	26:T:101:BCR:C18	2.57	0.72
26:B:618:BCR:H402	28:B:622:SQD:H82	1.71	0.72
1:A:50:ILE:HG22	26:A:610:BCR:H271	1.72	0.72
26:k:101:BCR:C36	26:k:101:BCR:C19	2.57	0.71
26:t:101:BCR:C20	26:t:101:BCR:C22	2.54	0.71
3:C:124:VAL:HG11	26:C:514:BCR:C17	2.18	0.71
1:a:106:LEU:HD21	26:a:610:BCR:H383	1.71	0.71
28:b:601:SQD:H62	11:l:7:ARG:HH21	1.53	0.71
10:k:34:ALA:HB1	26:k:101:BCR:C20	2.21	0.71
26:f:101:BCR:C36	26:f:101:BCR:C17	2.66	0.70
24:C:501:CLA:C1D	24:C:503:CLA:H2	2.21	0.70
4:D:279:LEU:HD22	25:D:401:PHO:HBC3	1.73	0.70
27:D:405:PL9:H411	11:L:29:LEU:HD23	1.74	0.70
10:K:17:ILE:H	10:K:17:ILE:HD13	1.56	0.70
26:B:620:BCR:C36	26:B:620:BCR:C19	2.63	0.69
3:c:213[B]:LEU:HD11	26:c:515:BCR:C22	2.22	0.69
26:F:101:BCR:C20	26:F:101:BCR:C22	2.57	0.69
7:h:38:PHE:HB2	26:h:101:BCR:H10C	1.73	0.69
28:A:614:SQD:H272	26:b:621:BCR:H19C	1.74	0.69
26:b:621:BCR:C21	26:b:621:BCR:H20C	2.16	0.68
26:B:619:BCR:H381	26:t:101:BCR:H341	1.75	0.68
1:a:214:MET:HG2	27:a:611:PL9:H102	1.74	0.68
26:c:521:BCR:C20	26:c:521:BCR:C18	2.63	0.68
28:A:614:SQD:C27	26:b:621:BCR:H19C	2.24	0.68
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.74	0.68
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.73	0.68
26:K:101:BCR:C22	26:K:101:BCR:C20	2.55	0.68
26:I:101:BCR:C36	26:I:101:BCR:C19	2.59	0.67
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.76	0.67
24:b:616:CLA:H18	29:b:622:LMG:H421	1.77	0.67
24:C:501:CLA:H192	24:C:506:CLA:C1B	2.24	0.67
26:H:101:BCR:C36	26:H:101:BCR:C19	2.61	0.67
26:c:514:BCR:C19	26:c:514:BCR:C36	2.62	0.67
5:E:23:HIS:NE2	33:E:103:HEM:ND	2.44	0.66
24:C:501:CLA:C2D	24:C:503:CLA:H2	2.25	0.66
24:C:513:CLA:HBB1	24:C:513:CLA:HMB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:x:31:ILE:HG23	28:x:101:SQD:H462	1.78	0.66
24:b:616:CLA:HMB1	24:b:616:CLA:HBB1	1.78	0.66
1:A:310:LYS:NZ	5:E:58:GLN:O	2.29	0.66
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.31	0.66
26:c:521:BCR:H391	10:k:36:ALA:HB2	1.78	0.66
28:L:102:SQD:O49	28:b:601:SQD:H461	1.94	0.65
30:a:616:LHG:H223	32:c:518:DGD:HBH2	1.79	0.65
26:b:619:BCR:C37	26:b:619:BCR:C20	2.74	0.65
26:F:101:BCR:H20C	26:F:101:BCR:C37	2.27	0.65
26:B:618:BCR:C36	26:B:618:BCR:C17	2.70	0.65
16:V:3:LEU:HD23	16:V:23:GLU:HG3	1.78	0.65
4:D:192:THR:HG23	24:D:403:CLA:HBC2	1.78	0.65
11:l:21:LEU:HD13	28:l:101:SQD:H312	1.78	0.65
26:B:618:BCR:C18	26:B:618:BCR:C20	2.59	0.65
24:b:612:CLA:OBD	24:b:612:CLA:H152	1.97	0.65
28:A:612:SQD:O7	3:C:28:GLN:NE2	2.24	0.65
2:b:113:TRP:CB	26:b:621:BCR:H21C	2.18	0.65
24:B:616:CLA:H51	26:B:620:BCR:H11C	1.77	0.64
2:B:450:TRP:CD1	24:B:608:CLA:HBA1	2.32	0.64
26:b:621:BCR:C18	26:b:621:BCR:C20	2.65	0.64
4:d:186:GLN:HB2	24:d:402:CLA:HBC1	1.80	0.64
26:K:102:BCR:C36	26:K:102:BCR:C19	2.62	0.64
4:d:315:TYR:CZ	4:d:319:LEU:HD11	2.33	0.64
2:B:383:PHE:O	13:O:166:SER:HA	1.97	0.64
26:h:101:BCR:C36	26:h:101:BCR:C17	2.71	0.64
3:C:213[B]:LEU:HD11	26:I:101:BCR:C22	2.27	0.64
24:a:607:CLA:H122	27:a:611:PL9:H23	1.79	0.64
3:C:406:SER:HA	3:C:420:VAL:HG23	1.79	0.64
4:d:87:HIS:ND1	32:h:102:DGD:O2D	2.27	0.64
26:F:101:BCR:C20	26:F:101:BCR:C18	2.61	0.63
2:B:464:PHE:HD2	24:B:612:CLA:HAC2	1.63	0.63
26:B:619:BCR:H17C	26:t:101:BCR:C17	2.28	0.63
3:C:71:GLU:HB3	3:C:86:LEU:HD22	1.79	0.63
4:D:141:TYR:OH	30:D:406:LHG:O4	2.16	0.63
26:h:101:BCR:C36	26:h:101:BCR:C19	2.64	0.63
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.78	0.63
26:f:101:BCR:C36	26:f:101:BCR:C19	2.63	0.63
28:L:102:SQD:H45	14:T:23:PHE:CD1	2.33	0.63
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.79	0.63
2:B:29:LEU:HD21	26:B:618:BCR:H19C	1.80	0.63
26:B:618:BCR:C36	26:B:618:BCR:C19	2.60	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:507:CLA:OBD	24:C:509:CLA:H122	1.99	0.62
1:a:308:ASP:HB2	5:e:52:PRO:O	1.98	0.62
24:A:609:CLA:HAC2	26:A:610:BCR:H362	1.82	0.62
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.81	0.62
14:T:1[B]:MET:HB3	14:T:4:ILE:HD12	1.81	0.62
26:c:521:BCR:H15C	26:k:101:BCR:H342	1.81	0.62
24:C:501:CLA:H193	24:C:507:CLA:HBB1	1.80	0.62
3:c:83:GLU:OE2	3:c:398:HIS:NE2	2.32	0.62
13:o:57:LYS:O	13:o:58:ASN:HB2	1.99	0.62
26:b:619:BCR:C36	26:b:619:BCR:C17	2.70	0.62
26:c:521:BCR:C37	26:c:521:BCR:C21	2.60	0.62
13:o:58:ASN:HA	13:o:60:ARG:NH2	2.15	0.62
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.82	0.62
26:c:515:BCR:H20C	26:c:515:BCR:C37	2.28	0.62
26:f:101:BCR:C22	26:f:101:BCR:C20	2.58	0.62
28:l:101:SQD:H342	14:t:12:CYS:HB3	1.81	0.62
24:C:506:CLA:HMB3	24:C:506:CLA:HBB1	1.80	0.62
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.81	0.62
30:l:102:LHG:H271	12:m:22:LEU:HD11	1.82	0.62
26:b:619:BCR:C37	26:b:619:BCR:H20C	2.30	0.61
3:C:443:TRP:CE2	24:C:508:CLA:HMD2	2.35	0.61
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.82	0.61
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.82	0.61
28:B:622:SQD:H442	28:l:101:SQD:O7	2.00	0.61
4:d:214:HIS:ND1	27:d:404:PL9:O2	2.28	0.61
26:C:514:BCR:H15C	29:C:519:LMG:H401	1.83	0.61
30:d:406:LHG:HC91	30:l:102:LHG:HC81	1.82	0.61
28:A:614:SQD:H132	26:T:101:BCR:HC41	1.82	0.61
30:A:615:LHG:H371	24:C:508:CLA:H92	1.82	0.61
24:B:614:CLA:H193	26:B:619:BCR:C5	2.31	0.61
26:B:618:BCR:H15C	26:B:619:BCR:H352	1.83	0.61
10:K:36:ALA:HB2	26:K:102:BCR:H391	1.83	0.61
1:a:132:GLU:O	1:a:136:ARG:HG2	2.00	0.61
24:C:501:CLA:C1C	24:C:503:CLA:H71	2.30	0.61
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.83	0.61
1:a:172:MET:HE1	24:a:615:CLA:CHC	2.31	0.61
13:o:58:ASN:HA	13:o:60:ARG:HH21	1.66	0.60
33:E:103:HEM:HBB2	33:E:103:HEM:HMB2	1.81	0.60
8:i:1[C]:MET:HE3	8:i:4:LEU:HB2	1.83	0.60
2:B:32:GLY:HA3	26:B:619:BCR:H19C	1.82	0.60
33:V:201:HEM:HMB1	33:V:201:HEM:HBB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:619:BCR:H333	12:m:13:LEU:HD12	1.83	0.60
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.02	0.60
6:F:20:TRP:CE2	6:F:24:HIS:CE1	2.90	0.60
1:A:42:LEU:HD13	26:A:610:BCR:H353	1.83	0.60
11:L:22:LEU:HD23	30:L:101:LHG:H162	1.84	0.60
24:b:614:CLA:H91	24:b:615:CLA:HBB1	1.84	0.59
33:v:201:HEM:HMC1	33:v:201:HEM:HBC2	1.84	0.59
24:B:612:CLA:H162	26:B:619:BCR:H342	1.84	0.59
26:B:619:BCR:C20	26:B:619:BCR:C22	2.60	0.59
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.85	0.59
3:C:324:LEU:HB3	15:U:32:ILE:HD13	1.84	0.59
24:D:404:CLA:H2	18:X:14:LEU:HA	1.83	0.59
26:c:514:BCR:C36	26:c:514:BCR:C17	2.74	0.59
1:A:84:PRO:HA	1:A:112:TYR:CG	2.37	0.59
24:A:607:CLA:H152	27:A:611:PL9:H262	1.83	0.59
14:T:8:PHE:CE1	24:b:616:CLA:H171	2.37	0.59
2:b:18:ARG:NH2	28:b:601:SQD:O9	2.36	0.59
26:T:101:BCR:C17	26:b:620:BCR:H17C	2.33	0.59
1:A:126:TYR:CZ	25:A:608:PHO:HBA1	2.38	0.59
24:C:511:CLA:HBB1	24:C:511:CLA:HMB3	1.84	0.59
29:D:408:LMG:H411	6:F:30:THR:HG21	1.85	0.59
1:A:269:ARG:NH1	4:D:222:LEU:HD13	2.18	0.59
1:A:308:ASP:HB2	5:E:52:PRO:O	2.02	0.59
2:B:30:VAL:HG22	24:B:614:CLA:C3C	2.33	0.58
3:C:165:LEU:HD21	24:C:506:CLA:HAB	1.85	0.58
24:b:616:CLA:H101	26:b:619:BCR:H362	1.84	0.58
3:c:213[B]:LEU:HD11	26:c:515:BCR:C21	2.32	0.58
33:e:102:HEM:HMB1	33:e:102:HEM:HBB2	1.84	0.58
3:c:210:PHE:HD2	3:c:213[B]:LEU:HD22	1.68	0.58
3:c:124:VAL:HG11	26:c:514:BCR:C17	2.33	0.58
4:d:123:ILE:HD11	32:h:102:DGD:HAH2	1.86	0.58
26:T:101:BCR:C37	26:T:101:BCR:H20C	2.32	0.58
1:a:323:ARG:HB3	4:d:329:MET:HA	1.84	0.58
15:U:27:LEU:HD21	15:U:82:PHE:CG	2.39	0.58
30:a:616:LHG:H132	30:a:616:LHG:H372	1.86	0.58
26:T:101:BCR:C37	26:T:101:BCR:C20	2.81	0.58
26:f:101:BCR:C37	26:f:101:BCR:C23	2.75	0.58
13:o:142:PHE:HB2	13:o:199:LEU:HB2	1.86	0.58
3:C:206:PRO:HG3	3:C:239:TRP:HZ2	1.69	0.58
26:K:102:BCR:C36	26:K:102:BCR:C16	2.82	0.58
24:a:615:CLA:H41	27:d:404:PL9:H202	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:t:101:BCR:C20	26:t:101:BCR:C18	2.65	0.58
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.86	0.57
24:C:501:CLA:C3D	24:C:503:CLA:H2	2.34	0.57
26:b:619:BCR:C19	26:b:619:BCR:C36	2.63	0.57
2:B:339:ALA:HB2	13:o:58:ASN:HB3	1.85	0.57
3:C:418:ASN:HB2	32:C:517:DGD:O4E	2.03	0.57
24:c:506:CLA:H162	26:c:515:BCR:H15C	1.84	0.57
26:F:101:BCR:C36	26:F:101:BCR:C19	2.65	0.57
30:a:616:LHG:H112	30:a:616:LHG:H382	1.85	0.57
5:E:56:TYR:O	16:V:1:ALA:N	2.23	0.57
24:b:606:CLA:H12	24:b:607:CLA:ND	2.19	0.57
1:a:215:HIS:HA	27:a:611:PL9:O1	2.05	0.57
26:B:620:BCR:C36	26:B:620:BCR:C17	2.72	0.57
6:F:34:LEU:HD21	26:F:101:BCR:H373	1.87	0.57
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.40	0.57
1:A:153:SER:HB2	24:A:606:CLA:H43	1.86	0.57
2:B:126:PRO:HB3	7:H:12[B]:ARG:NH1	2.19	0.57
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.87	0.57
8:I:20:VAL:HG13	26:I:101:BCR:HC41	1.86	0.57
13:O:57:LYS:O	13:O:58:ASN:HB2	2.03	0.57
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.86	0.57
3:C:334:PRO:HA	13:O:153:THR:OG1	2.05	0.57
4:d:257:PHE:O	30:d:407:LHG:H351	2.04	0.57
3:C:400:PRO:C	3:C:401:LEU:HD12	2.30	0.57
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.70	0.57
26:t:101:BCR:C37	26:t:101:BCR:H20C	2.35	0.57
16:v:41:HIS:CD2	33:v:201:HEM:NB	2.73	0.57
2:B:28:ALA:HB1	28:B:622:SQD:H221	1.87	0.57
32:E:101:DGD:O1B	32:E:101:DGD:O2D	2.21	0.57
4:d:67:TYR:O	29:j:101:LMG:O5	2.20	0.56
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.86	0.56
26:B:619:BCR:C36	26:B:619:BCR:C17	2.75	0.56
8:I:1[C]:MET:HE3	8:I:4:LEU:HB2	1.86	0.56
26:H:101:BCR:C36	26:H:101:BCR:C17	2.72	0.56
26:a:610:BCR:C36	26:a:610:BCR:C17	2.73	0.56
3:c:178:LYS:HB2	24:c:502:CLA:H141	1.88	0.56
24:B:605:CLA:H12	24:B:606:CLA:ND	2.21	0.56
10:K:35:LEU:HB2	26:K:101:BCR:H15C	1.85	0.56
1:a:129:ARG:NH2	4:d:255:GLN:O	2.39	0.56
2:b:475:PHE:CD2	4:d:140:PRO:HG3	2.41	0.56
3:c:429:SER:HA	32:c:517:DGD:HBE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:501:CLA:C2D	24:c:503:CLA:H2	2.36	0.56
1:A:332:HIS:HA	22:A:603:CL:CL	2.43	0.56
27:a:611:PL9:H221	25:d:401:PHO:HMA2	1.87	0.56
2:b:127:ARG:HG3	2:b:127:ARG:NH1	2.18	0.56
2:b:383:PHE:O	13:o:166:SER:HA	2.05	0.56
26:I:101:BCR:C36	26:I:101:BCR:C17	2.74	0.56
10:K:34:ALA:HB1	26:K:101:BCR:C20	2.35	0.56
28:L:102:SQD:H181	26:T:101:BCR:H351	1.88	0.56
2:b:479:PHE:O	4:d:139:ARG:NH2	2.33	0.56
24:b:613:CLA:HBB1	24:b:613:CLA:HMB1	1.88	0.56
24:c:508:CLA:HBC3	24:c:510:CLA:H71	1.88	0.56
1:A:74:GLY:O	4:D:301:GLN:NE2	2.39	0.55
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.21	0.55
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.36	0.55
3:c:406:SER:HA	3:c:420:VAL:HG23	1.87	0.55
7:h:65:LEU:HD12	7:h:66:GLY:H	1.72	0.55
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.89	0.55
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.40	0.55
3:C:216:SER:HB3	3:C:221:GLU:HG3	1.89	0.55
16:V:122:GLU:HG3	16:V:126:LEU:HD12	1.88	0.55
24:C:506:CLA:H162	26:I:101:BCR:H15C	1.89	0.55
7:H:35:MET:CG	26:H:101:BCR:HC42	2.37	0.55
10:K:25:LEU:HD21	26:K:101:BCR:HC41	1.89	0.55
1:A:195:HIS:CE1	1:A:197:PHE:HB2	2.41	0.55
24:A:607:CLA:H122	27:A:611:PL9:H23	1.88	0.55
14:T:8:PHE:HD1	26:T:101:BCR:H373	1.72	0.55
16:V:40:CYS:SG	33:V:201:HEM:CAC	2.95	0.55
4:d:149:PRO:HA	24:d:402:CLA:H41	1.88	0.55
11:l:14:ARG:HD3	28:l:101:SQD:H241	1.89	0.55
24:c:501:CLA:C1D	24:c:503:CLA:H2	2.36	0.55
26:K:102:BCR:C36	26:K:102:BCR:C17	2.73	0.55
28:L:102:SQD:H311	28:b:601:SQD:H292	1.84	0.55
16:V:41:HIS:CD2	33:V:201:HEM:NB	2.75	0.55
2:b:25:MET:HG2	26:b:619:BCR:C21	2.37	0.55
9:j:9:PRO:HD2	9:j:12:ILE:HD12	1.89	0.54
26:t:101:BCR:C36	26:t:101:BCR:C17	2.75	0.54
7:h:36:GLY:O	7:h:40:VAL:HG23	2.08	0.54
1:A:308:ASP:HB3	1:A:314:ILE:HD11	1.88	0.54
2:B:457:VAL:HG11	29:B:621:LMG:H211	1.89	0.54
15:U:76:ARG:HA	15:U:79:LEU:HG	1.89	0.54
4:D:269:PHE:CD2	30:D:406:LHG:HC11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.23	0.54
24:b:606:CLA:H2	24:b:607:CLA:C4C	2.37	0.54
26:k:101:BCR:H17C	17:y:33:PRO:HD3	1.88	0.54
15:u:27:LEU:HD21	15:u:82:PHE:CG	2.43	0.54
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.88	0.54
14:t:22:PHE:CE2	26:t:101:BCR:H333	2.43	0.54
30:A:615:LHG:H352	30:A:615:LHG:H151	1.90	0.54
2:b:460:LEU:O	2:b:463:PHE:HB3	2.08	0.54
4:d:193:LEU:O	11:l:34:TYR:OH	2.19	0.54
1:A:225:ARG:HA	2:B:480:SER:O	2.08	0.54
24:A:609:CLA:HMA2	29:A:613:LMG:H132	1.90	0.54
7:H:35:MET:HG2	26:H:101:BCR:HC42	1.90	0.54
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.88	0.54
1:A:276:ALA:HB1	30:A:615:LHG:H262	1.90	0.53
2:B:432:PHE:O	13:O:178:LYS:NZ	2.35	0.53
24:B:604:CLA:O1A	24:B:604:CLA:H3A	2.08	0.53
26:K:101:BCR:HC8	19:Z:20:VAL:HG21	1.90	0.53
24:c:509:CLA:HMB1	24:c:509:CLA:HBB1	1.90	0.53
1:A:105:TRP:HZ3	26:A:610:BCR:H24C	1.72	0.53
26:A:610:BCR:C36	26:A:610:BCR:C17	2.74	0.53
2:B:190:PHE:HB3	7:H:45:ILE:HG22	1.90	0.53
26:c:521:BCR:H24C	26:c:521:BCR:H371	1.91	0.53
26:f:101:BCR:H372	29:j:101:LMG:H292	1.90	0.53
1:A:132:GLU:O	1:A:136:ARG:HG2	2.07	0.53
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.88	0.53
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.89	0.53
1:a:210:LEU:HG	25:d:401:PHO:NC	2.22	0.53
26:I:101:BCR:H20C	26:I:101:BCR:C37	2.37	0.53
1:a:153:SER:HB3	24:a:606:CLA:HED1	1.90	0.53
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	1.88	0.53
5:E:8:ARG:O	6:F:19:ARG:NH2	2.34	0.53
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.89	0.53
1:A:24:THR:O	4:D:255:GLN:NE2	2.41	0.53
24:C:510:CLA:HBC3	24:C:510:CLA:H192	1.90	0.53
24:b:609:CLA:H102	29:b:622:LMG:H221	1.91	0.53
24:c:501:CLA:C1C	24:c:503:CLA:H71	2.39	0.53
2:B:274:GLN:HB3	2:B:280:PHE:CE2	2.43	0.53
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.91	0.53
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.91	0.53
4:D:303:ILE:HG21	12:M:2:GLU:HG3	1.89	0.53
20:a:601:OEX:O2	3:c:357:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:601:SQD:H82	26:b:619:BCR:H402	1.91	0.53
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.44	0.53
4:D:48:TRP:CD1	25:D:401:PHO:H162	2.43	0.53
5:E:51:ARG:N	5:E:54[B]:SER:OG	2.42	0.53
26:b:619:BCR:C20	26:b:619:BCR:C18	2.64	0.53
1:A:206:PHE:CZ	24:D:403:CLA:HAA1	2.44	0.52
6:F:37:ILE:HA	6:F:40:MET:SD	2.48	0.52
14:t:8:PHE:HD1	26:t:101:BCR:H373	1.74	0.52
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.13	0.52
1:a:201:GLY:HA3	1:a:286:ALA:HB2	1.91	0.52
3:c:223:TRP:CG	3:c:224:ILE:H	2.27	0.52
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.44	0.52
24:C:506:CLA:C2C	24:C:507:CLA:H122	2.39	0.52
2:b:101:ILE:HG23	26:b:620:BCR:C21	2.40	0.52
18:x:35:ASP:OD1	28:x:101:SQD:H1	2.09	0.52
24:c:506:CLA:CBB	24:c:507:CLA:HMA3	2.39	0.52
26:c:515:BCR:C20	26:c:515:BCR:C17	2.88	0.52
24:B:615:CLA:C12	26:B:618:BCR:H17C	2.40	0.52
28:L:102:SQD:H92	28:b:601:SQD:H251	1.91	0.52
30:a:616:LHG:H382	30:a:616:LHG:C11	2.40	0.52
2:b:137:LYS:NZ	7:h:17:GLU:OE2	2.31	0.52
3:c:327:ASN:HB3	13:o:99:ASP:OD2	2.09	0.52
11:L:21:LEU:HD22	28:L:102:SQD:H361	1.91	0.52
1:a:206:PHE:CZ	24:d:402:CLA:HAA1	2.43	0.52
1:A:176:ILE:O	1:A:179:THR:HB	2.09	0.52
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.92	0.52
24:B:617:CLA:H3A	26:B:620:BCR:H17C	1.91	0.52
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.45	0.52
14:t:8:PHE:CD1	26:t:101:BCR:H373	2.45	0.52
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.92	0.52
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.75	0.52
29:D:408:LMG:H172	26:F:101:BCR:H383	1.90	0.52
3:C:213[B]:LEU:HD11	26:I:101:BCR:C21	2.40	0.52
14:T:1[B]:MET:HE1	14:T:3:THR:HB	1.91	0.52
26:f:101:BCR:C37	26:f:101:BCR:C24	2.88	0.52
26:A:610:BCR:H392	26:A:610:BCR:H23C	1.92	0.52
3:c:233:VAL:O	3:c:237:HIS:ND1	2.38	0.52
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.92	0.52
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.45	0.51
24:C:506:CLA:HMC1	24:C:507:CLA:H102	1.92	0.51
4:D:49:LEU:HD22	26:F:101:BCR:H362	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:614:SQD:H132	26:t:101:BCR:HC41	1.92	0.51
24:b:612:CLA:H162	24:b:617:CLA:CAD	2.40	0.51
2:B:42:LEU:HD11	2:B:93:PHE:HB3	1.93	0.51
4:D:72:ASN:HA	29:D:408:LMG:HC1	1.92	0.51
29:D:408:LMG:H231	26:F:101:BCR:H381	1.91	0.51
10:k:21:LEU:O	10:k:25:LEU:HG	2.10	0.51
30:A:615:LHG:H223	32:C:517:DGD:HBH2	1.92	0.51
2:B:393:GLU:HB3	15:U:18:GLY:CA	2.40	0.51
28:B:622:SQD:C1	28:B:622:SQD:H462	2.41	0.51
30:a:616:LHG:H371	24:c:508:CLA:H92	1.91	0.51
2:b:24:LEU:HD21	24:b:618:CLA:CAB	2.40	0.51
2:b:384:ARG:HD3	15:u:102:LEU:HG	1.92	0.51
24:B:602:CLA:HAC1	26:H:101:BCR:H23C	1.93	0.51
32:d:405:DGD:HA72	26:f:101:BCR:C2	2.41	0.51
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.45	0.51
1:a:191:ASN:HB2	3:c:411:ALA:HB1	1.92	0.51
28:b:601:SQD:H121	24:b:616:CLA:C4	2.29	0.51
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.46	0.51
3:C:170:ILE:HD13	24:C:512:CLA:H111	1.92	0.51
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.45	0.51
7:H:38:PHE:CB	26:H:101:BCR:H10C	2.37	0.51
2:b:63:LEU:HA	2:b:66:MET:HE3	1.93	0.51
4:d:192:THR:HG23	24:d:402:CLA:HBC2	1.93	0.51
10:k:21:LEU:HD21	26:k:101:BCR:HC31	1.93	0.51
3:C:213[B]:LEU:HD21	26:I:101:BCR:C20	2.40	0.51
3:C:223:TRP:CG	3:C:224:ILE:H	2.28	0.51
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.92	0.51
24:a:607:CLA:HMB1	24:a:607:CLA:HBB1	1.93	0.51
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.46	0.51
2:B:200:ALA:HB3	24:B:603:CLA:HMB1	1.93	0.51
26:K:101:BCR:HC21	19:Z:13:VAL:HG13	1.93	0.51
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.93	0.51
24:c:501:CLA:C3D	24:c:503:CLA:H2	2.40	0.51
24:B:604:CLA:C1C	24:B:606:CLA:H71	2.40	0.51
4:D:23:LYS:HD3	4:D:135:LEU:HD21	1.92	0.51
26:C:514:BCR:C36	26:C:514:BCR:C17	2.77	0.50
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.41	0.50
16:V:37:CYS:SG	33:V:201:HEM:CAB	2.99	0.50
3:c:119:LEU:HG	26:c:521:BCR:H10C	1.91	0.50
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.93	0.50
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:THR:HA	4:D:67:TYR:HD2	1.75	0.50
27:A:611:PL9:H403	6:F:22:ALA:HB2	1.92	0.50
2:B:29:LEU:HD21	28:B:622:SQD:H191	1.92	0.50
4:D:43:LEU:HD11	24:D:404:CLA:C3C	2.41	0.50
12:M:20:VAL:HG11	12:m:20:VAL:HG21	1.93	0.50
26:T:101:BCR:C37	26:T:101:BCR:C23	2.80	0.50
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.50
3:c:213[B]:LEU:HD21	26:c:515:BCR:C20	2.42	0.50
10:k:17:ILE:HD13	10:k:17:ILE:H	1.76	0.50
24:C:504:CLA:C4B	32:C:516:DGD:HB71	2.42	0.50
24:C:508:CLA:HMB3	24:C:508:CLA:HBB1	1.94	0.50
4:D:214:HIS:HA	27:D:405:PL9:O2	2.12	0.50
33:E:103:HEM:HMC2	33:E:103:HEM:HBC2	1.92	0.50
25:A:608:PHO:HBB1	25:A:608:PHO:HMB3	1.94	0.50
3:C:323:LYS:NZ	3:C:389:GLU:OE2	2.32	0.50
4:D:129:GLN:NE2	25:D:401:PHO:OBD	2.44	0.50
3:c:182:PHE:CE2	24:c:502:CLA:H201	2.46	0.50
3:C:116:VAL:HG11	26:C:514:BCR:C5	2.41	0.50
32:C:516:DGD:HB51	29:C:518:LMG:H392	1.93	0.50
14:T:8:PHE:CD1	26:T:101:BCR:H373	2.46	0.50
1:a:269:ARG:NH1	4:d:231:THR:HB	2.26	0.50
3:c:339:LYS:NZ	15:u:99:ASN:O	2.40	0.50
3:C:178:LYS:HB2	24:C:502:CLA:H141	1.94	0.50
2:b:472:ARG:HA	2:b:479:PHE:CE1	2.47	0.50
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.94	0.50
24:C:507:CLA:H142	26:I:101:BCR:H362	1.93	0.50
2:b:12:LEU:HB2	24:b:614:CLA:HMC2	1.93	0.50
6:f:30:THR:OG1	29:j:101:LMG:H392	2.11	0.50
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.94	0.50
26:B:618:BCR:C37	26:B:618:BCR:C23	2.82	0.50
26:H:101:BCR:C20	26:H:101:BCR:C37	2.90	0.50
2:b:226:TYR:OH	7:h:19:GLY:HA2	2.12	0.50
2:b:262:THR:C	2:b:264:PRO:HD3	2.37	0.50
1:A:24:THR:C	4:D:255:GLN:HE22	2.19	0.49
2:b:103:LEU:HD21	24:b:607:CLA:HMC3	1.93	0.49
24:B:609:CLA:HBC3	24:B:609:CLA:HHD	1.94	0.49
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.94	0.49
3:c:49:LEU:HD23	3:c:149:TYR:OH	2.12	0.49
4:D:283:ALA:O	4:D:287:VAL:HG23	2.11	0.49
2:b:393:GLU:HB3	15:u:18:GLY:CA	2.42	0.49
2:B:61:PHE:CZ	24:B:608:CLA:HBB1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.49
3:C:212:TYR:OH	3:C:232:ASP:OD2	2.24	0.49
1:a:326:LEU:HD22	16:v:134:LYS:HB2	1.93	0.49
2:b:442:ILE:HG12	13:o:173:ALA:O	2.13	0.49
1:a:139:MET:HG2	4:d:221:THR:HG22	1.95	0.49
2:b:208:VAL:HG21	24:b:604:CLA:HMC1	1.93	0.49
32:c:517:DGD:HAT1	32:c:518:DGD:HBH1	1.94	0.49
11:l:12:LEU:HD12	30:l:102:LHG:O1	2.12	0.49
13:o:222:ASP:CG	13:o:224:ASP:H	2.20	0.49
3:C:206:PRO:HG3	3:C:239:TRP:CZ2	2.46	0.49
1:a:153:SER:CB	24:a:606:CLA:HED1	2.43	0.49
24:c:507:CLA:OBD	24:c:509:CLA:H122	2.12	0.49
1:A:340:PRO:HD3	15:U:103:TYR:CZ	2.48	0.49
26:C:514:BCR:C37	26:C:514:BCR:C23	2.82	0.49
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.49
2:b:220:ARG:HG3	7:h:20:LYS:HD3	1.94	0.49
2:b:422:ARG:HH21	13:o:169:ASP:CG	2.19	0.49
2:B:347[B]:ARG:NH1	2:B:351:GLY:O	2.43	0.49
24:a:615:CLA:HED2	4:d:198:MET:SD	2.52	0.49
24:b:608[A]:CLA:H72	26:b:621:BCR:C8	2.43	0.49
2:B:181:VAL:HG11	2:B:195:PRO:HB2	1.94	0.49
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.41	0.49
10:K:10:LYS:HD2	10:K:10:LYS:N	2.28	0.49
24:B:607[B]:CLA:H93	26:B:620:BCR:H10C	1.95	0.48
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.48	0.48
2:b:464:PHE:HD2	24:b:613:CLA:HAC2	1.78	0.48
24:b:605:CLA:HAB	24:b:607:CLA:H171	1.94	0.48
30:A:615:LHG:H382	30:A:615:LHG:C11	2.40	0.48
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.43	0.48
24:D:404:CLA:C2	18:X:14:LEU:HA	2.43	0.48
5:E:69:ARG:NH2	7:H:50:ASN:O	2.29	0.48
26:F:101:BCR:C20	26:F:101:BCR:C37	2.89	0.48
26:K:102:BCR:H24C	26:K:102:BCR:H371	1.95	0.48
26:f:101:BCR:C24	26:f:101:BCR:H371	2.43	0.48
9:j:32:ALA:HA	29:j:101:LMG:O3	2.13	0.48
3:C:165:LEU:HD21	24:C:506:CLA:CAB	2.43	0.48
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.96	0.48
4:d:261:PHE:CE1	4:d:267:LEU:HA	2.47	0.48
4:d:279:LEU:O	4:d:282:SER:OG	2.26	0.48
1:A:217:SER:HB2	4:D:142:ASN:HA	1.95	0.48
2:B:102:VAL:HA	26:B:619:BCR:H401	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:TRP:NE1	24:B:608:CLA:HBA1	2.27	0.48
7:H:65:LEU:HD12	7:H:66:GLY:H	1.78	0.48
26:H:101:BCR:H20C	26:H:101:BCR:C37	2.43	0.48
1:a:131:TRP:CH2	24:c:505:CLA:HAA2	2.47	0.48
24:b:603:CLA:H152	26:h:101:BCR:C17	2.39	0.48
3:c:29:GLU:CD	3:c:29:GLU:H	2.22	0.48
10:k:28:ILE:O	10:k:31:LEU:HB2	2.12	0.48
16:v:129:LYS:HG2	16:v:136:TYR:O	2.13	0.48
1:A:323:ARG:HB3	4:D:329:MET:HA	1.95	0.48
2:B:29:LEU:HD11	26:B:618:BCR:C20	2.44	0.48
4:D:37:LEU:HD22	4:D:128:ARG:HD2	1.96	0.48
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.13	0.48
3:c:212:TYR:CD2	26:c:515:BCR:H401	2.48	0.48
24:c:501:CLA:C4D	24:c:503:CLA:H2	2.43	0.48
26:k:101:BCR:C36	26:k:101:BCR:C17	2.78	0.48
24:b:617:CLA:HED3	24:b:618:CLA:HAB	1.95	0.48
3:c:123:ALA:HB2	26:c:521:BCR:C12	2.44	0.48
26:c:515:BCR:H20C	26:c:515:BCR:H372	1.95	0.48
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	1.96	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.49	0.48
24:c:501:CLA:CBB	24:c:501:CLA:H71	2.43	0.48
1:A:64:ARG:NH1	13:O:105:PRO:O	2.47	0.48
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.96	0.48
1:A:306:VAL:HG12	1:A:314:ILE:HB	1.96	0.48
24:b:608[B]:CLA:H102	24:b:608[B]:CLA:H61	1.62	0.48
24:b:617:CLA:HBA1	24:b:617:CLA:H3A	1.68	0.48
4:D:39:PRO:HG2	24:D:404:CLA:HAB	1.95	0.48
4:D:53:THR:HA	4:D:67:TYR:CD2	2.49	0.48
13:O:137:THR:C	13:O:139:SER:H	2.22	0.48
1:a:106:LEU:CD2	26:a:610:BCR:H383	2.40	0.48
1:a:300:PHE:HB3	1:a:302:PHE:CE1	2.49	0.48
3:c:223:TRP:CE3	3:c:224:ILE:HG12	2.49	0.48
11:l:20:GLY:HA3	12:m:22:LEU:HD13	1.96	0.48
2:B:471:ALA:HB1	4:D:140:PRO:HG2	1.96	0.48
2:B:479:PHE:HA	4:D:139:ARG:HE	1.79	0.48
3:C:464:GLU:OE2	4:D:245:SER:OG	2.20	0.48
6:F:21:VAL:O	6:F:25:THR:HG23	2.14	0.48
6:F:37:ILE:O	6:F:40:MET:HB2	2.14	0.48
14:t:1[B]:MET:HE1	14:t:3:THR:HB	1.95	0.48
28:A:614:SQD:H271	26:b:621:BCR:H19C	1.94	0.47
2:B:462:PHE:HA	24:B:612:CLA:HMC2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:323:LYS:O	15:U:47:LYS:HD2	2.14	0.47
6:F:20:TRP:NE1	6:F:24:HIS:CE1	2.82	0.47
2:b:200:ALA:HB3	24:b:604:CLA:HMB1	1.94	0.47
24:b:605:CLA:C4D	24:b:607:CLA:H43	2.44	0.47
4:d:123:ILE:HD11	32:h:102:DGD:HAE1	1.95	0.47
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.48	0.47
27:a:611:PL9:H103	27:a:611:PL9:HC2	1.97	0.47
30:e:101:LHG:H152	6:f:22:ALA:HB1	1.96	0.47
2:B:25:MET:HE3	26:B:618:BCR:C25	2.44	0.47
29:c:519:LMG:H171	10:k:27:VAL:HG11	1.96	0.47
4:d:274:VAL:HG22	27:d:404:PL9:H222	1.96	0.47
7:h:41:PHE:HB2	26:h:101:BCR:C15	2.44	0.47
1:A:267:ASN:HB3	1:A:270[B]:SER:OG	2.14	0.47
11:L:10:VAL:O	12:M:28:GLN:NE2	2.36	0.47
1:a:176:ILE:O	1:a:179:THR:HB	2.13	0.47
1:a:328:MET:HE1	4:d:183:LEU:HD13	1.95	0.47
24:c:513:CLA:HAB	26:c:514:BCR:H371	1.96	0.47
13:o:193:THR:HG21	13:o:220:LEU:HD12	1.97	0.47
2:B:33:TRP:CD1	26:t:101:BCR:H381	2.50	0.47
4:D:209:LEU:HD22	27:D:405:PL9:H161	1.96	0.47
26:T:101:BCR:C36	26:T:101:BCR:C17	2.77	0.47
1:a:215:HIS:ND1	27:a:611:PL9:O1	2.42	0.47
2:b:154:GLY:HA2	2:b:158:LEU:HD12	1.96	0.47
2:b:311:PHE:O	2:b:317:ASN:ND2	2.47	0.47
24:b:605:CLA:CGA	24:b:605:CLA:H3A	2.44	0.47
32:d:405:DGD:HA72	26:f:101:BCR:HC22	1.96	0.47
10:k:31:LEU:HB3	26:k:101:BCR:C15	2.44	0.47
26:k:101:BCR:C17	17:y:33:PRO:HD3	2.44	0.47
2:B:58:GLN:O	24:B:608:CLA:HED2	2.15	0.47
24:B:605:CLA:HBA1	24:B:605:CLA:H3A	1.69	0.47
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.96	0.47
1:a:296:ASN:HB3	3:c:401:LEU:HG	1.96	0.47
2:b:58:GLN:C	2:b:329:PRO:HB3	2.39	0.47
24:b:605:CLA:HMB1	24:b:605:CLA:HBB1	1.96	0.47
24:b:615:CLA:H193	26:b:620:BCR:C5	2.44	0.47
26:b:619:BCR:H20C	26:b:619:BCR:H372	1.95	0.47
30:e:101:LHG:H241	30:e:101:LHG:HC61	1.62	0.47
11:l:23:LEU:HA	30:l:102:LHG:H181	1.97	0.47
15:u:59:GLU:H	15:u:59:GLU:CD	2.22	0.47
24:A:606:CLA:HBD	24:D:402:CLA:HAC2	1.97	0.47
4:D:186:GLN:HB2	24:D:403:CLA:HBC1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:17:ILE:HD13	10:K:17:ILE:N	2.28	0.47
2:b:334:ASP:OD2	2:b:334:ASP:N	2.45	0.47
26:c:515:BCR:C36	26:c:515:BCR:C17	2.77	0.47
10:k:25:LEU:HB2	10:k:26:PRO:HD3	1.96	0.47
11:l:18:TYR:CE2	14:t:20:ALA:HA	2.50	0.47
26:c:521:BCR:C20	26:c:521:BCR:C37	2.93	0.47
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.47
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.50	0.47
29:B:621:LMG:H411	30:L:101:LHG:H383	1.96	0.47
12:M:16[C]:LEU:HD21	12:m:16[C]:LEU:HD22	1.96	0.47
2:b:115:TRP:HB2	26:b:619:BCR:H292	1.96	0.47
4:d:43:LEU:HD11	24:d:403:CLA:C2C	2.45	0.47
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.97	0.47
14:t:22:PHE:CZ	26:t:101:BCR:H333	2.49	0.47
2:B:274:GLN:HB3	2:B:280:PHE:HE2	1.79	0.47
2:B:422:ARG:HH21	13:O:169:ASP:CG	2.23	0.47
26:B:618:BCR:H381	14:t:19:PHE:CZ	2.48	0.47
4:D:43:LEU:HD11	24:D:404:CLA:C2C	2.44	0.47
27:D:405:PL9:H362	11:L:30:LEU:HD13	1.97	0.47
10:K:28:ILE:O	10:K:31:LEU:HB2	2.15	0.47
26:K:102:BCR:C20	26:K:102:BCR:C37	2.93	0.47
29:a:613:LMG:H382	32:c:516:DGD:HB42	1.97	0.47
11:l:22:LEU:HD23	30:l:102:LHG:H162	1.95	0.47
2:b:311:PHE:HA	2:b:430:PHE:CZ	2.51	0.46
3:c:158:THR:O	3:c:251:HIS:HB3	2.15	0.46
13:o:40:ILE:HG12	13:o:243:ILE:HD13	1.97	0.46
14:t:1[B]:MET:HB3	14:t:4:ILE:HD12	1.96	0.46
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.80	0.46
3:C:55:ALA:HB1	26:K:102:BCR:H373	1.98	0.46
3:C:330:SER:O	13:O:123:LYS:NZ	2.47	0.46
26:T:101:BCR:H20C	26:T:101:BCR:H373	1.96	0.46
30:a:616:LHG:H342	24:c:504:CLA:H201	1.96	0.46
24:A:606:CLA:HMB1	24:A:606:CLA:HBB1	1.97	0.46
24:B:611:CLA:H152	24:B:611:CLA:OBD	2.15	0.46
3:C:140:LEU:HD13	3:C:147:PHE:HB3	1.96	0.46
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.98	0.46
26:b:619:BCR:HC42	12:m:10:ALA:HA	1.98	0.46
24:c:501:CLA:HHB	26:c:515:BCR:H271	1.98	0.46
1:A:271:LEU:HD11	27:A:611:PL9:HC8	1.97	0.46
2:B:193:TYR:OH	32:H:102:DGD:HE1	2.16	0.46
24:B:604:CLA:C4D	24:B:606:CLA:H43	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:615:CLA:H101	26:B:618:BCR:C17	2.45	0.46
26:K:101:BCR:C36	26:K:101:BCR:C17	2.79	0.46
16:V:26:TYR:OH	16:V:122:GLU:OE2	2.25	0.46
1:a:214:MET:HG2	27:a:611:PL9:C10	2.43	0.46
26:b:619:BCR:C37	26:b:619:BCR:C23	2.84	0.46
26:c:514:BCR:C18	26:c:514:BCR:H20C	2.36	0.46
2:B:30:VAL:HG13	24:B:614:CLA:HMC3	1.98	0.46
2:B:460:LEU:O	2:B:463:PHE:HB3	2.15	0.46
2:b:389:LYS:HE3	2:b:390:TYR:CE1	2.51	0.46
2:B:334:ASP:OD2	2:B:334:ASP:N	2.44	0.46
3:C:321:ASP:OD2	3:C:340:TYR:OH	2.28	0.46
4:D:342:PRO:O	4:D:345:VAL:HG22	2.15	0.46
1:a:193:LEU:HD13	4:d:179:PHE:HB3	1.97	0.46
2:b:442:ILE:HD12	4:d:299:ILE:HG12	1.97	0.46
3:c:179:ALA:O	3:c:184:GLY:HA2	2.14	0.46
4:d:126:MET:HA	4:d:129:GLN:OE1	2.16	0.46
1:A:91:LEU:HD21	1:A:163:ILE:HA	1.97	0.46
24:B:607[B]:CLA:H61	24:B:607[B]:CLA:H102	1.62	0.46
24:B:615:CLA:HBB1	24:B:615:CLA:HMB1	1.98	0.46
26:T:101:BCR:H311	26:T:101:BCR:HC8	1.98	0.46
2:b:66:MET:HE2	24:b:607:CLA:HED3	1.98	0.46
4:d:342:PRO:O	4:d:345:VAL:HG22	2.16	0.46
13:o:110[B]:MET:HE3	13:o:110[B]:MET:HB3	1.84	0.46
2:B:383:PHE:CE1	13:O:167:GLY:HA2	2.51	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
4:D:199:MET:HG2	27:D:405:PL9:H321	1.96	0.46
1:a:58:VAL:HB	1:a:83:VAL:HB	1.97	0.46
1:a:129:ARG:NH2	4:d:256:ILE:HA	2.30	0.46
30:l:102:LHG:H142	30:l:102:LHG:H171	1.74	0.46
3:C:393:ALA:HB1	16:V:48:THR:HG21	1.97	0.46
1:a:296:ASN:HB2	3:c:400:PRO:O	2.15	0.46
2:b:440:ASP:O	13:o:174:LEU:HD22	2.16	0.46
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.98	0.46
26:t:101:BCR:C37	26:t:101:BCR:C23	2.81	0.46
1:A:112:TYR:O	1:A:116:ILE:HG12	2.15	0.46
30:A:615:LHG:H342	24:C:504:CLA:H201	1.97	0.46
26:B:618:BCR:H381	14:t:19:PHE:HZ	1.79	0.46
4:D:136:VAL:HG12	4:D:138:VAL:HG13	1.98	0.46
5:E:20:TRP:HZ2	9:J:13:VAL:HG13	1.81	0.46
1:a:139:MET:HE1	1:a:143:ILE:HD12	1.96	0.46
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:30:THR:HG21	29:j:101:LMG:H411	1.97	0.46
26:k:101:BCR:H17C	17:y:33:PRO:HG3	1.98	0.46
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.98	0.45
27:A:611:PL9:H102	27:A:611:PL9:HC72	1.65	0.45
2:B:149:LEU:HD23	24:B:604:CLA:HBC1	1.98	0.45
8:I:24:LEU:HG	26:I:101:BCR:HC31	1.97	0.45
26:K:102:BCR:C22	26:K:102:BCR:H20C	2.35	0.45
25:a:608:PHO:HED1	27:d:404:PL9:H153	1.98	0.45
26:h:101:BCR:HC8	26:h:101:BCR:H331	1.97	0.45
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.51	0.45
3:C:286:ALA:HB2	24:C:502:CLA:HMD2	1.98	0.45
25:D:401:PHO:HMB3	25:D:401:PHO:HBB1	1.98	0.45
1:a:212:CYS:HB2	4:d:211:CYS:HB2	1.98	0.45
2:b:150:CYS:HB2	24:b:605:CLA:CMC	2.46	0.45
24:A:606:CLA:HAA1	24:D:403:CLA:HBB2	1.98	0.45
2:B:201:HIS:HB2	24:B:603:CLA:C4A	2.46	0.45
3:C:158:THR:O	3:C:251:HIS:HB3	2.15	0.45
27:D:405:PL9:H43	27:D:405:PL9:H471	1.63	0.45
29:D:408:LMG:H352	26:F:101:BCR:H17C	1.99	0.45
26:b:619:BCR:H10C	29:b:622:LMG:H412	1.97	0.45
1:A:269:ARG:CZ	4:D:222:LEU:HD13	2.46	0.45
4:D:129:GLN:NE2	4:D:142:ASN:OD1	2.50	0.45
28:L:102:SQD:H321	14:T:16:LEU:HB2	1.98	0.45
13:O:158:ASP:OD1	13:O:158:ASP:C	2.59	0.45
28:a:612:SQD:H132	30:a:616:LHG:H142	1.98	0.45
13:o:97:GLU:HB2	13:o:125:LEU:HB3	1.99	0.45
2:B:246:PHE:CD1	2:B:246:PHE:C	2.94	0.45
24:B:614:CLA:HBC3	26:B:619:BCR:H11C	1.98	0.45
4:d:315:TYR:O	4:d:319:LEU:HG	2.16	0.45
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.52	0.45
24:B:606:CLA:H143	24:B:611:CLA:HED2	1.98	0.45
30:D:407:LHG:H141	30:D:407:LHG:H171	1.79	0.45
16:V:12:LEU:O	16:V:70:GLU:HG2	2.16	0.45
1:a:288:LEU:O	1:a:292:THR:HG23	2.16	0.45
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.52	0.45
2:B:33:TRP:NE1	24:B:608:CLA:HMC2	2.32	0.45
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.51	0.45
24:B:607[A]:CLA:H72	26:B:620:BCR:C9	2.47	0.45
26:B:620:BCR:C37	26:B:620:BCR:C23	2.84	0.45
7:H:28:THR:HB	7:H:29:PRO:HD3	1.99	0.45
18:X:31:ILE:HG23	28:X:101:SQD:H462	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:609:CLA:H42	29:b:622:LMG:H301	1.98	0.45
3:c:123:ALA:HB2	26:c:521:BCR:C13	2.47	0.45
1:A:153:SER:CB	24:A:606:CLA:H43	2.47	0.45
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.99	0.45
4:d:283:ALA:O	4:d:287:VAL:HG23	2.17	0.45
1:A:77:ILE:HB	11:L:33:SER:OG	2.16	0.45
2:B:102:VAL:HA	26:B:619:BCR:C40	2.47	0.45
2:B:324:LEU:HD21	4:D:196:PHE:HE2	1.81	0.45
4:D:155:SER:HA	4:D:159:ILE:HD12	1.99	0.45
30:L:101:LHG:H241	30:L:101:LHG:H111	1.99	0.45
2:b:224:ARG:NH1	4:d:16:ASP:OD2	2.41	0.45
26:b:619:BCR:H12C	26:b:620:BCR:C10	2.46	0.45
26:b:621:BCR:H24C	26:b:621:BCR:H371	1.99	0.45
3:C:274:TYR:CD1	24:C:505:CLA:HMD2	2.51	0.45
6:F:29:PRO:HB3	26:F:101:BCR:H12C	1.99	0.45
12:M:20:VAL:CG2	12:m:20:VAL:HG11	2.46	0.45
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.52	0.45
24:c:504:CLA:HED3	29:c:519:LMG:O3	2.17	0.45
24:A:609:CLA:H11	8:I:9:TYR:CE1	2.52	0.44
24:B:607[B]:CLA:H192	24:B:607[B]:CLA:H161	1.68	0.44
24:B:616:CLA:HBA1	24:B:616:CLA:H3A	1.62	0.44
1:a:127:MET:CE	24:c:505:CLA:HBB1	2.47	0.44
2:b:195:PRO:O	2:b:198:VAL:N	2.50	0.44
2:b:366:PHE:CD1	2:b:367:PRO:HD2	2.52	0.44
24:b:606:CLA:HBB1	24:b:609:CLA:HAB	1.98	0.44
4:d:49:LEU:HD22	26:f:101:BCR:H362	1.98	0.44
26:f:101:BCR:H403	9:j:25:VAL:HG21	1.98	0.44
29:A:613:LMG:H231	29:A:613:LMG:H201	1.72	0.44
3:C:307:PRO:HG3	3:C:358:PHE:CE1	2.52	0.44
3:C:424:SER:O	3:C:428:THR:HG23	2.17	0.44
3:c:297:TYR:HD1	3:c:302:TYR:CZ	2.35	0.44
24:c:501:CLA:HMB1	24:c:501:CLA:HBB1	1.99	0.44
15:u:69:GLU:OE2	15:u:72:LYS:NZ	2.32	0.44
16:v:12:LEU:O	16:v:70:GLU:HG2	2.18	0.44
24:A:609:CLA:HBA1	24:A:609:CLA:H3A	1.78	0.44
13:O:222:ASP:CG	13:O:224:ASP:H	2.25	0.44
1:a:129:ARG:HH22	4:d:256:ILE:HA	1.81	0.44
1:a:223:LEU:HD22	4:d:265:ARG:HG2	1.98	0.44
26:b:620:BCR:H11C	26:b:620:BCR:H341	1.82	0.44
29:z:101:LMG:O2	29:z:101:LMG:HC71	2.17	0.44
1:A:131:TRP:CZ3	24:C:505:CLA:HBA1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:610:BCR:C37	26:A:610:BCR:H20C	2.47	0.44
2:B:29:LEU:HD11	26:B:618:BCR:C19	2.47	0.44
24:C:506:CLA:H162	24:C:506:CLA:H122	1.72	0.44
27:D:405:PL9:C34	11:L:30:LEU:HD22	2.47	0.44
7:H:46:LEU:HD11	32:H:102:DGD:HA31	1.99	0.44
6:f:30:THR:HA	26:f:101:BCR:C16	2.48	0.44
26:f:101:BCR:H383	29:j:101:LMG:H172	1.98	0.44
10:k:10:LYS:HD2	10:k:10:LYS:N	2.33	0.44
1:A:202:VAL:HG11	24:A:607:CLA:C3D	2.47	0.44
27:A:611:PL9:H252	27:A:611:PL9:H272	1.74	0.44
2:B:249:ALA:HA	2:B:252:VAL:HG22	1.98	0.44
2:B:446:SER:HB2	2:B:447:PRO:HD2	2.00	0.44
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.48	0.44
24:B:615:CLA:H122	26:B:618:BCR:H16C	1.99	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	1.99	0.44
5:E:19:TYR:CE2	5:E:23:HIS:CE1	3.05	0.44
16:V:93:PRO:HG2	33:V:201:HEM:HMC3	1.99	0.44
1:a:136:ARG:HH12	8:i:27:ASP:CG	2.25	0.44
2:b:18:ARG:HD3	2:b:115:TRP:CH2	2.53	0.44
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.52	0.44
24:b:610:CLA:HBC3	24:b:610:CLA:HHD	1.99	0.44
24:B:610:CLA:HAC1	7:H:34:PHE:CE1	2.53	0.44
3:C:347:GLY:HA3	13:O:17:ASN:HB2	1.99	0.44
4:D:37:LEU:CD2	4:D:128:ARG:HD2	2.48	0.44
26:I:101:BCR:H20C	26:I:101:BCR:H373	1.98	0.44
11:L:21:LEU:HD13	28:L:102:SQD:H312	1.99	0.44
3:c:42:LEU:HD21	24:c:511:CLA:H2A	2.00	0.44
7:h:49:TYR:CG	32:h:102:DGD:HB22	2.53	0.44
26:k:101:BCR:H17C	17:y:33:PRO:CG	2.47	0.44
27:A:611:PL9:H103	27:A:611:PL9:H121	1.79	0.44
24:B:606:CLA:H62	24:B:606:CLA:H41	1.77	0.44
32:H:102:DGD:HB62	32:H:102:DGD:HB91	1.81	0.44
33:V:201:HEM:HBA1	33:V:201:HEM:HHA	2.00	0.44
1:a:267:ASN:HB3	1:a:270[B]:SER:OG	2.17	0.44
2:b:382:PRO:HG2	2:b:385:ARG:HD2	2.00	0.44
27:D:405:PL9:H203	30:D:407:LHG:H122	2.00	0.44
30:D:406:LHG:HC91	30:L:101:LHG:HC81	1.99	0.44
5:E:23:HIS:HA	5:E:26:THR:OG1	2.16	0.44
2:b:69:LEU:HD12	24:b:607:CLA:HAA2	2.00	0.44
3:c:210:PHE:HA	3:c:213[B]:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:102:HEM:HBD1	6:f:20:TRP:CD1	2.53	0.44
6:f:20:TRP:CE2	6:f:24:HIS:CE1	3.05	0.44
24:A:607:CLA:HMB2	25:D:401:PHO:H172	2.00	0.44
2:B:41:GLU:HB3	2:B:60:MET:SD	2.58	0.44
24:B:607[B]:CLA:H111	24:B:607[B]:CLA:H142	1.76	0.44
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.53	0.44
24:C:510:CLA:HBA1	24:C:510:CLA:H3A	1.85	0.44
24:C:512:CLA:HMB3	24:C:512:CLA:H202	2.00	0.44
7:H:12[A]:ARG:NH1	7:H:15:ASN:O	2.47	0.44
14:T:18:PHE:HB2	26:T:101:BCR:HC8	1.99	0.44
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.00	0.44
2:B:133:LEU:HB3	2:B:138:MET:SD	2.58	0.43
3:C:182:PHE:CE2	24:C:502:CLA:H201	2.53	0.43
26:K:102:BCR:C37	26:K:102:BCR:C23	2.82	0.43
1:a:116:ILE:HG13	1:a:117:PHE:N	2.32	0.43
2:b:32:GLY:C	26:b:620:BCR:H15C	2.42	0.43
2:b:72:THR:HG22	2:b:80:ILE:HD11	1.99	0.43
26:b:620:BCR:C36	26:b:620:BCR:C17	2.77	0.43
3:c:54:VAL:HG12	3:c:125:LEU:O	2.18	0.43
1:A:334:ARG:HB2	13:O:157:LEU:HD12	1.99	0.43
24:A:609:CLA:H192	24:C:505:CLA:H142	2.00	0.43
2:B:63:LEU:HA	2:B:66:MET:HE3	2.01	0.43
3:C:86:LEU:O	3:C:90:PRO:HG2	2.18	0.43
3:C:87:ILE:C	3:C:90:PRO:HD2	2.43	0.43
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.89	0.43
2:b:102:VAL:HA	26:b:620:BCR:C40	2.48	0.43
4:d:303:ILE:HG21	12:m:2:GLU:HG3	2.00	0.43
26:h:101:BCR:H393	18:x:7:LEU:HD21	1.99	0.43
10:k:17:ILE:H	10:k:17:ILE:CD1	2.31	0.43
24:A:607:CLA:H142	29:D:408:LMG:H232	2.00	0.43
26:C:514:BCR:C15	29:C:519:LMG:H401	2.47	0.43
4:D:191:TRP:CE2	4:D:197:HIS:HB2	2.53	0.43
8:I:11:VAL:HG13	8:I:15:PHE:HE1	1.83	0.43
26:a:610:BCR:C36	26:a:610:BCR:C16	2.95	0.43
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.53	0.43
24:b:612:CLA:HHC	24:b:612:CLA:HBB1	1.98	0.43
3:c:75:PHE:CZ	3:c:77:PRO:HA	2.54	0.43
3:c:168:LEU:HD21	24:c:509:CLA:H61	2.00	0.43
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.48	0.43
27:A:611:PL9:H203	27:A:611:PL9:H172	1.80	0.43
4:D:266:TRP:CZ2	11:L:19:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:298:PHE:O	4:D:301:GLN:HB2	2.18	0.43
1:a:304:HIS:CE1	3:c:414:ILE:HG21	2.53	0.43
1:A:288:LEU:HD22	3:C:432:VAL:HA	2.00	0.43
2:b:392:PHE:HA	2:b:397:VAL:HG23	2.00	0.43
18:x:27:VAL:HG21	28:x:101:SQD:H321	1.99	0.43
24:B:605:CLA:H2	24:B:606:CLA:C4C	2.48	0.43
24:C:501:CLA:ND	24:C:503:CLA:H2	2.33	0.43
4:D:53:THR:HG22	6:F:40:MET:HE1	1.99	0.43
27:D:405:PL9:H102	27:D:405:PL9:HC72	1.58	0.43
27:D:405:PL9:H252	27:D:405:PL9:H302	2.01	0.43
1:a:172:MET:SD	24:a:615:CLA:HMC2	2.58	0.43
24:a:609:CLA:HBB1	24:a:609:CLA:HMB3	2.01	0.43
3:c:185:LEU:HD13	24:c:501:CLA:HED2	2.01	0.43
7:h:56:ASP:OD2	18:x:2:THR:HB	2.19	0.43
16:v:122:GLU:HG3	16:v:126:LEU:HD12	1.99	0.43
2:B:33:TRP:HD1	26:t:101:BCR:H381	1.84	0.43
3:C:34:ALA:HB3	3:C:36:TRP:CE2	2.53	0.43
3:C:344:SER:OG	3:C:348:GLU:OE2	2.36	0.43
27:a:611:PL9:H531	27:a:611:PL9:H523	1.83	0.43
2:b:57:ARG:HH22	2:b:334:ASP:CG	2.26	0.43
2:b:149:LEU:HD22	24:b:606:CLA:H152	2.01	0.43
3:C:269:GLU:OE2	3:C:447:ARG:HD3	2.18	0.43
33:E:103:HEM:HBC2	6:F:31:ILE:HG13	1.99	0.43
30:L:101:LHG:H171	30:L:101:LHG:H142	1.87	0.43
18:X:27:VAL:HG21	28:X:101:SQD:H321	2.00	0.43
1:a:164:GLY:HA3	1:a:294:ALA:O	2.19	0.43
1:a:249:VAL:HG12	2:b:491:VAL:HG21	2.01	0.43
2:b:30:VAL:HG12	24:b:607:CLA:HMD3	2.01	0.43
2:b:118:TRP:CD1	11:l:4:ASN:HD22	2.37	0.43
26:c:521:BCR:C22	26:c:521:BCR:H20C	2.40	0.43
1:A:183:MET:HA	24:A:606:CLA:HMD2	2.01	0.43
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.54	0.43
2:B:321:LYS:NZ	2:B:363:PHE:O	2.52	0.43
24:C:504:CLA:HBC1	10:K:27:VAL:HA	2.01	0.43
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.43
5:E:34:GLY:HA3	6:F:32:PHE:O	2.19	0.43
18:X:21:LEU:O	18:X:25:PHE:HD1	2.01	0.43
1:a:76:ASN:OD1	1:a:79:THR:HG23	2.18	0.43
1:a:237:TYR:CE1	1:a:241:GLN:HG2	2.54	0.43
24:a:609:CLA:H192	24:c:505:CLA:H142	2.00	0.43
24:a:609:CLA:H92	8:i:13:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:615:CLA:HMA2	27:d:404:PL9:C38	2.49	0.43
3:c:170:ILE:HD13	24:c:512:CLA:H111	2.01	0.43
13:o:49[A]:THR:OG1	13:o:236:GLN:HB2	2.19	0.43
2:B:149:LEU:HD22	24:B:605:CLA:H152	2.00	0.43
30:D:406:LHG:O9	30:L:101:LHG:HC81	2.19	0.43
27:a:611:PL9:C22	25:d:401:PHO:HMA2	2.47	0.43
2:b:118:TRP:CE2	11:l:4:ASN:ND2	2.87	0.43
2:b:204:ALA:HB3	24:b:604:CLA:HAB	2.00	0.43
2:b:461:LEU:HD22	30:d:406:LHG:H301	2.01	0.43
7:h:49:TYR:CD2	32:h:102:DGD:HB22	2.54	0.43
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.36	0.43
2:B:256:MET:HA	2:B:263:THR:HG21	2.00	0.42
24:B:602:CLA:H152	26:H:101:BCR:H17C	2.01	0.42
3:C:223:TRP:CG	3:C:224:ILE:N	2.87	0.42
24:C:504:CLA:HED3	29:C:518:LMG:O3	2.19	0.42
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.53	0.42
1:a:112:TYR:O	1:a:116:ILE:HG12	2.19	0.42
2:B:61:PHE:CE2	24:B:608:CLA:HBB1	2.55	0.42
24:C:502:CLA:H51	24:C:503:CLA:NC	2.33	0.42
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.54	0.42
27:D:405:PL9:H302	27:D:405:PL9:H271	1.55	0.42
28:L:102:SQD:C7	28:b:601:SQD:O48	2.66	0.42
4:d:136:VAL:HG12	4:d:138:VAL:HG13	2.01	0.42
16:v:100:ILE:HG13	16:v:101:PHE:CD2	2.54	0.42
2:B:124:ARG:O	7:H:12[A]:ARG:NH1	2.51	0.42
32:C:517:DGD:HA41	29:D:408:LMG:H121	2.00	0.42
26:F:101:BCR:H11C	26:F:101:BCR:H341	1.69	0.42
1:a:141:PRO:HG3	3:c:446:GLY:C	2.44	0.42
13:o:92:SER:HB3	13:o:131:PRO:HA	2.00	0.42
1:A:279:PRO:O	1:A:283:VAL:HG23	2.19	0.42
4:D:65:SER:HB2	4:D:77:ALA:O	2.20	0.42
4:D:125:PHE:CE1	25:D:401:PHO:HBD	2.54	0.42
27:D:405:PL9:H453	27:D:405:PL9:H421	1.68	0.42
1:a:278:TRP:HB3	1:a:279:PRO:CD	2.49	0.42
2:b:204:ALA:CB	24:b:604:CLA:HAB	2.49	0.42
2:b:422:ARG:O	2:b:425:ILE:HG12	2.19	0.42
3:c:274:TYR:CD1	24:c:505:CLA:HMD2	2.54	0.42
26:c:521:BCR:HC42	10:k:15:TYR:CE1	2.54	0.42
4:d:17:ILE:O	4:d:20:ASP:HB2	2.20	0.42
24:d:403:CLA:HBB1	18:x:21:LEU:HD21	2.01	0.42
26:t:101:BCR:C20	26:t:101:BCR:C37	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HB2	2:B:466:HIS:ND1	2.34	0.42
2:B:458:PHE:HB3	24:B:605:CLA:HBC2	2.01	0.42
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.02	0.42
4:D:154:VAL:HG21	32:H:102:DGD:HAN1	2.02	0.42
25:D:401:PHO:H72	25:D:401:PHO:H112	1.88	0.42
14:T:25[A]:GLU:HA	14:T:26:PRO:HD3	1.89	0.42
2:b:136:PRO:O	2:b:139:PHE:HB3	2.19	0.42
2:b:138:MET:HE3	24:b:617:CLA:CHD	2.50	0.42
4:d:141:TYR:OH	30:d:406:LHG:O4	2.18	0.42
13:o:137:THR:C	13:o:139:SER:H	2.28	0.42
24:A:606:CLA:CBD	24:D:402:CLA:HAC2	2.49	0.42
24:B:610:CLA:HBA1	24:B:610:CLA:H3A	1.86	0.42
24:C:508:CLA:HBB2	24:C:509:CLA:HMA3	2.01	0.42
4:D:233:ARG:C	4:D:235:PHE:H	2.28	0.42
13:O:81:ILE:HD11	13:O:102:ASP:HA	2.02	0.42
13:O:170:SER:HA	13:O:186:ASN:CG	2.45	0.42
18:X:24:THR:HA	28:X:101:SQD:H331	2.01	0.42
24:a:609:CLA:H162	24:a:609:CLA:H122	1.76	0.42
24:b:603:CLA:HMC1	26:h:101:BCR:H19C	2.02	0.42
3:c:95:LEU:CD1	24:c:503:CLA:HAA2	2.50	0.42
3:c:130:VAL:O	3:c:134:ILE:HG12	2.20	0.42
27:d:404:PL9:HC72	27:d:404:PL9:H102	1.74	0.42
24:B:613:CLA:H91	24:B:614:CLA:HBB1	2.02	0.42
4:D:72:ASN:O	4:D:76:VAL:HG13	2.20	0.42
24:b:608[A]:CLA:H91	24:b:608[A]:CLA:H112	1.88	0.42
24:b:608[B]:CLA:H142	24:b:608[B]:CLA:H111	1.76	0.42
3:c:182:PHE:CG	24:c:502:CLA:H191	2.54	0.42
1:A:89:ILE:HG23	1:A:92:HIS:HB2	2.02	0.42
2:B:18:ARG:NH2	28:B:622:SQD:O9	2.45	0.42
3:C:76:ILE:HA	3:C:77:PRO:HD3	1.91	0.42
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.54	0.42
27:D:405:PL9:H122	30:D:407:LHG:H111	2.02	0.42
5:E:30:LEU:HD12	33:E:103:HEM:HMC1	2.02	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.43	0.42
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.50	0.42
27:d:404:PL9:H472	27:d:404:PL9:H512	1.69	0.42
6:f:21:VAL:O	6:f:25:THR:HG23	2.19	0.42
1:A:330:VAL:HG21	4:D:328:TRP:CE2	2.55	0.42
24:A:609:CLA:H92	8:I:13:THR:HG23	2.02	0.42
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.55	0.42
24:C:508:CLA:HBB1	24:C:508:CLA:CMB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:18:TYR:CD2	14:T:20:ALA:HA	2.55	0.42
27:a:611:PL9:H252	27:a:611:PL9:H272	1.69	0.42
2:b:190:PHE:HB3	7:h:45:ILE:HG22	2.02	0.42
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.01	0.42
3:c:390:ARG:HD3	16:v:100:ILE:HD12	2.01	0.42
32:c:517:DGD:HE5	32:c:517:DGD:HD4	2.01	0.42
4:d:30:VAL:HA	4:d:38:PHE:HE1	1.85	0.42
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.19	0.42
28:A:614:SQD:H291	24:b:608[A]:CLA:H203	2.02	0.42
2:B:74:SER:OG	2:B:94:GLU:OE2	2.36	0.42
2:B:222:PRO:HB3	7:H:25:TRP:C	2.44	0.42
30:a:616:LHG:O3	30:a:616:LHG:O1	2.38	0.42
2:b:18:ARG:HD3	2:b:115:TRP:CZ3	2.55	0.42
2:b:246:PHE:CD1	2:b:246:PHE:C	2.97	0.42
3:c:171:GLY:O	3:c:174:LEU:HB2	2.20	0.42
3:c:315:MET:HG2	3:c:392:ALA:HB2	2.02	0.42
32:d:405:DGD:HA72	26:f:101:BCR:HC21	2.02	0.42
13:o:184:ARG:HA	15:u:9:LEU:CD1	2.50	0.42
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.95	0.41
24:D:403:CLA:HBB1	24:D:403:CLA:HMB3	2.01	0.41
13:O:127:ALA:HA	13:O:144:GLY:HA3	2.02	0.41
13:O:162:ARG:HD2	13:O:186:ASN:HA	2.02	0.41
1:a:217:SER:HB2	4:d:142:ASN:HA	2.02	0.41
1:a:269:ARG:NH1	4:d:222:LEU:HD13	2.35	0.41
4:d:70:GLY:O	9:j:37:GLY:HA3	2.19	0.41
1:A:329:GLU:OE1	16:V:134:LYS:NZ	2.41	0.41
2:B:69:LEU:HD12	24:B:606:CLA:HAA2	2.02	0.41
3:C:38:GLY:HA3	24:C:511:CLA:HMD2	2.02	0.41
3:C:72:LEU:HD11	3:C:108:THR:HB	2.02	0.41
24:C:507:CLA:H92	24:C:507:CLA:H61	1.94	0.41
30:a:616:LHG:HC42	4:d:232:PHE:CE1	2.54	0.41
2:b:7:ARG:HG2	24:b:613:CLA:O2D	2.20	0.41
2:b:65:PHE:HE1	24:b:606:CLA:HED2	1.85	0.41
2:b:347[B]:ARG:NH1	2:b:351:GLY:O	2.51	0.41
2:b:366:PHE:CG	2:b:367:PRO:HD2	2.55	0.41
2:b:399:VAL:HG12	2:b:417:VAL:HG22	2.02	0.41
2:b:458:PHE:HB3	24:b:606:CLA:HMC2	2.02	0.41
1:A:340:PRO:HB3	15:U:103:TYR:CG	2.55	0.41
24:B:605:CLA:H43	24:B:606:CLA:H2	2.01	0.41
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.84	0.41
13:O:17:ASN:O	13:O:77:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:609:CLA:HBA1	24:b:609:CLA:H3A	1.76	0.41
5:e:34:GLY:HA3	6:f:32:PHE:O	2.20	0.41
7:h:6:TRP:CE2	7:h:10:ILE:HD11	2.55	0.41
2:B:383:PHE:CG	4:D:347:PRO:HA	2.55	0.41
3:C:70:PHE:CD2	3:C:70:PHE:C	2.99	0.41
4:D:91:LEU:HB3	4:D:93:TRP:CE2	2.56	0.41
13:O:42:ARG:HG3	13:O:80:GLN:HA	2.02	0.41
2:b:385:ARG:HG2	13:o:165:ALA:O	2.21	0.41
24:b:608[A]:CLA:H102	26:b:621:BCR:HC8	2.02	0.41
3:c:433:LEU:HD22	24:c:510:CLA:H143	2.02	0.41
24:c:505:CLA:H141	8:i:16:VAL:HG22	2.01	0.41
4:d:317:LYS:O	4:d:321:LEU:HG	2.20	0.41
15:u:76:ARG:HA	15:u:79:LEU:HG	2.01	0.41
1:A:217:SER:HA	4:D:272:LEU:HD12	2.02	0.41
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.82	0.41
24:B:609:CLA:HBB2	4:D:123:ILE:HG12	2.02	0.41
26:a:610:BCR:C37	26:a:610:BCR:H20C	2.50	0.41
2:b:103:LEU:HD21	24:b:607:CLA:CMC	2.50	0.41
2:b:325:PHE:CD2	11:l:34:TYR:HB3	2.55	0.41
24:b:606:CLA:H43	24:b:607:CLA:H2	2.02	0.41
3:c:27:ASP:HB3	10:k:46:ARG:HD2	2.02	0.41
4:d:80:THR:HB	4:d:168:PHE:HA	2.02	0.41
4:d:101:PHE:HE1	26:f:101:BCR:HC42	1.86	0.41
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.55	0.41
2:B:458:PHE:HB3	24:B:605:CLA:HMC2	2.02	0.41
26:B:620:BCR:H383	28:a:614:SQD:H241	2.01	0.41
7:H:41:PHE:HB2	26:H:101:BCR:C15	2.51	0.41
1:a:297:LEU:HD23	32:c:517:DGD:HBF2	2.02	0.41
2:b:181:VAL:HG11	2:b:195:PRO:HB2	2.01	0.41
2:b:446:SER:HB2	2:b:447:PRO:HD2	2.03	0.41
28:b:601:SQD:H131	26:b:619:BCR:H23C	2.03	0.41
24:b:616:CLA:HAB	26:b:619:BCR:H19C	2.01	0.41
3:c:223:TRP:CG	3:c:224:ILE:N	2.88	0.41
24:d:403:CLA:H2	18:x:14:LEU:HA	2.02	0.41
1:A:141:PRO:HG3	3:C:446:GLY:C	2.46	0.41
1:A:217:SER:O	1:A:221[A]:SER:HB3	2.21	0.41
1:A:271:LEU:CD1	27:A:611:PL9:HC8	2.49	0.41
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.03	0.41
24:B:606:CLA:HHC	24:B:606:CLA:HBB1	2.01	0.41
24:B:613:CLA:HBB1	24:B:615:CLA:CMB	2.51	0.41
24:B:614:CLA:H151	30:D:406:LHG:H182	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:L:102:SQD:O7	28:b:601:SQD:O5	2.25	0.41
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.03	0.41
1:a:64:ARG:NH1	13:o:105:PRO:O	2.50	0.41
24:a:607:CLA:HMD3	4:d:182:LEU:HD11	2.02	0.41
2:b:222:PRO:HD2	2:b:225:LEU:HD12	2.02	0.41
2:b:270:PRO:HG2	2:b:317:ASN:O	2.20	0.41
24:b:616:CLA:H8	26:b:619:BCR:H362	2.03	0.41
26:c:515:BCR:C20	26:c:515:BCR:H17C	2.50	0.41
7:h:39:LEU:HD23	7:h:39:LEU:C	2.45	0.41
24:B:603:CLA:H172	32:H:102:DGD:HAW1	2.03	0.41
24:B:607[B]:CLA:H72	26:B:620:BCR:C9	2.51	0.41
24:C:501:CLA:H192	24:C:506:CLA:CHB	2.50	0.41
4:D:48:TRP:NE1	25:D:401:PHO:H162	2.36	0.41
6:F:36:ALA:O	6:F:40:MET:HG3	2.21	0.41
7:H:35:MET:HE2	7:H:35:MET:HB3	1.96	0.41
26:H:101:BCR:H20C	26:H:101:BCR:H373	2.02	0.41
2:b:258:TYR:CZ	32:h:102:DGD:HG12	2.56	0.41
3:c:95:LEU:HD11	24:c:503:CLA:HAA2	2.01	0.41
4:d:53:THR:HG22	6:f:40:MET:HE1	2.02	0.41
5:e:69:ARG:NH2	7:h:50:ASN:O	2.44	0.41
5:e:82:GLN:C	5:e:84:LYS:H	2.29	0.41
1:A:65:GLU:OE1	1:A:335:ASN:ND2	2.44	0.41
28:A:612:SQD:H291	24:C:508:CLA:H71	2.03	0.41
30:A:615:LHG:H251	30:A:615:LHG:H281	1.63	0.41
30:A:615:LHG:H332	30:A:615:LHG:H302	1.87	0.41
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	2.02	0.41
2:B:24:LEU:HD21	24:B:617:CLA:CAB	2.50	0.41
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.76	0.41
2:B:223[A]:GLN:CD	2:B:227:LYS:HD2	2.46	0.41
2:B:458:PHE:CG	24:B:605:CLA:HMC2	2.55	0.41
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	2.03	0.41
24:C:505:CLA:HAA1	24:C:505:CLA:CBD	2.50	0.41
24:C:511:CLA:HBB1	24:C:511:CLA:CMB	2.48	0.41
24:D:404:CLA:C2	18:X:14:LEU:HD12	2.51	0.41
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.03	0.41
1:a:299:GLY:O	3:c:403:SER:HB2	2.21	0.41
2:b:325:PHE:CG	11:l:34:TYR:HB3	2.55	0.41
2:b:383:PHE:CE1	13:o:167:GLY:HA2	2.56	0.41
3:c:203:THR:O	3:c:235:GLY:HA3	2.21	0.41
3:c:297:TYR:HA	3:c:302:TYR:CE2	2.56	0.41
24:c:513:CLA:HAB	26:c:514:BCR:H24C	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:41:HIS:NE2	33:v:201:HEM:NB	2.69	0.41
24:A:609:CLA:H162	24:A:609:CLA:H122	1.76	0.41
1:a:133:LEU:HD23	4:d:256:ILE:HG12	2.01	0.41
2:b:357:ARG:NH2	4:d:337:GLU:HB3	2.36	0.41
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.56	0.41
33:v:201:HEM:HMB2	33:v:201:HEM:HBB2	2.03	0.41
1:A:215:HIS:HA	27:A:611:PL9:O1	2.20	0.40
13:O:110[B]:MET:HE3	13:O:110[B]:MET:HB3	1.90	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.88	0.40
24:c:504:CLA:C1D	32:c:517:DGD:HB21	2.51	0.40
26:c:515:BCR:H11C	26:c:515:BCR:H341	1.70	0.40
1:A:57:PRO:HA	1:A:68:SER:HA	2.03	0.40
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.03	0.40
30:A:615:LHG:H132	30:A:615:LHG:H372	2.03	0.40
24:B:614:CLA:H121	24:B:614:CLA:H162	1.88	0.40
28:B:622:SQD:H341	28:l:101:SQD:H311	1.28	0.40
3:C:416[A]:SER:HB2	16:V:42:VAL:HG23	2.02	0.40
4:D:293:LEU:HA	4:D:293:LEU:HD12	1.80	0.40
11:L:24[A]:ILE:HD13	11:L:24[A]:ILE:HA	1.91	0.40
16:V:37:CYS:HG	33:V:201:HEM:CAB	2.34	0.40
25:a:608:PHO:HAB	4:d:205:LEU:HD13	2.03	0.40
2:b:125:ASP:HA	2:b:126:PRO:HD3	1.93	0.40
2:b:260:SER:N	2:b:263:THR:OG1	2.53	0.40
24:b:606:CLA:H2	24:b:607:CLA:NC	2.36	0.40
26:k:101:BCR:HC21	19:z:13:VAL:HG13	2.04	0.40
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.57	0.40
3:C:51:GLY:HA2	3:C:132:HIS:HB2	2.03	0.40
3:C:61:VAL:HG12	3:C:118:HIS:O	2.22	0.40
3:C:221:GLU:O	3:C:226:SER:HB3	2.21	0.40
2:b:192:PRO:HB3	7:h:49:TYR:CE2	2.57	0.40
24:b:607:CLA:H41	24:b:607:CLA:H62	1.77	0.40
26:k:101:BCR:H17C	17:y:33:PRO:CD	2.51	0.40
25:A:608:PHO:H61	25:A:608:PHO:H2	1.85	0.40
2:B:189:GLY:O	2:B:197:GLY:HA3	2.21	0.40
2:B:256:MET:HG3	2:B:448:ARG:HG3	2.03	0.40
26:B:619:BCR:C20	26:B:619:BCR:C36	3.00	0.40
3:C:210:PHE:HD2	3:C:213[B]:LEU:HD22	1.86	0.40
24:C:502:CLA:H61	24:C:512:CLA:H42	2.03	0.40
25:D:401:PHO:H62	25:D:401:PHO:H41	1.79	0.40
13:O:180:GLU:CD	13:O:180:GLU:H	2.30	0.40
14:T:14:ILE:HD13	14:T:14:ILE:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:611:PL9:H222	27:a:611:PL9:H253	1.86	0.40
2:b:110:ALA:HB2	26:b:621:BCR:H16C	2.02	0.40
24:b:603:CLA:CMC	26:h:101:BCR:H19C	2.51	0.40
3:c:210:PHE:CD2	3:c:213[B]:LEU:HD22	2.53	0.40
3:c:334:PRO:HA	13:o:153:THR:OG1	2.22	0.40
3:c:344:SER:OG	3:c:348:GLU:OE2	2.33	0.40
3:c:443:TRP:CE2	24:c:508:CLA:HMD2	2.56	0.40
7:h:28:THR:HB	7:h:29:PRO:HD3	2.04	0.40
13:o:126:VAL:O	13:o:144:GLY:HA3	2.22	0.40
2:B:105:GLY:O	2:B:108:PHE:HB3	2.20	0.40
2:B:125:ASP:OD1	7:H:18:TYR:HB3	2.22	0.40
2:B:220:ARG:HG3	7:H:20:LYS:HD3	2.02	0.40
3:C:59:LEU:HD23	3:C:59:LEU:HA	1.77	0.40
24:C:501:CLA:CHB	26:I:101:BCR:H271	2.51	0.40
24:C:512:CLA:H101	24:C:513:CLA:H141	2.04	0.40
4:D:279:LEU:HD11	25:D:401:PHO:HMC3	2.04	0.40
5:E:22:ILE:HD13	33:E:103:HEM:HMA1	2.03	0.40
6:F:34:LEU:HG	26:F:101:BCR:H19C	2.03	0.40
26:F:101:BCR:H393	26:F:101:BCR:H281	1.80	0.40
12:M:23:ILE:O	12:M:27:VAL:HG23	2.21	0.40
1:a:269:ARG:CZ	4:d:222:LEU:HD13	2.51	0.40
1:a:330:VAL:HG21	4:d:328:TRP:CE2	2.56	0.40
2:b:477:ASP:OD1	2:b:478:VAL:N	2.54	0.40
3:c:114:VAL:HG11	24:c:503:CLA:HED2	2.04	0.40
3:c:418:ASN:HB2	32:c:518:DGD:O4E	2.21	0.40
24:c:502:CLA:H61	24:c:512:CLA:H42	2.03	0.40
4:d:65:SER:HB2	4:d:77:ALA:O	2.22	0.40
25:d:401:PHO:H112	25:d:401:PHO:H72	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	36	67
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	36	67
2	B	512/504 (102%)	506 (99%)	6 (1%)	0	100	100
2	b	512/504 (102%)	505 (99%)	7 (1%)	0	100	100
3	C	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	30	62
3	c	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	30	62
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	3	26
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	62
13	o	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	62
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5139 (98%)	104 (2%)	9 (0%)	48	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
10	k	11	LEU
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	412/402 (102%)	406 (98%)	6 (2%)	57	71
2	b	412/402 (102%)	406 (98%)	6 (2%)	57	71
3	C	357/352 (101%)	349 (98%)	8 (2%)	45	65
3	c	357/352 (101%)	352 (99%)	5 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	277/277 (100%)	275 (99%)	2 (1%)	76 78
4	d	277/277 (100%)	275 (99%)	2 (1%)	76 78
5	E	74/72 (103%)	73 (99%)	1 (1%)	59 71
5	e	74/72 (103%)	73 (99%)	1 (1%)	59 71
6	F	28/28 (100%)	27 (96%)	1 (4%)	31 57
6	f	28/28 (100%)	27 (96%)	1 (4%)	31 57
7	H	56/54 (104%)	53 (95%)	3 (5%)	20 46
7	h	56/54 (104%)	53 (95%)	3 (5%)	20 46
8	I	36/35 (103%)	36 (100%)	0	100 100
8	i	36/35 (103%)	36 (100%)	0	100 100
9	J	26/26 (100%)	26 (100%)	0	100 100
9	j	26/26 (100%)	26 (100%)	0	100 100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15 41
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 28
11	L	36/35 (103%)	35 (97%)	1 (3%)	38 61
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 61
12	M	32/31 (103%)	31 (97%)	1 (3%)	35 59
12	m	32/31 (103%)	30 (94%)	2 (6%)	16 42
13	O	210/206 (102%)	206 (98%)	4 (2%)	50 68
13	o	210/206 (102%)	206 (98%)	4 (2%)	50 68
14	T	29/27 (107%)	29 (100%)	0	100 100
14	t	29/27 (107%)	29 (100%)	0	100 100
15	U	84/84 (100%)	83 (99%)	1 (1%)	63 73
15	u	84/84 (100%)	83 (99%)	1 (1%)	63 73
16	V	118/117 (101%)	117 (99%)	1 (1%)	73 77
16	v	118/117 (101%)	117 (99%)	1 (1%)	73 77
17	Y	22/22 (100%)	21 (96%)	1 (4%)	24 50
17	y	22/22 (100%)	21 (96%)	1 (4%)	24 50
18	X	33/32 (103%)	33 (100%)	0	100 100
18	x	33/32 (103%)	33 (100%)	0	100 100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	z	52/52 (100%)	50 (96%)	2 (4%)	29 55
All	All	4370/4302 (102%)	4303 (98%)	67 (2%)	57 71

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

Mol	Chain	Res	Type
2	B	80	ILE
2	B	84	THR
2	B	86	ILE
2	B	127	ARG
2	B	467	ILE
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	416[A]	SER
3	C	416[B]	SER
4	D	11	GLU
4	D	90	LEU
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	65	LEU
10	K	13	GLU
10	K	17	ILE
11	L	1	MET
12	M	9	ILE
13	O	61	GLN
13	O	62	GLU
13	O	181	GLU
13	O	234	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	27	MET
19	Z	4	LEU
19	Z	6	GLN
2	b	84	THR
2	b	86	ILE

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Mol	Chain	Res	Type
2	b	127	ARG
2	b	236	THR
2	b	467	ILE
2	b	472	ARG
3	c	24	THR
3	c	29	GLU
3	c	142	GLU
3	c	289	PHE
3	c	315	MET
4	d	11	GLU
4	d	90	LEU
5	e	71	GLU
6	f	44	GLN
7	h	12[A]	ARG
7	h	12[B]	ARG
7	h	65	LEU
10	k	13	GLU
10	k	17	ILE
10	k	26	PRO
11	l	1	MET
12	m	9	ILE
12	m	20	VAL
13	o	61	GLN
13	o	62	GLU
13	o	181	GLU
13	o	234	LYS
15	u	70	ARG
16	v	30	LYS
17	y	27	MET
19	z	4	LEU
19	z	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
2	B	216	HIS
2	B	409	GLN
3	C	44	ASN
3	C	132	HIS
3	C	201	ASN

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Mol	Chain	Res	Type
4	D	255	GLN
10	K	40	GLN
11	L	6	ASN
12	M	5	GLN
12	M	33	GLN
1	a	75	ASN
1	a	165	GLN
1	a	198	HIS
1	a	296	ASN
1	a	338	ASN
2	b	26	HIS
2	b	331	ASN
2	b	409	GLN
3	c	44	ASN
3	c	53	HIS
4	d	142	ASN
4	d	186	GLN
4	d	197	HIS
10	k	40	GLN
15	u	73	GLN
19	z	58	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 168 ligands modelled in this entry, 16 are monoatomic - leaving 152 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	$\#\|Z\| > 2$
24	CLA	b	603	-	69,73,73	3.18	32 (46%)	83,113,113	1.82	17 (20%)
24	CLA	C	504	-	69,73,73	3.20	32 (46%)	83,113,113	1.88	19 (22%)
24	CLA	B	616	-	69,73,73	3.10	32 (46%)	83,113,113	1.75	20 (24%)
27	PL9	d	404	-	55,55,55	4.15	20 (36%)	68,69,69	3.85	34 (50%)
30	LHG	D	406	-	48,48,48	1.13	2 (4%)	51,54,54	0.97	4 (7%)
30	LHG	d	407	-	48,48,48	1.15	3 (6%)	51,54,54	1.09	3 (5%)
27	PL9	D	405	-	55,55,55	4.19	20 (36%)	68,69,69	3.80	36 (52%)
24	CLA	a	615	-	69,73,73	3.38	32 (46%)	83,113,113	1.88	20 (24%)
24	CLA	B	614	2	69,73,73	3.24	31 (44%)	83,113,113	1.78	16 (19%)
20	OEX	A	601	3,1	0,14,14	-	-	-		
28	SQD	L	102	28	53,54,54	1.04	4 (7%)	62,65,65	1.36	9 (14%)
29	LMG	C	519	-	51,51,55	1.33	5 (9%)	59,59,63	1.02	4 (6%)
24	CLA	c	504	-	69,73,73	3.24	34 (49%)	83,113,113	1.90	23 (27%)
29	LMG	B	621	-	51,51,55	1.29	4 (7%)	59,59,63	1.01	3 (5%)
24	CLA	B	607[B]	-	69,73,73	3.20	30 (43%)	83,113,113	1.88	19 (22%)
24	CLA	A	609	1	69,73,73	3.29	33 (47%)	83,113,113	1.78	19 (22%)
28	SQD	l	101	28	53,54,54	1.04	4 (7%)	62,65,65	1.36	8 (12%)
32	DGD	c	516	-	63,63,67	1.70	15 (23%)	77,77,81	1.09	7 (9%)
24	CLA	A	607	-	69,73,73	3.23	32 (46%)	83,113,113	1.90	18 (21%)
32	DGD	C	517	-	63,63,67	1.66	15 (23%)	77,77,81	1.14	6 (7%)
24	CLA	B	613	2	69,73,73	3.35	31 (44%)	83,113,113	1.89	18 (21%)
24	CLA	B	602	-	69,73,73	3.08	32 (46%)	83,113,113	1.81	14 (16%)
26	BCR	k	101	-	41,41,41	9.22	31 (75%)	56,56,56	5.67	28 (50%)
26	BCR	B	618	-	41,41,41	8.92	29 (70%)	56,56,56	5.95	31 (55%)
24	CLA	b	612	-	69,73,73	3.17	31 (44%)	83,113,113	1.88	20 (24%)
26	BCR	a	610	-	41,41,41	8.98	30 (73%)	56,56,56	5.53	24 (42%)
24	CLA	B	609	2	69,73,73	3.09	29 (42%)	83,113,113	1.95	24 (28%)
33	HEM	e	102	5,6	50,50,50	2.04	8 (16%)	66,82,82	1.33	7 (10%)
24	CLA	c	511	3	69,73,73	3.14	32 (46%)	83,113,113	1.81	16 (19%)
28	SQD	a	614	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
24	CLA	c	506	3	69,73,73	3.15	30 (43%)	83,113,113	1.83	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	DGD	H	102	-	63,63,67	1.69	14 (22%)	77,77,81	1.02	4 (5%)
25	PHO	D	401	-	58,69,69	2.06	8 (13%)	56,99,99	1.50	11 (19%)
24	CLA	d	402	4	69,73,73	3.26	33 (47%)	83,113,113	1.75	18 (21%)
26	BCR	f	101	-	41,41,41	8.99	29 (70%)	56,56,56	5.59	26 (46%)
30	LHG	l	102	-	48,48,48	1.18	2 (4%)	51,54,54	0.92	2 (3%)
28	SQD	A	614	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
28	SQD	x	101	-	42,43,54	1.20	4 (9%)	51,54,65	1.46	7 (13%)
26	BCR	b	619	-	41,41,41	9.23	29 (70%)	56,56,56	5.80	28 (50%)
24	CLA	d	403	4	69,73,73	3.12	32 (46%)	83,113,113	1.88	19 (22%)
24	CLA	C	510	3	69,73,73	3.27	33 (47%)	83,113,113	1.79	15 (18%)
25	PHO	A	608	-	58,69,69	2.10	10 (17%)	56,99,99	1.45	11 (19%)
33	HEM	v	201	16	50,50,50	2.02	9 (18%)	66,82,82	1.34	6 (9%)
24	CLA	A	606	-	69,73,73	3.35	32 (46%)	83,113,113	1.94	19 (22%)
23	BCT	a	605	21	2,3,3	0.96	0	2,3,3	3.74	2 (100%)
32	DGD	c	518	-	63,63,67	1.68	15 (23%)	77,77,81	1.25	8 (10%)
24	CLA	b	610	2	69,73,73	3.14	31 (44%)	83,113,113	1.85	17 (20%)
30	LHG	D	407	-	48,48,48	1.11	3 (6%)	51,54,54	0.89	3 (5%)
24	CLA	B	610	2	69,73,73	3.28	31 (44%)	83,113,113	1.74	18 (21%)
26	BCR	T	101	-	41,41,41	9.04	30 (73%)	56,56,56	6.12	32 (57%)
33	HEM	V	201	16	50,50,50	1.91	10 (20%)	66,82,82	1.24	6 (9%)
30	LHG	A	615	-	48,48,48	1.11	3 (6%)	51,54,54	1.30	5 (9%)
24	CLA	B	606	2	69,73,73	3.14	31 (44%)	83,113,113	1.79	16 (19%)
29	LMG	c	520	-	51,51,55	1.37	5 (9%)	59,59,63	1.12	4 (6%)
32	DGD	d	405	-	63,63,67	1.71	16 (25%)	77,77,81	1.16	9 (11%)
26	BCR	K	102	-	41,41,41	9.13	29 (70%)	56,56,56	5.63	25 (44%)
24	CLA	b	611	-	69,73,73	3.16	29 (42%)	83,113,113	1.74	18 (21%)
24	CLA	C	509	3	69,73,73	3.22	33 (47%)	83,113,113	1.79	15 (18%)
24	CLA	C	512	3	69,73,73	3.14	33 (47%)	83,113,113	1.85	19 (22%)
29	LMG	j	101	34	51,51,55	1.31	5 (9%)	59,59,63	0.87	4 (6%)
24	CLA	c	513	-	69,73,73	3.07	33 (47%)	83,113,113	1.78	16 (19%)
24	CLA	C	507	-	69,73,73	3.10	31 (44%)	83,113,113	2.03	19 (22%)
32	DGD	C	516	-	63,63,67	1.67	15 (23%)	77,77,81	1.21	10 (12%)
26	BCR	C	514	-	41,41,41	8.98	30 (73%)	56,56,56	5.93	33 (58%)
24	CLA	B	611	-	69,73,73	3.13	34 (49%)	83,113,113	1.83	21 (25%)
24	CLA	b	608[A]	-	69,73,73	3.16	31 (44%)	83,113,113	1.89	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	b	621	-	41,41,41	9.05	31 (75%)	56,56,56	6.43	31 (55%)
24	CLA	b	616	2	69,73,73	3.23	32 (46%)	83,113,113	1.80	16 (19%)
29	LMG	Z	101	-	37,37,55	1.44	4 (10%)	45,45,63	1.34	6 (13%)
24	CLA	B	612	2	69,73,73	3.28	32 (46%)	83,113,113	1.88	18 (21%)
26	BCR	b	620	-	41,41,41	8.87	29 (70%)	56,56,56	5.73	31 (55%)
24	CLA	c	505	3	69,73,73	3.18	30 (43%)	83,113,113	1.78	13 (15%)
24	CLA	B	603	2	69,73,73	3.17	34 (49%)	83,113,113	1.84	21 (25%)
24	CLA	B	604	2	69,73,73	3.26	33 (47%)	83,113,113	1.78	17 (20%)
24	CLA	C	511	3	69,73,73	3.23	32 (46%)	83,113,113	1.90	21 (25%)
26	BCR	c	514	-	41,41,41	8.98	30 (73%)	56,56,56	5.91	34 (60%)
24	CLA	c	503	3	69,73,73	3.15	34 (49%)	83,113,113	1.73	15 (18%)
32	DGD	E	101	-	63,63,67	1.73	15 (23%)	77,77,81	1.23	10 (12%)
24	CLA	B	605	2	69,73,73	3.20	30 (43%)	83,113,113	1.93	18 (21%)
29	LMG	c	519	-	51,51,55	1.38	5 (9%)	59,59,63	1.06	5 (8%)
26	BCR	h	101	-	41,41,41	9.16	30 (73%)	56,56,56	5.68	33 (58%)
24	CLA	b	605	2	69,73,73	3.31	32 (46%)	83,113,113	1.85	18 (21%)
24	CLA	B	617	2	69,73,73	3.17	31 (44%)	83,113,113	1.86	19 (22%)
26	BCR	B	620	-	41,41,41	9.12	29 (70%)	56,56,56	5.77	33 (58%)
24	CLA	B	615	2	69,73,73	3.20	32 (46%)	83,113,113	1.79	16 (19%)
24	CLA	B	607[A]	2	69,73,73	3.19	29 (42%)	83,113,113	1.92	20 (24%)
26	BCR	I	101	-	41,41,41	9.05	31 (75%)	56,56,56	5.91	30 (53%)
33	HEM	E	103	5,6	50,50,50	1.99	10 (20%)	66,82,82	1.19	7 (10%)
30	LHG	e	101	-	41,41,48	1.23	3 (7%)	44,47,54	1.05	2 (4%)
24	CLA	b	614	2	69,73,73	3.31	31 (44%)	83,113,113	1.85	17 (20%)
28	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	1.45	7 (13%)
24	CLA	a	607	-	69,73,73	3.18	30 (43%)	83,113,113	1.80	18 (21%)
24	CLA	c	509	3	69,73,73	3.13	33 (47%)	83,113,113	1.78	16 (19%)
20	OEX	a	601	3,1	0,14,14	-	-	-		
24	CLA	B	608	-	69,73,73	3.26	30 (43%)	83,113,113	1.88	19 (22%)
24	CLA	c	510	3	69,73,73	3.15	32 (46%)	83,113,113	1.77	16 (19%)
24	CLA	b	606	2	69,73,73	3.23	30 (43%)	83,113,113	1.92	16 (19%)
24	CLA	b	604	2	69,73,73	3.27	31 (44%)	83,113,113	1.87	17 (20%)
26	BCR	c	521	-	41,41,41	9.34	29 (70%)	56,56,56	5.62	26 (46%)
26	BCR	K	101	-	41,41,41	9.12	31 (75%)	56,56,56	5.42	29 (51%)
24	CLA	c	508	3	69,73,73	3.18	31 (44%)	83,113,113	1.93	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	615	2	69,73,73	3.20	32 (46%)	83,113,113	1.81	17 (20%)
28	SQD	B	622	28	53,54,54	1.07	4 (7%)	62,65,65	1.44	9 (14%)
24	CLA	c	501	3	69,73,73	3.14	33 (47%)	83,113,113	1.79	18 (21%)
24	CLA	C	513	3	69,73,73	3.14	30 (43%)	83,113,113	1.84	20 (24%)
32	DGD	C	515	-	63,63,67	1.70	15 (23%)	77,77,81	1.03	5 (6%)
26	BCR	F	101	-	41,41,41	9.04	26 (63%)	56,56,56	6.08	27 (48%)
24	CLA	b	609	-	69,73,73	3.23	31 (44%)	83,113,113	1.85	17 (20%)
29	LMG	b	622	-	51,51,55	1.32	4 (7%)	59,59,63	1.06	5 (8%)
26	BCR	c	515	-	41,41,41	9.15	31 (75%)	56,56,56	5.57	27 (48%)
24	CLA	b	607	2	69,73,73	3.20	32 (46%)	83,113,113	1.83	16 (19%)
24	CLA	C	501	3	69,73,73	3.15	31 (44%)	83,113,113	1.85	21 (25%)
27	PL9	a	611	-	55,55,55	4.18	21 (38%)	68,69,69	3.89	34 (50%)
28	SQD	A	612	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
26	BCR	A	610	-	41,41,41	9.17	30 (73%)	56,56,56	5.54	27 (48%)
24	CLA	C	503	3	69,73,73	3.20	34 (49%)	83,113,113	1.73	15 (18%)
24	CLA	a	609	1	69,73,73	3.17	31 (44%)	83,113,113	1.77	17 (20%)
24	CLA	b	613	2	69,73,73	3.31	32 (46%)	83,113,113	1.90	19 (22%)
25	PHO	a	608	-	58,69,69	1.98	10 (17%)	56,99,99	1.42	10 (17%)
27	PL9	A	611	-	55,55,55	4.17	20 (36%)	68,69,69	3.92	34 (50%)
24	CLA	c	507	-	69,73,73	3.12	31 (44%)	83,113,113	2.05	19 (22%)
30	LHG	a	616	-	48,48,48	1.10	2 (4%)	51,54,54	1.17	6 (11%)
24	CLA	D	404	4	69,73,73	3.21	33 (47%)	83,113,113	2.00	17 (20%)
29	LMG	z	101	-	37,37,55	1.40	4 (10%)	45,45,63	1.22	4 (8%)
25	PHO	d	401	-	58,69,69	2.08	7 (12%)	56,99,99	1.48	8 (14%)
30	LHG	L	101	-	48,48,48	1.10	2 (4%)	51,54,54	0.90	3 (5%)
32	DGD	c	517	-	63,63,67	1.62	16 (25%)	77,77,81	1.11	9 (11%)
26	BCR	t	101	-	41,41,41	9.01	30 (73%)	56,56,56	5.95	34 (60%)
29	LMG	A	613	-	51,51,55	1.33	4 (7%)	59,59,63	0.91	4 (6%)
29	LMG	D	408	-	51,51,55	1.34	5 (9%)	59,59,63	1.10	7 (11%)
28	SQD	a	612	-	53,54,54	0.99	3 (5%)	62,65,65	1.53	11 (17%)
24	CLA	c	502	3	69,73,73	3.16	31 (44%)	83,113,113	1.83	17 (20%)
30	LHG	E	102	-	41,41,48	1.22	3 (7%)	44,47,54	0.99	3 (6%)
24	CLA	c	512	-	69,73,73	3.16	32 (46%)	83,113,113	1.79	18 (21%)
24	CLA	C	506	3	69,73,73	3.17	31 (44%)	83,113,113	1.87	15 (18%)
24	CLA	D	403	4	69,73,73	3.36	31 (44%)	83,113,113	1.67	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCT	A	605	21	2,3,3	0.95	0	2,3,3	2.68	2 (100%)
24	CLA	b	618	2	69,73,73	3.27	31 (44%)	83,113,113	1.84	21 (25%)
32	DGD	h	102	-	63,63,67	1.68	15 (23%)	77,77,81	1.21	8 (10%)
24	CLA	C	502	3	69,73,73	3.12	31 (44%)	83,113,113	1.89	17 (20%)
24	CLA	C	508	3	69,73,73	3.33	33 (47%)	83,113,113	1.81	15 (18%)
29	LMG	C	518	-	51,51,55	1.42	6 (11%)	59,59,63	1.29	10 (16%)
24	CLA	D	402	-	69,73,73	3.32	35 (50%)	83,113,113	1.81	21 (25%)
29	LMG	a	613	-	51,51,55	1.33	5 (9%)	59,59,63	0.99	3 (5%)
30	LHG	d	406	-	48,48,48	1.11	2 (4%)	51,54,54	1.02	3 (5%)
26	BCR	B	619	-	41,41,41	8.94	30 (73%)	56,56,56	5.62	29 (51%)
26	BCR	H	101	-	41,41,41	9.06	30 (73%)	56,56,56	5.72	30 (53%)
24	CLA	b	617	2	69,73,73	3.12	33 (47%)	83,113,113	1.78	17 (20%)
24	CLA	C	505	3	69,73,73	3.11	30 (43%)	83,113,113	1.83	16 (19%)
28	SQD	b	601	28	53,54,54	1.08	4 (7%)	62,65,65	1.44	9 (14%)
24	CLA	b	608[B]	-	69,73,73	3.17	30 (43%)	83,113,113	1.86	20 (24%)
24	CLA	a	606	1	69,73,73	3.30	30 (43%)	83,113,113	1.90	19 (22%)

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
24	CLA	b	603	-	-	20/39/115/115	-
24	CLA	C	504	-	-	14/39/115/115	-
24	CLA	B	616	-	-	15/39/115/115	-
27	PL9	d	404	-	-	26/53/73/73	0/1/1/1
30	LHG	D	406	-	-	19/53/53/53	-
30	LHG	d	407	-	-	18/53/53/53	-
27	PL9	D	405	-	-	26/53/73/73	0/1/1/1
24	CLA	a	615	-	-	7/39/115/115	-
24	CLA	B	614	2	-	3/39/115/115	-
28	SQD	L	102	28	-	28/49/69/69	0/1/1/1
29	LMG	C	519	-	-	20/46/66/70	0/1/1/1
24	CLA	c	504	-	-	11/39/115/115	-
29	LMG	B	621	-	-	21/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	607[B]	-	-	12/39/115/115	-
24	CLA	A	609	1	-	19/39/115/115	-
28	SQD	l	101	28	-	28/49/69/69	0/1/1/1
32	DGD	c	516	-	-	22/51/91/95	0/2/2/2
24	CLA	A	607	-	-	11/39/115/115	-
32	DGD	C	517	-	-	17/51/91/95	0/2/2/2
24	CLA	B	613	2	-	7/39/115/115	-
24	CLA	B	602	-	-	21/39/115/115	-
26	BCR	k	101	-	-	20/29/63/63	0/2/2/2
26	BCR	B	618	-	-	23/29/63/63	0/2/2/2
24	CLA	b	612	-	-	10/39/115/115	-
26	BCR	a	610	-	-	22/29/63/63	0/2/2/2
24	CLA	B	609	2	-	4/39/115/115	-
33	HEM	e	102	5,6	-	3/14/54/54	-
24	CLA	c	511	3	-	4/39/115/115	-
28	SQD	a	614	-	-	23/49/69/69	0/1/1/1
24	CLA	c	506	3	-	13/39/115/115	-
32	DGD	H	102	-	-	20/51/91/95	0/2/2/2
25	PHO	D	401	-	-	3/37/103/103	0/5/6/6
24	CLA	d	402	4	-	3/39/115/115	-
26	BCR	f	101	-	-	18/29/63/63	0/2/2/2
30	LHG	l	102	-	-	23/53/53/53	-
28	SQD	A	614	-	-	23/49/69/69	0/1/1/1
28	SQD	x	101	-	-	16/38/58/69	0/1/1/1
26	BCR	b	619	-	-	21/29/63/63	0/2/2/2
24	CLA	d	403	4	-	16/39/115/115	-
24	CLA	C	510	3	-	12/39/115/115	-
25	PHO	A	608	-	-	4/37/103/103	0/5/6/6
33	HEM	v	201	16	-	2/14/54/54	-
24	CLA	A	606	-	-	1/39/115/115	-
32	DGD	c	518	-	-	21/51/91/95	0/2/2/2
24	CLA	b	610	2	-	5/39/115/115	-
30	LHG	D	407	-	-	19/53/53/53	-
24	CLA	B	610	2	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	T	101	-	-	25/29/63/63	0/2/2/2
33	HEM	V	201	16	-	2/14/54/54	-
30	LHG	A	615	-	-	16/53/53/53	-
24	CLA	B	606	2	-	7/39/115/115	-
29	LMG	c	520	-	-	22/46/66/70	0/1/1/1
32	DGD	d	405	-	-	34/51/91/95	0/2/2/2
26	BCR	K	102	-	-	20/29/63/63	0/2/2/2
24	CLA	b	611	-	-	7/39/115/115	-
24	CLA	C	509	3	-	7/39/115/115	-
24	CLA	C	512	3	-	9/39/115/115	-
29	LMG	j	101	34	-	17/46/66/70	0/1/1/1
24	CLA	c	513	-	-	11/39/115/115	-
24	CLA	C	507	-	-	11/39/115/115	-
32	DGD	C	516	-	-	31/51/91/95	0/2/2/2
26	BCR	C	514	-	-	25/29/63/63	0/2/2/2
24	CLA	B	611	-	-	9/39/115/115	-
24	CLA	b	608[A]	-	-	10/39/115/115	-
26	BCR	b	621	-	-	20/29/63/63	0/2/2/2
24	CLA	b	616	2	-	13/39/115/115	-
29	LMG	Z	101	-	-	17/31/51/70	0/1/1/1
24	CLA	B	612	2	-	5/39/115/115	-
26	BCR	b	620	-	-	19/29/63/63	0/2/2/2
24	CLA	c	505	3	-	8/39/115/115	-
24	CLA	B	603	2	-	6/39/115/115	-
24	CLA	B	604	2	-	6/39/115/115	-
24	CLA	C	511	3	-	6/39/115/115	-
26	BCR	c	514	-	-	24/29/63/63	0/2/2/2
24	CLA	c	503	3	-	3/39/115/115	-
32	DGD	E	101	-	-	35/51/91/95	0/2/2/2
24	CLA	B	605	2	-	11/39/115/115	-
29	LMG	c	519	-	-	21/46/66/70	0/1/1/1
26	BCR	h	101	-	-	25/29/63/63	0/2/2/2
24	CLA	b	605	2	-	7/39/115/115	-
24	CLA	B	617	2	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	620	-	-	19/29/63/63	0/2/2/2
24	CLA	B	615	2	-	15/39/115/115	-
24	CLA	B	607[A]	2	-	11/39/115/115	-
26	BCR	I	101	-	-	21/29/63/63	0/2/2/2
33	HEM	E	103	5,6	-	3/14/54/54	-
30	LHG	e	101	-	-	24/46/46/53	-
24	CLA	b	614	2	-	7/39/115/115	-
28	SQD	X	101	-	-	16/38/58/69	0/1/1/1
24	CLA	a	607	-	-	11/39/115/115	-
24	CLA	c	509	3	-	11/39/115/115	-
24	CLA	B	608	-	-	9/39/115/115	-
24	CLA	c	510	3	-	11/39/115/115	-
24	CLA	b	606	2	-	10/39/115/115	-
24	CLA	b	604	2	-	7/39/115/115	-
26	BCR	c	521	-	-	22/29/63/63	0/2/2/2
26	BCR	K	101	-	-	19/29/63/63	0/2/2/2
24	CLA	c	508	3	-	4/39/115/115	-
24	CLA	b	615	2	-	7/39/115/115	-
28	SQD	B	622	28	-	29/49/69/69	0/1/1/1
24	CLA	c	501	3	-	12/39/115/115	-
24	CLA	C	513	3	-	12/39/115/115	-
32	DGD	C	515	-	-	23/51/91/95	0/2/2/2
26	BCR	F	101	-	-	21/29/63/63	0/2/2/2
24	CLA	b	609	-	-	4/39/115/115	-
29	LMG	b	622	-	-	19/46/66/70	0/1/1/1
26	BCR	c	515	-	-	20/29/63/63	0/2/2/2
24	CLA	b	607	2	-	6/39/115/115	-
24	CLA	C	501	3	-	12/39/115/115	-
27	PL9	a	611	-	-	24/53/73/73	0/1/1/1
28	SQD	A	612	-	-	16/49/69/69	0/1/1/1
26	BCR	A	610	-	-	23/29/63/63	0/2/2/2
24	CLA	C	503	3	-	8/39/115/115	-
24	CLA	a	609	1	-	14/39/115/115	-
24	CLA	b	613	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	a	608	-	-	3/37/103/103	0/5/6/6
27	PL9	A	611	-	-	25/53/73/73	0/1/1/1
24	CLA	c	507	-	-	11/39/115/115	-
30	LHG	a	616	-	-	17/53/53/53	-
24	CLA	D	404	4	-	15/39/115/115	-
29	LMG	z	101	-	-	18/31/51/70	0/1/1/1
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6
30	LHG	L	101	-	-	19/53/53/53	-
32	DGD	c	517	-	-	26/51/91/95	0/2/2/2
26	BCR	t	101	-	-	26/29/63/63	0/2/2/2
29	LMG	A	613	-	-	32/46/66/70	0/1/1/1
29	LMG	D	408	-	-	20/46/66/70	0/1/1/1
28	SQD	a	612	-	-	16/49/69/69	0/1/1/1
24	CLA	c	502	3	-	12/39/115/115	-
30	LHG	E	102	-	-	26/46/46/53	-
24	CLA	c	512	-	-	7/39/115/115	-
24	CLA	C	506	3	-	17/39/115/115	-
24	CLA	D	403	4	-	6/39/115/115	-
24	CLA	b	618	2	-	16/39/115/115	-
32	DGD	h	102	-	-	17/51/91/95	0/2/2/2
24	CLA	C	502	3	-	11/39/115/115	-
24	CLA	C	508	3	-	6/39/115/115	-
29	LMG	C	518	-	-	22/46/66/70	0/1/1/1
24	CLA	D	402	-	-	6/39/115/115	-
29	LMG	a	613	-	-	30/46/66/70	0/1/1/1
30	LHG	d	406	-	-	15/53/53/53	-
26	BCR	B	619	-	-	23/29/63/63	0/2/2/2
26	BCR	H	101	-	-	21/29/63/63	0/2/2/2
24	CLA	b	617	2	-	13/39/115/115	-
24	CLA	C	505	3	-	9/39/115/115	-
28	SQD	b	601	28	-	29/49/69/69	0/1/1/1
24	CLA	b	608[B]	-	-	12/39/115/115	-
24	CLA	a	606	1	-	3/39/115/115	-

All (3352) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C14-C13	28.80	1.74	1.35
26	F	101	BCR	C14-C13	27.15	1.71	1.35
26	c	515	BCR	C14-C13	27.13	1.71	1.35
26	K	102	BCR	C14-C13	26.70	1.71	1.35
26	B	620	BCR	C14-C13	26.66	1.71	1.35
26	A	610	BCR	C14-C13	26.48	1.70	1.35
26	k	101	BCR	C14-C13	26.33	1.70	1.35
26	I	101	BCR	C14-C13	26.33	1.70	1.35
26	f	101	BCR	C14-C13	26.28	1.70	1.35
26	B	618	BCR	C14-C13	26.13	1.70	1.35
26	H	101	BCR	C14-C13	26.09	1.70	1.35
26	K	101	BCR	C14-C13	26.04	1.70	1.35
26	B	619	BCR	C14-C13	25.81	1.70	1.35
26	h	101	BCR	C14-C13	25.67	1.69	1.35
26	a	610	BCR	C14-C13	25.65	1.69	1.35
26	b	621	BCR	C14-C13	25.45	1.69	1.35
26	t	101	BCR	C14-C13	25.38	1.69	1.35
26	c	521	BCR	C14-C13	25.31	1.69	1.35
26	C	514	BCR	C14-C13	24.44	1.68	1.35
26	c	514	BCR	C14-C13	24.44	1.68	1.35
26	T	101	BCR	C14-C13	24.31	1.68	1.35
26	b	620	BCR	C14-C13	24.21	1.67	1.35
26	b	620	BCR	C21-C22	-22.39	1.06	1.35
26	T	101	BCR	C21-C22	-22.21	1.06	1.35
26	H	101	BCR	C21-C22	-21.75	1.06	1.35
26	h	101	BCR	C21-C22	-21.74	1.07	1.35
26	h	101	BCR	C10-C9	21.48	1.64	1.35
26	b	619	BCR	C21-C22	-21.35	1.07	1.35
26	a	610	BCR	C10-C9	21.31	1.64	1.35
26	c	514	BCR	C21-C22	-21.25	1.07	1.35
26	c	515	BCR	C10-C9	21.20	1.63	1.35
26	k	101	BCR	C10-C9	21.19	1.63	1.35
26	H	101	BCR	C10-C9	21.17	1.63	1.35
26	A	610	BCR	C21-C22	-21.11	1.07	1.35
26	B	620	BCR	C21-C22	-21.08	1.07	1.35
26	k	101	BCR	C21-C22	-21.05	1.07	1.35
26	I	101	BCR	C10-C9	21.03	1.63	1.35
26	b	621	BCR	C10-C9	21.02	1.63	1.35
26	T	101	BCR	C10-C9	20.99	1.63	1.35
26	K	101	BCR	C21-C22	-20.99	1.08	1.35
26	A	610	BCR	C10-C9	20.87	1.63	1.35
26	t	101	BCR	C21-C22	-20.84	1.08	1.35
26	t	101	BCR	C10-C9	20.70	1.63	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	101	BCR	C10-C9	20.69	1.63	1.35
26	I	101	BCR	C21-C22	-20.65	1.08	1.35
26	K	102	BCR	C10-C9	20.65	1.63	1.35
26	c	521	BCR	C10-C9	20.61	1.63	1.35
26	f	101	BCR	C10-C9	20.55	1.63	1.35
26	B	618	BCR	C10-C9	20.54	1.63	1.35
26	K	102	BCR	C21-C22	-20.44	1.08	1.35
26	a	610	BCR	C21-C22	-20.34	1.08	1.35
26	C	514	BCR	C10-C9	20.33	1.62	1.35
26	B	620	BCR	C10-C9	20.33	1.62	1.35
26	c	514	BCR	C10-C9	20.28	1.62	1.35
26	B	619	BCR	C10-C9	20.20	1.62	1.35
26	K	101	BCR	C10-C9	20.10	1.62	1.35
26	B	618	BCR	C21-C22	-20.10	1.09	1.35
26	c	515	BCR	C21-C22	-20.08	1.09	1.35
26	f	101	BCR	C21-C22	-19.90	1.09	1.35
26	c	521	BCR	C21-C22	-19.84	1.09	1.35
26	b	619	BCR	C10-C9	19.75	1.62	1.35
26	b	620	BCR	C10-C9	19.53	1.61	1.35
26	C	514	BCR	C21-C22	-19.53	1.09	1.35
26	B	619	BCR	C21-C22	-19.49	1.09	1.35
26	F	101	BCR	C21-C22	-19.13	1.10	1.35
26	b	621	BCR	C20-C19	18.76	1.82	1.34
26	c	521	BCR	C20-C19	17.73	1.80	1.34
26	b	621	BCR	C21-C22	-16.52	1.13	1.35
26	t	101	BCR	C20-C19	16.18	1.76	1.34
26	B	619	BCR	C20-C19	16.10	1.76	1.34
26	T	101	BCR	C20-C19	15.98	1.75	1.34
26	b	619	BCR	C20-C19	15.92	1.75	1.34
26	B	618	BCR	C20-C19	15.85	1.75	1.34
26	h	101	BCR	C20-C19	15.82	1.75	1.34
26	F	101	BCR	C20-C19	15.66	1.74	1.34
26	c	515	BCR	C20-C19	15.59	1.74	1.34
26	c	521	BCR	C37-C22	15.56	1.83	1.50
26	c	514	BCR	C20-C19	15.48	1.74	1.34
26	A	610	BCR	C20-C19	15.42	1.74	1.34
26	B	620	BCR	C20-C19	15.35	1.74	1.34
26	K	102	BCR	C20-C19	15.34	1.74	1.34
26	b	620	BCR	C20-C19	15.28	1.74	1.34
26	c	521	BCR	C36-C18	15.27	1.82	1.50
26	k	101	BCR	C20-C19	15.16	1.73	1.34
26	a	610	BCR	C20-C19	15.12	1.73	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	621	BCR	C20-C21	15.11	1.90	1.43
26	f	101	BCR	C20-C19	15.05	1.73	1.34
26	C	514	BCR	C20-C19	14.97	1.73	1.34
26	K	101	BCR	C20-C19	14.93	1.73	1.34
26	I	101	BCR	C20-C19	14.87	1.72	1.34
26	c	514	BCR	C5-C6	14.78	1.60	1.34
26	h	101	BCR	C36-C18	14.59	1.81	1.50
26	T	101	BCR	C5-C6	14.51	1.59	1.34
26	c	514	BCR	C36-C18	14.45	1.80	1.50
26	c	515	BCR	C5-C6	14.45	1.59	1.34
26	C	514	BCR	C5-C6	14.45	1.59	1.34
26	b	621	BCR	C5-C6	14.40	1.59	1.34
26	B	620	BCR	C36-C18	14.32	1.80	1.50
26	c	521	BCR	C5-C6	14.31	1.59	1.34
26	K	102	BCR	C36-C18	14.28	1.80	1.50
26	H	101	BCR	C20-C19	14.28	1.71	1.34
26	c	515	BCR	C36-C18	14.28	1.80	1.50
26	k	101	BCR	C5-C6	14.25	1.59	1.34
26	C	514	BCR	C36-C18	14.21	1.80	1.50
26	T	101	BCR	C16-C15	14.14	1.72	1.36
26	K	101	BCR	C16-C15	14.11	1.72	1.36
26	t	101	BCR	C16-C15	14.08	1.72	1.36
26	k	101	BCR	C36-C18	14.07	1.80	1.50
26	H	101	BCR	C36-C18	14.05	1.79	1.50
26	K	101	BCR	C5-C6	14.05	1.58	1.34
26	B	620	BCR	C16-C15	14.00	1.72	1.36
26	k	101	BCR	C16-C15	13.98	1.72	1.36
26	I	101	BCR	C36-C18	13.97	1.79	1.50
26	K	102	BCR	C5-C6	13.95	1.58	1.34
26	B	620	BCR	C5-C6	13.90	1.58	1.34
26	C	514	BCR	C16-C15	13.89	1.72	1.36
26	t	101	BCR	C5-C6	13.83	1.58	1.34
26	F	101	BCR	C16-C15	13.79	1.71	1.36
26	b	620	BCR	C36-C18	13.77	1.79	1.50
26	a	610	BCR	C16-C15	13.74	1.71	1.36
26	I	101	BCR	C5-C6	13.74	1.58	1.34
26	A	610	BCR	C36-C18	13.71	1.79	1.50
26	b	619	BCR	C36-C18	13.70	1.79	1.50
26	b	619	BCR	C16-C15	13.70	1.71	1.36
26	T	101	BCR	C36-C18	13.70	1.79	1.50
26	A	610	BCR	C16-C15	13.68	1.71	1.36
26	K	102	BCR	C16-C15	13.66	1.71	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	610	BCR	C5-C6	13.60	1.58	1.34
26	H	101	BCR	C16-C15	13.58	1.71	1.36
26	c	514	BCR	C16-C15	13.54	1.71	1.36
26	h	101	BCR	C16-C15	13.48	1.71	1.36
26	a	610	BCR	C36-C18	13.48	1.78	1.50
26	b	620	BCR	C16-C15	13.47	1.71	1.36
26	F	101	BCR	C5-C6	13.47	1.57	1.34
26	K	101	BCR	C36-C18	13.45	1.78	1.50
26	a	610	BCR	C5-C6	13.43	1.57	1.34
26	f	101	BCR	C5-C6	13.42	1.57	1.34
26	t	101	BCR	C36-C18	13.30	1.78	1.50
26	f	101	BCR	C36-C18	13.24	1.78	1.50
26	b	621	BCR	C36-C18	13.20	1.78	1.50
26	h	101	BCR	C5-C6	13.18	1.57	1.34
26	K	101	BCR	C19-C18	-13.18	1.17	1.45
26	b	621	BCR	C16-C15	13.13	1.70	1.36
26	I	101	BCR	C16-C15	13.12	1.70	1.36
26	c	515	BCR	C16-C15	13.07	1.70	1.36
26	c	521	BCR	C20-C21	13.06	1.83	1.43
26	f	101	BCR	C16-C15	13.06	1.70	1.36
26	b	621	BCR	C37-C22	13.03	1.77	1.50
26	B	618	BCR	C36-C18	13.00	1.77	1.50
26	B	619	BCR	C16-C15	13.00	1.69	1.36
26	B	618	BCR	C19-C18	-12.93	1.18	1.45
26	B	619	BCR	C5-C6	12.86	1.56	1.34
26	b	619	BCR	C5-C6	12.82	1.56	1.34
26	F	101	BCR	C36-C18	12.78	1.77	1.50
26	B	618	BCR	C5-C6	12.78	1.56	1.34
26	H	101	BCR	C5-C6	12.52	1.56	1.34
26	k	101	BCR	C19-C18	-12.46	1.19	1.45
26	a	610	BCR	C19-C18	-12.44	1.19	1.45
26	B	620	BCR	C37-C22	12.43	1.76	1.50
26	B	618	BCR	C16-C15	12.36	1.68	1.36
26	C	514	BCR	C37-C22	12.36	1.76	1.50
26	b	620	BCR	C5-C6	12.34	1.55	1.34
26	B	619	BCR	C36-C18	12.34	1.76	1.50
26	H	101	BCR	C19-C18	-12.27	1.19	1.45
26	c	515	BCR	C19-C18	-12.22	1.19	1.45
26	K	102	BCR	C37-C22	12.22	1.76	1.50
26	c	521	BCR	C16-C15	12.12	1.67	1.36
26	K	102	BCR	C19-C18	-12.10	1.19	1.45
26	A	610	BCR	C37-C22	12.09	1.75	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	610	BCR	C37-C22	12.06	1.75	1.50
26	B	619	BCR	C20-C21	12.01	1.80	1.43
26	C	514	BCR	C19-C18	-11.98	1.20	1.45
26	F	101	BCR	C20-C21	11.96	1.80	1.43
26	A	610	BCR	C19-C18	-11.90	1.20	1.45
26	t	101	BCR	C37-C22	11.87	1.75	1.50
26	b	619	BCR	C19-C18	-11.87	1.20	1.45
26	K	101	BCR	C37-C22	11.85	1.75	1.50
26	B	618	BCR	C20-C21	11.84	1.80	1.43
26	f	101	BCR	C19-C18	-11.79	1.20	1.45
26	f	101	BCR	C37-C22	11.79	1.75	1.50
26	K	102	BCR	C20-C21	11.77	1.79	1.43
26	I	101	BCR	C19-C18	-11.76	1.20	1.45
26	b	619	BCR	C20-C21	11.74	1.79	1.43
26	c	514	BCR	C19-C18	-11.74	1.20	1.45
26	B	618	BCR	C37-C22	11.74	1.75	1.50
26	k	101	BCR	C37-C22	11.70	1.75	1.50
26	B	620	BCR	C19-C18	-11.68	1.20	1.45
26	b	619	BCR	C37-C22	11.65	1.75	1.50
26	b	620	BCR	C19-C18	-11.65	1.20	1.45
26	B	619	BCR	C19-C18	-11.54	1.21	1.45
26	h	101	BCR	C19-C18	-11.53	1.21	1.45
26	k	101	BCR	C8-C7	11.53	1.67	1.33
26	t	101	BCR	C20-C21	11.49	1.79	1.43
26	t	101	BCR	C19-C18	-11.47	1.21	1.45
26	T	101	BCR	C37-C22	11.44	1.74	1.50
26	c	515	BCR	C20-C21	11.44	1.78	1.43
26	K	101	BCR	C20-C21	11.43	1.78	1.43
26	K	101	BCR	C8-C7	11.42	1.67	1.33
26	k	101	BCR	C20-C21	11.41	1.78	1.43
26	B	620	BCR	C20-C21	11.40	1.78	1.43
26	f	101	BCR	C20-C21	11.40	1.78	1.43
26	B	619	BCR	C37-C22	11.37	1.74	1.50
26	h	101	BCR	C20-C21	11.37	1.78	1.43
26	c	514	BCR	C37-C22	11.35	1.74	1.50
26	c	521	BCR	C19-C18	-11.34	1.21	1.45
26	c	515	BCR	C37-C22	11.34	1.74	1.50
26	c	521	BCR	C8-C7	11.33	1.67	1.33
26	F	101	BCR	C19-C18	-11.30	1.21	1.45
26	T	101	BCR	C20-C21	11.29	1.78	1.43
26	C	514	BCR	C20-C21	11.29	1.78	1.43
26	T	101	BCR	C19-C18	-11.29	1.21	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	514	BCR	C8-C7	11.22	1.67	1.33
26	F	101	BCR	C37-C22	11.20	1.74	1.50
24	c	510	CLA	C4B-NB	11.19	1.51	1.37
26	I	101	BCR	C20-C21	11.17	1.78	1.43
24	C	505	CLA	C4B-NB	11.16	1.51	1.37
24	C	502	CLA	C4B-NB	11.16	1.51	1.37
24	B	602	CLA	C4B-NB	11.13	1.51	1.37
26	b	620	BCR	C37-C22	11.12	1.73	1.50
24	a	609	CLA	C4B-NB	11.11	1.51	1.37
26	I	101	BCR	C37-C22	11.11	1.73	1.50
24	c	512	CLA	C4B-NB	11.09	1.51	1.37
26	A	610	BCR	C20-C21	11.09	1.77	1.43
24	b	603	CLA	C4B-NB	11.09	1.51	1.37
24	B	616	CLA	C4B-NB	11.07	1.51	1.37
24	b	615	CLA	C4B-NB	11.06	1.51	1.37
24	c	503	CLA	C4B-NB	11.06	1.51	1.37
26	C	514	BCR	C8-C7	11.06	1.66	1.33
26	h	101	BCR	C37-C22	11.05	1.73	1.50
26	b	621	BCR	C8-C7	11.03	1.66	1.33
26	A	610	BCR	C8-C7	11.03	1.66	1.33
24	c	505	CLA	C4B-NB	11.01	1.51	1.37
26	H	101	BCR	C8-C7	11.00	1.66	1.33
24	c	508	CLA	C4B-NB	10.99	1.51	1.37
24	B	617	CLA	C4B-NB	10.97	1.51	1.37
26	b	620	BCR	C20-C21	10.95	1.77	1.43
24	B	609	CLA	C4B-NB	10.95	1.51	1.37
24	B	610	CLA	C4B-NB	10.94	1.51	1.37
24	b	612	CLA	C4B-NB	10.93	1.51	1.37
26	a	610	BCR	C8-C7	10.92	1.66	1.33
24	b	605	CLA	C4B-NB	10.91	1.51	1.37
26	f	101	BCR	C8-C7	10.89	1.66	1.33
26	T	101	BCR	C8-C7	10.88	1.66	1.33
26	c	515	BCR	C8-C7	10.87	1.66	1.33
26	I	101	BCR	C8-C7	10.86	1.65	1.33
26	K	102	BCR	C8-C7	10.86	1.65	1.33
26	b	619	BCR	C8-C7	10.86	1.65	1.33
24	B	606	CLA	C4B-NB	10.86	1.51	1.37
24	c	502	CLA	C4B-NB	10.84	1.51	1.37
26	t	101	BCR	C8-C7	10.84	1.65	1.33
24	b	611	CLA	C4B-NB	10.83	1.51	1.37
26	F	101	BCR	C8-C7	10.83	1.65	1.33
24	B	611	CLA	C4B-NB	10.83	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	610	BCR	C20-C21	10.82	1.77	1.43
24	b	617	CLA	C4B-NB	10.82	1.51	1.37
24	b	613	CLA	C4B-NB	10.82	1.51	1.37
24	B	603	CLA	C4B-NB	10.82	1.51	1.37
24	c	501	CLA	C4B-NB	10.81	1.51	1.37
24	c	511	CLA	C4B-NB	10.80	1.51	1.37
26	h	101	BCR	C8-C7	10.79	1.65	1.33
24	C	511	CLA	C4B-NB	10.79	1.51	1.37
24	c	513	CLA	C4B-NB	10.79	1.51	1.37
24	b	608[A]	CLA	C4B-NB	10.76	1.51	1.37
26	B	618	BCR	C8-C7	10.76	1.65	1.33
24	B	607[A]	CLA	C4B-NB	10.73	1.51	1.37
26	B	619	BCR	C8-C7	10.72	1.65	1.33
24	D	402	CLA	C4B-NB	10.72	1.51	1.37
26	c	514	BCR	C20-C21	10.71	1.76	1.43
24	c	506	CLA	C4B-NB	10.68	1.50	1.37
26	b	620	BCR	C8-C7	10.68	1.65	1.33
24	b	608[B]	CLA	C4B-NB	10.66	1.50	1.37
24	a	607	CLA	C4B-NB	10.65	1.50	1.37
24	c	507	CLA	C4B-NB	10.63	1.50	1.37
24	b	618	CLA	C4B-NB	10.63	1.50	1.37
26	H	101	BCR	C20-C21	10.59	1.76	1.43
24	c	504	CLA	C4B-NB	10.58	1.50	1.37
24	B	607[B]	CLA	C4B-NB	10.58	1.50	1.37
24	B	608	CLA	C4B-NB	10.57	1.50	1.37
27	a	611	PL9	C18-C19	10.55	1.58	1.33
27	A	611	PL9	C18-C19	10.54	1.58	1.33
24	B	614	CLA	C4B-NB	10.53	1.50	1.37
24	b	610	CLA	C4B-NB	10.52	1.50	1.37
27	D	405	PL9	C18-C19	10.50	1.58	1.33
24	b	606	CLA	C4B-NB	10.48	1.50	1.37
24	C	503	CLA	C4B-NB	10.47	1.50	1.37
24	b	614	CLA	C4B-NB	10.46	1.50	1.37
24	c	509	CLA	C4B-NB	10.45	1.50	1.37
24	C	508	CLA	C4B-NB	10.45	1.50	1.37
24	d	403	CLA	C4B-NB	10.43	1.50	1.37
24	C	504	CLA	C4B-NB	10.40	1.50	1.37
26	B	620	BCR	C8-C7	10.39	1.64	1.33
24	B	612	CLA	C4B-NB	10.39	1.50	1.37
27	d	404	PL9	C18-C19	10.38	1.57	1.33
24	C	501	CLA	C4B-NB	10.37	1.50	1.37
24	A	606	CLA	C4B-NB	10.37	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C4B-NB	10.34	1.50	1.37
24	b	607	CLA	C4B-NB	10.34	1.50	1.37
24	C	512	CLA	C4B-NB	10.31	1.50	1.37
24	b	609	CLA	C4B-NB	10.28	1.50	1.37
24	D	404	CLA	C4B-NB	10.28	1.50	1.37
24	B	615	CLA	C4B-NB	10.26	1.50	1.37
24	b	604	CLA	C4B-NB	10.24	1.50	1.37
24	C	506	CLA	C4B-NB	10.19	1.50	1.37
24	C	513	CLA	C4B-NB	10.03	1.50	1.37
24	A	609	CLA	C4B-NB	10.02	1.50	1.37
24	C	507	CLA	C4B-NB	10.02	1.50	1.37
25	D	401	PHO	C1B-C2B	10.01	1.50	1.39
24	d	402	CLA	C4B-NB	9.96	1.50	1.37
27	D	405	PL9	C38-C39	9.94	1.56	1.33
24	a	615	CLA	C4B-NB	9.94	1.50	1.37
24	C	509	CLA	C4B-NB	9.91	1.50	1.37
26	C	514	BCR	C16-C17	9.90	1.74	1.43
24	A	607	CLA	C4B-NB	9.89	1.49	1.37
24	B	613	CLA	C4B-NB	9.86	1.49	1.37
24	B	604	CLA	C4B-NB	9.83	1.49	1.37
27	d	404	PL9	C38-C39	9.83	1.56	1.33
27	a	611	PL9	C38-C39	9.82	1.56	1.33
24	a	606	CLA	C4B-NB	9.80	1.49	1.37
27	D	405	PL9	C23-C24	9.78	1.56	1.33
25	A	608	PHO	C1B-C2B	9.73	1.50	1.39
26	T	101	BCR	C16-C17	9.70	1.73	1.43
26	B	619	BCR	C26-C25	9.69	1.51	1.34
26	H	101	BCR	C16-C17	9.68	1.73	1.43
26	K	101	BCR	C16-C17	9.68	1.73	1.43
27	A	611	PL9	C23-C24	9.68	1.56	1.33
24	b	616	CLA	C4B-NB	9.68	1.49	1.37
26	t	101	BCR	C16-C17	9.63	1.73	1.43
24	C	510	CLA	C4B-NB	9.61	1.49	1.37
26	f	101	BCR	C26-C25	9.58	1.51	1.34
26	h	101	BCR	C16-C17	9.53	1.73	1.43
27	a	611	PL9	C23-C24	9.53	1.55	1.33
25	a	608	PHO	C1B-C2B	9.52	1.50	1.39
26	k	101	BCR	C16-C17	9.51	1.72	1.43
26	b	621	BCR	C19-C18	-9.51	1.25	1.45
26	b	620	BCR	C26-C25	9.50	1.50	1.34
26	F	101	BCR	C26-C25	9.49	1.50	1.34
27	A	611	PL9	C38-C39	9.48	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	102	BCR	C16-C17	9.46	1.72	1.43
26	c	514	BCR	C16-C17	9.46	1.72	1.43
26	B	620	BCR	C16-C17	9.45	1.72	1.43
27	d	404	PL9	C23-C24	9.45	1.55	1.33
26	H	101	BCR	C37-C22	9.44	1.70	1.50
26	b	619	BCR	C16-C17	9.44	1.72	1.43
24	D	403	CLA	C4B-NB	9.38	1.49	1.37
26	A	610	BCR	C16-C17	9.31	1.72	1.43
26	b	621	BCR	C16-C17	9.23	1.72	1.43
26	I	101	BCR	C16-C17	9.20	1.71	1.43
26	F	101	BCR	C16-C17	9.13	1.71	1.43
26	a	610	BCR	C16-C17	9.10	1.71	1.43
26	b	620	BCR	C16-C17	9.04	1.71	1.43
25	d	401	PHO	C1B-C2B	8.98	1.49	1.39
26	c	521	BCR	C16-C17	8.97	1.71	1.43
27	d	404	PL9	C28-C29	8.97	1.54	1.33
26	f	101	BCR	C16-C17	8.93	1.71	1.43
24	C	508	CLA	C4D-ND	-8.92	1.25	1.37
26	c	515	BCR	C16-C17	8.85	1.70	1.43
27	a	611	PL9	C48-C49	8.83	1.57	1.32
25	d	401	PHO	C3B-C4B	8.82	1.51	1.41
27	D	405	PL9	C28-C29	8.81	1.54	1.33
26	B	619	BCR	C16-C17	8.78	1.70	1.43
27	A	611	PL9	C48-C49	8.77	1.57	1.32
27	d	404	PL9	C13-C14	8.75	1.54	1.33
27	D	405	PL9	C13-C14	8.75	1.54	1.33
26	B	618	BCR	C16-C17	8.70	1.70	1.43
26	A	610	BCR	C26-C25	8.65	1.49	1.34
26	h	101	BCR	C26-C25	8.64	1.49	1.34
26	H	101	BCR	C26-C25	8.58	1.49	1.34
24	a	615	CLA	C4D-ND	-8.55	1.26	1.37
27	a	611	PL9	C28-C29	8.52	1.53	1.33
27	D	405	PL9	C48-C49	8.50	1.56	1.32
27	A	611	PL9	C13-C14	8.50	1.53	1.33
27	D	405	PL9	C43-C44	8.50	1.53	1.33
24	D	402	CLA	C4D-ND	-8.49	1.26	1.37
27	d	404	PL9	C48-C49	8.47	1.56	1.32
24	b	604	CLA	C4D-ND	-8.45	1.26	1.37
27	A	611	PL9	C28-C29	8.44	1.53	1.33
26	I	101	BCR	C26-C25	8.42	1.49	1.34
27	a	611	PL9	C8-C9	8.41	1.53	1.33
24	b	613	CLA	C4D-ND	-8.41	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C4D-ND	-8.39	1.26	1.37
26	b	619	BCR	C26-C25	8.39	1.49	1.34
24	a	615	CLA	MG-ND	-8.37	1.89	2.05
27	d	404	PL9	C43-C44	8.34	1.53	1.33
24	B	613	CLA	C4D-ND	-8.33	1.26	1.37
27	D	405	PL9	C8-C9	8.30	1.52	1.33
24	B	606	CLA	C4D-ND	-8.30	1.26	1.37
27	A	611	PL9	C8-C9	8.29	1.52	1.33
27	a	611	PL9	C13-C14	8.29	1.52	1.33
24	A	606	CLA	MG-ND	-8.28	1.89	2.05
24	B	604	CLA	C4D-ND	-8.26	1.26	1.37
24	c	508	CLA	C4D-ND	-8.26	1.26	1.37
24	A	607	CLA	MG-ND	-8.26	1.89	2.05
26	k	101	BCR	C26-C25	8.26	1.48	1.34
24	A	609	CLA	C4D-ND	-8.24	1.26	1.37
27	A	611	PL9	C43-C44	8.23	1.52	1.33
24	b	606	CLA	C4D-ND	-8.22	1.26	1.37
27	a	611	PL9	C43-C44	8.21	1.52	1.33
33	v	201	HEM	C3D-C2D	8.18	1.54	1.36
24	D	403	CLA	C1B-NB	-8.18	1.27	1.37
24	a	606	CLA	C4D-ND	-8.17	1.26	1.37
24	D	403	CLA	C4D-ND	-8.17	1.26	1.37
24	B	615	CLA	C4D-ND	-8.14	1.26	1.37
26	A	610	BCR	C8-C9	8.13	1.63	1.45
27	d	404	PL9	O1-C4	8.12	1.41	1.23
24	b	605	CLA	C4D-ND	-8.08	1.26	1.37
27	d	404	PL9	C8-C9	8.08	1.52	1.33
24	a	606	CLA	MG-ND	-8.08	1.89	2.05
24	b	616	CLA	C4D-ND	-8.07	1.26	1.37
26	k	101	BCR	C8-C9	8.07	1.63	1.45
27	a	611	PL9	C33-C34	8.06	1.52	1.33
24	c	504	CLA	C4D-ND	-8.02	1.26	1.37
24	b	618	CLA	C4D-ND	-7.99	1.26	1.37
24	B	612	CLA	MG-ND	-7.97	1.90	2.05
24	b	609	CLA	C4D-ND	-7.97	1.26	1.37
24	A	606	CLA	C4D-ND	-7.96	1.26	1.37
24	C	506	CLA	C4D-ND	-7.95	1.26	1.37
24	B	612	CLA	C4D-ND	-7.95	1.26	1.37
24	b	614	CLA	C4D-ND	-7.94	1.26	1.37
27	A	611	PL9	C33-C34	7.93	1.52	1.33
24	B	613	CLA	MG-ND	-7.91	1.90	2.05
24	C	510	CLA	C4D-ND	-7.90	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	MG-ND	-7.89	1.90	2.05
26	K	102	BCR	C26-C25	7.89	1.48	1.34
26	c	515	BCR	C26-C25	7.89	1.48	1.34
24	D	404	CLA	MG-ND	-7.89	1.90	2.05
24	B	608	CLA	C4D-ND	-7.88	1.26	1.37
26	K	101	BCR	C8-C9	7.88	1.62	1.45
24	A	606	CLA	C3A-C2A	-7.88	1.32	1.54
24	A	609	CLA	MG-ND	-7.86	1.90	2.05
26	K	101	BCR	C26-C25	7.86	1.48	1.34
24	C	509	CLA	C4D-ND	-7.85	1.26	1.37
26	C	514	BCR	C26-C25	7.84	1.48	1.34
24	B	608	CLA	MG-ND	-7.81	1.90	2.05
27	A	611	PL9	O1-C4	7.81	1.40	1.23
24	a	606	CLA	C3A-C2A	-7.79	1.32	1.54
26	c	521	BCR	C8-C9	7.78	1.62	1.45
24	a	607	CLA	C4D-ND	-7.78	1.27	1.37
24	b	607	CLA	C4D-ND	-7.78	1.27	1.37
25	A	608	PHO	C3B-C4B	7.77	1.50	1.41
26	c	514	BCR	C8-C9	7.75	1.62	1.45
26	c	521	BCR	C26-C25	7.74	1.47	1.34
26	c	521	BCR	C17-C18	7.74	1.46	1.35
27	D	405	PL9	C33-C34	7.70	1.51	1.33
26	C	514	BCR	C8-C9	7.70	1.62	1.45
24	B	603	CLA	C4D-ND	-7.70	1.27	1.37
24	C	511	CLA	C4D-ND	-7.70	1.27	1.37
26	a	610	BCR	C8-C9	7.69	1.62	1.45
27	d	404	PL9	C33-C34	7.67	1.51	1.33
24	B	613	CLA	C1B-NB	-7.67	1.28	1.37
24	b	609	CLA	MG-ND	-7.66	1.90	2.05
24	B	613	CLA	C3A-C2A	-7.66	1.33	1.54
33	V	201	HEM	C3D-C2D	7.64	1.53	1.36
24	C	507	CLA	MG-ND	-7.63	1.90	2.05
24	D	402	CLA	C3A-C2A	-7.62	1.33	1.54
26	I	101	BCR	C8-C9	7.62	1.62	1.45
24	b	614	CLA	C3A-C2A	-7.62	1.33	1.54
24	B	608	CLA	C3A-C2A	-7.62	1.33	1.54
24	d	402	CLA	C4D-ND	-7.61	1.27	1.37
24	C	509	CLA	C1B-NB	-7.61	1.28	1.37
24	C	501	CLA	C4D-ND	-7.61	1.27	1.37
33	e	102	HEM	C3D-C2D	7.61	1.52	1.36
24	D	403	CLA	C3A-C2A	-7.60	1.33	1.54
24	C	503	CLA	C4D-ND	-7.60	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	C3A-C2A	-7.60	1.33	1.54
24	B	605	CLA	C4D-ND	-7.60	1.27	1.37
24	B	604	CLA	C1B-NB	-7.59	1.28	1.37
24	B	607[B]	CLA	C4D-ND	-7.59	1.27	1.37
24	C	511	CLA	MG-ND	-7.58	1.90	2.05
24	c	502	CLA	C4D-ND	-7.58	1.27	1.37
24	b	614	CLA	MG-ND	-7.58	1.90	2.05
24	b	605	CLA	C3A-C2A	-7.57	1.33	1.54
24	D	402	CLA	MG-ND	-7.57	1.90	2.05
24	c	505	CLA	C4D-ND	-7.56	1.27	1.37
25	D	401	PHO	C3B-C4B	7.56	1.50	1.41
24	c	503	CLA	C4D-ND	-7.56	1.27	1.37
24	C	504	CLA	C4D-ND	-7.56	1.27	1.37
24	a	609	CLA	MG-ND	-7.55	1.90	2.05
26	c	515	BCR	C8-C9	7.55	1.62	1.45
24	b	618	CLA	C3A-C2A	-7.55	1.33	1.54
24	B	611	CLA	C4D-ND	-7.54	1.27	1.37
24	b	613	CLA	MG-ND	-7.54	1.90	2.05
24	b	604	CLA	C3A-C2A	-7.53	1.33	1.54
24	B	612	CLA	C1B-NB	-7.53	1.28	1.37
24	B	607[A]	CLA	C3A-C2A	-7.53	1.33	1.54
24	B	607[B]	CLA	C3A-C2A	-7.53	1.33	1.54
24	B	609	CLA	C3A-C2A	-7.52	1.33	1.54
24	b	608[B]	CLA	C4D-ND	-7.52	1.27	1.37
24	D	404	CLA	C3A-C2A	-7.52	1.33	1.54
24	C	510	CLA	C3A-C2A	-7.51	1.33	1.54
24	b	614	CLA	C1B-NB	-7.51	1.28	1.37
24	c	506	CLA	C3A-C2A	-7.51	1.33	1.54
26	B	618	BCR	C26-C25	7.51	1.47	1.34
24	b	608[A]	CLA	C3A-C2A	-7.51	1.33	1.54
24	b	608[B]	CLA	C3A-C2A	-7.50	1.33	1.54
24	b	609	CLA	C3A-C2A	-7.49	1.33	1.54
24	C	509	CLA	MG-ND	-7.48	1.91	2.05
24	b	618	CLA	MG-ND	-7.48	1.91	2.05
26	b	621	BCR	C8-C9	7.48	1.62	1.45
24	b	612	CLA	C3A-C2A	-7.46	1.33	1.54
24	c	506	CLA	C4D-ND	-7.46	1.27	1.37
24	C	504	CLA	C3A-C2A	-7.46	1.33	1.54
24	b	611	CLA	C4D-ND	-7.44	1.27	1.37
24	C	501	CLA	C3A-C2A	-7.44	1.33	1.54
24	B	614	CLA	C3A-C2A	-7.44	1.33	1.54
24	B	615	CLA	C3A-C2A	-7.44	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	C4D-ND	-7.43	1.27	1.37
24	C	513	CLA	C4D-ND	-7.43	1.27	1.37
26	t	101	BCR	C8-C9	7.43	1.61	1.45
24	B	607[A]	CLA	C4D-ND	-7.41	1.27	1.37
24	C	509	CLA	C3A-C2A	-7.41	1.33	1.54
24	a	609	CLA	C3A-C2A	-7.41	1.33	1.54
24	C	513	CLA	MG-ND	-7.41	1.91	2.05
26	B	620	BCR	C26-C25	7.40	1.47	1.34
24	A	609	CLA	C3A-C2A	-7.40	1.33	1.54
24	a	609	CLA	C4D-ND	-7.40	1.27	1.37
24	a	607	CLA	MG-ND	-7.40	1.91	2.05
24	c	507	CLA	MG-ND	-7.40	1.91	2.05
24	c	512	CLA	C3A-C2A	-7.39	1.33	1.54
27	D	405	PL9	O1-C4	7.38	1.39	1.23
26	b	621	BCR	C26-C25	7.38	1.47	1.34
26	H	101	BCR	C8-C9	7.37	1.61	1.45
24	B	604	CLA	MG-ND	-7.37	1.91	2.05
26	f	101	BCR	C8-C9	7.37	1.61	1.45
24	c	511	CLA	C3A-C2A	-7.37	1.33	1.54
27	a	611	PL9	O1-C4	7.37	1.39	1.23
24	b	610	CLA	C4D-ND	-7.36	1.27	1.37
24	b	617	CLA	C4D-ND	-7.36	1.27	1.37
24	C	510	CLA	C1B-NB	-7.35	1.28	1.37
24	b	615	CLA	C3A-C2A	-7.35	1.33	1.54
24	b	608[A]	CLA	C4D-ND	-7.35	1.27	1.37
33	E	103	HEM	C3D-C2D	7.35	1.52	1.36
24	C	505	CLA	C4D-ND	-7.35	1.27	1.37
24	B	610	CLA	MG-ND	-7.35	1.91	2.05
26	T	101	BCR	C8-C9	7.35	1.61	1.45
24	B	603	CLA	C3A-C2A	-7.34	1.34	1.54
24	b	612	CLA	MG-ND	-7.34	1.91	2.05
24	a	615	CLA	C3A-C2A	-7.34	1.34	1.54
24	C	511	CLA	C3A-C2A	-7.33	1.34	1.54
24	a	606	CLA	C1B-NB	-7.33	1.28	1.37
24	c	504	CLA	C3A-C2A	-7.32	1.34	1.54
24	d	402	CLA	C1B-NB	-7.32	1.28	1.37
24	b	612	CLA	C4D-ND	-7.31	1.27	1.37
24	C	512	CLA	C3A-C2A	-7.31	1.34	1.54
24	C	502	CLA	C3A-C2A	-7.30	1.34	1.54
24	c	509	CLA	C3A-C2A	-7.30	1.34	1.54
24	C	508	CLA	C3A-C2A	-7.30	1.34	1.54
24	b	607	CLA	C3A-C2A	-7.30	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	502	CLA	C3A-C2A	-7.29	1.34	1.54
24	b	613	CLA	C3A-C2A	-7.29	1.34	1.54
24	D	403	CLA	MG-ND	-7.29	1.91	2.05
24	C	503	CLA	MG-ND	-7.29	1.91	2.05
24	d	402	CLA	C3A-C2A	-7.27	1.34	1.54
26	c	514	BCR	C26-C25	7.27	1.47	1.34
24	B	607[B]	CLA	MG-ND	-7.27	1.91	2.05
26	h	101	BCR	C8-C9	7.26	1.61	1.45
24	B	615	CLA	MG-ND	-7.25	1.91	2.05
26	b	619	BCR	C8-C9	7.25	1.61	1.45
24	b	606	CLA	C3A-C2A	-7.25	1.34	1.54
24	c	510	CLA	C3A-C2A	-7.25	1.34	1.54
24	d	402	CLA	MG-ND	-7.24	1.91	2.05
24	B	616	CLA	C4D-ND	-7.24	1.27	1.37
24	d	403	CLA	C3A-C2A	-7.23	1.34	1.54
24	b	615	CLA	MG-ND	-7.23	1.91	2.05
24	b	617	CLA	C3A-C2A	-7.22	1.34	1.54
26	f	101	BCR	C38-C26	7.22	1.62	1.50
24	b	616	CLA	C3A-C2A	-7.22	1.34	1.54
24	B	610	CLA	C3A-C2A	-7.22	1.34	1.54
24	b	611	CLA	C3A-C2A	-7.21	1.34	1.54
26	a	610	BCR	C26-C25	7.21	1.46	1.34
24	C	503	CLA	C3A-C2A	-7.20	1.34	1.54
26	b	620	BCR	C8-C9	7.20	1.61	1.45
24	b	603	CLA	MG-ND	-7.19	1.91	2.05
24	a	615	CLA	C1B-NB	-7.17	1.29	1.37
24	A	607	CLA	C3A-C2A	-7.17	1.34	1.54
24	c	508	CLA	C3A-C2A	-7.16	1.34	1.54
24	B	612	CLA	C3A-C2A	-7.16	1.34	1.54
24	c	504	CLA	C1B-NB	-7.16	1.29	1.37
24	C	505	CLA	C3A-C2A	-7.15	1.34	1.54
26	K	102	BCR	C8-C9	7.15	1.61	1.45
24	C	508	CLA	MG-ND	-7.14	1.91	2.05
24	c	505	CLA	C3A-C2A	-7.13	1.34	1.54
24	b	604	CLA	MG-ND	-7.13	1.91	2.05
24	B	614	CLA	MG-ND	-7.13	1.91	2.05
24	B	605	CLA	C3A-C2A	-7.12	1.34	1.54
24	B	617	CLA	C3A-C2A	-7.12	1.34	1.54
24	b	608[B]	CLA	MG-ND	-7.11	1.91	2.05
24	D	404	CLA	C4D-ND	-7.11	1.28	1.37
24	B	617	CLA	C4D-ND	-7.10	1.28	1.37
24	C	506	CLA	C3A-C2A	-7.10	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	607	CLA	C3A-C2A	-7.10	1.34	1.54
24	c	503	CLA	C3A-C2A	-7.10	1.34	1.54
24	C	507	CLA	C3A-C2A	-7.08	1.34	1.54
24	c	501	CLA	C3A-C2A	-7.08	1.34	1.54
24	c	512	CLA	C4D-ND	-7.07	1.28	1.37
24	b	606	CLA	MG-ND	-7.06	1.91	2.05
24	B	614	CLA	C4D-ND	-7.06	1.28	1.37
24	b	605	CLA	C1B-NB	-7.06	1.29	1.37
26	B	619	BCR	C8-C9	7.05	1.61	1.45
24	A	607	CLA	C4D-ND	-7.04	1.28	1.37
24	B	609	CLA	C4D-ND	-7.04	1.28	1.37
24	B	616	CLA	C3A-C2A	-7.03	1.34	1.54
24	b	605	CLA	MG-ND	-7.03	1.91	2.05
24	C	508	CLA	C1B-NB	-7.03	1.29	1.37
24	c	513	CLA	C3A-C2A	-7.03	1.34	1.54
24	B	605	CLA	C1B-NB	-7.02	1.29	1.37
24	B	604	CLA	C3A-C2A	-7.02	1.34	1.54
24	c	509	CLA	C4D-ND	-7.02	1.28	1.37
24	A	606	CLA	C1B-NB	-7.02	1.29	1.37
24	B	605	CLA	MG-ND	-7.02	1.91	2.05
24	B	611	CLA	C3A-C2A	-7.00	1.34	1.54
24	b	613	CLA	C1B-NB	-7.00	1.29	1.37
24	c	501	CLA	MG-ND	-6.99	1.91	2.05
26	B	618	BCR	C8-C9	6.99	1.61	1.45
24	C	512	CLA	MG-ND	-6.98	1.91	2.05
24	c	501	CLA	C4D-ND	-6.98	1.28	1.37
24	B	607[A]	CLA	MG-ND	-6.98	1.92	2.05
24	B	606	CLA	C3A-C2A	-6.97	1.35	1.54
24	b	603	CLA	C3A-C2A	-6.96	1.35	1.54
24	c	511	CLA	MG-ND	-6.96	1.92	2.05
24	c	507	CLA	C3A-C2A	-6.95	1.35	1.54
24	c	510	CLA	C4D-ND	-6.95	1.28	1.37
24	C	510	CLA	MG-ND	-6.95	1.92	2.05
25	a	608	PHO	C3B-C4B	6.95	1.49	1.41
24	C	504	CLA	C1B-NB	-6.94	1.29	1.37
24	C	506	CLA	MG-ND	-6.94	1.92	2.05
24	B	616	CLA	MG-ND	-6.90	1.92	2.05
24	B	602	CLA	C3A-C2A	-6.90	1.35	1.54
24	D	404	CLA	C1B-NB	-6.90	1.29	1.37
24	C	507	CLA	C4D-ND	-6.87	1.28	1.37
26	t	101	BCR	C26-C25	6.86	1.46	1.34
24	c	513	CLA	C4D-ND	-6.85	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C3A-C2A	-6.85	1.35	1.54
24	B	614	CLA	C1B-NB	-6.84	1.29	1.37
26	F	101	BCR	C8-C9	6.84	1.60	1.45
24	b	615	CLA	C4D-ND	-6.82	1.28	1.37
24	c	503	CLA	MG-ND	-6.82	1.92	2.05
24	c	510	CLA	MG-ND	-6.81	1.92	2.05
24	C	506	CLA	C1B-NB	-6.79	1.29	1.37
26	K	101	BCR	C34-C9	-6.79	1.36	1.50
24	b	608[A]	CLA	MG-ND	-6.78	1.92	2.05
24	b	618	CLA	C1B-NB	-6.78	1.29	1.37
24	C	504	CLA	MG-ND	-6.78	1.92	2.05
24	C	502	CLA	C4D-ND	-6.77	1.28	1.37
24	b	606	CLA	C1B-NB	-6.77	1.29	1.37
24	b	615	CLA	C1B-NB	-6.77	1.29	1.37
24	b	616	CLA	C1B-NB	-6.77	1.29	1.37
24	c	506	CLA	C1B-NB	-6.76	1.29	1.37
24	B	602	CLA	C4D-ND	-6.76	1.28	1.37
24	B	611	CLA	MG-ND	-6.75	1.92	2.05
24	c	501	CLA	C1B-NB	-6.75	1.29	1.37
24	b	604	CLA	C1B-NB	-6.74	1.29	1.37
26	B	619	BCR	C34-C9	-6.73	1.37	1.50
24	C	501	CLA	MG-ND	-6.72	1.92	2.05
24	b	610	CLA	MG-ND	-6.72	1.92	2.05
26	T	101	BCR	C26-C25	6.71	1.46	1.34
24	c	507	CLA	C4D-ND	-6.70	1.28	1.37
24	C	512	CLA	C1B-NB	-6.70	1.29	1.37
24	c	504	CLA	MG-ND	-6.70	1.92	2.05
26	h	101	BCR	C38-C26	6.70	1.61	1.50
24	A	607	CLA	C1B-NB	-6.70	1.29	1.37
24	c	511	CLA	C4D-ND	-6.70	1.28	1.37
26	F	101	BCR	C38-C26	6.70	1.61	1.50
24	A	609	CLA	C1B-NB	-6.69	1.29	1.37
27	a	611	PL9	O2-C1	6.68	1.42	1.24
26	B	620	BCR	C8-C9	6.67	1.60	1.45
24	c	512	CLA	MG-ND	-6.66	1.92	2.05
24	C	503	CLA	C1B-NB	-6.66	1.29	1.37
26	b	620	BCR	C38-C26	6.65	1.61	1.50
24	B	615	CLA	C1B-NB	-6.65	1.29	1.37
24	b	609	CLA	C1B-NB	-6.64	1.29	1.37
24	D	402	CLA	C1B-NB	-6.64	1.29	1.37
26	H	101	BCR	C38-C26	6.63	1.61	1.50
24	b	607	CLA	MG-ND	-6.60	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C1B-NB	-6.58	1.29	1.37
24	d	403	CLA	C4D-ND	-6.58	1.28	1.37
24	c	505	CLA	MG-ND	-6.58	1.92	2.05
24	d	403	CLA	MG-ND	-6.57	1.92	2.05
26	b	619	BCR	C34-C9	-6.55	1.37	1.50
27	A	611	PL9	O2-C1	6.55	1.42	1.24
24	b	608[B]	CLA	C1B-NB	-6.53	1.29	1.37
24	B	617	CLA	C1B-NB	-6.53	1.29	1.37
26	B	618	BCR	C34-C9	-6.53	1.37	1.50
24	B	617	CLA	MG-ND	-6.53	1.92	2.05
26	b	621	BCR	C34-C9	-6.52	1.37	1.50
24	C	513	CLA	C1B-NB	-6.51	1.29	1.37
26	I	101	BCR	C34-C9	-6.50	1.37	1.50
24	c	502	CLA	C1B-NB	-6.49	1.29	1.37
26	C	514	BCR	C34-C9	-6.49	1.37	1.50
24	B	603	CLA	C1B-NB	-6.49	1.29	1.37
24	b	611	CLA	MG-ND	-6.48	1.92	2.05
24	C	512	CLA	C4D-ND	-6.48	1.28	1.37
24	c	509	CLA	MG-ND	-6.47	1.93	2.05
24	B	609	CLA	MG-ND	-6.45	1.93	2.05
26	C	514	BCR	C17-C18	6.45	1.44	1.35
24	c	509	CLA	C1B-NB	-6.45	1.29	1.37
24	B	603	CLA	MG-ND	-6.44	1.93	2.05
26	c	514	BCR	C34-C9	-6.42	1.37	1.50
26	F	101	BCR	C34-C9	-6.42	1.37	1.50
24	b	608[A]	CLA	C1B-NB	-6.41	1.29	1.37
26	b	620	BCR	C34-C9	-6.41	1.37	1.50
24	B	607[B]	CLA	C1B-NB	-6.41	1.29	1.37
24	B	608	CLA	C1B-NB	-6.39	1.29	1.37
24	b	606	CLA	C1D-C2D	-6.37	1.32	1.45
24	C	502	CLA	C1B-NB	-6.36	1.30	1.37
24	c	508	CLA	MG-ND	-6.36	1.93	2.05
26	c	515	BCR	C34-C9	-6.35	1.37	1.50
24	a	607	CLA	C1B-NB	-6.34	1.30	1.37
24	b	617	CLA	MG-ND	-6.34	1.93	2.05
24	b	612	CLA	C1B-NB	-6.33	1.30	1.37
33	e	102	HEM	FE-ND	6.33	2.14	1.94
26	t	101	BCR	C34-C9	-6.32	1.37	1.50
24	b	610	CLA	C1B-NB	-6.31	1.30	1.37
26	I	101	BCR	C38-C26	6.31	1.61	1.50
24	B	602	CLA	MG-ND	-6.31	1.93	2.05
24	c	507	CLA	C1B-NB	-6.31	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	MG-NB	-6.30	1.93	2.05
24	d	403	CLA	C1B-NB	-6.30	1.30	1.37
24	C	502	CLA	MG-ND	-6.30	1.93	2.05
24	c	508	CLA	C1B-NB	-6.30	1.30	1.37
24	C	507	CLA	C1B-NB	-6.30	1.30	1.37
24	c	506	CLA	MG-ND	-6.29	1.93	2.05
24	B	607[A]	CLA	C1B-NB	-6.26	1.30	1.37
26	c	521	BCR	C34-C9	-6.26	1.37	1.50
24	B	606	CLA	MG-ND	-6.26	1.93	2.05
24	c	512	CLA	C1B-NB	-6.25	1.30	1.37
26	A	610	BCR	C38-C26	6.24	1.61	1.50
26	B	620	BCR	C34-C9	-6.24	1.38	1.50
27	d	404	PL9	O2-C1	6.23	1.41	1.24
27	D	405	PL9	O2-C1	6.23	1.41	1.24
26	f	101	BCR	C34-C9	-6.23	1.38	1.50
26	B	619	BCR	C24-C23	6.22	1.51	1.33
26	B	619	BCR	C38-C26	6.21	1.61	1.50
24	A	606	CLA	C1D-C2D	-6.21	1.33	1.45
26	c	521	BCR	C38-C26	6.17	1.61	1.50
24	c	505	CLA	C1B-NB	-6.16	1.30	1.37
26	K	102	BCR	C38-C26	6.16	1.61	1.50
24	c	513	CLA	C1B-NB	-6.16	1.30	1.37
24	c	502	CLA	MG-ND	-6.14	1.93	2.05
26	c	521	BCR	C11-C12	6.14	1.50	1.34
26	H	101	BCR	C34-C9	-6.13	1.38	1.50
33	v	201	HEM	FE-ND	6.13	2.13	1.94
24	C	501	CLA	C1B-NB	-6.13	1.30	1.37
26	K	102	BCR	C34-C9	-6.13	1.38	1.50
26	c	514	BCR	C38-C26	6.13	1.61	1.50
24	B	610	CLA	C1B-NB	-6.12	1.30	1.37
26	A	610	BCR	C34-C9	-6.10	1.38	1.50
26	k	101	BCR	C38-C26	6.10	1.60	1.50
26	k	101	BCR	C34-C9	-6.09	1.38	1.50
24	B	616	CLA	C1B-NB	-6.09	1.30	1.37
24	C	510	CLA	MG-NB	-6.09	1.93	2.05
26	B	620	BCR	C38-C26	6.07	1.60	1.50
26	T	101	BCR	C34-C9	-6.07	1.38	1.50
26	F	101	BCR	C23-C22	6.07	1.59	1.45
24	B	605	CLA	C1D-C2D	-6.05	1.33	1.45
26	b	621	BCR	C38-C26	6.04	1.60	1.50
26	F	101	BCR	C24-C23	6.04	1.51	1.33
26	I	101	BCR	C11-C12	6.04	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C1D-C2D	-6.03	1.33	1.45
26	h	101	BCR	C34-C9	-6.03	1.38	1.50
24	c	513	CLA	MG-ND	-6.00	1.93	2.05
24	B	613	CLA	C1D-C2D	-5.99	1.33	1.45
24	C	511	CLA	C1B-NB	-5.98	1.30	1.37
26	I	101	BCR	C17-C18	5.98	1.43	1.35
24	b	617	CLA	C1B-NB	-5.97	1.30	1.37
24	B	608	CLA	C1D-C2D	-5.97	1.33	1.45
24	C	505	CLA	MG-ND	-5.97	1.94	2.05
24	B	611	CLA	C1B-NB	-5.96	1.30	1.37
24	b	605	CLA	C1D-C2D	-5.95	1.33	1.45
24	a	606	CLA	C1D-C2D	-5.95	1.33	1.45
24	C	508	CLA	C1D-C2D	-5.94	1.33	1.45
24	c	510	CLA	C1B-NB	-5.93	1.30	1.37
26	b	619	BCR	C38-C26	5.93	1.60	1.50
26	B	618	BCR	C38-C26	5.92	1.60	1.50
26	c	515	BCR	C38-C26	5.92	1.60	1.50
24	c	503	CLA	C1B-NB	-5.91	1.30	1.37
26	a	610	BCR	C34-C9	-5.90	1.38	1.50
26	A	610	BCR	C11-C12	5.90	1.49	1.34
24	B	610	CLA	C1D-C2D	-5.89	1.33	1.45
24	B	613	CLA	MG-NB	-5.89	1.94	2.05
24	D	403	CLA	CHC-C4B	-5.89	1.26	1.39
24	C	505	CLA	C1B-NB	-5.87	1.30	1.37
24	b	613	CLA	C1D-C2D	-5.85	1.33	1.45
26	b	621	BCR	C11-C12	5.85	1.49	1.34
24	C	511	CLA	C1D-C2D	-5.85	1.33	1.45
24	C	506	CLA	C1D-C2D	-5.85	1.33	1.45
26	C	514	BCR	C38-C26	5.84	1.60	1.50
26	K	101	BCR	C38-C26	5.81	1.60	1.50
26	B	619	BCR	C23-C22	5.81	1.58	1.45
24	c	504	CLA	C1D-C2D	-5.80	1.33	1.45
26	h	101	BCR	C11-C12	5.79	1.49	1.34
26	t	101	BCR	C38-C26	5.79	1.60	1.50
24	c	505	CLA	C1D-C2D	-5.78	1.33	1.45
26	K	102	BCR	C11-C12	5.77	1.49	1.34
24	B	606	CLA	C1B-NB	-5.77	1.30	1.37
24	B	611	CLA	C1D-C2D	-5.77	1.33	1.45
24	b	616	CLA	C1D-C2D	-5.76	1.34	1.45
24	b	611	CLA	C1B-NB	-5.75	1.30	1.37
26	c	515	BCR	C11-C12	5.75	1.49	1.34
26	H	101	BCR	C24-C23	5.74	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	619	BCR	C11-C12	5.74	1.49	1.34
26	H	101	BCR	C11-C12	5.73	1.49	1.34
24	B	612	CLA	C1D-C2D	-5.73	1.34	1.45
24	c	511	CLA	C1B-NB	-5.72	1.30	1.37
24	a	615	CLA	C1D-C2D	-5.72	1.34	1.45
26	B	618	BCR	C23-C22	5.72	1.58	1.45
24	a	615	CLA	MG-NB	-5.72	1.94	2.05
24	A	609	CLA	C1D-C2D	-5.72	1.34	1.45
24	d	402	CLA	C1D-C2D	-5.71	1.34	1.45
24	B	602	CLA	C1B-NB	-5.71	1.30	1.37
24	B	609	CLA	C1B-NB	-5.70	1.30	1.37
26	b	621	BCR	C17-C18	5.70	1.43	1.35
26	C	514	BCR	C11-C12	5.70	1.49	1.34
24	b	604	CLA	C1D-C2D	-5.69	1.34	1.45
26	t	101	BCR	C11-C12	5.69	1.49	1.34
33	E	103	HEM	FE-ND	5.68	2.12	1.94
24	B	614	CLA	CHC-C4B	-5.68	1.26	1.39
26	T	101	BCR	C11-C12	5.67	1.49	1.34
24	a	609	CLA	C1D-C2D	-5.66	1.34	1.45
24	C	507	CLA	C1D-C2D	-5.66	1.34	1.45
24	B	617	CLA	CHC-C4B	-5.65	1.26	1.39
24	B	607[B]	CLA	C1D-C2D	-5.63	1.34	1.45
26	t	101	BCR	C23-C22	5.61	1.58	1.45
26	H	101	BCR	C17-C18	5.61	1.43	1.35
24	C	512	CLA	C1D-C2D	-5.61	1.34	1.45
26	a	610	BCR	C11-C12	5.60	1.49	1.34
26	c	521	BCR	C23-C22	5.60	1.58	1.45
26	c	514	BCR	C11-C12	5.60	1.49	1.34
24	D	403	CLA	C1D-C2D	-5.60	1.34	1.45
33	e	102	HEM	FE-NA	5.59	2.14	1.95
26	C	514	BCR	C23-C22	5.59	1.58	1.45
24	c	508	CLA	C1D-C2D	-5.59	1.34	1.45
24	B	604	CLA	CHC-C4B	-5.58	1.26	1.39
24	C	502	CLA	CHD-C1D	5.57	1.49	1.38
24	B	604	CLA	MG-NB	-5.57	1.94	2.05
26	A	610	BCR	C24-C23	5.57	1.49	1.33
26	a	610	BCR	C38-C26	5.57	1.60	1.50
24	b	605	CLA	MG-NB	-5.56	1.94	2.05
24	a	615	CLA	CHC-C4B	-5.56	1.26	1.39
26	a	610	BCR	C23-C22	5.55	1.57	1.45
24	b	603	CLA	C1D-C2D	-5.55	1.34	1.45
26	k	101	BCR	C11-C12	5.53	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C1D-C2D	-5.53	1.34	1.45
24	C	510	CLA	CHC-C4B	-5.53	1.27	1.39
24	b	614	CLA	C1D-C2D	-5.53	1.34	1.45
24	B	609	CLA	CHD-C1D	5.53	1.49	1.38
24	b	618	CLA	CHC-C4B	-5.53	1.27	1.39
24	D	402	CLA	C1D-C2D	-5.53	1.34	1.45
24	b	614	CLA	MG-NB	-5.53	1.94	2.05
26	K	101	BCR	C17-C18	5.53	1.43	1.35
24	C	503	CLA	C1D-C2D	-5.51	1.34	1.45
26	b	620	BCR	C24-C23	5.50	1.49	1.33
24	B	607[A]	CLA	C1D-C2D	-5.50	1.34	1.45
24	C	504	CLA	MG-NB	-5.49	1.94	2.05
24	B	603	CLA	C1D-C2D	-5.49	1.34	1.45
24	C	512	CLA	CHC-C4B	-5.49	1.27	1.39
24	b	605	CLA	CHC-C4B	-5.49	1.27	1.39
24	a	609	CLA	C1B-NB	-5.48	1.31	1.37
24	B	606	CLA	C1D-C2D	-5.48	1.34	1.45
26	T	101	BCR	C23-C22	5.47	1.57	1.45
27	D	405	PL9	C3-C4	-5.47	1.40	1.49
24	C	505	CLA	CHD-C1D	5.46	1.49	1.38
26	A	610	BCR	C23-C22	5.46	1.57	1.45
24	b	613	CLA	CHC-C4B	-5.45	1.27	1.39
26	f	101	BCR	C24-C23	5.45	1.49	1.33
24	b	611	CLA	C1D-C2D	-5.45	1.34	1.45
24	c	507	CLA	C1D-C2D	-5.44	1.34	1.45
26	B	619	BCR	C24-C25	5.44	1.64	1.45
33	V	201	HEM	FE-ND	5.43	2.11	1.94
24	B	615	CLA	C1D-C2D	-5.43	1.34	1.45
24	b	608[B]	CLA	C1D-C2D	-5.42	1.34	1.45
24	C	509	CLA	C1D-C2D	-5.42	1.34	1.45
24	B	612	CLA	MG-NB	-5.40	1.95	2.05
24	d	402	CLA	MG-NB	-5.38	1.95	2.05
26	B	620	BCR	C11-C12	5.38	1.48	1.34
26	h	101	BCR	C24-C23	5.37	1.49	1.33
24	C	513	CLA	C1D-C2D	-5.37	1.34	1.45
24	b	607	CLA	C1D-C2D	-5.36	1.34	1.45
26	B	618	BCR	C11-C12	5.36	1.48	1.34
24	B	613	CLA	CHC-C4B	-5.35	1.27	1.39
24	B	605	CLA	CHC-C4B	-5.35	1.27	1.39
24	C	508	CLA	MG-NB	-5.34	1.95	2.05
24	C	508	CLA	CHC-C4B	-5.33	1.27	1.39
26	T	101	BCR	C38-C26	5.33	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	CHD-C4C	-5.31	1.27	1.39
26	f	101	BCR	C23-C22	5.31	1.57	1.45
26	F	101	BCR	C11-C12	5.30	1.48	1.34
24	b	613	CLA	MG-NB	-5.30	1.95	2.05
24	A	609	CLA	MG-NB	-5.30	1.95	2.05
24	b	617	CLA	C1D-C2D	-5.30	1.34	1.45
26	H	101	BCR	C23-C22	5.29	1.57	1.45
24	A	606	CLA	MG-NB	-5.29	1.95	2.05
24	b	608[A]	CLA	C1D-C2D	-5.29	1.34	1.45
24	C	509	CLA	MG-NB	-5.28	1.95	2.05
24	c	506	CLA	MG-NB	-5.28	1.95	2.05
24	b	607	CLA	MG-NB	-5.28	1.95	2.05
26	h	101	BCR	C17-C18	5.27	1.42	1.35
24	a	606	CLA	CHC-C4B	-5.27	1.27	1.39
26	B	618	BCR	C24-C23	5.27	1.49	1.33
26	a	610	BCR	C24-C23	5.26	1.49	1.33
24	c	501	CLA	C1D-C2D	-5.26	1.34	1.45
24	c	509	CLA	C1D-C2D	-5.26	1.34	1.45
24	B	616	CLA	C1D-C2D	-5.25	1.35	1.45
24	c	503	CLA	C1D-C2D	-5.25	1.35	1.45
24	b	604	CLA	MG-NB	-5.25	1.95	2.05
24	c	502	CLA	MG-NB	-5.25	1.95	2.05
24	D	404	CLA	C1D-C2D	-5.24	1.35	1.45
24	b	603	CLA	C1B-NB	-5.24	1.31	1.37
24	C	509	CLA	CHC-C4B	-5.23	1.27	1.39
33	E	103	HEM	FE-NA	5.23	2.12	1.95
24	c	506	CLA	C1D-C2D	-5.23	1.35	1.45
24	C	511	CLA	CHB-C1B	5.22	1.51	1.39
26	b	619	BCR	C23-C22	5.22	1.57	1.45
24	B	617	CLA	CHB-C1B	5.22	1.51	1.39
24	B	609	CLA	CHC-C4B	-5.22	1.27	1.39
24	D	402	CLA	MG-NB	-5.22	1.95	2.05
24	b	612	CLA	CHD-C1D	5.21	1.48	1.38
24	C	505	CLA	C1D-C2D	-5.19	1.35	1.45
24	C	501	CLA	C1D-C2D	-5.19	1.35	1.45
24	C	506	CLA	MG-NB	-5.19	1.95	2.05
26	B	620	BCR	C17-C18	5.18	1.42	1.35
25	A	608	PHO	C1D-C2D	5.18	1.45	1.39
24	a	606	CLA	MG-NB	-5.18	1.95	2.05
26	K	101	BCR	C24-C23	5.17	1.48	1.33
24	b	609	CLA	C1D-C2D	-5.17	1.35	1.45
24	b	618	CLA	MG-NB	-5.17	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	C1D-C2D	-5.17	1.35	1.45
24	D	404	CLA	CHC-C4B	-5.17	1.27	1.39
24	C	506	CLA	CHC-C4B	-5.17	1.27	1.39
24	B	617	CLA	MG-NB	-5.15	1.95	2.05
24	b	610	CLA	C1D-C2D	-5.15	1.35	1.45
24	B	614	CLA	C1D-C2D	-5.15	1.35	1.45
24	c	510	CLA	C1D-C2D	-5.14	1.35	1.45
26	b	620	BCR	C11-C12	5.14	1.47	1.34
26	c	515	BCR	C24-C23	5.14	1.48	1.33
24	b	603	CLA	CHB-C1B	5.13	1.50	1.39
24	c	505	CLA	CHB-C1B	5.13	1.50	1.39
24	c	512	CLA	C1D-C2D	-5.13	1.35	1.45
24	c	504	CLA	CHC-C4B	-5.12	1.27	1.39
24	B	603	CLA	CHC-C1C	5.12	1.48	1.38
24	A	607	CLA	CHC-C4B	-5.11	1.27	1.39
24	c	511	CLA	C1D-C2D	-5.11	1.35	1.45
24	C	513	CLA	CHD-C1D	5.11	1.48	1.38
24	b	614	CLA	CHC-C4B	-5.11	1.27	1.39
24	c	513	CLA	CHD-C1D	5.10	1.48	1.38
26	b	619	BCR	C11-C12	5.10	1.47	1.34
24	c	513	CLA	C1D-C2D	-5.10	1.35	1.45
26	f	101	BCR	C11-C12	5.10	1.47	1.34
24	C	501	CLA	CHD-C1D	5.09	1.48	1.38
24	A	606	CLA	CHC-C4B	-5.09	1.28	1.39
24	b	618	CLA	CHB-C1B	5.08	1.50	1.39
24	b	606	CLA	CHC-C4B	-5.08	1.28	1.39
24	b	608[A]	CLA	CHD-C1D	5.08	1.48	1.38
24	b	611	CLA	MG-NB	-5.07	1.95	2.05
24	c	512	CLA	CHC-C4B	-5.07	1.28	1.39
24	c	506	CLA	CHD-C1D	5.07	1.48	1.38
24	c	505	CLA	CHC-C4B	-5.06	1.28	1.39
24	c	505	CLA	CHD-C1D	5.06	1.48	1.38
30	l	102	LHG	O8-C23	5.05	1.48	1.33
24	c	501	CLA	CHD-C1D	5.05	1.48	1.38
24	C	504	CLA	CHC-C4B	-5.04	1.28	1.39
24	B	614	CLA	CHB-C1B	5.04	1.50	1.39
24	A	607	CLA	C1D-C2D	-5.04	1.35	1.45
24	d	403	CLA	CHC-C4B	-5.04	1.28	1.39
26	C	514	BCR	C24-C23	5.03	1.48	1.33
24	b	608[B]	CLA	CHD-C1D	5.03	1.48	1.38
24	d	403	CLA	CHB-C1B	5.03	1.50	1.39
24	B	609	CLA	C1D-C2D	-5.03	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	606	CLA	CHD-C4C	-5.03	1.27	1.39
24	C	503	CLA	MG-NB	-5.03	1.95	2.05
24	B	609	CLA	CHB-C1B	5.03	1.50	1.39
24	C	504	CLA	CHD-C1D	5.03	1.48	1.38
24	c	502	CLA	C1D-C2D	-5.03	1.35	1.45
24	b	603	CLA	CHC-C4B	-5.02	1.28	1.39
26	b	619	BCR	C24-C23	5.02	1.48	1.33
24	B	602	CLA	C1D-C2D	-5.02	1.35	1.45
24	D	402	CLA	CHD-C1D	5.02	1.48	1.38
24	C	505	CLA	CHC-C4B	-5.01	1.28	1.39
29	c	520	LMG	O7-C10	5.00	1.48	1.34
24	b	607	CLA	CHC-C4B	-5.00	1.28	1.39
24	C	502	CLA	MG-NB	-4.99	1.95	2.05
26	B	620	BCR	C23-C22	4.99	1.56	1.45
24	a	609	CLA	CHB-C1B	4.99	1.50	1.39
24	b	615	CLA	CHC-C4B	-4.98	1.28	1.39
24	b	612	CLA	C1D-C2D	-4.98	1.35	1.45
29	C	518	LMG	O7-C10	4.97	1.48	1.34
24	c	504	CLA	MG-NB	-4.97	1.95	2.05
24	c	507	CLA	CHC-C4B	-4.97	1.28	1.39
24	c	502	CLA	CHD-C1D	4.97	1.48	1.38
24	d	403	CLA	C1D-C2D	-4.97	1.35	1.45
24	b	610	CLA	CHC-C4B	-4.97	1.28	1.39
24	C	502	CLA	CHC-C4B	-4.96	1.28	1.39
26	K	101	BCR	C11-C12	4.96	1.47	1.34
24	d	402	CLA	CHC-C4B	-4.96	1.28	1.39
24	b	617	CLA	CHC-C4B	-4.96	1.28	1.39
24	C	510	CLA	CHD-C1D	4.96	1.48	1.38
24	B	617	CLA	C1D-C2D	-4.95	1.35	1.45
24	c	506	CLA	CHC-C4B	-4.95	1.28	1.39
24	a	606	CLA	CHD-C4C	-4.95	1.27	1.39
24	b	617	CLA	C4C-C3C	-4.95	1.36	1.45
26	A	610	BCR	C24-C25	4.95	1.62	1.45
24	B	615	CLA	MG-NB	-4.94	1.96	2.05
24	a	607	CLA	C1D-C2D	-4.94	1.35	1.45
26	F	101	BCR	C24-C25	4.94	1.62	1.45
29	a	613	LMG	O7-C10	4.93	1.48	1.34
24	c	509	CLA	CHC-C4B	-4.93	1.28	1.39
24	B	607[A]	CLA	MG-NB	-4.93	1.96	2.05
24	b	612	CLA	CHC-C4B	-4.93	1.28	1.39
26	c	514	BCR	C24-C23	4.93	1.48	1.33
24	c	510	CLA	CHC-C4B	-4.92	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	CHD-C1D	4.92	1.48	1.38
26	c	515	BCR	C23-C22	4.92	1.56	1.45
26	K	101	BCR	C23-C22	4.92	1.56	1.45
24	B	608	CLA	CHC-C4B	-4.92	1.28	1.39
24	c	513	CLA	MG-NB	-4.92	1.96	2.05
24	c	511	CLA	CHB-C1B	4.92	1.50	1.39
26	k	101	BCR	C24-C23	4.92	1.47	1.33
24	D	403	CLA	C4C-C3C	-4.92	1.36	1.45
24	c	502	CLA	CHC-C4B	-4.91	1.28	1.39
24	B	617	CLA	CHD-C1D	4.91	1.47	1.38
24	a	607	CLA	CHD-C1D	4.91	1.47	1.38
24	B	610	CLA	CHC-C4B	-4.90	1.28	1.39
24	c	510	CLA	CHB-C1B	4.90	1.50	1.39
24	C	513	CLA	MG-NB	-4.90	1.96	2.05
24	C	507	CLA	CHC-C4B	-4.90	1.28	1.39
24	B	607[B]	CLA	CHC-C4B	-4.90	1.28	1.39
24	A	607	CLA	CHD-C4C	-4.90	1.28	1.39
24	C	511	CLA	CHC-C4B	-4.89	1.28	1.39
24	B	608	CLA	CHD-C4C	-4.89	1.28	1.39
24	C	510	CLA	C1D-C2D	-4.89	1.35	1.45
26	b	620	BCR	C24-C25	4.88	1.62	1.45
24	D	402	CLA	CHC-C4B	-4.88	1.28	1.39
24	b	603	CLA	C4C-C3C	-4.88	1.36	1.45
24	D	404	CLA	CHD-C1D	4.87	1.47	1.38
24	c	512	CLA	CHB-C1B	4.87	1.50	1.39
24	b	616	CLA	CHD-C4C	-4.87	1.28	1.39
24	c	507	CLA	CHD-C1D	4.87	1.47	1.38
26	t	101	BCR	C24-C23	4.87	1.47	1.33
24	d	403	CLA	C4C-C3C	-4.87	1.36	1.45
24	c	511	CLA	CHD-C1D	4.86	1.47	1.38
26	T	101	BCR	C24-C23	4.86	1.47	1.33
26	f	101	BCR	C24-C25	4.86	1.62	1.45
24	B	606	CLA	CHC-C4B	-4.85	1.28	1.39
24	C	505	CLA	CHB-C1B	4.85	1.50	1.39
24	b	604	CLA	CHD-C1D	4.85	1.47	1.38
24	C	503	CLA	CHD-C4C	-4.84	1.28	1.39
24	b	608[A]	CLA	MG-NB	-4.84	1.96	2.05
24	B	613	CLA	CHD-C1D	4.84	1.47	1.38
24	B	614	CLA	CHD-C1D	4.83	1.47	1.38
24	b	617	CLA	CHD-C4C	-4.83	1.28	1.39
24	b	615	CLA	CHD-C1D	4.83	1.47	1.38
26	k	101	BCR	C17-C18	4.83	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	CHB-C1B	4.83	1.50	1.39
24	b	609	CLA	CHD-C4C	-4.82	1.28	1.39
30	d	407	LHG	O8-C23	4.82	1.47	1.33
24	c	508	CLA	MG-NB	-4.81	1.96	2.05
24	b	606	CLA	CHC-C1C	4.81	1.48	1.38
24	B	602	CLA	CHD-C1D	4.81	1.47	1.38
24	c	501	CLA	MG-NB	-4.80	1.96	2.05
24	B	612	CLA	CHC-C4B	-4.80	1.28	1.39
24	C	501	CLA	CHC-C1C	4.80	1.48	1.38
24	C	502	CLA	CHB-C1B	4.80	1.50	1.39
24	b	608[B]	CLA	CHC-C4B	-4.80	1.28	1.39
24	b	616	CLA	CHC-C4B	-4.80	1.28	1.39
24	b	610	CLA	CHD-C1D	4.79	1.47	1.38
24	C	507	CLA	CHD-C4C	-4.79	1.28	1.39
24	C	504	CLA	C1D-C2D	-4.79	1.35	1.45
24	c	508	CLA	CHC-C4B	-4.79	1.28	1.39
24	c	512	CLA	CHD-C1D	4.79	1.47	1.38
24	b	609	CLA	CHC-C4B	-4.79	1.28	1.39
24	C	510	CLA	C1C-NC	-4.79	1.30	1.37
24	A	609	CLA	CHD-C4C	-4.78	1.28	1.39
24	B	602	CLA	CHC-C4B	-4.78	1.28	1.39
24	A	609	CLA	CHD-C1D	4.78	1.47	1.38
24	B	615	CLA	CHC-C4B	-4.78	1.28	1.39
24	c	513	CLA	CHC-C4B	-4.78	1.28	1.39
29	c	519	LMG	O7-C10	4.78	1.47	1.34
24	c	511	CLA	CHD-C4C	-4.77	1.28	1.39
24	d	403	CLA	CHD-C4C	-4.77	1.28	1.39
26	c	515	BCR	C17-C18	4.77	1.42	1.35
26	B	620	BCR	C24-C23	4.77	1.47	1.33
26	b	619	BCR	C17-C18	4.76	1.42	1.35
24	b	607	CLA	CHD-C4C	-4.76	1.28	1.39
30	D	406	LHG	O8-C23	4.76	1.47	1.33
24	a	609	CLA	CHD-C4C	-4.76	1.28	1.39
24	b	613	CLA	CHB-C1B	4.76	1.50	1.39
26	c	514	BCR	C17-C18	4.76	1.42	1.35
24	B	610	CLA	CHB-C1B	4.76	1.50	1.39
24	B	607[A]	CLA	CHC-C4B	-4.76	1.28	1.39
24	C	503	CLA	CHC-C1C	4.75	1.48	1.38
24	C	512	CLA	CHD-C4C	-4.75	1.28	1.39
26	b	620	BCR	C23-C22	4.75	1.56	1.45
26	h	101	BCR	C23-C22	4.74	1.56	1.45
24	b	612	CLA	CHB-C1B	4.74	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C4C-C3C	-4.74	1.36	1.45
26	K	102	BCR	C23-C22	4.74	1.56	1.45
24	b	610	CLA	MG-NB	-4.74	1.96	2.05
24	A	609	CLA	C4C-C3C	-4.73	1.36	1.45
24	D	404	CLA	MG-NB	-4.73	1.96	2.05
24	a	607	CLA	CHC-C4B	-4.73	1.28	1.39
24	B	612	CLA	CHD-C1D	4.73	1.47	1.38
24	B	614	CLA	C4C-C3C	-4.72	1.36	1.45
24	C	503	CLA	CHC-C4B	-4.72	1.28	1.39
26	I	101	BCR	C23-C22	4.72	1.56	1.45
24	B	607[A]	CLA	CHD-C1D	4.72	1.47	1.38
24	c	503	CLA	CHB-C1B	4.72	1.50	1.39
24	B	610	CLA	MG-NB	-4.72	1.96	2.05
24	a	615	CLA	CHD-C1D	4.72	1.47	1.38
24	b	604	CLA	CHC-C1C	4.72	1.48	1.38
24	c	508	CLA	CHD-C1D	4.71	1.47	1.38
24	c	501	CLA	CHB-C1B	4.71	1.50	1.39
24	B	605	CLA	CHD-C1D	4.71	1.47	1.38
24	A	607	CLA	CHD-C1D	4.71	1.47	1.38
24	D	404	CLA	CHD-C4C	-4.71	1.28	1.39
29	C	519	LMG	O7-C10	4.70	1.47	1.34
24	B	616	CLA	CHD-C4C	-4.70	1.28	1.39
26	I	101	BCR	C24-C23	4.69	1.47	1.33
26	B	619	BCR	C17-C18	4.69	1.42	1.35
24	b	617	CLA	MG-NB	-4.68	1.96	2.05
24	b	615	CLA	CHD-C4C	-4.68	1.28	1.39
24	b	611	CLA	CHD-C1D	4.68	1.47	1.38
24	B	602	CLA	MG-NB	-4.68	1.96	2.05
24	c	511	CLA	CHC-C4B	-4.68	1.28	1.39
24	B	603	CLA	CHD-C1D	4.68	1.47	1.38
24	b	611	CLA	CHD-C4C	-4.67	1.28	1.39
24	b	613	CLA	CHD-C4C	-4.67	1.28	1.39
24	C	509	CLA	CHD-C4C	-4.67	1.28	1.39
24	B	610	CLA	CHD-C4C	-4.67	1.28	1.39
24	b	612	CLA	MG-NB	-4.66	1.96	2.05
24	c	505	CLA	MG-NB	-4.66	1.96	2.05
24	a	607	CLA	CHD-C4C	-4.66	1.28	1.39
24	b	616	CLA	C4C-C3C	-4.66	1.37	1.45
24	A	607	CLA	C1C-NC	-4.66	1.30	1.37
24	B	607[B]	CLA	CHD-C1D	4.65	1.47	1.38
24	B	615	CLA	CHD-C1D	4.65	1.47	1.38
24	a	615	CLA	C1C-NC	-4.65	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	CHD-C1D	4.65	1.47	1.38
26	K	102	BCR	C24-C23	4.65	1.47	1.33
24	C	505	CLA	MG-NB	-4.65	1.96	2.05
24	a	607	CLA	CHC-C1C	4.65	1.48	1.38
24	b	608[A]	CLA	CHC-C4B	-4.64	1.29	1.39
24	b	609	CLA	CHD-C1D	4.64	1.47	1.38
24	C	512	CLA	CHB-C1B	4.64	1.49	1.39
24	d	402	CLA	CHD-C1D	4.64	1.47	1.38
24	b	615	CLA	C4C-C3C	-4.63	1.37	1.45
24	b	615	CLA	CHB-C1B	4.63	1.49	1.39
32	E	101	DGD	O2G-C1B	4.63	1.47	1.34
24	c	507	CLA	CHB-C1B	4.62	1.49	1.39
24	a	615	CLA	CHD-C4C	-4.62	1.28	1.39
24	A	607	CLA	MG-NB	-4.62	1.96	2.05
24	B	611	CLA	MG-NB	-4.62	1.96	2.05
27	a	611	PL9	C3-C4	-4.61	1.41	1.49
24	A	609	CLA	C1C-NC	-4.61	1.30	1.37
24	B	603	CLA	MG-NB	-4.61	1.96	2.05
24	B	606	CLA	MG-NB	-4.61	1.96	2.05
24	b	611	CLA	CHB-C1B	4.61	1.49	1.39
24	b	616	CLA	CHD-C1D	4.61	1.47	1.38
27	d	404	PL9	C3-C4	-4.60	1.41	1.49
26	c	514	BCR	C23-C22	4.60	1.55	1.45
24	c	503	CLA	CHD-C1D	4.60	1.47	1.38
24	C	513	CLA	CHB-C1B	4.60	1.49	1.39
24	b	611	CLA	CHC-C4B	-4.60	1.29	1.39
29	z	101	LMG	O7-C10	4.60	1.47	1.34
24	B	611	CLA	CHC-C4B	-4.59	1.29	1.39
24	c	507	CLA	MG-NB	-4.59	1.96	2.05
24	B	607[B]	CLA	MG-NB	-4.59	1.96	2.05
24	D	403	CLA	CHD-C4C	-4.59	1.28	1.39
24	c	510	CLA	CHD-C4C	-4.59	1.28	1.39
26	K	101	BCR	C24-C25	4.59	1.61	1.45
24	c	501	CLA	CHC-C4B	-4.59	1.29	1.39
24	B	612	CLA	CHD-C4C	-4.59	1.28	1.39
24	b	604	CLA	CHC-C4B	-4.58	1.29	1.39
24	B	603	CLA	CHC-C4B	-4.58	1.29	1.39
24	d	403	CLA	CHD-C1D	4.58	1.47	1.38
24	b	609	CLA	C4C-C3C	-4.58	1.37	1.45
24	b	603	CLA	C1C-NC	-4.58	1.31	1.37
32	d	405	DGD	O2G-C1B	4.57	1.47	1.34
24	A	609	CLA	CHC-C4B	-4.57	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	CHD-C4C	-4.57	1.28	1.39
24	C	513	CLA	CHC-C4B	-4.57	1.29	1.39
28	X	101	SQD	O48-C23	4.57	1.46	1.33
24	B	614	CLA	CHD-C4C	-4.56	1.28	1.39
24	b	606	CLA	CHD-C1D	4.56	1.47	1.38
24	D	402	CLA	CMA-C3A	-4.56	1.43	1.53
24	B	614	CLA	MG-NB	-4.56	1.96	2.05
24	c	503	CLA	CHC-C1C	4.56	1.47	1.38
24	C	513	CLA	CHC-C1C	4.55	1.47	1.38
24	b	616	CLA	CHC-C1C	4.55	1.47	1.38
29	A	613	LMG	O7-C10	4.55	1.47	1.34
24	b	609	CLA	CHC-C1C	4.55	1.47	1.38
24	B	611	CLA	CHD-C1D	4.55	1.47	1.38
24	B	602	CLA	CHD-C4C	-4.55	1.28	1.39
24	B	605	CLA	CHD-C4C	-4.55	1.28	1.39
24	b	606	CLA	CHD-C4C	-4.55	1.28	1.39
24	c	507	CLA	CHD-C4C	-4.54	1.28	1.39
26	c	521	BCR	C24-C23	4.54	1.46	1.33
24	c	501	CLA	CHC-C1C	4.54	1.47	1.38
24	C	504	CLA	C4C-C3C	-4.54	1.37	1.45
24	B	616	CLA	CHC-C1C	4.54	1.47	1.38
24	B	608	CLA	CHB-C1B	4.53	1.49	1.39
24	C	501	CLA	MG-NB	-4.53	1.96	2.05
24	B	607[B]	CLA	CHD-C4C	-4.53	1.28	1.39
24	c	511	CLA	C1C-NC	-4.53	1.31	1.37
24	B	616	CLA	CHC-C4B	-4.53	1.29	1.39
27	a	611	PL9	C7-C3	4.53	1.55	1.51
24	C	506	CLA	CHD-C1D	4.53	1.47	1.38
30	L	101	LHG	O8-C23	4.53	1.46	1.33
24	C	512	CLA	C4C-C3C	-4.53	1.37	1.45
24	c	509	CLA	CHD-C4C	-4.53	1.28	1.39
24	b	615	CLA	MG-NB	-4.53	1.96	2.05
24	b	608[B]	CLA	MG-NB	-4.53	1.96	2.05
24	c	509	CLA	CHB-C1B	4.53	1.49	1.39
24	b	605	CLA	CHD-C4C	-4.53	1.28	1.39
24	B	606	CLA	CHB-C1B	4.52	1.49	1.39
24	c	504	CLA	CHC-C1C	4.52	1.47	1.38
24	a	606	CLA	CHB-C1B	4.52	1.49	1.39
28	x	101	SQD	O48-C23	4.52	1.46	1.33
24	C	511	CLA	CHD-C4C	-4.52	1.28	1.39
24	b	614	CLA	CHB-C1B	4.52	1.49	1.39
24	c	503	CLA	CHC-C4B	-4.51	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	MG-NB	-4.51	1.96	2.05
24	b	618	CLA	CHD-C1D	4.51	1.47	1.38
24	A	609	CLA	CHB-C1B	4.51	1.49	1.39
26	K	102	BCR	C17-C18	4.50	1.41	1.35
26	H	101	BCR	C24-C25	4.50	1.61	1.45
24	c	509	CLA	CHD-C1D	4.50	1.47	1.38
24	a	609	CLA	CHC-C4B	-4.50	1.29	1.39
24	C	508	CLA	CHD-C4C	-4.50	1.28	1.39
30	E	102	LHG	O7-C7	4.50	1.47	1.34
24	c	511	CLA	CHC-C1C	4.49	1.47	1.38
24	C	512	CLA	MG-NB	-4.49	1.96	2.05
24	B	607[A]	CLA	CHD-C4C	-4.49	1.28	1.39
24	B	605	CLA	MG-NB	-4.49	1.96	2.05
24	d	403	CLA	C1C-NC	-4.49	1.31	1.37
24	A	606	CLA	CHB-C1B	4.49	1.49	1.39
26	T	101	BCR	C17-C18	4.49	1.41	1.35
24	C	503	CLA	C4C-C3C	-4.49	1.37	1.45
24	b	603	CLA	MG-NB	-4.48	1.96	2.05
24	c	503	CLA	MG-NB	-4.48	1.96	2.05
28	X	101	SQD	O47-C7	4.48	1.46	1.34
26	k	101	BCR	C24-C25	4.48	1.61	1.45
24	b	606	CLA	MG-NB	-4.48	1.96	2.05
24	b	618	CLA	CHD-C4C	-4.48	1.29	1.39
28	a	614	SQD	O48-C23	4.48	1.46	1.33
24	D	404	CLA	CHC-C1C	4.47	1.47	1.38
28	A	614	SQD	O48-C23	4.47	1.46	1.33
26	k	101	BCR	C23-C22	4.47	1.55	1.45
24	c	508	CLA	CHC-C1C	4.47	1.47	1.38
30	D	407	LHG	O7-C7	4.47	1.46	1.34
24	b	614	CLA	CHD-C4C	-4.46	1.29	1.39
24	c	510	CLA	CHC-C1C	4.46	1.47	1.38
24	C	501	CLA	CHC-C4B	-4.46	1.29	1.39
27	A	611	PL9	C3-C4	-4.46	1.42	1.49
24	D	403	CLA	CHD-C1D	4.46	1.47	1.38
24	b	609	CLA	C1C-NC	-4.46	1.31	1.37
24	c	511	CLA	C4C-C3C	-4.46	1.37	1.45
24	b	605	CLA	CHD-C1D	4.45	1.47	1.38
28	x	101	SQD	O47-C7	4.45	1.46	1.34
24	b	611	CLA	CHC-C1C	4.45	1.47	1.38
24	B	608	CLA	C4C-C3C	-4.44	1.37	1.45
24	B	607[B]	CLA	CHB-C1B	4.44	1.49	1.39
24	C	510	CLA	CHD-C4C	-4.44	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	608[B]	CLA	CHB-C1B	4.43	1.49	1.39
29	Z	101	LMG	O7-C10	4.43	1.46	1.34
24	c	512	CLA	MG-NB	-4.43	1.97	2.05
24	b	616	CLA	CHB-C1B	4.43	1.49	1.39
24	c	510	CLA	CHD-C1D	4.43	1.47	1.38
28	b	601	SQD	O47-C7	4.43	1.46	1.34
24	b	610	CLA	CHB-C1B	4.43	1.49	1.39
24	b	617	CLA	CHD-C1D	4.42	1.47	1.38
24	b	608[A]	CLA	CHB-C1B	4.42	1.49	1.39
24	B	617	CLA	CHD-C4C	-4.42	1.29	1.39
24	C	504	CLA	C1C-NC	-4.42	1.31	1.37
24	B	615	CLA	CHD-C4C	-4.42	1.29	1.39
30	e	101	LHG	O7-C7	4.42	1.46	1.34
24	c	503	CLA	CHD-C4C	-4.41	1.29	1.39
24	C	503	CLA	CHB-C1B	4.41	1.49	1.39
28	b	601	SQD	O48-C23	4.41	1.46	1.33
24	A	606	CLA	C4C-C3C	-4.41	1.37	1.45
28	l	101	SQD	O47-C7	4.41	1.46	1.34
28	B	622	SQD	O48-C23	4.40	1.46	1.33
24	d	402	CLA	C1C-NC	-4.40	1.31	1.37
28	B	622	SQD	O47-C7	4.40	1.46	1.34
24	A	607	CLA	CHB-C1B	4.40	1.49	1.39
26	B	620	BCR	C40-C30	4.40	1.62	1.53
24	B	610	CLA	CHD-C1D	4.39	1.46	1.38
24	b	616	CLA	MG-NB	-4.39	1.97	2.05
30	e	101	LHG	O8-C23	4.39	1.46	1.33
24	C	502	CLA	C1D-C2D	-4.39	1.36	1.45
26	K	102	BCR	C40-C30	4.39	1.62	1.53
24	c	502	CLA	CHB-C1B	4.39	1.49	1.39
24	B	604	CLA	CHB-C1B	4.39	1.49	1.39
24	B	616	CLA	CHD-C1D	4.39	1.46	1.38
24	c	512	CLA	CHD-C4C	-4.39	1.29	1.39
24	c	510	CLA	MG-NB	-4.39	1.97	2.05
24	C	501	CLA	CHB-C1B	4.39	1.49	1.39
28	L	102	SQD	O47-C7	4.38	1.46	1.34
24	B	616	CLA	C4C-C3C	-4.38	1.37	1.45
24	a	606	CLA	CHC-C1C	4.38	1.47	1.38
24	c	506	CLA	CHB-C1B	4.38	1.49	1.39
24	c	512	CLA	CHC-C1C	4.37	1.47	1.38
24	C	506	CLA	CHD-C4C	-4.37	1.29	1.39
24	d	402	CLA	CHD-C4C	-4.37	1.29	1.39
24	b	607	CLA	CHD-C1D	4.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	608[B]	CLA	CHC-C1C	4.37	1.47	1.38
24	C	508	CLA	C1D-ND	-4.37	1.32	1.37
24	C	511	CLA	CHD-C1D	4.37	1.46	1.38
24	D	404	CLA	CHB-C1B	4.36	1.49	1.39
24	C	507	CLA	MG-NB	-4.36	1.97	2.05
24	A	607	CLA	CHC-C1C	4.36	1.47	1.38
24	B	613	CLA	CHD-C4C	-4.36	1.29	1.39
24	B	602	CLA	CHB-C1B	4.36	1.49	1.39
24	B	608	CLA	MG-NB	-4.36	1.97	2.05
24	b	613	CLA	C1D-ND	-4.36	1.32	1.37
24	b	609	CLA	MG-NB	-4.36	1.97	2.05
24	B	608	CLA	CHD-C1D	4.36	1.46	1.38
24	c	509	CLA	C4C-C3C	-4.36	1.37	1.45
24	B	607[A]	CLA	CHB-C1B	4.36	1.49	1.39
24	c	504	CLA	CHD-C1D	4.35	1.46	1.38
24	B	606	CLA	C4C-C3C	-4.35	1.37	1.45
24	b	607	CLA	CHC-C1C	4.35	1.47	1.38
24	b	604	CLA	CHD-C4C	-4.35	1.29	1.39
24	b	604	CLA	C1C-NC	-4.35	1.31	1.37
24	c	509	CLA	CHC-C1C	4.35	1.47	1.38
30	E	102	LHG	O8-C23	4.35	1.46	1.33
32	C	515	DGD	O2G-C1B	4.35	1.46	1.34
24	a	609	CLA	CHC-C1C	4.35	1.47	1.38
24	b	618	CLA	C3B-C4B	-4.34	1.32	1.42
24	b	606	CLA	CHB-C1B	4.34	1.49	1.39
24	B	603	CLA	CHD-C4C	-4.34	1.29	1.39
24	C	508	CLA	CHB-C1B	4.34	1.49	1.39
24	b	617	CLA	CHB-C1B	4.34	1.49	1.39
24	C	509	CLA	CHD-C1D	4.34	1.46	1.38
24	a	607	CLA	C1C-NC	-4.34	1.31	1.37
24	c	506	CLA	CHC-C1C	4.33	1.47	1.38
30	a	616	LHG	O8-C23	4.33	1.46	1.33
24	b	614	CLA	CHC-C1C	4.33	1.47	1.38
24	B	611	CLA	CHD-C4C	-4.33	1.29	1.39
29	b	622	LMG	O7-C10	4.33	1.46	1.34
24	B	606	CLA	CHC-C1C	4.33	1.47	1.38
24	b	618	CLA	C4C-C3C	-4.33	1.37	1.45
24	B	616	CLA	CHB-C1B	4.32	1.49	1.39
26	I	101	BCR	C24-C25	4.32	1.60	1.45
24	C	510	CLA	C3B-C4B	-4.32	1.32	1.42
24	c	513	CLA	CHC-C1C	4.32	1.47	1.38
24	B	606	CLA	CHD-C1D	4.32	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	CHD-C4C	-4.32	1.29	1.39
24	b	608[A]	CLA	CHC-C1C	4.32	1.47	1.38
24	c	509	CLA	MG-NB	-4.32	1.97	2.05
24	B	616	CLA	MG-NB	-4.31	1.97	2.05
29	B	621	LMG	O7-C10	4.31	1.46	1.34
24	D	403	CLA	CMA-C3A	-4.31	1.43	1.53
24	c	513	CLA	C4C-C3C	-4.31	1.37	1.45
24	C	504	CLA	CMA-C3A	-4.31	1.43	1.53
24	a	607	CLA	CHB-C1B	4.31	1.49	1.39
24	B	604	CLA	C3B-C4B	-4.31	1.32	1.42
24	C	507	CLA	CHD-C1D	4.31	1.46	1.38
24	C	512	CLA	CHD-C1D	4.30	1.46	1.38
24	b	616	CLA	C1C-NC	-4.30	1.31	1.37
26	c	521	BCR	C40-C30	4.30	1.62	1.53
24	a	606	CLA	CHD-C1D	4.30	1.46	1.38
24	C	511	CLA	CHC-C1C	4.29	1.47	1.38
26	b	619	BCR	C24-C25	4.29	1.60	1.45
24	d	403	CLA	CHC-C1C	4.29	1.47	1.38
24	B	605	CLA	CHB-C1B	4.29	1.49	1.39
24	a	607	CLA	MG-NB	-4.29	1.97	2.05
24	a	609	CLA	CHD-C1D	4.29	1.46	1.38
24	b	613	CLA	CHD-C1D	4.29	1.46	1.38
28	A	614	SQD	O47-C7	4.28	1.46	1.34
24	B	605	CLA	C1C-NC	-4.28	1.31	1.37
24	c	505	CLA	C3B-C4B	-4.28	1.32	1.42
24	B	607[B]	CLA	CHC-C1C	4.28	1.47	1.38
28	a	614	SQD	O47-C7	4.28	1.46	1.34
24	B	611	CLA	CHC-C1C	4.28	1.47	1.38
24	D	403	CLA	CBD-CGD	-4.27	1.39	1.52
24	c	502	CLA	CHC-C1C	4.27	1.47	1.38
24	b	605	CLA	CMA-C3A	-4.27	1.44	1.53
24	B	608	CLA	CAA-C2A	-4.27	1.46	1.54
24	b	608[B]	CLA	CHD-C4C	-4.26	1.29	1.39
24	C	507	CLA	CHB-C1B	4.26	1.49	1.39
26	c	515	BCR	C24-C25	4.26	1.60	1.45
24	B	607[B]	CLA	CMA-C3A	-4.26	1.44	1.53
24	b	607	CLA	C1C-NC	-4.26	1.31	1.37
24	C	506	CLA	CHB-C1B	4.25	1.49	1.39
24	b	604	CLA	C3D-C4D	-4.25	1.34	1.44
24	c	504	CLA	CHD-C4C	-4.25	1.29	1.39
24	B	614	CLA	CMA-C3A	-4.24	1.44	1.53
32	h	102	DGD	O2G-C1B	4.24	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	CHC-C1C	4.24	1.47	1.38
24	B	612	CLA	C1C-NC	-4.24	1.31	1.37
24	b	616	CLA	C1A-CHA	-4.24	1.25	1.43
24	D	403	CLA	CHB-C1B	4.24	1.48	1.39
26	h	101	BCR	C24-C25	4.23	1.60	1.45
24	C	509	CLA	C1C-NC	-4.23	1.31	1.37
24	C	504	CLA	CHD-C4C	-4.23	1.29	1.39
24	B	608	CLA	CMA-C3A	-4.23	1.44	1.53
24	B	615	CLA	CHB-C1B	4.22	1.48	1.39
24	C	513	CLA	C4C-C3C	-4.22	1.37	1.45
24	C	509	CLA	CHB-C1B	4.22	1.48	1.39
24	C	507	CLA	CHC-C1C	4.22	1.47	1.38
24	d	403	CLA	O2A-CGA	4.22	1.45	1.33
26	B	618	BCR	C24-C25	4.22	1.60	1.45
24	B	607[A]	CLA	CMA-C3A	-4.22	1.44	1.53
26	B	620	BCR	C24-C25	4.22	1.60	1.45
24	C	513	CLA	CHD-C4C	-4.22	1.29	1.39
30	d	407	LHG	O7-C7	4.22	1.46	1.34
24	B	607[B]	CLA	C4C-C3C	-4.22	1.37	1.45
24	d	402	CLA	CHC-C1C	4.22	1.47	1.38
24	b	614	CLA	CMA-C3A	-4.22	1.44	1.53
24	D	404	CLA	CMA-C3A	-4.21	1.44	1.53
24	a	606	CLA	C3B-C4B	-4.21	1.33	1.42
24	B	613	CLA	CMA-C3A	-4.21	1.44	1.53
26	a	610	BCR	C24-C25	4.21	1.60	1.45
24	c	501	CLA	CHD-C4C	-4.21	1.29	1.39
24	c	504	CLA	CHB-C1B	4.21	1.48	1.39
24	B	613	CLA	C1C-NC	-4.21	1.31	1.37
24	C	508	CLA	CHC-C1C	4.21	1.47	1.38
24	c	509	CLA	CMA-C3A	-4.21	1.44	1.53
24	C	502	CLA	CHD-C4C	-4.20	1.29	1.39
24	A	606	CLA	CMA-C3A	-4.20	1.44	1.53
24	c	513	CLA	CHB-C1B	4.20	1.48	1.39
26	A	610	BCR	C17-C18	4.20	1.41	1.35
24	d	403	CLA	MG-NB	-4.19	1.97	2.05
24	b	615	CLA	CHC-C1C	4.19	1.47	1.38
24	a	615	CLA	CHB-C1B	4.19	1.48	1.39
24	B	602	CLA	C4C-C3C	-4.19	1.37	1.45
24	B	610	CLA	CHC-C1C	4.19	1.47	1.38
24	B	613	CLA	C1A-CHA	-4.19	1.25	1.43
32	H	102	DGD	O1G-C1A	4.19	1.45	1.33
24	C	502	CLA	C4C-C3C	-4.19	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	606	CLA	CHC-C1C	4.19	1.47	1.38
24	b	616	CLA	C3D-C4D	-4.19	1.34	1.44
30	d	406	LHG	O8-C23	4.18	1.45	1.33
24	B	614	CLA	C1C-NC	-4.18	1.31	1.37
24	B	613	CLA	C1D-ND	-4.18	1.32	1.37
32	c	517	DGD	O2G-C2G	-4.18	1.36	1.46
24	a	615	CLA	C3D-C4D	-4.17	1.34	1.44
24	c	506	CLA	CHD-C4C	-4.17	1.29	1.39
24	c	508	CLA	CHD-C4C	-4.17	1.29	1.39
32	c	518	DGD	O2G-C2G	-4.17	1.36	1.46
24	B	613	CLA	CHB-C1B	4.17	1.48	1.39
24	D	403	CLA	C3B-C4B	-4.17	1.33	1.42
24	B	617	CLA	C1C-NC	-4.17	1.31	1.37
24	C	507	CLA	C1C-NC	-4.17	1.31	1.37
24	b	617	CLA	CHC-C1C	4.17	1.47	1.38
24	b	617	CLA	C1C-NC	-4.17	1.31	1.37
24	B	605	CLA	CMA-C3A	-4.16	1.44	1.53
24	C	501	CLA	CMA-C3A	-4.16	1.44	1.53
24	b	606	CLA	O2A-CGA	4.16	1.45	1.33
24	c	508	CLA	CHB-C1B	4.16	1.48	1.39
24	D	403	CLA	C1C-NC	-4.16	1.31	1.37
24	c	503	CLA	C4C-C3C	-4.16	1.37	1.45
24	B	607[A]	CLA	CHC-C1C	4.16	1.47	1.38
24	b	610	CLA	CHD-C4C	-4.16	1.29	1.39
24	c	502	CLA	CHD-C4C	-4.16	1.29	1.39
24	b	603	CLA	CHD-C1D	4.16	1.46	1.38
24	B	611	CLA	CMA-C3A	-4.16	1.44	1.53
24	D	402	CLA	C3D-C4D	-4.16	1.34	1.44
24	C	506	CLA	C1C-NC	-4.16	1.31	1.37
30	l	102	LHG	O7-C7	4.16	1.46	1.34
24	B	607[A]	CLA	C4C-C3C	-4.16	1.37	1.45
24	c	511	CLA	MG-NB	-4.16	1.97	2.05
24	B	602	CLA	CHC-C1C	4.15	1.47	1.38
24	C	511	CLA	CMA-C3A	-4.15	1.44	1.53
24	B	608	CLA	C3D-C4D	-4.15	1.34	1.44
32	c	518	DGD	O2G-C1B	4.15	1.46	1.34
24	b	608[A]	CLA	CHD-C4C	-4.15	1.29	1.39
24	C	502	CLA	C1C-NC	-4.15	1.31	1.37
24	b	611	CLA	C4C-C3C	-4.15	1.37	1.45
24	A	609	CLA	C3D-C4D	-4.15	1.34	1.44
24	C	512	CLA	CHC-C1C	4.15	1.46	1.38
26	b	621	BCR	C40-C30	4.14	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	CHC-C1C	4.14	1.46	1.38
24	B	615	CLA	CHC-C1C	4.14	1.46	1.38
24	c	502	CLA	CMA-C3A	-4.14	1.44	1.53
26	c	521	BCR	C24-C25	4.14	1.59	1.45
24	b	605	CLA	O2A-CGA	4.14	1.45	1.33
25	d	401	PHO	C1D-C2D	4.14	1.44	1.39
24	C	501	CLA	CHD-C4C	-4.14	1.29	1.39
30	d	406	LHG	O7-C7	4.14	1.46	1.34
28	A	612	SQD	O47-C7	4.14	1.46	1.34
24	c	504	CLA	CMA-C3A	-4.14	1.44	1.53
24	d	402	CLA	CMA-C3A	-4.13	1.44	1.53
29	c	519	LMG	O8-C28	4.13	1.45	1.33
24	a	615	CLA	C4C-C3C	-4.13	1.37	1.45
24	C	510	CLA	CMA-C3A	-4.13	1.44	1.53
28	l	101	SQD	O48-C23	4.13	1.45	1.33
24	b	612	CLA	CHD-C4C	-4.13	1.29	1.39
28	a	612	SQD	O47-C7	4.13	1.45	1.34
30	A	615	LHG	O7-C7	4.13	1.45	1.34
24	b	613	CLA	C1C-NC	-4.13	1.31	1.37
32	C	516	DGD	O1G-C1A	4.13	1.45	1.33
24	c	505	CLA	CHC-C1C	4.13	1.46	1.38
24	b	608[A]	CLA	CMA-C3A	-4.13	1.44	1.53
24	C	504	CLA	CHB-C1B	4.12	1.48	1.39
26	F	101	BCR	C2-C3	4.12	1.62	1.52
24	c	511	CLA	CMA-C3A	-4.12	1.44	1.53
24	b	609	CLA	CMA-C3A	-4.12	1.44	1.53
24	A	609	CLA	CHC-C1C	4.12	1.46	1.38
26	C	514	BCR	C24-C25	4.12	1.59	1.45
24	C	502	CLA	CHC-C1C	4.12	1.46	1.38
29	C	518	LMG	O6-C1	4.12	1.52	1.41
26	k	101	BCR	C40-C30	4.12	1.61	1.53
24	D	403	CLA	C3D-C2D	-4.12	1.27	1.39
24	b	608[B]	CLA	CMA-C3A	-4.12	1.44	1.53
24	c	512	CLA	C4C-C3C	-4.12	1.37	1.45
24	B	617	CLA	C4C-C3C	-4.12	1.37	1.45
28	L	102	SQD	O48-C23	4.11	1.45	1.33
24	A	609	CLA	CMA-C3A	-4.11	1.44	1.53
29	j	101	LMG	O7-C10	4.11	1.45	1.34
24	c	507	CLA	C1C-NC	-4.11	1.31	1.37
24	C	502	CLA	CMA-C3A	-4.11	1.44	1.53
24	a	615	CLA	CMA-C3A	-4.11	1.44	1.53
24	c	506	CLA	CMA-C3A	-4.11	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	CHB-C1B	4.10	1.48	1.39
32	c	516	DGD	O2G-C2G	-4.10	1.36	1.46
24	B	605	CLA	CHC-C1C	4.10	1.46	1.38
32	c	516	DGD	O2G-C1B	4.10	1.45	1.34
24	B	605	CLA	C4C-C3C	-4.10	1.38	1.45
32	C	516	DGD	O2G-C1B	4.10	1.45	1.34
24	B	610	CLA	C3D-C4D	-4.10	1.34	1.44
24	d	402	CLA	C4C-C3C	-4.10	1.38	1.45
27	A	611	PL9	C7-C3	4.10	1.55	1.51
24	b	607	CLA	CHB-C1B	4.09	1.48	1.39
24	C	508	CLA	C4C-C3C	-4.09	1.38	1.45
25	D	401	PHO	C1D-C2D	4.09	1.44	1.39
24	a	606	CLA	C4C-C3C	-4.09	1.38	1.45
24	a	609	CLA	C1C-NC	-4.09	1.31	1.37
24	D	402	CLA	CHC-C1C	4.08	1.46	1.38
30	A	615	LHG	O8-C23	4.08	1.45	1.33
24	B	612	CLA	C4C-C3C	-4.08	1.38	1.45
32	c	517	DGD	O1G-C1A	4.08	1.45	1.33
30	D	407	LHG	O8-C23	4.08	1.45	1.33
24	c	513	CLA	CHD-C4C	-4.08	1.29	1.39
24	C	508	CLA	C3D-C4D	-4.08	1.35	1.44
24	b	607	CLA	CMA-C3A	-4.08	1.44	1.53
26	b	621	BCR	C24-C25	4.08	1.59	1.45
32	C	517	DGD	O2G-C2G	-4.07	1.36	1.46
24	B	602	CLA	C1C-NC	-4.07	1.31	1.37
32	E	101	DGD	O1G-C1A	4.07	1.45	1.33
24	d	402	CLA	CHB-C4A	-4.07	1.28	1.37
29	C	518	LMG	O8-C28	4.07	1.45	1.33
24	a	609	CLA	O2A-CGA	4.07	1.45	1.33
24	B	603	CLA	CHB-C1B	4.06	1.48	1.39
24	c	505	CLA	CHD-C4C	-4.06	1.29	1.39
24	B	604	CLA	C1C-NC	-4.06	1.31	1.37
24	B	610	CLA	C1D-ND	-4.06	1.32	1.37
24	D	404	CLA	O2A-CGA	4.06	1.45	1.33
24	B	615	CLA	C4C-C3C	-4.06	1.38	1.45
24	b	615	CLA	C1C-NC	-4.05	1.31	1.37
32	H	102	DGD	O2G-C2G	-4.05	1.36	1.46
24	C	503	CLA	CHD-C1D	4.05	1.46	1.38
26	K	102	BCR	C24-C25	4.05	1.59	1.45
24	b	610	CLA	CMA-C3A	-4.05	1.44	1.53
24	B	608	CLA	C1C-NC	-4.05	1.31	1.37
24	C	510	CLA	C4C-C3C	-4.05	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C1C-NC	-4.05	1.31	1.37
24	c	504	CLA	C4C-C3C	-4.05	1.38	1.45
28	a	612	SQD	O48-C23	4.04	1.45	1.33
26	f	101	BCR	C27-C26	4.04	1.59	1.51
32	c	516	DGD	O1G-C1A	4.04	1.45	1.33
32	d	405	DGD	O1G-C1A	4.04	1.45	1.33
24	b	604	CLA	C4C-C3C	-4.03	1.38	1.45
26	a	610	BCR	C17-C18	4.03	1.41	1.35
24	a	609	CLA	CMA-C3A	-4.03	1.44	1.53
24	C	501	CLA	C1A-CHA	-4.03	1.26	1.43
24	B	609	CLA	CMA-C3A	-4.03	1.44	1.53
24	b	605	CLA	C4C-C3C	-4.03	1.38	1.45
24	C	508	CLA	CHD-C1D	4.03	1.46	1.38
24	C	511	CLA	C4C-C3C	-4.03	1.38	1.45
24	B	615	CLA	C1C-NC	-4.03	1.31	1.37
24	b	613	CLA	C4C-C3C	-4.03	1.38	1.45
26	H	101	BCR	C40-C30	4.02	1.61	1.53
24	B	614	CLA	C3D-C4D	-4.02	1.35	1.44
24	c	504	CLA	O2A-CGA	4.02	1.45	1.33
30	L	101	LHG	O7-C7	4.02	1.45	1.34
27	D	405	PL9	C6-C1	-4.02	1.41	1.48
29	c	520	LMG	O8-C28	4.02	1.45	1.33
32	C	517	DGD	O1G-C1A	4.02	1.45	1.33
24	c	512	CLA	C1C-NC	-4.02	1.31	1.37
24	b	604	CLA	CMA-C3A	-4.01	1.44	1.53
24	a	609	CLA	C4C-C3C	-4.01	1.38	1.45
24	B	606	CLA	C3D-C2D	-4.01	1.28	1.39
24	b	603	CLA	CHC-C1C	4.01	1.46	1.38
24	D	402	CLA	CHD-C4C	-4.01	1.30	1.39
24	b	610	CLA	CHC-C1C	4.01	1.46	1.38
24	B	612	CLA	CMA-C3A	-4.01	1.44	1.53
30	a	616	LHG	O7-C7	4.01	1.45	1.34
26	c	521	BCR	C12-C13	4.00	1.54	1.45
24	B	610	CLA	CMA-C3A	-4.00	1.44	1.53
29	D	408	LMG	O7-C10	4.00	1.45	1.34
32	C	517	DGD	O2G-C1B	4.00	1.45	1.34
24	B	604	CLA	C3D-C4D	-4.00	1.35	1.44
24	a	606	CLA	CMA-C3A	-4.00	1.44	1.53
24	B	612	CLA	C1A-CHA	-4.00	1.26	1.43
24	B	613	CLA	CHC-C1C	4.00	1.46	1.38
24	c	509	CLA	C1C-NC	-3.99	1.31	1.37
24	C	509	CLA	C4C-C3C	-3.99	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	CHC-C1C	3.99	1.46	1.38
24	d	402	CLA	C3D-C4D	-3.99	1.35	1.44
24	D	402	CLA	CHB-C1B	3.99	1.48	1.39
24	c	508	CLA	C1C-NC	-3.98	1.31	1.37
24	B	614	CLA	C3B-C4B	-3.98	1.33	1.42
24	C	505	CLA	C3B-C4B	-3.98	1.33	1.42
28	A	612	SQD	O48-C23	3.97	1.44	1.33
24	D	402	CLA	C1C-NC	-3.97	1.31	1.37
24	C	507	CLA	O2A-CGA	3.97	1.44	1.33
24	b	606	CLA	CMA-C3A	-3.97	1.44	1.53
24	b	614	CLA	C3D-C2D	-3.97	1.28	1.39
24	b	611	CLA	C1C-NC	-3.97	1.31	1.37
24	b	613	CLA	CMA-C3A	-3.97	1.44	1.53
24	c	510	CLA	C4C-C3C	-3.97	1.38	1.45
24	c	502	CLA	C1C-NC	-3.97	1.31	1.37
24	B	615	CLA	CMA-C3A	-3.97	1.44	1.53
24	B	612	CLA	C3D-C4D	-3.97	1.35	1.44
24	B	605	CLA	C3B-C4B	-3.97	1.33	1.42
24	C	513	CLA	C3D-C4D	-3.96	1.35	1.44
24	c	507	CLA	O2A-CGA	3.96	1.44	1.33
24	A	606	CLA	C1C-NC	-3.96	1.31	1.37
24	b	612	CLA	CMA-C3A	-3.96	1.44	1.53
24	C	505	CLA	CHC-C1C	3.96	1.46	1.38
24	b	611	CLA	CMA-C3A	-3.96	1.44	1.53
24	B	613	CLA	C3B-C4B	-3.96	1.33	1.42
24	B	612	CLA	CHB-C1B	3.96	1.48	1.39
24	D	403	CLA	C3D-C4D	-3.95	1.35	1.44
24	C	505	CLA	CMA-C3A	-3.95	1.44	1.53
24	C	509	CLA	CMA-C3A	-3.95	1.44	1.53
24	B	615	CLA	C3D-C2D	-3.95	1.28	1.39
24	b	615	CLA	CMA-C3A	-3.95	1.44	1.53
24	B	614	CLA	C3D-C2D	-3.95	1.28	1.39
24	b	606	CLA	C3D-C4D	-3.95	1.35	1.44
24	C	512	CLA	C1C-NC	-3.95	1.31	1.37
24	A	607	CLA	C3D-C4D	-3.95	1.35	1.44
24	c	507	CLA	C4C-C3C	-3.95	1.38	1.45
24	a	615	CLA	C3B-C4B	-3.95	1.33	1.42
26	c	514	BCR	C24-C25	3.94	1.59	1.45
26	B	618	BCR	C2-C3	3.94	1.62	1.52
24	b	609	CLA	C3D-C4D	-3.94	1.35	1.44
32	c	518	DGD	O6E-C5E	3.94	1.53	1.44
26	T	101	BCR	C2-C3	3.94	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	606	CLA	C1A-CHA	-3.94	1.26	1.43
24	c	512	CLA	CMA-C3A	-3.94	1.44	1.53
33	e	102	HEM	FE-NB	3.94	2.07	1.94
24	b	605	CLA	C1C-NC	-3.94	1.31	1.37
24	C	508	CLA	C1C-NC	-3.93	1.31	1.37
24	b	606	CLA	C1C-NC	-3.93	1.31	1.37
24	b	614	CLA	C1A-CHA	-3.93	1.26	1.43
24	A	609	CLA	C1A-CHA	-3.93	1.26	1.43
24	d	403	CLA	CMA-C3A	-3.93	1.44	1.53
24	C	502	CLA	O2A-CGA	3.93	1.44	1.33
24	b	616	CLA	CMA-C3A	-3.93	1.44	1.53
24	b	617	CLA	CMA-C3A	-3.93	1.44	1.53
32	c	518	DGD	O1G-C1A	3.93	1.44	1.33
32	C	516	DGD	O2G-C2G	-3.93	1.36	1.46
29	D	408	LMG	O6-C1	3.93	1.51	1.41
32	h	102	DGD	O1G-C1A	3.92	1.44	1.33
24	D	404	CLA	C1C-NC	-3.92	1.31	1.37
24	B	607[B]	CLA	C1C-NC	-3.92	1.32	1.37
24	b	610	CLA	C1C-NC	-3.92	1.32	1.37
24	a	609	CLA	MG-NB	-3.92	1.98	2.05
24	C	511	CLA	C3D-C4D	-3.92	1.35	1.44
24	a	606	CLA	C3D-C4D	-3.91	1.35	1.44
24	B	602	CLA	O2A-CGA	3.91	1.44	1.33
24	B	610	CLA	C1C-NC	-3.91	1.32	1.37
24	c	508	CLA	C4C-C3C	-3.91	1.38	1.45
24	D	402	CLA	CBD-CGD	-3.91	1.40	1.52
24	C	508	CLA	CMA-C3A	-3.91	1.44	1.53
24	B	607[A]	CLA	C1C-NC	-3.91	1.32	1.37
24	b	612	CLA	C1C-NC	-3.91	1.32	1.37
24	c	510	CLA	CMA-C3A	-3.90	1.44	1.53
24	C	509	CLA	C3B-C4B	-3.90	1.33	1.42
24	B	606	CLA	CMA-C3A	-3.90	1.44	1.53
32	E	101	DGD	O6E-C5E	3.90	1.53	1.44
30	D	406	LHG	O7-C7	3.90	1.45	1.34
24	c	507	CLA	CHC-C1C	3.90	1.46	1.38
32	C	515	DGD	O1G-C1A	3.90	1.44	1.33
24	C	503	CLA	C3D-C2D	-3.90	1.28	1.39
26	t	101	BCR	C24-C25	3.90	1.58	1.45
24	D	402	CLA	C1A-CHA	-3.90	1.26	1.43
24	A	607	CLA	O2A-CGA	3.90	1.44	1.33
24	B	609	CLA	MG-NB	-3.90	1.98	2.05
24	B	617	CLA	O2A-CGA	3.90	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C1A-CHA	-3.90	1.26	1.43
24	D	402	CLA	CHB-C4A	-3.89	1.28	1.37
24	c	501	CLA	CMA-C3A	-3.89	1.44	1.53
24	c	510	CLA	CAA-C2A	-3.89	1.46	1.54
24	c	505	CLA	CMA-C3A	-3.89	1.44	1.53
24	B	604	CLA	C1D-ND	-3.89	1.33	1.37
24	a	615	CLA	C1A-CHA	-3.89	1.27	1.43
24	a	607	CLA	C3D-C4D	-3.89	1.35	1.44
24	B	617	CLA	C3B-C4B	-3.89	1.33	1.42
24	b	604	CLA	CAA-C2A	-3.88	1.46	1.54
24	b	612	CLA	CHC-C1C	3.88	1.46	1.38
24	A	606	CLA	CHD-C1D	3.88	1.45	1.38
24	c	508	CLA	CMA-C3A	-3.88	1.44	1.53
24	C	503	CLA	C3D-C4D	-3.88	1.35	1.44
32	h	102	DGD	O2G-C2G	-3.88	1.36	1.46
24	B	607[B]	CLA	C3D-C4D	-3.88	1.35	1.44
27	d	404	PL9	C6-C1	-3.88	1.41	1.48
29	A	613	LMG	O8-C28	3.87	1.44	1.33
24	C	511	CLA	C3D-C2D	-3.87	1.28	1.39
24	a	606	CLA	C3D-C2D	-3.87	1.28	1.39
24	B	611	CLA	CHB-C1B	3.87	1.48	1.39
24	b	613	CLA	CBD-CGD	-3.87	1.40	1.52
29	j	101	LMG	O6-C1	3.86	1.51	1.41
24	c	502	CLA	C4C-C3C	-3.86	1.38	1.45
24	b	608[B]	CLA	C3D-C4D	-3.86	1.35	1.44
24	a	606	CLA	C1C-NC	-3.86	1.32	1.37
24	C	503	CLA	C1C-NC	-3.86	1.32	1.37
24	C	508	CLA	C1A-CHA	-3.86	1.27	1.43
24	c	506	CLA	C1C-NC	-3.86	1.32	1.37
24	c	503	CLA	CMA-C3A	-3.86	1.44	1.53
24	C	513	CLA	C1C-NC	-3.85	1.32	1.37
24	B	606	CLA	C1C-NC	-3.85	1.32	1.37
24	b	609	CLA	C1A-CHA	-3.85	1.27	1.43
29	a	613	LMG	O8-C28	3.85	1.44	1.33
24	A	609	CLA	CBD-CGD	-3.85	1.40	1.52
24	B	603	CLA	C3D-C4D	-3.85	1.35	1.44
26	c	515	BCR	C12-C13	3.85	1.54	1.45
29	b	622	LMG	O6-C1	3.85	1.51	1.41
32	h	102	DGD	O6E-C5E	3.84	1.53	1.44
26	b	619	BCR	C40-C30	3.84	1.61	1.53
24	b	618	CLA	C3D-C4D	-3.84	1.35	1.44
24	b	609	CLA	C3D-C2D	-3.84	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	CAA-C2A	-3.84	1.47	1.54
26	T	101	BCR	C24-C25	3.84	1.58	1.45
24	b	611	CLA	C1D-ND	-3.84	1.33	1.37
26	I	101	BCR	C12-C13	3.83	1.54	1.45
24	B	603	CLA	C4C-C3C	-3.83	1.38	1.45
26	f	101	BCR	C2-C3	3.83	1.62	1.52
24	C	506	CLA	C4C-C3C	-3.83	1.38	1.45
32	H	102	DGD	O2G-C1B	3.83	1.45	1.34
24	b	613	CLA	C3D-C2D	-3.83	1.28	1.39
24	b	605	CLA	C1D-ND	-3.83	1.33	1.37
32	C	516	DGD	O6E-C5E	3.83	1.53	1.44
24	b	606	CLA	C3D-C2D	-3.83	1.28	1.39
24	A	607	CLA	C4C-C3C	-3.82	1.38	1.45
24	b	606	CLA	C4C-C3C	-3.82	1.38	1.45
24	b	614	CLA	C3D-C4D	-3.82	1.35	1.44
24	a	615	CLA	C3D-C2D	-3.82	1.28	1.39
24	d	402	CLA	C1D-ND	-3.82	1.33	1.37
24	A	606	CLA	C1D-ND	-3.82	1.33	1.37
26	B	619	BCR	C2-C3	3.82	1.62	1.52
24	b	610	CLA	C3B-C4B	-3.81	1.34	1.42
24	b	613	CLA	C3D-C4D	-3.81	1.35	1.44
26	c	521	BCR	C2-C3	3.81	1.62	1.52
24	b	608[B]	CLA	C4C-C3C	-3.81	1.38	1.45
24	b	611	CLA	O2D-CGD	3.81	1.42	1.33
24	B	608	CLA	C1A-CHA	-3.81	1.27	1.43
24	C	501	CLA	O2A-CGA	3.81	1.44	1.33
24	b	618	CLA	CAA-C2A	-3.80	1.47	1.54
24	B	603	CLA	CMA-C3A	-3.80	1.45	1.53
24	c	504	CLA	C1C-NC	-3.80	1.32	1.37
24	b	618	CLA	C1C-NC	-3.80	1.32	1.37
24	D	402	CLA	C3D-C2D	-3.80	1.28	1.39
24	B	614	CLA	CHC-C1C	3.80	1.46	1.38
24	A	606	CLA	C3D-C4D	-3.80	1.35	1.44
24	B	602	CLA	CMA-C3A	-3.80	1.45	1.53
24	C	507	CLA	C4C-C3C	-3.80	1.38	1.45
24	C	504	CLA	C1A-CHA	-3.80	1.27	1.43
24	B	604	CLA	O2A-CGA	3.80	1.44	1.33
24	B	605	CLA	C3D-C4D	-3.79	1.35	1.44
24	c	505	CLA	C1C-NC	-3.79	1.32	1.37
24	c	507	CLA	CMA-C3A	-3.79	1.45	1.53
26	c	514	BCR	C40-C30	3.79	1.61	1.53
32	C	515	DGD	O6E-C5E	3.79	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	CLA	C3D-C4D	-3.79	1.35	1.44
24	B	609	CLA	CHC-C1C	3.78	1.46	1.38
24	a	607	CLA	C4C-C3C	-3.78	1.38	1.45
24	C	506	CLA	O2D-CGD	3.78	1.42	1.33
24	a	607	CLA	CMA-C3A	-3.78	1.45	1.53
24	B	613	CLA	C3D-C4D	-3.78	1.35	1.44
24	c	513	CLA	CMA-C3A	-3.78	1.45	1.53
24	b	614	CLA	C1D-ND	-3.78	1.33	1.37
24	C	510	CLA	CHB-C1B	3.78	1.47	1.39
24	D	404	CLA	C4C-C3C	-3.77	1.38	1.45
26	t	101	BCR	C17-C18	3.77	1.40	1.35
29	c	519	LMG	O6-C1	3.77	1.51	1.41
24	b	614	CLA	C1C-NC	-3.77	1.32	1.37
24	b	618	CLA	CMA-C3A	-3.77	1.45	1.53
24	B	613	CLA	CAA-C2A	-3.76	1.47	1.54
32	c	517	DGD	O2G-C1B	3.76	1.44	1.34
24	b	606	CLA	C3B-C4B	-3.76	1.34	1.42
24	C	505	CLA	CAA-C2A	-3.76	1.47	1.54
26	c	515	BCR	C40-C30	3.76	1.61	1.53
24	C	506	CLA	C3D-C4D	-3.76	1.35	1.44
24	C	513	CLA	O2A-CGA	3.76	1.44	1.33
32	C	515	DGD	O2G-C2G	-3.76	1.37	1.46
26	C	514	BCR	C40-C30	3.76	1.61	1.53
29	B	621	LMG	O8-C28	3.76	1.44	1.33
24	c	505	CLA	C3D-C4D	-3.76	1.35	1.44
24	b	608[A]	CLA	C3D-C4D	-3.76	1.35	1.44
24	b	610	CLA	C4C-C3C	-3.75	1.38	1.45
24	C	509	CLA	CHC-C1C	3.75	1.46	1.38
24	C	506	CLA	CHB-C4A	-3.75	1.28	1.37
24	B	604	CLA	CHC-C1C	3.75	1.46	1.38
24	b	615	CLA	CAA-C2A	-3.75	1.47	1.54
24	b	605	CLA	C3B-C4B	-3.75	1.34	1.42
24	C	508	CLA	C3D-C2D	-3.75	1.28	1.39
24	B	603	CLA	C1C-NC	-3.75	1.32	1.37
24	B	604	CLA	C4C-C3C	-3.75	1.38	1.45
24	c	512	CLA	O2A-CGA	3.75	1.44	1.33
24	b	618	CLA	CHC-C1C	3.75	1.46	1.38
26	F	101	BCR	C40-C30	3.75	1.61	1.53
24	c	506	CLA	O2A-CGA	3.75	1.44	1.33
29	b	622	LMG	O8-C28	3.75	1.44	1.33
24	B	607[A]	CLA	C3D-C4D	-3.75	1.35	1.44
24	c	509	CLA	O2A-CGA	3.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	C1C-NC	-3.74	1.32	1.37
24	b	604	CLA	CHB-C1B	3.74	1.47	1.39
24	c	504	CLA	C3D-C2D	-3.74	1.28	1.39
32	d	405	DGD	O6E-C5E	3.73	1.53	1.44
26	B	620	BCR	C2-C3	3.73	1.61	1.52
24	c	509	CLA	C3B-C4B	-3.73	1.34	1.42
24	B	610	CLA	O2A-CGA	3.72	1.44	1.33
24	c	511	CLA	O2A-CGA	3.72	1.44	1.33
24	A	607	CLA	C1A-CHA	-3.72	1.27	1.43
24	D	404	CLA	C3B-C4B	-3.72	1.34	1.42
24	b	604	CLA	C1A-CHA	-3.72	1.27	1.43
24	c	503	CLA	CBD-CGD	-3.72	1.40	1.52
24	C	511	CLA	O2A-CGA	3.72	1.44	1.33
24	b	616	CLA	C3B-C4B	-3.72	1.34	1.42
29	D	408	LMG	O8-C28	3.72	1.44	1.33
24	B	609	CLA	C3D-C4D	-3.71	1.35	1.44
24	A	606	CLA	C3B-C4B	-3.71	1.34	1.42
24	c	505	CLA	C1D-ND	-3.71	1.33	1.37
24	B	616	CLA	C1C-NC	-3.71	1.32	1.37
24	a	615	CLA	C1D-ND	-3.71	1.33	1.37
27	A	611	PL9	C6-C1	-3.71	1.42	1.48
24	b	605	CLA	C3D-C4D	-3.71	1.35	1.44
24	C	510	CLA	C1D-ND	-3.70	1.33	1.37
24	c	502	CLA	O2A-CGA	3.70	1.44	1.33
24	B	610	CLA	C4C-C3C	-3.70	1.38	1.45
29	C	519	LMG	O8-C28	3.70	1.44	1.33
32	H	102	DGD	O6E-C5E	3.70	1.53	1.44
24	C	507	CLA	CMA-C3A	-3.70	1.45	1.53
24	c	508	CLA	C3D-C4D	-3.70	1.35	1.44
24	b	604	CLA	CHB-C4A	-3.70	1.29	1.37
24	b	608[A]	CLA	O2A-CGA	3.70	1.44	1.33
24	b	605	CLA	C3D-C2D	-3.69	1.29	1.39
24	c	503	CLA	O2A-CGA	3.69	1.44	1.33
26	K	102	BCR	C2-C3	3.69	1.61	1.52
24	c	511	CLA	C3D-C4D	-3.69	1.35	1.44
24	b	614	CLA	C4C-C3C	-3.69	1.38	1.45
24	B	609	CLA	C1C-NC	-3.69	1.32	1.37
24	A	609	CLA	C3D-C2D	-3.69	1.29	1.39
24	B	615	CLA	C3D-C4D	-3.69	1.35	1.44
24	b	608[A]	CLA	C4C-C3C	-3.68	1.38	1.45
24	B	606	CLA	C3D-C4D	-3.68	1.35	1.44
24	b	613	CLA	CHC-C1C	3.68	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	607	CLA	C3D-C2D	-3.68	1.29	1.39
26	B	618	BCR	C40-C30	3.68	1.61	1.53
24	b	609	CLA	CAA-C2A	-3.68	1.47	1.54
24	a	615	CLA	CBD-CGD	-3.68	1.40	1.52
32	C	517	DGD	O6E-C5E	3.68	1.53	1.44
24	A	606	CLA	CAA-C2A	-3.68	1.47	1.54
26	c	515	BCR	C2-C3	3.68	1.61	1.52
24	c	501	CLA	C1C-NC	-3.68	1.32	1.37
24	C	503	CLA	CMA-C3A	-3.68	1.45	1.53
24	b	612	CLA	C3D-C4D	-3.67	1.35	1.44
27	a	611	PL9	C36-C34	3.67	1.58	1.51
24	B	614	CLA	C1A-CHA	-3.67	1.27	1.43
24	b	612	CLA	C1A-CHA	-3.67	1.27	1.43
24	a	609	CLA	C3D-C4D	-3.67	1.35	1.44
24	B	608	CLA	C3D-C2D	-3.67	1.29	1.39
24	C	513	CLA	C3B-C4B	-3.67	1.34	1.42
24	C	510	CLA	C3D-C2D	-3.67	1.29	1.39
24	b	611	CLA	CAA-C2A	-3.67	1.47	1.54
24	B	614	CLA	CBD-CGD	-3.66	1.40	1.52
24	B	611	CLA	CHB-C4A	-3.66	1.29	1.37
24	c	503	CLA	C3D-C4D	-3.66	1.35	1.44
24	D	404	CLA	CBD-CGD	-3.66	1.41	1.52
24	C	513	CLA	C1A-CHA	-3.66	1.27	1.43
26	K	102	BCR	C12-C13	3.66	1.53	1.45
24	b	614	CLA	C3B-C4B	-3.66	1.34	1.42
24	B	613	CLA	MG-NA	-3.66	1.97	2.06
24	B	605	CLA	C1A-CHA	-3.66	1.27	1.43
24	C	513	CLA	CMA-C3A	-3.66	1.45	1.53
24	A	607	CLA	CMA-C3A	-3.66	1.45	1.53
26	I	101	BCR	C40-C30	3.66	1.61	1.53
24	C	511	CLA	C1C-NC	-3.66	1.32	1.37
24	b	608[A]	CLA	CBD-CGD	-3.66	1.41	1.52
24	d	403	CLA	CBD-CGD	-3.66	1.41	1.52
24	b	608[B]	CLA	C1A-CHA	-3.65	1.28	1.43
24	C	503	CLA	CBD-CGD	-3.65	1.41	1.52
26	B	619	BCR	C27-C26	3.65	1.58	1.51
24	d	402	CLA	C1A-CHA	-3.65	1.28	1.43
24	b	618	CLA	O2A-CGA	3.65	1.44	1.33
24	c	505	CLA	C4C-C3C	-3.65	1.38	1.45
24	b	603	CLA	C3D-C2D	-3.65	1.29	1.39
24	b	612	CLA	O2A-CGA	3.65	1.44	1.33
24	C	509	CLA	CBD-CGD	-3.65	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z	101	LMG	O6-C1	3.65	1.51	1.41
24	b	608[B]	CLA	O2A-CGA	3.64	1.44	1.33
24	a	615	CLA	MG-NA	-3.64	1.97	2.06
24	b	603	CLA	CMA-C3A	-3.64	1.45	1.53
26	A	610	BCR	C12-C13	3.64	1.53	1.45
24	B	614	CLA	CAA-C2A	-3.64	1.47	1.54
24	C	505	CLA	CHD-C4C	-3.64	1.30	1.39
24	a	606	CLA	C1A-CHA	-3.64	1.28	1.43
24	b	611	CLA	C3D-C4D	-3.64	1.36	1.44
24	a	615	CLA	CAA-C2A	-3.64	1.47	1.54
24	C	510	CLA	CHB-C4A	-3.64	1.29	1.37
24	C	504	CLA	CHC-C1C	3.64	1.45	1.38
24	C	506	CLA	C3B-C4B	-3.63	1.34	1.42
24	B	609	CLA	C3B-C4B	-3.63	1.34	1.42
24	B	604	CLA	C1A-CHA	-3.63	1.28	1.43
24	B	612	CLA	C1D-ND	-3.63	1.33	1.37
24	a	615	CLA	CHC-C1C	3.63	1.45	1.38
24	C	506	CLA	CMA-C3A	-3.63	1.45	1.53
24	b	605	CLA	CHC-C1C	3.63	1.45	1.38
24	c	508	CLA	CHB-C4A	-3.63	1.29	1.37
24	C	510	CLA	C1A-CHA	-3.63	1.28	1.43
24	c	510	CLA	C3D-C2D	-3.62	1.29	1.39
24	b	603	CLA	C3D-C4D	-3.62	1.36	1.44
24	C	512	CLA	CMA-C3A	-3.62	1.45	1.53
24	b	608[B]	CLA	CBD-CGD	-3.62	1.41	1.52
24	c	503	CLA	C3D-C2D	-3.62	1.29	1.39
27	a	611	PL9	C6-C1	-3.61	1.42	1.48
24	C	510	CLA	CHC-C1C	3.61	1.45	1.38
24	b	604	CLA	C3D-C2D	-3.61	1.29	1.39
24	b	608[B]	CLA	C1C-NC	-3.61	1.32	1.37
26	a	610	BCR	C2-C3	3.61	1.61	1.52
24	c	503	CLA	C1C-NC	-3.61	1.32	1.37
24	b	613	CLA	O2A-CGA	3.61	1.43	1.33
24	B	602	CLA	CBD-CGD	-3.61	1.41	1.52
24	B	607[A]	CLA	O2A-CGA	3.61	1.43	1.33
29	C	519	LMG	O6-C1	3.61	1.51	1.41
24	B	616	CLA	CMA-C3A	-3.61	1.45	1.53
24	A	607	CLA	MG-NA	-3.61	1.97	2.06
24	B	609	CLA	CHD-C4C	-3.61	1.31	1.39
29	z	101	LMG	O6-C1	3.61	1.51	1.41
24	c	501	CLA	C3D-C4D	-3.61	1.36	1.44
32	d	405	DGD	O2G-C2G	-3.60	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	CAA-C2A	-3.60	1.47	1.54
32	c	517	DGD	O6E-C5E	3.60	1.53	1.44
26	B	618	BCR	C1-C6	-3.60	1.48	1.53
26	b	620	BCR	C2-C3	3.60	1.61	1.52
26	b	621	BCR	C2-C3	3.60	1.61	1.52
24	A	607	CLA	CBD-CGD	-3.60	1.41	1.52
24	C	511	CLA	O2D-CGD	3.60	1.42	1.33
24	b	603	CLA	O2A-CGA	3.60	1.43	1.33
24	b	604	CLA	C1D-ND	-3.60	1.33	1.37
24	b	608[A]	CLA	C1A-CHA	-3.60	1.28	1.43
24	c	504	CLA	C3D-C4D	-3.60	1.36	1.44
24	b	608[B]	CLA	C3D-C2D	-3.60	1.29	1.39
25	a	608	PHO	C1D-C2D	3.60	1.43	1.39
24	c	512	CLA	C1A-CHA	-3.60	1.28	1.43
24	B	603	CLA	C1A-CHA	-3.60	1.28	1.43
27	A	611	PL9	C36-C34	3.60	1.58	1.51
26	b	621	BCR	C24-C23	3.59	1.43	1.33
24	B	611	CLA	C3D-C4D	-3.59	1.36	1.44
24	a	609	CLA	C3D-C2D	-3.59	1.29	1.39
24	c	501	CLA	O2A-CGA	3.59	1.43	1.33
26	h	101	BCR	C2-C3	3.59	1.61	1.52
24	d	402	CLA	C3D-C2D	-3.59	1.29	1.39
24	D	403	CLA	CHC-C1C	3.59	1.45	1.38
24	b	610	CLA	C3D-C4D	-3.59	1.36	1.44
24	b	604	CLA	O2D-CGD	3.59	1.42	1.33
24	C	511	CLA	C3B-C4B	-3.59	1.34	1.42
24	D	404	CLA	C1A-CHA	-3.59	1.28	1.43
24	c	508	CLA	CAA-C2A	-3.59	1.47	1.54
24	c	505	CLA	C3D-C2D	-3.59	1.29	1.39
24	d	403	CLA	C1A-CHA	-3.58	1.28	1.43
26	c	514	BCR	C2-C3	3.58	1.61	1.52
24	C	508	CLA	C3B-C4B	-3.58	1.34	1.42
24	b	608[A]	CLA	C3D-C2D	-3.58	1.29	1.39
24	b	607	CLA	C3D-C4D	-3.58	1.36	1.44
24	b	618	CLA	C1A-CHA	-3.58	1.28	1.43
24	d	402	CLA	CHB-C1B	3.58	1.47	1.39
24	c	506	CLA	C3B-C4B	-3.58	1.34	1.42
24	b	615	CLA	C3B-C4B	-3.58	1.34	1.42
29	c	520	LMG	O6-C1	3.58	1.51	1.41
24	b	618	CLA	C1D-ND	-3.58	1.33	1.37
24	b	615	CLA	C3D-C4D	-3.57	1.36	1.44
24	C	505	CLA	C1C-NC	-3.57	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	515	DGD	O6D-C5D	3.57	1.53	1.44
24	C	508	CLA	O2A-CGA	3.57	1.43	1.33
24	B	606	CLA	O2A-CGA	3.57	1.43	1.33
24	b	613	CLA	C1A-CHA	-3.57	1.28	1.43
24	B	607[A]	CLA	C1A-CHA	-3.57	1.28	1.43
24	B	613	CLA	CHB-C4A	-3.57	1.29	1.37
24	a	615	CLA	CHB-C4A	-3.57	1.29	1.37
24	c	511	CLA	C3D-C2D	-3.57	1.29	1.39
24	C	509	CLA	C3D-C2D	-3.57	1.29	1.39
26	b	619	BCR	C2-C3	3.56	1.61	1.52
24	B	607[B]	CLA	C1A-CHA	-3.56	1.28	1.43
26	C	514	BCR	C4-C5	3.56	1.58	1.51
24	b	610	CLA	CHB-C4A	-3.56	1.29	1.37
26	A	610	BCR	C2-C3	3.56	1.61	1.52
24	D	402	CLA	O2A-CGA	3.56	1.43	1.33
26	K	101	BCR	C40-C30	3.56	1.60	1.53
24	a	606	CLA	CAA-C2A	-3.56	1.47	1.54
24	D	402	CLA	C4C-C3C	-3.56	1.38	1.45
24	C	507	CLA	C3D-C4D	-3.56	1.36	1.44
24	A	607	CLA	C1D-ND	-3.56	1.33	1.37
24	d	402	CLA	MG-NA	-3.55	1.97	2.06
26	a	610	BCR	C40-C30	3.55	1.60	1.53
24	B	604	CLA	C3D-C2D	-3.55	1.29	1.39
24	b	607	CLA	C3D-C2D	-3.55	1.29	1.39
24	c	510	CLA	C1C-NC	-3.55	1.32	1.37
24	B	607[B]	CLA	CAA-C2A	-3.55	1.47	1.54
24	C	511	CLA	C1A-CHA	-3.55	1.28	1.43
24	A	606	CLA	O2A-CGA	3.54	1.43	1.33
26	F	101	BCR	C27-C26	3.54	1.58	1.51
26	t	101	BCR	C2-C3	3.54	1.61	1.52
24	c	504	CLA	C1A-CHA	-3.54	1.28	1.43
24	b	607	CLA	CAA-C2A	-3.54	1.47	1.54
24	B	606	CLA	O2D-CGD	3.54	1.41	1.33
24	D	404	CLA	C3D-C4D	-3.54	1.36	1.44
24	b	610	CLA	C1A-CHA	-3.54	1.28	1.43
24	B	610	CLA	CAA-C2A	-3.54	1.47	1.54
24	c	501	CLA	C4C-C3C	-3.53	1.38	1.45
24	C	506	CLA	C3D-C2D	-3.53	1.29	1.39
24	b	607	CLA	O2A-CGA	3.53	1.43	1.33
24	A	607	CLA	CAA-C2A	-3.53	1.47	1.54
24	B	607[B]	CLA	O2A-CGA	3.53	1.43	1.33
26	T	101	BCR	C40-C30	3.53	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	607	CLA	C3D-C2D	-3.53	1.29	1.39
24	D	403	CLA	C1A-CHA	-3.53	1.28	1.43
24	c	506	CLA	CHB-C4A	-3.53	1.29	1.37
24	c	502	CLA	C3B-C4B	-3.53	1.34	1.42
24	c	507	CLA	C3D-C4D	-3.53	1.36	1.44
24	a	607	CLA	C1A-CHA	-3.53	1.28	1.43
24	C	501	CLA	C1C-NC	-3.53	1.32	1.37
24	C	510	CLA	C3D-C4D	-3.52	1.36	1.44
33	v	201	HEM	CAB-C3B	3.52	1.57	1.47
24	a	607	CLA	CBD-CGD	-3.52	1.41	1.52
24	a	607	CLA	O2A-CGA	3.52	1.43	1.33
24	D	403	CLA	C1D-ND	-3.52	1.33	1.37
24	B	615	CLA	C3B-C4B	-3.52	1.34	1.42
24	D	402	CLA	C1D-ND	-3.52	1.33	1.37
24	C	510	CLA	CAA-C2A	-3.52	1.47	1.54
24	B	608	CLA	C3B-C4B	-3.52	1.34	1.42
24	B	617	CLA	CHC-C1C	3.52	1.45	1.38
32	E	101	DGD	O2G-C2G	-3.51	1.37	1.46
24	c	506	CLA	C4C-C3C	-3.51	1.39	1.45
24	c	504	CLA	CHB-C4A	-3.51	1.29	1.37
26	H	101	BCR	C2-C3	3.51	1.61	1.52
24	B	616	CLA	C1A-CHA	-3.51	1.28	1.43
24	B	612	CLA	CHB-C4A	-3.50	1.29	1.37
24	b	608[A]	CLA	C1C-NC	-3.50	1.32	1.37
26	f	101	BCR	C40-C30	3.50	1.60	1.53
26	C	514	BCR	C2-C3	3.50	1.61	1.52
26	A	610	BCR	C27-C26	3.50	1.57	1.51
24	b	607	CLA	C3B-C4B	-3.50	1.34	1.42
24	D	402	CLA	C3B-C4B	-3.50	1.34	1.42
24	C	510	CLA	MG-NA	-3.49	1.98	2.06
24	D	402	CLA	MG-NA	-3.49	1.98	2.06
33	V	201	HEM	FE-NB	3.49	2.05	1.94
24	B	611	CLA	O2A-CGA	3.49	1.43	1.33
24	C	502	CLA	C3B-C4B	-3.49	1.34	1.42
24	a	606	CLA	O2A-CGA	3.49	1.43	1.33
24	C	509	CLA	C3D-C4D	-3.49	1.36	1.44
24	c	501	CLA	O2D-CGD	3.49	1.41	1.33
26	h	101	BCR	C40-C30	3.49	1.60	1.53
24	B	617	CLA	CAA-C2A	-3.49	1.47	1.54
24	B	603	CLA	O2A-CGA	3.48	1.43	1.33
24	C	504	CLA	CHB-C4A	-3.48	1.29	1.37
24	b	617	CLA	C3D-C2D	-3.48	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607[B]	CLA	C3D-C2D	-3.48	1.29	1.39
24	B	617	CLA	CMA-C3A	-3.48	1.45	1.53
24	b	605	CLA	CBD-CGD	-3.48	1.41	1.52
24	A	609	CLA	O2A-CGA	3.48	1.43	1.33
24	B	615	CLA	CHB-C4A	-3.48	1.29	1.37
24	b	606	CLA	C1A-CHA	-3.48	1.28	1.43
24	b	617	CLA	O2A-CGA	3.48	1.43	1.33
24	D	403	CLA	CHB-C4A	-3.47	1.29	1.37
24	d	402	CLA	CAA-C2A	-3.47	1.47	1.54
26	b	620	BCR	C27-C26	3.47	1.57	1.51
24	B	616	CLA	CBD-CGD	-3.47	1.41	1.52
24	C	512	CLA	CAA-C2A	-3.47	1.47	1.54
24	B	616	CLA	O2A-CGA	3.47	1.43	1.33
26	F	101	BCR	C12-C13	3.46	1.53	1.45
24	b	609	CLA	CBD-CGD	-3.46	1.41	1.52
24	c	507	CLA	C3B-C4B	-3.46	1.34	1.42
24	c	508	CLA	C1A-CHA	-3.46	1.28	1.43
24	b	616	CLA	C1D-ND	-3.46	1.33	1.37
24	C	508	CLA	CHB-C4A	-3.45	1.29	1.37
24	C	513	CLA	O2D-CGD	3.45	1.41	1.33
24	C	502	CLA	C1A-CHA	-3.45	1.28	1.43
24	C	508	CLA	CAA-C2A	-3.45	1.47	1.54
24	c	512	CLA	C3D-C4D	-3.45	1.36	1.44
32	c	518	DGD	C3D-C2D	-3.45	1.43	1.52
24	D	404	CLA	C3D-C2D	-3.45	1.29	1.39
24	C	512	CLA	C3B-C4B	-3.44	1.34	1.42
24	C	512	CLA	O2A-CGA	3.44	1.43	1.33
24	b	617	CLA	C3D-C4D	-3.44	1.36	1.44
24	b	608[A]	CLA	C3B-C4B	-3.44	1.34	1.42
29	B	621	LMG	O6-C1	3.44	1.50	1.41
24	c	509	CLA	CAA-C2A	-3.44	1.47	1.54
32	c	516	DGD	O6E-C5E	3.44	1.52	1.44
24	B	611	CLA	CBD-CGD	-3.44	1.41	1.52
24	B	607[A]	CLA	C3D-C2D	-3.44	1.29	1.39
32	c	516	DGD	C3D-C2D	-3.44	1.43	1.52
24	c	509	CLA	C1A-CHA	-3.43	1.28	1.43
26	I	101	BCR	C2-C3	3.43	1.61	1.52
24	B	609	CLA	C1A-CHA	-3.43	1.28	1.43
24	c	513	CLA	CHB-C4A	-3.43	1.29	1.37
24	b	607	CLA	C1A-CHA	-3.43	1.28	1.43
24	B	617	CLA	CBD-CGD	-3.43	1.41	1.52
24	A	609	CLA	C1D-ND	-3.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C3D-C2D	-3.43	1.29	1.39
24	b	606	CLA	O2D-CGD	3.42	1.41	1.33
24	b	613	CLA	C3B-C4B	-3.42	1.34	1.42
24	c	502	CLA	CHB-C4A	-3.42	1.29	1.37
24	B	607[A]	CLA	CAA-C2A	-3.42	1.47	1.54
32	C	515	DGD	C3D-C2D	-3.42	1.43	1.52
33	V	201	HEM	CAC-C3C	3.42	1.56	1.47
24	B	615	CLA	C1A-CHA	-3.42	1.28	1.43
26	f	101	BCR	C4-C5	3.41	1.57	1.51
24	B	610	CLA	C3B-C4B	-3.41	1.34	1.42
26	t	101	BCR	C40-C30	3.41	1.60	1.53
24	B	616	CLA	C3D-C4D	-3.41	1.36	1.44
27	A	611	PL9	C21-C19	3.41	1.58	1.51
24	B	612	CLA	CBD-CGD	-3.41	1.41	1.52
24	c	507	CLA	C1A-CHA	-3.41	1.29	1.43
24	c	506	CLA	CAA-C2A	-3.41	1.47	1.54
24	C	504	CLA	C3B-C4B	-3.41	1.34	1.42
24	b	611	CLA	O2A-CGA	3.41	1.43	1.33
24	C	505	CLA	C3D-C4D	-3.41	1.36	1.44
26	k	101	BCR	C4-C5	3.41	1.57	1.51
24	B	607[A]	CLA	C3B-C4B	-3.40	1.34	1.42
24	d	402	CLA	CBD-CGD	-3.40	1.41	1.52
24	c	502	CLA	C3D-C2D	-3.40	1.29	1.39
24	a	606	CLA	CBD-CGD	-3.40	1.41	1.52
32	H	102	DGD	C3D-C2D	-3.40	1.43	1.52
24	b	618	CLA	O2D-CGD	3.40	1.41	1.33
24	b	615	CLA	C1A-CHA	-3.40	1.29	1.43
24	A	606	CLA	CHB-C4A	-3.39	1.29	1.37
24	B	602	CLA	C3D-C2D	-3.39	1.29	1.39
24	C	504	CLA	CAA-C2A	-3.39	1.47	1.54
24	b	616	CLA	CAA-C2A	-3.39	1.47	1.54
24	d	402	CLA	O2A-CGA	3.39	1.43	1.33
33	v	201	HEM	FE-NC	3.39	2.06	1.95
24	b	614	CLA	O2A-CGA	3.39	1.43	1.33
24	B	617	CLA	C1A-CHA	-3.39	1.29	1.43
24	B	610	CLA	C3D-C2D	-3.39	1.29	1.39
24	B	605	CLA	O2A-CGA	3.39	1.43	1.33
24	B	612	CLA	C3D-C2D	-3.39	1.29	1.39
24	B	603	CLA	C3D-C2D	-3.39	1.29	1.39
24	c	508	CLA	C1D-ND	-3.38	1.33	1.37
24	C	503	CLA	O2A-CGA	3.38	1.43	1.33
24	B	604	CLA	CMA-C3A	-3.38	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	CBD-CGD	-3.38	1.41	1.52
26	K	101	BCR	C2-C3	3.38	1.60	1.52
24	c	503	CLA	C1A-CHA	-3.38	1.29	1.43
32	C	517	DGD	O6D-C5D	3.38	1.52	1.44
29	A	613	LMG	O6-C1	3.37	1.50	1.41
24	B	609	CLA	CAA-C2A	-3.37	1.47	1.54
24	c	510	CLA	C3D-C4D	-3.37	1.36	1.44
24	c	509	CLA	O2D-CGD	3.37	1.41	1.33
24	c	510	CLA	C3B-C4B	-3.37	1.35	1.42
24	C	503	CLA	C1A-CHA	-3.37	1.29	1.43
26	H	101	BCR	C27-C26	3.37	1.57	1.51
24	A	606	CLA	C3D-C2D	-3.37	1.29	1.39
24	D	403	CLA	O2A-CGA	3.37	1.43	1.33
24	c	511	CLA	C1A-CHA	-3.37	1.29	1.43
24	C	507	CLA	C3D-C2D	-3.37	1.29	1.39
24	C	512	CLA	C3D-C4D	-3.36	1.36	1.44
24	c	513	CLA	C3B-C4B	-3.36	1.35	1.42
24	c	513	CLA	C3D-C4D	-3.36	1.36	1.44
24	c	502	CLA	C1A-CHA	-3.36	1.29	1.43
24	c	501	CLA	C1A-CHA	-3.36	1.29	1.43
24	d	403	CLA	C3B-C4B	-3.35	1.35	1.42
33	v	201	HEM	FE-NA	3.35	2.06	1.95
24	B	615	CLA	CBD-CGD	-3.35	1.41	1.52
24	c	505	CLA	C1A-CHA	-3.35	1.29	1.43
24	C	504	CLA	CBD-CGD	-3.35	1.41	1.52
24	B	615	CLA	C1D-ND	-3.35	1.33	1.37
24	b	607	CLA	CHB-C4A	-3.35	1.29	1.37
24	B	604	CLA	CBD-CGD	-3.35	1.41	1.52
24	c	505	CLA	CAA-C2A	-3.35	1.47	1.54
25	D	401	PHO	C4D-ND	-3.35	1.33	1.38
24	C	510	CLA	CBD-CGD	-3.35	1.41	1.52
24	B	608	CLA	O2A-CGA	3.34	1.43	1.33
24	b	608[B]	CLA	C3B-C4B	-3.34	1.35	1.42
24	c	508	CLA	O2D-CGD	3.34	1.41	1.33
26	B	620	BCR	C1-C6	-3.34	1.49	1.53
24	b	612	CLA	C3B-C4B	-3.34	1.35	1.42
24	C	509	CLA	C1D-ND	-3.34	1.33	1.37
24	b	617	CLA	CAA-C2A	-3.34	1.47	1.54
24	A	607	CLA	C3B-C4B	-3.34	1.35	1.42
27	d	404	PL9	C36-C34	3.34	1.58	1.51
24	C	511	CLA	C1D-ND	-3.33	1.33	1.37
24	B	605	CLA	CBD-CGD	-3.33	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	O2D-CGD	3.33	1.41	1.33
29	j	101	LMG	O8-C28	3.33	1.43	1.33
24	c	512	CLA	CBD-CGD	-3.33	1.42	1.52
26	b	621	BCR	C23-C22	3.33	1.53	1.45
24	b	604	CLA	O2A-CGA	3.33	1.43	1.33
24	c	513	CLA	C1A-CHA	-3.32	1.29	1.43
24	B	615	CLA	CAA-C2A	-3.32	1.47	1.54
24	B	607[A]	CLA	CHB-C4A	-3.32	1.29	1.37
24	c	509	CLA	C3D-C4D	-3.32	1.36	1.44
26	b	621	BCR	C4-C5	3.32	1.57	1.51
24	c	508	CLA	C3B-C4B	-3.32	1.35	1.42
24	b	612	CLA	CAA-C2A	-3.32	1.47	1.54
24	C	508	CLA	CBD-CGD	-3.32	1.42	1.52
27	D	405	PL9	C21-C19	3.32	1.58	1.51
24	B	606	CLA	C1D-ND	-3.32	1.33	1.37
24	c	513	CLA	O2D-CGD	3.32	1.41	1.33
24	C	512	CLA	C1A-CHA	-3.32	1.29	1.43
32	d	405	DGD	O6D-C5D	3.32	1.52	1.44
24	B	607[B]	CLA	C3B-C4B	-3.32	1.35	1.42
24	C	507	CLA	C3B-C4B	-3.32	1.35	1.42
24	D	402	CLA	CAA-C2A	-3.32	1.47	1.54
33	v	201	HEM	CAC-C3C	3.31	1.56	1.47
24	a	615	CLA	O2A-CGA	3.31	1.43	1.33
24	C	504	CLA	O2A-CGA	3.31	1.43	1.33
24	b	606	CLA	C1D-ND	-3.31	1.33	1.37
24	C	509	CLA	O2A-CGA	3.31	1.43	1.33
24	B	613	CLA	C4C-C3C	-3.31	1.39	1.45
24	b	615	CLA	CBD-CGD	-3.31	1.42	1.52
24	B	613	CLA	O2A-CGA	3.31	1.43	1.33
24	C	504	CLA	C3D-C4D	-3.30	1.36	1.44
24	b	603	CLA	O2D-CGD	3.30	1.41	1.33
24	C	505	CLA	C1A-CHA	-3.30	1.29	1.43
24	D	403	CLA	CAA-C2A	-3.30	1.48	1.54
24	B	607[A]	CLA	C1D-ND	-3.30	1.33	1.37
24	c	502	CLA	C3D-C4D	-3.29	1.36	1.44
24	c	504	CLA	CAA-C2A	-3.29	1.48	1.54
24	C	508	CLA	O2D-CGD	3.29	1.41	1.33
29	b	622	LMG	O7-C8	-3.29	1.38	1.46
24	B	612	CLA	C3B-C4B	-3.29	1.35	1.42
24	c	513	CLA	O2A-CGA	3.29	1.42	1.33
24	c	501	CLA	C3B-C4B	-3.29	1.35	1.42
24	c	506	CLA	C3D-C4D	-3.28	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	C3D-C2D	-3.28	1.30	1.39
24	c	509	CLA	CBD-CGD	-3.28	1.42	1.52
24	b	611	CLA	C1A-CHA	-3.28	1.29	1.43
24	B	609	CLA	O2D-CGD	3.28	1.41	1.33
24	b	605	CLA	C1A-CHA	-3.28	1.29	1.43
24	c	505	CLA	O2D-CGD	3.28	1.41	1.33
24	B	602	CLA	CHB-C4A	-3.28	1.30	1.37
24	a	607	CLA	CHB-C4A	-3.28	1.30	1.37
24	B	612	CLA	CAA-C2A	-3.28	1.48	1.54
26	K	101	BCR	C4-C5	3.28	1.57	1.51
24	B	613	CLA	C3D-C2D	-3.28	1.30	1.39
24	b	607	CLA	CBD-CGD	-3.28	1.42	1.52
26	b	621	BCR	C12-C13	3.27	1.53	1.45
24	b	614	CLA	MG-NA	-3.27	1.98	2.06
24	b	615	CLA	C3D-C2D	-3.27	1.30	1.39
32	h	102	DGD	C3D-C2D	-3.27	1.44	1.52
32	E	101	DGD	O6D-C5D	3.27	1.52	1.44
24	d	403	CLA	C3D-C4D	-3.26	1.36	1.44
24	a	606	CLA	C1D-ND	-3.26	1.33	1.37
26	A	610	BCR	C40-C30	3.26	1.60	1.53
24	b	617	CLA	C3B-C4B	-3.26	1.35	1.42
24	C	505	CLA	CHB-C4A	-3.26	1.30	1.37
24	c	508	CLA	C3D-C2D	-3.26	1.30	1.39
24	B	617	CLA	C3D-C4D	-3.26	1.36	1.44
24	B	603	CLA	CHB-C4A	-3.26	1.30	1.37
24	B	607[A]	CLA	O2D-CGD	3.25	1.41	1.33
24	C	501	CLA	CAA-C2A	-3.25	1.48	1.54
24	c	502	CLA	CBD-CGD	-3.25	1.42	1.52
24	C	509	CLA	C1A-CHA	-3.25	1.29	1.43
24	c	504	CLA	C3B-C4B	-3.25	1.35	1.42
24	B	603	CLA	C1D-ND	-3.25	1.33	1.37
26	H	101	BCR	C12-C13	3.25	1.52	1.45
24	C	512	CLA	CBD-CGD	-3.25	1.42	1.52
33	E	103	HEM	CAC-C3C	3.24	1.56	1.47
26	b	620	BCR	C17-C18	3.24	1.40	1.35
24	C	505	CLA	C4C-C3C	-3.24	1.39	1.45
24	b	616	CLA	MG-NA	-3.24	1.98	2.06
33	V	201	HEM	CAB-C3B	3.24	1.56	1.47
24	b	609	CLA	CHB-C4A	-3.24	1.30	1.37
24	b	612	CLA	CBD-CGD	-3.24	1.42	1.52
24	C	506	CLA	CAA-C2A	-3.24	1.48	1.54
24	B	615	CLA	O2A-CGA	3.24	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	O2A-CGA	3.23	1.42	1.33
24	c	510	CLA	C1D-ND	-3.23	1.33	1.37
24	B	613	CLA	CBD-CGD	-3.23	1.42	1.52
24	d	402	CLA	C3B-C4B	-3.23	1.35	1.42
24	B	605	CLA	C3D-C2D	-3.23	1.30	1.39
24	b	609	CLA	C3B-C4B	-3.23	1.35	1.42
24	C	513	CLA	C1D-ND	-3.23	1.33	1.37
24	c	512	CLA	C3D-C2D	-3.23	1.30	1.39
24	B	614	CLA	O2A-CGA	3.22	1.42	1.33
24	c	511	CLA	O2D-CGD	3.22	1.41	1.33
24	b	618	CLA	C3D-C2D	-3.22	1.30	1.39
24	C	507	CLA	C1A-CHA	-3.22	1.29	1.43
24	c	501	CLA	C3D-C2D	-3.22	1.30	1.39
26	k	101	BCR	C2-C3	3.22	1.60	1.52
24	B	607[B]	CLA	O2D-CGD	3.22	1.41	1.33
24	b	603	CLA	C1A-CHA	-3.22	1.29	1.43
24	c	502	CLA	O2D-CGD	3.22	1.41	1.33
24	b	607	CLA	C1D-ND	-3.22	1.33	1.37
24	B	610	CLA	O2D-CGD	3.21	1.41	1.33
24	C	511	CLA	MG-NA	-3.21	1.98	2.06
29	D	408	LMG	O7-C8	-3.21	1.38	1.46
24	B	605	CLA	O2D-CGD	3.21	1.41	1.33
24	c	510	CLA	O2A-CGA	3.21	1.42	1.33
32	c	518	DGD	O6D-C5D	3.21	1.52	1.44
24	b	608[B]	CLA	CAA-C2A	-3.21	1.48	1.54
24	C	501	CLA	O2D-CGD	3.20	1.41	1.33
26	c	515	BCR	C4-C5	3.20	1.57	1.51
27	a	611	PL9	C21-C19	3.20	1.57	1.51
24	B	607[B]	CLA	CHB-C4A	-3.20	1.30	1.37
26	h	101	BCR	C27-C26	3.20	1.57	1.51
24	B	612	CLA	O2D-CGD	3.19	1.41	1.33
24	B	612	CLA	O2A-CGA	3.19	1.42	1.33
24	a	609	CLA	C1A-CHA	-3.19	1.29	1.43
24	B	614	CLA	C1D-ND	-3.18	1.33	1.37
24	c	510	CLA	O2D-CGD	3.18	1.41	1.33
24	B	611	CLA	C3D-C2D	-3.18	1.30	1.39
24	B	606	CLA	C3B-C4B	-3.18	1.35	1.42
24	C	506	CLA	C1D-ND	-3.18	1.33	1.37
24	B	608	CLA	CBD-CGD	-3.18	1.42	1.52
24	b	606	CLA	CHB-C4A	-3.18	1.30	1.37
24	b	605	CLA	CAA-C2A	-3.18	1.48	1.54
24	c	501	CLA	CAA-C2A	-3.17	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	514	BCR	C4-C5	3.17	1.57	1.51
24	b	603	CLA	C3B-C4B	-3.17	1.35	1.42
24	c	512	CLA	C3B-C4B	-3.17	1.35	1.42
26	h	101	BCR	C12-C13	3.17	1.52	1.45
24	b	605	CLA	O2D-CGD	3.17	1.40	1.33
24	B	611	CLA	C1A-CHA	-3.17	1.30	1.43
24	B	607[A]	CLA	CBD-CGD	-3.17	1.42	1.52
24	C	505	CLA	O2D-CGD	3.17	1.40	1.33
24	B	611	CLA	C4C-C3C	-3.17	1.39	1.45
33	E	103	HEM	CAB-C3B	3.16	1.56	1.47
24	c	505	CLA	O2A-CGA	3.16	1.42	1.33
24	b	604	CLA	MG-NA	-3.16	1.98	2.06
26	B	619	BCR	C12-C13	3.16	1.52	1.45
24	b	617	CLA	O2D-CGD	3.16	1.40	1.33
24	B	612	CLA	MG-NA	-3.16	1.98	2.06
24	b	610	CLA	C3D-C2D	-3.16	1.30	1.39
24	C	507	CLA	O2D-CGD	3.15	1.40	1.33
24	B	609	CLA	CBD-CGD	-3.15	1.42	1.52
24	b	603	CLA	C1D-ND	-3.15	1.33	1.37
24	c	511	CLA	CAA-C2A	-3.15	1.48	1.54
32	C	517	DGD	C3D-C2D	-3.15	1.44	1.52
24	B	609	CLA	C3D-C2D	-3.15	1.30	1.39
24	C	503	CLA	C1D-ND	-3.15	1.33	1.37
32	h	102	DGD	O6D-C5D	3.15	1.52	1.44
27	D	405	PL9	C36-C34	3.14	1.57	1.51
24	C	502	CLA	C3D-C4D	-3.14	1.37	1.44
24	C	505	CLA	O2A-CGA	3.14	1.42	1.33
24	C	505	CLA	C1D-ND	-3.14	1.33	1.37
24	b	612	CLA	O2D-CGD	3.14	1.40	1.33
26	k	101	BCR	C12-C13	3.14	1.52	1.45
24	C	513	CLA	MG-NA	-3.13	1.98	2.06
26	B	620	BCR	C4-C5	3.13	1.57	1.51
24	d	403	CLA	C3D-C2D	-3.13	1.30	1.39
24	C	501	CLA	C3B-C4B	-3.13	1.35	1.42
24	b	611	CLA	C3D-C2D	-3.13	1.30	1.39
24	a	607	CLA	O2D-CGD	3.13	1.40	1.33
24	a	609	CLA	C3B-C4B	-3.13	1.35	1.42
24	A	609	CLA	C3B-C4B	-3.13	1.35	1.42
26	T	101	BCR	C4-C5	3.13	1.57	1.51
26	b	619	BCR	C1-C6	-3.13	1.49	1.53
24	c	510	CLA	C1A-CHA	-3.13	1.30	1.43
24	C	507	CLA	CAA-C2A	-3.13	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CAA-C2A	-3.12	1.48	1.54
24	B	606	CLA	CAA-C2A	-3.12	1.48	1.54
24	A	606	CLA	MG-NA	-3.12	1.98	2.06
24	B	613	CLA	C2A-C1A	-3.12	1.45	1.52
24	B	607[B]	CLA	CBD-CGD	-3.12	1.42	1.52
24	C	506	CLA	O2A-CGA	3.12	1.42	1.33
24	b	608[A]	CLA	CHB-C4A	-3.12	1.30	1.37
24	C	505	CLA	C3D-C2D	-3.12	1.30	1.39
24	B	602	CLA	C3D-C4D	-3.12	1.37	1.44
24	b	613	CLA	CHB-C4A	-3.11	1.30	1.37
24	B	609	CLA	O2A-CGA	3.11	1.42	1.33
24	C	501	CLA	C4C-C3C	-3.11	1.39	1.45
33	e	102	HEM	CAB-C3B	3.11	1.55	1.47
24	D	404	CLA	CHB-C4A	-3.11	1.30	1.37
24	B	603	CLA	O2D-CGD	3.11	1.40	1.33
24	a	607	CLA	MG-NA	-3.11	1.98	2.06
26	b	620	BCR	C1-C6	-3.11	1.49	1.53
26	k	101	BCR	C27-C26	3.11	1.57	1.51
24	c	509	CLA	C3D-C2D	-3.11	1.30	1.39
33	e	102	HEM	CAC-C3C	3.10	1.55	1.47
24	b	612	CLA	C4C-C3C	-3.10	1.39	1.45
26	h	101	BCR	C4-C5	3.10	1.57	1.51
24	b	617	CLA	C1A-CHA	-3.10	1.30	1.43
24	b	609	CLA	O2D-CGD	3.10	1.40	1.33
24	c	513	CLA	CAA-C2A	-3.09	1.48	1.54
24	b	615	CLA	O2A-CGA	3.09	1.42	1.33
32	E	101	DGD	C3D-C2D	-3.09	1.44	1.52
24	A	606	CLA	O2D-CGD	3.09	1.40	1.33
24	C	513	CLA	C3D-C2D	-3.08	1.30	1.39
29	a	613	LMG	O6-C1	3.08	1.49	1.41
24	B	610	CLA	MG-NA	-3.08	1.99	2.06
24	C	502	CLA	C3D-C2D	-3.08	1.30	1.39
24	C	503	CLA	C3B-C4B	-3.07	1.35	1.42
24	B	615	CLA	O2D-CGD	3.07	1.40	1.33
24	c	507	CLA	CBD-CGD	-3.07	1.42	1.52
24	a	607	CLA	C3B-C4B	-3.07	1.35	1.42
24	b	614	CLA	CHB-C4A	-3.07	1.30	1.37
24	a	606	CLA	CHB-C4A	-3.06	1.30	1.37
24	B	617	CLA	O2D-CGD	3.06	1.40	1.33
24	B	607[B]	CLA	C1D-ND	-3.06	1.34	1.37
24	B	611	CLA	C1D-ND	-3.06	1.34	1.37
24	B	606	CLA	CHB-C4A	-3.06	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	CHB-C4A	-3.06	1.30	1.37
32	E	101	DGD	O5D-C1E	3.06	1.45	1.40
24	b	608[A]	CLA	CAA-C2A	-3.06	1.48	1.54
24	b	612	CLA	C3D-C2D	-3.05	1.30	1.39
24	c	502	CLA	C1D-ND	-3.05	1.34	1.37
24	a	609	CLA	C1D-ND	-3.05	1.34	1.37
24	b	614	CLA	C2A-C1A	-3.05	1.45	1.52
24	c	503	CLA	CHB-C4A	-3.05	1.30	1.37
24	C	508	CLA	MG-NA	-3.04	1.99	2.06
24	b	615	CLA	CHB-C4A	-3.04	1.30	1.37
32	H	102	DGD	C6E-C5E	-3.04	1.41	1.51
26	C	514	BCR	C27-C26	3.04	1.57	1.51
24	C	503	CLA	CHB-C4A	-3.04	1.30	1.37
32	E	101	DGD	O6E-C1E	3.03	1.49	1.41
24	A	609	CLA	CHB-C4A	-3.03	1.30	1.37
24	B	606	CLA	C1A-CHA	-3.03	1.30	1.43
24	c	513	CLA	C3D-CAD	3.03	1.55	1.45
24	C	501	CLA	CBD-CGD	-3.03	1.42	1.52
24	C	510	CLA	C2A-C1A	-3.03	1.45	1.52
32	c	517	DGD	C3D-C2D	-3.02	1.44	1.52
24	B	604	CLA	O2D-CGD	3.02	1.40	1.33
24	b	612	CLA	C1D-ND	-3.02	1.34	1.37
24	B	609	CLA	CHB-C4A	-3.02	1.30	1.37
25	d	401	PHO	C4D-CHA	3.02	1.44	1.39
26	a	610	BCR	C35-C13	-3.02	1.44	1.50
24	c	510	CLA	CBD-CGD	-3.02	1.43	1.52
24	b	611	CLA	C3B-C4B	-3.02	1.35	1.42
24	B	602	CLA	C1A-CHA	-3.02	1.30	1.43
24	b	608[B]	CLA	CHB-C4A	-3.01	1.30	1.37
24	B	616	CLA	C3D-C2D	-3.01	1.30	1.39
24	c	504	CLA	MG-NA	-3.01	1.99	2.06
24	a	609	CLA	O2D-CGD	3.01	1.40	1.33
26	c	521	BCR	C4-C5	3.01	1.56	1.51
24	b	617	CLA	CHB-C4A	-3.01	1.30	1.37
24	B	608	CLA	CHB-C4A	-3.00	1.30	1.37
24	c	504	CLA	C1D-ND	-3.00	1.34	1.37
24	C	504	CLA	C3D-C2D	-3.00	1.30	1.39
24	b	609	CLA	MG-NA	-3.00	1.99	2.06
24	b	605	CLA	CHB-C4A	-3.00	1.30	1.37
24	c	507	CLA	C3D-C2D	-3.00	1.30	1.39
24	c	501	CLA	C1D-ND	-2.99	1.34	1.37
24	B	616	CLA	O2D-CGD	2.99	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C12-C13	2.99	1.52	1.45
24	b	612	CLA	CHB-C4A	-2.99	1.30	1.37
24	C	501	CLA	C1D-ND	-2.99	1.34	1.37
24	C	501	CLA	C3D-CAD	2.99	1.55	1.45
29	Z	101	LMG	O7-C8	-2.99	1.39	1.46
24	C	501	CLA	CHB-C4A	-2.99	1.30	1.37
24	c	504	CLA	CBD-CGD	-2.99	1.43	1.52
24	B	608	CLA	C1D-ND	-2.99	1.34	1.37
24	b	607	CLA	MG-NA	-2.98	1.99	2.06
26	t	101	BCR	C4-C5	2.98	1.56	1.51
24	b	604	CLA	C3B-C4B	-2.98	1.35	1.42
32	H	102	DGD	O6D-C5D	2.98	1.51	1.44
27	d	404	PL9	C41-C39	2.98	1.57	1.51
24	A	606	CLA	C3D-CAD	2.98	1.55	1.45
26	B	618	BCR	C12-C13	2.98	1.52	1.45
24	C	502	CLA	CHB-C4A	-2.98	1.30	1.37
24	B	605	CLA	CHB-C4A	-2.98	1.30	1.37
24	B	617	CLA	C3D-CAD	2.98	1.55	1.45
24	C	502	CLA	C3D-CAD	2.98	1.55	1.45
24	b	607	CLA	O2D-CGD	2.98	1.40	1.33
24	b	603	CLA	CBD-CGD	-2.97	1.43	1.52
24	b	611	CLA	MG-NA	-2.97	1.99	2.06
24	C	502	CLA	CBD-CGD	-2.97	1.43	1.52
29	j	101	LMG	O7-C8	-2.97	1.39	1.46
24	b	608[A]	CLA	C1D-ND	-2.97	1.34	1.37
24	b	611	CLA	CHB-C4A	-2.96	1.30	1.37
24	a	607	CLA	C1D-ND	-2.96	1.34	1.37
24	B	603	CLA	MG-NA	-2.96	1.99	2.06
24	C	509	CLA	O2D-CGD	2.96	1.40	1.33
24	c	511	CLA	CHB-C4A	-2.96	1.30	1.37
24	c	508	CLA	O2A-CGA	2.95	1.42	1.33
24	C	501	CLA	C3D-C2D	-2.95	1.31	1.39
24	B	615	CLA	MG-NA	-2.95	1.99	2.06
24	C	509	CLA	CHB-C4A	-2.95	1.30	1.37
24	A	609	CLA	CAA-C2A	-2.94	1.48	1.54
24	C	509	CLA	CAA-C2A	-2.94	1.48	1.54
32	d	405	DGD	C3D-C2D	-2.94	1.44	1.52
24	b	610	CLA	C1D-ND	-2.94	1.34	1.37
24	d	402	CLA	C2A-C1A	-2.94	1.45	1.52
26	K	101	BCR	C12-C13	2.94	1.52	1.45
24	b	610	CLA	C3D-CAD	2.94	1.55	1.45
24	c	513	CLA	C3D-C2D	-2.93	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	MG-NC	-2.93	1.99	2.06
24	b	614	CLA	O2D-CGD	2.93	1.40	1.33
24	B	603	CLA	CAA-C2A	-2.93	1.48	1.54
24	B	604	CLA	CHB-C4A	-2.93	1.30	1.37
24	b	610	CLA	O2A-CGA	2.93	1.41	1.33
24	C	507	CLA	C1D-ND	-2.93	1.34	1.37
24	c	503	CLA	C3B-C4B	-2.93	1.36	1.42
24	B	604	CLA	MG-NA	-2.92	1.99	2.06
24	c	512	CLA	CHB-C4A	-2.92	1.30	1.37
24	B	604	CLA	CAA-C2A	-2.92	1.48	1.54
32	C	516	DGD	O6E-C1E	2.92	1.49	1.41
24	b	609	CLA	O2A-CGA	2.92	1.41	1.33
24	a	606	CLA	O2D-CGD	2.92	1.40	1.33
26	B	619	BCR	C40-C30	2.92	1.59	1.53
32	C	517	DGD	C3E-C2E	-2.92	1.44	1.52
24	b	604	CLA	C2A-C1A	-2.91	1.45	1.52
24	b	609	CLA	C2A-C1A	-2.91	1.45	1.52
24	b	616	CLA	CHB-C4A	-2.91	1.30	1.37
24	B	613	CLA	O2D-CGD	2.91	1.40	1.33
24	B	603	CLA	C3B-C4B	-2.91	1.36	1.42
26	H	101	BCR	C4-C5	2.91	1.56	1.51
24	C	512	CLA	C3D-C2D	-2.91	1.31	1.39
24	C	506	CLA	C1A-CHA	-2.91	1.31	1.43
24	C	511	CLA	CBD-CGD	-2.91	1.43	1.52
24	C	507	CLA	MG-NA	-2.91	1.99	2.06
26	K	101	BCR	C27-C26	2.91	1.56	1.51
24	c	508	CLA	C3D-CAD	2.90	1.55	1.45
24	c	506	CLA	C1A-CHA	-2.90	1.31	1.43
24	a	615	CLA	O2D-CGD	2.90	1.40	1.33
24	c	509	CLA	CHB-C4A	-2.90	1.30	1.37
24	c	508	CLA	MG-NA	-2.90	1.99	2.06
26	T	101	BCR	C35-C13	-2.90	1.44	1.50
26	c	514	BCR	C27-C26	2.90	1.56	1.51
24	b	613	CLA	MG-NA	-2.90	1.99	2.06
26	C	514	BCR	C31-C1	-2.89	1.48	1.53
26	c	514	BCR	C35-C13	-2.89	1.44	1.50
24	c	506	CLA	O2D-CGD	2.89	1.40	1.33
24	a	609	CLA	CBD-CGD	-2.89	1.43	1.52
24	b	611	CLA	C3D-CAD	2.89	1.54	1.45
24	b	604	CLA	CBD-CGD	-2.89	1.43	1.52
25	a	608	PHO	CAC-C3C	-2.89	1.46	1.51
24	C	503	CLA	CAA-C2A	-2.88	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	620	BCR	C27-C26	2.88	1.56	1.51
24	C	509	CLA	MG-NA	-2.88	1.99	2.06
24	b	606	CLA	CBD-CGD	-2.88	1.43	1.52
24	b	615	CLA	O2D-CGD	2.88	1.40	1.33
24	C	504	CLA	C3D-CAD	2.88	1.54	1.45
24	B	609	CLA	C4C-C3C	-2.88	1.40	1.45
24	D	404	CLA	O2D-CED	-2.87	1.38	1.45
24	C	512	CLA	O2D-CGD	2.87	1.40	1.33
24	C	512	CLA	C1D-ND	-2.87	1.34	1.37
32	C	516	DGD	O2D-C2D	2.87	1.49	1.43
24	C	510	CLA	O2D-CGD	2.87	1.40	1.33
24	c	504	CLA	O2D-CGD	2.86	1.40	1.33
24	C	513	CLA	CHB-C4A	-2.86	1.30	1.37
24	B	616	CLA	C3B-C4B	-2.86	1.36	1.42
27	d	404	PL9	C21-C19	2.86	1.57	1.51
26	b	621	BCR	C31-C1	-2.86	1.48	1.53
24	B	616	CLA	CHB-C4A	-2.86	1.30	1.37
26	f	101	BCR	C12-C13	2.86	1.52	1.45
24	a	606	CLA	O2D-CED	-2.86	1.38	1.45
26	K	102	BCR	C27-C26	2.86	1.56	1.51
24	c	501	CLA	C3D-CAD	2.86	1.54	1.45
24	B	602	CLA	C3B-C4B	-2.86	1.36	1.42
24	A	609	CLA	CAB-C3B	2.86	1.55	1.47
24	A	607	CLA	CHB-C4A	-2.85	1.30	1.37
26	c	514	BCR	C31-C1	-2.85	1.48	1.53
24	c	502	CLA	CAA-C2A	-2.85	1.48	1.54
24	c	503	CLA	CAA-C2A	-2.85	1.48	1.54
24	c	512	CLA	CAA-C2A	-2.85	1.48	1.54
29	C	518	LMG	O7-C8	-2.85	1.39	1.46
24	b	615	CLA	C1D-ND	-2.85	1.34	1.37
24	a	606	CLA	MG-NA	-2.85	1.99	2.06
24	c	507	CLA	O2D-CGD	2.84	1.40	1.33
24	B	602	CLA	O2D-CGD	2.84	1.40	1.33
26	b	620	BCR	C40-C30	2.84	1.59	1.53
24	c	510	CLA	CHB-C4A	-2.84	1.31	1.37
26	K	102	BCR	C4-C5	2.84	1.56	1.51
24	c	507	CLA	CHB-C4A	-2.84	1.31	1.37
24	c	510	CLA	MG-NA	-2.83	1.99	2.06
24	c	507	CLA	C3D-CAD	2.83	1.54	1.45
24	B	611	CLA	MG-NA	-2.83	1.99	2.06
24	B	611	CLA	C3B-C4B	-2.83	1.36	1.42
24	c	503	CLA	O2D-CED	-2.83	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	MG-NA	-2.83	1.99	2.06
24	B	608	CLA	O2D-CGD	2.83	1.40	1.33
24	A	606	CLA	MG-NC	-2.83	1.99	2.06
24	B	611	CLA	O2D-CGD	2.83	1.40	1.33
24	b	615	CLA	C3D-CAD	2.83	1.54	1.45
24	c	511	CLA	C3B-C4B	-2.83	1.36	1.42
24	C	505	CLA	C3D-CAD	2.83	1.54	1.45
26	B	620	BCR	C31-C1	-2.83	1.48	1.53
24	C	512	CLA	CHB-C4A	-2.82	1.31	1.37
24	B	608	CLA	C2A-C1A	-2.82	1.45	1.52
24	c	505	CLA	CHB-C4A	-2.82	1.31	1.37
24	c	509	CLA	C3D-CAD	2.82	1.54	1.45
24	c	501	CLA	CHB-C4A	-2.82	1.31	1.37
24	C	513	CLA	CAA-C2A	-2.82	1.48	1.54
26	h	101	BCR	C31-C1	-2.81	1.48	1.53
29	c	519	LMG	O7-C8	-2.81	1.39	1.46
24	b	618	CLA	C3D-CAD	2.81	1.54	1.45
26	f	101	BCR	C17-C18	2.81	1.39	1.35
24	C	504	CLA	O2D-CGD	2.81	1.40	1.33
24	C	513	CLA	C3D-CAD	2.81	1.54	1.45
32	c	516	DGD	O6D-C5D	2.80	1.51	1.44
26	c	514	BCR	C12-C13	2.80	1.52	1.45
24	B	613	CLA	C3D-CAD	2.80	1.54	1.45
24	b	616	CLA	C2A-C1A	-2.80	1.45	1.52
24	C	512	CLA	C3D-CAD	2.80	1.54	1.45
26	t	101	BCR	C12-C13	2.80	1.51	1.45
26	H	101	BCR	C1-C6	-2.79	1.49	1.53
28	A	612	SQD	C6-S	-2.79	1.67	1.77
24	B	610	CLA	CBD-CGD	-2.79	1.43	1.52
32	c	516	DGD	C6E-C5E	-2.79	1.42	1.51
24	B	611	CLA	O2D-CED	-2.79	1.38	1.45
32	H	102	DGD	O5D-C1E	2.78	1.44	1.40
24	c	506	CLA	CBD-CGD	-2.78	1.43	1.52
32	c	518	DGD	O5D-C1E	2.78	1.44	1.40
29	A	613	LMG	O7-C8	-2.78	1.39	1.46
29	B	621	LMG	O7-C8	-2.78	1.39	1.46
32	c	516	DGD	O6E-C1E	2.77	1.48	1.41
28	a	612	SQD	C6-S	-2.77	1.67	1.77
24	C	507	CLA	CHB-C4A	-2.77	1.31	1.37
24	B	617	CLA	C3D-C2D	-2.77	1.31	1.39
26	a	610	BCR	C4-C5	2.77	1.56	1.51
26	k	101	BCR	C31-C1	-2.77	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	405	PL9	C41-C39	2.77	1.57	1.51
24	d	403	CLA	C3D-CAD	2.77	1.54	1.45
26	F	101	BCR	C4-C5	2.77	1.56	1.51
24	b	608[A]	CLA	O2D-CGD	2.77	1.40	1.33
24	C	505	CLA	CBD-CGD	-2.76	1.43	1.52
24	c	502	CLA	MG-NA	-2.76	1.99	2.06
26	b	620	BCR	C4-C5	2.76	1.56	1.51
24	B	606	CLA	CBD-CGD	-2.76	1.43	1.52
32	d	405	DGD	O3G-C1D	2.76	1.44	1.40
24	B	610	CLA	C2A-C1A	-2.75	1.46	1.52
24	b	613	CLA	O2D-CGD	2.75	1.39	1.33
32	d	405	DGD	O6E-C1E	2.75	1.48	1.41
24	A	607	CLA	MG-NC	-2.75	1.99	2.06
24	b	613	CLA	CAA-C2A	-2.75	1.49	1.54
26	B	619	BCR	C4-C5	2.75	1.56	1.51
24	C	504	CLA	MG-NA	-2.75	1.99	2.06
24	A	607	CLA	C3D-CAD	2.75	1.54	1.45
26	A	610	BCR	C4-C5	2.75	1.56	1.51
32	h	102	DGD	C6E-C5E	-2.74	1.42	1.51
24	B	602	CLA	C3D-CAD	2.74	1.54	1.45
26	k	101	BCR	C7-C6	2.74	1.54	1.45
24	a	609	CLA	CHB-C4A	-2.74	1.31	1.37
24	c	511	CLA	CBD-CGD	-2.74	1.43	1.52
24	B	609	CLA	C3D-CAD	2.74	1.54	1.45
24	B	608	CLA	MG-NA	-2.74	1.99	2.06
32	c	516	DGD	C3E-C2E	-2.74	1.45	1.52
24	C	507	CLA	C3D-CAD	2.74	1.54	1.45
24	B	610	CLA	C3D-CAD	2.74	1.54	1.45
24	A	606	CLA	O2D-CED	-2.73	1.38	1.45
26	C	514	BCR	C12-C13	2.73	1.51	1.45
24	c	512	CLA	C1D-ND	-2.73	1.34	1.37
24	A	606	CLA	C2A-C1A	-2.73	1.46	1.52
26	K	102	BCR	C31-C1	-2.73	1.48	1.53
24	C	502	CLA	CAA-C2A	-2.73	1.49	1.54
24	c	505	CLA	CBD-CGD	-2.73	1.43	1.52
24	C	502	CLA	O2D-CGD	2.73	1.39	1.33
24	D	404	CLA	O2D-CGD	2.73	1.39	1.33
24	c	506	CLA	C1D-ND	-2.73	1.34	1.37
26	I	101	BCR	C27-C26	2.73	1.56	1.51
33	E	103	HEM	FE-NB	2.73	2.03	1.94
24	b	618	CLA	CHB-C4A	-2.73	1.31	1.37
24	D	402	CLA	O2D-CED	-2.73	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	H	102	DGD	O6E-C1E	2.73	1.48	1.41
26	B	619	BCR	C35-C13	-2.72	1.45	1.50
32	C	516	DGD	O5D-C1E	2.72	1.44	1.40
24	B	616	CLA	C3D-CAD	2.71	1.54	1.45
24	c	502	CLA	C3D-CAD	2.71	1.54	1.45
24	C	511	CLA	CAA-C2A	-2.71	1.49	1.54
24	B	603	CLA	C3D-CAD	2.71	1.54	1.45
26	b	619	BCR	C27-C26	2.71	1.56	1.51
24	D	403	CLA	MG-NA	-2.71	1.99	2.06
24	B	612	CLA	C3D-CAD	2.70	1.54	1.45
24	B	609	CLA	C1D-ND	-2.70	1.34	1.37
32	C	515	DGD	C1D-C2D	-2.70	1.44	1.52
24	b	608[B]	CLA	O2D-CGD	2.70	1.39	1.33
24	B	617	CLA	C1D-ND	-2.70	1.34	1.37
24	B	605	CLA	C1D-ND	-2.70	1.34	1.37
24	B	611	CLA	C3D-CAD	2.69	1.54	1.45
24	C	501	CLA	C2A-C1A	-2.69	1.46	1.52
24	C	504	CLA	C2A-C1A	-2.69	1.46	1.52
26	B	620	BCR	C12-C13	2.69	1.51	1.45
24	b	608[B]	CLA	C1D-ND	-2.69	1.34	1.37
24	d	403	CLA	O2D-CED	-2.69	1.39	1.45
24	B	616	CLA	CAA-C2A	-2.69	1.49	1.54
24	c	509	CLA	MG-NA	-2.69	1.99	2.06
32	c	517	DGD	O6D-C5D	2.69	1.50	1.44
28	A	614	SQD	C6-S	-2.68	1.67	1.77
28	a	614	SQD	C6-S	-2.68	1.67	1.77
24	D	403	CLA	O2D-CED	-2.68	1.39	1.45
26	t	101	BCR	C27-C26	2.68	1.56	1.51
26	c	521	BCR	C7-C6	2.68	1.54	1.45
24	c	507	CLA	CAA-C2A	-2.67	1.49	1.54
24	B	603	CLA	CBD-CGD	-2.67	1.44	1.52
32	h	102	DGD	C3E-C2E	-2.67	1.45	1.52
24	b	612	CLA	C3D-CAD	2.67	1.54	1.45
24	b	614	CLA	CBD-CGD	-2.67	1.44	1.52
24	C	505	CLA	MG-NA	-2.67	1.99	2.06
26	K	101	BCR	C31-C1	-2.67	1.48	1.53
26	b	619	BCR	C4-C5	2.66	1.56	1.51
32	C	516	DGD	C3D-C2D	-2.66	1.45	1.52
24	C	509	CLA	C3D-CAD	2.66	1.54	1.45
32	c	517	DGD	C6E-C5E	-2.66	1.42	1.51
24	b	617	CLA	CBD-CGD	-2.66	1.44	1.52
32	C	515	DGD	C6E-C5E	-2.65	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	V	201	HEM	CMC-C2C	2.65	1.56	1.50
24	B	612	CLA	C2A-C1A	-2.65	1.46	1.52
25	A	608	PHO	C4D-ND	-2.65	1.34	1.38
24	a	607	CLA	CAA-C2A	-2.65	1.49	1.54
32	C	517	DGD	O2D-C2D	2.65	1.49	1.43
29	z	101	LMG	O7-C8	-2.65	1.40	1.46
24	A	607	CLA	O2D-CGD	2.65	1.39	1.33
24	C	503	CLA	O2D-CED	-2.65	1.39	1.45
26	b	620	BCR	C31-C1	-2.64	1.48	1.53
24	A	609	CLA	O2D-CGD	2.64	1.39	1.33
32	c	518	DGD	C6E-C5E	-2.64	1.43	1.51
24	d	403	CLA	CHB-C4A	-2.64	1.31	1.37
24	d	403	CLA	O2D-CGD	2.64	1.39	1.33
24	d	402	CLA	CAB-C3B	2.64	1.54	1.47
26	b	621	BCR	C27-C26	2.64	1.56	1.51
24	B	614	CLA	O2D-CED	-2.64	1.39	1.45
24	B	607[A]	CLA	C3D-CAD	2.64	1.54	1.45
24	a	615	CLA	C2A-C1A	-2.63	1.46	1.52
24	c	506	CLA	C3D-CAD	2.63	1.54	1.45
32	c	518	DGD	O2D-C2D	2.63	1.49	1.43
24	B	614	CLA	MG-NC	-2.63	2.00	2.06
24	c	512	CLA	O2D-CGD	2.63	1.39	1.33
24	C	511	CLA	CHB-C4A	-2.63	1.31	1.37
24	B	607[A]	CLA	MG-NA	-2.63	2.00	2.06
28	X	101	SQD	C6-S	-2.63	1.67	1.77
24	a	609	CLA	CAA-C2A	-2.63	1.49	1.54
24	C	503	CLA	MG-NA	-2.63	2.00	2.06
24	a	609	CLA	O2D-CED	-2.63	1.39	1.45
24	b	610	CLA	C2A-C1A	-2.63	1.46	1.52
24	a	615	CLA	MG-NC	-2.63	2.00	2.06
28	x	101	SQD	C6-S	-2.62	1.67	1.77
24	B	607[B]	CLA	C2A-C1A	-2.62	1.46	1.52
32	C	517	DGD	C6E-C5E	-2.62	1.43	1.51
24	C	508	CLA	C2A-C1A	-2.62	1.46	1.52
24	b	615	CLA	MG-NA	-2.61	2.00	2.06
24	b	603	CLA	CHB-C4A	-2.61	1.31	1.37
24	b	609	CLA	C1D-ND	-2.61	1.34	1.37
24	C	502	CLA	O2D-CED	-2.61	1.39	1.45
24	b	616	CLA	O2A-CGA	2.61	1.41	1.33
26	c	515	BCR	C27-C26	2.61	1.56	1.51
26	c	521	BCR	C27-C26	2.60	1.56	1.51
24	a	607	CLA	C3D-CAD	2.60	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	C3D-CAD	2.60	1.54	1.45
24	C	501	CLA	CMC-C2C	2.60	1.56	1.50
26	T	101	BCR	C27-C26	2.60	1.56	1.51
24	B	614	CLA	CHB-C4A	-2.60	1.31	1.37
25	a	608	PHO	CMD-C2D	-2.60	1.46	1.51
26	h	101	BCR	C35-C13	-2.60	1.45	1.50
32	d	405	DGD	C6E-C5E	-2.60	1.43	1.51
25	d	401	PHO	C4D-ND	-2.59	1.34	1.38
26	b	620	BCR	C12-C13	2.59	1.51	1.45
24	D	402	CLA	O2D-CGD	2.59	1.39	1.33
24	A	606	CLA	CBD-CGD	-2.59	1.44	1.52
24	B	607[B]	CLA	C3D-CAD	2.59	1.53	1.45
24	D	403	CLA	MG-NC	-2.59	2.00	2.06
24	C	506	CLA	C3D-CAD	2.59	1.53	1.45
24	b	603	CLA	CAA-C2A	-2.59	1.49	1.54
24	C	505	CLA	C2A-C1A	-2.59	1.46	1.52
26	k	101	BCR	C1-C6	-2.59	1.50	1.53
24	A	609	CLA	OBD-CAD	-2.59	1.18	1.22
24	C	513	CLA	CBD-CGD	-2.59	1.44	1.52
24	B	614	CLA	MG-NA	-2.58	2.00	2.06
24	a	607	CLA	CAB-C3B	2.58	1.54	1.47
24	b	616	CLA	O2D-CGD	2.58	1.39	1.33
24	c	505	CLA	C2A-C1A	-2.58	1.46	1.52
24	d	402	CLA	O2D-CGD	2.57	1.39	1.33
24	C	506	CLA	MG-NA	-2.57	2.00	2.06
24	D	402	CLA	OBD-CAD	-2.57	1.18	1.22
24	D	402	CLA	C2A-C1A	-2.57	1.46	1.52
24	B	607[A]	CLA	C2A-C1A	-2.57	1.46	1.52
25	a	608	PHO	C4D-ND	-2.57	1.35	1.38
24	b	608[B]	CLA	O2D-CED	-2.56	1.39	1.45
24	d	402	CLA	C3D-CAD	2.56	1.53	1.45
24	b	618	CLA	MG-NA	-2.56	2.00	2.06
24	b	613	CLA	CAB-C3B	2.56	1.54	1.47
27	D	405	PL9	C26-C24	2.56	1.56	1.51
32	c	516	DGD	O2D-C2D	2.56	1.49	1.43
24	b	607	CLA	C2A-C1A	-2.56	1.46	1.52
24	b	606	CLA	MG-NA	-2.55	2.00	2.06
24	B	614	CLA	OBD-CAD	-2.55	1.18	1.22
24	c	510	CLA	C3D-CAD	2.55	1.53	1.45
32	h	102	DGD	C1D-C2D	-2.55	1.45	1.52
28	b	601	SQD	C6-S	-2.55	1.68	1.77
24	D	404	CLA	C3D-CAD	2.55	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	CAA-C2A	-2.55	1.49	1.54
24	A	609	CLA	MG-NA	-2.55	2.00	2.06
24	C	503	CLA	CMC-C2C	2.55	1.56	1.50
33	v	201	HEM	FE-NB	2.54	2.02	1.94
24	B	606	CLA	MG-NA	-2.54	2.00	2.06
32	C	516	DGD	C6D-C5D	-2.54	1.43	1.51
24	c	513	CLA	MG-NA	-2.54	2.00	2.06
24	d	403	CLA	CAA-C2A	-2.53	1.49	1.54
25	a	608	PHO	C4D-CHA	2.53	1.43	1.39
32	C	515	DGD	C3E-C2E	-2.53	1.45	1.52
24	c	501	CLA	CBD-CGD	-2.53	1.44	1.52
26	f	101	BCR	C35-C13	-2.53	1.45	1.50
29	C	519	LMG	O7-C8	-2.53	1.40	1.46
24	c	503	CLA	O2D-CGD	2.53	1.39	1.33
24	c	501	CLA	CAB-C3B	2.53	1.54	1.47
32	E	101	DGD	O3G-C1D	2.52	1.44	1.40
24	b	606	CLA	CAA-C2A	-2.52	1.49	1.54
26	B	618	BCR	C27-C26	2.52	1.56	1.51
32	h	102	DGD	O6E-C1E	2.52	1.48	1.41
26	t	101	BCR	C35-C13	-2.52	1.45	1.50
24	c	507	CLA	C1D-ND	-2.52	1.34	1.37
32	d	405	DGD	O6D-C1D	2.52	1.48	1.41
24	b	613	CLA	MG-NC	-2.52	2.00	2.06
24	A	609	CLA	O2D-CED	-2.52	1.39	1.45
24	c	507	CLA	MG-NA	-2.52	2.00	2.06
24	b	603	CLA	C3D-CAD	2.52	1.53	1.45
24	c	511	CLA	C3D-CAD	2.52	1.53	1.45
26	H	101	BCR	C31-C1	-2.51	1.48	1.53
32	d	405	DGD	O5D-C1E	2.51	1.44	1.40
24	C	504	CLA	C1D-ND	-2.51	1.34	1.37
24	c	501	CLA	MG-NA	-2.51	2.00	2.06
24	c	504	CLA	CMC-C2C	2.51	1.56	1.50
28	B	622	SQD	C6-S	-2.51	1.68	1.77
24	c	504	CLA	MG-NC	-2.51	2.00	2.06
24	a	609	CLA	C3D-CAD	2.51	1.53	1.45
24	c	504	CLA	C3D-CAD	2.51	1.53	1.45
32	H	102	DGD	O2D-C2D	2.50	1.48	1.43
24	A	607	CLA	O2D-CED	-2.50	1.39	1.45
24	c	506	CLA	O2D-CED	-2.50	1.39	1.45
24	D	404	CLA	CAA-C2A	-2.50	1.49	1.54
24	B	617	CLA	CHB-C4A	-2.50	1.31	1.37
24	c	511	CLA	O2D-CED	-2.50	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	MG-NA	-2.50	2.00	2.06
26	a	610	BCR	C12-C13	2.50	1.51	1.45
24	C	503	CLA	OBD-CAD	-2.50	1.18	1.22
26	b	621	BCR	C35-C13	-2.50	1.45	1.50
24	C	507	CLA	CBD-CGD	-2.50	1.44	1.52
24	C	504	CLA	CAB-C3B	2.50	1.54	1.47
24	d	402	CLA	O2D-CED	-2.49	1.39	1.45
24	b	612	CLA	MG-NA	-2.49	2.00	2.06
26	C	514	BCR	C33-C5	2.49	1.55	1.50
24	B	616	CLA	C1D-ND	-2.49	1.34	1.37
24	c	508	CLA	C2A-C1A	-2.49	1.46	1.52
24	b	608[A]	CLA	O2D-CED	-2.49	1.39	1.45
24	C	508	CLA	C3D-CAD	2.49	1.53	1.45
24	b	618	CLA	CBD-CGD	-2.49	1.44	1.52
24	C	510	CLA	C3D-CAD	2.48	1.53	1.45
32	d	405	DGD	O2D-C2D	2.48	1.48	1.43
24	B	603	CLA	C2A-C1A	-2.48	1.46	1.52
24	b	610	CLA	CBD-CGD	-2.48	1.44	1.52
32	c	517	DGD	O6E-C1E	2.48	1.48	1.41
24	b	610	CLA	MG-NA	-2.48	2.00	2.06
24	B	608	CLA	O2D-CED	-2.48	1.39	1.45
24	c	503	CLA	CMC-C2C	2.47	1.56	1.50
24	B	607[B]	CLA	MG-NA	-2.47	2.00	2.06
24	D	403	CLA	O2D-CGD	2.47	1.39	1.33
26	B	618	BCR	C31-C1	-2.47	1.48	1.53
32	c	516	DGD	O5D-C1E	2.47	1.44	1.40
24	b	611	CLA	C2A-C1A	-2.47	1.46	1.52
24	c	512	CLA	O2D-CED	-2.47	1.39	1.45
24	b	604	CLA	OBD-CAD	-2.47	1.18	1.22
26	K	101	BCR	C7-C6	2.47	1.53	1.45
24	B	614	CLA	C2A-C1A	-2.47	1.46	1.52
24	B	605	CLA	C3D-CAD	2.47	1.53	1.45
28	l	101	SQD	C6-S	-2.47	1.68	1.77
26	K	101	BCR	C1-C6	-2.47	1.50	1.53
24	B	616	CLA	O2D-CED	-2.46	1.39	1.45
24	B	602	CLA	C1D-ND	-2.46	1.34	1.37
24	D	403	CLA	OBD-CAD	-2.46	1.18	1.22
25	d	401	PHO	C3D-C4D	2.46	1.44	1.41
24	B	602	CLA	O2D-CED	-2.46	1.39	1.45
24	c	501	CLA	CMC-C2C	2.46	1.56	1.50
24	C	501	CLA	MG-NA	-2.46	2.00	2.06
24	D	403	CLA	CAB-C3B	2.46	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	515	DGD	O6E-C1E	2.46	1.48	1.41
24	b	605	CLA	CAB-C3B	2.46	1.54	1.47
32	E	101	DGD	O3D-C3D	2.45	1.48	1.43
24	A	607	CLA	C2A-C1A	-2.45	1.46	1.52
24	C	509	CLA	MG-NC	-2.45	2.00	2.06
32	C	516	DGD	O6D-C5D	2.45	1.50	1.44
24	c	504	CLA	CAB-C3B	2.45	1.54	1.47
26	C	514	BCR	C35-C13	-2.45	1.45	1.50
24	B	617	CLA	O2D-CED	-2.45	1.39	1.45
24	c	505	CLA	MG-NA	-2.45	2.00	2.06
26	a	610	BCR	C31-C1	-2.45	1.48	1.53
24	C	509	CLA	O2D-CED	-2.45	1.39	1.45
24	c	512	CLA	CAB-C3B	2.44	1.54	1.47
28	L	102	SQD	C6-S	-2.44	1.68	1.77
24	B	605	CLA	C2A-C1A	-2.44	1.46	1.52
26	A	610	BCR	C7-C6	2.44	1.53	1.45
32	c	518	DGD	O6E-C1E	2.44	1.48	1.41
24	c	509	CLA	C2A-C1A	-2.44	1.46	1.52
24	b	615	CLA	O2D-CED	-2.44	1.39	1.45
24	c	513	CLA	CBD-CGD	-2.44	1.44	1.52
26	k	101	BCR	C35-C13	-2.44	1.45	1.50
24	C	513	CLA	C2A-C1A	-2.44	1.46	1.52
24	c	511	CLA	C1D-ND	-2.44	1.34	1.37
24	D	403	CLA	C2A-C1A	-2.44	1.46	1.52
24	d	403	CLA	MG-NA	-2.43	2.00	2.06
29	a	613	LMG	O7-C8	-2.43	1.40	1.46
24	b	616	CLA	C3D-CAD	2.43	1.53	1.45
24	b	608[A]	CLA	C3D-CAD	2.43	1.53	1.45
26	B	619	BCR	C1-C6	-2.43	1.50	1.53
29	c	520	LMG	O7-C8	-2.42	1.40	1.46
26	I	101	BCR	C35-C13	-2.42	1.45	1.50
24	c	503	CLA	CAB-C3B	2.42	1.54	1.47
26	K	101	BCR	C35-C13	-2.42	1.45	1.50
26	c	521	BCR	C31-C1	-2.42	1.49	1.53
26	B	619	BCR	C30-C25	2.42	1.57	1.53
24	c	503	CLA	C3D-CAD	2.42	1.53	1.45
24	C	504	CLA	O2D-CED	-2.42	1.39	1.45
24	C	508	CLA	OBD-CAD	-2.42	1.18	1.22
24	b	614	CLA	C3D-CAD	2.42	1.53	1.45
32	C	517	DGD	O3D-C3D	2.42	1.48	1.43
26	a	610	BCR	C7-C6	2.41	1.53	1.45
24	b	609	CLA	MG-NC	-2.41	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	O2D-CGD	2.41	1.39	1.33
32	h	102	DGD	O2D-C2D	2.41	1.48	1.43
24	b	608[B]	CLA	C3D-CAD	2.41	1.53	1.45
26	K	102	BCR	C7-C6	2.41	1.53	1.45
24	b	607	CLA	C3D-CAD	2.41	1.53	1.45
24	c	504	CLA	O2D-CED	-2.41	1.39	1.45
27	d	404	PL9	C7-C3	2.41	1.53	1.51
24	d	403	CLA	MG-NC	-2.40	2.00	2.06
32	E	101	DGD	O6D-C1D	2.40	1.48	1.41
32	h	102	DGD	O5D-C1E	2.40	1.44	1.40
24	b	605	CLA	MG-NA	-2.40	2.00	2.06
24	a	615	CLA	O2D-CED	-2.40	1.39	1.45
26	t	101	BCR	C7-C6	2.40	1.53	1.45
24	c	507	CLA	O2D-CED	-2.40	1.39	1.45
26	B	618	BCR	C4-C5	2.39	1.55	1.51
24	a	606	CLA	C3D-CAD	2.39	1.53	1.45
24	b	605	CLA	C3D-CAD	2.39	1.53	1.45
24	b	608[A]	CLA	MG-NA	-2.39	2.00	2.06
32	c	516	DGD	C6D-C5D	-2.39	1.44	1.51
24	C	510	CLA	O2D-CED	-2.39	1.39	1.45
24	c	513	CLA	C2A-C1A	-2.39	1.46	1.52
24	b	612	CLA	OBD-CAD	-2.39	1.18	1.22
32	c	518	DGD	O3D-C3D	2.39	1.48	1.43
24	b	617	CLA	CAB-C3B	2.39	1.53	1.47
26	b	621	BCR	C1-C6	-2.38	1.50	1.53
32	E	101	DGD	C6E-C5E	-2.38	1.43	1.51
24	b	610	CLA	O2D-CED	-2.38	1.39	1.45
24	c	505	CLA	C3D-CAD	2.38	1.53	1.45
24	C	503	CLA	MG-NC	-2.38	2.00	2.06
29	C	518	LMG	O6-C5	2.38	1.50	1.44
26	I	101	BCR	C4-C5	2.38	1.55	1.51
24	B	602	CLA	CAB-C3B	2.37	1.53	1.47
24	B	609	CLA	O2D-CED	-2.37	1.39	1.45
26	H	101	BCR	C7-C6	2.37	1.53	1.45
24	B	608	CLA	CMC-C2C	2.37	1.55	1.50
24	C	512	CLA	CMC-C2C	2.37	1.55	1.50
32	C	515	DGD	O2D-C2D	2.37	1.48	1.43
32	C	517	DGD	C1E-C2E	-2.37	1.45	1.52
26	f	101	BCR	C7-C6	2.37	1.53	1.45
26	c	515	BCR	C7-C6	2.37	1.53	1.45
26	T	101	BCR	C12-C13	2.37	1.51	1.45
32	C	515	DGD	O6D-C1D	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	516	DGD	O6D-C1D	2.37	1.47	1.41
26	T	101	BCR	C7-C6	2.36	1.53	1.45
32	c	517	DGD	O2D-C2D	2.36	1.48	1.43
24	B	610	CLA	O2D-CED	-2.36	1.39	1.45
24	C	503	CLA	CAB-C3B	2.36	1.53	1.47
24	B	605	CLA	OBD-CAD	-2.36	1.18	1.22
25	a	608	PHO	CMC-C2C	-2.36	1.46	1.50
25	A	608	PHO	C4D-CHA	2.36	1.43	1.39
32	H	102	DGD	O3D-C3D	2.36	1.48	1.43
25	A	608	PHO	CMB-C2B	-2.36	1.46	1.51
24	d	402	CLA	C3A-C4A	-2.35	1.44	1.51
26	c	515	BCR	C35-C13	-2.35	1.46	1.50
24	C	502	CLA	C1D-ND	-2.35	1.34	1.37
24	D	404	CLA	MG-NA	-2.35	2.00	2.06
24	B	603	CLA	O2D-CED	-2.35	1.39	1.45
24	b	612	CLA	O2D-CED	-2.35	1.39	1.45
24	b	617	CLA	O2D-CED	-2.35	1.39	1.45
32	C	516	DGD	C6E-C5E	-2.35	1.44	1.51
29	z	101	LMG	O8-C28	2.34	1.45	1.33
24	B	617	CLA	C4D-CHA	2.34	1.46	1.38
24	c	504	CLA	C2A-C1A	-2.34	1.46	1.52
26	t	101	BCR	C31-C1	-2.34	1.49	1.53
33	V	201	HEM	FE-NC	2.34	2.03	1.95
24	B	610	CLA	CAB-C3B	2.34	1.53	1.47
24	C	512	CLA	MG-NC	-2.34	2.00	2.06
24	C	507	CLA	CMC-C2C	2.34	1.55	1.50
24	b	618	CLA	C2A-C1A	-2.34	1.47	1.52
24	b	613	CLA	C3D-CAD	2.34	1.53	1.45
26	c	514	BCR	C7-C6	2.34	1.53	1.45
24	b	617	CLA	C3D-CAD	2.34	1.53	1.45
24	c	511	CLA	MG-NC	-2.34	2.00	2.06
29	Z	101	LMG	O8-C28	2.33	1.44	1.33
24	B	607[B]	CLA	O2D-CED	-2.33	1.39	1.45
32	d	405	DGD	O3D-C3D	2.33	1.48	1.43
24	C	504	CLA	MG-NC	-2.33	2.00	2.06
24	B	602	CLA	CMC-C2C	2.33	1.55	1.50
25	A	608	PHO	CMC-C2C	-2.33	1.46	1.50
26	a	610	BCR	C27-C26	2.33	1.55	1.51
24	b	608[B]	CLA	MG-NA	-2.33	2.00	2.06
24	B	607[A]	CLA	O2D-CED	-2.33	1.39	1.45
24	c	509	CLA	MG-NC	-2.33	2.00	2.06
24	a	607	CLA	CMC-C2C	2.33	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	O2D-CED	-2.33	1.39	1.45
24	B	603	CLA	MG-NC	-2.32	2.00	2.06
26	b	619	BCR	C31-C1	-2.32	1.49	1.53
24	b	616	CLA	O2D-CED	-2.32	1.39	1.45
24	c	510	CLA	O2D-CED	-2.32	1.39	1.45
25	d	401	PHO	CMC-C2C	-2.32	1.46	1.50
24	b	603	CLA	MG-NC	-2.32	2.00	2.06
24	b	614	CLA	O2D-CED	-2.32	1.39	1.45
30	e	101	LHG	C8-C7	2.32	1.57	1.50
24	b	614	CLA	CAB-C3B	2.32	1.53	1.47
26	b	621	BCR	C7-C6	2.32	1.53	1.45
24	B	615	CLA	C3D-CAD	2.32	1.53	1.45
24	C	503	CLA	C3D-CAD	2.31	1.53	1.45
24	B	617	CLA	MG-NC	-2.31	2.00	2.06
26	b	620	BCR	C35-C13	-2.31	1.46	1.50
24	B	617	CLA	C2A-C1A	-2.31	1.47	1.52
24	C	501	CLA	CAB-C3B	2.31	1.53	1.47
32	E	101	DGD	O2D-C2D	2.31	1.48	1.43
24	a	607	CLA	O2D-CED	-2.31	1.39	1.45
24	c	506	CLA	C4D-CHA	2.31	1.46	1.38
26	h	101	BCR	C7-C6	2.31	1.53	1.45
26	B	620	BCR	C33-C5	2.31	1.54	1.50
24	B	615	CLA	CMC-C2C	2.31	1.55	1.50
24	C	505	CLA	O2D-CED	-2.31	1.39	1.45
24	B	602	CLA	CAA-C2A	-2.31	1.49	1.54
24	C	512	CLA	CAB-C3B	2.31	1.53	1.47
33	e	102	HEM	CMA-C3A	2.30	1.55	1.50
24	d	402	CLA	MG-NC	-2.30	2.00	2.06
24	b	617	CLA	C2A-C1A	-2.30	1.47	1.52
25	D	401	PHO	CMC-C2C	-2.30	1.46	1.50
24	D	404	CLA	CMC-C2C	2.30	1.55	1.50
24	B	613	CLA	O2D-CED	-2.30	1.39	1.45
24	B	608	CLA	C3D-CAD	2.30	1.52	1.45
26	A	610	BCR	C31-C1	-2.29	1.49	1.53
24	b	615	CLA	C2A-C1A	-2.29	1.47	1.52
24	D	402	CLA	C3A-C4A	-2.29	1.44	1.51
24	b	607	CLA	O2D-CED	-2.29	1.39	1.45
26	K	101	BCR	C33-C5	2.29	1.54	1.50
24	c	513	CLA	CAB-C3B	2.29	1.53	1.47
24	b	605	CLA	O2D-CED	-2.29	1.39	1.45
24	b	608[B]	CLA	C2A-C1A	-2.29	1.47	1.52
27	a	611	PL9	C41-C39	2.29	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C3D-CAD	2.29	1.52	1.45
24	b	603	CLA	O2D-CED	-2.28	1.39	1.45
24	D	404	CLA	CAB-C3B	2.28	1.53	1.47
24	A	609	CLA	MG-NC	-2.28	2.00	2.06
32	c	517	DGD	O5D-C1E	2.28	1.44	1.40
32	C	517	DGD	O6E-C1E	2.28	1.47	1.41
24	d	403	CLA	C2A-C1A	-2.28	1.47	1.52
24	a	615	CLA	C3D-CAD	2.28	1.52	1.45
32	C	515	DGD	O5D-C1E	2.28	1.44	1.40
32	C	515	DGD	C1E-C2E	-2.28	1.45	1.52
24	b	611	CLA	CAB-C3B	2.28	1.53	1.47
24	d	402	CLA	OBD-CAD	-2.28	1.18	1.22
33	E	103	HEM	CMB-C2B	2.28	1.55	1.50
24	a	609	CLA	C4D-CHA	2.28	1.46	1.38
26	c	514	BCR	C33-C5	2.28	1.54	1.50
24	b	605	CLA	MG-NC	-2.28	2.00	2.06
24	b	613	CLA	O2D-CED	-2.28	1.40	1.45
26	f	101	BCR	C1-C6	-2.27	1.50	1.53
24	D	404	CLA	C1D-ND	-2.27	1.35	1.37
24	A	609	CLA	C3D-CAD	2.27	1.52	1.45
24	c	512	CLA	CMC-C2C	2.27	1.55	1.50
24	C	511	CLA	CBA-CGA	2.27	1.57	1.50
24	B	616	CLA	CAB-C3B	2.27	1.53	1.47
24	B	604	CLA	C3D-CAD	2.27	1.52	1.45
24	C	510	CLA	CAB-C3B	2.26	1.53	1.47
32	C	516	DGD	O3D-C3D	2.26	1.48	1.43
24	B	604	CLA	O2D-CED	-2.26	1.40	1.45
24	B	606	CLA	O2D-CED	-2.26	1.40	1.45
24	C	509	CLA	OBD-CAD	-2.26	1.18	1.22
24	b	611	CLA	C4D-CHA	2.26	1.46	1.38
29	C	518	LMG	C11-C10	2.26	1.57	1.50
24	c	501	CLA	C4D-CHA	2.26	1.46	1.38
32	c	516	DGD	O3D-C3D	2.26	1.48	1.43
26	c	515	BCR	C31-C1	-2.26	1.49	1.53
24	c	510	CLA	CAB-C3B	2.26	1.53	1.47
24	b	604	CLA	C3D-CAD	2.26	1.52	1.45
24	A	607	CLA	CMC-C2C	2.25	1.55	1.50
24	c	510	CLA	C2A-C1A	-2.25	1.47	1.52
24	A	607	CLA	CAB-C3B	2.25	1.53	1.47
33	E	103	HEM	CMA-C3A	2.25	1.55	1.50
24	b	612	CLA	C2A-C1A	-2.25	1.47	1.52
24	c	508	CLA	CBD-CGD	-2.25	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	CMC-C2C	2.25	1.55	1.50
24	C	510	CLA	MG-NC	-2.25	2.00	2.06
24	a	609	CLA	CBA-CGA	2.25	1.57	1.50
32	d	405	DGD	C6D-C5D	-2.25	1.44	1.51
24	b	606	CLA	CAB-C3B	2.25	1.53	1.47
24	c	512	CLA	C2A-C1A	-2.25	1.47	1.52
24	b	618	CLA	O2D-CED	-2.25	1.40	1.45
24	B	616	CLA	MG-NA	-2.25	2.00	2.06
24	b	603	CLA	MG-NA	-2.25	2.00	2.06
24	B	611	CLA	OBD-CAD	-2.24	1.18	1.22
32	C	516	DGD	C3E-C2E	-2.24	1.46	1.52
26	A	610	BCR	C1-C6	-2.24	1.50	1.53
24	B	606	CLA	CAB-C3B	2.24	1.53	1.47
24	c	503	CLA	OBD-CAD	-2.24	1.18	1.22
24	C	506	CLA	C4D-CHA	2.24	1.46	1.38
32	C	517	DGD	C1D-C2D	-2.24	1.46	1.52
24	b	606	CLA	C3D-CAD	2.24	1.52	1.45
24	D	402	CLA	C3D-CAD	2.24	1.52	1.45
24	C	512	CLA	MG-NA	-2.24	2.00	2.06
29	c	520	LMG	C7-C8	2.24	1.57	1.50
26	c	521	BCR	C35-C13	-2.24	1.46	1.50
24	C	512	CLA	C4D-CHA	2.24	1.46	1.38
24	C	506	CLA	MG-NC	-2.24	2.01	2.06
33	V	201	HEM	CMD-C2D	2.24	1.55	1.50
24	c	513	CLA	C4D-CHA	2.23	1.46	1.38
24	C	510	CLA	CMC-C2C	2.23	1.55	1.50
24	a	606	CLA	C2A-C1A	-2.23	1.47	1.52
24	c	511	CLA	CAB-C3B	2.23	1.53	1.47
24	C	512	CLA	O2D-CED	-2.23	1.40	1.45
24	c	512	CLA	MG-NA	-2.23	2.01	2.06
24	D	402	CLA	CAB-C3B	2.23	1.53	1.47
24	B	602	CLA	MG-NA	-2.23	2.01	2.06
24	b	615	CLA	C4D-CHA	2.23	1.46	1.38
26	b	619	BCR	C7-C6	2.23	1.53	1.45
32	H	102	DGD	C3E-C2E	-2.23	1.46	1.52
24	d	403	CLA	C4D-CHA	2.23	1.46	1.38
24	c	502	CLA	C2A-C1A	-2.23	1.47	1.52
25	A	608	PHO	C3B-C2B	-2.22	1.37	1.40
33	e	102	HEM	CMB-C2B	2.22	1.55	1.50
24	c	503	CLA	C1D-ND	-2.22	1.35	1.37
24	b	603	CLA	CMB-C2B	2.22	1.55	1.50
26	b	621	BCR	C33-C5	2.22	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	O2D-CED	-2.22	1.40	1.45
30	E	102	LHG	C8-C7	2.22	1.57	1.50
24	c	509	CLA	O2D-CED	-2.22	1.40	1.45
26	I	101	BCR	C1-C6	-2.21	1.50	1.53
32	H	102	DGD	C6D-C5D	-2.21	1.44	1.51
27	D	405	PL9	C22-C23	2.21	1.57	1.50
24	A	609	CLA	C2A-C1A	-2.21	1.47	1.52
29	c	519	LMG	C11-C10	2.21	1.57	1.50
24	b	605	CLA	CMC-C2C	2.21	1.55	1.50
24	B	615	CLA	O2D-CED	-2.21	1.40	1.45
26	I	101	BCR	C7-C6	2.20	1.52	1.45
24	B	610	CLA	CMB-C2B	2.20	1.55	1.50
26	T	101	BCR	C32-C1	2.20	1.58	1.53
33	E	103	HEM	CAA-C2A	2.20	1.57	1.51
24	c	505	CLA	CAB-C3B	2.20	1.53	1.47
24	B	604	CLA	CMC-C2C	2.20	1.55	1.50
24	c	506	CLA	MG-NA	-2.20	2.01	2.06
24	C	509	CLA	CMC-C2C	2.20	1.55	1.50
24	D	404	CLA	C4D-CHA	2.20	1.46	1.38
24	b	608[B]	CLA	CMC-C2C	2.20	1.55	1.50
24	B	613	CLA	CAB-C3B	2.20	1.53	1.47
24	c	508	CLA	CAB-C3B	2.20	1.53	1.47
24	c	513	CLA	CMC-C2C	2.19	1.55	1.50
24	C	502	CLA	C4D-CHA	2.19	1.46	1.38
24	C	508	CLA	O2D-CED	-2.19	1.40	1.45
24	c	505	CLA	O2D-CED	-2.19	1.40	1.45
32	c	518	DGD	C1D-C2D	-2.19	1.46	1.52
33	V	201	HEM	C2A-C3A	-2.19	1.33	1.38
27	A	611	PL9	C41-C39	2.19	1.55	1.51
24	B	606	CLA	CMC-C2C	2.19	1.55	1.50
24	c	502	CLA	O2D-CED	-2.19	1.40	1.45
33	v	201	HEM	CMD-C2D	2.19	1.55	1.50
24	b	609	CLA	C3D-CAD	2.19	1.52	1.45
24	D	404	CLA	CBA-CGA	2.19	1.57	1.50
24	d	403	CLA	CAB-C3B	2.19	1.53	1.47
25	a	608	PHO	CMB-C2B	-2.18	1.47	1.51
25	A	608	PHO	C3D-C4D	2.18	1.44	1.41
24	B	612	CLA	MG-NC	-2.18	2.01	2.06
24	B	611	CLA	C3A-C4A	-2.18	1.44	1.51
24	b	618	CLA	MG-NC	-2.18	2.01	2.06
24	b	616	CLA	OBD-CAD	-2.18	1.18	1.22
26	H	101	BCR	C35-C13	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	O2D-CED	-2.18	1.40	1.45
29	C	519	LMG	C7-C8	2.18	1.57	1.50
26	a	610	BCR	C1-C6	-2.18	1.50	1.53
24	c	509	CLA	C1D-ND	-2.18	1.35	1.37
24	C	506	CLA	CBD-CGD	-2.18	1.45	1.52
27	a	611	PL9	C2-C3	2.18	1.40	1.34
24	C	511	CLA	C3D-CAD	2.17	1.52	1.45
32	E	101	DGD	C3G-C2G	2.17	1.57	1.50
24	b	615	CLA	OBD-CAD	-2.17	1.18	1.22
24	b	606	CLA	OBD-CAD	-2.17	1.18	1.22
24	B	604	CLA	C2A-C1A	-2.17	1.47	1.52
24	C	507	CLA	C4D-CHA	2.17	1.46	1.38
24	b	603	CLA	CAB-C3B	2.17	1.53	1.47
24	c	506	CLA	CAB-C3B	2.17	1.53	1.47
24	B	612	CLA	O2D-CED	-2.17	1.40	1.45
32	c	517	DGD	C1E-C2E	-2.17	1.46	1.52
24	B	606	CLA	MG-NC	-2.17	2.01	2.06
24	c	511	CLA	C4D-CHA	2.17	1.46	1.38
32	c	518	DGD	C3E-C2E	-2.17	1.46	1.52
24	b	613	CLA	OBD-CAD	-2.17	1.18	1.22
24	b	609	CLA	O2D-CED	-2.17	1.40	1.45
24	b	617	CLA	MG-NA	-2.16	2.01	2.06
26	C	514	BCR	C7-C6	2.16	1.52	1.45
25	D	401	PHO	CMD-C2D	-2.16	1.47	1.51
24	b	608[A]	CLA	C2A-C1A	-2.16	1.47	1.52
26	c	515	BCR	C1-C6	-2.16	1.50	1.53
24	C	509	CLA	C4D-CHA	2.16	1.46	1.38
24	c	513	CLA	O2D-CED	-2.16	1.40	1.45
24	c	503	CLA	MG-NC	-2.16	2.01	2.06
26	K	102	BCR	C1-C6	-2.16	1.50	1.53
24	C	502	CLA	MG-NA	-2.16	2.01	2.06
24	c	507	CLA	C4D-CHA	2.16	1.46	1.38
24	B	602	CLA	C4D-CHA	2.15	1.46	1.38
24	B	604	CLA	OBD-CAD	-2.15	1.18	1.22
27	A	611	PL9	C22-C23	2.15	1.57	1.50
32	c	516	DGD	C1D-C2D	-2.15	1.46	1.52
28	B	622	SQD	O6-C1	2.15	1.43	1.40
24	B	614	CLA	C3D-CAD	2.15	1.52	1.45
24	c	512	CLA	CBA-CGA	2.15	1.57	1.50
24	a	609	CLA	CAB-C3B	2.15	1.53	1.47
24	b	603	CLA	C4D-CHA	2.15	1.46	1.38
24	c	504	CLA	OBD-CAD	-2.15	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	102	SQD	O6-C1	2.15	1.43	1.40
24	B	614	CLA	O2D-CGD	2.14	1.38	1.33
27	D	405	PL9	C37-C38	2.14	1.57	1.50
24	b	604	CLA	CAB-C3B	2.14	1.53	1.47
24	B	604	CLA	CAB-C3B	2.14	1.53	1.47
24	C	502	CLA	C2A-C1A	-2.14	1.47	1.52
24	C	511	CLA	C2A-C1A	-2.14	1.47	1.52
26	c	515	BCR	C33-C5	2.14	1.54	1.50
24	b	618	CLA	C4D-CHA	2.14	1.46	1.38
24	C	511	CLA	OBD-CAD	-2.14	1.18	1.22
24	c	510	CLA	C4D-CHA	2.14	1.46	1.38
24	B	615	CLA	CAB-C3B	2.13	1.53	1.47
24	D	402	CLA	MG-NC	-2.13	2.01	2.06
24	C	513	CLA	O2D-CED	-2.13	1.40	1.45
24	B	611	CLA	CAB-C3B	2.13	1.53	1.47
24	B	604	CLA	MG-NC	-2.13	2.01	2.06
24	c	509	CLA	C4D-CHA	2.13	1.46	1.38
25	A	608	PHO	CMD-C2D	-2.13	1.47	1.51
24	b	616	CLA	MG-NC	-2.13	2.01	2.06
32	C	516	DGD	O6D-C1D	2.13	1.47	1.41
32	H	102	DGD	O6D-C1D	2.13	1.47	1.41
26	B	618	BCR	C17-C18	2.13	1.38	1.35
24	b	617	CLA	C4D-CHA	2.13	1.46	1.38
26	B	618	BCR	C35-C13	-2.13	1.46	1.50
24	a	615	CLA	CAB-C3B	2.13	1.53	1.47
27	d	404	PL9	C37-C38	2.13	1.57	1.50
24	b	608[A]	CLA	OBD-CAD	-2.12	1.18	1.22
28	b	601	SQD	O6-C1	2.12	1.43	1.40
29	D	408	LMG	O6-C5	2.12	1.49	1.44
24	B	607[B]	CLA	MG-NC	-2.12	2.01	2.06
24	b	607	CLA	MG-NC	-2.12	2.01	2.06
24	b	617	CLA	MG-NC	-2.12	2.01	2.06
24	d	403	CLA	CBA-CGA	2.12	1.56	1.50
32	E	101	DGD	C6D-C5D	-2.12	1.45	1.51
24	b	612	CLA	CMC-C2C	2.12	1.55	1.50
32	c	518	DGD	O6D-C1D	2.12	1.47	1.41
24	B	609	CLA	C2A-C1A	-2.12	1.47	1.52
24	b	614	CLA	CMC-C2C	2.11	1.55	1.50
32	C	517	DGD	O6D-C1D	2.11	1.47	1.41
32	c	517	DGD	C6D-C5D	-2.11	1.45	1.51
24	c	503	CLA	MG-NA	-2.11	2.01	2.06
24	B	603	CLA	OBD-CAD	-2.11	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	CAB-C3B	2.11	1.53	1.47
24	c	508	CLA	MG-NC	-2.11	2.01	2.06
24	C	502	CLA	CAB-C3B	2.11	1.53	1.47
24	a	606	CLA	CMC-C2C	2.11	1.55	1.50
24	C	508	CLA	CAB-C3B	2.11	1.53	1.47
32	d	405	DGD	C3G-C2G	2.11	1.57	1.50
24	B	602	CLA	CBA-CGA	2.10	1.56	1.50
27	A	611	PL9	C2-C3	2.10	1.40	1.34
27	d	404	PL9	C26-C24	2.10	1.55	1.51
24	B	611	CLA	CMC-C2C	2.10	1.55	1.50
24	b	617	CLA	OBD-CAD	-2.10	1.18	1.22
32	h	102	DGD	O3D-C3D	2.10	1.47	1.43
24	c	513	CLA	C1D-ND	-2.10	1.35	1.37
24	a	609	CLA	CMC-C2C	2.10	1.55	1.50
24	c	501	CLA	C2A-C1A	-2.10	1.47	1.52
32	c	517	DGD	C3E-C2E	-2.10	1.47	1.52
32	h	102	DGD	C6D-C5D	-2.10	1.45	1.51
24	a	615	CLA	C3A-C4A	-2.09	1.45	1.51
24	b	607	CLA	OBD-CAD	-2.09	1.18	1.22
24	b	608[A]	CLA	CMC-C2C	2.09	1.55	1.50
28	l	101	SQD	O6-C1	2.09	1.43	1.40
24	C	513	CLA	OBD-CAD	-2.09	1.18	1.22
25	D	401	PHO	C4C-NC	2.09	1.44	1.37
32	h	102	DGD	O6D-C1D	2.09	1.47	1.41
26	T	101	BCR	C31-C1	-2.09	1.49	1.53
24	C	501	CLA	O2D-CED	-2.09	1.40	1.45
24	b	610	CLA	CMC-C2C	2.09	1.55	1.50
24	C	512	CLA	C2A-C1A	-2.09	1.47	1.52
24	b	609	CLA	CAB-C3B	2.09	1.53	1.47
32	C	515	DGD	O3D-C3D	2.09	1.47	1.43
24	b	615	CLA	CAB-C3B	2.08	1.53	1.47
26	A	610	BCR	C35-C13	-2.08	1.46	1.50
24	C	506	CLA	CAB-C3B	2.08	1.53	1.47
24	c	502	CLA	CBA-CGA	2.08	1.56	1.50
24	C	509	CLA	CAB-C3B	2.08	1.53	1.47
24	B	615	CLA	OBD-CAD	-2.08	1.18	1.22
24	b	616	CLA	CBD-CHA	-2.08	1.42	1.52
32	c	517	DGD	C1D-C2D	-2.08	1.46	1.52
24	B	612	CLA	CAB-C3B	2.08	1.53	1.47
26	F	101	BCR	C7-C6	2.08	1.52	1.45
24	B	603	CLA	CMC-C2C	2.08	1.55	1.50
30	A	615	LHG	C8-C7	2.08	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	CMC-C2C	2.07	1.55	1.50
24	C	504	CLA	CMC-C2C	2.07	1.55	1.50
24	B	611	CLA	C4D-CHA	2.07	1.45	1.38
24	c	503	CLA	CMB-C2B	2.07	1.55	1.50
24	C	506	CLA	O2D-CED	-2.07	1.40	1.45
24	C	507	CLA	MG-NC	-2.07	2.01	2.06
27	a	611	PL9	C37-C38	2.07	1.57	1.50
24	B	605	CLA	CAB-C3B	2.07	1.53	1.47
24	c	509	CLA	CMC-C2C	2.07	1.55	1.50
24	A	606	CLA	CMC-C2C	2.06	1.55	1.50
24	D	402	CLA	CMC-C2C	2.06	1.55	1.50
27	D	405	PL9	C17-C18	2.06	1.57	1.50
24	b	605	CLA	C4D-CHA	2.06	1.45	1.38
24	B	615	CLA	MG-NC	-2.06	2.01	2.06
26	k	101	BCR	C33-C5	2.06	1.54	1.50
24	c	501	CLA	O2D-CED	-2.06	1.40	1.45
24	c	501	CLA	MG-NC	-2.06	2.01	2.06
32	c	517	DGD	O3G-C1D	2.06	1.43	1.40
27	d	404	PL9	C22-C23	2.05	1.57	1.50
24	b	604	CLA	C3A-C4A	-2.05	1.45	1.51
33	v	201	HEM	CMA-C3A	2.05	1.55	1.50
24	B	609	CLA	CMC-C2C	2.05	1.55	1.50
24	A	606	CLA	C4D-CHA	2.05	1.45	1.38
24	b	617	CLA	C1D-ND	-2.05	1.35	1.37
27	a	611	PL9	C17-C18	2.05	1.57	1.50
29	a	613	LMG	C7-C8	2.04	1.57	1.50
27	a	611	PL9	C22-C23	2.04	1.57	1.50
24	D	404	CLA	MG-NC	-2.04	2.01	2.06
30	D	407	LHG	C8-C7	2.04	1.56	1.50
24	c	513	CLA	MG-NC	-2.04	2.01	2.06
24	b	613	CLA	C2A-C1A	-2.04	1.47	1.52
24	C	510	CLA	OBD-CAD	-2.04	1.19	1.22
24	D	402	CLA	CBD-CHA	-2.04	1.42	1.52
24	c	503	CLA	C4D-CHA	2.04	1.45	1.38
24	c	504	CLA	C4D-CHA	2.04	1.45	1.38
24	c	507	CLA	CMC-C2C	2.04	1.55	1.50
28	X	101	SQD	O6-C1	2.04	1.43	1.40
29	j	101	LMG	O8-C9	-2.03	1.40	1.45
24	c	511	CLA	CMB-C2B	2.03	1.55	1.50
24	A	609	CLA	CBD-CHA	-2.03	1.42	1.52
24	B	616	CLA	MG-NC	-2.03	2.01	2.06
26	B	619	BCR	C31-C1	-2.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I	101	BCR	C32-C1	2.03	1.57	1.53
24	B	612	CLA	OBD-CAD	-2.03	1.19	1.22
30	d	407	LHG	C8-C7	2.03	1.56	1.50
24	B	611	CLA	CBA-CGA	2.03	1.56	1.50
24	c	507	CLA	CAB-C3B	2.03	1.53	1.47
24	c	502	CLA	CAB-C3B	2.03	1.53	1.47
24	c	509	CLA	CAB-C3B	2.03	1.52	1.47
24	B	617	CLA	CAB-C3B	2.02	1.52	1.47
24	C	511	CLA	CAB-C3B	2.02	1.52	1.47
25	a	608	PHO	C3B-CAB	-2.02	1.43	1.47
26	h	101	BCR	C1-C6	-2.02	1.51	1.53
26	t	101	BCR	C39-C30	-2.02	1.49	1.53
32	C	517	DGD	O3G-C3G	-2.02	1.40	1.43
33	V	201	HEM	C1B-NB	-2.02	1.36	1.40
32	d	405	DGD	C3E-C2E	-2.02	1.47	1.52
24	B	616	CLA	C2A-C1A	-2.01	1.47	1.52
24	C	503	CLA	C4D-CHA	2.01	1.45	1.38
24	C	503	CLA	CMB-C2B	2.01	1.55	1.50
26	I	101	BCR	C31-C1	-2.01	1.49	1.53
28	x	101	SQD	O6-C1	2.01	1.43	1.40
24	b	607	CLA	CAB-C3B	2.01	1.52	1.47
24	C	508	CLA	CMC-C2C	2.01	1.55	1.50
27	A	611	PL9	C17-C18	2.01	1.57	1.50
32	c	518	DGD	O3G-C3G	-2.01	1.40	1.43
24	b	610	CLA	C4D-CHA	2.01	1.45	1.38
33	E	103	HEM	CMC-C2C	2.01	1.55	1.50
24	B	603	CLA	C4D-CHA	2.01	1.45	1.38
32	c	517	DGD	O6D-C1D	2.01	1.47	1.41
24	b	606	CLA	O2D-CED	-2.00	1.40	1.45
25	D	401	PHO	O2D-CGD	2.00	1.38	1.33
24	C	505	CLA	CAB-C3B	2.00	1.52	1.47
24	B	616	CLA	C4D-CHA	2.00	1.45	1.38
32	C	516	DGD	C1D-C2D	-2.00	1.46	1.52

All (2390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	621	BCR	C15-C16-C17	25.00	174.68	123.47
26	k	101	BCR	C15-C16-C17	24.97	174.62	123.47
26	T	101	BCR	C15-C16-C17	24.91	174.50	123.47
26	t	101	BCR	C15-C16-C17	24.76	174.19	123.47
26	A	610	BCR	C15-C16-C17	23.82	172.26	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C15-C16-C17	23.09	170.76	123.47
26	I	101	BCR	C15-C16-C17	23.08	170.75	123.47
26	F	101	BCR	C15-C16-C17	23.06	170.72	123.47
26	C	514	BCR	C15-C16-C17	22.99	170.57	123.47
26	B	618	BCR	C15-C16-C17	22.79	170.16	123.47
26	c	521	BCR	C15-C16-C17	22.79	170.15	123.47
26	H	101	BCR	C15-C16-C17	22.69	169.95	123.47
26	c	515	BCR	C15-C16-C17	22.57	169.72	123.47
26	K	102	BCR	C15-C16-C17	22.45	169.46	123.47
26	b	620	BCR	C15-C16-C17	22.32	169.19	123.47
26	B	619	BCR	C15-C16-C17	22.09	168.72	123.47
26	f	101	BCR	C15-C16-C17	21.73	167.99	123.47
26	h	101	BCR	C15-C16-C17	21.61	167.74	123.47
26	c	514	BCR	C15-C16-C17	21.60	167.72	123.47
26	b	619	BCR	C15-C16-C17	21.27	167.04	123.47
26	K	101	BCR	C15-C16-C17	21.21	166.92	123.47
26	a	610	BCR	C15-C16-C17	20.30	165.06	123.47
26	b	619	BCR	C21-C20-C19	18.01	179.43	123.22
26	T	101	BCR	C21-C20-C19	17.74	178.57	123.22
26	a	610	BCR	C21-C20-C19	17.43	177.61	123.22
26	c	514	BCR	C21-C20-C19	17.42	177.57	123.22
26	I	101	BCR	C21-C20-C19	17.33	177.31	123.22
26	c	515	BCR	C21-C20-C19	17.25	177.04	123.22
26	K	102	BCR	C21-C20-C19	17.18	176.83	123.22
26	h	101	BCR	C21-C20-C19	17.14	176.72	123.22
26	t	101	BCR	C21-C20-C19	17.11	176.60	123.22
26	A	610	BCR	C21-C20-C19	17.08	176.52	123.22
26	b	621	BCR	C21-C20-C19	16.91	175.99	123.22
26	b	620	BCR	C21-C20-C19	16.82	175.72	123.22
26	F	101	BCR	C21-C20-C19	16.80	175.63	123.22
26	B	618	BCR	C21-C20-C19	16.78	175.59	123.22
26	C	514	BCR	C21-C20-C19	16.69	175.30	123.22
26	c	521	BCR	C21-C20-C19	16.52	174.78	123.22
26	B	619	BCR	C21-C20-C19	16.31	174.13	123.22
26	k	101	BCR	C21-C20-C19	16.06	173.33	123.22
26	f	101	BCR	C21-C20-C19	15.91	172.85	123.22
26	K	101	BCR	C21-C20-C19	15.82	172.58	123.22
26	B	620	BCR	C21-C20-C19	15.49	171.57	123.22
26	F	101	BCR	C33-C5-C6	-15.38	107.26	124.53
26	B	618	BCR	C33-C5-C6	-15.09	107.59	124.53
26	T	101	BCR	C38-C26-C25	-14.94	107.75	124.53
26	B	618	BCR	C38-C26-C25	-14.58	108.15	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	619	BCR	C33-C5-C6	-14.40	108.36	124.53
26	f	101	BCR	C33-C5-C6	-14.22	108.56	124.53
26	H	101	BCR	C21-C20-C19	14.16	167.40	123.22
26	b	621	BCR	C38-C26-C25	-14.09	108.71	124.53
26	H	101	BCR	C33-C5-C6	-13.87	108.95	124.53
26	b	620	BCR	C33-C5-C6	-13.84	108.98	124.53
26	B	620	BCR	C38-C26-C25	-13.71	109.14	124.53
26	C	514	BCR	C38-C26-C25	-13.66	109.18	124.53
26	K	101	BCR	C38-C26-C25	-13.55	109.31	124.53
26	k	101	BCR	C33-C5-C6	-13.45	109.42	124.53
26	B	619	BCR	C33-C5-C6	-13.32	109.57	124.53
26	t	101	BCR	C38-C26-C25	-13.30	109.59	124.53
26	c	515	BCR	C38-C26-C25	-13.23	109.68	124.53
26	b	621	BCR	C15-C14-C13	-13.22	108.44	127.31
26	K	101	BCR	C33-C5-C6	-13.09	109.83	124.53
26	a	610	BCR	C33-C5-C6	-13.06	109.86	124.53
26	A	610	BCR	C33-C5-C6	-13.03	109.90	124.53
26	I	101	BCR	C38-C26-C25	-13.02	109.91	124.53
26	c	514	BCR	C38-C26-C25	-12.94	110.00	124.53
26	k	101	BCR	C38-C26-C25	-12.82	110.13	124.53
26	a	610	BCR	C38-C26-C25	-12.66	110.31	124.53
26	b	619	BCR	C38-C26-C25	-12.64	110.33	124.53
26	K	102	BCR	C33-C5-C6	-12.54	110.45	124.53
26	A	610	BCR	C38-C26-C25	-12.37	110.63	124.53
26	T	101	BCR	C33-C5-C6	-12.35	110.66	124.53
26	t	101	BCR	C33-C5-C6	-12.25	110.78	124.53
26	h	101	BCR	C33-C5-C6	-11.94	111.12	124.53
26	b	620	BCR	C24-C23-C22	-11.64	108.64	126.23
26	F	101	BCR	C16-C17-C18	-11.63	110.72	127.31
26	b	621	BCR	C16-C17-C18	-11.59	110.77	127.31
26	H	101	BCR	C38-C26-C25	-11.50	111.62	124.53
27	D	405	PL9	C7-C8-C9	-11.45	107.74	126.79
26	c	521	BCR	C33-C5-C6	-11.44	111.69	124.53
26	C	514	BCR	C33-C5-C6	-11.44	111.69	124.53
26	K	102	BCR	C16-C17-C18	-11.36	111.09	127.31
26	h	101	BCR	C38-C26-C25	-11.36	111.78	124.53
26	b	619	BCR	C16-C17-C18	-11.34	111.13	127.31
27	d	404	PL9	C7-C8-C9	-11.29	108.00	126.79
26	b	621	BCR	C33-C5-C6	-11.27	111.88	124.53
26	c	514	BCR	C16-C17-C18	-11.24	111.27	127.31
26	c	521	BCR	C38-C26-C25	-11.20	111.95	124.53
26	c	521	BCR	C20-C21-C22	-11.09	111.48	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	f	101	BCR	C16-C17-C18	-11.08	111.49	127.31
26	B	620	BCR	C33-C5-C6	-11.07	112.10	124.53
26	b	621	BCR	C24-C23-C22	-10.99	109.62	126.23
26	c	514	BCR	C33-C5-C6	-10.81	112.39	124.53
26	b	621	BCR	C20-C21-C22	-10.77	111.94	127.31
26	c	521	BCR	C24-C23-C22	-10.57	110.26	126.23
26	B	620	BCR	C16-C17-C18	-10.55	112.26	127.31
26	h	101	BCR	C15-C14-C13	-10.25	112.69	127.31
26	c	514	BCR	C24-C23-C22	-10.24	110.77	126.23
26	F	101	BCR	C7-C8-C9	-10.18	110.85	126.23
26	I	101	BCR	C4-C5-C6	-10.16	107.98	122.73
26	F	101	BCR	C11-C10-C9	-10.16	112.81	127.31
26	t	101	BCR	C24-C23-C22	-10.15	110.89	126.23
26	c	521	BCR	C16-C17-C18	-10.13	112.85	127.31
26	c	515	BCR	C33-C5-C6	-10.00	113.30	124.53
26	a	610	BCR	C16-C17-C18	-9.95	113.11	127.31
26	B	619	BCR	C11-C10-C9	-9.82	113.30	127.31
26	h	101	BCR	C16-C17-C18	-9.81	113.31	127.31
26	B	619	BCR	C16-C17-C18	-9.75	113.40	127.31
26	K	102	BCR	C38-C26-C25	-9.72	113.61	124.53
26	T	101	BCR	C24-C23-C22	-9.72	111.55	126.23
26	F	101	BCR	C36-C18-C17	-9.54	109.56	122.92
26	I	101	BCR	C33-C5-C6	-9.46	113.91	124.53
26	I	101	BCR	C24-C23-C22	-9.45	111.95	126.23
26	f	101	BCR	C30-C25-C26	-9.34	109.45	122.61
26	C	514	BCR	C11-C10-C9	-9.29	114.05	127.31
26	I	101	BCR	C11-C10-C9	-9.22	114.15	127.31
26	B	620	BCR	C8-C7-C6	-9.20	101.36	127.20
26	H	101	BCR	C37-C22-C21	-9.18	110.06	122.92
26	B	618	BCR	C16-C17-C18	-9.12	114.30	127.31
26	H	101	BCR	C15-C14-C13	-9.09	114.33	127.31
26	K	102	BCR	C24-C23-C22	-9.04	112.57	126.23
26	A	610	BCR	C16-C17-C18	-8.98	114.50	127.31
26	t	101	BCR	C30-C25-C26	-8.97	109.97	122.61
26	b	620	BCR	C38-C26-C25	-8.89	114.55	124.53
26	f	101	BCR	C4-C5-C6	-8.84	109.90	122.73
26	c	515	BCR	C11-C10-C9	-8.83	114.71	127.31
26	I	101	BCR	C16-C17-C18	-8.81	114.74	127.31
26	F	101	BCR	C24-C23-C22	-8.80	112.94	126.23
26	T	101	BCR	C16-C17-C18	-8.74	114.84	127.31
26	T	101	BCR	C30-C25-C26	-8.64	110.44	122.61
26	b	619	BCR	C11-C10-C9	-8.62	115.01	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	I	101	BCR	C7-C8-C9	-8.58	113.27	126.23
26	b	619	BCR	C4-C5-C6	-8.58	110.28	122.73
26	b	620	BCR	C8-C7-C6	-8.57	103.13	127.20
26	B	619	BCR	C38-C26-C25	-8.52	114.97	124.53
26	F	101	BCR	C38-C26-C25	-8.51	114.97	124.53
26	k	101	BCR	C16-C17-C18	-8.50	115.18	127.31
26	b	620	BCR	C11-C10-C9	-8.44	115.27	127.31
26	F	101	BCR	C4-C5-C6	-8.43	110.50	122.73
24	A	606	CLA	C4A-NA-C1A	-8.34	102.96	106.71
26	K	101	BCR	C30-C25-C26	-8.32	110.90	122.61
26	B	619	BCR	C7-C8-C9	-8.28	113.73	126.23
26	F	101	BCR	C30-C25-C26	-8.27	110.96	122.61
24	C	510	CLA	C4A-NA-C1A	-8.27	102.99	106.71
26	b	619	BCR	C7-C8-C9	-8.22	113.82	126.23
26	K	102	BCR	C20-C21-C22	-8.17	115.66	127.31
26	C	514	BCR	C7-C8-C9	-8.16	113.90	126.23
26	t	101	BCR	C27-C26-C25	-8.16	110.88	122.73
26	b	620	BCR	C15-C14-C13	-8.15	115.68	127.31
26	a	610	BCR	C27-C26-C25	-8.14	110.91	122.73
26	T	101	BCR	C27-C26-C25	-8.11	110.96	122.73
26	B	618	BCR	C7-C8-C9	-8.06	114.06	126.23
26	T	101	BCR	C15-C14-C13	-8.05	115.83	127.31
26	H	101	BCR	C16-C17-C18	-8.05	115.83	127.31
27	A	611	PL9	C37-C38-C39	-8.03	108.31	127.66
26	C	514	BCR	C16-C17-C18	-8.01	115.88	127.31
26	c	515	BCR	C24-C23-C22	-7.98	114.18	126.23
26	c	515	BCR	C4-C5-C6	-7.96	111.17	122.73
26	c	514	BCR	C11-C10-C9	-7.95	115.97	127.31
26	a	610	BCR	C4-C5-C6	-7.95	111.19	122.73
27	A	611	PL9	C42-C43-C44	-7.91	108.62	127.66
26	H	101	BCR	C24-C23-C22	-7.84	114.38	126.23
26	C	514	BCR	C20-C21-C22	-7.81	116.17	127.31
26	f	101	BCR	C38-C26-C25	-7.79	115.78	124.53
26	C	514	BCR	C24-C23-C22	-7.76	114.50	126.23
26	B	619	BCR	C8-C7-C6	-7.76	105.41	127.20
27	a	611	PL9	C7-C8-C9	-7.73	113.93	126.79
27	a	611	PL9	C37-C38-C39	-7.70	109.11	127.66
27	A	611	PL9	C7-C8-C9	-7.70	113.98	126.79
26	K	101	BCR	C11-C10-C9	-7.70	116.33	127.31
26	B	620	BCR	C27-C26-C25	-7.69	111.56	122.73
26	I	101	BCR	C27-C26-C25	-7.66	111.61	122.73
26	C	514	BCR	C15-C14-C13	-7.63	116.41	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	514	BCR	C15-C14-C13	-7.62	116.44	127.31
26	B	618	BCR	C11-C10-C9	-7.58	116.49	127.31
26	f	101	BCR	C11-C10-C9	-7.57	116.51	127.31
27	d	404	PL9	C12-C13-C14	-7.57	109.44	127.66
27	a	611	PL9	C16-C14-C13	-7.55	105.84	121.12
27	D	405	PL9	C32-C33-C34	-7.54	109.51	127.66
26	t	101	BCR	C7-C6-C5	-7.54	103.20	121.46
26	T	101	BCR	C7-C8-C9	-7.53	114.86	126.23
26	H	101	BCR	C8-C7-C6	-7.50	106.14	127.20
26	b	621	BCR	C36-C18-C19	-7.49	106.28	118.08
26	f	101	BCR	C24-C23-C22	-7.48	114.93	126.23
27	D	405	PL9	C22-C23-C24	-7.47	109.67	127.66
26	B	618	BCR	C4-C5-C6	-7.45	111.92	122.73
26	A	610	BCR	C4-C5-C6	-7.41	111.97	122.73
27	A	611	PL9	C16-C14-C13	-7.37	106.19	121.12
26	b	620	BCR	C4-C5-C6	-7.37	112.03	122.73
26	I	101	BCR	C1-C6-C5	-7.35	112.26	122.61
26	b	621	BCR	C8-C7-C6	-7.30	106.71	127.20
26	k	101	BCR	C24-C23-C22	-7.30	115.21	126.23
26	a	610	BCR	C30-C25-C26	-7.29	112.35	122.61
26	H	101	BCR	C4-C5-C6	-7.29	112.15	122.73
26	c	514	BCR	C30-C25-C26	-7.29	112.35	122.61
27	a	611	PL9	C27-C28-C29	-7.24	110.22	127.66
24	C	505	CLA	C3A-C2A-C1A	7.23	112.17	101.34
27	a	611	PL9	C42-C43-C44	-7.22	110.26	127.66
27	a	611	PL9	C22-C23-C24	-7.22	110.29	127.66
26	t	101	BCR	C11-C10-C9	-7.21	117.02	127.31
26	f	101	BCR	C7-C8-C9	-7.19	115.37	126.23
27	D	405	PL9	C27-C28-C29	-7.17	110.39	127.66
27	A	611	PL9	C27-C28-C29	-7.17	110.39	127.66
26	f	101	BCR	C1-C6-C5	-7.17	112.51	122.61
26	K	102	BCR	C30-C25-C26	-7.16	112.52	122.61
26	c	515	BCR	C7-C8-C9	-7.15	115.42	126.23
27	d	404	PL9	C32-C33-C34	-7.14	110.47	127.66
26	c	515	BCR	C27-C26-C25	-7.09	112.44	122.73
27	d	404	PL9	C22-C23-C24	-7.02	110.75	127.66
26	B	620	BCR	C30-C25-C26	-7.02	112.72	122.61
26	k	101	BCR	C30-C25-C26	-6.99	112.77	122.61
26	b	620	BCR	C16-C17-C18	-6.96	117.37	127.31
26	b	619	BCR	C1-C6-C5	-6.96	112.82	122.61
24	D	404	CLA	C4A-NA-C1A	-6.95	103.58	106.71
26	b	621	BCR	C11-C10-C9	-6.93	117.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	611	PL9	C41-C39-C38	-6.93	107.10	121.12
26	T	101	BCR	C7-C6-C5	-6.91	104.73	121.46
27	D	405	PL9	C16-C14-C13	-6.90	107.15	121.12
26	B	618	BCR	C1-C6-C5	-6.90	112.89	122.61
26	c	514	BCR	C20-C21-C22	-6.86	117.52	127.31
26	c	514	BCR	C27-C26-C25	-6.85	112.79	122.73
26	c	515	BCR	C1-C6-C5	-6.83	112.99	122.61
24	C	507	CLA	O2D-CGD-CBD	6.83	123.40	111.27
26	a	610	BCR	C1-C6-C5	-6.79	113.05	122.61
26	c	514	BCR	C34-C9-C10	-6.76	113.46	122.92
27	d	404	PL9	C46-C44-C43	-6.75	107.47	121.12
26	c	515	BCR	C15-C14-C13	-6.72	117.72	127.31
26	K	102	BCR	C27-C26-C25	-6.72	112.97	122.73
26	B	619	BCR	C7-C6-C5	-6.71	105.20	121.46
27	A	611	PL9	C17-C18-C19	-6.71	111.51	127.66
26	h	101	BCR	C36-C18-C17	-6.68	113.56	122.92
27	a	611	PL9	C17-C18-C19	-6.63	111.70	127.66
24	c	505	CLA	C3A-C2A-C1A	6.63	111.27	101.34
26	c	521	BCR	C30-C25-C26	-6.62	113.29	122.61
26	t	101	BCR	C15-C14-C13	-6.61	117.88	127.31
26	c	515	BCR	C16-C17-C18	-6.60	117.89	127.31
26	B	619	BCR	C19-C18-C17	6.59	129.06	118.94
24	C	512	CLA	C3A-C2A-C1A	6.58	111.20	101.34
24	b	604	CLA	O2D-CGD-CBD	6.58	122.97	111.27
26	B	620	BCR	C4-C5-C6	-6.57	113.19	122.73
24	b	614	CLA	O2D-CGD-CBD	6.56	122.92	111.27
24	a	606	CLA	C4A-NA-C1A	-6.53	103.77	106.71
27	a	611	PL9	C32-C33-C34	-6.53	111.94	127.66
27	d	404	PL9	C16-C14-C13	-6.52	107.93	121.12
26	f	101	BCR	C27-C26-C25	-6.50	113.30	122.73
26	f	101	BCR	C36-C18-C17	-6.49	113.83	122.92
26	A	610	BCR	C15-C14-C13	-6.45	118.11	127.31
24	C	506	CLA	C3A-C2A-C1A	6.43	110.97	101.34
26	a	610	BCR	C24-C23-C22	-6.42	116.53	126.23
26	B	618	BCR	C20-C21-C22	-6.42	118.15	127.31
24	C	505	CLA	O2D-CGD-CBD	6.41	122.66	111.27
27	d	404	PL9	C21-C19-C18	-6.41	108.14	121.12
26	K	101	BCR	C8-C7-C6	-6.41	109.21	127.20
26	K	101	BCR	C27-C26-C25	-6.40	113.44	122.73
24	c	507	CLA	C4A-NA-C1A	-6.39	103.83	106.71
24	B	603	CLA	O2D-CGD-CBD	6.39	122.62	111.27
27	A	611	PL9	C22-C23-C24	-6.38	112.31	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CHB-C1B-NB	6.38	131.01	124.26
27	A	611	PL9	C26-C24-C23	-6.37	108.22	121.12
26	b	621	BCR	C27-C26-C25	-6.36	113.50	122.73
26	b	619	BCR	C36-C18-C17	-6.36	114.01	122.92
26	k	101	BCR	C27-C26-C25	-6.36	113.50	122.73
26	h	101	BCR	C24-C23-C22	-6.36	116.63	126.23
26	c	514	BCR	C8-C7-C6	-6.35	109.38	127.20
26	f	101	BCR	C15-C14-C13	-6.34	118.27	127.31
26	F	101	BCR	C27-C26-C25	-6.30	113.59	122.73
27	d	404	PL9	C11-C9-C8	-6.29	108.39	121.12
26	k	101	BCR	C8-C7-C6	-6.29	109.55	127.20
24	D	404	CLA	CHB-C1B-NB	6.29	130.91	124.26
24	c	511	CLA	C3A-C2A-C1A	6.28	110.74	101.34
26	t	101	BCR	C16-C17-C18	-6.27	118.37	127.31
26	b	620	BCR	C12-C13-C14	-6.24	109.37	118.94
26	A	610	BCR	C11-C10-C9	-6.23	118.41	127.31
27	a	611	PL9	C40-C39-C38	-6.22	107.73	123.68
27	d	404	PL9	C17-C18-C19	-6.21	112.70	127.66
26	B	619	BCR	C15-C14-C13	-6.20	118.46	127.31
26	F	101	BCR	C23-C22-C21	6.20	128.45	118.94
27	a	611	PL9	C12-C13-C14	-6.19	112.76	127.66
26	H	101	BCR	C1-C6-C5	-6.17	113.92	122.61
24	c	510	CLA	C3A-C2A-C1A	6.17	110.58	101.34
27	A	611	PL9	C12-C13-C14	-6.16	112.83	127.66
26	I	101	BCR	C37-C22-C21	-6.14	114.32	122.92
27	d	404	PL9	C27-C28-C29	-6.14	112.87	127.66
27	A	611	PL9	C40-C39-C38	-6.13	107.95	123.68
27	A	611	PL9	C32-C33-C34	-6.13	112.90	127.66
26	C	514	BCR	C23-C24-C25	-6.12	110.00	127.20
26	B	620	BCR	C24-C23-C22	-6.12	116.98	126.23
24	C	506	CLA	CHB-C1B-NB	6.11	130.73	124.26
26	C	514	BCR	C8-C7-C6	-6.09	110.08	127.20
26	A	610	BCR	C1-C6-C5	-6.08	114.04	122.61
27	a	611	PL9	C45-C44-C43	-6.07	108.11	123.68
26	B	620	BCR	C15-C14-C13	-6.05	118.67	127.31
24	b	617	CLA	C3A-C2A-C1A	6.05	110.41	101.34
26	B	619	BCR	C24-C23-C22	-6.05	117.09	126.23
24	c	506	CLA	C3A-C2A-C1A	6.05	110.40	101.34
26	B	620	BCR	C36-C18-C17	-6.04	114.46	122.92
24	c	507	CLA	O2D-CGD-CBD	6.04	122.00	111.27
24	B	609	CLA	C3A-C2A-C1A	6.03	110.38	101.34
26	h	101	BCR	C1-C6-C5	-6.02	114.14	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d	404	PL9	C37-C38-C39	-6.01	113.19	127.66
24	b	610	CLA	C3A-C2A-C1A	6.00	110.33	101.34
26	b	620	BCR	C1-C6-C5	-6.00	114.16	122.61
26	C	514	BCR	C30-C25-C26	-5.99	114.17	122.61
24	c	501	CLA	C3A-C2A-C1A	5.99	110.31	101.34
27	A	611	PL9	C10-C9-C8	-5.98	108.33	123.68
24	c	508	CLA	C3A-C2A-C1A	5.98	110.30	101.34
27	d	404	PL9	C42-C43-C44	-5.98	113.26	127.66
26	k	101	BCR	C34-C9-C10	-5.98	114.55	122.92
27	A	611	PL9	C45-C44-C43	-5.96	108.40	123.68
26	B	620	BCR	C11-C10-C9	-5.95	118.81	127.31
24	b	616	CLA	C3A-C2A-C1A	5.95	110.25	101.34
27	a	611	PL9	C11-C9-C8	-5.95	109.08	121.12
24	C	509	CLA	C4A-NA-C1A	-5.93	104.04	106.71
24	b	612	CLA	C4A-NA-C1A	-5.93	104.04	106.71
26	H	101	BCR	C36-C18-C17	-5.93	114.62	122.92
26	H	101	BCR	C31-C1-C6	-5.90	100.72	110.30
24	B	610	CLA	C3A-C2A-C1A	5.90	110.18	101.34
24	b	615	CLA	C3A-C2A-C1A	5.90	110.18	101.34
26	c	521	BCR	C11-C10-C9	-5.90	118.89	127.31
24	b	610	CLA	CHB-C1B-NB	5.90	130.50	124.26
24	b	618	CLA	C3A-C2A-C1A	5.89	110.17	101.34
24	C	511	CLA	C3A-C2A-C1A	5.89	110.16	101.34
27	A	611	PL9	C11-C9-C8	-5.89	109.21	121.12
24	b	607	CLA	C3A-C2A-C1A	5.88	110.15	101.34
24	C	502	CLA	C4A-NA-C1A	-5.88	104.06	106.71
26	h	101	BCR	C20-C21-C22	-5.88	118.92	127.31
26	b	620	BCR	C7-C6-C5	-5.88	107.23	121.46
26	K	101	BCR	C34-C9-C10	-5.86	114.71	122.92
24	b	613	CLA	O2D-CGD-CBD	5.86	121.68	111.27
24	b	606	CLA	C4A-NA-C1A	-5.86	104.07	106.71
26	b	621	BCR	C4-C5-C6	-5.86	114.23	122.73
26	c	514	BCR	C24-C25-C26	-5.85	107.28	121.46
26	k	101	BCR	C1-C6-C5	-5.85	114.38	122.61
24	b	611	CLA	C3A-C2A-C1A	5.84	110.09	101.34
26	A	610	BCR	C30-C25-C26	-5.82	114.42	122.61
24	C	502	CLA	CHB-C1B-NB	5.81	130.41	124.26
24	b	608[B]	CLA	C2A-C3A-C4A	5.81	111.25	101.87
26	c	515	BCR	C30-C25-C26	-5.81	114.44	122.61
24	B	606	CLA	C3A-C2A-C1A	5.80	110.02	101.34
26	K	101	BCR	C7-C8-C9	-5.79	117.49	126.23
24	B	615	CLA	C3A-C2A-C1A	5.79	110.01	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	O2D-CGD-CBD	5.79	121.55	111.27
26	c	521	BCR	C27-C26-C25	-5.79	114.33	122.73
27	A	611	PL9	C46-C44-C43	-5.78	109.43	121.12
24	b	604	CLA	C3A-C2A-C1A	5.77	109.99	101.34
24	B	613	CLA	C2A-C3A-C4A	5.77	111.19	101.87
27	D	405	PL9	C17-C18-C19	-5.77	113.77	127.66
24	c	508	CLA	CHB-C1B-NB	5.77	130.37	124.26
26	a	610	BCR	C20-C21-C22	-5.76	119.09	127.31
27	a	611	PL9	C10-C9-C8	-5.76	108.91	123.68
27	d	404	PL9	C35-C34-C33	-5.75	108.93	123.68
27	D	405	PL9	C11-C9-C8	-5.74	109.50	121.12
26	B	618	BCR	C27-C26-C25	-5.74	114.40	122.73
26	b	620	BCR	C20-C21-C22	-5.73	119.13	127.31
26	b	619	BCR	C38-C26-C27	-5.72	102.62	113.62
27	D	405	PL9	C21-C19-C18	-5.72	109.54	121.12
27	a	611	PL9	C40-C39-C41	-5.72	105.65	115.27
24	C	503	CLA	C3A-C2A-C1A	5.72	109.90	101.34
24	B	613	CLA	C4A-NA-C1A	-5.71	104.14	106.71
26	k	101	BCR	C15-C14-C13	-5.71	119.16	127.31
26	a	610	BCR	C7-C8-C9	-5.70	117.62	126.23
26	F	101	BCR	C7-C6-C5	-5.70	107.66	121.46
24	c	513	CLA	CHB-C1B-NB	5.70	130.29	124.26
27	a	611	PL9	C26-C24-C23	-5.70	109.59	121.12
24	C	501	CLA	C2A-C3A-C4A	5.69	111.07	101.87
26	K	102	BCR	C15-C14-C13	-5.69	119.19	127.31
24	b	608[A]	CLA	C2A-C3A-C4A	5.69	111.06	101.87
24	C	501	CLA	O2D-CGD-CBD	5.68	121.36	111.27
24	c	502	CLA	CHB-C1B-NB	5.68	130.27	124.26
26	h	101	BCR	C7-C6-C5	-5.67	107.72	121.46
26	a	610	BCR	C15-C14-C13	-5.67	119.22	127.31
24	B	616	CLA	C2A-C3A-C4A	5.65	111.00	101.87
24	b	617	CLA	C2A-C3A-C4A	5.65	110.99	101.87
26	B	618	BCR	C8-C7-C6	-5.64	111.35	127.20
24	c	512	CLA	O2D-CGD-CBD	5.64	121.30	111.27
26	b	619	BCR	C20-C21-C22	-5.64	119.26	127.31
24	C	504	CLA	CHB-C1B-NB	5.63	130.22	124.26
24	c	509	CLA	C2A-C3A-C4A	5.63	110.96	101.87
24	c	502	CLA	C3A-C2A-C1A	5.62	109.76	101.34
24	c	507	CLA	CHB-C1B-NB	5.62	130.21	124.26
24	c	513	CLA	C3A-C2A-C1A	5.62	109.76	101.34
26	t	101	BCR	C7-C8-C9	-5.62	117.74	126.23
24	b	611	CLA	C2A-C3A-C4A	5.62	110.94	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	610	BCR	C11-C10-C9	-5.61	119.30	127.31
24	b	605	CLA	C2A-C3A-C4A	5.61	110.93	101.87
26	I	101	BCR	C20-C21-C22	-5.61	119.31	127.31
24	B	617	CLA	C3A-C2A-C1A	5.60	109.73	101.34
26	c	521	BCR	C4-C5-C6	-5.60	114.60	122.73
26	B	619	BCR	C4-C5-C6	-5.59	114.62	122.73
24	B	607[B]	CLA	C2A-C3A-C4A	5.59	110.89	101.87
24	A	607	CLA	O2D-CGD-CBD	5.59	121.19	111.27
27	a	611	PL9	C35-C34-C33	-5.58	109.36	123.68
26	K	102	BCR	C7-C6-C5	-5.58	107.95	121.46
24	D	402	CLA	CHB-C1B-NB	5.58	130.16	124.26
26	K	102	BCR	C11-C10-C9	-5.57	119.36	127.31
24	C	508	CLA	C3A-C2A-C1A	5.57	109.69	101.34
24	C	512	CLA	O2D-CGD-CBD	5.57	121.17	111.27
26	B	618	BCR	C15-C14-C13	-5.57	119.36	127.31
27	a	611	PL9	C15-C14-C13	-5.57	109.39	123.68
30	A	615	LHG	O7-C7-C8	5.57	123.50	111.50
24	B	608	CLA	C2A-C3A-C4A	5.57	110.86	101.87
26	B	618	BCR	C37-C22-C21	-5.55	115.15	122.92
24	C	508	CLA	CHB-C1B-NB	5.54	130.13	124.26
24	b	603	CLA	C3A-C2A-C1A	5.54	109.64	101.34
24	B	608	CLA	C3A-C2A-C1A	5.54	109.64	101.34
26	h	101	BCR	C2-C1-C6	5.54	119.00	110.48
24	B	612	CLA	O2D-CGD-CBD	5.53	121.09	111.27
24	c	509	CLA	C3A-C2A-C1A	5.53	109.61	101.34
26	c	514	BCR	C7-C6-C5	-5.52	108.09	121.46
24	b	613	CLA	C3A-C2A-C1A	5.52	109.60	101.34
24	c	505	CLA	O2D-CGD-CBD	5.52	121.07	111.27
26	B	618	BCR	C24-C23-C22	-5.51	117.90	126.23
24	C	513	CLA	CHB-C1B-NB	5.51	130.09	124.26
24	B	602	CLA	C3A-C2A-C1A	5.50	109.58	101.34
26	C	514	BCR	C7-C6-C5	-5.50	108.14	121.46
24	C	507	CLA	C3A-C2A-C1A	5.50	109.58	101.34
26	b	619	BCR	C24-C23-C22	-5.49	117.93	126.23
24	B	611	CLA	CHB-C1B-NB	5.49	130.07	124.26
27	D	405	PL9	C42-C43-C44	-5.49	114.45	127.66
24	B	614	CLA	C3A-C2A-C1A	5.48	109.55	101.34
24	b	614	CLA	C2A-C3A-C4A	5.47	110.71	101.87
26	H	101	BCR	C29-C30-C25	5.47	118.90	110.48
24	B	607[B]	CLA	C3A-C2A-C1A	5.47	109.53	101.34
24	B	617	CLA	C4A-NA-C1A	-5.45	104.25	106.71
24	B	607[A]	CLA	C2A-C3A-C4A	5.45	110.67	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	605	CLA	C2A-C1A-CHA	5.44	133.37	123.86
27	D	405	PL9	C46-C44-C43	-5.44	110.11	121.12
24	C	504	CLA	C2A-C3A-C4A	5.43	110.65	101.87
24	c	503	CLA	C3A-C2A-C1A	5.43	109.47	101.34
26	T	101	BCR	C11-C10-C9	-5.42	119.57	127.31
24	C	509	CLA	C2A-C3A-C4A	5.41	110.61	101.87
24	c	507	CLA	C2A-C3A-C4A	5.41	110.61	101.87
24	B	610	CLA	C2A-C3A-C4A	5.41	110.60	101.87
24	b	606	CLA	C3A-C2A-C1A	5.40	109.43	101.34
24	C	507	CLA	C2A-C3A-C4A	5.40	110.59	101.87
26	C	514	BCR	C16-C15-C14	-5.40	112.42	123.47
26	C	514	BCR	C2-C1-C6	5.40	118.79	110.48
26	h	101	BCR	C4-C5-C6	-5.39	114.90	122.73
24	b	605	CLA	C3A-C2A-C1A	5.39	109.42	101.34
24	a	615	CLA	CHB-C1B-NB	5.38	129.96	124.26
26	K	102	BCR	C8-C7-C6	-5.38	112.10	127.20
24	B	607[A]	CLA	C3A-C2A-C1A	5.38	109.39	101.34
27	D	405	PL9	C30-C29-C28	-5.37	109.90	123.68
24	C	506	CLA	C2A-C1A-CHA	5.37	133.24	123.86
24	b	609	CLA	C2A-C3A-C4A	5.36	110.53	101.87
24	c	508	CLA	O2D-CGD-CBD	5.36	120.80	111.27
26	K	101	BCR	C7-C6-C5	-5.36	108.47	121.46
27	D	405	PL9	C37-C38-C39	-5.36	114.76	127.66
26	c	521	BCR	C8-C7-C6	-5.36	112.16	127.20
24	C	504	CLA	C4A-NA-C1A	-5.35	104.30	106.71
24	c	501	CLA	O2D-CGD-CBD	5.35	120.78	111.27
26	F	101	BCR	C1-C6-C5	-5.35	115.08	122.61
24	B	607[A]	CLA	CHB-C1B-NB	5.34	129.91	124.26
27	A	611	PL9	C15-C14-C13	-5.34	109.97	123.68
24	b	612	CLA	O2D-CGD-CBD	5.33	120.73	111.27
24	A	609	CLA	CHB-C1B-NB	5.33	129.90	124.26
24	B	614	CLA	C2A-C3A-C4A	5.33	110.47	101.87
26	c	521	BCR	C7-C6-C5	-5.32	108.57	121.46
26	B	619	BCR	C34-C9-C10	-5.32	115.47	122.92
24	B	602	CLA	CHB-C1B-NB	5.32	129.88	124.26
24	c	506	CLA	CHB-C1B-NB	5.31	129.88	124.26
24	a	606	CLA	CHB-C1B-NB	5.31	129.88	124.26
24	b	613	CLA	CHB-C1B-NB	5.30	129.87	124.26
24	C	511	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	c	506	CLA	C2A-C1A-CHA	5.30	133.13	123.86
24	B	606	CLA	C2A-C3A-C4A	5.30	110.43	101.87
24	a	609	CLA	C3A-C2A-C1A	5.29	109.27	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	607	CLA	C2A-C3A-C4A	5.29	110.41	101.87
24	b	609	CLA	C3A-C2A-C1A	5.29	109.25	101.34
24	C	502	CLA	C2A-C3A-C4A	5.28	110.40	101.87
26	B	620	BCR	C7-C6-C5	-5.27	108.69	121.46
24	b	608[A]	CLA	CHB-C1B-NB	5.27	129.84	124.26
24	B	612	CLA	C3A-C2A-C1A	5.26	109.22	101.34
24	b	609	CLA	C4A-NA-C1A	-5.26	104.34	106.71
24	B	605	CLA	C2A-C3A-C4A	5.26	110.36	101.87
26	b	621	BCR	C30-C25-C26	-5.26	115.21	122.61
24	B	610	CLA	O2D-CGD-CBD	5.26	120.61	111.27
24	B	612	CLA	C2A-C3A-C4A	5.25	110.36	101.87
24	B	606	CLA	C2A-C1A-CHA	5.25	133.04	123.86
24	c	512	CLA	C3A-C2A-C1A	5.25	109.21	101.34
27	D	405	PL9	C25-C24-C23	-5.25	110.22	123.68
24	A	607	CLA	C3A-C2A-C1A	5.24	109.19	101.34
26	K	102	BCR	C36-C18-C17	-5.24	115.58	122.92
26	B	619	BCR	C38-C26-C27	-5.24	103.55	113.62
27	D	405	PL9	C10-C9-C8	-5.24	110.23	123.68
26	I	101	BCR	C16-C15-C14	-5.24	112.75	123.47
26	C	514	BCR	C27-C26-C25	-5.23	115.13	122.73
24	b	608[B]	CLA	C3A-C2A-C1A	5.23	109.18	101.34
24	a	615	CLA	O2D-CGD-CBD	5.23	120.56	111.27
27	A	611	PL9	C21-C19-C18	-5.23	110.53	121.12
27	d	404	PL9	C25-C24-C23	-5.23	110.26	123.68
26	b	621	BCR	C35-C13-C14	-5.23	115.60	122.92
26	C	514	BCR	C24-C25-C26	-5.23	108.80	121.46
24	A	609	CLA	C3A-C2A-C1A	5.22	109.16	101.34
24	A	606	CLA	CHB-C1B-NB	5.22	129.78	124.26
27	D	405	PL9	C45-C44-C43	-5.22	110.30	123.68
26	K	101	BCR	C16-C17-C18	-5.22	119.87	127.31
24	B	602	CLA	C2A-C3A-C4A	5.22	110.29	101.87
27	a	611	PL9	C46-C44-C43	-5.20	110.59	121.12
24	C	511	CLA	C2A-C1A-CHA	5.20	132.95	123.86
24	d	403	CLA	C2A-C3A-C4A	5.20	110.27	101.87
26	h	101	BCR	C27-C26-C25	-5.20	115.19	122.73
26	H	101	BCR	C27-C26-C25	-5.20	115.19	122.73
24	b	616	CLA	CHB-C1B-NB	5.20	129.76	124.26
24	B	605	CLA	C3A-C2A-C1A	5.19	109.11	101.34
24	B	605	CLA	CHB-C1B-NB	5.18	129.74	124.26
27	D	405	PL9	C15-C14-C13	-5.17	110.41	123.68
24	b	603	CLA	C2A-C1A-CHA	5.17	132.90	123.86
24	a	607	CLA	C2A-C1A-CHA	5.17	132.90	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	403	CLA	CHB-C1B-NB	5.17	129.73	124.26
26	I	101	BCR	C34-C9-C10	-5.16	115.69	122.92
24	b	606	CLA	CHB-C1B-NB	5.16	129.72	124.26
24	c	504	CLA	C2A-C3A-C4A	5.16	110.20	101.87
24	B	614	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	b	608[A]	CLA	C3A-C2A-C1A	5.15	109.05	101.34
27	a	611	PL9	C25-C24-C23	-5.14	110.49	123.68
33	v	201	HEM	C4D-ND-C1D	5.14	110.38	105.07
27	d	404	PL9	C15-C14-C13	-5.14	110.50	123.68
26	B	620	BCR	C7-C8-C9	-5.13	118.48	126.23
24	b	615	CLA	CHB-C1B-NB	5.13	129.69	124.26
26	B	618	BCR	C30-C25-C26	-5.13	115.38	122.61
26	T	101	BCR	C23-C24-C25	-5.13	112.80	127.20
24	b	614	CLA	C3A-C2A-C1A	5.12	109.01	101.34
26	t	101	BCR	C35-C13-C12	-5.11	110.02	118.08
24	c	502	CLA	C2A-C3A-C4A	5.11	110.12	101.87
26	b	621	BCR	C37-C22-C23	5.11	126.13	118.08
24	b	617	CLA	O2D-CGD-CBD	5.11	120.34	111.27
24	B	604	CLA	C3A-C2A-C1A	5.10	108.98	101.34
24	d	402	CLA	C3A-C2A-C1A	5.10	108.97	101.34
24	b	608[B]	CLA	CHB-C1B-NB	5.10	129.65	124.26
26	h	101	BCR	C7-C8-C9	-5.09	118.54	126.23
24	D	404	CLA	C2A-C1A-CHA	5.09	132.76	123.86
24	B	616	CLA	C3A-C2A-C1A	5.08	108.95	101.34
24	C	509	CLA	C3A-C2A-C1A	5.08	108.94	101.34
27	A	611	PL9	C35-C34-C33	-5.07	110.67	123.68
27	D	405	PL9	C20-C19-C18	-5.07	110.67	123.68
24	B	615	CLA	C2A-C1A-CHA	5.07	132.72	123.86
24	C	513	CLA	C3A-C2A-C1A	5.07	108.93	101.34
24	c	503	CLA	C2A-C3A-C4A	5.06	110.05	101.87
24	a	615	CLA	C3A-C2A-C1A	5.06	108.92	101.34
27	d	404	PL9	C26-C24-C23	-5.06	110.88	121.12
24	c	503	CLA	CHB-C1B-NB	5.06	129.61	124.26
26	B	620	BCR	C20-C19-C18	-5.05	112.22	126.42
24	C	507	CLA	CHB-C1B-NB	5.05	129.60	124.26
26	B	619	BCR	C1-C6-C5	-5.05	115.50	122.61
24	B	609	CLA	O2D-CGD-CBD	5.05	120.23	111.27
24	B	605	CLA	O1D-CGD-CBD	-5.04	114.17	124.48
27	d	404	PL9	C10-C9-C8	-5.04	110.75	123.68
24	D	403	CLA	C2A-C3A-C4A	5.04	110.00	101.87
24	C	502	CLA	C3A-C2A-C1A	5.03	108.87	101.34
24	d	402	CLA	O2D-CGD-CBD	5.03	120.20	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	405	PL9	C40-C39-C38	-5.03	110.78	123.68
26	c	514	BCR	C7-C8-C9	-5.03	118.64	126.23
24	B	609	CLA	C2A-C1A-CHA	5.02	132.65	123.86
24	B	609	CLA	CHB-C1B-NB	5.02	129.57	124.26
24	b	603	CLA	C2A-C3A-C4A	5.02	109.98	101.87
26	K	101	BCR	C38-C26-C27	-5.02	103.97	113.62
24	C	501	CLA	C3A-C2A-C1A	5.01	108.85	101.34
27	a	611	PL9	C41-C39-C38	-5.01	110.98	121.12
24	a	607	CLA	C3A-C2A-C1A	5.00	108.83	101.34
24	B	607[B]	CLA	CHB-C1B-NB	5.00	129.55	124.26
24	B	611	CLA	C2A-C3A-C4A	5.00	109.94	101.87
27	d	404	PL9	C45-C44-C43	-4.99	110.88	123.68
26	t	101	BCR	C4-C5-C6	-4.99	115.49	122.73
26	c	514	BCR	C4-C5-C6	-4.98	115.50	122.73
26	T	101	BCR	C8-C7-C6	-4.98	113.23	127.20
27	D	405	PL9	C47-C48-C49	-4.97	110.76	127.75
26	c	514	BCR	C23-C24-C25	-4.97	113.24	127.20
27	a	611	PL9	C30-C29-C28	-4.97	110.93	123.68
24	c	506	CLA	C2A-C3A-C4A	4.97	109.89	101.87
24	a	607	CLA	CHB-C1B-NB	4.96	129.51	124.26
24	b	612	CLA	C3A-C2A-C1A	4.96	108.77	101.34
24	C	503	CLA	CHB-C1B-NB	4.96	129.51	124.26
24	c	510	CLA	C2A-C1A-CHA	4.95	132.52	123.86
33	e	102	HEM	C4D-ND-C1D	4.95	110.19	105.07
24	B	604	CLA	CHB-C1B-NB	4.95	129.50	124.26
24	B	607[A]	CLA	O2D-CGD-CBD	4.95	120.07	111.27
24	c	510	CLA	O2D-CGD-CBD	4.95	120.07	111.27
24	C	503	CLA	C2A-C3A-C4A	4.95	109.86	101.87
24	c	511	CLA	C2A-C1A-CHA	4.94	132.50	123.86
24	b	608[A]	CLA	C2A-C1A-CHA	4.94	132.50	123.86
26	b	619	BCR	C23-C24-C25	-4.94	113.33	127.20
24	A	609	CLA	C2A-C3A-C4A	4.94	109.85	101.87
24	B	611	CLA	C3A-C2A-C1A	4.94	108.73	101.34
24	d	402	CLA	CHB-C1B-NB	4.93	129.47	124.26
24	D	404	CLA	C2A-C3A-C4A	4.92	109.82	101.87
24	B	604	CLA	C2A-C3A-C4A	4.92	109.82	101.87
25	A	608	PHO	C4D-CHA-CBD	-4.92	106.29	108.52
24	B	613	CLA	O2D-CGD-CBD	4.92	120.01	111.27
26	h	101	BCR	C29-C30-C25	4.92	118.05	110.48
26	t	101	BCR	C8-C7-C6	-4.91	113.40	127.20
24	b	610	CLA	O2D-CGD-CBD	4.91	119.99	111.27
24	c	512	CLA	C4A-NA-C1A	-4.90	104.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607[B]	CLA	O2D-CGD-CBD	4.90	119.98	111.27
26	H	101	BCR	C2-C1-C6	4.90	118.02	110.48
26	b	619	BCR	C34-C9-C10	-4.90	116.07	122.92
26	h	101	BCR	C8-C7-C6	-4.89	113.46	127.20
24	c	506	CLA	O2D-CGD-CBD	4.89	119.96	111.27
26	A	610	BCR	C24-C23-C22	-4.89	118.84	126.23
30	a	616	LHG	O7-C7-C8	4.89	122.04	111.50
24	C	513	CLA	C2A-C3A-C4A	4.89	109.77	101.87
24	A	607	CLA	C2A-C3A-C4A	4.89	109.77	101.87
24	c	501	CLA	C2A-C3A-C4A	4.89	109.76	101.87
24	b	606	CLA	C2A-C1A-CHA	4.89	132.40	123.86
30	d	407	LHG	O7-C7-C8	4.88	122.03	111.50
26	I	101	BCR	C36-C18-C17	-4.88	116.09	122.92
24	b	615	CLA	C2A-C3A-C4A	4.88	109.75	101.87
26	H	101	BCR	C24-C25-C26	-4.87	109.65	121.46
24	c	511	CLA	O2D-CGD-CBD	4.87	119.92	111.27
24	b	606	CLA	C2A-C3A-C4A	4.87	109.73	101.87
26	K	101	BCR	C1-C6-C5	-4.87	115.76	122.61
26	T	101	BCR	C35-C13-C12	-4.87	110.41	118.08
26	h	101	BCR	C35-C13-C14	-4.86	116.12	122.92
24	B	602	CLA	C4A-NA-C1A	-4.86	104.52	106.71
24	b	613	CLA	C2A-C3A-C4A	4.85	109.71	101.87
26	b	621	BCR	C24-C25-C26	-4.85	109.72	121.46
27	D	405	PL9	C35-C34-C33	-4.84	111.25	123.68
26	B	618	BCR	C7-C6-C5	-4.84	109.74	121.46
24	B	611	CLA	C2A-C1A-CHA	4.83	132.30	123.86
24	d	403	CLA	C2A-C1A-CHA	4.82	132.29	123.86
26	C	514	BCR	C4-C5-C6	-4.82	115.73	122.73
26	B	618	BCR	C24-C25-C26	-4.82	109.78	121.46
24	a	609	CLA	C2A-C1A-CHA	4.82	132.29	123.86
24	c	513	CLA	O2D-CGD-CBD	4.82	119.83	111.27
27	D	405	PL9	C12-C13-C14	-4.82	116.06	127.66
26	k	101	BCR	C11-C10-C9	-4.81	120.45	127.31
24	a	606	CLA	C2A-C1A-CHA	4.81	132.27	123.86
27	d	404	PL9	C30-C29-C28	-4.80	111.35	123.68
24	C	502	CLA	O2D-CGD-CBD	4.80	119.79	111.27
24	B	615	CLA	C4A-NA-C1A	-4.79	104.55	106.71
24	c	513	CLA	C2A-C3A-C4A	4.78	109.60	101.87
24	D	402	CLA	C3A-C2A-C1A	4.77	108.49	101.34
26	B	620	BCR	C20-C21-C22	-4.77	120.50	127.31
26	b	620	BCR	C7-C8-C9	-4.77	119.03	126.23
26	K	101	BCR	C15-C14-C13	-4.76	120.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	CHB-C1B-NB	4.76	129.30	124.26
24	c	504	CLA	C3A-C2A-C1A	4.75	108.46	101.34
24	c	504	CLA	C4A-NA-C1A	-4.75	104.57	106.71
26	C	514	BCR	C31-C1-C6	-4.75	102.59	110.30
24	c	507	CLA	C3A-C2A-C1A	4.75	108.45	101.34
24	B	603	CLA	C2A-C1A-CHA	4.75	132.16	123.86
26	k	101	BCR	C7-C6-C5	-4.74	109.98	121.46
24	b	608[B]	CLA	C2A-C1A-CHA	4.74	132.15	123.86
30	e	101	LHG	O7-C7-C8	4.74	121.71	111.50
26	K	102	BCR	C7-C8-C9	-4.74	119.08	126.23
27	A	611	PL9	C30-C29-C28	-4.74	111.53	123.68
24	B	608	CLA	C2A-C1A-CHA	4.73	132.14	123.86
24	b	606	CLA	O2D-CGD-CBD	4.73	119.67	111.27
26	b	621	BCR	C31-C1-C6	-4.73	102.64	110.30
24	B	605	CLA	C2A-C1A-CHA	4.72	132.12	123.86
24	C	508	CLA	C2A-C3A-C4A	4.72	109.49	101.87
24	d	403	CLA	C3A-C2A-C1A	4.72	108.41	101.34
27	d	404	PL9	C47-C48-C49	-4.72	111.63	127.75
27	d	404	PL9	C40-C39-C38	-4.72	111.58	123.68
24	C	510	CLA	CHB-C1B-NB	4.72	129.25	124.26
24	C	507	CLA	C2A-C1A-CHA	4.71	132.10	123.86
26	c	515	BCR	C38-C26-C27	-4.71	104.56	113.62
24	b	615	CLA	C2A-C1A-CHA	4.71	132.10	123.86
24	c	503	CLA	C4A-NA-C1A	-4.71	104.59	106.71
24	b	607	CLA	O2D-CGD-CBD	4.70	119.62	111.27
24	A	607	CLA	C2A-C1A-CHA	4.70	132.07	123.86
32	c	518	DGD	O2G-C1B-C2B	4.69	121.62	111.50
24	B	602	CLA	C2A-C1A-CHA	4.69	132.05	123.86
26	K	102	BCR	C1-C6-C5	-4.69	116.01	122.61
28	A	612	SQD	O6-C1-C2	4.68	115.62	108.30
26	b	621	BCR	C7-C6-C5	-4.68	110.12	121.46
26	I	101	BCR	C33-C5-C4	-4.68	104.62	113.62
26	h	101	BCR	C23-C24-C25	-4.68	114.06	127.20
24	C	513	CLA	O2D-CGD-CBD	4.68	119.58	111.27
24	D	404	CLA	C3A-C2A-C1A	4.68	108.35	101.34
24	a	606	CLA	C3A-C2A-C1A	4.68	108.34	101.34
24	B	617	CLA	CHB-C1B-NB	4.67	129.20	124.26
28	a	612	SQD	O6-C1-C2	4.67	115.59	108.30
27	A	611	PL9	C20-C19-C18	-4.66	111.72	123.68
24	C	507	CLA	C4A-NA-C1A	-4.66	104.61	106.71
24	C	512	CLA	CHB-C1B-NB	4.65	129.18	124.26
26	H	101	BCR	C7-C6-C5	-4.65	110.20	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	604	CLA	C2A-C3A-C4A	4.65	109.38	101.87
26	t	101	BCR	C24-C25-C26	-4.64	110.21	121.46
24	B	605	CLA	O2D-CGD-O1D	-4.64	114.76	123.84
26	H	101	BCR	C38-C26-C27	-4.64	104.70	113.62
24	b	612	CLA	C2A-C3A-C4A	4.64	109.36	101.87
24	B	609	CLA	C2A-C3A-C4A	4.64	109.36	101.87
26	T	101	BCR	C11-C12-C13	-4.63	113.42	126.42
26	K	101	BCR	C24-C23-C22	-4.63	119.25	126.23
26	c	514	BCR	C36-C18-C17	-4.62	116.45	122.92
26	t	101	BCR	C11-C12-C13	-4.62	113.44	126.42
24	C	510	CLA	C3A-C2A-C1A	4.62	108.25	101.34
27	A	611	PL9	C40-C39-C41	-4.62	107.51	115.27
26	c	521	BCR	C38-C26-C27	-4.61	104.75	113.62
24	a	609	CLA	C2A-C3A-C4A	4.61	109.32	101.87
24	C	510	CLA	C2A-C3A-C4A	4.61	109.32	101.87
24	B	606	CLA	O2D-CGD-CBD	4.61	119.46	111.27
28	l	101	SQD	O6-C1-C2	4.60	115.49	108.30
28	L	102	SQD	O6-C1-C2	4.60	115.49	108.30
24	c	508	CLA	C2A-C3A-C4A	4.60	109.30	101.87
24	B	608	CLA	CHB-C1B-NB	4.60	129.13	124.26
24	c	512	CLA	C2A-C3A-C4A	4.59	109.28	101.87
26	K	101	BCR	C4-C5-C6	-4.59	116.07	122.73
24	B	613	CLA	CHB-C1B-NB	4.59	129.11	124.26
24	a	609	CLA	O2D-CGD-CBD	4.58	119.42	111.27
24	b	609	CLA	CHB-C1B-NB	4.58	129.11	124.26
32	h	102	DGD	O2G-C1B-C2B	4.58	121.38	111.50
26	a	610	BCR	C7-C6-C5	-4.58	110.37	121.46
24	B	606	CLA	CHB-C1B-NB	4.58	129.10	124.26
26	F	101	BCR	C15-C14-C13	-4.57	120.78	127.31
24	C	508	CLA	C2A-C1A-CHA	4.57	131.86	123.86
26	B	618	BCR	C34-C9-C10	-4.57	116.52	122.92
26	F	101	BCR	C8-C7-C6	-4.57	114.36	127.20
27	D	405	PL9	C45-C44-C46	-4.57	107.58	115.27
26	B	620	BCR	C31-C1-C6	-4.57	102.89	110.30
26	h	101	BCR	C38-C26-C27	-4.57	104.84	113.62
24	b	610	CLA	C2A-C3A-C4A	4.56	109.24	101.87
24	c	502	CLA	O2D-CGD-CBD	4.56	119.37	111.27
24	c	504	CLA	C2A-C1A-CHA	4.56	131.83	123.86
24	c	504	CLA	O2D-CGD-CBD	4.56	119.37	111.27
24	B	607[A]	CLA	C4A-NA-C1A	-4.56	104.66	106.71
24	C	512	CLA	C4A-NA-C1A	-4.55	104.66	106.71
24	C	506	CLA	O2D-CGD-CBD	4.55	119.35	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	402	CLA	C2A-C3A-C4A	4.54	109.21	101.87
24	b	607	CLA	CHB-C1B-NB	4.54	129.07	124.26
24	b	616	CLA	C2A-C3A-C4A	4.54	109.20	101.87
24	C	511	CLA	C2A-C3A-C4A	4.53	109.19	101.87
26	K	102	BCR	C4-C5-C6	-4.52	116.17	122.73
24	D	403	CLA	C3A-C2A-C1A	4.52	108.11	101.34
26	c	515	BCR	C8-C7-C6	-4.52	114.51	127.20
24	b	611	CLA	O2D-CGD-CBD	4.51	119.29	111.27
24	b	603	CLA	C4A-NA-C1A	-4.51	104.68	106.71
26	A	610	BCR	C7-C8-C9	-4.51	119.42	126.23
24	C	511	CLA	C4A-NA-C1A	-4.51	104.68	106.71
27	a	611	PL9	C21-C19-C18	-4.50	112.01	121.12
24	b	613	CLA	C2A-C1A-CHA	4.49	131.71	123.86
24	c	509	CLA	C2A-C1A-CHA	4.49	131.71	123.86
27	A	611	PL9	C25-C24-C23	-4.49	112.17	123.68
24	b	603	CLA	CHB-C1B-NB	4.48	129.00	124.26
26	B	619	BCR	C30-C25-C26	-4.48	116.30	122.61
24	B	617	CLA	CHC-C1C-NC	4.48	131.00	124.20
24	c	512	CLA	CHB-C1B-NB	4.47	128.99	124.26
24	B	613	CLA	C3A-C2A-C1A	4.47	108.04	101.34
24	C	512	CLA	C2A-C3A-C4A	4.46	109.08	101.87
26	a	610	BCR	C38-C26-C27	-4.46	105.05	113.62
26	c	514	BCR	C2-C1-C6	4.46	117.34	110.48
24	A	609	CLA	O2D-CGD-CBD	4.46	119.19	111.27
24	B	615	CLA	C2A-C3A-C4A	4.46	109.07	101.87
24	C	504	CLA	O2D-CGD-CBD	4.45	119.18	111.27
24	b	612	CLA	C2A-C1A-CHA	4.45	131.65	123.86
24	c	511	CLA	C4A-NA-C1A	-4.45	104.70	106.71
24	c	505	CLA	C2A-C1A-CHA	4.45	131.63	123.86
24	c	509	CLA	CHB-C1B-NB	4.45	128.96	124.26
24	b	604	CLA	CHB-C1B-NB	4.44	128.96	124.26
24	c	502	CLA	C2A-C1A-CHA	4.44	131.63	123.86
26	b	619	BCR	C7-C6-C5	-4.44	110.70	121.46
24	A	606	CLA	C2A-C1A-CHA	4.44	131.63	123.86
29	c	520	LMG	O7-C10-C11	4.44	121.07	111.50
24	D	402	CLA	C2A-C3A-C4A	4.44	109.04	101.87
26	c	521	BCR	C1-C6-C5	-4.44	116.36	122.61
26	K	102	BCR	C38-C26-C27	-4.43	105.10	113.62
24	A	607	CLA	C4D-CHA-C1A	-4.43	115.86	121.25
24	b	618	CLA	CHB-C1B-NB	4.43	128.94	124.26
24	C	504	CLA	C3A-C2A-C1A	4.42	107.96	101.34
24	c	511	CLA	C2A-C3A-C4A	4.42	109.00	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	T	101	BCR	C4-C5-C6	-4.41	116.33	122.73
27	a	611	PL9	C20-C19-C18	-4.41	112.37	123.68
26	T	101	BCR	C35-C13-C14	-4.41	116.75	122.92
27	A	611	PL9	C36-C34-C33	-4.40	112.20	121.12
24	c	504	CLA	CHB-C1B-NB	4.39	128.91	124.26
24	B	614	CLA	C2A-C1A-CHA	4.39	131.53	123.86
24	b	612	CLA	CHB-C1B-NB	4.38	128.89	124.26
24	B	605	CLA	O2D-CGD-CBD	4.38	119.04	111.27
24	b	610	CLA	C2A-C1A-CHA	4.37	131.51	123.86
24	b	607	CLA	C2A-C1A-CHA	4.37	131.51	123.86
24	c	510	CLA	C2A-C3A-C4A	4.37	108.93	101.87
26	c	521	BCR	C15-C14-C13	-4.37	121.07	127.31
26	H	101	BCR	C30-C25-C26	-4.37	116.46	122.61
26	k	101	BCR	C38-C26-C27	-4.37	105.22	113.62
24	a	606	CLA	C2A-C3A-C4A	4.37	108.92	101.87
24	b	618	CLA	C2A-C3A-C4A	4.37	108.92	101.87
24	A	606	CLA	O2D-CGD-CBD	4.36	119.02	111.27
24	B	607[A]	CLA	C2A-C1A-CHA	4.36	131.48	123.86
28	a	612	SQD	O9-S-C6	4.35	112.11	106.94
24	c	505	CLA	C2A-C3A-C4A	4.34	108.88	101.87
24	c	508	CLA	C2A-C1A-CHA	4.33	131.44	123.86
24	C	501	CLA	C4A-NA-C1A	-4.33	104.76	106.71
24	b	615	CLA	O2D-CGD-CBD	4.33	118.96	111.27
24	a	607	CLA	C2A-C3A-C4A	4.33	108.86	101.87
26	h	101	BCR	C24-C25-C26	-4.33	110.98	121.46
28	a	612	SQD	O47-C7-C8	4.32	120.82	111.50
26	I	101	BCR	C30-C25-C26	-4.32	116.52	122.61
24	b	617	CLA	CHB-C1B-NB	4.32	128.83	124.26
24	D	402	CLA	CHA-C1A-NA	-4.32	116.50	126.40
26	T	101	BCR	C24-C25-C26	-4.32	111.00	121.46
28	A	612	SQD	O47-C7-C8	4.31	120.80	111.50
28	A	612	SQD	O9-S-C6	4.31	112.06	106.94
24	c	507	CLA	C2A-C1A-CHA	4.31	131.39	123.86
26	b	620	BCR	C38-C26-C27	-4.30	105.35	113.62
30	d	406	LHG	O7-C7-C8	4.30	120.77	111.50
24	C	502	CLA	C2A-C1A-CHA	4.30	131.38	123.86
24	B	617	CLA	C2A-C3A-C4A	4.30	108.81	101.87
26	b	619	BCR	C37-C22-C21	-4.30	116.90	122.92
26	B	619	BCR	C36-C18-C19	-4.29	111.32	118.08
26	T	101	BCR	C20-C21-C22	-4.28	121.20	127.31
26	f	101	BCR	C8-C7-C6	-4.27	115.20	127.20
24	b	616	CLA	O2D-CGD-CBD	4.27	118.86	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	505	CLA	C2A-C1A-CHA	4.27	131.32	123.86
24	c	511	CLA	CHB-C1B-NB	4.26	128.77	124.26
26	b	621	BCR	C37-C22-C21	-4.26	116.95	122.92
24	C	506	CLA	C2A-C3A-C4A	4.26	108.75	101.87
24	c	509	CLA	O2D-CGD-CBD	4.26	118.83	111.27
24	b	608[A]	CLA	O2D-CGD-CBD	4.25	118.83	111.27
26	H	101	BCR	C23-C24-C25	-4.25	115.26	127.20
24	B	604	CLA	O2D-CGD-CBD	4.25	118.82	111.27
24	d	403	CLA	C1-O2A-CGA	4.25	127.59	116.44
26	B	620	BCR	C23-C22-C21	-4.24	112.43	118.94
26	C	514	BCR	C20-C19-C18	-4.24	114.50	126.42
24	b	608[A]	CLA	C4A-NA-C1A	-4.24	104.80	106.71
26	A	610	BCR	C7-C6-C5	-4.23	111.21	121.46
24	C	513	CLA	C4A-NA-C1A	-4.23	104.80	106.71
24	C	508	CLA	O2D-CGD-CBD	4.23	118.78	111.27
28	B	622	SQD	O6-C1-C2	4.22	114.90	108.30
28	b	601	SQD	O6-C1-C2	4.22	114.89	108.30
32	c	516	DGD	O2G-C1B-C2B	4.22	120.60	111.50
24	B	616	CLA	C2A-C1A-CHA	4.22	131.24	123.86
26	t	101	BCR	C23-C24-C25	-4.22	115.36	127.20
25	d	401	PHO	CMB-C2B-C3B	4.21	132.56	124.68
24	b	608[B]	CLA	O2D-CGD-CBD	4.21	118.75	111.27
24	C	504	CLA	C2A-C1A-CHA	4.21	131.22	123.86
24	c	513	CLA	C2A-C1A-CHA	4.20	131.21	123.86
26	f	101	BCR	C7-C6-C5	-4.20	111.28	121.46
24	B	603	CLA	CHB-C1B-NB	4.20	128.71	124.26
24	c	510	CLA	CHB-C1B-NB	4.20	128.71	124.26
24	b	616	CLA	C4A-NA-C1A	-4.20	104.82	106.71
27	d	404	PL9	C20-C19-C18	-4.19	112.92	123.68
24	B	608	CLA	C4A-NA-C1A	-4.19	104.82	106.71
26	C	514	BCR	C36-C18-C17	-4.18	117.07	122.92
24	B	615	CLA	O2D-CGD-CBD	4.18	118.70	111.27
30	E	102	LHG	O7-C7-C8	4.18	120.50	111.50
27	d	404	PL9	C31-C29-C28	-4.17	112.67	121.12
24	C	505	CLA	C2A-C3A-C4A	4.17	108.61	101.87
24	c	503	CLA	C2A-C1A-CHA	4.17	131.15	123.86
26	B	619	BCR	C20-C19-C18	-4.17	114.70	126.42
24	b	616	CLA	C2A-C1A-CHA	4.17	131.15	123.86
24	B	607[B]	CLA	C2A-C1A-CHA	4.16	131.14	123.86
24	c	501	CLA	C2A-C1A-CHA	4.16	131.13	123.86
26	c	521	BCR	C35-C13-C14	-4.16	117.10	122.92
26	b	621	BCR	C38-C26-C27	-4.15	105.64	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	607	CLA	C4A-NA-C1A	-4.14	104.84	106.71
26	A	610	BCR	C39-C30-C25	4.14	117.01	110.30
24	d	403	CLA	C4A-NA-C1A	-4.13	104.85	106.71
27	d	404	PL9	C36-C34-C33	-4.13	112.76	121.12
32	d	405	DGD	O2G-C1B-C2B	4.12	120.39	111.50
24	D	402	CLA	O1D-CGD-CBD	-4.12	116.05	124.48
24	b	609	CLA	O2D-CGD-CBD	4.12	118.58	111.27
24	B	603	CLA	C2A-C3A-C4A	4.12	108.52	101.87
28	X	101	SQD	O6-C1-C2	4.12	114.73	108.30
27	A	611	PL9	C47-C48-C49	-4.11	113.70	127.75
26	a	610	BCR	C24-C25-C26	-4.11	111.51	121.46
24	C	510	CLA	O2D-CGD-CBD	4.11	118.57	111.27
26	C	514	BCR	C38-C26-C27	-4.11	105.72	113.62
26	B	618	BCR	C36-C18-C17	-4.11	117.17	122.92
28	x	101	SQD	O6-C1-C2	4.10	114.71	108.30
24	C	511	CLA	CHB-C1B-NB	4.10	128.60	124.26
26	a	610	BCR	C36-C18-C17	-4.10	117.19	122.92
24	B	614	CLA	CHC-C1C-NC	4.09	130.41	124.20
26	k	101	BCR	C23-C24-C25	-4.09	115.71	127.20
26	c	514	BCR	C16-C15-C14	-4.09	115.10	123.47
26	B	618	BCR	C23-C24-C25	-4.08	115.73	127.20
29	C	518	LMG	O7-C10-C11	4.08	120.30	111.50
26	K	101	BCR	C23-C22-C21	-4.08	112.68	118.94
26	B	619	BCR	C11-C12-C13	-4.07	114.99	126.42
27	D	405	PL9	C7-C3-C4	4.07	120.18	116.88
24	a	609	CLA	CHB-C1B-NB	4.06	128.56	124.26
24	C	512	CLA	CHC-C1C-NC	4.06	130.36	124.20
26	F	101	BCR	C37-C22-C21	-4.06	117.24	122.92
27	a	611	PL9	C47-C48-C49	-4.06	113.88	127.75
26	A	610	BCR	C34-C9-C10	-4.05	117.25	122.92
24	A	607	CLA	CHB-C1B-NB	4.05	128.54	124.26
26	K	102	BCR	C23-C24-C25	-4.04	115.85	127.20
24	B	603	CLA	CHC-C1C-NC	4.04	130.34	124.20
26	k	101	BCR	C4-C5-C6	-4.04	116.87	122.73
27	a	611	PL9	C31-C29-C28	-4.03	112.95	121.12
27	A	611	PL9	C31-C29-C28	-4.03	112.96	121.12
24	a	615	CLA	C2A-C3A-C4A	4.03	108.38	101.87
32	C	515	DGD	O2G-C1B-C2B	4.03	120.18	111.50
26	a	610	BCR	C8-C7-C6	-4.03	115.89	127.20
26	F	101	BCR	C36-C18-C19	4.02	124.41	118.08
24	b	613	CLA	C4A-NA-C1A	-4.02	104.90	106.71
24	D	402	CLA	C2A-C1A-CHA	4.01	130.87	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	CAC-C3C-C4C	4.00	130.00	124.81
24	A	609	CLA	C2A-C1A-CHA	4.00	130.85	123.86
24	C	501	CLA	CHB-C1B-NB	3.99	128.48	124.26
26	B	619	BCR	C35-C13-C14	-3.99	117.33	122.92
23	a	605	BCT	O2-C-O1	-3.99	109.19	119.55
26	I	101	BCR	C38-C26-C27	-3.99	105.96	113.62
24	D	404	CLA	C1-O2A-CGA	3.99	126.91	116.44
24	a	607	CLA	O1D-CGD-CBD	-3.98	116.33	124.48
24	a	609	CLA	CHA-C1A-NA	-3.98	117.29	126.40
26	c	515	BCR	C20-C21-C22	-3.97	121.64	127.31
27	D	405	PL9	C51-C49-C48	-3.97	111.17	122.65
24	c	508	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
28	b	601	SQD	O47-C7-C8	3.97	120.06	111.50
28	B	622	SQD	O47-C7-C8	3.97	120.05	111.50
32	E	101	DGD	O2G-C1B-C2B	3.97	120.05	111.50
26	B	618	BCR	C33-C5-C4	-3.96	106.00	113.62
26	b	620	BCR	C37-C22-C21	-3.96	117.38	122.92
24	c	503	CLA	O2D-CGD-CBD	3.96	118.30	111.27
24	B	615	CLA	CHB-C1B-NB	3.96	128.44	124.26
32	C	517	DGD	O2G-C1B-C2B	3.95	120.02	111.50
24	c	508	CLA	C4D-C3D-CAD	-3.95	103.44	108.10
24	b	618	CLA	CHC-C1C-NC	3.94	130.19	124.20
24	c	510	CLA	CHC-C1C-NC	3.94	130.18	124.20
24	b	611	CLA	C2A-C1A-CHA	3.93	130.73	123.86
24	B	606	CLA	C4-C3-C5	3.93	121.88	115.27
24	C	507	CLA	C1D-ND-C4D	-3.92	103.55	106.33
24	d	403	CLA	C1D-ND-C4D	-3.92	103.55	106.33
24	C	508	CLA	CHC-C1C-NC	3.92	130.15	124.20
28	b	601	SQD	O7-S-C6	3.92	111.60	106.94
24	c	501	CLA	CHB-C1B-NB	3.92	128.40	124.26
24	a	615	CLA	CHC-C1C-NC	3.91	130.13	124.20
24	B	617	CLA	O2D-CGD-CBD	3.90	118.21	111.27
24	b	607	CLA	C4-C3-C5	3.90	121.83	115.27
24	C	505	CLA	CHB-C1B-NB	3.89	128.38	124.26
28	B	622	SQD	O7-S-C6	3.89	111.56	106.94
25	D	401	PHO	O2D-CGD-O1D	-3.89	116.23	123.84
26	b	619	BCR	C30-C25-C26	-3.88	117.15	122.61
30	l	102	LHG	O7-C7-C8	3.88	119.86	111.50
24	b	603	CLA	O2D-CGD-CBD	3.88	118.16	111.27
26	b	621	BCR	C19-C18-C17	3.87	124.88	118.94
27	D	405	PL9	C41-C39-C38	-3.87	113.29	121.12
26	b	620	BCR	C30-C25-C26	-3.87	117.17	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	607	CLA	CHC-C1C-NC	3.86	130.06	124.20
26	h	101	BCR	C31-C1-C6	-3.86	104.04	110.30
24	c	502	CLA	C4A-NA-C1A	-3.86	104.97	106.71
24	b	614	CLA	CHB-C1B-NB	3.86	128.34	124.26
29	C	519	LMG	O7-C10-C11	3.86	119.82	111.50
26	f	101	BCR	C37-C22-C23	-3.86	112.00	118.08
24	A	606	CLA	CHC-C1C-NC	3.85	130.05	124.20
27	d	404	PL9	C50-C49-C48	-3.85	111.52	122.65
24	b	614	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
24	B	612	CLA	C4A-NA-C1A	-3.84	104.98	106.71
26	K	101	BCR	C35-C13-C14	-3.84	117.54	122.92
24	b	613	CLA	CHC-C1C-NC	3.84	130.03	124.20
27	A	611	PL9	C50-C49-C48	-3.84	111.55	122.65
26	A	610	BCR	C23-C22-C21	-3.84	113.05	118.94
24	B	607[B]	CLA	CHC-C1C-NC	3.84	130.02	124.20
24	C	503	CLA	C2A-C1A-CHA	3.83	130.56	123.86
28	B	622	SQD	C3-C4-C5	3.83	117.07	110.24
24	D	403	CLA	CHB-C1B-NB	3.82	128.30	124.26
28	b	601	SQD	C3-C4-C5	3.82	117.05	110.24
27	d	404	PL9	C41-C39-C38	-3.82	113.39	121.12
26	h	101	BCR	C40-C30-C25	-3.82	104.11	110.30
24	C	506	CLA	CED-O2D-CGD	3.81	124.56	115.94
26	A	610	BCR	C8-C7-C6	-3.81	116.52	127.20
33	e	102	HEM	CBD-CAD-C3D	-3.80	102.08	112.63
27	A	611	PL9	C7-C3-C4	3.79	119.96	116.88
24	b	603	CLA	CHC-C1C-NC	3.79	129.95	124.20
26	b	621	BCR	C2-C1-C6	3.78	116.30	110.48
26	B	618	BCR	C38-C26-C27	-3.78	106.36	113.62
26	c	521	BCR	C24-C25-C26	-3.78	112.31	121.46
24	b	605	CLA	CHB-C4A-NA	-3.78	119.29	124.51
26	b	619	BCR	C8-C7-C6	-3.77	116.60	127.20
28	X	101	SQD	O47-C7-C8	3.77	119.63	111.50
29	Z	101	LMG	O1-C1-C2	3.77	114.19	108.30
24	C	503	CLA	C4A-NA-C1A	-3.77	105.01	106.71
32	c	518	DGD	O3G-C3G-C2G	-3.77	101.80	110.90
28	x	101	SQD	O47-C7-C8	3.77	119.62	111.50
27	D	405	PL9	C10-C9-C11	-3.77	108.93	115.27
26	A	610	BCR	C36-C18-C17	-3.77	117.64	122.92
25	d	401	PHO	CBC-CAC-C3C	3.77	118.40	112.88
24	b	604	CLA	O1D-CGD-CBD	-3.77	116.78	124.48
24	a	615	CLA	O2A-CGA-CBA	3.76	123.72	111.91
33	v	201	HEM	C3B-C2B-C1B	3.76	109.28	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607[A]	CLA	CHC-C1C-NC	3.76	129.91	124.20
24	b	605	CLA	O1D-CGD-CBD	-3.76	116.80	124.48
25	D	401	PHO	CMB-C2B-C3B	3.76	131.70	124.68
26	C	514	BCR	C34-C9-C10	-3.75	117.66	122.92
29	a	613	LMG	O7-C10-C11	3.75	119.59	111.50
24	C	511	CLA	CHC-C1C-NC	3.74	129.87	124.20
24	b	607	CLA	C1-O2A-CGA	3.73	126.24	116.44
27	a	611	PL9	C7-C3-C4	3.73	119.91	116.88
24	c	505	CLA	CHB-C1B-NB	3.73	128.21	124.26
33	E	103	HEM	C4D-ND-C1D	3.73	108.93	105.07
24	c	504	CLA	C1D-ND-C4D	-3.73	103.68	106.33
24	d	403	CLA	CHC-C1C-NC	3.73	129.86	124.20
26	B	620	BCR	C38-C26-C27	-3.73	106.45	113.62
24	C	501	CLA	C2A-C1A-CHA	3.73	130.37	123.86
28	L	102	SQD	O47-C7-C8	3.72	119.52	111.50
26	B	620	BCR	C24-C25-C26	-3.71	112.47	121.46
26	h	101	BCR	C33-C5-C4	-3.71	106.49	113.62
26	c	514	BCR	C20-C19-C18	-3.71	116.00	126.42
24	B	604	CLA	C2A-C1A-CHA	3.70	130.34	123.86
32	C	517	DGD	O3G-C3G-C2G	-3.70	101.96	110.90
24	D	404	CLA	O2D-CGD-CBD	3.70	117.84	111.27
26	B	619	BCR	C37-C22-C21	-3.69	117.75	122.92
24	B	614	CLA	CHB-C1B-NB	3.69	128.16	124.26
28	L	102	SQD	O7-S-C6	3.68	111.31	106.94
26	B	620	BCR	C16-C15-C14	-3.67	115.95	123.47
24	c	507	CLA	CHC-C1C-NC	3.67	129.78	124.20
28	l	101	SQD	O7-S-C6	3.67	111.31	106.94
28	l	101	SQD	O47-C7-C8	3.67	119.42	111.50
33	E	103	HEM	CBD-CAD-C3D	-3.66	102.45	112.63
27	a	611	PL9	C45-C44-C46	-3.66	109.11	115.27
24	A	607	CLA	C4A-NA-C1A	-3.65	105.06	106.71
24	a	615	CLA	C2A-C1A-CHA	3.65	130.24	123.86
24	a	606	CLA	CHC-C1C-NC	3.65	129.74	124.20
26	I	101	BCR	C8-C7-C6	-3.65	116.96	127.20
24	B	605	CLA	C4D-C3D-CAD	-3.63	103.81	108.10
24	b	605	CLA	CHB-C1B-NB	3.63	128.10	124.26
24	B	607[B]	CLA	C4A-NA-C1A	-3.63	105.08	106.71
24	b	608[A]	CLA	C3B-C4B-NB	-3.63	107.15	110.52
24	c	503	CLA	C1D-ND-C4D	-3.62	103.76	106.33
27	d	404	PL9	C51-C49-C48	-3.62	112.17	122.65
24	B	604	CLA	CHB-C4A-NA	-3.62	119.50	124.51
24	B	616	CLA	O2D-CGD-CBD	3.61	117.69	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	515	BCR	C23-C24-C25	-3.61	117.06	127.20
26	c	515	BCR	C34-C9-C10	-3.61	117.86	122.92
24	b	615	CLA	CHC-C1C-NC	3.61	129.68	124.20
26	I	101	BCR	C20-C19-C18	-3.61	116.28	126.42
26	h	101	BCR	C30-C25-C26	-3.61	117.53	122.61
24	B	603	CLA	C4A-NA-C1A	-3.61	105.08	106.71
29	z	101	LMG	O7-C10-C11	3.60	119.25	111.50
24	b	609	CLA	C1D-ND-C4D	-3.60	103.78	106.33
27	D	405	PL9	C50-C49-C48	-3.59	112.26	122.65
27	a	611	PL9	C50-C49-C48	-3.59	112.26	122.65
24	a	609	CLA	C4-C3-C5	3.59	121.30	115.27
26	I	101	BCR	C7-C6-C5	-3.59	112.78	121.46
24	B	607[A]	CLA	C3B-C4B-NB	-3.58	107.19	110.52
26	c	515	BCR	C7-C6-C5	-3.58	112.79	121.46
24	A	609	CLA	C4-C3-C5	3.58	121.29	115.27
29	Z	101	LMG	O7-C10-C11	3.57	119.20	111.50
26	t	101	BCR	C34-C9-C10	-3.57	117.93	122.92
33	V	201	HEM	C4D-ND-C1D	3.56	108.75	105.07
24	C	502	CLA	C1-O2A-CGA	3.56	125.79	116.44
24	a	607	CLA	CHA-C1A-NA	-3.56	118.24	126.40
24	d	402	CLA	C2A-C1A-CHA	3.56	130.09	123.86
24	a	615	CLA	CHA-C1A-NA	-3.56	118.25	126.40
26	K	102	BCR	C33-C5-C4	-3.56	106.78	113.62
24	C	509	CLA	CHB-C1B-NB	3.55	128.02	124.26
24	D	403	CLA	C4A-NA-C1A	-3.55	105.11	106.71
24	C	503	CLA	O2D-CGD-CBD	3.54	117.56	111.27
26	k	101	BCR	C24-C25-C26	-3.54	112.89	121.46
30	D	407	LHG	O7-C7-C8	3.53	119.12	111.50
29	c	519	LMG	O7-C10-C11	3.53	119.11	111.50
26	c	515	BCR	C33-C5-C4	-3.53	106.83	113.62
26	a	610	BCR	C34-C9-C10	-3.53	117.98	122.92
24	b	617	CLA	CHC-C1C-NC	3.52	129.55	124.20
26	A	610	BCR	C33-C5-C4	-3.52	106.85	113.62
24	c	510	CLA	C4A-NA-C1A	-3.52	105.12	106.71
24	B	613	CLA	CHB-C4A-NA	-3.52	119.65	124.51
33	V	201	HEM	C3B-C2B-C1B	3.52	109.09	106.49
29	D	408	LMG	O6-C5-C4	3.52	116.08	109.69
24	c	509	CLA	CHC-C1C-NC	3.51	129.53	124.20
24	b	605	CLA	CHC-C1C-NC	3.51	129.53	124.20
26	k	101	BCR	C20-C21-C22	-3.51	122.31	127.31
27	A	611	PL9	C15-C14-C16	-3.50	109.38	115.27
24	b	613	CLA	O1D-CGD-CBD	-3.50	117.32	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	CHC-C1C-NC	3.50	129.51	124.20
24	B	617	CLA	C4D-C3D-CAD	-3.50	103.98	108.10
24	B	610	CLA	CHC-C1C-NC	3.50	129.51	124.20
24	b	608[B]	CLA	C4A-NA-C1A	-3.49	105.14	106.71
26	K	102	BCR	C24-C25-C26	-3.49	113.00	121.46
27	A	611	PL9	C45-C44-C46	-3.49	109.40	115.27
24	A	607	CLA	O2A-CGA-CBA	3.49	122.86	111.91
24	B	616	CLA	CHC-C1C-NC	3.49	129.50	124.20
24	b	611	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
24	c	509	CLA	C1D-ND-C4D	-3.49	103.86	106.33
27	a	611	PL9	C36-C34-C33	-3.48	114.08	121.12
26	A	610	BCR	C16-C15-C14	-3.48	116.35	123.47
24	d	403	CLA	O2D-CGD-CBD	3.47	117.44	111.27
23	a	605	BCT	O3-C-O1	-3.47	110.55	119.55
24	b	611	CLA	CHB-C1B-NB	3.47	127.93	124.26
24	B	604	CLA	O1D-CGD-CBD	-3.47	117.39	124.48
24	D	404	CLA	CHA-C1A-NA	-3.46	118.47	126.40
24	B	610	CLA	C2A-C1A-CHA	3.46	129.91	123.86
24	c	508	CLA	CHC-C1C-NC	3.46	129.45	124.20
25	d	401	PHO	C4D-CHA-CBD	-3.46	106.95	108.52
26	I	101	BCR	C30-C25-C24	-3.46	106.00	115.78
28	A	614	SQD	O9-S-C6	3.46	111.05	106.94
24	b	616	CLA	C4-C3-C5	3.45	121.08	115.27
24	c	508	CLA	C4A-NA-C1A	-3.45	105.16	106.71
26	K	102	BCR	C40-C30-C25	3.45	115.89	110.30
24	B	610	CLA	CHB-C1B-NB	3.44	127.90	124.26
24	B	615	CLA	C4-C3-C5	3.44	121.06	115.27
24	b	616	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
26	b	619	BCR	C24-C25-C26	-3.44	113.13	121.46
24	C	507	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
24	C	509	CLA	C2A-C1A-CHA	3.44	129.87	123.86
24	c	505	CLA	C4A-NA-C1A	-3.44	105.16	106.71
26	b	620	BCR	C16-C15-C14	-3.44	116.44	123.47
24	B	609	CLA	CHC-C1C-NC	3.44	129.41	124.20
24	a	615	CLA	C4D-CHA-C1A	-3.43	117.07	121.25
26	b	620	BCR	C27-C26-C25	-3.43	117.75	122.73
24	A	606	CLA	C3A-C2A-C1A	3.42	106.47	101.34
24	A	606	CLA	C2A-C3A-C4A	3.42	107.40	101.87
24	c	506	CLA	CHB-C4A-NA	-3.42	119.78	124.51
30	L	101	LHG	O7-C7-C8	3.42	118.87	111.50
24	B	602	CLA	O2D-CGD-CBD	3.41	117.34	111.27
24	C	503	CLA	C1D-ND-C4D	-3.41	103.91	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	603	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
28	a	614	SQD	O9-S-C6	3.41	110.99	106.94
24	b	608[B]	CLA	C3B-C4B-NB	-3.40	107.36	110.52
26	t	101	BCR	C1-C6-C5	-3.40	117.82	122.61
24	b	610	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
27	a	611	PL9	C15-C14-C16	-3.39	109.56	115.27
24	c	507	CLA	C1-O2A-CGA	3.39	125.35	116.44
24	b	606	CLA	C1-O2A-CGA	3.39	125.34	116.44
24	a	607	CLA	C1-O2A-CGA	3.39	125.33	116.44
28	A	614	SQD	O47-C7-C8	3.37	118.77	111.50
28	a	614	SQD	O47-C7-C8	3.37	118.77	111.50
24	b	605	CLA	O2A-C1-C2	3.37	117.50	108.64
25	a	608	PHO	C4D-CHA-CBD	-3.37	106.99	108.52
24	A	609	CLA	CHA-C1A-NA	-3.36	118.70	126.40
29	C	518	LMG	O8-C28-C29	3.36	122.44	111.91
24	b	604	CLA	C2A-C1A-CHA	3.36	129.73	123.86
26	b	621	BCR	C1-C6-C5	-3.35	117.89	122.61
29	D	408	LMG	O7-C10-C11	3.35	118.73	111.50
28	A	612	SQD	O8-S-C6	3.35	111.08	105.74
25	A	608	PHO	CMB-C2B-C3B	3.34	130.93	124.68
24	b	605	CLA	O2D-CGD-CBD	3.34	117.20	111.27
27	A	611	PL9	C51-C49-C48	-3.34	113.00	122.65
24	b	617	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
24	C	508	CLA	C4D-C3D-CAD	-3.34	104.16	108.10
24	B	602	CLA	C1D-ND-C4D	-3.34	103.97	106.33
24	a	607	CLA	CHC-C1C-NC	3.33	129.26	124.20
28	a	612	SQD	C1-C2-C3	-3.33	103.06	110.00
33	V	201	HEM	CBA-CAA-C2A	-3.33	103.38	112.63
32	c	517	DGD	O2G-C1B-C2B	3.33	118.67	111.50
24	C	501	CLA	C4D-C3D-CAD	-3.32	104.19	108.10
24	A	607	CLA	O1D-CGD-CBD	-3.32	117.70	124.48
28	a	612	SQD	O8-S-C6	3.31	111.02	105.74
28	A	612	SQD	C1-C2-C3	-3.31	103.10	110.00
32	E	101	DGD	C4E-C3E-C2E	3.31	116.60	110.82
24	b	609	CLA	C2A-C1A-CHA	3.31	129.64	123.86
25	a	608	PHO	CMB-C2B-C3B	3.31	130.86	124.68
24	B	607[B]	CLA	C3B-C4B-NB	-3.30	107.45	110.52
26	t	101	BCR	C35-C13-C14	-3.30	118.30	122.92
24	C	512	CLA	C4-C3-C5	3.30	120.82	115.27
27	D	405	PL9	C15-C14-C16	-3.30	109.72	115.27
24	c	512	CLA	CHC-C1C-NC	3.29	129.20	124.20
24	c	504	CLA	CHC-C1C-NC	3.29	129.20	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C37-C22-C21	-3.29	118.31	122.92
24	c	505	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
26	c	521	BCR	C34-C9-C10	-3.28	118.32	122.92
24	C	507	CLA	CHC-C1C-NC	3.28	129.19	124.20
24	c	512	CLA	C4-C3-C5	3.28	120.80	115.27
24	C	509	CLA	CHC-C1C-NC	3.28	129.18	124.20
24	b	608[B]	CLA	CHC-C1C-NC	3.28	129.18	124.20
32	C	516	DGD	O1G-C1A-C2A	3.28	122.20	111.91
25	a	608	PHO	C1C-C2C-C3C	-3.28	105.88	108.61
24	D	402	CLA	CHC-C1C-NC	3.28	129.18	124.20
24	C	505	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
26	B	620	BCR	C12-C13-C14	-3.27	113.92	118.94
26	T	101	BCR	C37-C22-C21	-3.27	118.34	122.92
26	F	101	BCR	C20-C21-C22	-3.27	122.64	127.31
24	c	501	CLA	CHC-C1C-NC	3.27	129.16	124.20
24	c	511	CLA	CHC-C1C-NC	3.27	129.16	124.20
26	k	101	BCR	C23-C22-C21	-3.26	113.94	118.94
26	K	101	BCR	C11-C12-C13	-3.26	117.27	126.42
24	a	607	CLA	C1D-ND-C4D	-3.25	104.02	106.33
24	C	502	CLA	CHC-C1C-NC	3.25	129.14	124.20
24	c	509	CLA	O1D-CGD-CBD	-3.25	117.83	124.48
24	b	614	CLA	C4-C3-C5	3.25	120.74	115.27
24	a	606	CLA	O2D-CGD-CBD	3.25	117.04	111.27
24	b	604	CLA	CHC-C1C-NC	3.25	129.13	124.20
26	h	101	BCR	C20-C19-C18	-3.25	117.30	126.42
24	b	614	CLA	CHC-C1C-NC	3.25	129.13	124.20
24	B	611	CLA	C4A-NA-C1A	-3.25	105.25	106.71
26	h	101	BCR	C37-C22-C21	-3.24	118.38	122.92
24	B	614	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	b	604	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
26	K	101	BCR	C23-C24-C25	-3.24	118.10	127.20
24	C	501	CLA	O2A-CGA-CBA	3.24	122.06	111.91
26	t	101	BCR	C16-C15-C14	-3.24	116.85	123.47
26	T	101	BCR	C16-C15-C14	-3.23	116.85	123.47
24	B	603	CLA	C3A-C2A-C1A	3.23	106.18	101.34
26	t	101	BCR	C38-C26-C27	-3.23	107.42	113.62
24	B	615	CLA	C1D-ND-C4D	-3.22	104.05	106.33
26	K	101	BCR	C37-C22-C21	-3.22	118.41	122.92
26	T	101	BCR	C33-C5-C4	-3.22	107.43	113.62
24	c	502	CLA	CHC-C1C-NC	3.22	129.09	124.20
26	K	101	BCR	C33-C5-C4	-3.22	107.44	113.62
28	x	101	SQD	O7-S-C6	3.22	110.76	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	606	CLA	O1D-CGD-CBD	-3.21	117.91	124.48
24	B	613	CLA	C4-C3-C5	3.21	120.68	115.27
24	C	513	CLA	C3B-C4B-NB	-3.21	107.53	110.52
27	D	405	PL9	C7-C3-C2	-3.21	119.08	123.30
27	D	405	PL9	C31-C29-C28	-3.21	114.62	121.12
24	B	608	CLA	CHB-C4A-NA	-3.21	120.08	124.51
25	D	401	PHO	CBA-CAA-C2A	-3.21	104.44	113.81
25	D	401	PHO	C4D-CHA-CBD	-3.21	107.07	108.52
24	B	613	CLA	CBA-CAA-C2A	-3.21	104.40	113.86
24	C	509	CLA	O2D-CGD-CBD	3.20	116.96	111.27
24	b	615	CLA	C4A-NA-C1A	-3.20	105.27	106.71
24	c	512	CLA	C1-O2A-CGA	3.20	124.83	116.44
26	b	621	BCR	C20-C19-C18	-3.20	117.44	126.42
26	b	619	BCR	C27-C26-C25	-3.20	118.09	122.73
24	B	603	CLA	C4-C3-C5	3.19	120.64	115.27
26	k	101	BCR	C33-C5-C4	-3.19	107.48	113.62
26	b	621	BCR	C7-C8-C9	-3.19	121.41	126.23
24	b	604	CLA	C3B-C4B-NB	-3.19	107.56	110.52
26	k	101	BCR	C37-C22-C21	-3.19	118.46	122.92
24	B	613	CLA	C4D-C3D-CAD	-3.18	104.34	108.10
26	b	619	BCR	C30-C25-C24	-3.18	106.78	115.78
24	C	510	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
24	b	617	CLA	C1D-ND-C4D	-3.18	104.08	106.33
24	b	614	CLA	C4A-NA-C1A	-3.17	105.28	106.71
24	B	602	CLA	O2A-CGA-CBA	3.17	121.86	111.91
28	X	101	SQD	O7-S-C6	3.17	110.71	106.94
24	b	606	CLA	CHC-C1C-NC	3.17	129.01	124.20
24	d	402	CLA	CHC-C1C-NC	3.17	129.01	124.20
24	D	403	CLA	CHC-C1C-NC	3.17	129.01	124.20
24	C	513	CLA	C4D-C3D-CAD	-3.16	104.37	108.10
24	C	510	CLA	CHC-C1C-NC	3.16	129.00	124.20
24	c	504	CLA	C1-O2A-CGA	3.16	124.74	116.44
26	T	101	BCR	C38-C26-C27	-3.16	107.54	113.62
32	C	516	DGD	O6D-C5D-C4D	-3.16	103.96	109.69
24	B	609	CLA	CHD-C4C-C3C	3.16	129.48	124.84
24	b	604	CLA	C4-C3-C5	3.16	120.58	115.27
32	d	405	DGD	C4E-C3E-C2E	3.16	116.33	110.82
24	d	403	CLA	C4D-C3D-CAD	-3.15	104.38	108.10
23	A	605	BCT	O2-C-O1	-3.15	111.37	119.55
26	a	610	BCR	C11-C12-C13	-3.15	117.57	126.42
24	a	607	CLA	C4-C3-C5	3.15	120.57	115.27
32	C	516	DGD	C3E-C4E-C5E	3.15	115.86	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d	404	PL9	C7-C3-C2	-3.15	119.16	123.30
24	a	609	CLA	C4A-NA-C1A	-3.15	105.29	106.71
26	b	620	BCR	C20-C19-C18	-3.15	117.58	126.42
24	B	607[A]	CLA	C1-O2A-CGA	3.14	124.69	116.44
24	b	604	CLA	CHB-C4A-NA	-3.14	120.17	124.51
26	A	610	BCR	C38-C26-C27	-3.14	107.58	113.62
33	v	201	HEM	C1B-NB-C4B	3.14	108.31	105.07
24	D	404	CLA	O1D-CGD-CBD	-3.13	118.07	124.48
24	A	607	CLA	C4-C3-C5	3.13	120.54	115.27
24	B	606	CLA	CHC-C1C-NC	3.13	128.95	124.20
26	B	619	BCR	C27-C26-C25	-3.13	118.19	122.73
24	C	513	CLA	C2A-C1A-CHA	3.13	129.33	123.86
30	d	406	LHG	C5-O7-C7	-3.13	110.10	117.79
28	a	614	SQD	O6-C1-C2	3.13	113.18	108.30
29	A	613	LMG	O7-C10-C11	3.12	118.23	111.50
24	C	513	CLA	C4D-CHA-C1A	-3.12	117.45	121.25
24	B	608	CLA	CHC-C1C-NC	3.12	128.94	124.20
24	c	507	CLA	C4-C3-C5	3.12	120.52	115.27
27	D	405	PL9	C26-C24-C23	-3.12	114.80	121.12
24	C	505	CLA	C4D-C3D-CAD	-3.12	104.42	108.10
25	d	401	PHO	CMA-C3A-C4A	-3.12	107.54	114.38
24	D	404	CLA	CHC-C1C-NC	3.12	128.94	124.20
32	C	516	DGD	O2G-C1B-C2B	3.12	118.22	111.50
24	C	506	CLA	C4-C3-C5	3.12	120.52	115.27
24	D	403	CLA	CMC-C2C-C1C	3.12	129.79	125.04
24	B	606	CLA	C1D-ND-C4D	-3.12	104.12	106.33
24	b	612	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
29	B	621	LMG	C6-C5-C4	-3.11	105.72	113.00
28	X	101	SQD	O9-S-C6	3.10	110.63	106.94
24	b	608[A]	CLA	CHC-C1C-NC	3.10	128.91	124.20
24	B	609	CLA	O1D-CGD-CBD	-3.10	118.14	124.48
24	c	505	CLA	C2B-C1B-NB	-3.10	108.15	110.23
24	c	501	CLA	C4A-NA-C1A	-3.10	105.31	106.71
26	H	101	BCR	C8-C9-C10	-3.10	114.19	118.94
24	B	613	CLA	C2A-C1A-CHA	3.09	129.27	123.86
29	b	622	LMG	O7-C10-C11	3.09	118.17	111.50
24	c	506	CLA	C4-C3-C5	3.09	120.47	115.27
24	d	403	CLA	CHA-C1A-NA	-3.09	119.33	126.40
24	b	607	CLA	CHC-C1C-NC	3.08	128.88	124.20
24	B	611	CLA	C4D-C3D-CAD	-3.08	104.46	108.10
26	f	101	BCR	C36-C18-C19	3.08	122.93	118.08
28	x	101	SQD	O9-S-C6	3.08	110.60	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H	101	BCR	C35-C13-C14	-3.08	118.61	122.92
24	B	612	CLA	C2A-C1A-CHA	3.08	129.24	123.86
24	A	606	CLA	O2A-CGA-CBA	3.08	121.56	111.91
26	f	101	BCR	C34-C9-C10	-3.08	118.61	122.92
24	C	507	CLA	O2A-CGA-CBA	3.08	121.56	111.91
27	a	611	PL9	C53-C6-C1	3.08	121.28	114.99
24	B	608	CLA	O2D-CGD-CBD	3.07	116.73	111.27
27	d	404	PL9	C7-C3-C4	3.07	119.37	116.88
26	I	101	BCR	C15-C14-C13	-3.07	122.93	127.31
24	b	617	CLA	C2A-C1A-CHA	3.07	129.22	123.86
24	b	614	CLA	CHA-C1A-NA	-3.07	119.37	126.40
24	C	507	CLA	C2D-C1D-ND	3.07	112.36	110.10
24	B	604	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
28	A	614	SQD	O6-C1-C2	3.06	113.09	108.30
29	b	622	LMG	C6-C5-C4	-3.06	105.83	113.00
24	b	610	CLA	C4A-NA-C1A	-3.06	105.33	106.71
24	a	615	CLA	O1D-CGD-CBD	-3.06	118.22	124.48
24	B	612	CLA	CHA-C1A-NA	-3.06	119.39	126.40
26	H	101	BCR	C10-C11-C12	-3.06	113.67	123.22
32	E	101	DGD	C3E-C4E-C5E	3.06	115.69	110.24
24	B	610	CLA	C4D-C3D-CAD	-3.05	104.50	108.10
27	D	405	PL9	C36-C34-C33	-3.05	114.94	121.12
24	b	613	CLA	C1-O2A-CGA	3.05	124.45	116.44
24	B	617	CLA	O2A-CGA-CBA	3.05	121.48	111.91
24	c	507	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	B	604	CLA	CHC-C1C-NC	3.05	128.83	124.20
26	b	620	BCR	C34-C9-C10	-3.05	118.65	122.92
26	B	620	BCR	C23-C24-C25	-3.05	118.65	127.20
24	B	611	CLA	CHC-C1C-NC	3.05	128.82	124.20
25	a	608	PHO	C2B-C1B-NB	-3.05	107.42	109.53
24	C	507	CLA	C4-C3-C5	3.04	120.39	115.27
24	b	610	CLA	C3B-C4B-NB	-3.04	107.69	110.52
24	B	612	CLA	O1D-CGD-CBD	-3.04	118.26	124.48
24	C	504	CLA	C4-C3-C5	3.04	120.38	115.27
26	A	610	BCR	C27-C26-C25	-3.04	118.32	122.73
26	F	101	BCR	C12-C13-C14	-3.03	114.29	118.94
32	c	517	DGD	O6D-C5D-C4D	-3.03	104.19	109.69
27	a	611	PL9	C51-C49-C48	-3.03	113.90	122.65
24	b	603	CLA	CHA-C1A-NA	-3.03	119.47	126.40
24	B	604	CLA	C4-C3-C5	3.03	120.36	115.27
24	A	609	CLA	C4A-NA-C1A	-3.03	105.35	106.71
24	b	605	CLA	C4-C3-C5	3.02	120.36	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	515	BCR	C36-C18-C17	-3.02	118.69	122.92
26	c	521	BCR	C33-C5-C4	-3.02	107.81	113.62
26	c	514	BCR	C3-C4-C5	-3.02	108.69	114.08
24	B	611	CLA	O2A-CGA-CBA	3.02	121.38	111.91
24	b	618	CLA	C2A-C1A-CHA	3.02	129.13	123.86
24	B	609	CLA	CAC-C3C-C2C	-3.01	122.37	127.53
24	a	609	CLA	C1-O2A-CGA	3.01	124.35	116.44
24	C	504	CLA	C4D-C3D-CAD	-3.01	104.55	108.10
24	b	612	CLA	O2A-CGA-CBA	3.01	121.36	111.91
25	a	608	PHO	O1D-CGD-CBD	3.01	129.75	124.74
32	c	517	DGD	O1G-C1A-C2A	3.01	121.34	111.91
24	c	504	CLA	C4-C3-C5	3.00	120.33	115.27
30	A	615	LHG	O8-C23-O10	-3.00	116.01	123.59
24	C	503	CLA	CHC-C1C-NC	3.00	128.76	124.20
24	c	506	CLA	C4A-NA-C1A	-2.99	105.36	106.71
24	c	513	CLA	C4D-C3D-CAD	-2.99	104.57	108.10
24	B	611	CLA	O2D-CGD-CBD	2.99	116.58	111.27
29	Z	101	LMG	O2-C2-C3	-2.99	103.44	110.35
24	b	606	CLA	C4D-C3D-CAD	-2.99	104.57	108.10
24	C	510	CLA	CHA-C1A-NA	-2.99	119.56	126.40
26	t	101	BCR	C20-C21-C22	-2.99	123.05	127.31
24	C	505	CLA	CHC-C1C-NC	2.99	128.73	124.20
26	c	515	BCR	C24-C25-C26	-2.99	114.23	121.46
24	C	511	CLA	C1-O2A-CGA	2.98	124.27	116.44
24	B	617	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
30	A	615	LHG	C5-O7-C7	-2.98	110.45	117.79
24	C	509	CLA	C4D-C3D-CAD	-2.98	104.58	108.10
24	B	612	CLA	C4D-C3D-CAD	-2.98	104.58	108.10
24	c	502	CLA	O1D-CGD-CBD	-2.98	118.39	124.48
24	B	612	CLA	CHC-C1C-NC	2.98	128.72	124.20
24	b	604	CLA	C4D-C3D-CAD	-2.98	104.59	108.10
26	a	610	BCR	C33-C5-C4	-2.98	107.90	113.62
26	c	514	BCR	C31-C1-C6	-2.97	105.48	110.30
24	c	505	CLA	O2A-C1-C2	2.97	116.44	108.64
24	c	511	CLA	C1D-ND-C4D	-2.96	104.23	106.33
24	C	506	CLA	CHC-C1C-NC	2.96	128.70	124.20
24	C	504	CLA	CHC-C1C-NC	2.96	128.70	124.20
24	d	402	CLA	C3C-C4C-NC	-2.96	107.25	110.57
26	t	101	BCR	C2-C1-C6	2.96	115.04	110.48
24	D	403	CLA	O2A-CGA-CBA	2.96	121.19	111.91
24	b	613	CLA	CHA-C1A-NA	-2.96	119.63	126.40
26	b	620	BCR	C35-C13-C14	-2.96	118.78	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C1D-ND-C4D	-2.96	104.23	106.33
24	B	607[B]	CLA	C1-O2A-CGA	2.96	124.20	116.44
30	D	406	LHG	O7-C7-C8	2.95	117.86	111.50
26	t	101	BCR	C36-C18-C17	-2.95	118.79	122.92
24	A	607	CLA	CHA-C1A-NA	-2.95	119.64	126.40
24	a	606	CLA	CHA-C1A-NA	-2.95	119.65	126.40
26	B	620	BCR	C1-C6-C7	-2.95	107.44	115.78
24	b	605	CLA	CHA-C1A-NA	-2.95	119.65	126.40
24	B	608	CLA	C1-C2-C3	-2.94	120.95	126.04
24	a	615	CLA	CHC-C1C-C2C	-2.94	118.55	126.73
24	B	616	CLA	C3B-C4B-NB	-2.94	107.78	110.52
24	b	618	CLA	C4D-C3D-CAD	-2.94	104.63	108.10
28	a	614	SQD	O48-C23-C24	2.94	121.13	111.91
24	B	607[B]	CLA	C4-C3-C5	2.94	120.21	115.27
28	X	101	SQD	O48-C23-C24	2.94	121.12	111.91
24	b	610	CLA	CHC-C1C-NC	2.94	128.66	124.20
26	H	101	BCR	C33-C5-C4	-2.94	107.98	113.62
28	x	101	SQD	O48-C23-C24	2.93	121.11	111.91
24	b	608[B]	CLA	C4-C3-C5	2.93	120.20	115.27
29	C	518	LMG	C4-C3-C2	2.93	115.94	110.82
24	a	607	CLA	CMD-C2D-C1D	2.93	129.88	124.71
24	b	610	CLA	C4D-C3D-CAD	-2.93	104.65	108.10
32	C	516	DGD	C1D-O6D-C5D	-2.92	107.95	113.69
24	B	613	CLA	CHC-C1C-NC	2.92	128.64	124.20
27	a	611	PL9	C25-C24-C26	-2.92	110.36	115.27
25	D	401	PHO	C1-C2-C3	-2.92	120.99	126.04
28	A	614	SQD	O48-C23-C24	2.92	121.08	111.91
24	B	607[A]	CLA	C4-C3-C5	2.92	120.18	115.27
32	C	516	DGD	C4E-C3E-C2E	2.92	115.92	110.82
24	A	609	CLA	O1D-CGD-CBD	-2.92	118.51	124.48
26	a	610	BCR	C23-C24-C25	-2.92	119.01	127.20
26	F	101	BCR	C37-C22-C23	-2.91	113.49	118.08
24	c	502	CLA	CED-O2D-CGD	2.91	122.52	115.94
32	C	516	DGD	O6E-C5E-C6E	2.91	113.67	106.44
32	c	516	DGD	O6D-C5D-C4D	-2.91	104.41	109.69
24	C	505	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
24	b	617	CLA	C3B-C4B-NB	-2.91	107.82	110.52
24	b	609	CLA	CHC-C1C-NC	2.91	128.62	124.20
26	H	101	BCR	C34-C9-C8	2.91	122.66	118.08
24	b	616	CLA	CHC-C1C-NC	2.91	128.61	124.20
26	A	610	BCR	C20-C19-C18	-2.91	118.25	126.42
27	d	404	PL9	C45-C44-C46	-2.91	110.38	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	609	CLA	C1-C2-C3	-2.90	121.02	126.04
24	c	507	CLA	O2A-CGA-CBA	2.90	121.02	111.91
24	B	611	CLA	C1D-ND-C4D	-2.90	104.27	106.33
24	B	616	CLA	O2A-CGA-CBA	2.90	121.02	111.91
24	b	608[A]	CLA	C1-O2A-CGA	2.90	124.05	116.44
25	d	401	PHO	C1-C2-C3	-2.90	121.03	126.04
33	e	102	HEM	C4C-NC-C1C	2.89	108.18	105.35
26	c	514	BCR	C19-C18-C17	2.89	123.38	118.94
29	C	518	LMG	O6-C5-C4	2.89	114.93	109.69
24	b	608[A]	CLA	O1D-CGD-CBD	-2.88	118.58	124.48
26	K	101	BCR	C24-C25-C26	-2.88	114.48	121.46
24	B	611	CLA	CED-O2D-CGD	2.88	122.45	115.94
24	b	608[A]	CLA	C4-C3-C5	2.88	120.11	115.27
24	c	506	CLA	CHC-C1C-NC	2.88	128.57	124.20
24	a	615	CLA	C4-C3-C5	2.87	120.11	115.27
24	D	403	CLA	O2D-CGD-CBD	2.87	116.37	111.27
24	B	612	CLA	C1-C2-C3	-2.87	121.08	126.04
24	D	402	CLA	C4A-NA-C1A	-2.87	105.42	106.71
24	B	617	CLA	C2A-C1A-CHA	2.87	128.88	123.86
24	c	502	CLA	C4D-C3D-CAD	-2.87	104.72	108.10
24	b	614	CLA	O2A-CGA-CBA	2.87	120.90	111.91
24	c	512	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
24	b	606	CLA	CHA-C1A-NA	-2.86	119.84	126.40
28	A	612	SQD	C45-O47-C7	-2.86	110.75	117.79
24	A	606	CLA	CHA-C1A-NA	-2.86	119.84	126.40
24	C	511	CLA	C2B-C1B-NB	-2.86	108.31	110.23
24	C	502	CLA	C4D-C3D-CAD	-2.86	104.72	108.10
24	C	505	CLA	C1-O2A-CGA	2.86	123.95	116.44
28	a	612	SQD	C45-O47-C7	-2.86	110.76	117.79
24	b	616	CLA	C1D-ND-C4D	-2.85	104.31	106.33
24	c	509	CLA	C4D-C3D-CAD	-2.85	104.73	108.10
29	c	519	LMG	O8-C28-C29	2.85	120.86	111.91
24	c	507	CLA	C1D-ND-C4D	-2.85	104.31	106.33
26	B	618	BCR	C29-C30-C25	2.85	114.86	110.48
24	B	608	CLA	C4-C3-C5	2.85	120.06	115.27
24	b	613	CLA	C1-C2-C3	-2.85	121.12	126.04
29	c	520	LMG	O8-C28-C29	2.84	120.83	111.91
24	a	606	CLA	CHB-C4A-NA	-2.84	120.58	124.51
24	D	402	CLA	C4-C3-C5	2.84	120.05	115.27
26	c	514	BCR	C10-C11-C12	-2.84	114.35	123.22
24	b	612	CLA	CHC-C1C-NC	2.84	128.51	124.20
26	B	620	BCR	C1-C6-C5	-2.84	118.62	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CHB-C1B-C2B	-2.84	119.23	127.24
24	b	612	CLA	O1D-CGD-CBD	-2.83	118.69	124.48
24	B	609	CLA	C4A-NA-C1A	-2.83	105.43	106.71
26	H	101	BCR	C20-C19-C18	-2.83	118.46	126.42
24	c	501	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	b	619	BCR	C2-C3-C4	2.83	117.70	111.38
24	D	403	CLA	CHB-C4A-NA	-2.83	120.60	124.51
24	b	615	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	c	513	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	c	512	CLA	O2A-CGA-CBA	2.83	120.77	111.91
24	a	609	CLA	CHC-C1C-NC	2.82	128.49	124.20
32	h	102	DGD	C4D-C3D-C2D	2.82	115.75	110.82
24	b	609	CLA	C4-C3-C5	2.82	120.02	115.27
24	b	618	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
32	C	517	DGD	C3G-C2G-C1G	-2.82	105.12	111.79
24	B	614	CLA	CHC-C1C-C2C	-2.81	118.91	126.73
24	B	611	CLA	CMA-C3A-C4A	-2.81	104.22	111.77
24	B	616	CLA	C1D-ND-C4D	-2.81	104.34	106.33
32	E	101	DGD	C1E-C2E-C3E	2.81	115.84	110.00
24	c	505	CLA	CHC-C1C-NC	2.81	128.46	124.20
24	d	403	CLA	O2A-CGA-CBA	2.81	120.72	111.91
24	b	611	CLA	CHC-C1C-NC	2.81	128.46	124.20
24	c	504	CLA	C4D-C3D-CAD	-2.81	104.79	108.10
24	b	611	CLA	O2A-CGA-CBA	2.80	120.70	111.91
24	b	605	CLA	C4D-C3D-CAD	-2.80	104.79	108.10
26	k	101	BCR	C35-C13-C14	-2.80	119.00	122.92
24	c	501	CLA	O2A-CGA-CBA	2.80	120.70	111.91
28	a	612	SQD	C44-O6-C1	-2.80	108.27	113.74
26	C	514	BCR	C37-C22-C21	-2.80	119.00	122.92
24	b	613	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
26	B	618	BCR	C30-C25-C24	-2.79	107.88	115.78
28	l	101	SQD	C1-O5-C5	-2.79	108.21	113.69
24	B	617	CLA	C2B-C1B-NB	-2.79	108.36	110.23
24	c	508	CLA	CHB-C1B-C2B	-2.79	119.37	127.24
24	b	606	CLA	CED-O2D-CGD	2.79	122.24	115.94
26	f	101	BCR	C19-C18-C17	2.78	123.21	118.94
28	L	102	SQD	C1-O5-C5	-2.78	108.22	113.69
26	b	621	BCR	C23-C24-C25	-2.78	119.39	127.20
28	A	612	SQD	C44-O6-C1	-2.78	108.31	113.74
27	d	404	PL9	C30-C29-C31	-2.78	110.60	115.27
24	b	605	CLA	C1-O2A-CGA	2.78	123.73	116.44
24	d	402	CLA	O2D-CGD-O1D	-2.78	118.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	502	CLA	C1D-ND-C4D	-2.78	104.36	106.33
24	c	513	CLA	C1D-ND-C4D	-2.78	104.36	106.33
26	I	101	BCR	C1-C6-C7	-2.78	107.93	115.78
24	B	604	CLA	C4D-C3D-CAD	-2.77	104.83	108.10
33	V	201	HEM	C1D-C2D-C3D	-2.77	104.04	106.96
24	b	605	CLA	CED-O2D-CGD	2.77	122.20	115.94
30	D	406	LHG	O8-C23-C24	2.77	120.58	111.91
24	b	606	CLA	C4-C3-C5	2.76	119.92	115.27
24	C	508	CLA	C4-C3-C5	2.76	119.92	115.27
24	c	507	CLA	C4D-C3D-CAD	-2.76	104.84	108.10
24	c	508	CLA	C4-C3-C5	2.76	119.91	115.27
24	C	506	CLA	CHB-C1B-C2B	-2.76	119.45	127.24
24	b	608[B]	CLA	C1-O2A-CGA	2.76	123.68	116.44
25	d	401	PHO	O1D-CGD-CBD	2.76	129.33	124.74
25	D	401	PHO	O1D-CGD-CBD	2.76	129.33	124.74
24	c	507	CLA	CHC-C1C-C2C	-2.75	119.09	126.73
24	B	609	CLA	C4D-C3D-CAD	-2.75	104.85	108.10
25	a	608	PHO	C1-C2-C3	-2.75	121.29	126.04
24	b	609	CLA	CMD-C2D-C1D	2.75	129.56	124.71
24	C	513	CLA	O2A-CGA-CBA	2.75	120.53	111.91
24	D	402	CLA	C4D-C3D-CAD	-2.75	104.86	108.10
24	b	611	CLA	CED-O2D-CGD	2.75	122.15	115.94
24	C	506	CLA	CHB-C4A-NA	-2.75	120.72	124.51
24	b	610	CLA	C1D-ND-C4D	-2.74	104.39	106.33
24	B	614	CLA	C4A-NA-C1A	-2.74	105.47	106.71
24	B	608	CLA	C1D-ND-C4D	-2.74	104.39	106.33
24	B	605	CLA	C4-C3-C5	2.74	119.89	115.27
24	c	513	CLA	CHC-C1C-NC	2.74	128.36	124.20
27	A	611	PL9	C53-C6-C1	2.74	120.59	114.99
24	B	608	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
28	B	622	SQD	O48-C23-C24	2.74	120.50	111.91
24	A	609	CLA	C4D-C3D-CAD	-2.74	104.87	108.10
24	C	502	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
27	D	405	PL9	C40-C39-C41	-2.73	110.68	115.27
26	b	620	BCR	C10-C11-C12	-2.73	114.71	123.22
24	c	513	CLA	C4A-NA-C1A	-2.72	105.48	106.71
24	B	603	CLA	C4D-C3D-CAD	-2.72	104.89	108.10
24	b	616	CLA	C4D-C3D-CAD	-2.72	104.89	108.10
28	b	601	SQD	O48-C23-C24	2.72	120.44	111.91
30	E	102	LHG	O8-C23-C24	2.72	120.44	111.91
24	b	615	CLA	C4D-C3D-CAD	-2.72	104.89	108.10
30	l	102	LHG	O8-C23-C24	2.72	120.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	O1D-CGD-CBD	-2.72	118.93	124.48
30	D	406	LHG	C5-O7-C7	-2.71	111.11	117.79
28	L	102	SQD	O48-C23-C24	2.71	120.42	111.91
26	H	101	BCR	C19-C18-C17	2.71	123.10	118.94
26	T	101	BCR	C1-C6-C5	-2.71	118.80	122.61
25	D	401	PHO	O2D-CGD-CBD	2.71	114.43	111.00
24	c	506	CLA	C4D-C3D-CAD	-2.71	104.90	108.10
28	l	101	SQD	O48-C23-C24	2.71	120.41	111.91
24	c	509	CLA	CED-O2D-CGD	2.71	122.06	115.94
24	B	614	CLA	C1D-ND-C4D	-2.71	104.41	106.33
29	b	622	LMG	O8-C28-C29	2.71	120.40	111.91
24	C	504	CLA	CED-O2D-CGD	2.71	122.06	115.94
26	A	610	BCR	C24-C25-C26	-2.70	114.91	121.46
26	h	101	BCR	C11-C12-C13	-2.70	118.82	126.42
24	b	612	CLA	CHB-C4A-NA	-2.70	120.78	124.51
24	b	618	CLA	CHA-C1A-NA	-2.70	120.21	126.40
24	D	403	CLA	CHA-C1A-NA	-2.70	120.21	126.40
26	b	621	BCR	C34-C9-C10	-2.70	119.14	122.92
24	C	507	CLA	C3B-C4B-NB	-2.70	108.01	110.52
24	C	512	CLA	O2A-CGA-CBA	2.70	120.37	111.91
24	c	513	CLA	CHB-C1B-C2B	-2.70	119.62	127.24
24	B	603	CLA	CHC-C4B-NB	-2.69	121.40	124.26
24	D	403	CLA	C4-C3-C5	2.69	119.80	115.27
24	c	503	CLA	C4-C3-C5	2.69	119.80	115.27
26	I	101	BCR	C24-C25-C26	-2.69	114.94	121.46
26	B	618	BCR	C36-C18-C19	2.69	122.32	118.08
28	L	102	SQD	O8-S-C6	2.69	110.03	105.74
28	b	601	SQD	O9-S-C6	2.69	110.14	106.94
24	D	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	e	101	LHG	O8-C23-C24	2.69	120.35	111.91
26	K	101	BCR	C35-C13-C12	2.69	122.31	118.08
24	c	503	CLA	CHC-C1C-NC	2.69	128.28	124.20
24	c	512	CLA	CHA-C1A-NA	-2.69	120.24	126.40
25	d	401	PHO	O2D-CGD-O1D	-2.69	118.58	123.84
24	a	607	CLA	O2D-CGD-CBD	2.69	116.04	111.27
24	a	606	CLA	O2A-CGA-CBA	2.69	120.34	111.91
28	b	601	SQD	C4-C3-C2	2.68	115.50	110.82
26	K	102	BCR	C16-C15-C14	-2.68	117.98	123.47
24	b	603	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
30	d	406	LHG	O8-C23-C24	2.68	120.32	111.91
25	A	608	PHO	C1C-C2C-C3C	-2.68	106.38	108.61
24	c	511	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	504	CLA	C1D-ND-C4D	-2.68	104.43	106.33
24	B	611	CLA	CHB-C1B-C2B	-2.68	119.67	127.24
24	b	612	CLA	C4D-C3D-CAD	-2.68	104.94	108.10
24	C	508	CLA	CHB-C1B-C2B	-2.68	119.68	127.24
28	B	622	SQD	O9-S-C6	2.68	110.12	106.94
24	B	603	CLA	C3B-C4B-NB	-2.68	108.03	110.52
32	c	518	DGD	C3G-O3G-C1D	-2.68	108.51	113.74
29	c	520	LMG	C3-C4-C5	2.67	115.01	110.24
28	B	622	SQD	C4-C3-C2	2.67	115.49	110.82
24	d	402	CLA	C4-C3-C5	2.67	119.76	115.27
24	b	607	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	C	508	CLA	CED-O2D-CGD	2.67	121.97	115.94
24	b	607	CLA	C3B-C4B-NB	-2.67	108.04	110.52
24	b	617	CLA	C4D-C3D-CAD	-2.67	104.95	108.10
24	B	607[A]	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
24	b	618	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	c	511	CLA	O2A-CGA-CBA	2.67	120.28	111.91
24	B	611	CLA	C3B-C4B-NB	-2.67	108.04	110.52
24	b	603	CLA	O2A-CGA-CBA	2.66	120.27	111.91
24	A	606	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
28	l	101	SQD	O8-S-C6	2.66	109.98	105.74
24	C	503	CLA	C4-C3-C5	2.66	119.75	115.27
26	c	515	BCR	C1-C6-C7	-2.66	108.24	115.78
26	I	101	BCR	C8-C9-C10	2.66	123.03	118.94
32	c	518	DGD	C2G-O2G-C1B	-2.66	111.24	117.79
24	b	608[B]	CLA	C1-C2-C3	-2.66	121.45	126.04
24	A	606	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
26	b	619	BCR	C36-C18-C19	2.66	122.26	118.08
24	D	404	CLA	C4D-C3D-CAD	-2.65	104.97	108.10
24	C	513	CLA	CHA-C1A-NA	-2.65	120.32	126.40
32	E	101	DGD	O1G-C1A-C2A	2.65	120.23	111.91
24	b	608[B]	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
25	A	608	PHO	O2D-CGD-O1D	-2.65	118.66	123.84
24	B	602	CLA	CHB-C1B-C2B	-2.65	119.76	127.24
24	d	402	CLA	O2A-CGA-CBA	2.65	120.21	111.91
24	B	607[B]	CLA	C1-C2-C3	-2.65	121.47	126.04
26	b	619	BCR	C33-C5-C4	-2.65	108.53	113.62
26	C	514	BCR	C12-C13-C14	-2.65	114.88	118.94
30	D	407	LHG	O8-C23-C24	2.64	120.20	111.91
24	C	509	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
27	d	404	PL9	C15-C14-C16	-2.64	110.83	115.27
24	B	611	CLA	O2A-CGA-O1A	-2.64	116.93	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	407	LHG	C5-O7-C7	-2.64	111.30	117.79
26	c	521	BCR	C7-C8-C9	-2.64	122.25	126.23
24	b	607	CLA	C1D-ND-C4D	-2.64	104.46	106.33
24	C	513	CLA	CED-O2D-CGD	2.63	121.89	115.94
24	b	608[A]	CLA	CHA-C1A-NA	-2.63	120.37	126.40
24	c	509	CLA	O2A-CGA-CBA	2.63	120.16	111.91
24	A	607	CLA	C1D-ND-C4D	-2.63	104.47	106.33
24	B	606	CLA	CED-O2D-CGD	2.63	121.88	115.94
26	c	514	BCR	C29-C30-C25	2.63	114.53	110.48
24	c	504	CLA	C2D-C1D-ND	2.62	112.04	110.10
24	C	513	CLA	CHC-C1C-NC	2.62	128.18	124.20
24	C	511	CLA	CED-O2D-CGD	2.62	121.87	115.94
26	t	101	BCR	C30-C25-C24	-2.62	108.36	115.78
24	c	502	CLA	C4-C3-C5	2.62	119.68	115.27
24	C	508	CLA	C4A-NA-C1A	-2.62	105.53	106.71
26	T	101	BCR	C20-C19-C18	-2.62	119.06	126.42
32	d	405	DGD	O1G-C1A-C2A	2.62	120.13	111.91
26	t	101	BCR	C29-C30-C25	2.62	114.51	110.48
26	h	101	BCR	C30-C25-C24	-2.62	108.37	115.78
24	c	506	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	C	501	CLA	CHD-C4C-C3C	2.61	128.68	124.84
24	C	504	CLA	CHB-C1B-C2B	-2.61	119.86	127.24
24	C	511	CLA	C4-C3-C5	2.61	119.66	115.27
24	A	607	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
24	b	612	CLA	C3B-C4B-NB	-2.61	108.09	110.52
26	K	101	BCR	C16-C15-C14	-2.61	118.13	123.47
32	C	517	DGD	O2E-C2E-C3E	-2.61	104.31	110.35
24	C	509	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
24	b	609	CLA	O1D-CGD-CBD	-2.61	119.15	124.48
27	D	405	PL9	C53-C6-C1	2.61	120.32	114.99
24	b	617	CLA	C4-C3-C5	2.61	119.65	115.27
24	D	402	CLA	CHB-C1B-C2B	-2.61	119.88	127.24
24	a	609	CLA	O2A-CGA-CBA	2.60	120.08	111.91
24	b	615	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
25	a	608	PHO	CBC-CAC-C3C	-2.60	109.07	112.88
24	b	605	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
33	e	102	HEM	CHD-C4C-NC	2.60	127.25	124.44
30	D	406	LHG	O7-C7-O9	-2.59	117.43	123.70
26	B	619	BCR	C29-C30-C25	2.59	114.47	110.48
24	B	613	CLA	O2A-CGA-CBA	2.59	120.03	111.91
26	t	101	BCR	C8-C9-C10	-2.58	114.97	118.94
24	B	604	CLA	O2A-CGA-CBA	2.58	120.02	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
33	v	201	HEM	CMB-C2B-C1B	-2.58	121.11	125.04
24	B	611	CLA	O2A-C1-C2	2.58	115.42	108.64
26	k	101	BCR	C36-C18-C17	-2.58	119.31	122.92
24	c	511	CLA	C4-C3-C5	2.58	119.61	115.27
24	C	502	CLA	C4-C3-C5	2.58	119.61	115.27
24	C	509	CLA	C1-O2A-CGA	2.58	123.21	116.44
24	c	501	CLA	C4D-C3D-CAD	-2.58	105.06	108.10
24	B	616	CLA	C4-C3-C5	2.58	119.61	115.27
26	c	514	BCR	C38-C26-C27	-2.58	108.67	113.62
24	c	512	CLA	C1-C2-C3	-2.58	121.59	126.04
32	h	102	DGD	O1G-C1A-C2A	2.57	119.99	111.91
26	B	620	BCR	C33-C5-C4	-2.57	108.67	113.62
24	B	611	CLA	C4-C3-C5	2.57	119.60	115.27
33	v	201	HEM	CAA-CBA-CGA	-2.57	108.07	113.60
24	B	603	CLA	C1-O2A-CGA	2.57	123.19	116.44
24	b	615	CLA	C4-C3-C5	2.57	119.60	115.27
24	C	512	CLA	CHC-C1C-C2C	-2.57	119.59	126.73
26	c	521	BCR	C19-C18-C17	2.57	122.88	118.94
24	a	615	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
26	F	101	BCR	C34-C9-C10	-2.56	119.33	122.92
26	B	619	BCR	C36-C18-C17	-2.56	119.33	122.92
26	c	521	BCR	C29-C28-C27	2.56	117.10	111.38
24	D	402	CLA	C4D-CHA-C1A	-2.56	118.13	121.25
24	b	611	CLA	CHB-C4A-NA	-2.56	120.97	124.51
24	B	610	CLA	C1-O2A-CGA	2.56	123.16	116.44
24	B	614	CLA	C4-C3-C5	2.56	119.58	115.27
24	c	512	CLA	C2A-C1A-CHA	2.56	128.33	123.86
24	B	602	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
30	a	616	LHG	O8-C23-C24	2.56	119.93	111.91
24	b	613	CLA	CHB-C4A-NA	-2.56	120.98	124.51
24	C	502	CLA	CHA-C1A-NA	-2.55	120.55	126.40
24	b	603	CLA	CED-O2D-CGD	2.55	121.71	115.94
24	D	404	CLA	CHB-C1B-C2B	-2.55	120.03	127.24
24	D	403	CLA	C2A-C1A-CHA	2.55	128.32	123.86
32	C	515	DGD	O6D-C5D-C6D	2.55	111.81	106.67
26	c	515	BCR	C30-C25-C24	-2.55	108.57	115.78
28	a	614	SQD	O8-S-C6	2.55	109.80	105.74
26	c	514	BCR	C30-C25-C24	-2.55	108.57	115.78
29	c	520	LMG	O6-C5-C4	2.55	114.32	109.69
28	A	612	SQD	C1-O5-C5	-2.55	108.69	113.69
24	c	501	CLA	CHA-C1A-NA	-2.54	120.57	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	609	CLA	CED-O2D-CGD	2.54	121.69	115.94
26	C	514	BCR	C1-C6-C5	-2.54	119.03	122.61
24	D	402	CLA	O2A-CGA-CBA	2.54	119.88	111.91
24	b	609	CLA	CHB-C1B-C2B	-2.54	120.06	127.24
24	C	512	CLA	C1-C2-C3	-2.54	121.65	126.04
24	b	608[B]	CLA	CHA-C1A-NA	-2.54	120.58	126.40
24	b	618	CLA	CHB-C4A-NA	-2.54	121.00	124.51
24	b	615	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
26	a	610	BCR	C20-C19-C18	-2.54	119.29	126.42
28	A	614	SQD	O8-S-C6	2.53	109.78	105.74
32	c	517	DGD	O3G-C1D-C2D	2.53	112.26	108.30
24	B	607[A]	CLA	CHB-C1B-C2B	-2.53	120.08	127.24
24	B	602	CLA	CHC-C1C-NC	2.53	128.04	124.20
26	B	620	BCR	C2-C1-C6	2.53	114.38	110.48
32	c	516	DGD	C2G-O2G-C1B	-2.53	111.56	117.79
24	C	512	CLA	C4D-C3D-CAD	-2.53	105.11	108.10
24	C	513	CLA	C3C-C4C-NC	-2.53	107.73	110.57
32	c	517	DGD	O6E-C5E-C6E	2.53	112.72	106.44
29	z	101	LMG	O2-C2-C3	-2.53	104.51	110.35
24	B	609	CLA	CHB-C4A-NA	-2.53	121.02	124.51
24	a	615	CLA	CHB-C1B-C2B	-2.53	120.10	127.24
24	C	512	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
24	d	403	CLA	C4-C3-C5	2.53	119.52	115.27
24	D	404	CLA	C4-C3-C5	2.52	119.52	115.27
24	B	615	CLA	CHA-C1A-NA	-2.52	120.62	126.40
32	c	516	DGD	O3G-C3G-C2G	-2.52	104.81	110.90
24	B	606	CLA	C3B-C4B-NB	-2.52	108.17	110.52
26	T	101	BCR	C36-C18-C17	-2.52	119.39	122.92
26	t	101	BCR	C3-C4-C5	-2.52	109.57	114.08
24	b	606	CLA	O2A-CGA-CBA	2.52	119.82	111.91
24	b	610	CLA	CHB-C1B-C2B	-2.52	120.12	127.24
24	C	507	CLA	CHB-C1B-C2B	-2.52	120.12	127.24
24	B	605	CLA	C4A-NA-C1A	-2.52	105.57	106.71
25	A	608	PHO	CMA-C3A-C4A	-2.52	108.86	114.38
24	c	507	CLA	C3B-C4B-NB	-2.52	108.18	110.52
24	c	502	CLA	C1-O2A-CGA	2.51	123.04	116.44
24	C	501	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
32	E	101	DGD	C6D-C5D-C4D	-2.51	106.85	112.09
24	c	510	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
24	b	603	CLA	C1D-ND-C4D	-2.51	104.55	106.33
26	I	101	BCR	C23-C22-C21	-2.51	115.09	118.94
24	c	510	CLA	C1D-ND-C4D	-2.51	104.55	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	CHA-C1A-NA	-2.51	120.66	126.40
24	B	607[B]	CLA	CHC-C1C-C2C	-2.51	119.77	126.73
24	b	612	CLA	C4-C3-C5	2.50	119.48	115.27
24	c	505	CLA	C4D-C3D-CAD	-2.50	105.15	108.10
32	d	405	DGD	O2G-C1B-O1B	-2.50	117.66	123.70
28	a	612	SQD	C1-O5-C5	-2.50	108.78	113.69
24	B	616	CLA	CHA-C1A-NA	-2.50	120.68	126.40
24	b	604	CLA	CED-O2D-CGD	2.50	121.58	115.94
24	B	607[B]	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
24	a	606	CLA	CHC-C1C-C2C	-2.49	119.80	126.73
24	C	504	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
24	b	616	CLA	CHB-C1B-C2B	-2.49	120.20	127.24
24	C	501	CLA	C1-O2A-CGA	2.49	122.98	116.44
27	A	611	PL9	C7-C3-C2	-2.49	120.02	123.30
24	b	615	CLA	C1D-ND-C4D	-2.49	104.57	106.33
24	c	513	CLA	C3B-C4B-NB	-2.49	108.21	110.52
30	a	616	LHG	C5-O7-C7	-2.49	111.67	117.79
24	D	402	CLA	CHC-C1C-C2C	-2.49	119.82	126.73
24	C	511	CLA	CHC-C1C-C2C	-2.49	119.82	126.73
24	b	613	CLA	C4D-C3D-CAD	-2.49	105.17	108.10
26	B	618	BCR	C2-C1-C6	-2.49	106.66	110.48
24	b	612	CLA	CHC-C1C-C2C	-2.48	119.83	126.73
24	b	611	CLA	C4D-C3D-CAD	-2.48	105.17	108.10
26	A	610	BCR	C40-C30-C25	-2.48	106.27	110.30
26	c	515	BCR	C8-C9-C10	2.48	122.74	118.94
24	C	506	CLA	C4D-C3D-CAD	-2.48	105.18	108.10
25	A	608	PHO	CBC-CAC-C3C	2.48	116.50	112.88
24	c	501	CLA	C4D-CHA-C1A	-2.47	118.24	121.25
25	a	608	PHO	O2A-CGA-O1A	-2.47	117.35	123.59
24	B	613	CLA	CAC-C3C-C4C	2.47	128.02	124.81
24	b	611	CLA	C1-C2-C3	-2.47	121.77	126.04
24	D	404	CLA	C1D-ND-C4D	-2.47	104.58	106.33
24	B	604	CLA	C4A-NA-C1A	-2.47	105.60	106.71
24	B	615	CLA	CHC-C1C-NC	2.47	127.94	124.20
24	B	612	CLA	CED-O2D-CGD	2.47	121.52	115.94
24	b	608[A]	CLA	CHB-C1B-C2B	-2.47	120.27	127.24
24	C	510	CLA	C2A-C1A-CHA	2.46	128.17	123.86
26	C	514	BCR	C30-C25-C24	-2.46	108.81	115.78
32	h	102	DGD	O2G-C1B-O1B	-2.46	117.75	123.70
24	b	618	CLA	CBA-CAA-C2A	-2.46	106.59	113.86
32	E	101	DGD	O6D-C5D-C6D	2.46	111.64	106.67
26	b	621	BCR	C11-C12-C13	-2.46	119.50	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	608	PHO	C4D-ND-C1D	-2.46	106.33	108.83
24	c	502	CLA	CHB-C1B-C2B	-2.46	120.29	127.24
24	b	608[A]	CLA	C1-C2-C3	-2.46	121.79	126.04
24	B	603	CLA	CHB-C1B-C2B	-2.46	120.29	127.24
24	c	512	CLA	C4D-C3D-CAD	-2.46	105.20	108.10
24	D	403	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
24	C	512	CLA	O1D-CGD-CBD	-2.46	119.46	124.48
26	c	515	BCR	C16-C15-C14	-2.46	118.44	123.47
24	B	609	CLA	CHC-C1C-C2C	-2.46	119.91	126.73
24	b	612	CLA	CHA-C1A-NA	-2.46	120.78	126.40
33	E	103	HEM	C1D-C2D-C3D	-2.45	104.38	106.96
24	B	609	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
24	B	609	CLA	O2A-CGA-CBA	2.45	119.60	111.91
24	B	607[A]	CLA	CHC-C1C-C2C	-2.45	119.92	126.73
24	B	615	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
32	d	405	DGD	O6D-C5D-C6D	2.45	111.60	106.67
24	C	508	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
32	c	518	DGD	C3G-C2G-C1G	-2.45	106.00	111.79
24	c	504	CLA	CHA-C1A-NA	-2.45	120.80	126.40
24	b	606	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
24	C	507	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
24	d	402	CLA	C4D-C3D-CAD	-2.44	105.22	108.10
24	b	614	CLA	CAC-C3C-C4C	2.44	127.98	124.81
24	B	604	CLA	CHA-C1A-NA	-2.44	120.81	126.40
29	D	408	LMG	O7-C10-O9	-2.44	117.80	123.70
24	B	612	CLA	C3B-C4B-NB	-2.44	108.25	110.52
24	b	604	CLA	CHA-C1A-NA	-2.44	120.81	126.40
24	C	513	CLA	C4-C3-C5	2.44	119.37	115.27
24	c	513	CLA	C4-C3-C5	2.44	119.37	115.27
24	C	501	CLA	C1D-ND-C4D	-2.44	104.60	106.33
24	b	603	CLA	CHC-C1C-C2C	-2.44	119.96	126.73
26	A	610	BCR	C34-C9-C8	2.43	121.91	118.08
26	c	514	BCR	C33-C5-C4	-2.43	108.94	113.62
24	B	605	CLA	CED-O2D-CGD	2.43	121.44	115.94
24	b	617	CLA	C1D-CHD-C4C	-2.43	120.81	126.06
26	B	619	BCR	C24-C25-C26	-2.43	115.57	121.46
26	b	619	BCR	C19-C18-C17	2.43	122.67	118.94
24	B	605	CLA	O2A-CGA-CBA	2.43	119.53	111.91
24	D	403	CLA	C1D-CHD-C4C	-2.43	120.81	126.06
24	c	513	CLA	O2A-CGA-CBA	2.43	119.53	111.91
24	B	607[A]	CLA	C1-C2-C3	-2.43	121.84	126.04
24	C	507	CLA	CHC-C1C-C2C	-2.43	119.98	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	CHB-C1B-C2B	-2.43	120.38	127.24
24	c	504	CLA	CHB-C4A-NA	-2.43	121.16	124.51
24	B	605	CLA	C1D-ND-C4D	-2.43	104.61	106.33
26	B	619	BCR	C12-C13-C14	2.42	122.66	118.94
26	T	101	BCR	C2-C1-C6	2.42	114.21	110.48
29	D	408	LMG	O8-C28-O10	-2.42	117.48	123.59
24	C	511	CLA	CHA-C1A-NA	-2.42	120.85	126.40
24	a	615	CLA	C4A-NA-C1A	-2.42	105.62	106.71
24	B	609	CLA	C3B-C4B-NB	-2.42	108.27	110.52
32	C	517	DGD	O6E-C5E-C6E	2.42	112.45	106.44
24	b	614	CLA	C1D-ND-C4D	-2.42	104.62	106.33
24	C	512	CLA	C1-O2A-CGA	2.42	122.78	116.44
26	b	621	BCR	C33-C5-C4	-2.41	108.98	113.62
24	B	610	CLA	C1-C2-C3	-2.41	121.87	126.04
29	a	613	LMG	O8-C28-C29	2.41	119.47	111.91
24	b	604	CLA	CHB-C1B-C2B	-2.41	120.43	127.24
26	K	101	BCR	C34-C9-C8	2.41	121.88	118.08
24	C	510	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
26	b	620	BCR	C34-C9-C8	2.41	121.87	118.08
24	C	501	CLA	CAC-C3C-C4C	2.40	127.93	124.81
32	C	515	DGD	O3G-C3G-C2G	-2.40	105.10	110.90
24	b	607	CLA	C4D-C3D-CAD	-2.40	105.26	108.10
24	c	511	CLA	CHA-C1A-NA	-2.40	120.90	126.40
24	b	608[B]	CLA	CHB-C1B-C2B	-2.40	120.45	127.24
24	a	609	CLA	C1D-ND-C4D	-2.40	104.63	106.33
24	C	503	CLA	CHA-C1A-NA	-2.40	120.90	126.40
24	B	612	CLA	C1D-ND-C4D	-2.40	104.63	106.33
24	D	402	CLA	C1D-ND-C4D	-2.40	104.63	106.33
24	C	512	CLA	CHA-C1A-NA	-2.40	120.90	126.40
24	B	608	CLA	CHC-C1C-C2C	-2.40	120.07	126.73
24	b	611	CLA	CBA-CAA-C2A	-2.40	106.79	113.86
24	c	512	CLA	C1D-ND-C4D	-2.40	104.63	106.33
26	f	101	BCR	C30-C25-C24	-2.39	109.00	115.78
24	c	508	CLA	C1D-ND-C4D	-2.39	104.63	106.33
32	H	102	DGD	C1D-C2D-C3D	2.39	114.98	110.00
26	K	101	BCR	C1-C6-C7	-2.39	109.01	115.78
24	b	618	CLA	O2A-CGA-CBA	2.39	119.42	111.91
24	d	403	CLA	C2D-C1D-ND	2.39	111.86	110.10
26	h	101	BCR	C10-C11-C12	-2.39	115.76	123.22
24	C	504	CLA	O2A-CGA-CBA	2.39	119.40	111.91
26	B	619	BCR	C40-C30-C25	2.39	114.17	110.30
24	c	502	CLA	C3B-C4B-NB	-2.39	108.30	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	C1-O2A-CGA	2.39	122.70	116.44
24	B	613	CLA	CHA-C1A-NA	-2.39	120.93	126.40
24	b	618	CLA	C2B-C1B-NB	-2.39	108.63	110.23
29	C	518	LMG	C1-C2-C3	2.38	114.96	110.00
24	C	501	CLA	CHC-C1C-NC	2.38	127.82	124.20
24	c	506	CLA	CHB-C1B-C2B	-2.38	120.51	127.24
24	c	504	CLA	C4D-CHA-C1A	-2.38	118.35	121.25
24	B	617	CLA	CED-O2D-CGD	2.38	121.32	115.94
26	h	101	BCR	C11-C10-C9	-2.38	123.91	127.31
24	b	611	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
24	B	603	CLA	C1-C2-C3	-2.38	121.93	126.04
27	d	404	PL9	C53-C6-C1	2.38	119.85	114.99
24	B	613	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	C	510	CLA	C4D-C3D-CAD	-2.38	105.30	108.10
24	c	503	CLA	CHB-C1B-C2B	-2.38	120.53	127.24
26	B	618	BCR	C1-C6-C7	-2.38	109.06	115.78
24	c	507	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
24	b	615	CLA	C2B-C1B-NB	-2.37	108.64	110.23
24	b	607	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
24	c	503	CLA	C4D-C3D-CAD	-2.37	105.30	108.10
24	B	616	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
24	D	402	CLA	CHD-C4C-C3C	2.37	128.33	124.84
24	C	501	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
24	b	608[A]	CLA	C4D-C3D-CAD	-2.37	105.30	108.10
24	b	618	CLA	C4B-CHC-C1C	-2.37	120.72	126.34
24	b	614	CLA	CHC-C1C-C2C	-2.37	120.15	126.73
24	C	509	CLA	CHA-C1A-NA	-2.37	120.98	126.40
24	b	614	CLA	CBA-CAA-C2A	-2.37	106.88	113.86
24	b	618	CLA	C3B-C4B-NB	-2.36	108.32	110.52
24	B	616	CLA	C4D-C3D-CAD	-2.36	105.31	108.10
26	B	618	BCR	C2-C3-C4	2.36	116.66	111.38
26	k	101	BCR	C12-C13-C14	-2.36	115.31	118.94
24	A	606	CLA	C1D-CHD-C4C	-2.36	120.96	126.06
24	c	513	CLA	C3C-C4C-NC	-2.36	107.92	110.57
24	B	607[B]	CLA	CHB-C1B-C2B	-2.36	120.57	127.24
24	B	602	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	C	512	CLA	CHB-C1B-C2B	-2.36	120.57	127.24
25	A	608	PHO	C1-C2-C3	-2.36	121.97	126.04
24	b	612	CLA	CED-O2D-CGD	2.36	121.27	115.94
26	c	514	BCR	C12-C13-C14	-2.36	115.33	118.94
29	B	621	LMG	C3-C4-C5	2.35	114.44	110.24
24	C	503	CLA	CHB-C1B-C2B	-2.35	120.59	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	O2A-CGA-CBA	2.35	119.29	111.91
24	B	604	CLA	CHC-C1C-C2C	-2.35	120.19	126.73
24	C	513	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
25	A	608	PHO	C3D-C4D-ND	2.35	110.92	107.72
24	B	617	CLA	C3B-C4B-NB	-2.35	108.33	110.52
30	A	615	LHG	O7-C7-O9	-2.35	118.02	123.70
26	h	101	BCR	C1-C6-C7	-2.35	109.13	115.78
24	c	504	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	C	501	CLA	CHA-C1A-NA	-2.35	121.02	126.40
24	b	615	CLA	C1-O2A-CGA	2.35	122.61	116.44
24	B	605	CLA	CHC-C1C-C2C	-2.35	120.21	126.73
24	B	603	CLA	O1D-CGD-CBD	-2.35	119.69	124.48
24	B	610	CLA	CHC-C1C-C2C	-2.35	120.22	126.73
32	c	516	DGD	O1G-C1A-O1A	-2.35	117.67	123.59
24	C	508	CLA	CHC-C1C-C2C	-2.34	120.22	126.73
24	a	615	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
24	c	504	CLA	CED-O2D-CGD	2.34	121.23	115.94
26	c	521	BCR	C16-C15-C14	-2.34	118.68	123.47
24	c	504	CLA	CHB-C1B-C2B	-2.34	120.63	127.24
24	b	605	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
24	b	604	CLA	O2A-CGA-CBA	2.34	119.25	111.91
29	A	613	LMG	O1-C1-C2	2.34	111.95	108.30
24	c	507	CLA	CHB-C1B-C2B	-2.34	120.63	127.24
24	B	602	CLA	CHA-C1A-NA	-2.34	121.04	126.40
24	c	501	CLA	C1-O2A-CGA	2.34	122.57	116.44
24	b	609	CLA	CED-O2D-CGD	2.34	121.22	115.94
24	A	606	CLA	C1-O2A-CGA	2.33	122.57	116.44
24	b	604	CLA	C1-C2-C3	-2.33	122.01	126.04
26	T	101	BCR	C1-C6-C7	-2.33	109.18	115.78
24	b	618	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
24	a	607	CLA	CHB-C1B-C2B	-2.33	120.66	127.24
24	C	513	CLA	CHB-C1B-C2B	-2.33	120.66	127.24
24	A	609	CLA	C1-O2A-CGA	2.33	122.55	116.44
29	c	519	LMG	O7-C10-O9	-2.33	118.08	123.70
24	c	501	CLA	CHC-C1C-C2C	-2.33	120.27	126.73
32	C	517	DGD	C2G-O2G-C1B	-2.33	112.06	117.79
26	f	101	BCR	C16-C15-C14	-2.32	118.71	123.47
25	A	608	PHO	O1D-CGD-CBD	2.32	128.61	124.74
24	d	403	CLA	CHB-C4A-NA	-2.32	121.30	124.51
24	B	612	CLA	CHC-C1C-C2C	-2.32	120.28	126.73
24	a	607	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
26	F	101	BCR	C8-C9-C10	2.32	122.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607[A]	CLA	O2A-CGA-CBA	2.32	119.19	111.91
32	h	102	DGD	O6D-C5D-C6D	2.32	111.35	106.67
24	B	608	CLA	C4D-C3D-CAD	-2.32	105.36	108.10
24	b	617	CLA	O2A-CGA-CBA	2.32	119.19	111.91
24	c	506	CLA	CHA-C1A-NA	-2.32	121.09	126.40
24	B	607[A]	CLA	C4D-C3D-CAD	-2.32	105.36	108.10
25	D	401	PHO	C2B-C1B-NB	-2.32	107.92	109.53
32	H	102	DGD	O5E-C6E-C5E	-2.32	103.34	111.29
24	C	511	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
24	B	606	CLA	CMD-C2D-C1D	2.31	128.79	124.71
24	C	502	CLA	CHB-C1B-C2B	-2.31	120.70	127.24
24	C	510	CLA	CHB-C1B-C2B	-2.31	120.70	127.24
24	B	616	CLA	C4A-NA-C1A	-2.31	105.67	106.71
24	D	403	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
24	d	402	CLA	CHB-C1B-C2B	-2.31	120.71	127.24
24	B	610	CLA	CED-O2D-CGD	2.31	121.16	115.94
24	B	616	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
24	c	510	CLA	CHA-C1A-NA	-2.31	121.11	126.40
25	a	608	PHO	C3D-C4D-ND	2.31	110.86	107.72
24	C	507	CLA	C4D-C3D-CAD	-2.31	105.38	108.10
24	C	504	CLA	C3C-C4C-NC	-2.31	107.98	110.57
28	a	614	SQD	C3-C4-C5	2.31	114.36	110.24
24	b	616	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
24	b	618	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
24	C	511	CLA	CHB-C4A-NA	-2.31	121.32	124.51
26	B	620	BCR	C11-C12-C13	-2.30	119.95	126.42
24	B	610	CLA	CHA-C1A-NA	-2.30	121.13	126.40
24	D	402	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
26	C	514	BCR	C11-C12-C13	-2.30	119.95	126.42
29	Z	101	LMG	O6-C5-C4	2.30	113.87	109.69
24	B	608	CLA	CHA-C1A-NA	-2.30	121.13	126.40
24	C	503	CLA	O2A-C1-C2	2.30	114.67	108.64
24	B	610	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
24	C	506	CLA	C1D-ND-C4D	-2.30	104.70	106.33
26	c	515	BCR	C35-C13-C14	-2.30	119.71	122.92
24	b	611	CLA	C3B-C4B-NB	-2.29	108.39	110.52
29	D	408	LMG	O8-C28-C29	2.29	119.11	111.91
26	t	101	BCR	C33-C5-C4	-2.29	109.21	113.62
24	b	613	CLA	C1D-ND-C4D	-2.29	104.71	106.33
24	C	507	CLA	C1-O2A-CGA	2.29	122.46	116.44
24	b	608[B]	CLA	CHC-C1C-C2C	-2.29	120.36	126.73
24	b	610	CLA	C4-C3-C5	2.29	119.12	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	404	CLA	O2A-CGA-CBA	2.29	119.09	111.91
32	d	405	DGD	C1E-C2E-C3E	2.29	114.77	110.00
24	B	607[A]	CLA	CHA-C1A-NA	-2.29	121.15	126.40
32	c	516	DGD	O6D-C5D-C6D	2.29	111.29	106.67
24	C	513	CLA	C1-O2A-CGA	2.29	122.45	116.44
24	d	402	CLA	CMA-C3A-C4A	-2.29	105.63	111.77
24	C	507	CLA	CHA-C1A-NA	-2.29	121.16	126.40
29	c	519	LMG	O6-C5-C4	2.29	113.84	109.69
24	C	505	CLA	CHD-C4C-C3C	2.28	128.20	124.84
32	E	101	DGD	O2G-C1B-O1B	-2.28	118.18	123.70
33	e	102	HEM	C1B-NB-C4B	2.28	107.43	105.07
24	B	609	CLA	C4-C3-C5	2.28	119.11	115.27
32	C	516	DGD	O1G-C1A-O1A	-2.28	117.83	123.59
30	d	407	LHG	O8-C23-C24	2.28	119.07	111.91
24	B	606	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
24	b	610	CLA	C11-C12-C13	-2.28	108.55	115.92
24	A	606	CLA	C4-C3-C5	2.28	119.11	115.27
24	A	606	CLA	C3C-C4C-NC	-2.28	108.01	110.57
25	D	401	PHO	C4A-C3A-C2A	-2.28	100.67	102.84
26	K	102	BCR	C39-C30-C25	-2.28	106.61	110.30
24	a	609	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
33	E	103	HEM	CHC-C1C-NC	2.27	126.90	124.44
24	A	606	CLA	CHB-C1B-C2B	-2.27	120.83	127.24
26	k	101	BCR	C11-C12-C13	-2.27	120.04	126.42
24	C	501	CLA	CHB-C1B-C2B	-2.27	120.83	127.24
27	a	611	PL9	C3-C4-C5	2.27	121.55	118.60
24	d	402	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
24	B	606	CLA	CHB-C1B-C2B	-2.27	120.83	127.24
24	b	613	CLA	CHB-C1B-C2B	-2.27	120.84	127.24
28	A	614	SQD	C3-C4-C5	2.26	114.28	110.24
24	C	511	CLA	C3B-C4B-NB	-2.26	108.42	110.52
30	A	615	LHG	O8-C23-C24	2.26	119.01	111.91
24	A	607	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
32	d	405	DGD	C3E-C4E-C5E	2.26	114.28	110.24
24	a	606	CLA	C2B-C1B-NB	-2.26	108.72	110.23
24	B	610	CLA	CAC-C3C-C4C	2.26	127.74	124.81
24	d	403	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
24	B	611	CLA	CHA-C1A-NA	-2.26	121.22	126.40
32	c	518	DGD	O4D-C4D-C3D	-2.26	105.13	110.35
24	C	504	CLA	CHC-C1C-C2C	-2.26	120.45	126.73
24	a	609	CLA	CED-O2D-CGD	2.26	121.05	115.94
24	B	605	CLA	CHA-C1A-NA	-2.26	121.23	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	F	101	BCR	C30-C25-C24	-2.26	109.39	115.78
24	a	607	CLA	CHC-C1C-C2C	-2.26	120.47	126.73
29	C	518	LMG	O1-C7-C8	-2.25	105.46	110.90
24	A	609	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
25	a	608	PHO	O2D-CGD-O1D	-2.25	119.43	123.84
24	B	607[B]	CLA	C3C-C4C-NC	-2.25	108.05	110.57
24	B	604	CLA	CHD-C4C-C3C	2.25	128.15	124.84
24	A	609	CLA	CHB-C1B-C2B	-2.25	120.88	127.24
24	c	504	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
24	A	609	CLA	CHC-C1C-NC	2.25	127.61	124.20
24	B	616	CLA	CHC-C1C-C2C	-2.25	120.48	126.73
24	b	608[B]	CLA	C1D-ND-C4D	-2.25	104.74	106.33
24	B	609	CLA	C11-C12-C13	-2.25	108.65	115.92
24	c	504	CLA	C3C-C4C-NC	-2.25	108.05	110.57
29	A	613	LMG	O8-C28-O10	-2.25	117.92	123.59
24	c	513	CLA	CHA-C1A-NA	-2.24	121.26	126.40
24	B	613	CLA	CHD-C4C-C3C	2.24	128.14	124.84
24	C	511	CLA	O2A-CGA-CBA	2.24	118.95	111.91
26	k	101	BCR	C20-C19-C18	-2.24	120.11	126.42
29	j	101	LMG	O8-C28-O10	-2.24	117.93	123.59
24	a	606	CLA	C4-C3-C5	2.24	119.04	115.27
29	D	408	LMG	C1-O6-C5	2.24	118.09	113.69
24	D	402	CLA	C3C-C4C-NC	-2.24	108.06	110.57
24	b	614	CLA	C2A-C1A-CHA	2.24	127.78	123.86
24	A	609	CLA	CHD-C4C-C3C	2.24	128.13	124.84
24	c	510	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
32	C	515	DGD	C3G-C2G-C1G	-2.24	106.49	111.79
26	F	101	BCR	C38-C26-C27	-2.24	109.32	113.62
24	c	503	CLA	CHA-C1A-NA	-2.24	121.27	126.40
24	b	607	CLA	CED-O2D-CGD	2.24	121.00	115.94
24	B	611	CLA	CHC-C1C-C2C	-2.24	120.52	126.73
24	B	608	CLA	CHB-C1B-C2B	-2.24	120.92	127.24
24	B	608	CLA	O2A-CGA-CBA	2.24	118.92	111.91
24	B	610	CLA	CHD-C4C-C3C	2.24	128.13	124.84
24	B	609	CLA	CHB-C1B-C2B	-2.23	120.92	127.24
32	C	516	DGD	C1E-C2E-C3E	2.23	114.65	110.00
33	V	201	HEM	C4B-C3B-C2B	-2.23	105.34	107.11
25	D	401	PHO	C3D-C4D-ND	2.23	110.76	107.72
24	c	502	CLA	CHA-C1A-NA	-2.23	121.28	126.40
24	a	606	CLA	C4D-C3D-CAD	-2.23	105.47	108.10
24	b	605	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
24	B	614	CLA	CMD-C2D-C1D	2.23	128.65	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	609	CLA	O2A-CGA-CBA	2.23	118.91	111.91
24	C	512	CLA	C2A-C1A-CHA	2.23	127.76	123.86
24	B	610	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
29	C	518	LMG	O4-C4-C5	2.23	114.83	109.30
24	A	607	CLA	CHB-C1B-C2B	-2.23	120.95	127.24
24	B	617	CLA	C4B-CHC-C1C	-2.23	121.06	126.34
24	C	503	CLA	C1D-CHD-C4C	-2.23	121.25	126.06
24	B	615	CLA	CMD-C2D-C1D	2.23	128.63	124.71
24	C	505	CLA	C4D-CHA-C1A	-2.23	118.54	121.25
33	e	102	HEM	C4A-NA-C1A	2.22	107.53	105.35
24	B	616	CLA	CED-O2D-CGD	2.22	120.96	115.94
26	f	101	BCR	C28-C27-C26	-2.22	110.11	114.08
24	C	502	CLA	CHC-C1C-C2C	-2.22	120.57	126.73
29	a	613	LMG	O8-C28-O10	-2.22	118.00	123.59
29	B	621	LMG	O7-C10-C11	2.22	116.28	111.50
24	b	603	CLA	CHB-C1B-C2B	-2.22	120.98	127.24
24	C	504	CLA	C3B-C4B-NB	-2.21	108.46	110.52
24	b	615	CLA	C1-C2-C3	-2.21	122.21	126.04
28	A	612	SQD	O48-C23-C24	2.21	118.86	111.91
28	x	101	SQD	O48-C23-O10	-2.21	118.01	123.59
24	B	609	CLA	C1D-ND-C4D	-2.21	104.76	106.33
26	B	618	BCR	C16-C15-C14	-2.21	118.94	123.47
26	A	610	BCR	C1-C6-C7	-2.21	109.52	115.78
26	C	514	BCR	C8-C9-C10	2.21	122.33	118.94
24	b	615	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	j	101	LMG	O7-C10-C11	2.21	116.26	111.50
26	c	514	BCR	C37-C22-C21	-2.21	119.83	122.92
32	c	517	DGD	O2G-C1B-O1B	-2.21	118.37	123.70
24	D	404	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
28	X	101	SQD	O48-C23-O10	-2.21	118.03	123.59
24	B	607[B]	CLA	O2A-CGA-CBA	2.20	118.83	111.91
32	E	101	DGD	O6E-C5E-C6E	2.20	111.91	106.44
33	e	102	HEM	CHC-C1C-NC	2.20	126.82	124.44
24	A	607	CLA	CHD-C4C-C3C	2.20	128.08	124.84
24	B	603	CLA	O2A-CGA-CBA	2.20	118.81	111.91
24	D	403	CLA	CED-O2D-CGD	2.20	120.91	115.94
24	B	614	CLA	C1-O2A-CGA	2.20	122.22	116.44
28	a	612	SQD	O48-C23-C24	2.20	118.81	111.91
26	I	101	BCR	C23-C24-C25	-2.20	121.03	127.20
26	T	101	BCR	C30-C25-C24	-2.20	109.56	115.78
24	C	503	CLA	CMD-C2D-C1D	2.20	128.59	124.71
24	c	509	CLA	CHC-C1C-C2C	-2.20	120.62	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Z	101	LMG	O7-C10-O9	-2.20	118.39	123.70
24	b	608[A]	CLA	CHC-C1C-C2C	-2.20	120.63	126.73
24	B	614	CLA	C1-C2-C3	-2.20	122.25	126.04
24	B	607[A]	CLA	C3C-C4C-NC	-2.20	108.11	110.57
26	B	620	BCR	C3-C4-C5	-2.19	110.16	114.08
24	B	602	CLA	C1-O2A-CGA	2.19	122.20	116.44
24	c	501	CLA	CHD-C4C-C3C	2.19	128.06	124.84
24	b	611	CLA	CHC-C4B-NB	-2.19	121.94	124.26
24	c	510	CLA	CED-O2D-CGD	2.19	120.89	115.94
24	B	614	CLA	C4B-CHC-C1C	-2.19	121.14	126.34
26	H	101	BCR	C11-C12-C13	-2.19	120.26	126.42
33	V	201	HEM	CAD-C3D-C4D	2.19	128.49	124.66
24	C	511	CLA	C1D-ND-C4D	-2.19	104.78	106.33
24	d	403	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
29	A	613	LMG	O8-C28-C29	2.19	118.78	111.91
24	c	503	CLA	O2A-CGA-CBA	2.19	118.78	111.91
29	C	518	LMG	O8-C28-O10	-2.19	118.07	123.59
24	b	609	CLA	CHA-C1A-NA	-2.19	121.39	126.40
24	C	501	CLA	C4-C3-C5	2.19	118.95	115.27
24	c	501	CLA	CED-O2D-CGD	2.18	120.88	115.94
33	E	103	HEM	CMD-C2D-C1D	2.18	128.37	125.04
24	A	607	CLA	CMD-C2D-C1D	2.18	128.56	124.71
24	C	502	CLA	C1D-ND-C4D	-2.18	104.78	106.33
24	a	606	CLA	C1D-CHD-C4C	-2.18	121.35	126.06
24	C	501	CLA	C3B-C4B-NB	-2.18	108.49	110.52
26	h	101	BCR	C2-C3-C4	2.18	116.25	111.38
26	b	620	BCR	C29-C30-C25	2.18	113.84	110.48
28	a	612	SQD	O48-C23-O10	-2.18	118.09	123.59
32	d	405	DGD	C6D-C5D-C4D	-2.18	107.54	112.09
24	c	506	CLA	O2A-CGA-CBA	2.18	118.75	111.91
26	t	101	BCR	C39-C30-C25	-2.18	106.76	110.30
24	c	501	CLA	C4-C3-C5	2.18	118.94	115.27
24	b	606	CLA	CHB-C1B-C2B	-2.18	121.09	127.24
24	c	511	CLA	CHB-C1B-C2B	-2.18	121.09	127.24
24	a	609	CLA	CHC-C1C-C2C	-2.18	120.69	126.73
24	C	511	CLA	C3C-C4C-NC	-2.17	108.13	110.57
24	b	609	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	b	617	CLA	CHC-C1C-C2C	-2.17	120.69	126.73
26	I	101	BCR	C19-C18-C17	2.17	122.27	118.94
26	B	619	BCR	C28-C27-C26	2.17	117.95	114.08
24	C	508	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	B	615	CLA	CHB-C1B-C2B	-2.17	121.11	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	620	BCR	C28-C27-C26	2.17	117.95	114.08
28	A	612	SQD	O48-C23-O10	-2.17	118.12	123.59
24	c	507	CLA	C4B-CHC-C1C	-2.17	121.20	126.34
24	c	512	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
26	T	101	BCR	C3-C4-C5	-2.17	110.21	114.08
26	f	101	BCR	C20-C19-C18	-2.17	120.33	126.42
26	c	514	BCR	C35-C13-C12	2.17	121.49	118.08
24	b	608[B]	CLA	CHD-C4C-C3C	2.17	128.02	124.84
24	c	508	CLA	C3C-C4C-NC	-2.16	108.14	110.57
24	c	509	CLA	C2D-C1D-ND	2.16	111.70	110.10
26	t	101	BCR	C1-C6-C7	-2.16	109.66	115.78
24	c	510	CLA	CMD-C2D-C1D	2.16	128.52	124.71
24	A	606	CLA	C4D-C3D-CAD	-2.16	105.55	108.10
24	B	612	CLA	CHD-C4C-C3C	2.16	128.01	124.84
30	D	407	LHG	O8-C23-O10	-2.16	118.15	123.59
29	D	408	LMG	C3-C4-C5	2.15	114.08	110.24
29	C	519	LMG	O8-C28-C29	2.15	118.66	111.91
24	B	607[B]	CLA	C1D-ND-C4D	-2.15	104.81	106.33
24	B	606	CLA	CHA-C1A-NA	-2.15	121.47	126.40
24	b	618	CLA	C4A-NA-C1A	-2.15	105.74	106.71
24	c	503	CLA	C3B-C4B-NB	-2.15	108.52	110.52
32	d	405	DGD	O1G-C1A-O1A	-2.15	118.17	123.59
24	c	508	CLA	O2A-CGA-CBA	2.15	118.65	111.91
24	c	511	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
24	B	614	CLA	CHA-C1A-NA	-2.15	121.48	126.40
24	B	611	CLA	C2D-C1D-ND	2.15	111.69	110.10
24	b	612	CLA	CHD-C4C-C3C	2.14	127.99	124.84
24	a	607	CLA	CED-O2D-CGD	2.14	120.78	115.94
24	a	609	CLA	C3B-C4B-NB	-2.14	108.53	110.52
24	b	614	CLA	CAC-C3C-C2C	-2.14	123.87	127.53
28	b	601	SQD	O47-C7-O49	-2.14	118.53	123.70
26	c	521	BCR	C23-C24-C25	-2.14	121.19	127.20
24	B	617	CLA	CAC-C3C-C4C	2.14	127.59	124.81
24	b	608[A]	CLA	O2A-CGA-CBA	2.14	118.62	111.91
24	C	506	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
24	b	607	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
26	C	514	BCR	C1-C6-C7	-2.14	109.73	115.78
29	C	519	LMG	C3-C4-C5	2.14	114.05	110.24
24	C	505	CLA	C3B-C4B-NB	-2.14	108.53	110.52
24	B	607[B]	CLA	CHA-C1A-NA	-2.14	121.51	126.40
26	C	514	BCR	C35-C13-C14	-2.14	119.93	122.92
26	T	101	BCR	C23-C22-C21	2.13	122.22	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	615	CLA	C4B-CHC-C1C	-2.13	121.28	126.34
24	B	617	CLA	CHA-C1A-NA	-2.13	121.51	126.40
24	C	505	CLA	CHA-C1A-NA	-2.13	121.51	126.40
24	B	617	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
24	C	513	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
28	B	622	SQD	O47-C7-O49	-2.13	118.55	123.70
24	B	613	CLA	CHC-C1C-C2C	-2.13	120.81	126.73
24	c	504	CLA	C7-C6-C5	-2.13	107.58	113.36
24	B	608	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
24	b	609	CLA	CHC-C4B-NB	-2.12	122.01	124.26
24	A	609	CLA	C3B-C4B-NB	-2.12	108.55	110.52
32	c	516	DGD	O2G-C1B-O1B	-2.12	118.58	123.70
24	B	608	CLA	C4D-CHA-C1A	-2.12	118.67	121.25
24	b	616	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	c	509	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	B	607[B]	CLA	C4D-C3D-CAD	-2.12	105.60	108.10
24	C	504	CLA	C7-C6-C5	-2.12	107.61	113.36
24	C	509	CLA	O2A-CGA-CBA	2.12	118.55	111.91
26	K	101	BCR	C20-C21-C22	-2.12	124.29	127.31
32	C	515	DGD	O1G-C1A-O1A	-2.11	118.25	123.59
30	L	101	LHG	O8-C23-C24	2.11	118.54	111.91
25	d	401	PHO	CMD-C2D-C3D	2.11	128.63	124.68
24	b	608[A]	CLA	C1D-ND-C4D	-2.11	104.83	106.33
24	C	512	CLA	CED-O2D-CGD	2.11	120.72	115.94
24	b	616	CLA	C3B-C4B-NB	-2.11	108.56	110.52
24	a	607	CLA	C4D-C3D-CAD	-2.11	105.61	108.10
24	C	508	CLA	C1D-ND-C4D	-2.11	104.83	106.33
28	b	601	SQD	O5-C1-C2	-2.11	105.88	110.35
24	B	603	CLA	CHC-C1C-C2C	-2.11	120.87	126.73
24	c	505	CLA	CHD-C4C-C3C	2.11	127.94	124.84
24	d	402	CLA	CHD-C4C-C3C	2.11	127.94	124.84
24	c	509	CLA	CHB-C1B-C2B	-2.11	121.28	127.24
26	c	514	BCR	C37-C22-C23	-2.11	114.76	118.08
24	C	504	CLA	CHA-C1A-NA	-2.11	121.57	126.40
24	b	618	CLA	C4-C3-C5	2.10	118.81	115.27
24	b	603	CLA	CHB-C4A-NA	-2.10	121.60	124.51
24	a	615	CLA	C4D-C3D-CAD	-2.10	105.62	108.10
24	c	509	CLA	C4-C3-C5	2.10	118.81	115.27
24	B	617	CLA	C4-C3-C5	2.10	118.81	115.27
24	C	510	CLA	CHC-C1C-C2C	-2.10	120.89	126.73
25	D	401	PHO	CMA-C3A-C4A	-2.10	109.78	114.38
24	d	403	CLA	CHB-C1B-C2B	-2.10	121.31	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	z	101	LMG	O1-C1-C2	2.10	111.58	108.30
24	A	606	CLA	C1D-ND-C4D	-2.10	104.84	106.33
28	B	622	SQD	O5-C1-C2	-2.10	105.91	110.35
30	L	101	LHG	O8-C23-O10	-2.10	118.30	123.59
24	b	612	CLA	C1D-ND-C4D	-2.10	104.85	106.33
24	c	502	CLA	CHC-C1C-C2C	-2.10	120.91	126.73
23	A	605	BCT	O3-C-O1	-2.10	114.11	119.55
24	b	614	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
24	C	501	CLA	C1-C2-C3	-2.09	122.42	126.04
24	C	510	CLA	CMD-C2D-C1D	2.09	128.40	124.71
24	C	511	CLA	C4D-C3D-CAD	-2.09	105.63	108.10
26	C	514	BCR	C3-C4-C5	-2.09	110.34	114.08
26	t	101	BCR	C19-C18-C17	2.09	122.15	118.94
24	B	605	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
24	C	512	CLA	C1D-CHD-C4C	-2.09	121.55	126.06
32	c	517	DGD	C4E-C3E-C2E	2.09	114.47	110.82
24	B	609	CLA	C11-C10-C8	-2.09	109.17	115.92
24	b	610	CLA	C11-C10-C8	-2.09	109.17	115.92
24	a	606	CLA	CBA-CAA-C2A	-2.09	107.71	113.86
24	b	618	CLA	CED-O2D-CGD	2.09	120.65	115.94
24	c	501	CLA	C1-C2-C3	-2.08	122.44	126.04
24	B	611	CLA	CHD-C4C-C3C	2.08	127.90	124.84
24	b	617	CLA	C11-C10-C8	-2.08	109.18	115.92
24	C	509	CLA	C4-C3-C5	2.08	118.77	115.27
24	c	512	CLA	CHC-C1C-C2C	-2.08	120.95	126.73
24	B	603	CLA	CHB-C4A-NA	-2.08	121.64	124.51
28	X	101	SQD	C3-C4-C5	2.08	113.95	110.24
26	b	620	BCR	C36-C18-C17	-2.08	120.01	122.92
24	B	605	CLA	C1-O2A-CGA	2.08	121.90	116.44
24	B	615	CLA	CED-O2D-CGD	2.08	120.64	115.94
24	D	403	CLA	CHC-C1C-C2C	-2.08	120.96	126.73
26	b	619	BCR	C35-C13-C14	2.08	125.83	122.92
26	B	618	BCR	C39-C30-C25	-2.08	106.93	110.30
30	a	616	LHG	C9-C8-C7	-2.07	106.08	113.62
24	D	402	CLA	C3B-C4B-NB	-2.07	108.59	110.52
24	c	504	CLA	CHC-C4B-NB	-2.07	122.06	124.26
24	b	617	CLA	CHB-C1B-C2B	-2.07	121.38	127.24
24	c	510	CLA	CHB-C1B-C2B	-2.07	121.38	127.24
24	b	605	CLA	O2A-CGA-CBA	2.07	118.41	111.91
24	B	616	CLA	C11-C10-C8	-2.07	109.23	115.92
32	h	102	DGD	O3G-C3G-C2G	-2.07	105.90	110.90
29	C	519	LMG	O6-C5-C4	2.07	113.45	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	620	BCR	C32-C1-C6	-2.07	106.94	110.30
24	C	501	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	b	620	BCR	C11-C12-C13	-2.07	120.60	126.42
33	E	103	HEM	CHD-C4C-NC	2.07	126.68	124.44
24	b	608[B]	CLA	O2A-CGA-CBA	2.07	118.40	111.91
24	b	608[B]	CLA	C3C-C4C-NC	-2.07	108.25	110.57
27	D	405	PL9	C20-C19-C21	-2.07	111.79	115.27
27	d	404	PL9	C10-C9-C11	-2.07	111.79	115.27
24	d	402	CLA	C1D-ND-C4D	-2.07	104.87	106.33
24	C	503	CLA	O2A-CGA-CBA	2.07	118.39	111.91
24	a	606	CLA	CHB-C1B-C2B	-2.07	121.40	127.24
24	A	606	CLA	C3B-C4B-NB	-2.07	108.60	110.52
29	b	622	LMG	O1-C7-C8	-2.06	105.92	110.90
24	b	610	CLA	CHB-C4A-NA	-2.06	121.66	124.51
24	B	606	CLA	CBA-CAA-C2A	-2.06	107.77	113.86
26	F	101	BCR	C28-C27-C26	-2.06	110.39	114.08
25	A	608	PHO	O2A-CGA-O1A	-2.06	118.39	123.59
33	E	103	HEM	C4C-NC-C1C	2.06	107.36	105.35
24	B	615	CLA	CHC-C1C-C2C	-2.06	121.01	126.73
26	b	620	BCR	C35-C13-C12	2.06	121.32	118.08
24	c	503	CLA	CMD-C2D-C1D	2.06	128.34	124.71
32	c	518	DGD	C3D-C4D-C5D	2.06	113.91	110.24
24	C	510	CLA	C4-C3-C5	2.06	118.73	115.27
24	b	611	CLA	CHA-C1A-NA	-2.06	121.69	126.40
24	C	506	CLA	C4A-NA-C1A	-2.06	105.78	106.71
29	j	101	LMG	O7-C10-O9	-2.05	118.74	123.70
24	B	603	CLA	C3C-C4C-NC	-2.05	108.27	110.57
24	a	606	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
28	A	612	SQD	O5-C1-C2	-2.05	106.00	110.35
26	b	621	BCR	C1-C6-C7	-2.05	109.97	115.78
29	j	101	LMG	O6-C5-C4	2.05	113.42	109.69
24	b	617	CLA	CHA-C1A-NA	-2.05	121.70	126.40
24	B	616	CLA	C3C-C4C-NC	-2.05	108.27	110.57
24	B	604	CLA	CHB-C1B-C2B	-2.05	121.45	127.24
26	f	101	BCR	C12-C13-C14	-2.05	115.80	118.94
30	a	616	LHG	O7-C7-O9	-2.05	118.75	123.70
24	C	502	CLA	O2A-CGA-CBA	2.05	118.34	111.91
26	k	101	BCR	C8-C9-C10	-2.05	115.80	118.94
28	x	101	SQD	C3-C4-C5	2.05	113.89	110.24
24	a	615	CLA	CMA-C3A-C4A	-2.05	106.27	111.77
24	b	610	CLA	CHC-C1C-C2C	-2.05	121.05	126.73
24	d	402	CLA	CHB-C4A-NA	-2.05	121.68	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	403	CLA	C6-C7-C8	-2.04	109.31	115.92
26	c	521	BCR	C36-C18-C19	-2.04	114.86	118.08
24	B	609	CLA	C4B-CHC-C1C	-2.04	121.49	126.34
24	D	402	CLA	O2D-CGD-CBD	2.04	114.90	111.27
24	a	609	CLA	C4D-C3D-CAD	-2.04	105.69	108.10
24	b	616	CLA	C1-O2A-CGA	2.04	121.80	116.44
26	H	101	BCR	C35-C13-C12	2.04	121.29	118.08
29	C	518	LMG	O6-C5-C6	2.04	111.51	106.44
32	c	518	DGD	O2G-C1B-O1B	-2.04	118.77	123.70
24	a	615	CLA	CHD-C4C-C3C	2.04	127.84	124.84
28	l	101	SQD	C4-C3-C2	2.04	114.38	110.82
24	b	608[B]	CLA	C4D-C3D-CAD	-2.04	105.69	108.10
32	c	517	DGD	C1E-O6E-C5E	-2.04	109.69	113.69
24	B	603	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	b	612	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
27	A	611	PL9	C25-C24-C26	-2.03	111.85	115.27
32	c	517	DGD	O1G-C1A-O1A	-2.03	118.46	123.59
29	b	622	LMG	C8-O7-C10	-2.03	112.78	117.79
24	b	603	CLA	CMD-C2D-C1D	2.03	128.30	124.71
28	L	102	SQD	C4-C3-C2	2.03	114.37	110.82
24	a	606	CLA	C1D-ND-C4D	-2.03	104.89	106.33
27	D	405	PL9	C3-C2-C1	-2.03	118.70	122.52
24	B	613	CLA	CHD-C1D-ND	2.03	126.32	124.45
24	B	610	CLA	CHB-C4A-NA	-2.03	121.70	124.51
24	b	613	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
28	a	612	SQD	O5-C1-C2	-2.03	106.05	110.35
24	c	508	CLA	CHC-C1C-C2C	-2.03	121.10	126.73
24	c	510	CLA	C1-O2A-CGA	2.03	121.76	116.44
24	c	510	CLA	C4-C3-C5	2.03	118.68	115.27
24	B	609	CLA	C3C-C4C-NC	-2.03	108.30	110.57
29	C	518	LMG	O7-C10-O9	-2.03	118.80	123.70
24	C	513	CLA	CMC-C2C-C1C	2.03	128.12	125.04
24	D	404	CLA	C6-C7-C8	-2.03	109.37	115.92
32	E	101	DGD	O1B-C1B-C2B	-2.03	115.83	123.73
28	L	102	SQD	O9-S-C6	2.02	109.34	106.94
32	C	516	DGD	O2G-C1B-O1B	-2.02	118.82	123.70
32	H	102	DGD	O6D-C1D-C2D	2.02	114.63	110.35
26	b	619	BCR	C39-C30-C25	-2.02	107.02	110.30
26	f	101	BCR	C28-C29-C30	-2.02	107.38	114.60
26	B	620	BCR	C10-C11-C12	-2.02	116.91	123.22
28	l	101	SQD	O9-S-C6	2.02	109.34	106.94
24	B	606	CLA	CHC-C1C-C2C	-2.02	121.12	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	505	CLA	CHC-C1C-C2C	-2.02	121.12	126.73
24	B	607[A]	CLA	C1D-ND-C4D	-2.02	104.90	106.33
24	C	505	CLA	C1D-ND-C4D	-2.02	104.90	106.33
24	b	603	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
24	b	611	CLA	CHC-C1C-C2C	-2.02	121.12	126.73
24	c	504	CLA	CHC-C1C-C2C	-2.02	121.13	126.73
29	c	519	LMG	O1-C7-C8	-2.02	106.03	110.90
24	b	613	CLA	CHD-C4C-C3C	2.02	127.80	124.84
30	E	102	LHG	O7-C7-O9	-2.02	118.83	123.70
26	K	102	BCR	C1-C6-C7	-2.02	110.07	115.78
24	b	608[A]	CLA	CHD-C4C-C3C	2.01	127.80	124.84
24	c	508	CLA	CED-O2D-CGD	2.01	120.49	115.94
24	C	506	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	d	402	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	A	609	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
29	Z	101	LMG	C6-C5-C4	-2.01	108.30	113.00
32	h	102	DGD	C2G-O2G-C1B	-2.01	112.84	117.79
24	b	613	CLA	O2A-CGA-CBA	2.01	118.21	111.91
26	B	620	BCR	C34-C9-C8	2.01	121.24	118.08
32	H	102	DGD	O3D-C3D-C2D	-2.01	105.71	110.35
24	B	607[A]	CLA	CED-O2D-CGD	2.01	120.48	115.94
29	z	101	LMG	C4-C3-C2	2.01	114.33	110.82
24	b	607	CLA	C4A-NA-C1A	-2.01	105.80	106.71
28	L	102	SQD	O47-C7-O49	-2.01	118.86	123.70
32	h	102	DGD	O5D-C1E-C2E	2.00	111.43	108.30
24	B	615	CLA	C1-O2A-CGA	2.00	121.70	116.44
24	c	512	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
30	a	616	LHG	O8-C23-O10	-2.00	118.54	123.59
24	c	511	CLA	CHB-C4A-NA	-2.00	121.74	124.51
24	C	502	CLA	C2B-C1B-NB	-2.00	108.89	110.23
24	c	511	CLA	CHC-C1C-C2C	-2.00	121.17	126.73
24	B	617	CLA	CHB-C4A-NA	-2.00	121.75	124.51
33	v	201	HEM	C2B-C1B-NB	-2.00	107.47	109.84

There are no chirality outliers.

All (2210) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	607	CLA	CHA-CBD-CGD-O2D
24	A	609	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607[A]	CLA	CHA-CBD-CGD-O2D
24	B	607[B]	CLA	CHA-CBD-CGD-O2D
24	B	608	CLA	C1A-C2A-CAA-CBA
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	C1A-C2A-CAA-CBA
24	C	512	CLA	C1A-C2A-CAA-CBA
24	a	615	CLA	CHA-CBD-CGD-O1D
24	a	615	CLA	CHA-CBD-CGD-O2D
24	b	603	CLA	C1A-C2A-CAA-CBA
24	b	603	CLA	CHA-CBD-CGD-O1D
24	b	603	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	C2-C3-C5-C6
24	b	607	CLA	C4-C3-C5-C6
24	b	608[A]	CLA	CHA-CBD-CGD-O2D
24	b	608[B]	CLA	CHA-CBD-CGD-O2D
24	b	609	CLA	C1A-C2A-CAA-CBA
24	b	609	CLA	C3A-C2A-CAA-CBA
24	b	611	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CHA-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	C2B-C3B-CAB-CBB
24	b	617	CLA	C4B-C3B-CAB-CBB
24	c	502	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	C2B-C3B-CAB-CBB
24	c	507	CLA	C4B-C3B-CAB-CBB
24	c	508	CLA	CHA-CBD-CGD-O1D
26	A	610	BCR	C11-C12-C13-C14
26	A	610	BCR	C12-C13-C14-C15
26	A	610	BCR	C35-C13-C14-C15
26	A	610	BCR	C13-C14-C15-C16
26	A	610	BCR	C14-C15-C16-C17
26	A	610	BCR	C16-C17-C18-C19
26	A	610	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
26	A	610	BCR	C17-C18-C19-C20
26	A	610	BCR	C18-C19-C20-C21
26	A	610	BCR	C20-C21-C22-C37
26	A	610	BCR	C23-C24-C25-C30
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C9-C10-C11-C12
26	B	618	BCR	C10-C11-C12-C13
26	B	618	BCR	C11-C12-C13-C14
26	B	618	BCR	C11-C12-C13-C35
26	B	618	BCR	C14-C15-C16-C17
26	B	618	BCR	C15-C16-C17-C18
26	B	618	BCR	C16-C17-C18-C19
26	B	618	BCR	C16-C17-C18-C36
26	B	618	BCR	C36-C18-C19-C20
26	B	618	BCR	C20-C21-C22-C23
26	B	618	BCR	C20-C21-C22-C37
26	B	618	BCR	C21-C22-C23-C24
26	B	618	BCR	C22-C23-C24-C25
26	B	618	BCR	C23-C24-C25-C26
26	B	619	BCR	C5-C6-C7-C8
26	B	619	BCR	C7-C8-C9-C34
26	B	619	BCR	C11-C10-C9-C8
26	B	619	BCR	C11-C10-C9-C34
26	B	619	BCR	C10-C11-C12-C13
26	B	619	BCR	C14-C15-C16-C17
26	B	619	BCR	C16-C17-C18-C19
26	B	619	BCR	C16-C17-C18-C36
26	B	619	BCR	C18-C19-C20-C21
26	B	619	BCR	C20-C21-C22-C23
26	B	619	BCR	C20-C21-C22-C37
26	B	619	BCR	C21-C22-C23-C24
26	B	620	BCR	C5-C6-C7-C8
26	B	620	BCR	C11-C10-C9-C8
26	B	620	BCR	C10-C11-C12-C13
26	B	620	BCR	C11-C12-C13-C14
26	B	620	BCR	C14-C15-C16-C17
26	B	620	BCR	C16-C17-C18-C19
26	B	620	BCR	C16-C17-C18-C36
26	B	620	BCR	C17-C18-C19-C20
26	B	620	BCR	C36-C18-C19-C20
26	B	620	BCR	C18-C19-C20-C21
26	B	620	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
26	B	620	BCR	C20-C21-C22-C23
26	B	620	BCR	C20-C21-C22-C37
26	B	620	BCR	C37-C22-C23-C24
26	C	514	BCR	C5-C6-C7-C8
26	C	514	BCR	C11-C10-C9-C8
26	C	514	BCR	C11-C10-C9-C34
26	C	514	BCR	C10-C11-C12-C13
26	C	514	BCR	C13-C14-C15-C16
26	C	514	BCR	C14-C15-C16-C17
26	C	514	BCR	C16-C17-C18-C19
26	C	514	BCR	C16-C17-C18-C36
26	C	514	BCR	C36-C18-C19-C20
26	C	514	BCR	C18-C19-C20-C21
26	C	514	BCR	C20-C21-C22-C23
26	C	514	BCR	C20-C21-C22-C37
26	C	514	BCR	C22-C23-C24-C25
26	C	514	BCR	C23-C24-C25-C26
26	F	101	BCR	C10-C11-C12-C13
26	F	101	BCR	C11-C12-C13-C14
26	F	101	BCR	C12-C13-C14-C15
26	F	101	BCR	C35-C13-C14-C15
26	F	101	BCR	C13-C14-C15-C16
26	F	101	BCR	C14-C15-C16-C17
26	F	101	BCR	C16-C17-C18-C19
26	F	101	BCR	C16-C17-C18-C36
26	F	101	BCR	C36-C18-C19-C20
26	F	101	BCR	C18-C19-C20-C21
26	F	101	BCR	C21-C22-C23-C24
26	F	101	BCR	C37-C22-C23-C24
26	F	101	BCR	C22-C23-C24-C25
26	H	101	BCR	C5-C6-C7-C8
26	H	101	BCR	C11-C10-C9-C8
26	H	101	BCR	C11-C10-C9-C34
26	H	101	BCR	C10-C11-C12-C13
26	H	101	BCR	C11-C12-C13-C35
26	H	101	BCR	C14-C15-C16-C17
26	H	101	BCR	C15-C16-C17-C18
26	H	101	BCR	C16-C17-C18-C19
26	H	101	BCR	C16-C17-C18-C36
26	H	101	BCR	C36-C18-C19-C20
26	H	101	BCR	C18-C19-C20-C21
26	H	101	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	H	101	BCR	C20-C21-C22-C37
26	H	101	BCR	C22-C23-C24-C25
26	I	101	BCR	C6-C7-C8-C9
26	I	101	BCR	C7-C8-C9-C34
26	I	101	BCR	C11-C10-C9-C8
26	I	101	BCR	C12-C13-C14-C15
26	I	101	BCR	C35-C13-C14-C15
26	I	101	BCR	C14-C15-C16-C17
26	I	101	BCR	C36-C18-C19-C20
26	I	101	BCR	C18-C19-C20-C21
26	I	101	BCR	C20-C21-C22-C23
26	K	101	BCR	C7-C8-C9-C10
26	K	101	BCR	C7-C8-C9-C34
26	K	101	BCR	C10-C11-C12-C13
26	K	101	BCR	C11-C12-C13-C35
26	K	101	BCR	C12-C13-C14-C15
26	K	101	BCR	C14-C15-C16-C17
26	K	101	BCR	C16-C17-C18-C19
26	K	101	BCR	C16-C17-C18-C36
26	K	101	BCR	C17-C18-C19-C20
26	K	101	BCR	C36-C18-C19-C20
26	K	101	BCR	C20-C21-C22-C37
26	K	102	BCR	C6-C7-C8-C9
26	K	102	BCR	C7-C8-C9-C10
26	K	102	BCR	C7-C8-C9-C34
26	K	102	BCR	C10-C11-C12-C13
26	K	102	BCR	C11-C12-C13-C14
26	K	102	BCR	C13-C14-C15-C16
26	K	102	BCR	C14-C15-C16-C17
26	K	102	BCR	C17-C18-C19-C20
26	K	102	BCR	C18-C19-C20-C21
26	K	102	BCR	C20-C21-C22-C37
26	K	102	BCR	C21-C22-C23-C24
26	K	102	BCR	C37-C22-C23-C24
26	K	102	BCR	C22-C23-C24-C25
26	T	101	BCR	C6-C7-C8-C9
26	T	101	BCR	C11-C10-C9-C8
26	T	101	BCR	C11-C10-C9-C34
26	T	101	BCR	C10-C11-C12-C13
26	T	101	BCR	C11-C12-C13-C14
26	T	101	BCR	C12-C13-C14-C15
26	T	101	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	T	101	BCR	C16-C17-C18-C19
26	T	101	BCR	C16-C17-C18-C36
26	T	101	BCR	C18-C19-C20-C21
26	T	101	BCR	C37-C22-C23-C24
26	T	101	BCR	C22-C23-C24-C25
26	a	610	BCR	C7-C8-C9-C10
26	a	610	BCR	C11-C10-C9-C34
26	a	610	BCR	C11-C12-C13-C14
26	a	610	BCR	C12-C13-C14-C15
26	a	610	BCR	C35-C13-C14-C15
26	a	610	BCR	C14-C15-C16-C17
26	a	610	BCR	C15-C16-C17-C18
26	a	610	BCR	C17-C18-C19-C20
26	a	610	BCR	C18-C19-C20-C21
26	a	610	BCR	C20-C21-C22-C23
26	a	610	BCR	C20-C21-C22-C37
26	a	610	BCR	C21-C22-C23-C24
26	b	619	BCR	C9-C10-C11-C12
26	b	619	BCR	C10-C11-C12-C13
26	b	619	BCR	C11-C12-C13-C14
26	b	619	BCR	C11-C12-C13-C35
26	b	619	BCR	C12-C13-C14-C15
26	b	619	BCR	C35-C13-C14-C15
26	b	619	BCR	C14-C15-C16-C17
26	b	619	BCR	C15-C16-C17-C18
26	b	619	BCR	C16-C17-C18-C19
26	b	619	BCR	C16-C17-C18-C36
26	b	619	BCR	C18-C19-C20-C21
26	b	619	BCR	C19-C20-C21-C22
26	b	619	BCR	C21-C22-C23-C24
26	b	619	BCR	C22-C23-C24-C25
26	b	620	BCR	C5-C6-C7-C8
26	b	620	BCR	C11-C12-C13-C35
26	b	620	BCR	C12-C13-C14-C15
26	b	620	BCR	C14-C15-C16-C17
26	b	620	BCR	C16-C17-C18-C19
26	b	620	BCR	C16-C17-C18-C36
26	b	620	BCR	C17-C18-C19-C20
26	b	620	BCR	C36-C18-C19-C20
26	b	620	BCR	C18-C19-C20-C21
26	b	620	BCR	C20-C21-C22-C23
26	b	620	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
26	b	620	BCR	C21-C22-C23-C24
26	b	621	BCR	C5-C6-C7-C8
26	b	621	BCR	C7-C8-C9-C34
26	b	621	BCR	C11-C10-C9-C8
26	b	621	BCR	C11-C10-C9-C34
26	b	621	BCR	C12-C13-C14-C15
26	b	621	BCR	C35-C13-C14-C15
26	b	621	BCR	C14-C15-C16-C17
26	b	621	BCR	C16-C17-C18-C19
26	b	621	BCR	C16-C17-C18-C36
26	b	621	BCR	C36-C18-C19-C20
26	b	621	BCR	C18-C19-C20-C21
26	b	621	BCR	C19-C20-C21-C22
26	b	621	BCR	C20-C21-C22-C23
26	b	621	BCR	C20-C21-C22-C37
26	c	514	BCR	C5-C6-C7-C8
26	c	514	BCR	C6-C7-C8-C9
26	c	514	BCR	C7-C8-C9-C10
26	c	514	BCR	C11-C10-C9-C8
26	c	514	BCR	C11-C10-C9-C34
26	c	514	BCR	C10-C11-C12-C13
26	c	514	BCR	C12-C13-C14-C15
26	c	514	BCR	C35-C13-C14-C15
26	c	514	BCR	C14-C15-C16-C17
26	c	514	BCR	C15-C16-C17-C18
26	c	514	BCR	C16-C17-C18-C19
26	c	514	BCR	C16-C17-C18-C36
26	c	514	BCR	C17-C18-C19-C20
26	c	514	BCR	C36-C18-C19-C20
26	c	514	BCR	C18-C19-C20-C21
26	c	514	BCR	C20-C21-C22-C23
26	c	514	BCR	C20-C21-C22-C37
26	c	514	BCR	C21-C22-C23-C24
26	c	514	BCR	C22-C23-C24-C25
26	c	514	BCR	C23-C24-C25-C26
26	c	515	BCR	C6-C7-C8-C9
26	c	515	BCR	C12-C13-C14-C15
26	c	515	BCR	C35-C13-C14-C15
26	c	515	BCR	C14-C15-C16-C17
26	c	515	BCR	C16-C17-C18-C36
26	c	515	BCR	C36-C18-C19-C20
26	c	515	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	c	515	BCR	C20-C21-C22-C23
26	c	515	BCR	C37-C22-C23-C24
26	c	521	BCR	C6-C7-C8-C9
26	c	521	BCR	C7-C8-C9-C34
26	c	521	BCR	C11-C10-C9-C8
26	c	521	BCR	C10-C11-C12-C13
26	c	521	BCR	C12-C13-C14-C15
26	c	521	BCR	C13-C14-C15-C16
26	c	521	BCR	C14-C15-C16-C17
26	c	521	BCR	C18-C19-C20-C21
26	c	521	BCR	C20-C21-C22-C37
26	c	521	BCR	C22-C23-C24-C25
26	c	521	BCR	C23-C24-C25-C30
26	f	101	BCR	C10-C11-C12-C13
26	f	101	BCR	C11-C12-C13-C35
26	f	101	BCR	C12-C13-C14-C15
26	f	101	BCR	C35-C13-C14-C15
26	f	101	BCR	C14-C15-C16-C17
26	f	101	BCR	C16-C17-C18-C19
26	f	101	BCR	C16-C17-C18-C36
26	f	101	BCR	C18-C19-C20-C21
26	f	101	BCR	C20-C21-C22-C37
26	f	101	BCR	C22-C23-C24-C25
26	f	101	BCR	C23-C24-C25-C26
26	h	101	BCR	C6-C7-C8-C9
26	h	101	BCR	C7-C8-C9-C34
26	h	101	BCR	C11-C10-C9-C8
26	h	101	BCR	C11-C10-C9-C34
26	h	101	BCR	C10-C11-C12-C13
26	h	101	BCR	C11-C12-C13-C14
26	h	101	BCR	C12-C13-C14-C15
26	h	101	BCR	C13-C14-C15-C16
26	h	101	BCR	C14-C15-C16-C17
26	h	101	BCR	C16-C17-C18-C19
26	h	101	BCR	C16-C17-C18-C36
26	h	101	BCR	C36-C18-C19-C20
26	h	101	BCR	C18-C19-C20-C21
26	h	101	BCR	C20-C21-C22-C23
26	h	101	BCR	C20-C21-C22-C37
26	h	101	BCR	C21-C22-C23-C24
26	k	101	BCR	C7-C8-C9-C34
26	k	101	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	k	101	BCR	C10-C11-C12-C13
26	k	101	BCR	C11-C12-C13-C35
26	k	101	BCR	C12-C13-C14-C15
26	k	101	BCR	C16-C17-C18-C19
26	k	101	BCR	C16-C17-C18-C36
26	k	101	BCR	C36-C18-C19-C20
26	k	101	BCR	C20-C21-C22-C23
26	k	101	BCR	C20-C21-C22-C37
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C10-C9-C8
26	t	101	BCR	C11-C12-C13-C14
26	t	101	BCR	C12-C13-C14-C15
26	t	101	BCR	C35-C13-C14-C15
26	t	101	BCR	C14-C15-C16-C17
26	t	101	BCR	C16-C17-C18-C19
26	t	101	BCR	C16-C17-C18-C36
26	t	101	BCR	C18-C19-C20-C21
26	t	101	BCR	C21-C22-C23-C24
26	t	101	BCR	C37-C22-C23-C24
26	t	101	BCR	C22-C23-C24-C25
26	t	101	BCR	C23-C24-C25-C30
27	A	611	PL9	C7-C8-C9-C10
27	A	611	PL9	C12-C11-C9-C10
27	A	611	PL9	C12-C13-C14-C15
27	A	611	PL9	C14-C16-C17-C18
27	A	611	PL9	C19-C21-C22-C23
27	A	611	PL9	C22-C23-C24-C25
27	A	611	PL9	C32-C33-C34-C35
27	A	611	PL9	C35-C34-C36-C37
27	D	405	PL9	C7-C8-C9-C10
27	D	405	PL9	C12-C13-C14-C15
27	D	405	PL9	C17-C18-C19-C20
27	D	405	PL9	C22-C23-C24-C25
27	D	405	PL9	C42-C43-C44-C46
27	D	405	PL9	C44-C46-C47-C48
27	a	611	PL9	C12-C11-C9-C10
27	a	611	PL9	C12-C13-C14-C15
27	a	611	PL9	C14-C16-C17-C18
27	a	611	PL9	C18-C19-C21-C22
27	a	611	PL9	C19-C21-C22-C23
27	a	611	PL9	C22-C23-C24-C25
27	a	611	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
27	a	611	PL9	C24-C26-C27-C28
27	d	404	PL9	C17-C18-C19-C20
27	d	404	PL9	C25-C24-C26-C27
27	d	404	PL9	C27-C28-C29-C30
27	d	404	PL9	C42-C43-C44-C46
28	A	614	SQD	O6-C44-C45-O47
28	B	622	SQD	O5-C1-O6-C44
28	B	622	SQD	C8-C7-O47-C45
28	B	622	SQD	O5-C5-C6-S
28	L	102	SQD	C8-C7-O47-C45
28	L	102	SQD	O5-C5-C6-S
28	X	101	SQD	C2-C1-O6-C44
28	X	101	SQD	O5-C1-O6-C44
28	a	614	SQD	O6-C44-C45-O47
28	b	601	SQD	O5-C1-O6-C44
28	b	601	SQD	C8-C7-O47-C45
28	b	601	SQD	O5-C5-C6-S
28	l	101	SQD	C8-C7-O47-C45
28	l	101	SQD	O5-C5-C6-S
28	x	101	SQD	C2-C1-O6-C44
28	x	101	SQD	O5-C1-O6-C44
29	Z	101	LMG	O6-C1-O1-C7
29	Z	101	LMG	O1-C7-C8-O7
29	Z	101	LMG	O9-C10-O7-C8
29	Z	101	LMG	C11-C10-O7-C8
29	z	101	LMG	O6-C1-O1-C7
29	z	101	LMG	O1-C7-C8-O7
29	z	101	LMG	O9-C10-O7-C8
29	z	101	LMG	C11-C10-O7-C8
30	D	407	LHG	O1-C1-C2-C3
30	D	407	LHG	O2-C2-C3-O3
30	D	407	LHG	C3-O3-P-O5
30	D	407	LHG	C4-O6-P-O4
30	D	407	LHG	C4-O6-P-O5
30	L	101	LHG	C4-O6-P-O4
30	d	407	LHG	O1-C1-C2-C3
30	d	407	LHG	C3-O3-P-O4
30	d	407	LHG	C3-O3-P-O5
30	e	101	LHG	C8-C7-O7-C5
30	e	101	LHG	C24-C23-O8-C6
30	l	102	LHG	C4-O6-P-O4
32	C	515	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
32	E	101	DGD	C2B-C1B-O2G-C2G
32	d	405	DGD	C2B-C1B-O2G-C2G
32	d	405	DGD	O1B-C1B-O2G-C2G
32	d	405	DGD	C2E-C1E-O5D-C6D
29	z	101	LMG	C29-C28-O8-C9
24	b	611	CLA	CBD-CGD-O2D-CED
28	X	101	SQD	O10-C23-O48-C46
28	x	101	SQD	O10-C23-O48-C46
30	E	102	LHG	O10-C23-O8-C6
30	e	101	LHG	O10-C23-O8-C6
24	b	611	CLA	O1D-CGD-O2D-CED
28	X	101	SQD	C24-C23-O48-C46
28	x	101	SQD	C24-C23-O48-C46
30	E	102	LHG	C24-C23-O8-C6
29	Z	101	LMG	C29-C28-O8-C9
24	C	503	CLA	CBD-CGD-O2D-CED
24	b	606	CLA	CBD-CGD-O2D-CED
24	B	617	CLA	O1A-CGA-O2A-C1
24	b	618	CLA	O1A-CGA-O2A-C1
29	Z	101	LMG	O10-C28-O8-C9
29	z	101	LMG	O10-C28-O8-C9
24	b	612	CLA	O1D-CGD-O2D-CED
28	B	622	SQD	O49-C7-O47-C45
28	b	601	SQD	O49-C7-O47-C45
29	A	613	LMG	O9-C10-O7-C8
32	E	101	DGD	O1B-C1B-O2G-C2G
24	B	615	CLA	C3-C5-C6-C7
24	b	616	CLA	C3-C5-C6-C7
24	B	609	CLA	C2C-C3C-CAC-CBC
30	E	102	LHG	C8-C7-O7-C5
24	c	510	CLA	CBD-CGD-O2D-CED
29	C	519	LMG	O6-C5-C6-O5
27	A	611	PL9	C25-C24-C26-C27
27	A	611	PL9	C18-C19-C21-C22
24	b	612	CLA	CBD-CGD-O2D-CED
24	B	607[A]	CLA	C2A-CAA-CBA-CGA
24	B	607[B]	CLA	C2A-CAA-CBA-CGA
24	b	608[A]	CLA	C2A-CAA-CBA-CGA
24	b	608[B]	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	C3-C5-C6-C7
24	b	603	CLA	C3-C5-C6-C7
24	b	618	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	A	611	PL9	C27-C28-C29-C30
27	A	611	PL9	C37-C38-C39-C40
27	A	611	PL9	C42-C43-C44-C45
27	D	405	PL9	C32-C33-C34-C35
27	D	405	PL9	C37-C38-C39-C40
27	a	611	PL9	C7-C8-C9-C10
27	a	611	PL9	C27-C28-C29-C30
27	a	611	PL9	C32-C33-C34-C35
27	a	611	PL9	C37-C38-C39-C40
27	a	611	PL9	C42-C43-C44-C45
27	d	404	PL9	C7-C8-C9-C10
27	d	404	PL9	C12-C13-C14-C15
27	d	404	PL9	C22-C23-C24-C25
27	d	404	PL9	C32-C33-C34-C35
27	d	404	PL9	C37-C38-C39-C40
24	B	602	CLA	O1D-CGD-O2D-CED
24	b	607	CLA	O1D-CGD-O2D-CED
28	L	102	SQD	O49-C7-O47-C45
28	l	101	SQD	O49-C7-O47-C45
30	E	102	LHG	O9-C7-O7-C5
26	A	610	BCR	C9-C10-C11-C12
26	B	619	BCR	C15-C16-C17-C18
26	B	620	BCR	C13-C14-C15-C16
26	C	514	BCR	C15-C16-C17-C18
26	F	101	BCR	C15-C16-C17-C18
26	H	101	BCR	C19-C20-C21-C22
26	I	101	BCR	C13-C14-C15-C16
26	I	101	BCR	C19-C20-C21-C22
26	T	101	BCR	C15-C16-C17-C18
26	c	514	BCR	C19-C20-C21-C22
26	f	101	BCR	C13-C14-C15-C16
26	h	101	BCR	C15-C16-C17-C18
26	k	101	BCR	C15-C16-C17-C18
32	H	102	DGD	O6E-C5E-C6E-O5E
24	A	609	CLA	CBD-CGD-O2D-CED
24	B	605	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	CBD-CGD-O2D-CED
24	b	607	CLA	CBD-CGD-O2D-CED
24	b	609	CLA	CBD-CGD-O2D-CED
24	c	503	CLA	CBD-CGD-O2D-CED
30	d	407	LHG	O2-C2-C3-O3
24	B	617	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	j	101	LMG	O6-C5-C6-O5
24	a	606	CLA	O1D-CGD-O2D-CED
24	B	602	CLA	CBD-CGD-O2D-CED
24	b	616	CLA	CBD-CGD-O2D-CED
29	D	408	LMG	O6-C5-C6-O5
32	c	516	DGD	C4D-C5D-C6D-O5D
29	c	520	LMG	O6-C5-C6-O5
27	A	611	PL9	C47-C48-C49-C51
27	D	405	PL9	C47-C48-C49-C50
27	A	611	PL9	C38-C39-C41-C42
27	a	611	PL9	C38-C39-C41-C42
30	D	407	LHG	C14-C15-C16-C17
24	c	505	CLA	O1A-CGA-O2A-C1
32	H	102	DGD	O6E-C1E-O5D-C6D
27	A	611	PL9	C24-C26-C27-C28
27	d	404	PL9	C29-C31-C32-C33
27	d	404	PL9	C44-C46-C47-C48
32	H	102	DGD	C6B-C7B-C8B-C9B
27	A	611	PL9	C17-C18-C19-C20
24	B	616	CLA	O1D-CGD-O2D-CED
30	D	407	LHG	C1-C2-C3-O3
30	d	407	LHG	C1-C2-C3-O3
32	c	516	DGD	O6E-C5E-C6E-O5E
29	C	519	LMG	C4-C5-C6-O5
29	c	520	LMG	C4-C5-C6-O5
24	C	509	CLA	O1D-CGD-O2D-CED
28	L	102	SQD	C24-C23-O48-C46
28	l	101	SQD	C24-C23-O48-C46
32	c	518	DGD	C2A-C1A-O1G-C1G
32	h	102	DGD	O6E-C5E-C6E-O5E
24	B	612	CLA	CBD-CGD-O2D-CED
24	a	606	CLA	CBD-CGD-O2D-CED
32	h	102	DGD	C6B-C7B-C8B-C9B
26	B	620	BCR	C15-C16-C17-C18
26	a	610	BCR	C13-C14-C15-C16
26	h	101	BCR	C19-C20-C21-C22
32	H	102	DGD	C4E-C5E-C6E-O5E
29	Z	101	LMG	C2-C1-O1-C7
29	z	101	LMG	C2-C1-O1-C7
32	c	518	DGD	O1A-C1A-O1G-C1G
24	B	602	CLA	C11-C10-C8-C9
24	C	501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	C	502	CLA	C14-C13-C15-C16
24	C	504	CLA	C11-C12-C13-C14
24	C	509	CLA	C6-C7-C8-C9
24	b	603	CLA	C11-C10-C8-C9
24	c	501	CLA	C11-C12-C13-C14
24	c	502	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C12-C13-C14
24	c	509	CLA	C6-C7-C8-C9
26	A	610	BCR	C11-C12-C13-C35
26	A	610	BCR	C36-C18-C19-C20
26	A	610	BCR	C37-C22-C23-C24
26	B	618	BCR	C37-C22-C23-C24
26	B	619	BCR	C36-C18-C19-C20
26	C	514	BCR	C37-C22-C23-C24
26	F	101	BCR	C11-C12-C13-C35
26	I	101	BCR	C37-C22-C23-C24
26	T	101	BCR	C7-C8-C9-C34
26	b	620	BCR	C7-C8-C9-C34
26	c	514	BCR	C7-C8-C9-C34
26	c	515	BCR	C7-C8-C9-C34
26	f	101	BCR	C36-C18-C19-C20
26	h	101	BCR	C11-C12-C13-C35
26	C	514	BCR	C7-C8-C9-C10
26	C	514	BCR	C17-C18-C19-C20
26	C	514	BCR	C21-C22-C23-C24
26	H	101	BCR	C17-C18-C19-C20
26	b	620	BCR	C7-C8-C9-C10
26	b	621	BCR	C7-C8-C9-C10
26	t	101	BCR	C7-C8-C9-C10
29	A	613	LMG	O6-C5-C6-O5
29	B	621	LMG	O9-C10-O7-C8
29	a	613	LMG	O9-C10-O7-C8
24	B	609	CLA	C4C-C3C-CAC-CBC
32	C	516	DGD	C4E-C5E-C6E-O5E
29	a	613	LMG	C28-C29-C30-C31
27	a	611	PL9	C47-C48-C49-C51
27	d	404	PL9	C47-C48-C49-C51
28	L	102	SQD	O10-C23-O48-C46
28	l	101	SQD	O10-C23-O48-C46
29	a	613	LMG	O10-C28-O8-C9
24	A	609	CLA	C10-C11-C12-C13
24	B	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	a	609	CLA	C10-C11-C12-C13
24	b	617	CLA	C5-C6-C7-C8
24	B	616	CLA	CBD-CGD-O2D-CED
32	C	516	DGD	O6E-C5E-C6E-O5E
29	D	408	LMG	C4-C5-C6-O5
24	A	609	CLA	C13-C15-C16-C17
24	B	602	CLA	C10-C11-C12-C13
24	a	609	CLA	C13-C15-C16-C17
24	b	603	CLA	C10-C11-C12-C13
32	c	516	DGD	C2A-C3A-C4A-C5A
32	C	516	DGD	C1B-C2B-C3B-C4B
32	d	405	DGD	C1A-C2A-C3A-C4A
24	B	608	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
32	c	516	DGD	O6D-C5D-C6D-O5D
24	B	615	CLA	C5-C6-C7-C8
24	B	615	CLA	C10-C11-C12-C13
24	C	509	CLA	C8-C10-C11-C12
24	b	616	CLA	C5-C6-C7-C8
24	b	616	CLA	C10-C11-C12-C13
24	c	509	CLA	C8-C10-C11-C12
32	h	102	DGD	C4E-C5E-C6E-O5E
24	c	510	CLA	O1D-CGD-O2D-CED
30	D	407	LHG	O1-C1-C2-O2
30	d	407	LHG	O1-C1-C2-O2
27	a	611	PL9	C17-C18-C19-C20
28	B	622	SQD	C7-C8-C9-C10
28	b	601	SQD	C7-C8-C9-C10
29	B	621	LMG	C10-C11-C12-C13
29	C	518	LMG	C28-C29-C30-C31
29	Z	101	LMG	C10-C11-C12-C13
29	c	520	LMG	C28-C29-C30-C31
32	E	101	DGD	C1B-C2B-C3B-C4B
32	c	517	DGD	C1A-C2A-C3A-C4A
32	c	517	DGD	C1B-C2B-C3B-C4B
32	d	405	DGD	C1B-C2B-C3B-C4B
24	B	613	CLA	CBD-CGD-O2D-CED
24	B	607[A]	CLA	C13-C15-C16-C17
24	b	608[A]	CLA	C13-C15-C16-C17
30	e	101	LHG	O9-C7-O7-C5
24	C	506	CLA	C5-C6-C7-C8
24	D	404	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	d	403	CLA	C8-C10-C11-C12
28	A	614	SQD	C23-C24-C25-C26
28	a	614	SQD	C23-C24-C25-C26
29	A	613	LMG	C28-C29-C30-C31
29	C	519	LMG	C28-C29-C30-C31
32	C	516	DGD	C1A-C2A-C3A-C4A
32	E	101	DGD	C1A-C2A-C3A-C4A
24	c	506	CLA	C5-C6-C7-C8
24	C	513	CLA	O1D-CGD-O2D-CED
26	a	610	BCR	C9-C10-C11-C12
26	a	610	BCR	C19-C20-C21-C22
26	b	620	BCR	C13-C14-C15-C16
26	b	621	BCR	C9-C10-C11-C12
26	c	514	BCR	C13-C14-C15-C16
26	c	521	BCR	C15-C16-C17-C18
26	c	521	BCR	C19-C20-C21-C22
29	z	101	LMG	C10-C11-C12-C13
24	b	604	CLA	O1D-CGD-O2D-CED
24	B	607[A]	CLA	C15-C16-C17-C18
24	D	404	CLA	C10-C11-C12-C13
24	b	608[A]	CLA	C15-C16-C17-C18
24	d	403	CLA	C10-C11-C12-C13
24	C	504	CLA	O1A-CGA-O2A-C1
24	C	511	CLA	O1A-CGA-O2A-C1
32	d	405	DGD	O6E-C1E-O5D-C6D
24	A	607	CLA	C13-C15-C16-C17
24	a	607	CLA	C13-C15-C16-C17
27	A	611	PL9	C9-C11-C12-C13
27	D	405	PL9	C9-C11-C12-C13
27	D	405	PL9	C14-C16-C17-C18
27	D	405	PL9	C29-C31-C32-C33
27	d	404	PL9	C9-C11-C12-C13
27	d	404	PL9	C39-C41-C42-C43
29	C	518	LMG	C10-C11-C12-C13
29	c	519	LMG	C28-C29-C30-C31
26	I	101	BCR	C10-C11-C12-C13
26	c	515	BCR	C10-C11-C12-C13
27	d	404	PL9	C47-C48-C49-C50
30	l	102	LHG	O2-C2-C3-O3
29	j	101	LMG	C4-C5-C6-O5
24	C	509	CLA	C13-C15-C16-C17
24	c	509	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	z	101	LMG	C4-C5-C6-O5
24	A	609	CLA	C15-C16-C17-C18
24	B	612	CLA	C15-C16-C17-C18
24	a	609	CLA	C15-C16-C17-C18
24	b	613	CLA	C15-C16-C17-C18
29	A	613	LMG	C11-C10-O7-C8
24	B	607[B]	CLA	C10-C11-C12-C13
24	B	617	CLA	C10-C11-C12-C13
24	C	501	CLA	C15-C16-C17-C18
24	C	506	CLA	C10-C11-C12-C13
24	b	608[B]	CLA	C10-C11-C12-C13
24	b	618	CLA	C10-C11-C12-C13
24	c	501	CLA	C15-C16-C17-C18
24	c	506	CLA	C10-C11-C12-C13
30	D	407	LHG	C4-O6-P-O3
30	L	101	LHG	C4-O6-P-O3
30	d	407	LHG	C3-O3-P-O6
30	l	102	LHG	C4-O6-P-O3
24	c	505	CLA	CBA-CGA-O2A-C1
24	A	607	CLA	C16-C17-C18-C20
24	a	607	CLA	C16-C17-C18-C20
29	a	613	LMG	C29-C28-O8-C9
30	A	615	LHG	C24-C23-O8-C6
26	k	101	BCR	C14-C15-C16-C17
26	B	618	BCR	C13-C14-C15-C16
26	B	618	BCR	C19-C20-C21-C22
26	C	514	BCR	C19-C20-C21-C22
26	T	101	BCR	C19-C20-C21-C22
26	b	619	BCR	C13-C14-C15-C16
26	f	101	BCR	C19-C20-C21-C22
28	X	101	SQD	C29-C30-C31-C32
29	D	408	LMG	C16-C17-C18-C19
32	H	102	DGD	CBA-CCA-CDA-CEA
24	b	603	CLA	O1D-CGD-O2D-CED
24	c	513	CLA	CBD-CGD-O2D-CED
29	a	613	LMG	C11-C10-O7-C8
26	A	610	BCR	C11-C10-C9-C34
26	B	618	BCR	C35-C13-C14-C15
26	B	620	BCR	C11-C10-C9-C34
26	I	101	BCR	C16-C17-C18-C36
26	a	610	BCR	C16-C17-C18-C36
26	c	515	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
26	t	101	BCR	C11-C10-C9-C34
28	A	612	SQD	C11-C12-C13-C14
28	A	614	SQD	C15-C16-C17-C18
28	L	102	SQD	C15-C16-C17-C18
28	X	101	SQD	C26-C27-C28-C29
28	X	101	SQD	C34-C35-C36-C37
28	a	612	SQD	C11-C12-C13-C14
28	a	614	SQD	C15-C16-C17-C18
28	l	101	SQD	C11-C10-C9-C8
28	l	101	SQD	C10-C11-C12-C13
28	l	101	SQD	C15-C16-C17-C18
28	x	101	SQD	C26-C27-C28-C29
28	x	101	SQD	C29-C30-C31-C32
28	x	101	SQD	C34-C35-C36-C37
29	b	622	LMG	C32-C33-C34-C35
29	b	622	LMG	C34-C35-C36-C37
29	c	519	LMG	C15-C16-C17-C18
29	c	520	LMG	C29-C30-C31-C32
30	D	406	LHG	C29-C30-C31-C32
30	E	102	LHG	C15-C16-C17-C18
32	E	101	DGD	C7B-C8B-C9B-CAB
32	H	102	DGD	C7A-C8A-C9A-CAA
32	c	516	DGD	C5B-C6B-C7B-C8B
32	d	405	DGD	CCA-CDA-CEA-CFA
24	C	506	CLA	C16-C17-C18-C19
27	D	405	PL9	C47-C48-C49-C51
33	V	201	HEM	C2D-C3D-CAD-CBD
28	A	612	SQD	C28-C29-C30-C31
28	L	102	SQD	C11-C10-C9-C8
28	L	102	SQD	C10-C11-C12-C13
28	a	612	SQD	C28-C29-C30-C31
29	A	613	LMG	C18-C19-C20-C21
29	D	408	LMG	C38-C39-C40-C41
29	b	622	LMG	C17-C18-C19-C20
29	j	101	LMG	C14-C15-C16-C17
30	E	102	LHG	C24-C25-C26-C27
30	d	406	LHG	C32-C33-C34-C35
30	l	102	LHG	C11-C12-C13-C14
30	l	102	LHG	C31-C32-C33-C34
32	d	405	DGD	C9B-CAB-CBB-CCB
28	L	102	SQD	C46-C45-O47-C7
28	l	101	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
32	c	517	DGD	C3A-C4A-C5A-C6A
32	c	517	DGD	C9A-CAA-CBA-CCA
32	c	517	DGD	C6B-C7B-C8B-C9B
24	c	511	CLA	O1A-CGA-O2A-C1
29	z	101	LMG	O6-C5-C6-O5
28	A	612	SQD	C12-C13-C14-C15
28	A	612	SQD	C15-C16-C17-C18
28	a	612	SQD	C12-C13-C14-C15
28	a	612	SQD	C15-C16-C17-C18
29	B	621	LMG	C12-C13-C14-C15
29	C	519	LMG	C30-C31-C32-C33
30	E	102	LHG	C14-C15-C16-C17
30	L	101	LHG	C33-C34-C35-C36
30	e	101	LHG	C18-C19-C20-C21
32	C	516	DGD	C6B-C7B-C8B-C9B
32	C	516	DGD	CAB-CBB-CCB-CDB
32	E	101	DGD	C9A-CAA-CBA-CCA
32	E	101	DGD	C9B-CAB-CBB-CCB
32	c	518	DGD	C6A-C7A-C8A-C9A
28	L	102	SQD	C12-C13-C14-C15
28	l	101	SQD	C12-C13-C14-C15
29	a	613	LMG	C13-C14-C15-C16
29	j	101	LMG	C16-C17-C18-C19
30	e	101	LHG	C7-C8-C9-C10
24	C	508	CLA	O1D-CGD-O2D-CED
26	B	618	BCR	C11-C10-C9-C8
26	B	618	BCR	C12-C13-C14-C15
26	B	619	BCR	C12-C13-C14-C15
26	C	514	BCR	C12-C13-C14-C15
26	F	101	BCR	C20-C21-C22-C23
26	H	101	BCR	C12-C13-C14-C15
26	K	101	BCR	C11-C10-C9-C8
26	K	102	BCR	C12-C13-C14-C15
26	K	102	BCR	C20-C21-C22-C23
26	T	101	BCR	C20-C21-C22-C23
26	a	610	BCR	C11-C10-C9-C8
26	a	610	BCR	C16-C17-C18-C19
26	b	619	BCR	C20-C21-C22-C23
26	c	515	BCR	C16-C17-C18-C19
26	c	521	BCR	C16-C17-C18-C19
26	c	521	BCR	C20-C21-C22-C23
26	t	101	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
32	C	516	DGD	C2E-C1E-O5D-C6D
32	E	101	DGD	C2D-C1D-O3G-C3G
32	E	101	DGD	C2E-C1E-O5D-C6D
32	d	405	DGD	C2D-C1D-O3G-C3G
28	L	102	SQD	C17-C18-C19-C20
28	L	102	SQD	C24-C25-C26-C27
28	l	101	SQD	C17-C18-C19-C20
28	l	101	SQD	C18-C19-C20-C21
29	C	518	LMG	C15-C16-C17-C18
29	j	101	LMG	C12-C13-C14-C15
30	D	406	LHG	C32-C33-C34-C35
30	L	101	LHG	C34-C35-C36-C37
30	e	101	LHG	C24-C25-C26-C27
30	l	102	LHG	C33-C34-C35-C36
32	E	101	DGD	CCA-CDA-CEA-CFA
32	c	517	DGD	CAA-CBA-CCA-CDA
24	B	614	CLA	C15-C16-C17-C18
24	b	615	CLA	C15-C16-C17-C18
24	D	404	CLA	C16-C17-C18-C19
24	c	506	CLA	C16-C17-C18-C19
24	d	403	CLA	C16-C17-C18-C19
27	D	405	PL9	C27-C28-C29-C30
28	L	102	SQD	C18-C19-C20-C21
28	X	101	SQD	C24-C25-C26-C27
28	l	101	SQD	C24-C25-C26-C27
29	A	613	LMG	C14-C15-C16-C17
29	B	621	LMG	C37-C38-C39-C40
29	C	519	LMG	C31-C32-C33-C34
32	c	516	DGD	C4B-C5B-C6B-C7B
32	c	518	DGD	C9B-CAB-CBB-CCB
24	B	604	CLA	C6-C7-C8-C9
24	b	605	CLA	C6-C7-C8-C9
28	B	622	SQD	C34-C35-C36-C37
28	L	102	SQD	C29-C30-C31-C32
28	b	601	SQD	C34-C35-C36-C37
28	l	101	SQD	C29-C30-C31-C32
28	x	101	SQD	C24-C25-C26-C27
29	A	613	LMG	C12-C13-C14-C15
29	D	408	LMG	C12-C13-C14-C15
29	D	408	LMG	C15-C16-C17-C18
29	b	622	LMG	C37-C38-C39-C40
29	c	520	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	E	102	LHG	C25-C26-C27-C28
30	d	406	LHG	C29-C30-C31-C32
32	H	102	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	C2A-C3A-C4A-C5A
32	d	405	DGD	CBA-CCA-CDA-CEA
24	B	617	CLA	C8-C10-C11-C12
24	b	618	CLA	C8-C10-C11-C12
32	c	516	DGD	C4E-C5E-C6E-O5E
26	C	514	BCR	C7-C8-C9-C34
26	H	101	BCR	C37-C22-C23-C24
26	b	619	BCR	C37-C22-C23-C24
26	c	514	BCR	C37-C22-C23-C24
28	A	612	SQD	C16-C17-C18-C19
28	B	622	SQD	C31-C32-C33-C34
28	a	612	SQD	C16-C17-C18-C19
29	C	519	LMG	C29-C30-C31-C32
29	j	101	LMG	C30-C31-C32-C33
29	j	101	LMG	C39-C40-C41-C42
30	E	102	LHG	C13-C14-C15-C16
30	L	101	LHG	C11-C12-C13-C14
32	d	405	DGD	CCB-CDB-CEB-CFB
30	D	406	LHG	O1-C1-C2-C3
30	a	616	LHG	O1-C1-C2-C3
26	B	619	BCR	C7-C8-C9-C10
26	B	619	BCR	C17-C18-C19-C20
26	I	101	BCR	C21-C22-C23-C24
26	T	101	BCR	C7-C8-C9-C10
26	T	101	BCR	C21-C22-C23-C24
26	c	515	BCR	C17-C18-C19-C20
26	f	101	BCR	C11-C12-C13-C14
26	f	101	BCR	C17-C18-C19-C20
26	h	101	BCR	C17-C18-C19-C20
26	k	101	BCR	C7-C8-C9-C10
26	k	101	BCR	C17-C18-C19-C20
24	c	503	CLA	O1D-CGD-O2D-CED
24	b	610	CLA	C2C-C3C-CAC-CBC
28	B	622	SQD	C11-C12-C13-C14
28	L	102	SQD	C27-C28-C29-C30
28	b	601	SQD	C31-C32-C33-C34
28	l	101	SQD	C27-C28-C29-C30
29	B	621	LMG	C38-C39-C40-C41
29	Z	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	a	613	LMG	C34-C35-C36-C37
29	b	622	LMG	C14-C15-C16-C17
29	j	101	LMG	C15-C16-C17-C18
30	L	101	LHG	C13-C14-C15-C16
30	d	406	LHG	C25-C26-C27-C28
30	e	101	LHG	C25-C26-C27-C28
32	C	515	DGD	C6B-C7B-C8B-C9B
29	c	519	LMG	C10-C11-C12-C13
30	E	102	LHG	C7-C8-C9-C10
28	A	614	SQD	C16-C17-C18-C19
28	B	622	SQD	C11-C10-C9-C8
28	L	102	SQD	C32-C33-C34-C35
28	a	614	SQD	C16-C17-C18-C19
28	b	601	SQD	C11-C10-C9-C8
28	b	601	SQD	C11-C12-C13-C14
28	l	101	SQD	C14-C15-C16-C17
29	B	621	LMG	C16-C17-C18-C19
29	D	408	LMG	C14-C15-C16-C17
29	c	520	LMG	C17-C18-C19-C20
29	c	520	LMG	C30-C31-C32-C33
29	j	101	LMG	C13-C14-C15-C16
29	z	101	LMG	C12-C13-C14-C15
30	e	101	LHG	C14-C15-C16-C17
32	C	515	DGD	C6A-C7A-C8A-C9A
32	C	516	DGD	C3A-C4A-C5A-C6A
32	C	517	DGD	C6A-C7A-C8A-C9A
32	E	101	DGD	C2A-C3A-C4A-C5A
32	E	101	DGD	C5B-C6B-C7B-C8B
32	c	517	DGD	C4A-C5A-C6A-C7A
32	c	517	DGD	CAB-CBB-CCB-CDB
32	c	517	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	C9A-CAA-CBA-CCA
32	h	102	DGD	CBA-CCA-CDA-CEA
24	B	605	CLA	C4B-C3B-CAB-CBB
24	B	616	CLA	C4B-C3B-CAB-CBB
24	B	617	CLA	C4B-C3B-CAB-CBB
24	C	504	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	C4B-C3B-CAB-CBB
24	b	615	CLA	C4B-C3B-CAB-CBB
32	E	101	DGD	O6D-C1D-O3G-C3G
32	E	101	DGD	O6E-C1E-O5D-C6D
32	d	405	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
28	A	612	SQD	C9-C10-C11-C12
28	A	614	SQD	C26-C27-C28-C29
28	B	622	SQD	C24-C25-C26-C27
28	L	102	SQD	C14-C15-C16-C17
28	a	612	SQD	C9-C10-C11-C12
28	a	614	SQD	C26-C27-C28-C29
28	b	601	SQD	C24-C25-C26-C27
28	l	101	SQD	C32-C33-C34-C35
29	B	621	LMG	C14-C15-C16-C17
29	C	518	LMG	C16-C17-C18-C19
29	a	613	LMG	C38-C39-C40-C41
29	j	101	LMG	C36-C37-C38-C39
29	z	101	LMG	C19-C20-C21-C22
32	C	515	DGD	CAB-CBB-CCB-CDB
32	C	516	DGD	C9A-CAA-CBA-CCA
32	C	517	DGD	C2A-C3A-C4A-C5A
32	c	517	DGD	C9B-CAB-CBB-CCB
32	d	405	DGD	C7B-C8B-C9B-CAB
24	C	505	CLA	CBD-CGD-O2D-CED
28	A	614	SQD	C28-C29-C30-C31
29	A	613	LMG	C36-C37-C38-C39
29	B	621	LMG	C32-C33-C34-C35
29	c	519	LMG	C16-C17-C18-C19
29	z	101	LMG	C16-C17-C18-C19
30	L	101	LHG	C25-C26-C27-C28
30	e	101	LHG	C13-C14-C15-C16
32	C	515	DGD	C4B-C5B-C6B-C7B
32	C	516	DGD	CAA-CBA-CCA-CDA
32	C	516	DGD	C5B-C6B-C7B-C8B
32	c	516	DGD	C6A-C7A-C8A-C9A
32	c	516	DGD	C6B-C7B-C8B-C9B
28	a	614	SQD	C28-C29-C30-C31
29	D	408	LMG	C20-C21-C22-C23
30	E	102	LHG	C27-C28-C29-C30
30	a	616	LHG	C15-C16-C17-C18
30	l	102	LHG	C13-C14-C15-C16
32	c	518	DGD	C2A-C3A-C4A-C5A
29	c	520	LMG	C18-C19-C20-C21
30	L	101	LHG	C12-C13-C14-C15
30	a	616	LHG	C27-C28-C29-C30
24	c	504	CLA	O1D-CGD-O2D-CED
28	L	102	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	X	101	SQD	C31-C32-C33-C34
28	l	101	SQD	C16-C17-C18-C19
28	l	101	SQD	C28-C29-C30-C31
28	x	101	SQD	C31-C32-C33-C34
29	B	621	LMG	C17-C18-C19-C20
29	b	622	LMG	C31-C32-C33-C34
29	c	519	LMG	C29-C30-C31-C32
30	A	615	LHG	C15-C16-C17-C18
30	a	616	LHG	C30-C31-C32-C33
30	d	406	LHG	C13-C14-C15-C16
32	C	515	DGD	C5B-C6B-C7B-C8B
32	E	101	DGD	CCB-CDB-CEB-CFB
24	C	510	CLA	O1A-CGA-O2A-C1
29	A	613	LMG	O10-C28-O8-C9
30	d	407	LHG	O10-C23-O8-C6
24	a	615	CLA	C2C-C3C-CAC-CBC
28	B	622	SQD	C10-C11-C12-C13
28	L	102	SQD	C28-C29-C30-C31
28	b	601	SQD	C10-C11-C12-C13
29	A	613	LMG	C31-C32-C33-C34
29	a	613	LMG	C14-C15-C16-C17
29	a	613	LMG	C32-C33-C34-C35
30	L	101	LHG	C31-C32-C33-C34
32	H	102	DGD	CCA-CDA-CEA-CFA
32	c	518	DGD	C8B-C9B-CAB-CBB
32	h	102	DGD	C7B-C8B-C9B-CAB
24	D	402	CLA	O1D-CGD-O2D-CED
32	h	102	DGD	O1G-C1G-C2G-C3G
29	a	613	LMG	C12-C13-C14-C15
29	c	519	LMG	C19-C20-C21-C22
29	c	519	LMG	C38-C39-C40-C41
32	C	515	DGD	O6D-C5D-C6D-O5D
32	E	101	DGD	O6D-C5D-C6D-O5D
29	b	622	LMG	C16-C17-C18-C19
29	c	520	LMG	C33-C34-C35-C36
27	D	405	PL9	C45-C44-C46-C47
27	d	404	PL9	C30-C29-C31-C32
24	c	511	CLA	CBA-CGA-O2A-C1
27	D	405	PL9	C28-C29-C31-C32
27	D	405	PL9	C43-C44-C46-C47
27	d	404	PL9	C28-C29-C31-C32
28	X	101	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	x	101	SQD	C30-C31-C32-C33
30	A	615	LHG	C12-C13-C14-C15
32	c	518	DGD	C9A-CAA-CBA-CCA
29	A	613	LMG	C30-C31-C32-C33
29	a	613	LMG	C31-C32-C33-C34
29	b	622	LMG	C12-C13-C14-C15
30	E	102	LHG	C18-C19-C20-C21
32	C	516	DGD	C3B-C4B-C5B-C6B
32	c	516	DGD	CAB-CBB-CCB-CDB
32	c	517	DGD	C8B-C9B-CAB-CBB
24	C	507	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
29	b	622	LMG	C36-C37-C38-C39
24	B	605	CLA	C2B-C3B-CAB-CBB
24	B	608	CLA	C2B-C3B-CAB-CBB
24	B	616	CLA	C2B-C3B-CAB-CBB
24	B	617	CLA	C2B-C3B-CAB-CBB
24	C	504	CLA	C2B-C3B-CAB-CBB
24	C	507	CLA	C2B-C3B-CAB-CBB
24	b	615	CLA	C2B-C3B-CAB-CBB
24	c	502	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
24	B	605	CLA	C13-C15-C16-C17
29	C	518	LMG	C13-C14-C15-C16
29	Z	101	LMG	C19-C20-C21-C22
30	l	102	LHG	C16-C17-C18-C19
28	A	612	SQD	C32-C33-C34-C35
32	C	516	DGD	CBB-CCB-CDB-CEB
24	b	606	CLA	C13-C15-C16-C17
30	l	102	LHG	C1-C2-C3-O3
28	a	612	SQD	C32-C33-C34-C35
29	b	622	LMG	C38-C39-C40-C41
30	A	615	LHG	C10-C11-C12-C13
32	H	102	DGD	CCB-CDB-CEB-CFB
29	C	519	LMG	C38-C39-C40-C41
29	c	519	LMG	C32-C33-C34-C35
29	j	101	LMG	C20-C21-C22-C23
30	e	101	LHG	C12-C13-C14-C15
32	C	515	DGD	C7B-C8B-C9B-CAB
32	c	516	DGD	C4A-C5A-C6A-C7A
32	c	516	DGD	CAA-CBA-CCA-CDA
29	D	408	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
30	d	406	LHG	C33-C34-C35-C36
30	l	102	LHG	C12-C13-C14-C15
26	A	610	BCR	C5-C6-C7-C8
26	A	610	BCR	C23-C24-C25-C26
26	B	619	BCR	C23-C24-C25-C30
26	B	620	BCR	C23-C24-C25-C30
26	F	101	BCR	C5-C6-C7-C8
26	F	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C26
26	I	101	BCR	C5-C6-C7-C8
26	I	101	BCR	C23-C24-C25-C26
26	K	101	BCR	C5-C6-C7-C8
26	K	101	BCR	C23-C24-C25-C26
26	K	102	BCR	C5-C6-C7-C8
26	K	102	BCR	C23-C24-C25-C30
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C23-C24-C25-C26
26	a	610	BCR	C1-C6-C7-C8
26	a	610	BCR	C23-C24-C25-C26
26	b	619	BCR	C1-C6-C7-C8
26	b	620	BCR	C23-C24-C25-C30
26	b	621	BCR	C23-C24-C25-C26
26	c	515	BCR	C5-C6-C7-C8
26	c	515	BCR	C23-C24-C25-C26
26	c	521	BCR	C5-C6-C7-C8
26	f	101	BCR	C1-C6-C7-C8
26	h	101	BCR	C5-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C26
26	k	101	BCR	C1-C6-C7-C8
26	k	101	BCR	C5-C6-C7-C8
26	t	101	BCR	C1-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
29	A	613	LMG	C13-C14-C15-C16
29	a	613	LMG	C30-C31-C32-C33
30	D	406	LHG	C33-C34-C35-C36
28	A	614	SQD	C24-C23-O48-C46
28	a	614	SQD	C24-C23-O48-C46
30	a	616	LHG	C24-C23-O8-C6
24	C	506	CLA	C13-C15-C16-C17
24	c	506	CLA	C13-C15-C16-C17
28	X	101	SQD	C8-C7-O47-C45
28	x	101	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
32	C	517	DGD	C9B-CAB-CBB-CCB
32	d	405	DGD	O6E-C5E-C6E-O5E
30	D	406	LHG	C23-C24-C25-C26
28	B	622	SQD	C32-C33-C34-C35
28	b	601	SQD	C32-C33-C34-C35
32	C	515	DGD	CAA-CBA-CCA-CDA
32	c	516	DGD	C8B-C9B-CAB-CBB
27	a	611	PL9	C47-C48-C49-C50
29	D	408	LMG	C13-C14-C15-C16
30	d	406	LHG	C11-C10-C9-C8
30	d	406	LHG	C31-C32-C33-C34
30	e	101	LHG	C27-C28-C29-C30
24	B	606	CLA	O1D-CGD-O2D-CED
24	A	607	CLA	C6-C7-C8-C10
24	B	604	CLA	C6-C7-C8-C10
24	B	611	CLA	C12-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C10
24	C	504	CLA	C11-C12-C13-C15
24	C	510	CLA	C2-C3-C5-C6
24	a	607	CLA	C6-C7-C8-C10
24	b	605	CLA	C6-C7-C8-C10
24	b	612	CLA	C12-C13-C15-C16
24	b	618	CLA	C6-C7-C8-C10
24	c	504	CLA	C11-C12-C13-C15
24	c	510	CLA	C2-C3-C5-C6
24	A	609	CLA	O1A-CGA-O2A-C1
28	B	622	SQD	C29-C30-C31-C32
28	b	601	SQD	C29-C30-C31-C32
30	e	101	LHG	C17-C18-C19-C20
32	d	405	DGD	C5B-C6B-C7B-C8B
24	C	504	CLA	C13-C15-C16-C17
24	c	504	CLA	C13-C15-C16-C17
26	A	610	BCR	C19-C20-C21-C22
29	c	520	LMG	O9-C10-O7-C8
28	L	102	SQD	C7-C8-C9-C10
28	l	101	SQD	C7-C8-C9-C10
24	C	504	CLA	CBA-CGA-O2A-C1
29	D	408	LMG	C29-C28-O8-C9
30	L	101	LHG	C27-C28-C29-C30
32	C	516	DGD	C4A-C5A-C6A-C7A
24	C	503	CLA	C2A-CAA-CBA-CGA
24	C	503	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	d	401	PHO	C2C-C3C-CAC-CBC
28	b	601	SQD	C18-C19-C20-C21
32	c	517	DGD	C3B-C4B-C5B-C6B
28	B	622	SQD	C18-C19-C20-C21
30	d	406	LHG	C23-C24-C25-C26
29	C	519	LMG	C15-C16-C17-C18
30	A	615	LHG	C29-C30-C31-C32
30	E	102	LHG	C11-C10-C9-C8
32	E	101	DGD	C8B-C9B-CAB-CBB
27	D	405	PL9	C42-C43-C44-C45
28	a	612	SQD	C30-C31-C32-C33
29	C	518	LMG	C32-C33-C34-C35
32	C	517	DGD	C6B-C7B-C8B-C9B
32	c	518	DGD	C2B-C3B-C4B-C5B
26	B	619	BCR	C6-C7-C8-C9
26	C	514	BCR	C6-C7-C8-C9
26	h	101	BCR	C22-C23-C24-C25
32	C	515	DGD	O6E-C1E-O5D-C6D
32	C	516	DGD	O6E-C1E-O5D-C6D
32	c	517	DGD	O6E-C1E-O5D-C6D
24	C	501	CLA	C13-C15-C16-C17
24	c	501	CLA	C13-C15-C16-C17
27	a	611	PL9	C9-C11-C12-C13
28	A	612	SQD	C30-C31-C32-C33
29	A	613	LMG	C29-C30-C31-C32
29	j	101	LMG	C38-C39-C40-C41
30	l	102	LHG	C34-C35-C36-C37
32	c	517	DGD	C7B-C8B-C9B-CAB
32	d	405	DGD	C5A-C6A-C7A-C8A
29	B	621	LMG	C11-C10-O7-C8
30	D	406	LHG	C8-C7-O7-C5
26	t	101	BCR	C10-C11-C12-C13
29	C	519	LMG	C17-C18-C19-C20
30	a	616	LHG	C29-C30-C31-C32
24	B	607[A]	CLA	CBD-CGD-O2D-CED
32	d	405	DGD	C8B-C9B-CAB-CBB
28	X	101	SQD	O49-C7-O47-C45
28	x	101	SQD	O49-C7-O47-C45
29	j	101	LMG	C19-C20-C21-C22
32	h	102	DGD	C7A-C8A-C9A-CAA
32	d	405	DGD	O1A-C1A-O1G-C1G
32	C	517	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
32	d	405	DGD	C3A-C4A-C5A-C6A
24	C	510	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
27	D	405	PL9	C30-C29-C31-C32
29	b	622	LMG	C10-C11-C12-C13
29	b	622	LMG	C28-C29-C30-C31
27	A	611	PL9	C4-C3-C7-C8
27	a	611	PL9	C4-C3-C7-C8
29	A	613	LMG	C34-C35-C36-C37
24	A	607	CLA	C6-C7-C8-C9
24	B	611	CLA	C14-C13-C15-C16
24	B	616	CLA	C14-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C9
24	D	404	CLA	C11-C10-C8-C9
24	a	607	CLA	C6-C7-C8-C9
24	b	612	CLA	C14-C13-C15-C16
24	b	617	CLA	C14-C13-C15-C16
24	b	618	CLA	C6-C7-C8-C9
24	d	403	CLA	C11-C10-C8-C9
29	C	518	LMG	C38-C39-C40-C41
30	l	102	LHG	C32-C33-C34-C35
24	b	616	CLA	C2A-CAA-CBA-CGA
28	A	614	SQD	C18-C19-C20-C21
28	a	614	SQD	C18-C19-C20-C21
29	a	613	LMG	C18-C19-C20-C21
33	V	201	HEM	C4D-C3D-CAD-CBD
26	a	610	BCR	C36-C18-C19-C20
26	b	619	BCR	C36-C18-C19-C20
26	c	521	BCR	C37-C22-C23-C24
28	X	101	SQD	C23-C24-C25-C26
28	A	612	SQD	C34-C35-C36-C37
32	C	517	DGD	C3B-C4B-C5B-C6B
26	T	101	BCR	C17-C18-C19-C20
26	c	521	BCR	C11-C12-C13-C14
26	c	521	BCR	C17-C18-C19-C20
28	A	614	SQD	O10-C23-O48-C46
28	a	614	SQD	O10-C23-O48-C46
24	C	506	CLA	C1A-C2A-CAA-CBA
24	D	402	CLA	C1A-C2A-CAA-CBA
24	a	615	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	B	605	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	C	506	CLA	C16-C17-C18-C20
24	D	404	CLA	C16-C17-C18-C20
24	b	606	CLA	C16-C17-C18-C20
24	d	403	CLA	C16-C17-C18-C20
29	b	622	LMG	O9-C10-O7-C8
28	a	612	SQD	C34-C35-C36-C37
32	c	518	DGD	C4A-C5A-C6A-C7A
26	B	619	BCR	C13-C14-C15-C16
26	I	101	BCR	C9-C10-C11-C12
26	b	621	BCR	C15-C16-C17-C18
26	f	101	BCR	C15-C16-C17-C18
24	B	607[B]	CLA	C15-C16-C17-C18
24	C	507	CLA	C5-C6-C7-C8
24	b	608[B]	CLA	C15-C16-C17-C18
24	c	507	CLA	C5-C6-C7-C8
30	D	407	LHG	C3-O3-P-O6
30	e	101	LHG	C3-O3-P-O6
29	c	519	LMG	C11-C12-C13-C14
30	D	406	LHG	C25-C26-C27-C28
32	C	516	DGD	C6A-C7A-C8A-C9A
28	x	101	SQD	C23-C24-C25-C26
29	C	518	LMG	C17-C18-C19-C20
24	D	404	CLA	C13-C15-C16-C17
24	d	403	CLA	C13-C15-C16-C17
29	C	519	LMG	C29-C28-O8-C9
29	b	622	LMG	C33-C34-C35-C36
29	c	520	LMG	C38-C39-C40-C41
32	C	515	DGD	O6E-C5E-C6E-O5E
24	A	609	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C20
28	B	622	SQD	C27-C28-C29-C30
28	b	601	SQD	C27-C28-C29-C30
30	l	102	LHG	C27-C28-C29-C30
32	C	515	DGD	C4A-C5A-C6A-C7A
29	C	518	LMG	C11-C12-C13-C14
29	D	408	LMG	C35-C36-C37-C38
29	Z	101	LMG	C12-C13-C14-C15
29	a	613	LMG	C15-C16-C17-C18
30	a	616	LHG	C12-C13-C14-C15
28	B	622	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	C18-C19-C20-C21
30	a	616	LHG	C16-C17-C18-C19
30	e	101	LHG	C11-C10-C9-C8
32	C	515	DGD	C4D-C5D-C6D-O5D
29	A	613	LMG	C4-C5-C6-O5
28	b	601	SQD	C28-C29-C30-C31
29	b	622	LMG	C15-C16-C17-C18
29	c	520	LMG	C15-C16-C17-C18
32	C	516	DGD	C7B-C8B-C9B-CAB
28	a	612	SQD	C27-C28-C29-C30
29	B	621	LMG	C36-C37-C38-C39
30	d	406	LHG	C24-C25-C26-C27
32	C	517	DGD	C4A-C5A-C6A-C7A
32	E	101	DGD	CBA-CCA-CDA-CEA
28	A	612	SQD	C27-C28-C29-C30
29	c	519	LMG	C13-C14-C15-C16
33	v	201	HEM	C2D-C3D-CAD-CBD
24	A	607	CLA	C16-C17-C18-C19
24	a	607	CLA	C16-C17-C18-C19
24	a	609	CLA	C16-C17-C18-C19
28	A	614	SQD	O6-C44-C45-C46
28	X	101	SQD	C35-C36-C37-C38
28	a	614	SQD	O6-C44-C45-C46
29	Z	101	LMG	O1-C7-C8-C9
29	a	613	LMG	C7-C8-C9-O8
29	b	622	LMG	C18-C19-C20-C21
29	z	101	LMG	O1-C7-C8-C9
24	C	509	CLA	C10-C11-C12-C13
24	c	509	CLA	C10-C11-C12-C13
28	x	101	SQD	C35-C36-C37-C38
32	E	101	DGD	CAB-CBB-CCB-CDB
33	v	201	HEM	C4D-C3D-CAD-CBD
29	c	520	LMG	C8-C7-O1-C1
32	c	517	DGD	C5D-C6D-O5D-C1E
24	C	502	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	O1D-CGD-O2D-CED
30	d	407	LHG	C34-C35-C36-C37
32	h	102	DGD	C9A-CAA-CBA-CCA
32	h	102	DGD	CCB-CDB-CEB-CFB
28	B	622	SQD	C13-C14-C15-C16
28	B	622	SQD	C35-C36-C37-C38
28	b	601	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
28	b	601	SQD	C35-C36-C37-C38
32	C	517	DGD	C8B-C9B-CAB-CBB
29	D	408	LMG	O6-C1-O1-C7
24	C	511	CLA	O1D-CGD-O2D-CED
28	A	614	SQD	C19-C20-C21-C22
32	c	517	DGD	C5B-C6B-C7B-C8B
26	A	610	BCR	C15-C16-C17-C18
28	a	614	SQD	C19-C20-C21-C22
32	h	102	DGD	CCA-CDA-CEA-CFA
30	a	616	LHG	O10-C23-O8-C6
29	B	621	LMG	C28-C29-C30-C31
29	C	518	LMG	C29-C30-C31-C32
30	D	406	LHG	C24-C25-C26-C27
32	h	102	DGD	CBB-CCB-CDB-CEB
28	A	612	SQD	C35-C36-C37-C38
28	a	612	SQD	C35-C36-C37-C38
30	e	101	LHG	C15-C16-C17-C18
32	E	101	DGD	C3A-C4A-C5A-C6A
24	b	614	CLA	C13-C15-C16-C17
26	h	101	BCR	C35-C13-C14-C15
25	A	608	PHO	C4-C3-C5-C6
29	B	621	LMG	C15-C16-C17-C18
24	C	511	CLA	CBA-CGA-O2A-C1
24	A	609	CLA	C5-C6-C7-C8
32	h	102	DGD	CDB-CEB-CFB-CGB
24	a	609	CLA	C5-C6-C7-C8
24	c	509	CLA	C2-C1-O2A-CGA
32	d	405	DGD	CAA-CBA-CCA-CDA
29	B	621	LMG	C30-C31-C32-C33
30	D	407	LHG	C9-C10-C11-C12
30	a	616	LHG	C10-C11-C12-C13
32	H	102	DGD	CAA-CBA-CCA-CDA
24	B	608	CLA	O1A-CGA-O2A-C1
28	L	102	SQD	C19-C20-C21-C22
28	l	101	SQD	C19-C20-C21-C22
30	e	101	LHG	C26-C27-C28-C29
32	C	516	DGD	C8B-C9B-CAB-CBB
24	B	613	CLA	C13-C15-C16-C17
30	A	615	LHG	C25-C26-C27-C28
32	c	518	DGD	CBA-CCA-CDA-CEA
26	A	610	BCR	C11-C10-C9-C8
32	C	515	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
32	c	517	DGD	C2E-C1E-O5D-C6D
29	c	519	LMG	C34-C35-C36-C37
30	A	615	LHG	C33-C34-C35-C36
24	b	614	CLA	O1A-CGA-O2A-C1
24	a	609	CLA	C16-C17-C18-C20
32	C	516	DGD	CDA-CEA-CFA-CGA
32	E	101	DGD	C6A-C7A-C8A-C9A
29	c	519	LMG	C39-C40-C41-C42
29	z	101	LMG	C15-C16-C17-C18
24	A	609	CLA	C11-C10-C8-C7
24	B	602	CLA	C6-C7-C8-C10
24	B	602	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	B	617	CLA	C11-C12-C13-C15
24	C	501	CLA	C11-C12-C13-C15
24	C	506	CLA	C11-C12-C13-C15
24	C	508	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C10-C8-C7
24	C	513	CLA	C6-C7-C8-C10
24	D	404	CLA	C11-C10-C8-C7
24	a	609	CLA	C11-C10-C8-C7
24	b	603	CLA	C6-C7-C8-C10
24	b	603	CLA	C11-C10-C8-C7
24	b	617	CLA	C12-C13-C15-C16
24	b	618	CLA	C11-C12-C13-C15
24	c	501	CLA	C11-C12-C13-C15
24	c	506	CLA	C11-C12-C13-C15
24	c	508	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C10-C8-C7
24	c	513	CLA	C6-C7-C8-C10
24	d	403	CLA	C11-C10-C8-C7
27	d	404	PL9	C13-C14-C16-C17
24	c	504	CLA	O1A-CGA-O2A-C1
24	B	617	CLA	C11-C12-C13-C14
24	C	501	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	C	508	CLA	C11-C10-C8-C9
24	C	513	CLA	C11-C12-C13-C14
24	b	618	CLA	C11-C12-C13-C14
24	c	501	CLA	C14-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C14
24	c	508	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	513	CLA	C11-C12-C13-C14
26	K	101	BCR	C15-C16-C17-C18
26	K	102	BCR	C15-C16-C17-C18
26	t	101	BCR	C15-C16-C17-C18
28	A	612	SQD	C14-C15-C16-C17
28	a	612	SQD	C14-C15-C16-C17
29	Z	101	LMG	C13-C14-C15-C16
30	E	102	LHG	C26-C27-C28-C29
26	t	101	BCR	C36-C18-C19-C20
24	A	609	CLA	C16-C17-C18-C20
24	B	605	CLA	C16-C17-C18-C19
24	B	617	CLA	C16-C17-C18-C20
24	b	606	CLA	C16-C17-C18-C19
24	b	618	CLA	C16-C17-C18-C20
28	A	614	SQD	C25-C26-C27-C28
29	A	613	LMG	C22-C23-C24-C25
26	F	101	BCR	C17-C18-C19-C20
26	c	521	BCR	C21-C22-C23-C24
28	a	614	SQD	C25-C26-C27-C28
29	A	613	LMG	C21-C22-C23-C24
32	E	101	DGD	C4B-C5B-C6B-C7B
32	E	101	DGD	O1A-C1A-O1G-C1G
28	B	622	SQD	C24-C23-O48-C46
28	b	601	SQD	C24-C23-O48-C46
28	A	612	SQD	C19-C20-C21-C22
28	a	612	SQD	C19-C20-C21-C22
29	B	621	LMG	C31-C32-C33-C34
30	E	102	LHG	C9-C10-C11-C12
32	c	517	DGD	CDA-CEA-CFA-CGA
29	Z	101	LMG	C4-C5-C6-O5
29	D	408	LMG	C30-C31-C32-C33
30	A	615	LHG	C17-C18-C19-C20
32	C	517	DGD	C5B-C6B-C7B-C8B
26	B	618	BCR	C6-C7-C8-C9
26	c	515	BCR	C22-C23-C24-C25
24	a	607	CLA	CBD-CGD-O2D-CED
28	a	614	SQD	C31-C32-C33-C34
24	B	603	CLA	C4B-C3B-CAB-CBB
24	B	608	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
24	D	404	CLA	C4B-C3B-CAB-CBB
24	b	608[A]	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	b	608[B]	CLA	C4B-C3B-CAB-CBB
24	b	618	CLA	C4B-C3B-CAB-CBB
24	c	502	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C4B-C3B-CAB-CBB
28	A	614	SQD	O5-C1-O6-C44
28	a	614	SQD	O5-C1-O6-C44
30	L	101	LHG	O6-C4-C5-C6
30	l	102	LHG	O6-C4-C5-C6
28	A	614	SQD	C31-C32-C33-C34
30	d	407	LHG	C13-C14-C15-C16
29	c	519	LMG	C20-C21-C22-C23
27	A	611	PL9	C28-C29-C31-C32
27	d	404	PL9	C43-C44-C46-C47
24	D	403	CLA	O1D-CGD-O2D-CED
24	B	609	CLA	C13-C15-C16-C17
24	b	610	CLA	C13-C15-C16-C17
24	B	604	CLA	C16-C17-C18-C20
24	b	605	CLA	C16-C17-C18-C20
29	z	101	LMG	C13-C14-C15-C16
32	E	101	DGD	CAA-CBA-CCA-CDA
29	C	518	LMG	C14-C15-C16-C17
24	B	602	CLA	C3A-C2A-CAA-CBA
24	B	605	CLA	C4C-C3C-CAC-CBC
29	C	519	LMG	C33-C34-C35-C36
28	l	101	SQD	C35-C36-C37-C38
24	C	508	CLA	C5-C6-C7-C8
24	b	617	CLA	C13-C15-C16-C17
24	c	508	CLA	C5-C6-C7-C8
28	L	102	SQD	C35-C36-C37-C38
29	C	518	LMG	C34-C35-C36-C37
30	D	406	LHG	C27-C28-C29-C30
30	l	102	LHG	C14-C15-C16-C17
28	A	614	SQD	C32-C33-C34-C35
28	a	614	SQD	C32-C33-C34-C35
30	D	406	LHG	C31-C32-C33-C34
28	B	622	SQD	C44-C45-C46-O48
28	L	102	SQD	C44-C45-C46-O48
28	b	601	SQD	C44-C45-C46-O48
28	l	101	SQD	C44-C45-C46-O48
29	D	408	LMG	C7-C8-C9-O8
29	C	519	LMG	O9-C10-O7-C8
32	C	516	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
29	a	613	LMG	C39-C40-C41-C42
30	A	615	LHG	C24-C25-C26-C27
24	B	616	CLA	C13-C15-C16-C17
30	E	102	LHG	C19-C20-C21-C22
32	C	515	DGD	CBA-CCA-CDA-CEA
30	A	615	LHG	C27-C28-C29-C30
24	B	605	CLA	C2C-C3C-CAC-CBC
24	b	606	CLA	C2C-C3C-CAC-CBC
30	A	615	LHG	C18-C19-C20-C21
32	C	516	DGD	C9B-CAB-CBB-CCB
30	E	102	LHG	C3-O3-P-O6
30	D	407	LHG	O10-C23-O8-C6
24	B	613	CLA	O1D-CGD-O2D-CED
24	D	404	CLA	C2B-C3B-CAB-CBB
24	b	608[A]	CLA	C2B-C3B-CAB-CBB
24	b	608[B]	CLA	C2B-C3B-CAB-CBB
24	b	618	CLA	C2B-C3B-CAB-CBB
28	A	614	SQD	C35-C36-C37-C38
28	a	614	SQD	C35-C36-C37-C38
32	C	516	DGD	CDB-CEB-CFB-CGB
32	E	101	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	C6A-C7A-C8A-C9A
24	B	616	CLA	C10-C11-C12-C13
24	b	617	CLA	C10-C11-C12-C13
24	B	602	CLA	O1A-CGA-O2A-C1
30	D	406	LHG	C15-C16-C17-C18
28	B	622	SQD	O47-C45-C46-O48
28	L	102	SQD	O47-C45-C46-O48
28	b	601	SQD	O47-C45-C46-O48
28	l	101	SQD	O47-C45-C46-O48
32	E	101	DGD	O1G-C1G-C2G-O2G
32	d	405	DGD	O1G-C1G-C2G-O2G
24	b	615	CLA	O1D-CGD-O2D-CED
28	L	102	SQD	C30-C31-C32-C33
26	I	101	BCR	C15-C16-C17-C18
26	c	515	BCR	C15-C16-C17-C18
29	c	520	LMG	C11-C10-O7-C8
24	B	602	CLA	C16-C17-C18-C20
24	b	603	CLA	C16-C17-C18-C20
28	l	101	SQD	C30-C31-C32-C33
27	D	405	PL9	C39-C41-C42-C43
24	b	603	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	D	405	PL9	C13-C14-C16-C17
30	d	407	LHG	C32-C33-C34-C35
24	B	615	CLA	C11-C12-C13-C14
24	B	615	CLA	C14-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C9
24	b	616	CLA	C11-C12-C13-C14
24	b	616	CLA	C14-C13-C15-C16
24	c	507	CLA	C11-C10-C8-C9
29	B	621	LMG	C33-C34-C35-C36
29	B	621	LMG	C34-C35-C36-C37
29	c	520	LMG	C11-C12-C13-C14
24	B	602	CLA	C15-C16-C17-C18
24	B	607[A]	CLA	C8-C10-C11-C12
24	b	603	CLA	C15-C16-C17-C18
24	b	608[A]	CLA	C8-C10-C11-C12
30	A	615	LHG	C2-C3-O3-P
29	C	518	LMG	C20-C21-C22-C23
30	L	101	LHG	C32-C33-C34-C35
32	H	102	DGD	C5A-C6A-C7A-C8A
24	B	606	CLA	CBD-CGD-O2D-CED
26	K	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	b	619	BCR	C23-C24-C25-C26
26	k	101	BCR	C23-C24-C25-C30
29	a	613	LMG	C22-C23-C24-C25
32	H	102	DGD	O2G-C1B-C2B-C3B
26	K	102	BCR	C36-C18-C19-C20
27	A	611	PL9	C47-C48-C49-C50
28	B	622	SQD	C16-C17-C18-C19
24	B	612	CLA	O1D-CGD-O2D-CED
26	H	101	BCR	C21-C22-C23-C24
26	k	101	BCR	C21-C22-C23-C24
24	C	502	CLA	C15-C16-C17-C18
24	c	502	CLA	C15-C16-C17-C18
28	b	601	SQD	C16-C17-C18-C19
30	l	102	LHG	C25-C26-C27-C28
24	a	615	CLA	C4C-C3C-CAC-CBC
29	c	520	LMG	C40-C41-C42-C43
30	D	406	LHG	C13-C14-C15-C16
24	B	607[B]	CLA	C16-C17-C18-C19
24	C	501	CLA	C16-C17-C18-C19
24	C	502	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	b	608[B]	CLA	C16-C17-C18-C19
24	c	501	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C20
30	D	407	LHG	O6-C4-C5-C6
24	B	612	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	B	616	CLA	C11-C10-C8-C7
24	B	617	CLA	C12-C13-C15-C16
24	C	501	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	C	513	CLA	C11-C12-C13-C15
24	D	404	CLA	C6-C7-C8-C10
24	b	613	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C12-C13-C15
24	b	617	CLA	C11-C10-C8-C7
24	b	618	CLA	C12-C13-C15-C16
24	c	501	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C12-C13-C15
24	d	403	CLA	C6-C7-C8-C10
28	b	601	SQD	O10-C23-O48-C46
32	c	516	DGD	O1A-C1A-O1G-C1G
29	A	613	LMG	C15-C16-C17-C18
26	F	101	BCR	C19-C20-C21-C22
26	H	101	BCR	C13-C14-C15-C16
26	b	620	BCR	C15-C16-C17-C18
26	t	101	BCR	C9-C10-C11-C12
24	B	617	CLA	C16-C17-C18-C19
28	B	622	SQD	O10-C23-O48-C46
26	I	101	BCR	C11-C10-C9-C34
26	c	521	BCR	C16-C17-C18-C36
30	L	101	LHG	C24-C25-C26-C27
32	d	405	DGD	O6D-C5D-C6D-O5D
32	H	102	DGD	CDB-CEB-CFB-CGB
24	b	618	CLA	C16-C17-C18-C19
24	A	609	CLA	CBA-CGA-O2A-C1
30	D	407	LHG	C24-C23-O8-C6
32	E	101	DGD	C4D-C5D-C6D-O5D
28	x	101	SQD	C11-C10-C9-C8
29	c	519	LMG	C30-C31-C32-C33
30	d	406	LHG	C34-C35-C36-C37
32	c	518	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
32	d	405	DGD	CAB-CBB-CCB-CDB
24	C	503	CLA	C8-C10-C11-C12
24	c	503	CLA	C8-C10-C11-C12
24	A	606	CLA	CAD-CBD-CGD-O2D
24	A	609	CLA	CAD-CBD-CGD-O2D
24	C	501	CLA	CAD-CBD-CGD-O2D
24	C	509	CLA	CAD-CBD-CGD-O2D
24	b	603	CLA	CAD-CBD-CGD-O2D
24	c	513	CLA	CAD-CBD-CGD-O2D
25	A	608	PHO	CAD-CBD-CGD-O2D
29	c	519	LMG	O9-C10-O7-C8
28	X	101	SQD	C11-C10-C9-C8
32	C	517	DGD	C7A-C8A-C9A-CAA
30	D	406	LHG	C11-C10-C9-C8
26	B	620	BCR	C6-C7-C8-C9
29	A	613	LMG	C7-C8-C9-O8
32	E	101	DGD	O1G-C1G-C2G-C3G
32	H	102	DGD	O1G-C1G-C2G-C3G
24	B	606	CLA	O1A-CGA-O2A-C1
30	L	101	LHG	O6-C4-C5-O7
28	A	614	SQD	C24-C25-C26-C27
28	a	614	SQD	C24-C25-C26-C27
24	C	510	CLA	CBA-CGA-O2A-C1
24	B	615	CLA	C2A-CAA-CBA-CGA
24	B	604	CLA	C16-C17-C18-C19
24	b	605	CLA	C16-C17-C18-C19
29	C	518	LMG	C22-C23-C24-C25
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	604	CLA	CHA-CBD-CGD-O2D
24	B	607[A]	CLA	CHA-CBD-CGD-O1D
24	B	607[B]	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	610	CLA	CHA-CBD-CGD-O1D
24	B	610	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	b	604	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	b	608[A]	CLA	CHA-CBD-CGD-O1D
24	b	608[B]	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
32	C	515	DGD	CBB-CCB-CDB-CEB
28	A	614	SQD	C2-C1-O6-C44
28	a	614	SQD	C2-C1-O6-C44
29	C	519	LMG	C11-C12-C13-C14
32	C	515	DGD	CDA-CEA-CFA-CGA
32	C	517	DGD	CAB-CBB-CCB-CDB
29	a	613	LMG	O7-C8-C9-O8
30	d	407	LHG	C10-C11-C12-C13
24	b	609	CLA	O1A-CGA-O2A-C1
32	C	517	DGD	O1A-C1A-O1G-C1G
28	A	614	SQD	C29-C30-C31-C32
28	a	614	SQD	C29-C30-C31-C32
29	B	621	LMG	C18-C19-C20-C21
24	B	602	CLA	C16-C17-C18-C19
24	C	501	CLA	C16-C17-C18-C20
24	b	603	CLA	C16-C17-C18-C19
24	c	501	CLA	C16-C17-C18-C20
30	E	102	LHG	C12-C13-C14-C15
32	c	517	DGD	CDB-CEB-CFB-CGB
27	a	611	PL9	C15-C14-C16-C17
32	C	516	DGD	CCA-CDA-CEA-CFA
32	C	515	DGD	O1A-C1A-O1G-C1G
25	A	608	PHO	C2-C3-C5-C6
27	a	611	PL9	C28-C29-C31-C32
28	A	614	SQD	C27-C28-C29-C30
28	a	614	SQD	C27-C28-C29-C30
24	A	609	CLA	C11-C12-C13-C14
24	B	612	CLA	C14-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C9
24	a	609	CLA	C11-C12-C13-C14
24	b	613	CLA	C14-C13-C15-C16
24	d	403	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	512	CLA	O1D-CGD-O2D-CED
29	c	519	LMG	C14-C15-C16-C17
29	a	613	LMG	O6-C5-C6-O5
32	C	516	DGD	C8A-C9A-CAA-CBA
32	C	516	DGD	CBA-CCA-CDA-CEA
26	T	101	BCR	C36-C18-C19-C20
26	c	521	BCR	C36-C18-C19-C20
30	E	102	LHG	O1-C1-C2-C3
26	I	101	BCR	C17-C18-C19-C20
26	b	619	BCR	C17-C18-C19-C20
26	b	621	BCR	C17-C18-C19-C20
26	t	101	BCR	C17-C18-C19-C20
24	b	612	CLA	C8-C10-C11-C12
29	j	101	LMG	C17-C18-C19-C20
24	B	602	CLA	C2-C1-O2A-CGA
24	a	606	CLA	C2-C1-O2A-CGA
24	b	618	CLA	C2-C1-O2A-CGA
29	A	613	LMG	C11-C12-C13-C14
29	C	518	LMG	C19-C20-C21-C22
26	T	101	BCR	C9-C10-C11-C12
30	E	102	LHG	C4-O6-P-O3
30	a	616	LHG	C11-C10-C9-C8
24	b	606	CLA	C4C-C3C-CAC-CBC
24	B	614	CLA	C13-C15-C16-C17
30	a	616	LHG	C2-C3-O3-P
29	C	518	LMG	C31-C32-C33-C34
30	L	101	LHG	C14-C15-C16-C17
32	C	516	DGD	C7A-C8A-C9A-CAA
30	D	407	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O5
30	e	101	LHG	C3-O3-P-O4
30	l	102	LHG	C4-O6-P-O5
24	B	611	CLA	C16-C17-C18-C19
24	b	612	CLA	C16-C17-C18-C19
30	d	406	LHG	C15-C16-C17-C18
32	c	516	DGD	C9A-CAA-CBA-CCA
32	c	516	DGD	O6D-C1D-O3G-C3G
24	B	611	CLA	C8-C10-C11-C12
24	b	615	CLA	C13-C15-C16-C17
29	A	613	LMG	C29-C28-O8-C9
24	B	615	CLA	CBD-CGD-O2D-CED
29	c	519	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
28	a	614	SQD	C9-C10-C11-C12
28	A	614	SQD	C9-C10-C11-C12
29	j	101	LMG	C11-C12-C13-C14
32	C	515	DGD	C5A-C6A-C7A-C8A
29	Z	101	LMG	C18-C19-C20-C21
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	510	CLA	CAD-CBD-CGD-O1D
24	b	603	CLA	CAD-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
28	A	612	SQD	C23-C24-C25-C26
28	a	612	SQD	C23-C24-C25-C26
29	a	613	LMG	C29-C30-C31-C32
32	H	102	DGD	C8A-C9A-CAA-CBA
32	c	517	DGD	C5A-C6A-C7A-C8A
24	B	605	CLA	C3-C5-C6-C7
24	b	606	CLA	C3-C5-C6-C7
24	D	402	CLA	C2C-C3C-CAC-CBC
28	B	622	SQD	C19-C20-C21-C22
28	b	601	SQD	C19-C20-C21-C22
28	X	101	SQD	C28-C29-C30-C31
32	c	517	DGD	C6A-C7A-C8A-C9A
24	B	602	CLA	CBA-CGA-O2A-C1
24	b	603	CLA	CBA-CGA-O2A-C1
28	x	101	SQD	C28-C29-C30-C31
32	c	518	DGD	CAB-CBB-CCB-CDB
24	b	617	CLA	C16-C17-C18-C20
24	c	502	CLA	CBD-CGD-O2D-CED
24	A	607	CLA	C11-C10-C8-C7
24	B	615	CLA	C12-C13-C15-C16
24	C	504	CLA	C12-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C10
24	C	509	CLA	C6-C7-C8-C10
24	D	404	CLA	C11-C12-C13-C15
24	D	404	CLA	C12-C13-C15-C16
24	a	607	CLA	C11-C10-C8-C7
24	b	616	CLA	C12-C13-C15-C16
24	c	504	CLA	C12-C13-C15-C16
24	c	506	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	C6-C7-C8-C10
24	d	403	CLA	C12-C13-C15-C16
29	a	613	LMG	C10-C11-C12-C13
30	l	102	LHG	O6-C4-C5-O7
32	C	515	DGD	C9A-CAA-CBA-CCA
32	c	516	DGD	C5A-C6A-C7A-C8A
32	c	518	DGD	CDB-CEB-CFB-CGB
27	A	611	PL9	C2-C3-C7-C8
29	A	613	LMG	C10-C11-C12-C13
29	A	613	LMG	C17-C18-C19-C20
29	j	101	LMG	C34-C35-C36-C37
30	a	616	LHG	C17-C18-C19-C20
32	h	102	DGD	C5A-C6A-C7A-C8A
24	B	616	CLA	C16-C17-C18-C20
29	C	519	LMG	C40-C41-C42-C43
29	C	519	LMG	C16-C17-C18-C19
29	a	613	LMG	O1-C7-C8-C9
30	A	615	LHG	C30-C31-C32-C33
32	c	518	DGD	C3B-C4B-C5B-C6B
32	c	518	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	O1G-C1G-C2G-C3G
29	A	613	LMG	O1-C7-C8-O7
29	A	613	LMG	O7-C8-C9-O8
29	D	408	LMG	O7-C8-C9-O8
29	a	613	LMG	O1-C7-C8-O7
30	E	102	LHG	O7-C5-C6-O8
32	h	102	DGD	O1G-C1G-C2G-O2G
30	e	101	LHG	C9-C10-C11-C12
29	C	519	LMG	C8-C7-O1-C1
32	C	516	DGD	C2G-C3G-O3G-C1D
32	C	516	DGD	C5D-C6D-O5D-C1E
32	c	517	DGD	C2G-C3G-O3G-C1D
24	c	513	CLA	C3-C5-C6-C7
27	A	611	PL9	C15-C14-C16-C17
29	a	613	LMG	C33-C34-C35-C36
29	A	613	LMG	C39-C40-C41-C42
32	d	405	DGD	CBB-CCB-CDB-CEB
24	A	607	CLA	C11-C10-C8-C9
24	A	609	CLA	C11-C10-C8-C9
24	B	617	CLA	C14-C13-C15-C16
24	C	504	CLA	C14-C13-C15-C16
24	a	607	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	618	CLA	C14-C13-C15-C16
24	c	504	CLA	C14-C13-C15-C16
24	c	512	CLA	C11-C10-C8-C9
26	t	101	BCR	C6-C7-C8-C9
24	C	513	CLA	C3-C5-C6-C7
28	l	101	SQD	C13-C14-C15-C16
30	E	102	LHG	O1-C1-C2-O2
29	b	622	LMG	C35-C36-C37-C38
30	E	102	LHG	C17-C18-C19-C20
30	d	407	LHG	C11-C10-C9-C8
26	c	515	BCR	C13-C14-C15-C16
28	L	102	SQD	C13-C14-C15-C16
29	a	613	LMG	C17-C18-C19-C20
29	D	408	LMG	C11-C12-C13-C14
24	B	603	CLA	C2B-C3B-CAB-CBB
24	B	607[A]	CLA	C2B-C3B-CAB-CBB
24	B	607[B]	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C2B-C3B-CAB-CBB
24	C	503	CLA	C2B-C3B-CAB-CBB
24	C	505	CLA	C2B-C3B-CAB-CBB
24	b	611	CLA	C2B-C3B-CAB-CBB
28	B	622	SQD	C14-C15-C16-C17
28	b	601	SQD	C14-C15-C16-C17
29	B	621	LMG	C39-C40-C41-C42
29	C	519	LMG	C36-C37-C38-C39
29	Z	101	LMG	C15-C16-C17-C18
32	c	518	DGD	C7A-C8A-C9A-CAA
28	B	622	SQD	C46-C45-O47-C7
28	b	601	SQD	C46-C45-O47-C7
29	c	520	LMG	C16-C17-C18-C19
29	C	518	LMG	O9-C10-O7-C8
24	B	617	CLA	C2-C1-O2A-CGA
24	C	506	CLA	C2-C1-O2A-CGA
29	C	518	LMG	C30-C31-C32-C33
29	c	519	LMG	C29-C28-O8-C9
26	K	102	BCR	C19-C20-C21-C22
30	L	101	LHG	O10-C23-O8-C6
30	D	407	LHG	O6-C4-C5-O7
24	B	603	CLA	O1D-CGD-O2D-CED
27	a	611	PL9	C35-C34-C36-C37
29	c	520	LMG	C36-C37-C38-C39
32	c	517	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
26	A	610	BCR	C1-C6-C7-C8
26	F	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C23-C24-C25-C30
26	t	101	BCR	C23-C24-C25-C26
24	b	603	CLA	CAA-CBA-CGA-O2A
29	B	621	LMG	O8-C28-C29-C30
30	l	102	LHG	C28-C29-C30-C31
24	C	512	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C19
24	b	612	CLA	C2A-CAA-CBA-CGA
26	K	101	BCR	C20-C21-C22-C23
29	A	613	LMG	C2-C1-O1-C7
30	D	406	LHG	C3-O3-P-O6
30	e	101	LHG	C4-O6-P-O3
29	A	613	LMG	O1-C7-C8-C9
29	b	622	LMG	C30-C31-C32-C33
24	C	506	CLA	C12-C13-C15-C16
24	c	506	CLA	C12-C13-C15-C16
24	d	403	CLA	C11-C12-C13-C15
32	c	516	DGD	CBA-CCA-CDA-CEA
24	B	602	CLA	C6-C7-C8-C9
24	B	616	CLA	C11-C10-C8-C9
24	C	506	CLA	C6-C7-C8-C9
24	C	512	CLA	C11-C10-C8-C9
24	C	513	CLA	C6-C7-C8-C9
24	a	609	CLA	C11-C10-C8-C9
24	b	603	CLA	C6-C7-C8-C9
24	b	617	CLA	C11-C10-C8-C9
24	c	506	CLA	C6-C7-C8-C9
24	c	513	CLA	C6-C7-C8-C9
26	B	619	BCR	C19-C20-C21-C22
24	B	611	CLA	C16-C17-C18-C20
24	b	612	CLA	C16-C17-C18-C20
29	A	613	LMG	C19-C20-C21-C22
30	l	102	LHG	C9-C10-C11-C12
24	C	502	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C19
29	C	519	LMG	C39-C40-C41-C42
32	E	101	DGD	C5A-C6A-C7A-C8A
27	D	405	PL9	C36-C37-C38-C39
30	D	406	LHG	O1-C1-C2-O2
24	B	616	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	b	617	CLA	C16-C17-C18-C19
24	c	504	CLA	CBA-CGA-O2A-C1
32	d	405	DGD	C2A-C1A-O1G-C1G
30	d	406	LHG	C17-C18-C19-C20
24	a	609	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	CBD-CGD-O2D-CED
32	C	515	DGD	CCA-CDA-CEA-CFA
32	E	101	DGD	CDB-CEB-CFB-CGB
24	C	501	CLA	O1A-CGA-O2A-C1
24	b	615	CLA	O1A-CGA-O2A-C1
24	B	607[A]	CLA	C4B-C3B-CAB-CBB
24	B	607[B]	CLA	C4B-C3B-CAB-CBB
24	C	502	CLA	C4B-C3B-CAB-CBB
29	A	613	LMG	O6-C1-O1-C7
26	b	620	BCR	C9-C10-C11-C12
24	b	613	CLA	O1A-CGA-O2A-C1
24	A	607	CLA	C2C-C3C-CAC-CBC
24	A	607	CLA	C4C-C3C-CAC-CBC
29	B	621	LMG	C13-C14-C15-C16
32	h	102	DGD	C8B-C9B-CAB-CBB
26	k	101	BCR	C18-C19-C20-C21
24	d	403	CLA	O1A-CGA-O2A-C1
32	H	102	DGD	C7B-C8B-C9B-CAB
27	d	404	PL9	C15-C14-C16-C17
24	B	611	CLA	C13-C15-C16-C17
24	b	612	CLA	C13-C15-C16-C17
29	c	519	LMG	C21-C22-C23-C24
30	L	101	LHG	C16-C17-C18-C19
32	c	518	DGD	O6D-C5D-C6D-O5D
28	a	614	SQD	C10-C11-C12-C13
28	A	614	SQD	C10-C11-C12-C13
27	d	404	PL9	C42-C43-C44-C45
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
24	c	509	CLA	C2A-CAA-CBA-CGA
32	C	516	DGD	C2B-C3B-C4B-C5B
24	B	616	CLA	C3A-C2A-CAA-CBA
24	b	603	CLA	C3A-C2A-CAA-CBA
29	z	101	LMG	C14-C15-C16-C17
30	e	101	LHG	C19-C20-C21-C22
33	e	102	HEM	CAD-CBD-CGD-O1D
29	c	519	LMG	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
24	B	617	CLA	C13-C15-C16-C17
26	B	619	BCR	C35-C13-C14-C15
30	A	615	LHG	C13-C14-C15-C16
24	C	512	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C20
24	C	506	CLA	CBA-CGA-O2A-C1
24	C	510	CLA	C8-C10-C11-C12
24	b	618	CLA	C13-C15-C16-C17
24	c	510	CLA	C8-C10-C11-C12
24	c	505	CLA	CBD-CGD-O2D-CED
29	C	519	LMG	C12-C13-C14-C15
27	d	404	PL9	C35-C34-C36-C37
24	B	603	CLA	C1A-C2A-CAA-CBA
24	B	611	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C1A-C2A-CAA-CBA
24	D	403	CLA	C1A-C2A-CAA-CBA
29	b	622	LMG	C39-C40-C41-C42
24	A	609	CLA	C12-C13-C15-C16
24	B	607[B]	CLA	C11-C10-C8-C7
24	C	502	CLA	C12-C13-C15-C16
24	C	504	CLA	C11-C10-C8-C7
24	a	609	CLA	C12-C13-C15-C16
24	b	608[B]	CLA	C11-C10-C8-C7
24	c	502	CLA	C12-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C7
24	C	505	CLA	C2A-CAA-CBA-CGA
29	a	613	LMG	C21-C22-C23-C24
30	D	407	LHG	C35-C36-C37-C38
29	Z	101	LMG	O6-C5-C6-O5
24	B	608	CLA	CBA-CGA-O2A-C1
33	e	102	HEM	CAD-CBD-CGD-O2D
27	a	611	PL9	C45-C44-C46-C47
27	d	404	PL9	C12-C11-C9-C10
32	C	515	DGD	C1B-C2B-C3B-C4B
24	b	604	CLA	C2B-C3B-CAB-CBB
24	c	513	CLA	C2B-C3B-CAB-CBB
24	C	513	CLA	C16-C17-C18-C19
24	c	513	CLA	C16-C17-C18-C19
29	c	520	LMG	C39-C40-C41-C42
30	d	406	LHG	C11-C12-C13-C14
29	C	518	LMG	C33-C34-C35-C36
28	A	612	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
28	a	612	SQD	O6-C44-C45-O47
32	E	101	DGD	O2G-C2G-C3G-O3G
32	H	102	DGD	O1G-C1G-C2G-O2G
30	d	407	LHG	C26-C27-C28-C29
32	C	517	DGD	CBA-CCA-CDA-CEA
24	c	502	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	C6-C7-C8-C9
29	c	520	LMG	C32-C33-C34-C35
24	c	501	CLA	C2A-CAA-CBA-CGA
24	c	505	CLA	C2A-CAA-CBA-CGA
26	B	619	BCR	C1-C6-C7-C8
26	C	514	BCR	C1-C6-C7-C8
26	K	101	BCR	C23-C24-C25-C30
26	a	610	BCR	C23-C24-C25-C30
26	c	515	BCR	C1-C6-C7-C8
24	b	610	CLA	C4C-C3C-CAC-CBC
32	d	405	DGD	CDB-CEB-CFB-CGB
29	c	520	LMG	C37-C38-C39-C40
24	C	513	CLA	C4-C3-C5-C6
24	c	513	CLA	C4-C3-C5-C6
25	a	608	PHO	C4-C3-C5-C6
27	A	611	PL9	C45-C44-C46-C47
32	E	101	DGD	O6E-C5E-C6E-O5E
26	K	101	BCR	C21-C22-C23-C24
30	d	407	LHG	C16-C17-C18-C19
24	B	610	CLA	C2-C3-C5-C6
24	b	611	CLA	C2-C3-C5-C6
25	a	608	PHO	C2-C3-C5-C6
24	B	602	CLA	CAA-CBA-CGA-O2A
29	A	613	LMG	C20-C21-C22-C23
30	e	101	LHG	O6-C4-C5-O7
32	c	516	DGD	CCA-CDA-CEA-CFA
32	h	102	DGD	CDA-CEA-CFA-CGA
24	C	506	CLA	CBD-CGD-O2D-CED
24	B	613	CLA	CBA-CGA-O2A-C1
24	B	615	CLA	CBA-CGA-O2A-C1
32	d	405	DGD	C4E-C5E-C6E-O5E
24	C	505	CLA	C4B-C3B-CAB-CBB
24	b	603	CLA	C4B-C3B-CAB-CBB
24	b	604	CLA	C4B-C3B-CAB-CBB
24	b	611	CLA	C4B-C3B-CAB-CBB
25	D	401	PHO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	c	507	CLA	C4-C3-C5-C6
27	D	405	PL9	C19-C21-C22-C23
26	b	620	BCR	C19-C20-C21-C22
33	E	103	HEM	CAD-CBD-CGD-O1D
32	H	102	DGD	CDA-CEA-CFA-CGA
30	a	616	LHG	O7-C5-C6-O8
32	C	515	DGD	C8B-C9B-CAB-CBB
24	a	615	CLA	C2A-CAA-CBA-CGA
25	D	401	PHO	C5-C6-C7-C8
30	D	407	LHG	C25-C26-C27-C28
30	l	102	LHG	C17-C18-C19-C20
26	k	101	BCR	C35-C13-C14-C15
30	D	407	LHG	C13-C14-C15-C16
32	C	517	DGD	C2B-C3B-C4B-C5B
24	C	507	CLA	C4-C3-C5-C6
24	a	609	CLA	C4-C3-C5-C6
27	D	405	PL9	C12-C11-C9-C10
29	C	518	LMG	C29-C28-O8-C9
30	l	102	LHG	O7-C7-C8-C9
28	b	601	SQD	C33-C34-C35-C36
32	c	518	DGD	C6B-C7B-C8B-C9B
24	B	607[A]	CLA	C11-C12-C13-C14
24	B	607[B]	CLA	C11-C10-C8-C9
24	D	404	CLA	C11-C12-C13-C14
24	b	608[A]	CLA	C11-C12-C13-C14
24	b	608[B]	CLA	C11-C10-C8-C9
24	c	510	CLA	C6-C7-C8-C9
24	d	403	CLA	C11-C12-C13-C14
28	B	622	SQD	C33-C34-C35-C36
32	c	516	DGD	C3B-C4B-C5B-C6B
24	b	605	CLA	C13-C15-C16-C17
24	A	609	CLA	C3A-C2A-CAA-CBA
24	C	512	CLA	C3A-C2A-CAA-CBA
24	b	617	CLA	C3A-C2A-CAA-CBA
24	B	604	CLA	C13-C15-C16-C17
24	C	510	CLA	CAA-CBA-CGA-O2A
24	D	403	CLA	CAA-CBA-CGA-O2A
30	E	102	LHG	O7-C7-C8-C9
32	d	405	DGD	C4B-C5B-C6B-C7B
24	B	606	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	606	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	c	501	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CAD-CBD-CGD-O2D
24	D	402	CLA	C4C-C3C-CAC-CBC
30	D	406	LHG	C17-C18-C19-C20
28	B	622	SQD	C17-C18-C19-C20
28	L	102	SQD	O48-C23-C24-C25
24	A	609	CLA	C4-C3-C5-C6
28	l	101	SQD	O48-C23-C24-C25
29	j	101	LMG	O7-C10-C11-C12
30	L	101	LHG	O7-C7-C8-C9
28	b	601	SQD	C17-C18-C19-C20
26	A	610	BCR	C21-C22-C23-C24
26	C	514	BCR	C11-C12-C13-C14
26	h	101	BCR	C7-C8-C9-C10
29	c	520	LMG	C14-C15-C16-C17
30	d	406	LHG	C27-C28-C29-C30
30	E	102	LHG	C4-C5-C6-O8
27	A	611	PL9	C21-C22-C23-C24
24	c	510	CLA	CAA-CBA-CGA-O2A
32	c	518	DGD	O1G-C1A-C2A-C3A
24	B	605	CLA	O2A-C1-C2-C3
24	C	512	CLA	O2A-C1-C2-C3
24	D	403	CLA	O2A-C1-C2-C3
24	b	604	CLA	O2A-C1-C2-C3
24	b	606	CLA	O2A-C1-C2-C3
24	c	509	CLA	O2A-C1-C2-C3
24	c	512	CLA	O2A-C1-C2-C3
24	d	402	CLA	O2A-C1-C2-C3
25	A	608	PHO	O2A-C1-C2-C3
25	a	608	PHO	O2A-C1-C2-C3
32	c	518	DGD	C5B-C6B-C7B-C8B
24	A	607	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	D	402	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	a	607	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	CHA-CBD-CGD-O2D
24	c	505	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O1D
29	a	613	LMG	C19-C20-C21-C22
24	B	607[A]	CLA	C16-C17-C18-C20
24	b	608[A]	CLA	C16-C17-C18-C20
27	a	611	PL9	C2-C3-C7-C8
32	C	517	DGD	O1G-C1A-C2A-C3A
30	D	406	LHG	O7-C5-C6-O8
24	a	607	CLA	C4C-C3C-CAC-CBC
24	b	614	CLA	CAA-CBA-CGA-O2A
29	D	408	LMG	O7-C10-C11-C12
29	a	613	LMG	C16-C17-C18-C19
30	d	406	LHG	C10-C11-C12-C13
24	C	501	CLA	C2A-CAA-CBA-CGA
24	b	605	CLA	C2A-CAA-CBA-CGA
25	D	401	PHO	CHA-CBD-CGD-O1D
25	d	401	PHO	CHA-CBD-CGD-O1D
30	a	616	LHG	O1-C1-C2-O2
32	C	517	DGD	CDB-CEB-CFB-CGB
32	h	102	DGD	O2G-C1B-C2B-C3B
27	d	404	PL9	C36-C37-C38-C39
24	B	610	CLA	C4-C3-C5-C6
24	A	609	CLA	C11-C12-C13-C15
24	a	609	CLA	C11-C12-C13-C15
32	H	102	DGD	C9B-CAB-CBB-CCB
24	B	614	CLA	CAA-CBA-CGA-O2A
30	e	101	LHG	O7-C7-C8-C9
24	B	605	CLA	C6-C7-C8-C9
24	C	504	CLA	C11-C10-C8-C9
24	C	505	CLA	C14-C13-C15-C16
24	C	506	CLA	C14-C13-C15-C16
24	D	404	CLA	C14-C13-C15-C16
24	b	606	CLA	C6-C7-C8-C9
24	c	504	CLA	C11-C10-C8-C9
24	c	505	CLA	C14-C13-C15-C16
24	c	506	CLA	C14-C13-C15-C16
24	d	403	CLA	C14-C13-C15-C16
30	A	615	LHG	O10-C23-C24-C25
26	t	101	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
24	c	501	CLA	C2B-C3B-CAB-CBB
32	E	101	DGD	C3B-C4B-C5B-C6B
28	A	612	SQD	C18-C19-C20-C21
28	a	612	SQD	C18-C19-C20-C21
29	D	408	LMG	C32-C33-C34-C35
32	d	405	DGD	C3B-C4B-C5B-C6B
32	c	517	DGD	O1B-C1B-C2B-C3B
30	D	406	LHG	C34-C35-C36-C37
33	E	103	HEM	CAD-CBD-CGD-O2D
24	C	513	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C20
24	b	611	CLA	C4-C3-C5-C6
29	C	518	LMG	C21-C22-C23-C24
24	a	607	CLA	C2C-C3C-CAC-CBC
30	e	101	LHG	O9-C7-C8-C9
24	B	609	CLA	C1A-C2A-CAA-CBA
24	b	604	CLA	C1A-C2A-CAA-CBA
24	b	610	CLA	C1A-C2A-CAA-CBA
24	b	612	CLA	C1A-C2A-CAA-CBA
24	c	505	CLA	C1A-C2A-CAA-CBA
32	c	516	DGD	C7B-C8B-C9B-CAB
32	C	516	DGD	O1B-C1B-C2B-C3B
24	c	509	CLA	O1D-CGD-O2D-CED
24	B	608	CLA	C2-C1-O2A-CGA
24	d	402	CLA	C2-C1-O2A-CGA
28	A	614	SQD	C11-C12-C13-C14
29	c	519	LMG	C17-C18-C19-C20
32	E	101	DGD	C2A-C1A-O1G-C1G
32	E	101	DGD	C1G-C2G-C3G-O3G
28	a	614	SQD	C11-C12-C13-C14
24	D	403	CLA	CAA-CBA-CGA-O1A
24	B	606	CLA	C13-C15-C16-C17
24	b	607	CLA	C13-C15-C16-C17
32	c	517	DGD	C8A-C9A-CAA-CBA
27	D	405	PL9	C18-C19-C21-C22
33	E	103	HEM	CAA-CBA-CGA-O2A
32	c	516	DGD	C2E-C1E-O5D-C6D
30	A	615	LHG	C4-O6-P-O5
30	d	407	LHG	C4-O6-P-O5
28	L	102	SQD	O10-C23-C24-C25
30	a	616	LHG	O8-C23-C24-C25
24	B	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	l	101	SQD	O10-C23-C24-C25
29	z	101	LMG	O7-C10-C11-C12
24	c	512	CLA	CAA-CBA-CGA-O2A
29	A	613	LMG	O10-C28-C29-C30
27	d	404	PL9	C45-C44-C46-C47
30	D	406	LHG	C28-C29-C30-C31
27	d	404	PL9	C38-C39-C41-C42
24	B	610	CLA	CAD-CBD-CGD-O1D
24	B	613	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
24	A	609	CLA	C14-C13-C15-C16
24	B	607[B]	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
24	D	402	CLA	C11-C12-C13-C14
24	a	609	CLA	C14-C13-C15-C16
24	a	615	CLA	C11-C12-C13-C14
24	b	608[B]	CLA	C14-C13-C15-C16
24	c	511	CLA	C6-C7-C8-C9
29	a	613	LMG	C36-C37-C38-C39
24	c	501	CLA	CAA-CBA-CGA-O2A
29	D	408	LMG	C19-C20-C21-C22
24	B	616	CLA	C15-C16-C17-C18
33	e	102	HEM	CAA-CBA-CGA-O1A
32	H	102	DGD	C5B-C6B-C7B-C8B
28	B	622	SQD	C45-C46-O48-C23
28	b	601	SQD	C45-C46-O48-C23
24	b	604	CLA	C2A-CAA-CBA-CGA
24	C	505	CLA	CAA-CBA-CGA-O2A
32	C	516	DGD	O2G-C1B-C2B-C3B
27	D	405	PL9	C25-C24-C26-C27
24	b	617	CLA	C15-C16-C17-C18
24	B	607[B]	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C10-C8-C7
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C15
24	C	510	CLA	C6-C7-C8-C10
24	C	511	CLA	C6-C7-C8-C10
24	D	403	CLA	C12-C13-C15-C16
24	b	608[B]	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	c	505	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	c	507	CLA	C11-C12-C13-C15
24	c	510	CLA	C6-C7-C8-C10
24	c	511	CLA	C6-C7-C8-C10
24	d	402	CLA	C12-C13-C15-C16
24	C	501	CLA	CAA-CBA-CGA-O1A
32	c	517	DGD	O2G-C1B-C2B-C3B
32	C	517	DGD	CCA-CDA-CEA-CFA
30	d	407	LHG	C12-C13-C14-C15
26	B	618	BCR	C17-C18-C19-C20
26	b	621	BCR	C21-C22-C23-C24
24	B	613	CLA	CAA-CBA-CGA-O1A
24	B	613	CLA	C8-C10-C11-C12
24	b	614	CLA	C8-C10-C11-C12
32	c	518	DGD	O6E-C5E-C6E-O5E
29	C	518	LMG	O8-C28-C29-C30
24	C	506	CLA	C15-C16-C17-C18
24	c	506	CLA	C15-C16-C17-C18
30	E	102	LHG	O9-C7-C8-C9
30	a	616	LHG	O10-C23-C24-C25
30	l	102	LHG	O9-C7-C8-C9
32	d	405	DGD	O1A-C1A-C2A-C3A
30	d	407	LHG	O8-C23-C24-C25

There are no ring outliers.

144 monomers are involved in 796 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	603	CLA	4	0
24	C	504	CLA	4	0
24	B	616	CLA	3	0
27	d	404	PL9	7	0
30	D	406	LHG	5	0
30	d	407	LHG	1	0
27	D	405	PL9	13	0
24	a	615	CLA	5	0
24	B	614	CLA	7	0
28	L	102	SQD	12	0
29	C	519	LMG	2	0
24	c	504	CLA	3	0
29	B	621	LMG	2	0
24	B	607[B]	CLA	5	0
24	A	609	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	l	101	SQD	5	0
32	c	516	DGD	1	0
24	A	607	CLA	5	0
32	C	517	DGD	3	0
24	B	613	CLA	4	0
24	B	602	CLA	3	0
26	k	101	BCR	18	0
26	B	618	BCR	24	0
24	b	612	CLA	3	0
26	a	610	BCR	13	0
24	B	609	CLA	2	0
33	e	102	HEM	2	0
24	c	511	CLA	1	0
28	a	614	SQD	2	0
24	c	506	CLA	3	0
32	H	102	DGD	6	0
25	D	401	PHO	10	0
24	d	402	CLA	4	0
26	f	101	BCR	21	0
30	l	102	LHG	6	0
28	A	614	SQD	5	0
28	x	101	SQD	4	0
26	b	619	BCR	26	0
24	d	403	CLA	3	0
24	C	510	CLA	3	0
25	A	608	PHO	3	0
33	v	201	HEM	4	0
24	A	606	CLA	7	0
32	c	518	DGD	3	0
24	b	610	CLA	1	0
30	D	407	LHG	3	0
24	B	610	CLA	2	0
26	T	101	BCR	22	0
33	V	201	HEM	7	0
30	A	615	LHG	10	0
24	B	606	CLA	11	0
32	d	405	DGD	4	0
26	K	102	BCR	15	0
24	C	509	CLA	3	0
24	C	512	CLA	4	0
29	j	101	LMG	6	0
24	c	513	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	507	CLA	6	0
32	C	516	DGD	2	0
26	C	514	BCR	14	0
24	B	611	CLA	4	0
24	b	608[A]	CLA	4	0
26	b	621	BCR	19	0
24	b	616	CLA	8	0
24	B	612	CLA	3	0
26	b	620	BCR	15	0
24	c	505	CLA	5	0
24	B	603	CLA	3	0
24	B	604	CLA	5	0
24	C	511	CLA	4	0
26	c	514	BCR	14	0
24	c	503	CLA	8	0
32	E	101	DGD	1	0
24	B	605	CLA	8	0
29	c	519	LMG	2	0
26	h	101	BCR	17	0
24	b	605	CLA	5	0
24	B	617	CLA	4	0
26	B	620	BCR	16	0
24	B	615	CLA	6	0
24	B	607[A]	CLA	1	0
26	I	101	BCR	18	0
33	E	103	HEM	6	0
30	e	101	LHG	2	0
24	b	614	CLA	2	0
28	X	101	SQD	3	0
24	a	607	CLA	4	0
24	c	509	CLA	3	0
20	a	601	OEX	1	0
24	B	608	CLA	6	0
24	c	510	CLA	3	0
24	b	606	CLA	8	0
24	b	604	CLA	4	0
26	c	521	BCR	19	0
26	K	101	BCR	14	0
24	c	508	CLA	3	0
24	b	615	CLA	2	0
28	B	622	SQD	8	0
24	c	501	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	513	CLA	2	0
26	F	101	BCR	20	0
24	b	609	CLA	5	0
29	b	622	LMG	4	0
26	c	515	BCR	20	0
24	b	607	CLA	12	0
24	C	501	CLA	10	0
27	a	611	PL9	12	0
28	A	612	SQD	2	0
26	A	610	BCR	14	0
24	C	503	CLA	7	0
24	a	609	CLA	5	0
24	b	613	CLA	3	0
25	a	608	PHO	2	0
27	A	611	PL9	11	0
24	c	507	CLA	3	0
30	a	616	LHG	10	0
24	D	404	CLA	6	0
29	z	101	LMG	1	0
25	d	401	PHO	4	0
30	L	101	LHG	6	0
32	c	517	DGD	5	0
26	t	101	BCR	23	0
29	A	613	LMG	2	0
29	D	408	LMG	7	0
28	a	612	SQD	1	0
24	c	502	CLA	4	0
24	c	512	CLA	2	0
24	C	506	CLA	9	0
24	D	403	CLA	5	0
24	b	618	CLA	2	0
32	h	102	DGD	6	0
24	C	502	CLA	5	0
24	C	508	CLA	6	0
29	C	518	LMG	2	0
24	D	402	CLA	2	0
29	a	613	LMG	1	0
30	d	406	LHG	3	0
26	B	619	BCR	20	0
26	H	101	BCR	16	0
24	b	617	CLA	4	0
24	C	505	CLA	6	0

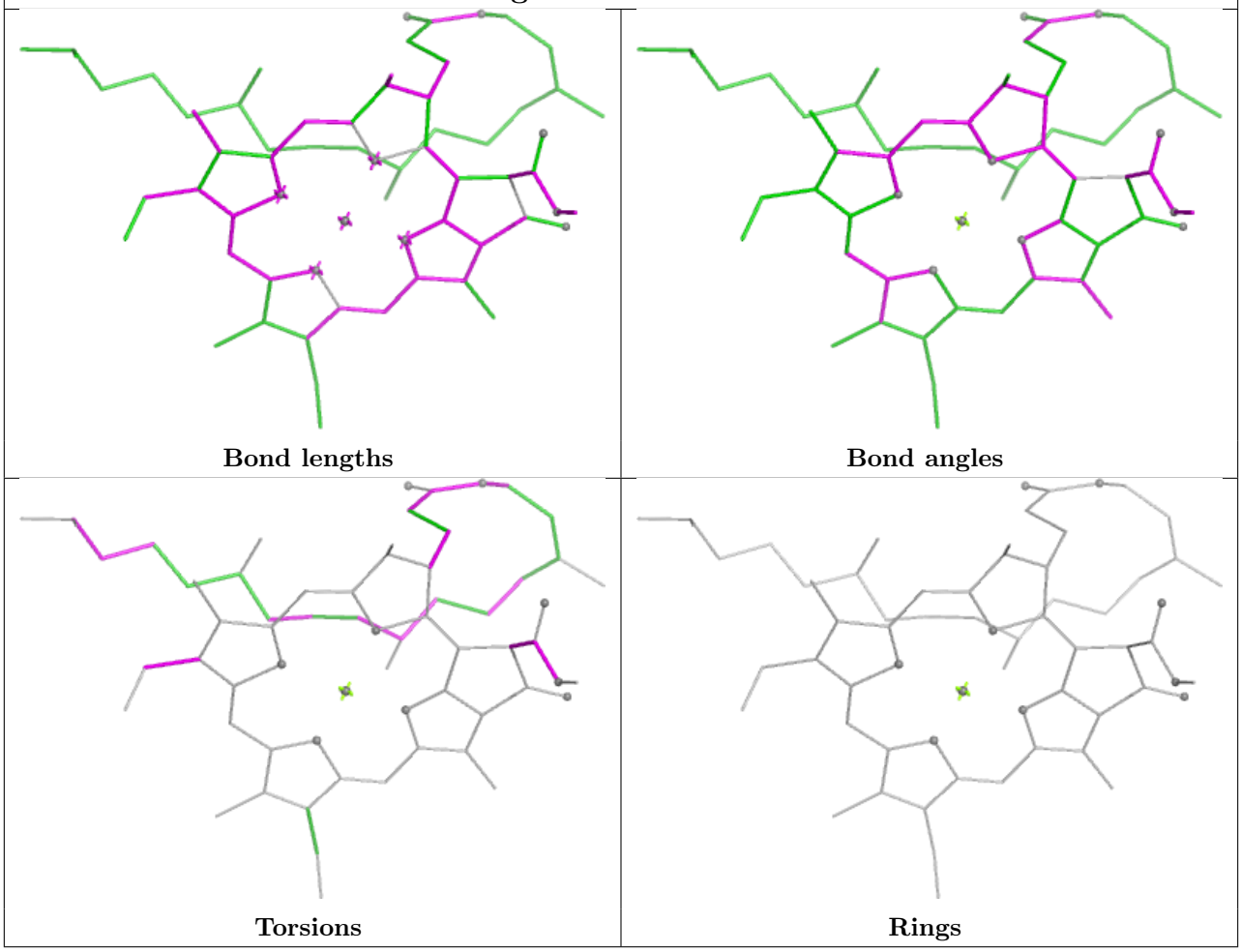
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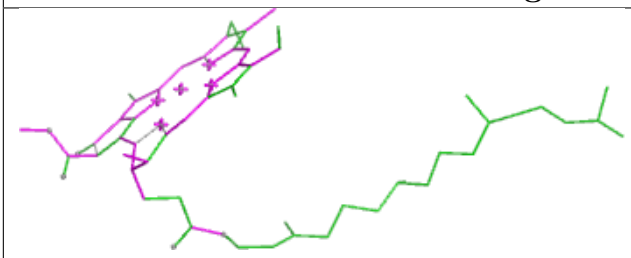
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	601	SQD	12	0
24	b	608[B]	CLA	2	0
24	a	606	CLA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

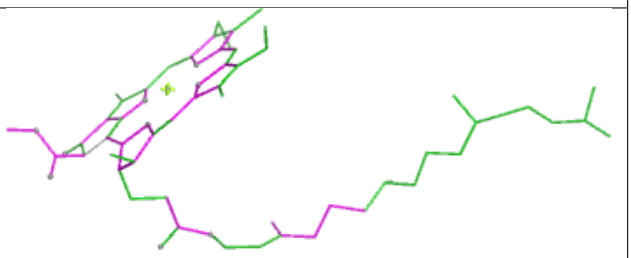
Ligand CLA b 603



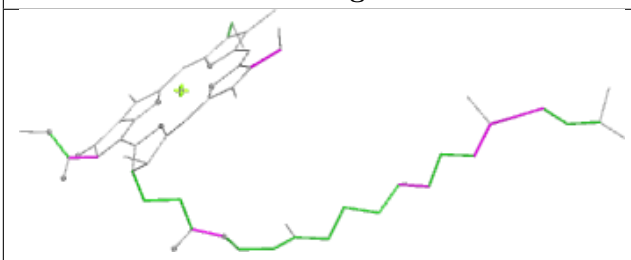
Ligand CLA C 504



Bond lengths



Bond angles

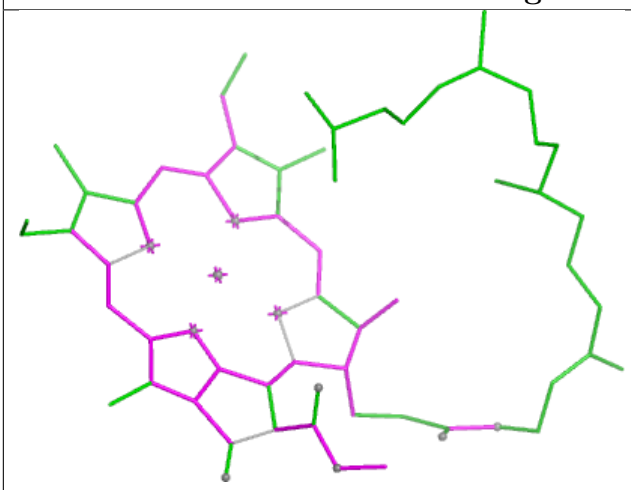


Torsions

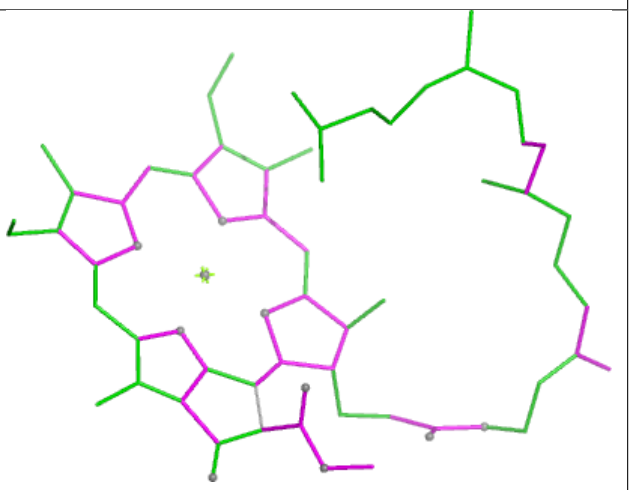


Rings

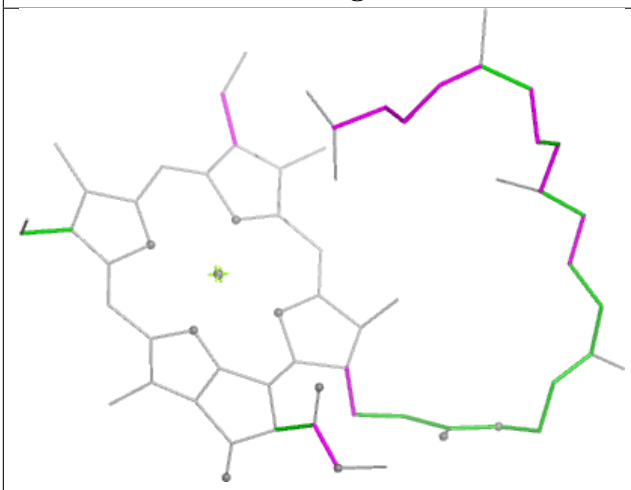
Ligand CLA B 616



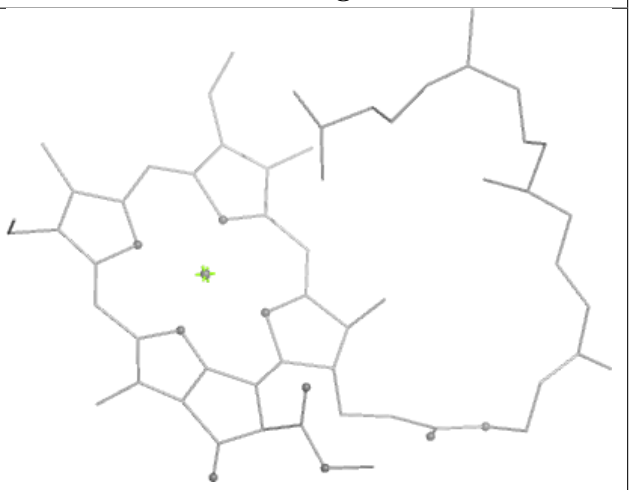
Bond lengths



Bond angles

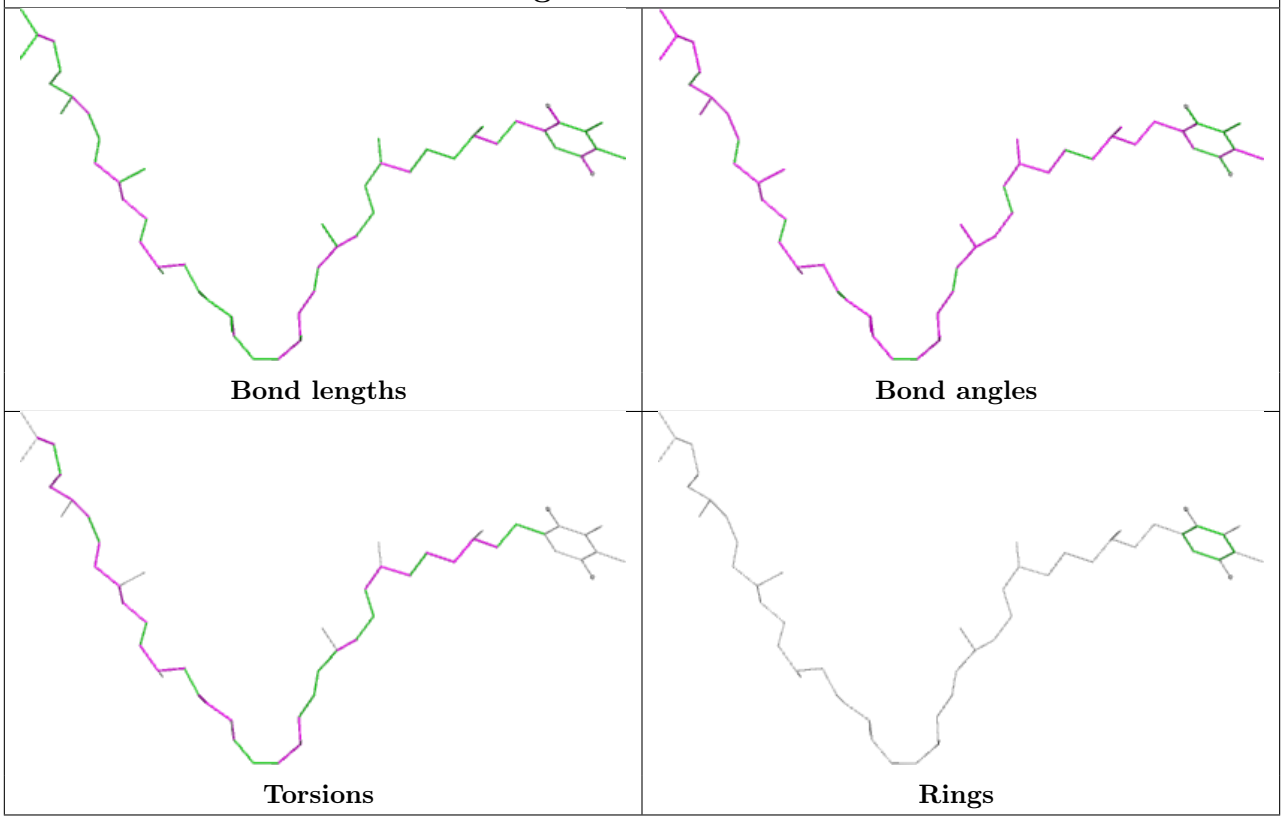


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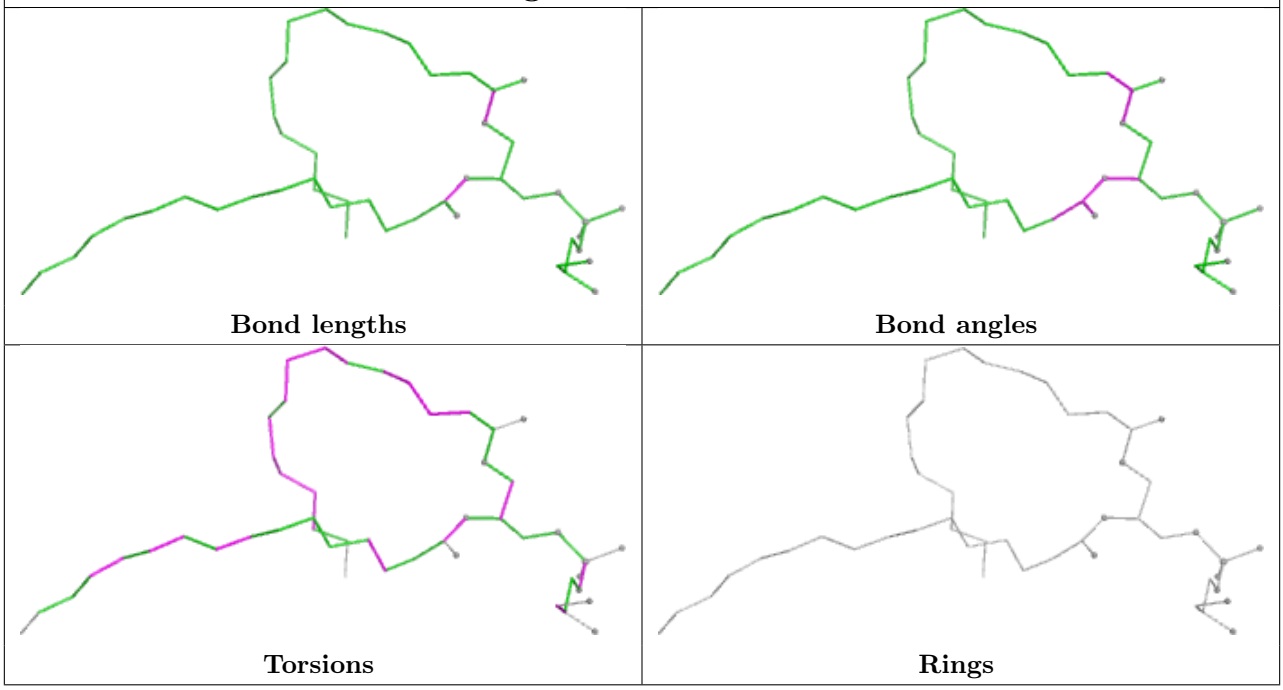


Rings

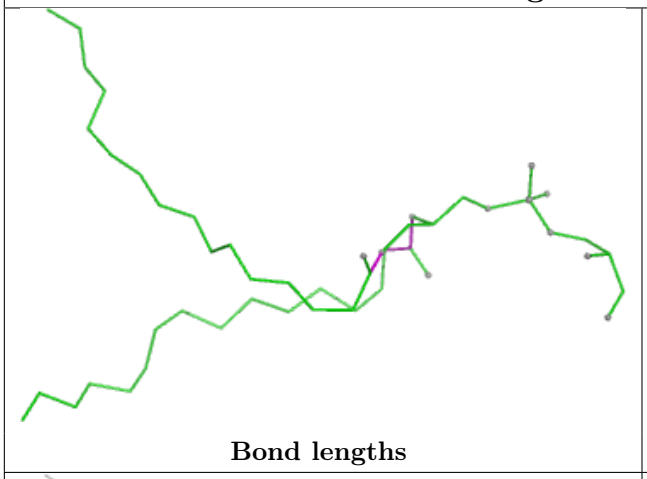
Ligand PL9 d 404



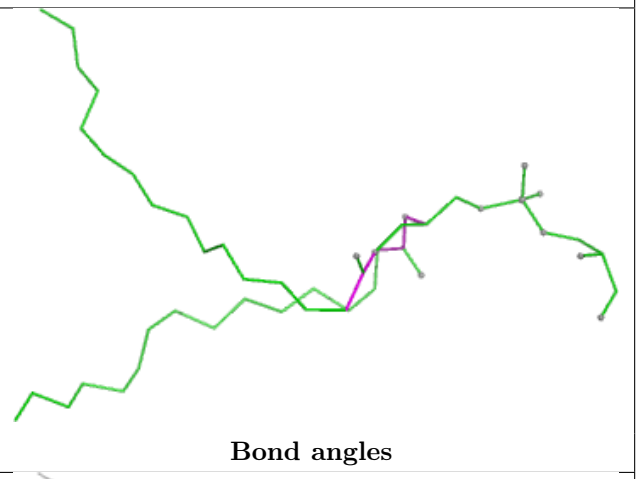
Ligand LHG D 406



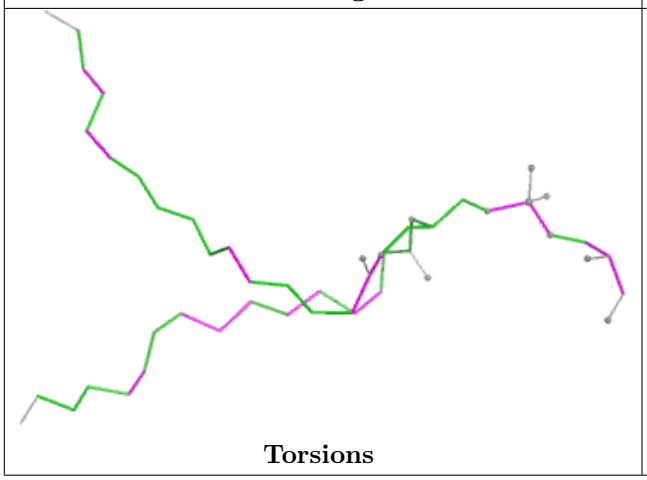
Ligand LHG d 407



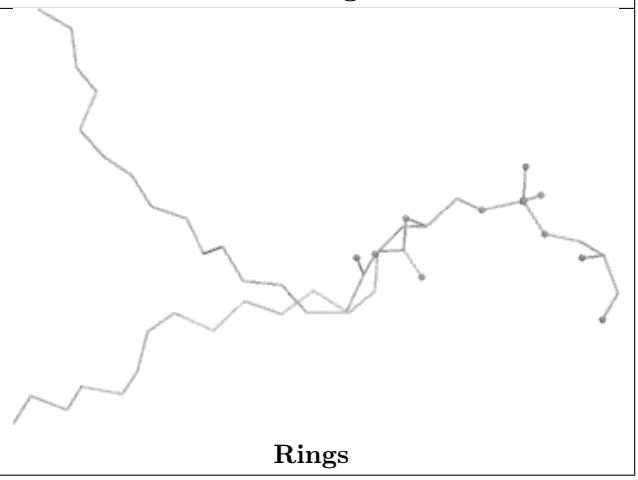
Bond lengths



Bond angles

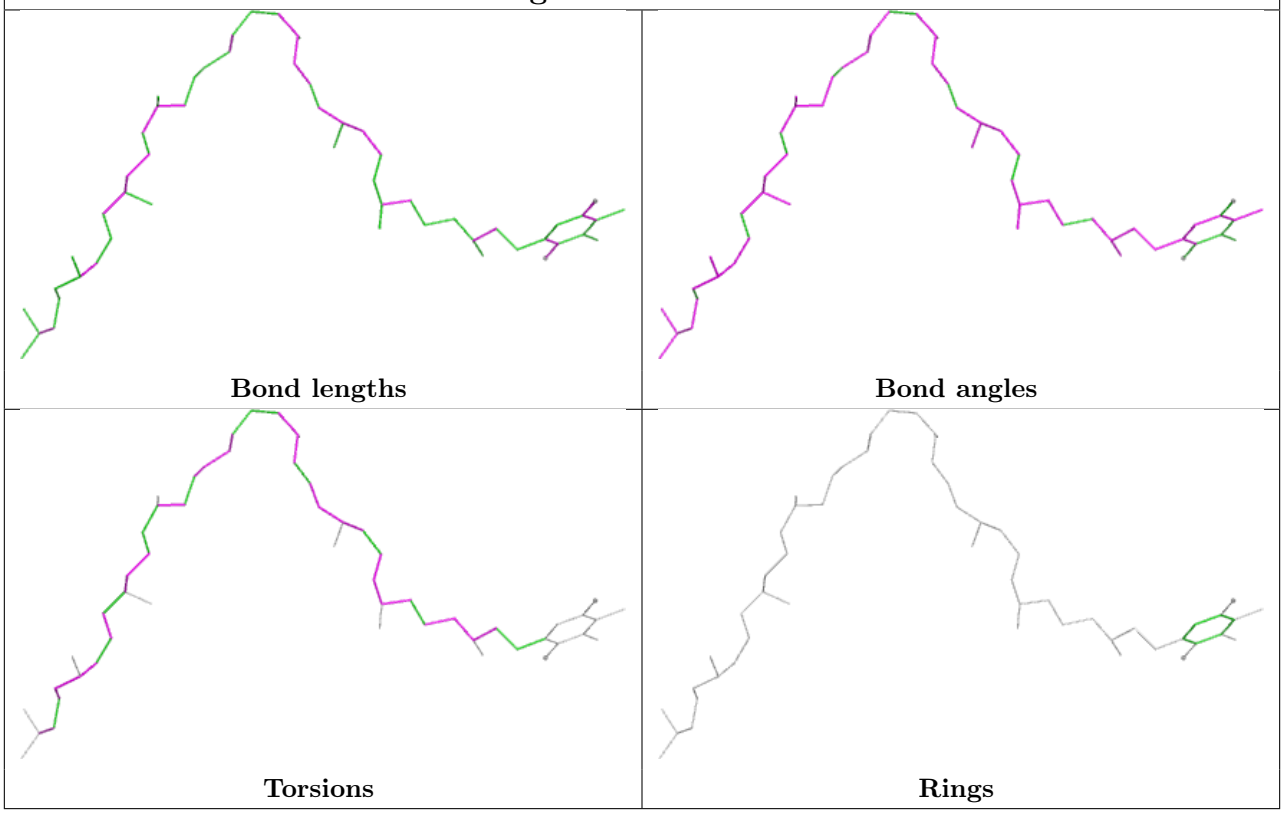


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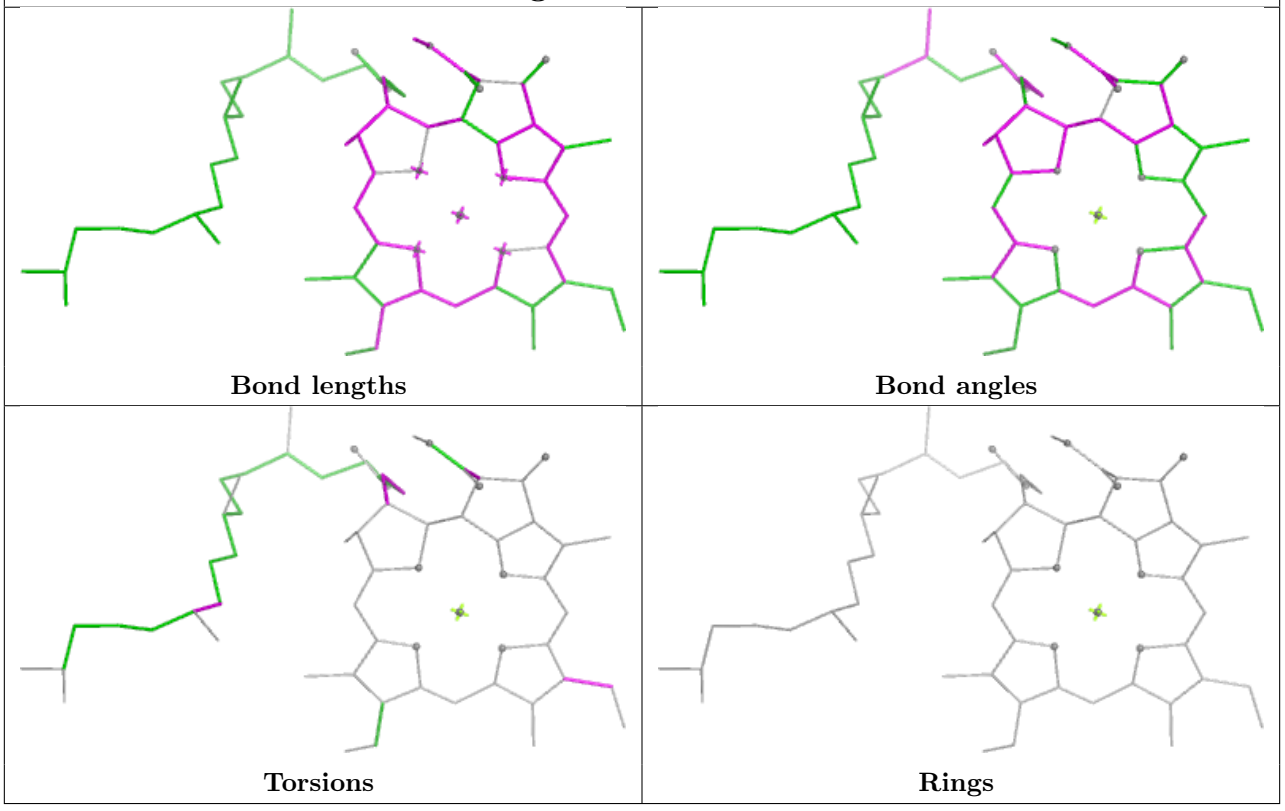


Rings

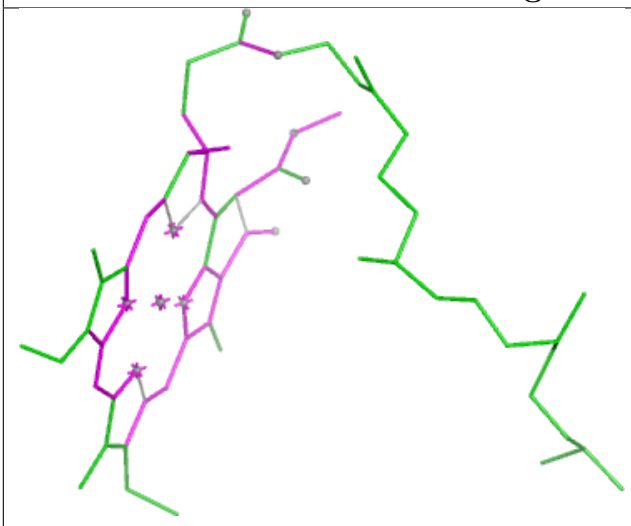
Ligand PL9 D 405



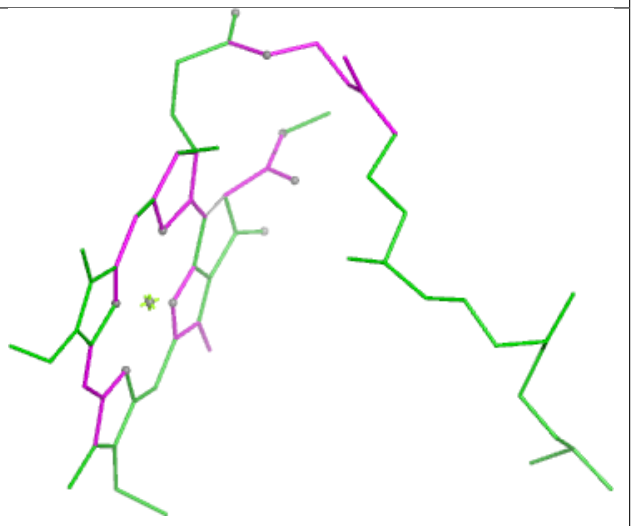
Ligand CLA a 615



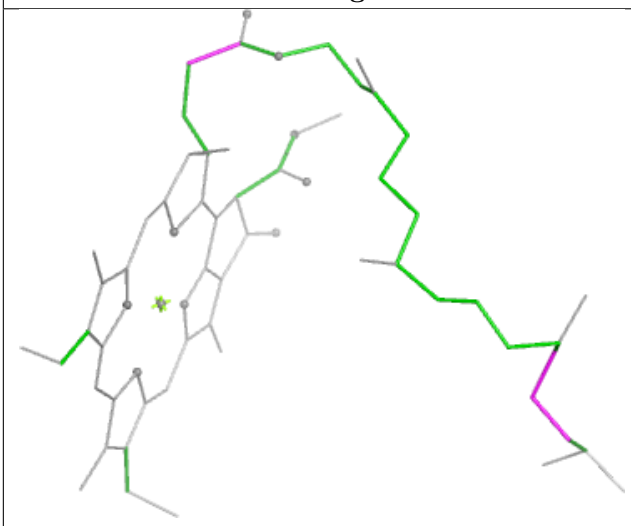
Ligand CLA B 614



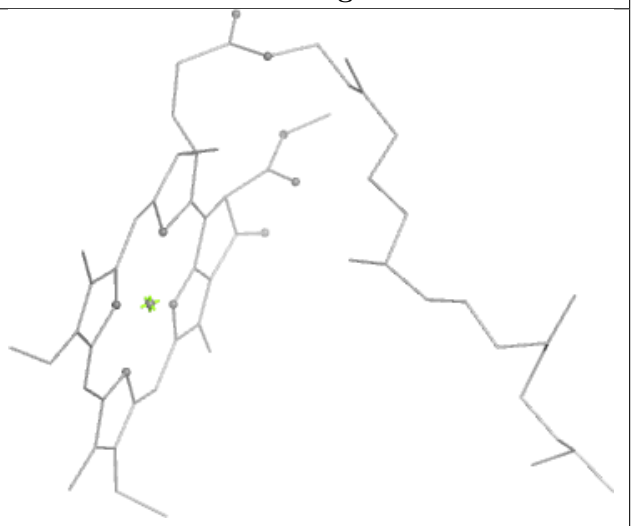
Bond lengths



Bond angles

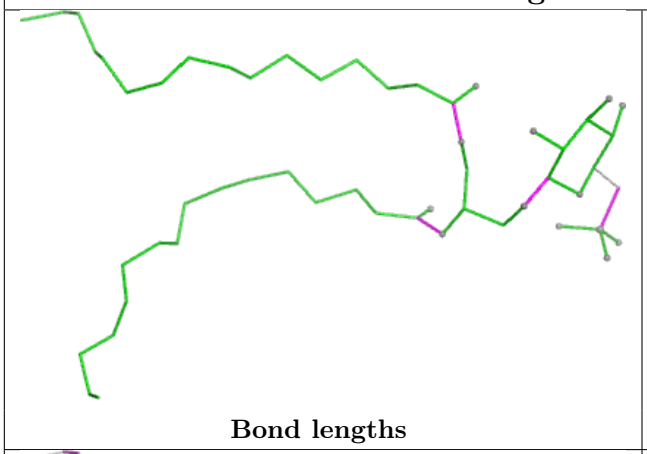


Torsions

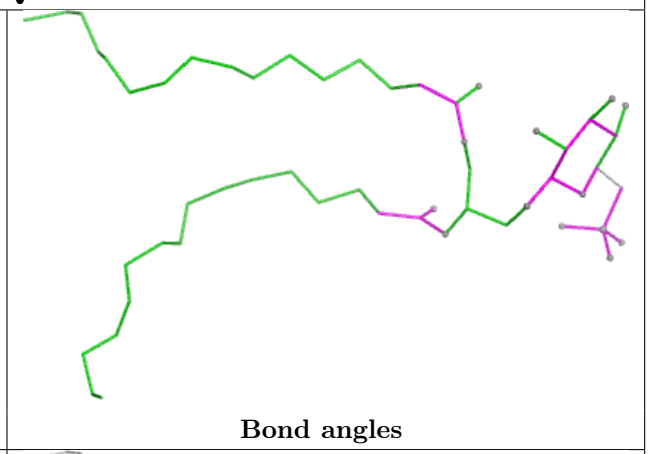


Rings

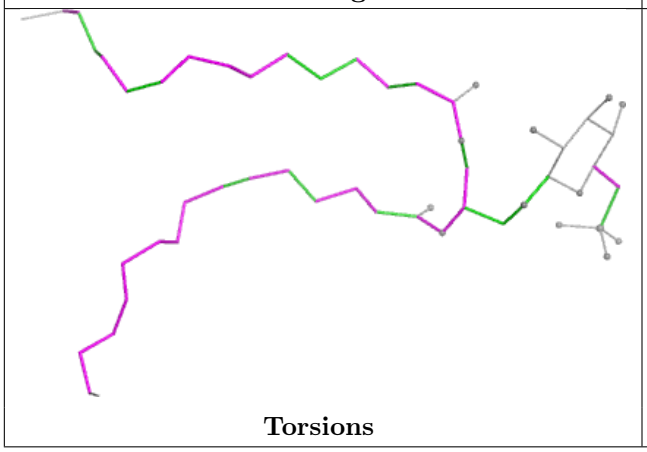
Ligand SQD L 102



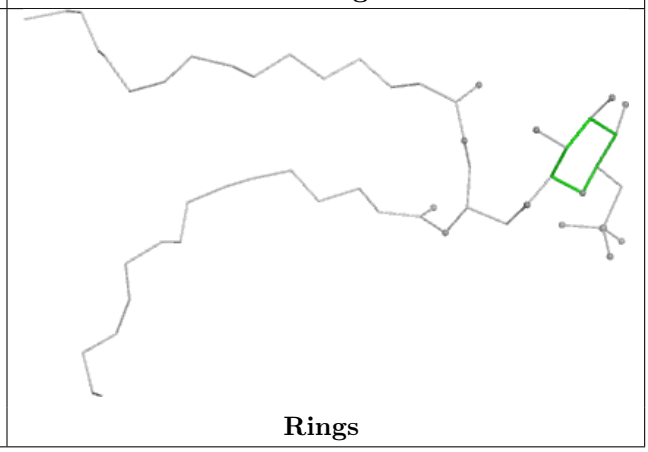
Bond lengths



Bond angles

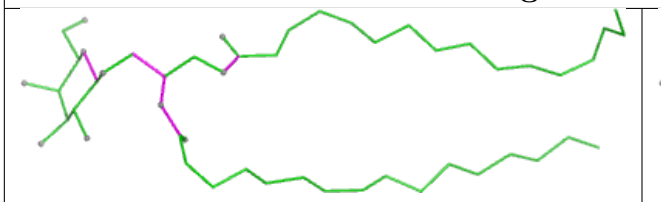


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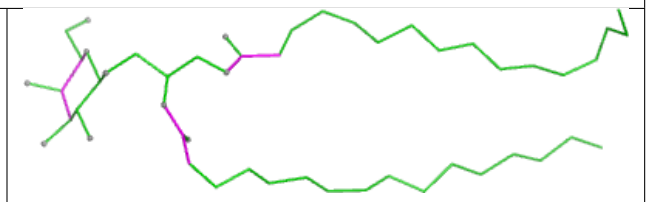


Rings

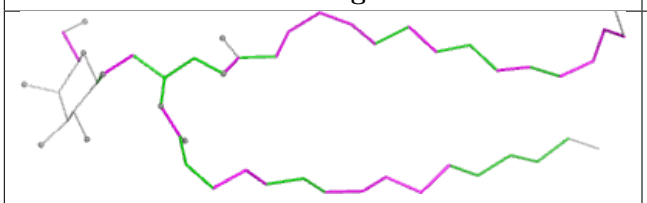
Ligand LMG C 519



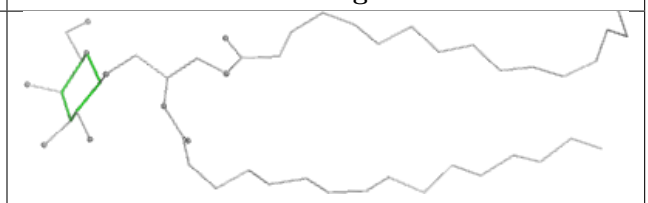
Bond lengths



Bond angles

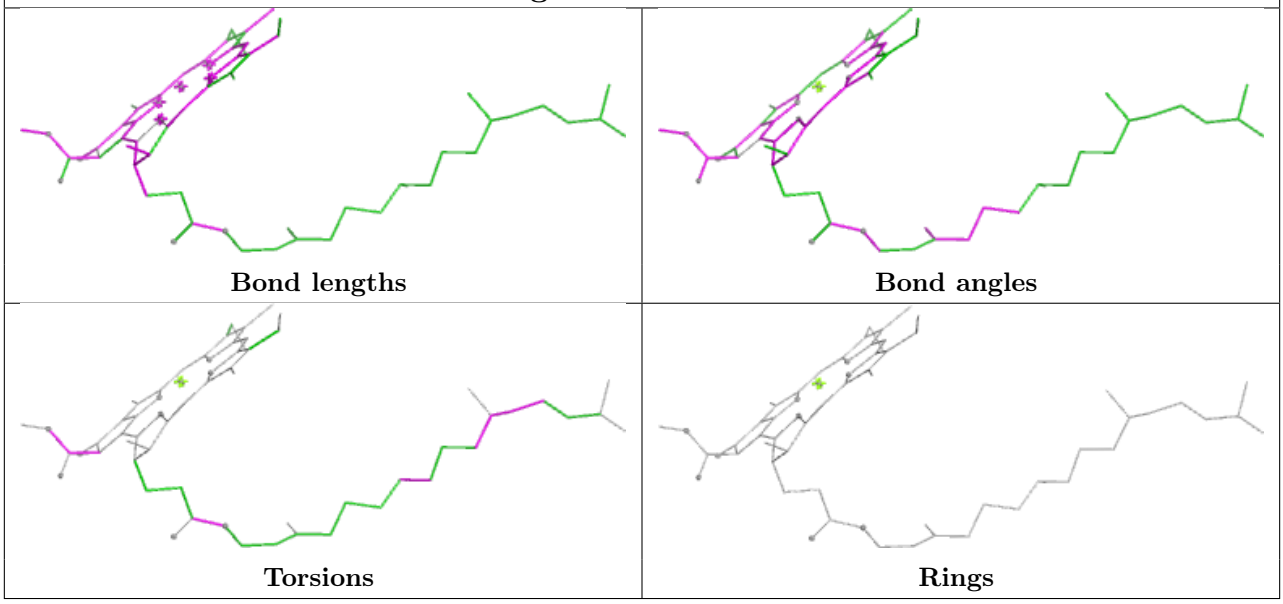


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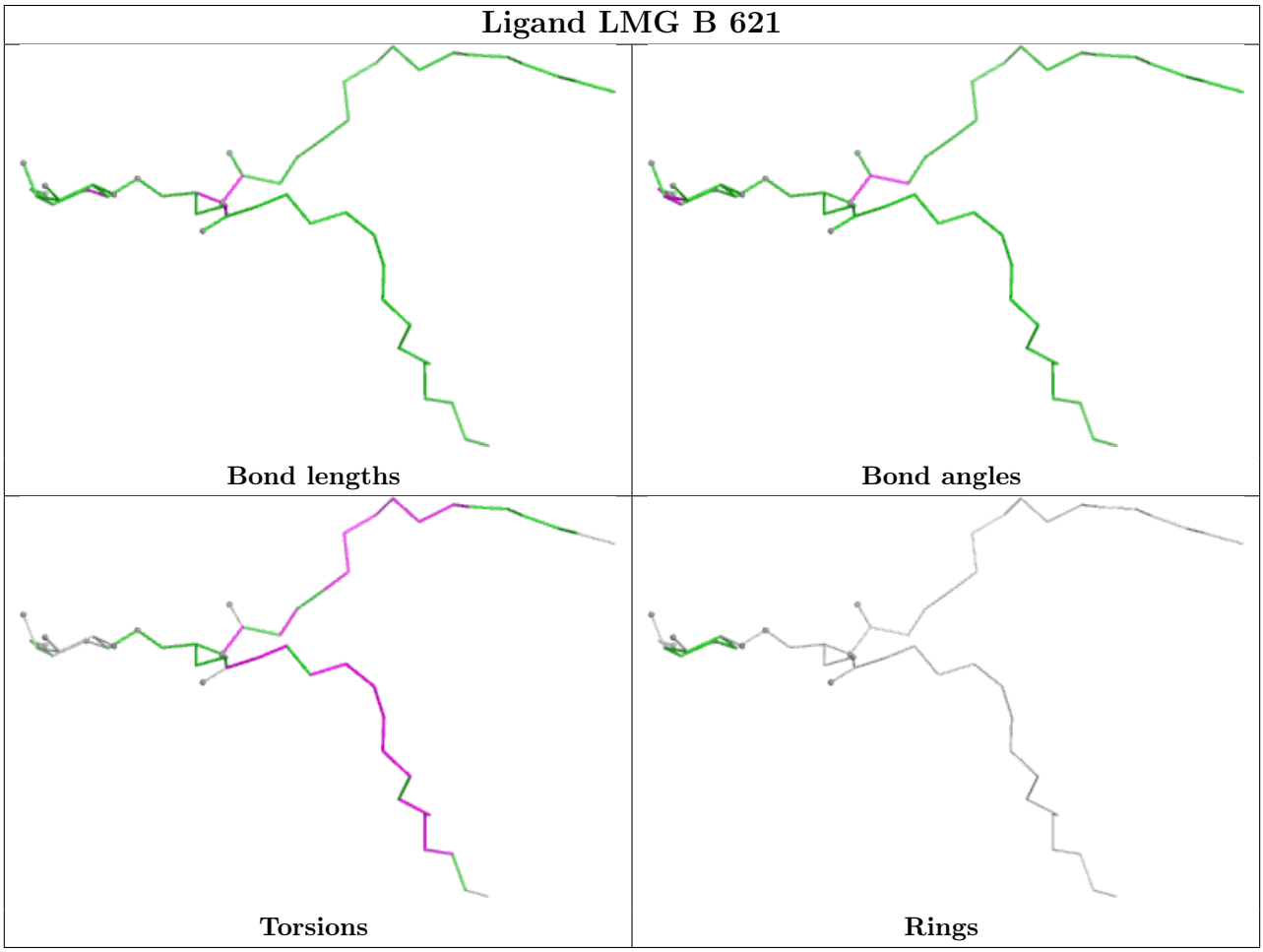


Rings

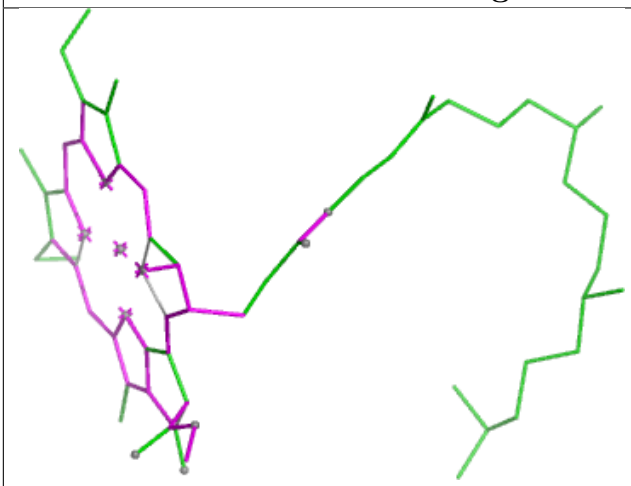
Ligand CLA c 504



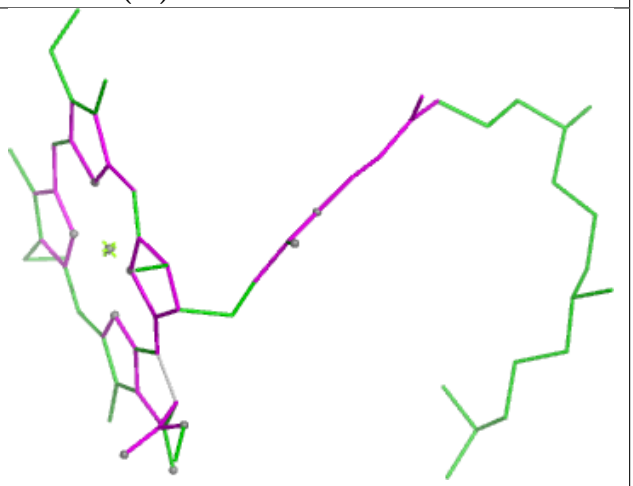
Ligand LMG B 621



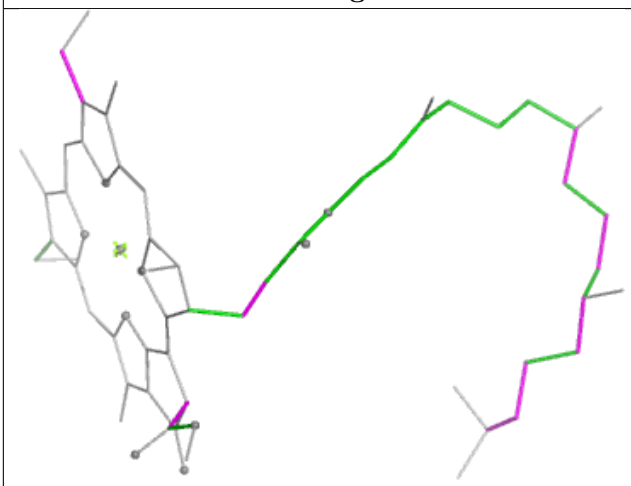
Ligand CLA B 607 (B)



Bond lengths



Bond angles

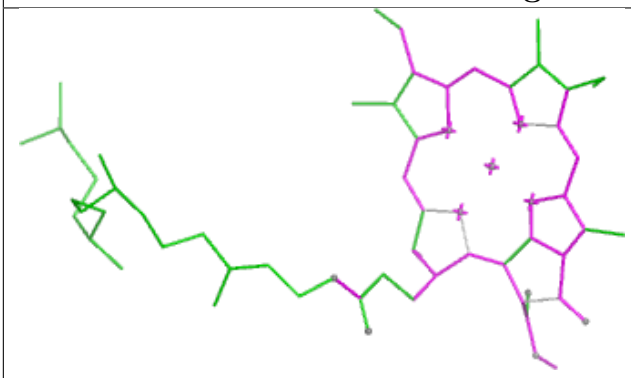


Torsions

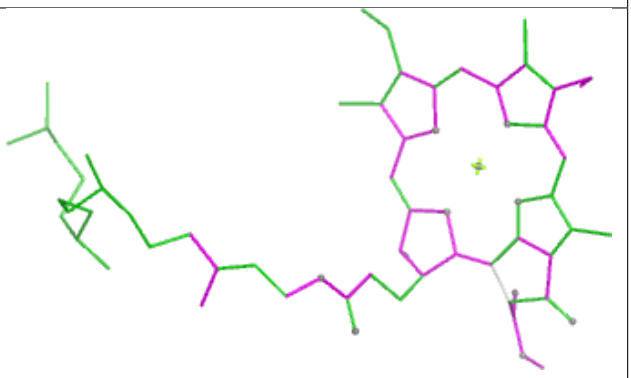


Rings

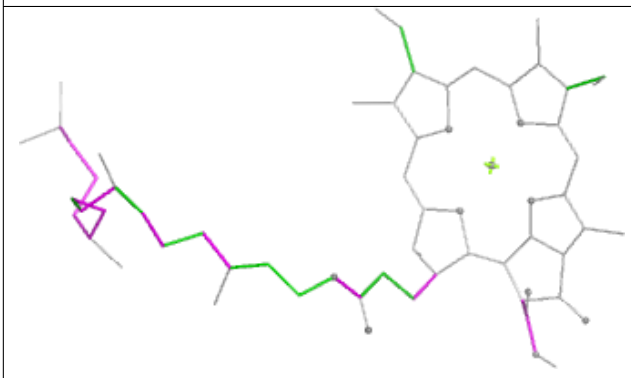
Ligand CLA A 609



Bond lengths



Bond angles

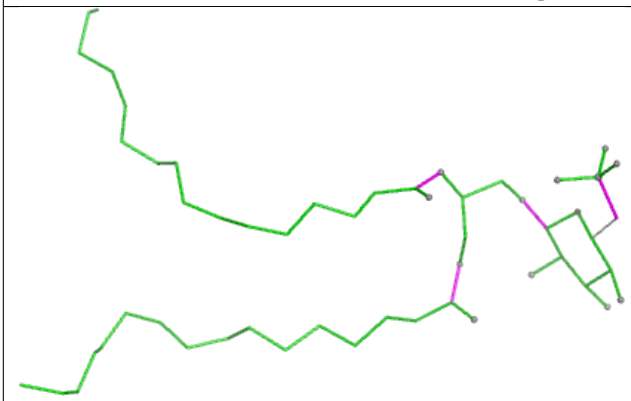


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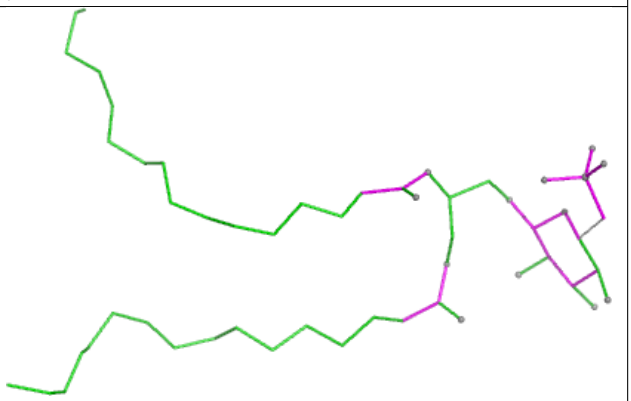


Rings

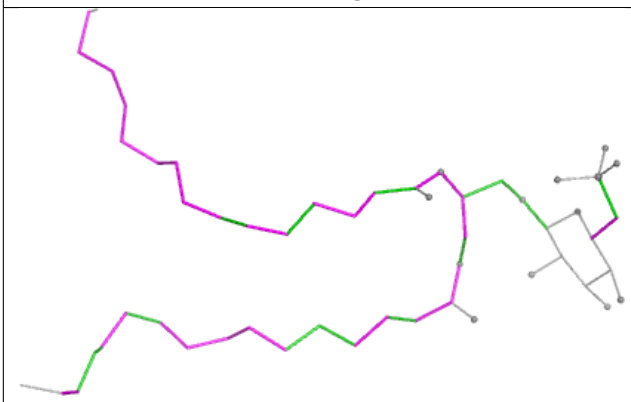
Ligand SQD l 101



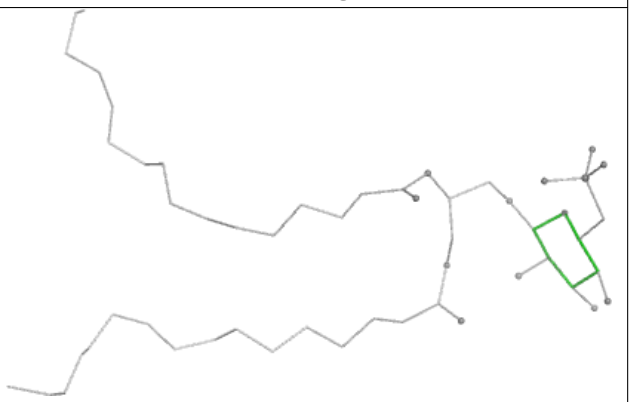
Bond lengths



Bond angles

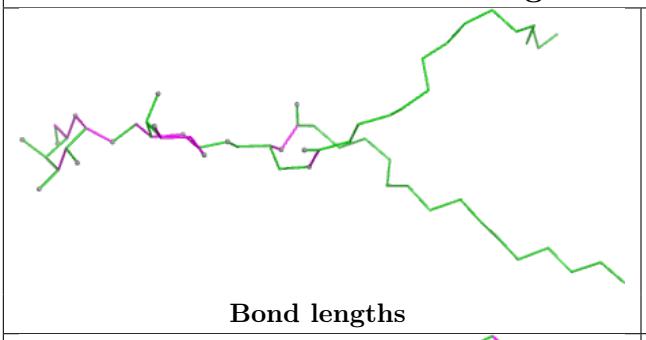


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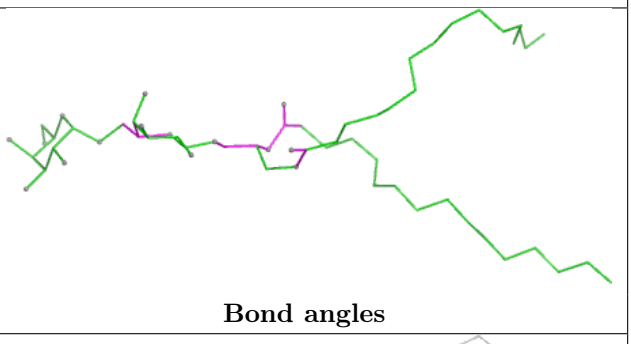


Rings

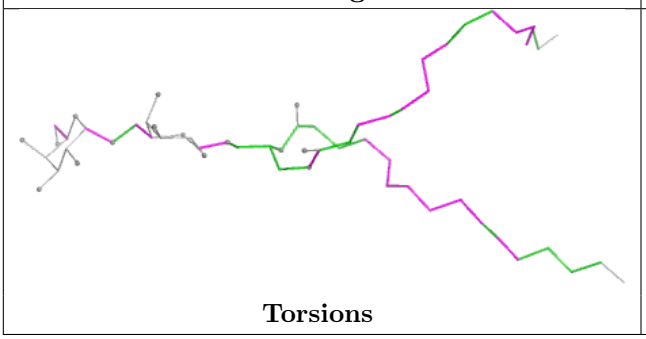
Ligand DGD c 516



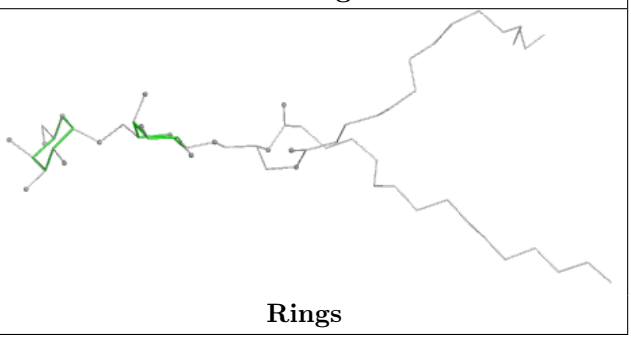
Bond lengths



Bond angles

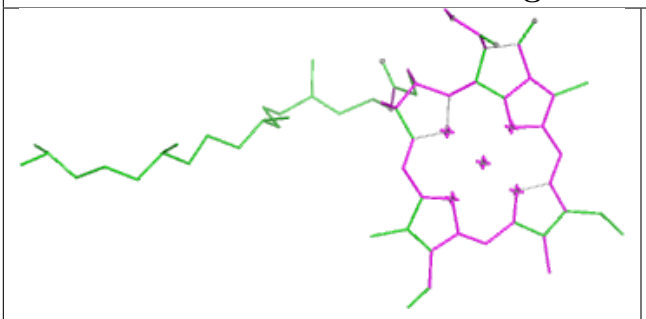


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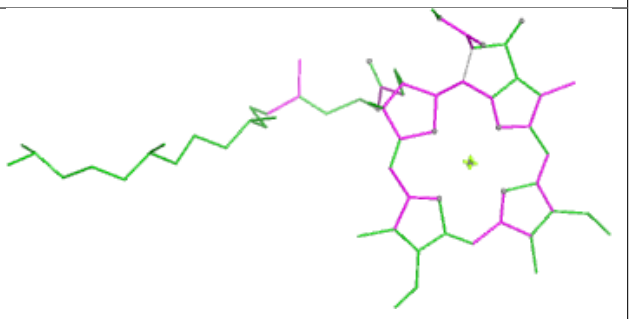


Rings

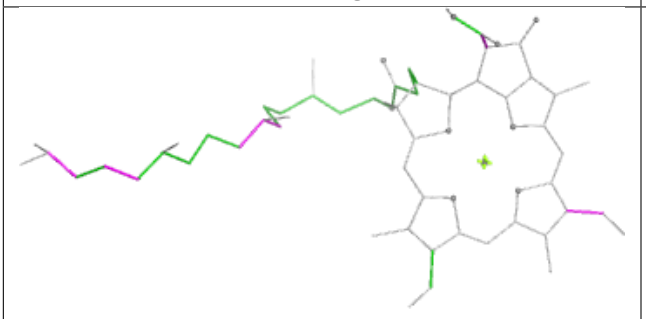
Ligand CLA A 607



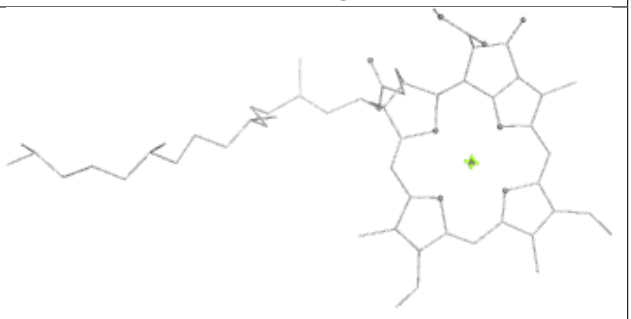
Bond lengths



Bond angles

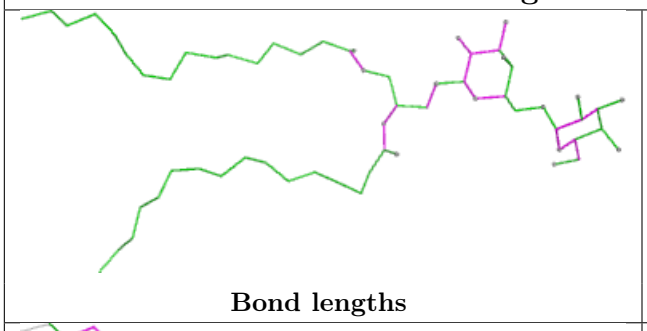


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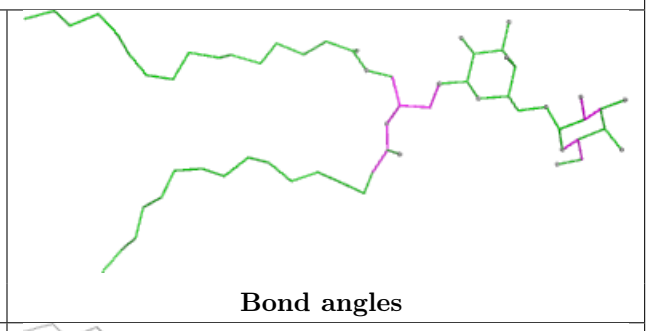


Rings

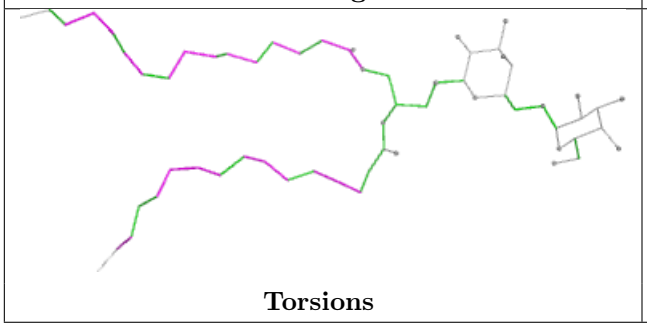
Ligand DGD C 517



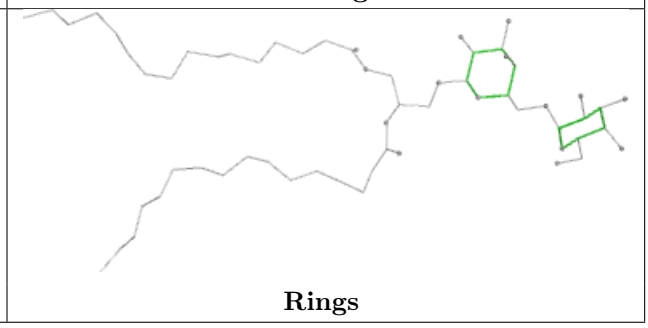
Bond lengths



Bond angles

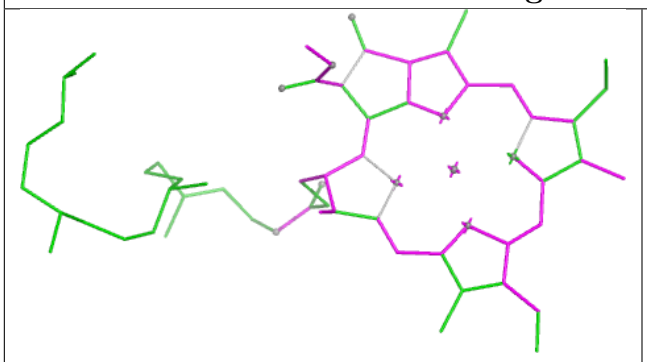


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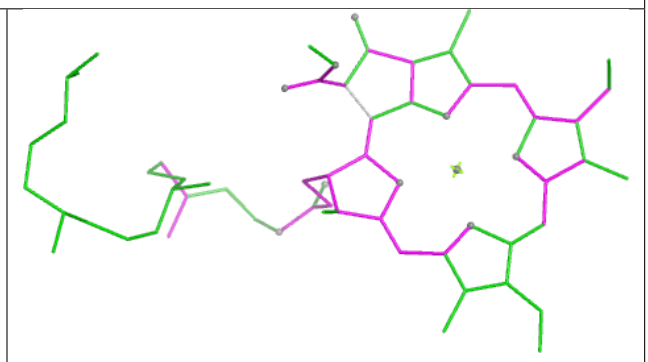


Rings

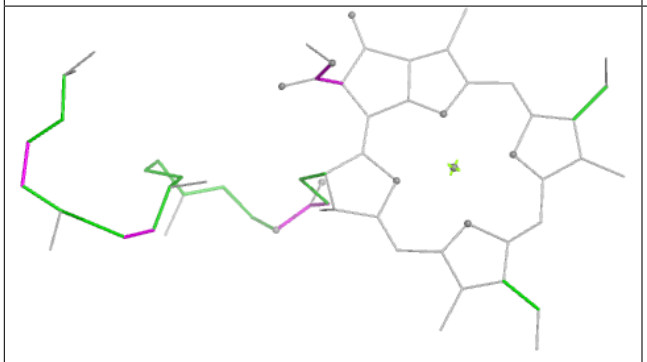
Ligand CLA B 613



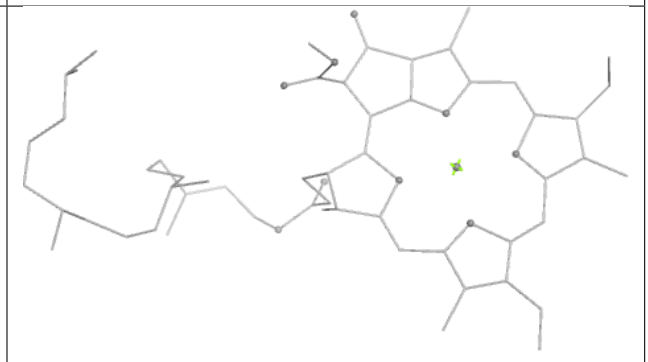
Bond lengths



Bond angles

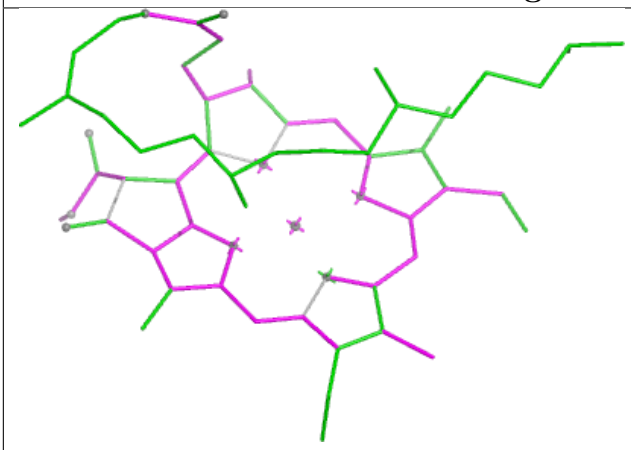


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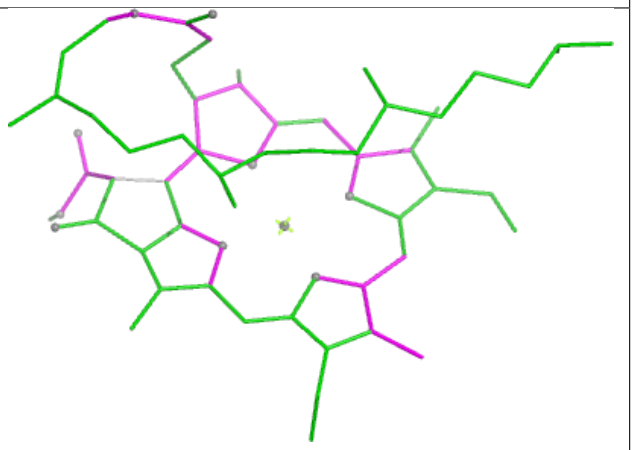


Rings

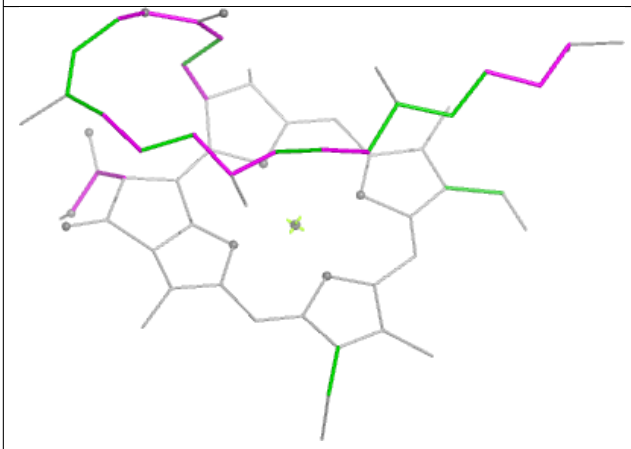
Ligand CLA B 602



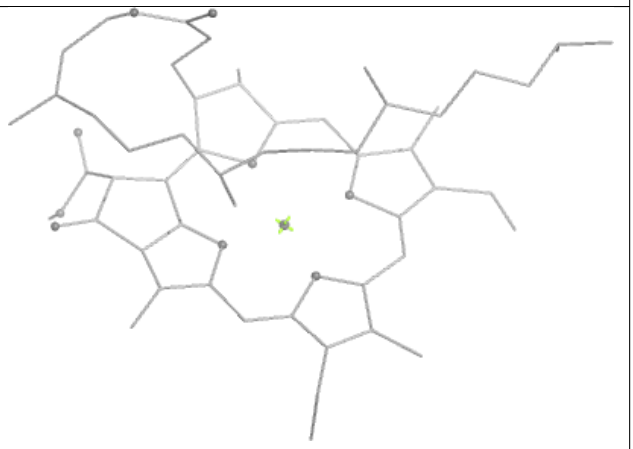
Bond lengths



Bond angles

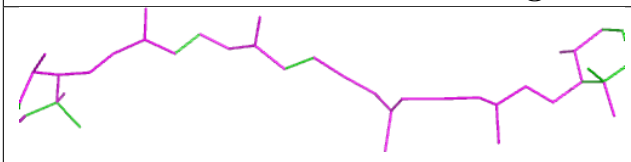


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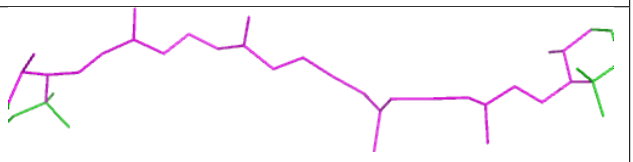


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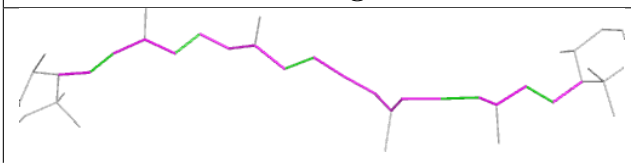
Ligand BCR k 101



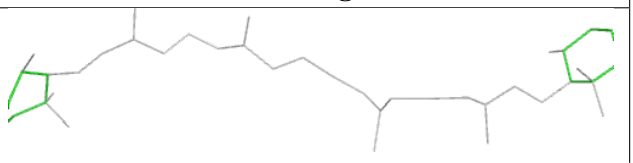
Bond lengths



Bond angles

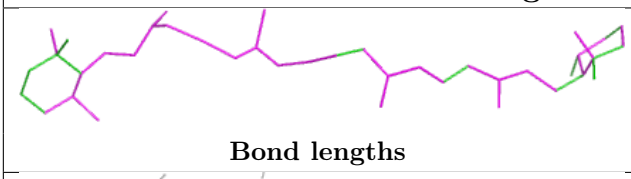


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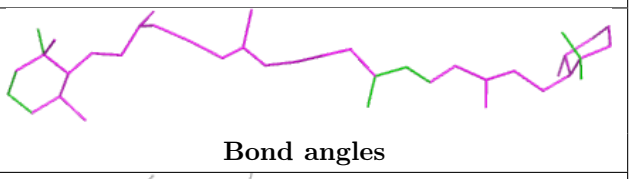


Rings

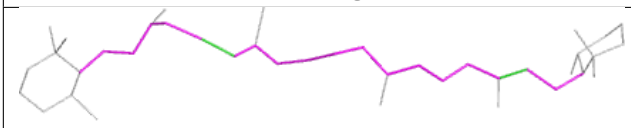
Ligand BCR B 618



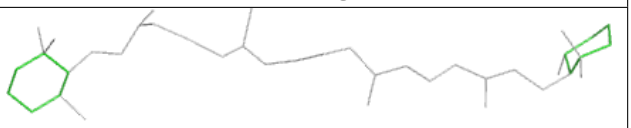
Bond lengths



Bond angles

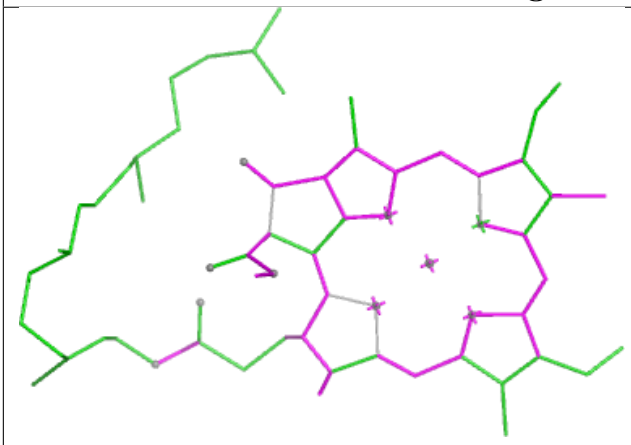


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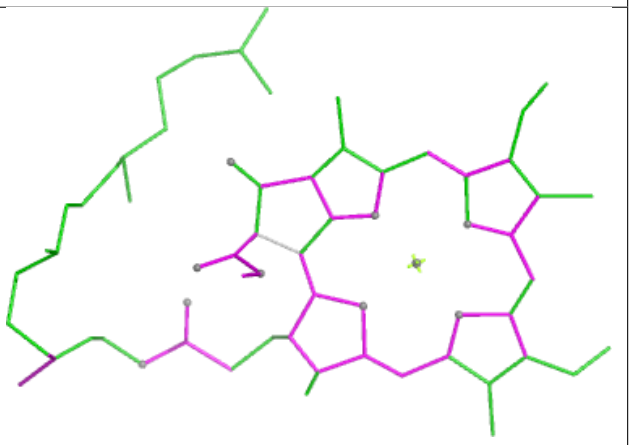


Rings

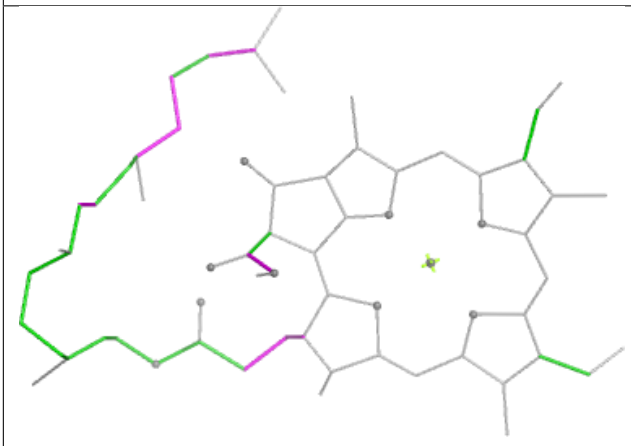
Ligand CLA b 612



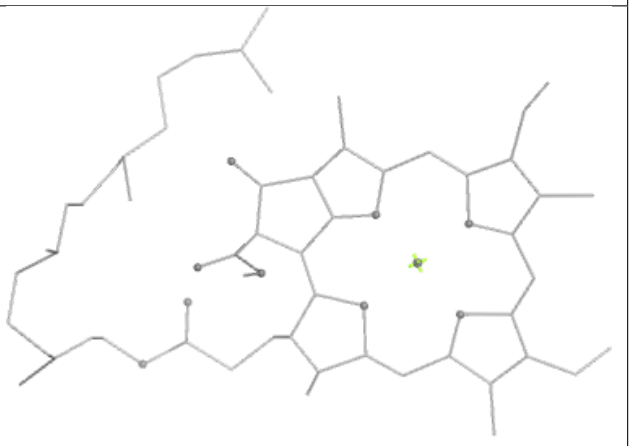
Bond lengths



Bond angles

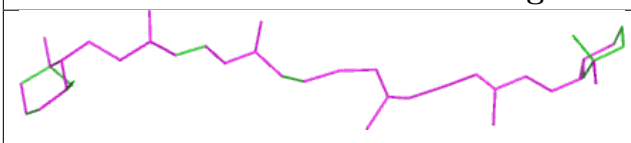


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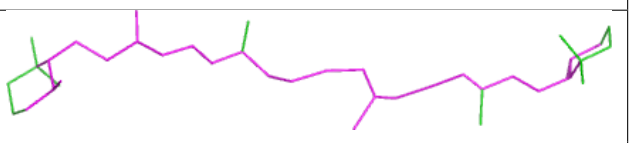


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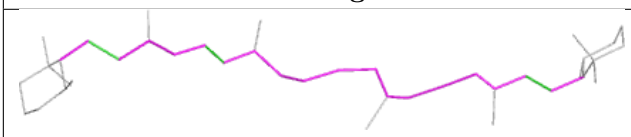
Ligand BCR a 610



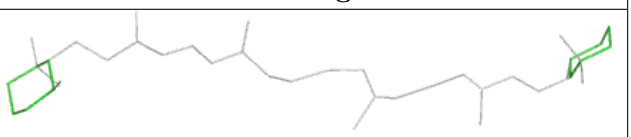
Bond lengths



Bond angles

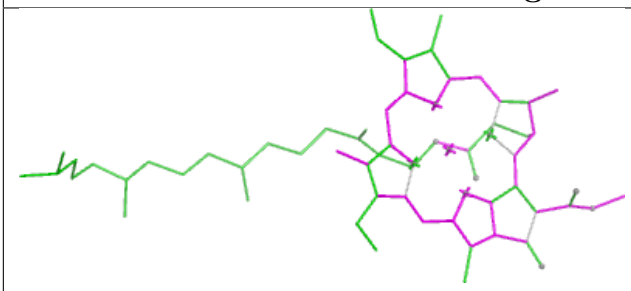


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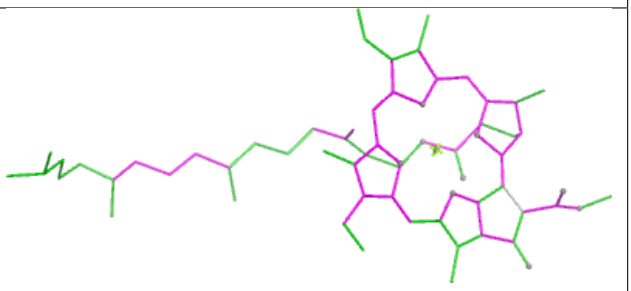


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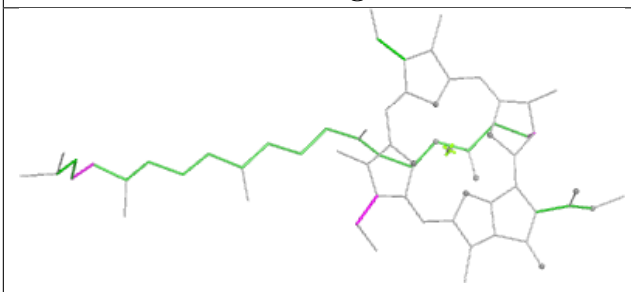
Ligand CLA B 609



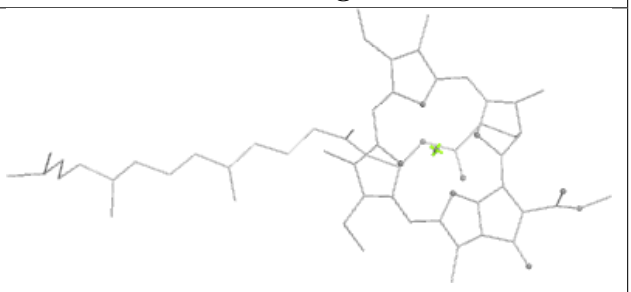
Bond lengths



Bond angles

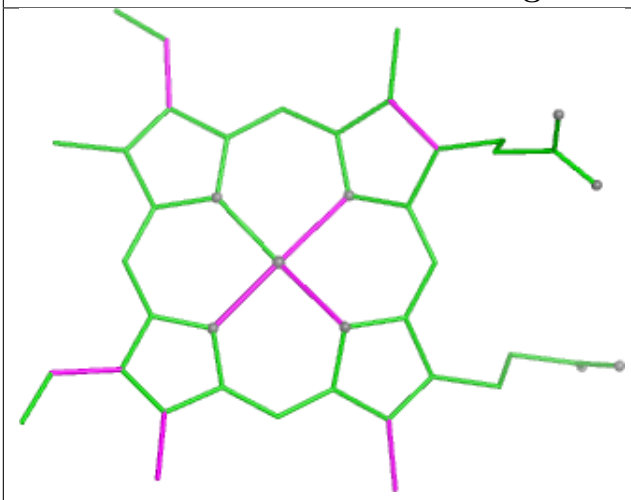


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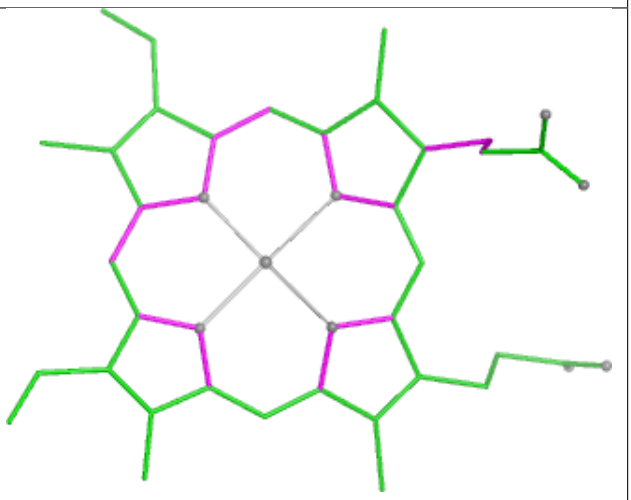


Rings

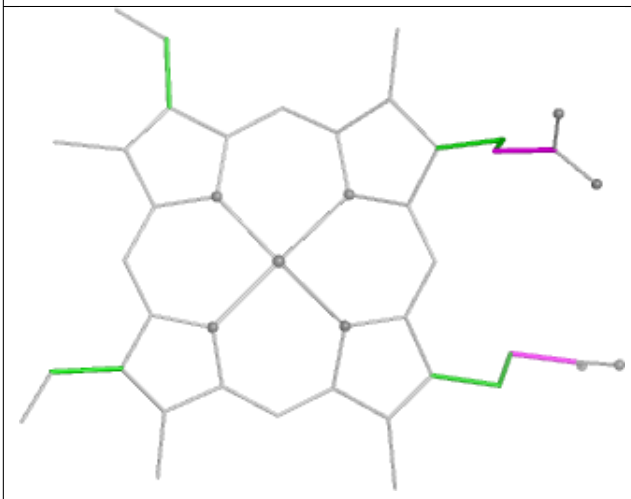
Ligand HEM e 102



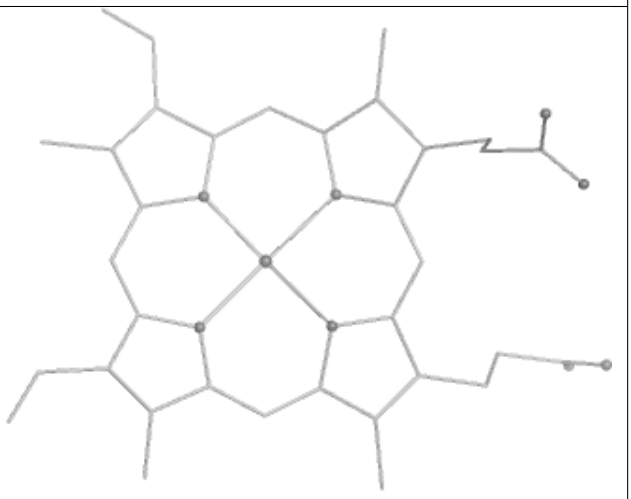
Bond lengths



Bond angles

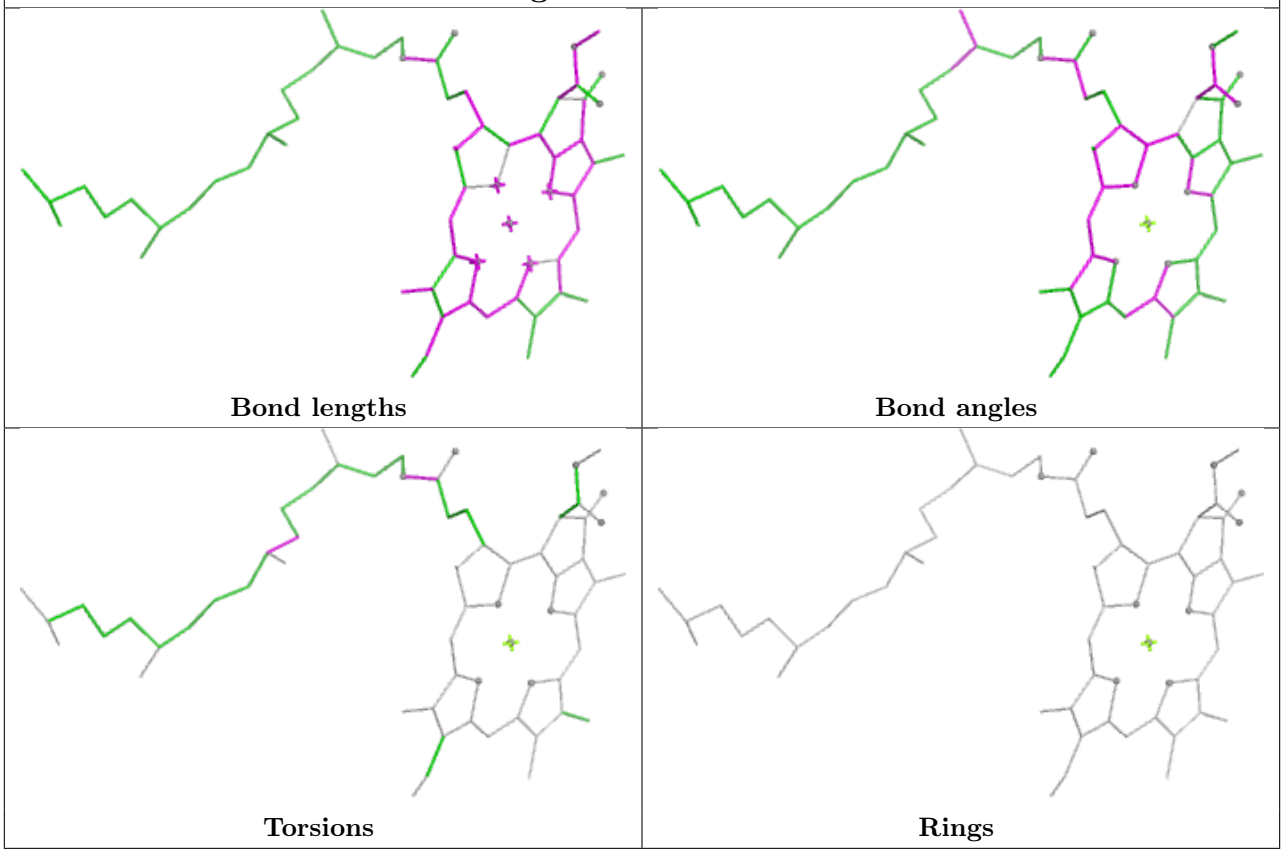


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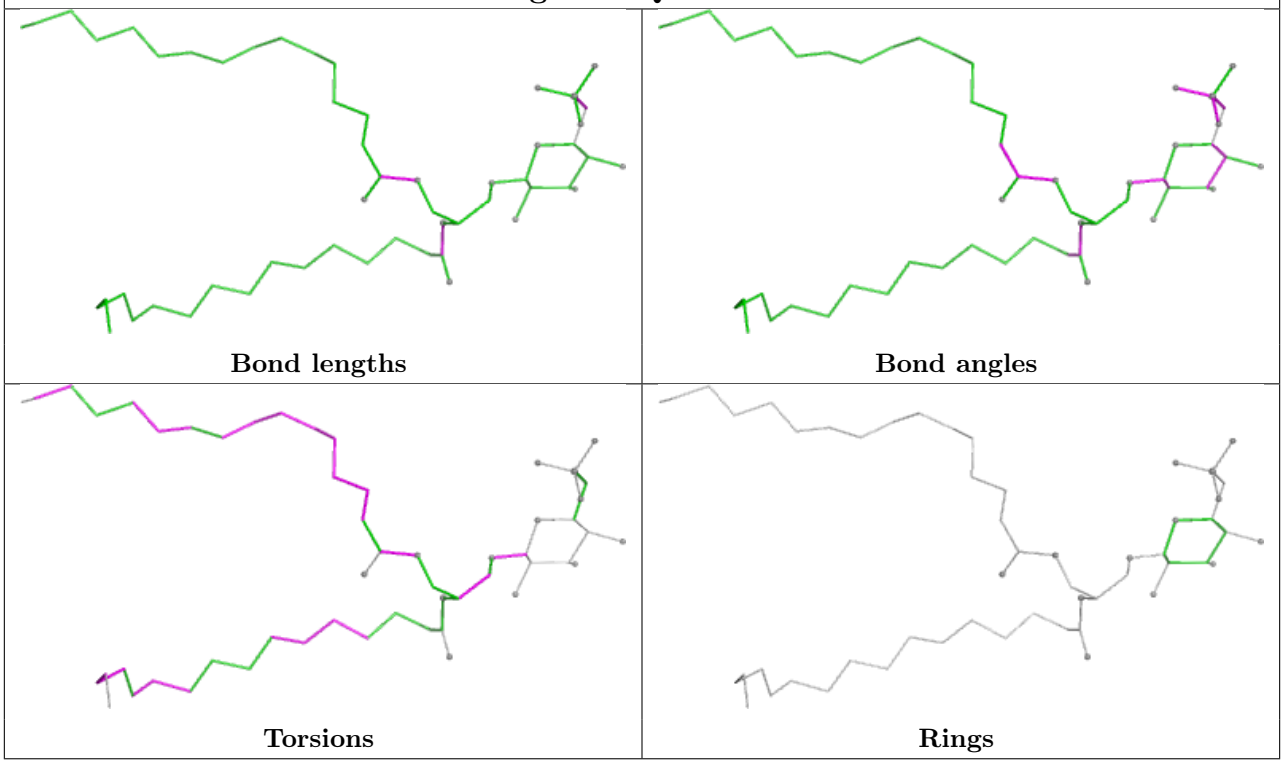


Rings

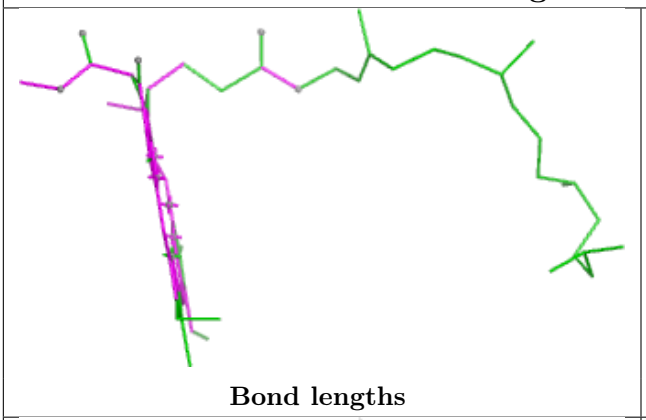
Ligand CLA c 511



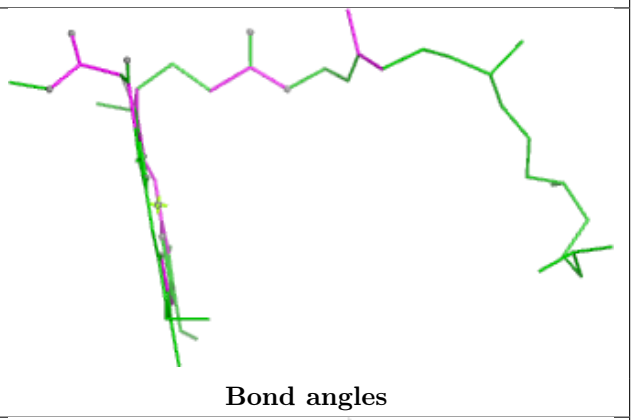
Ligand SQD a 614



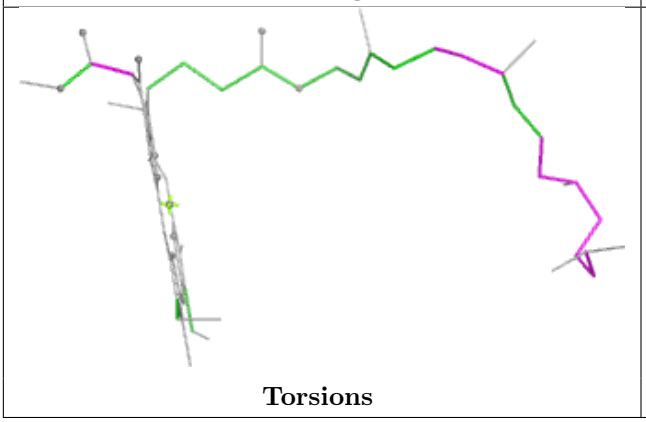
Ligand CLA c 506



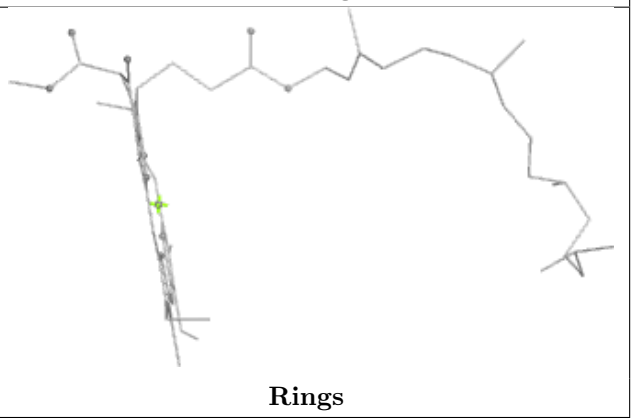
Bond lengths



Bond angles

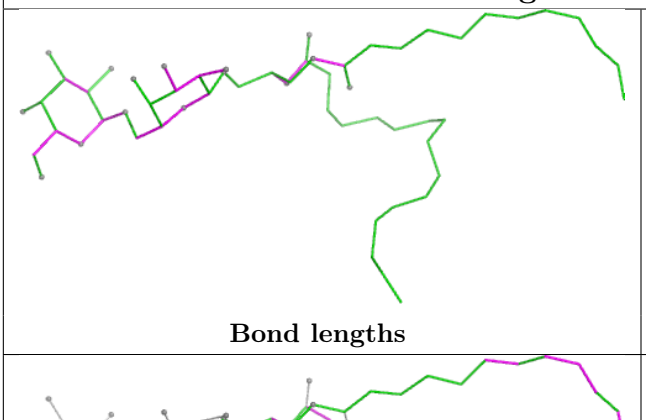


Torsions

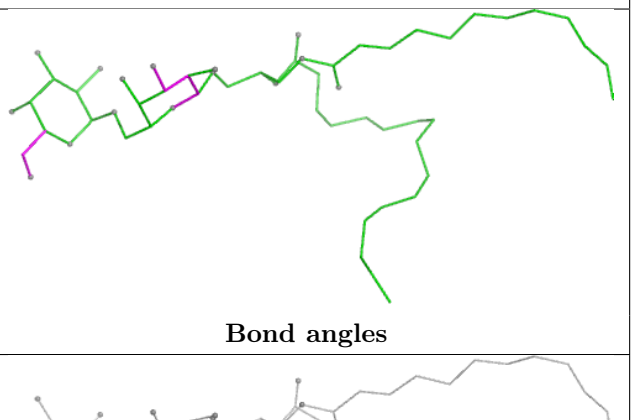


Rings

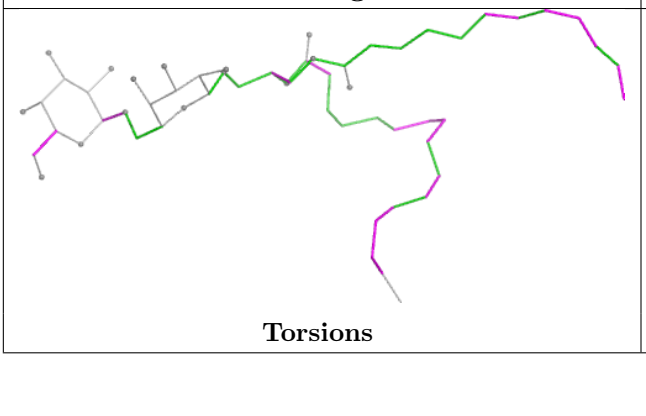
Ligand DGD H 102



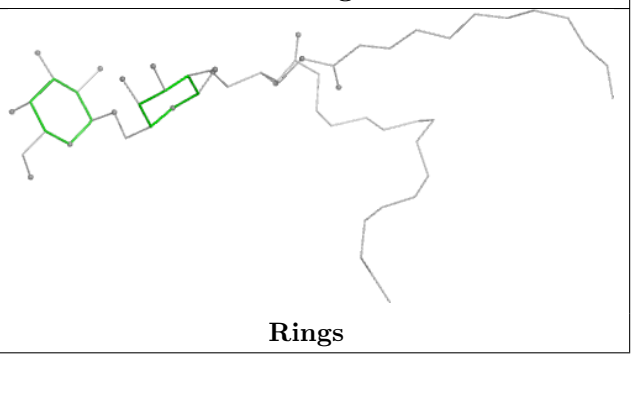
Bond lengths



Bond angles

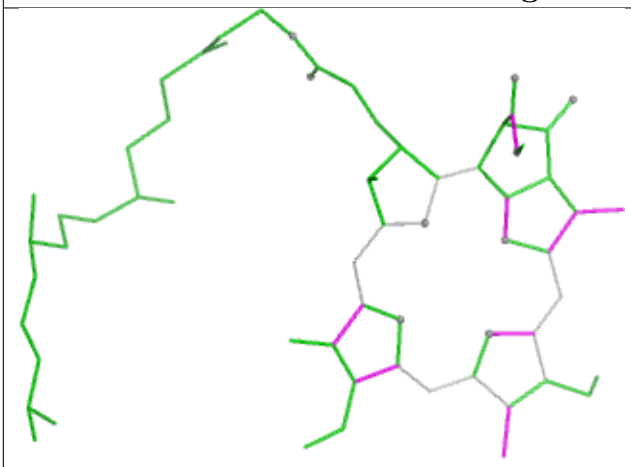


Torsions

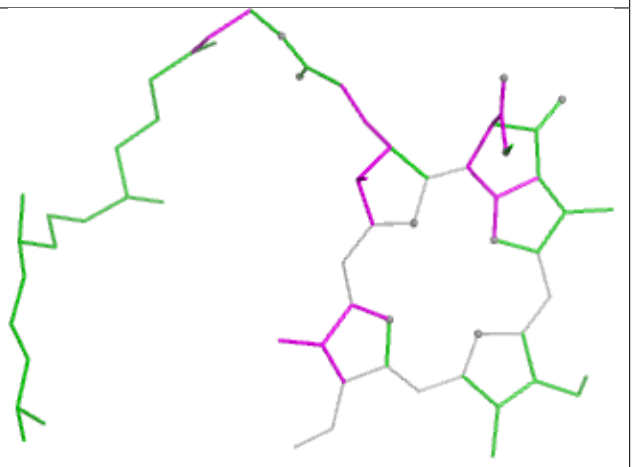


Rings

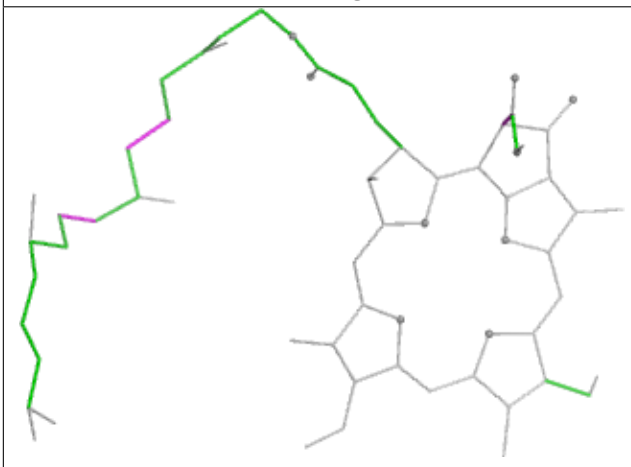
Ligand PHO D 401



Bond lengths



Bond angles

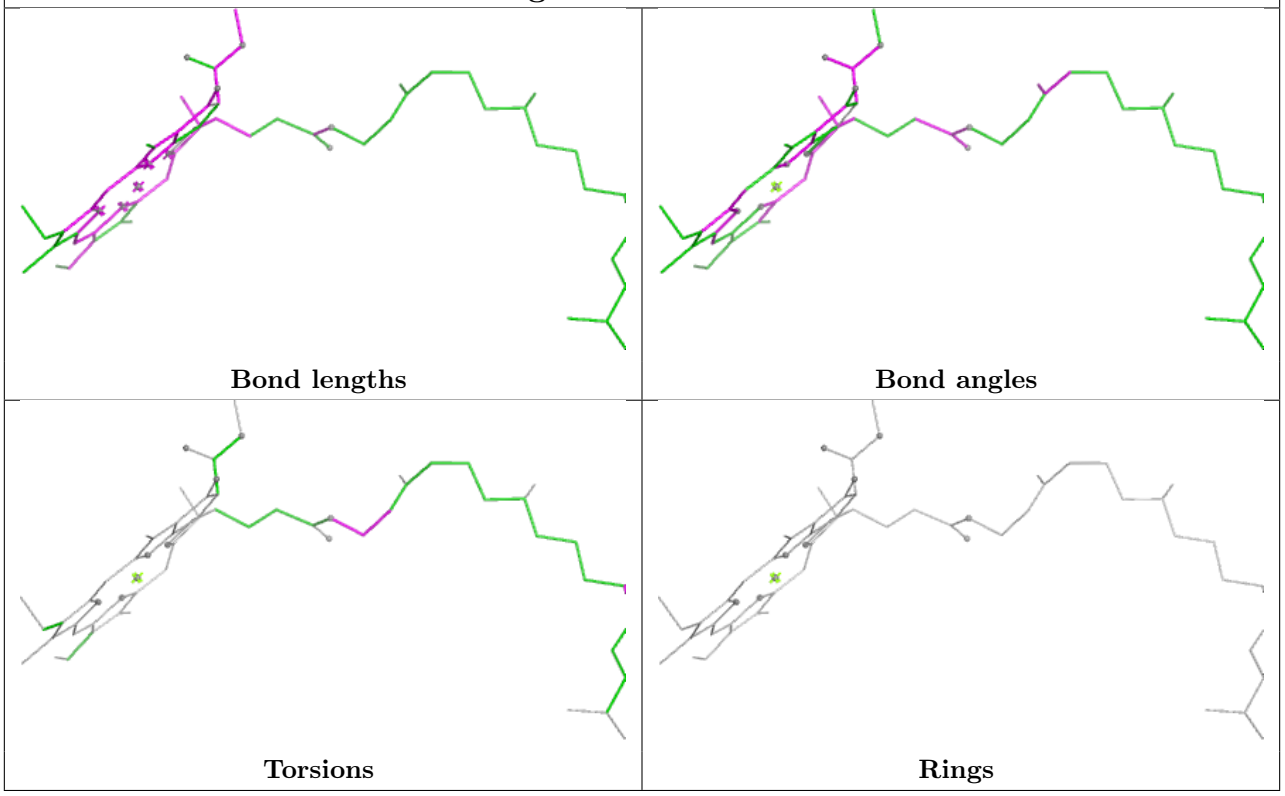


Torsions

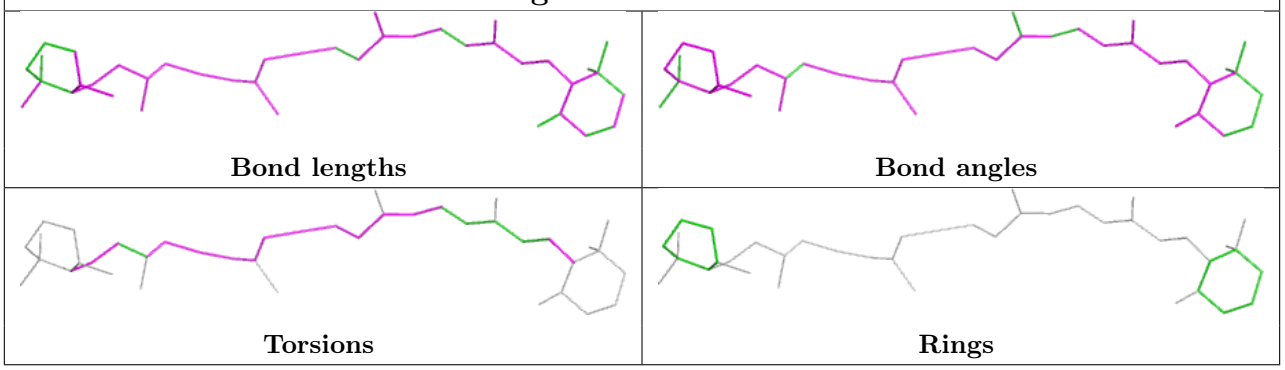


Rings

Ligand CLA d 402



Ligand BCR f 101



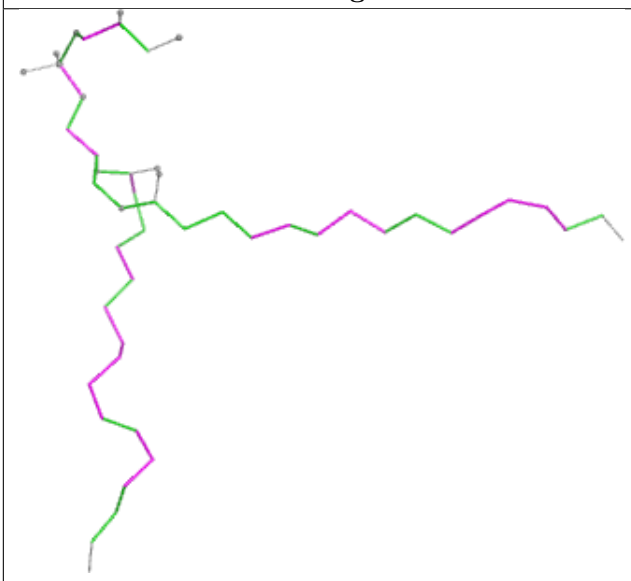
Ligand LHG l 102



Bond lengths



Bond angles

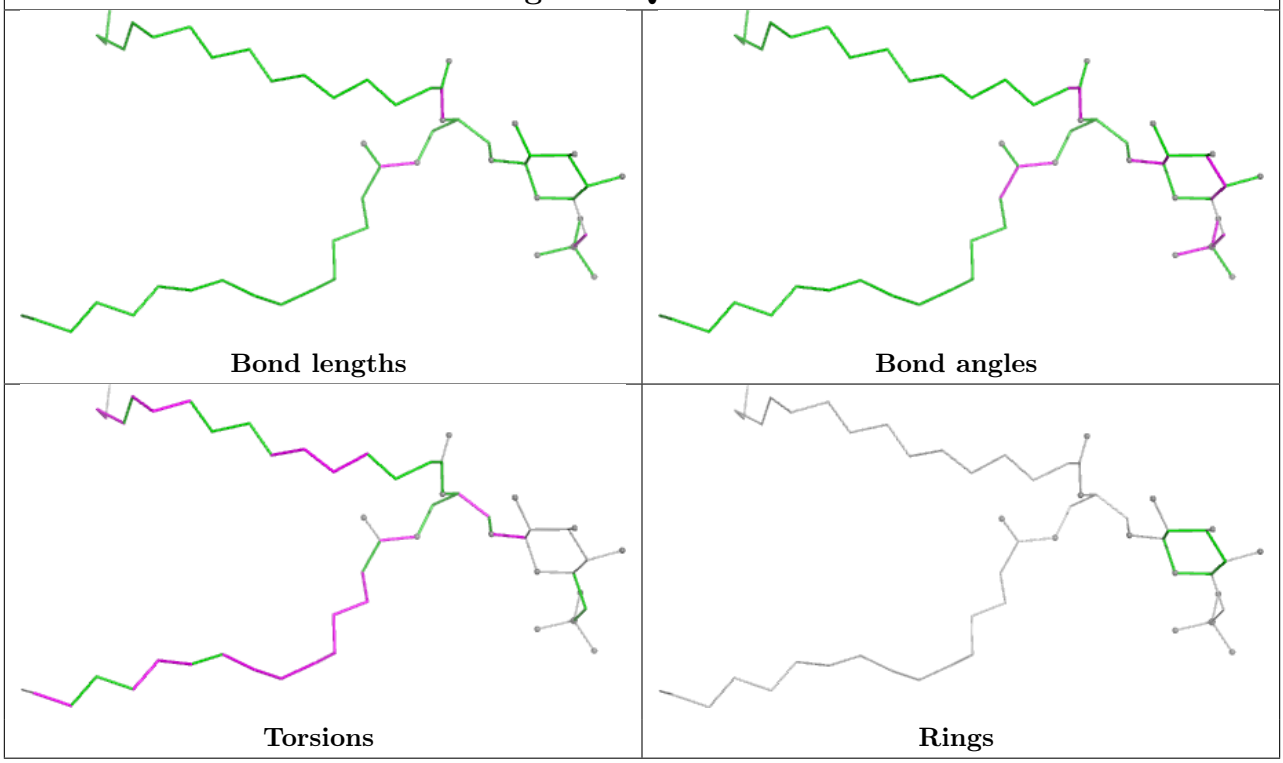


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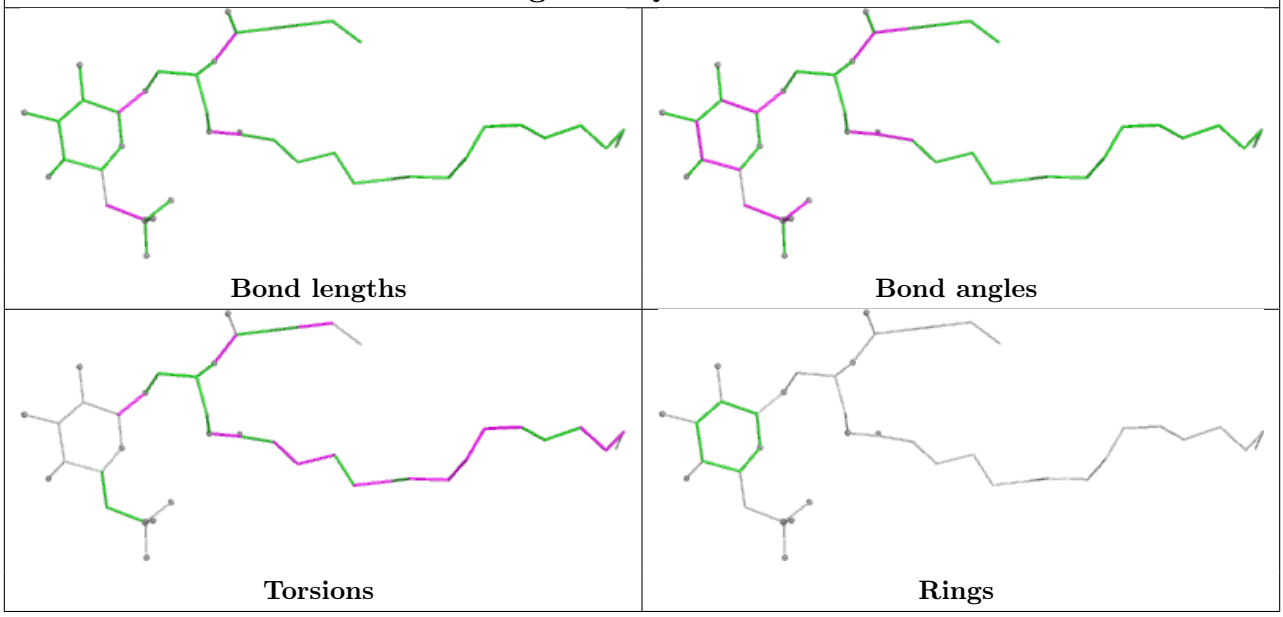


Rings

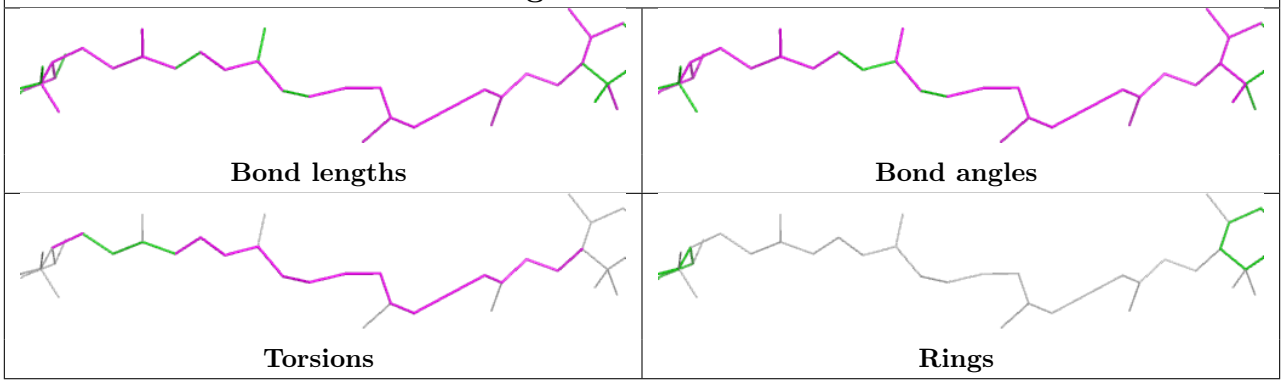
Ligand SQD A 614



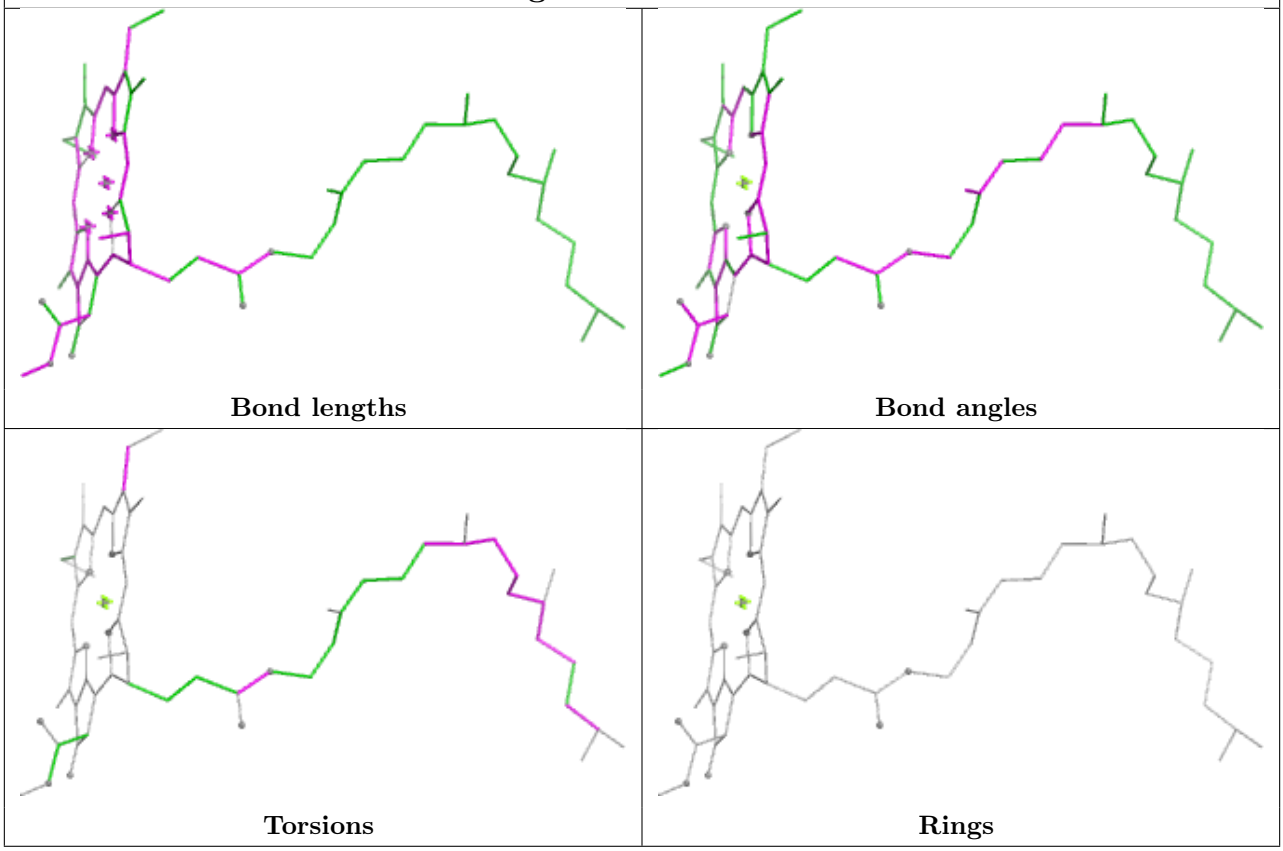
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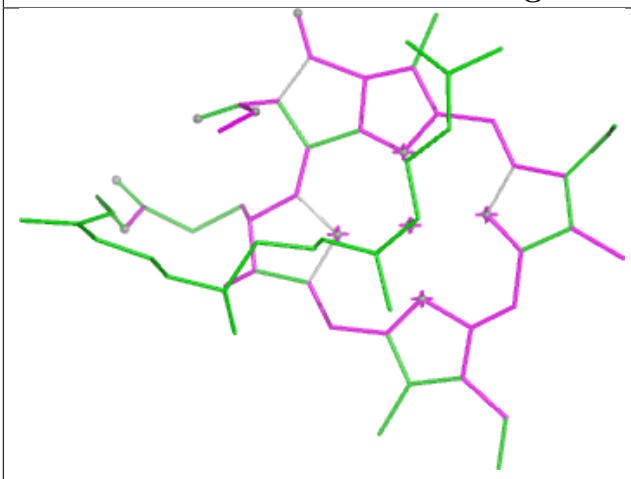
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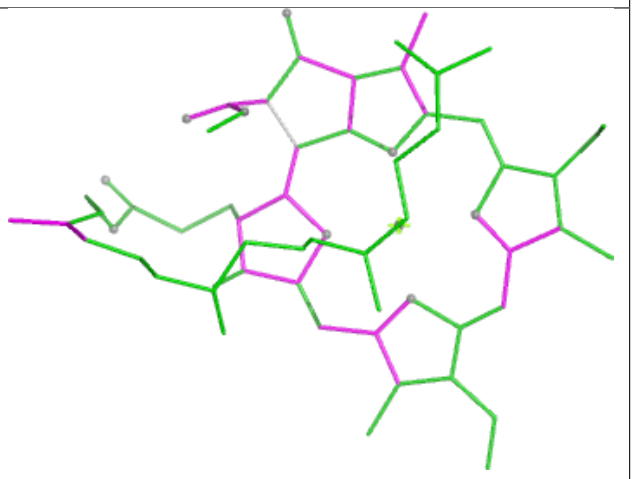
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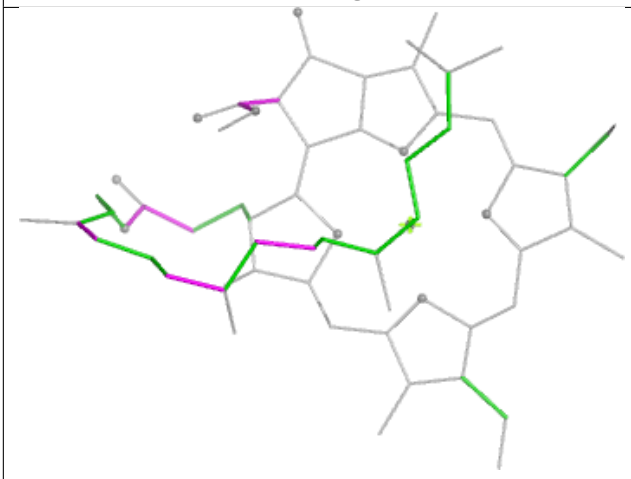
Ligand CLA C 510



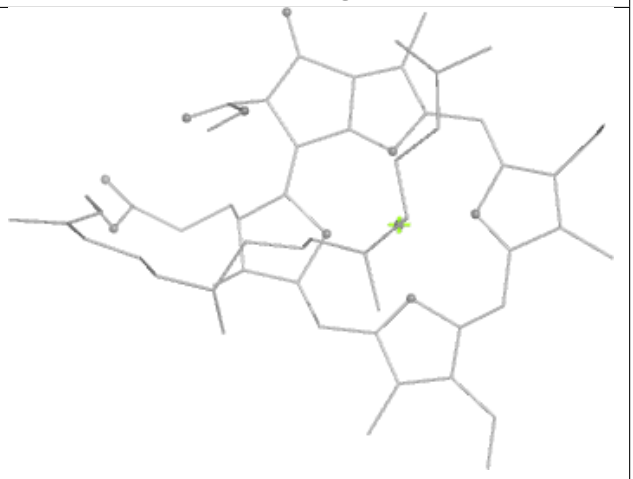
Bond lengths



Bond angles

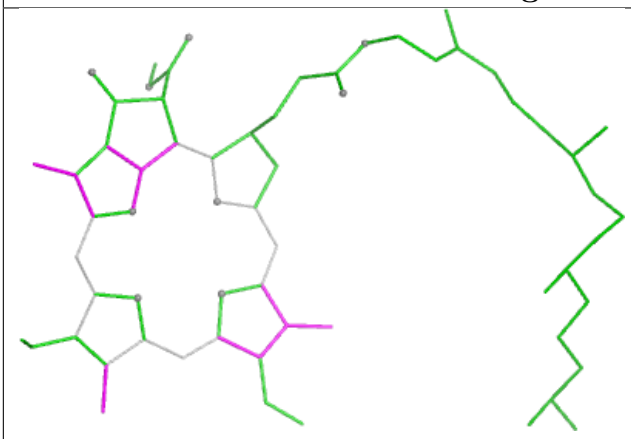


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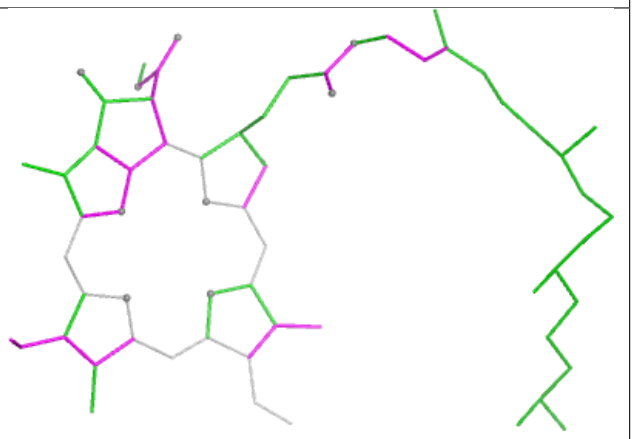


Rings

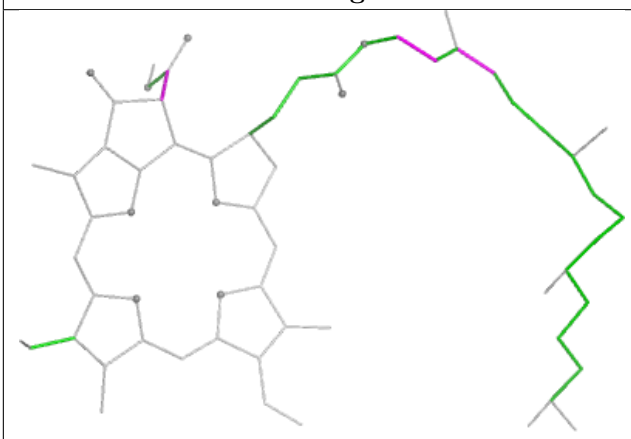
Ligand PHO A 608



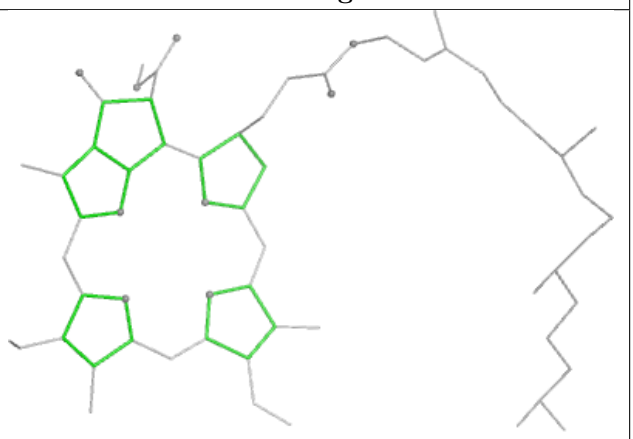
Bond lengths



Bond angles

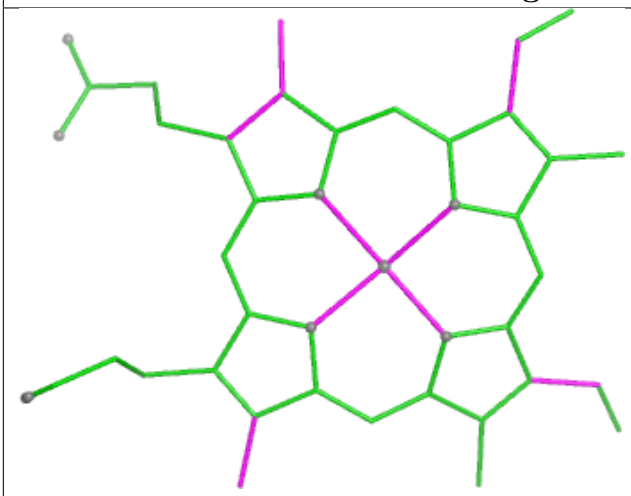


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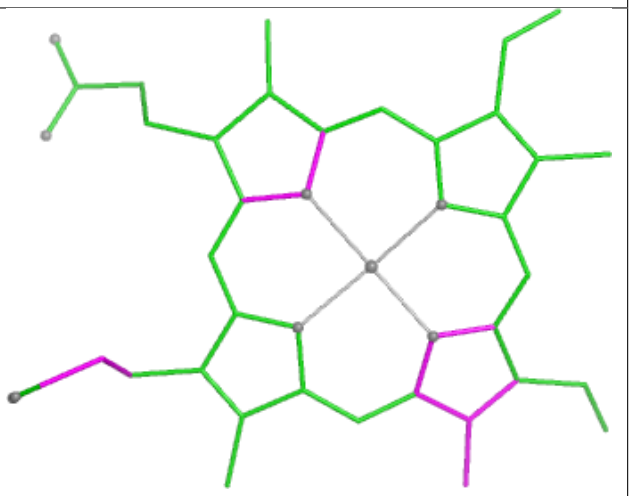


Rings

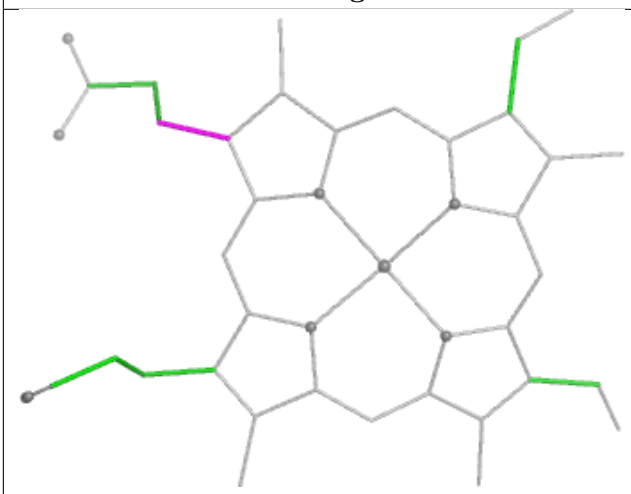
Ligand HEM v 201



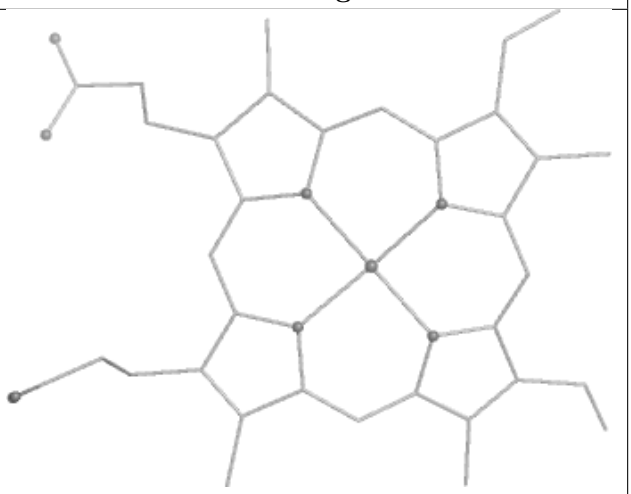
Bond lengths



Bond angles

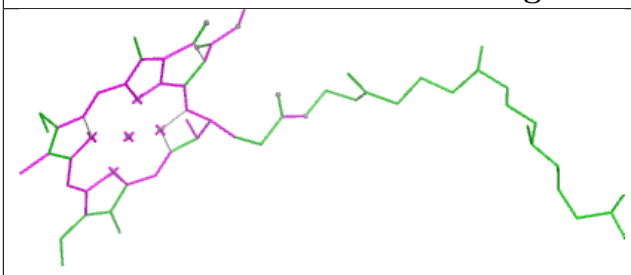


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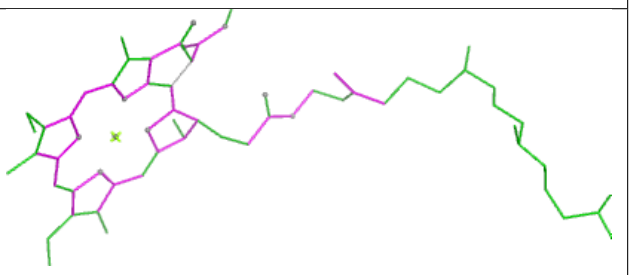


Rings

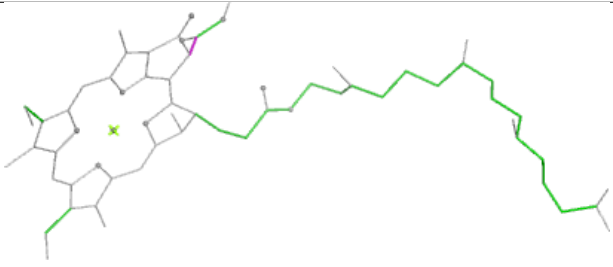
Ligand CLA A 606



Bond lengths



Bond angles

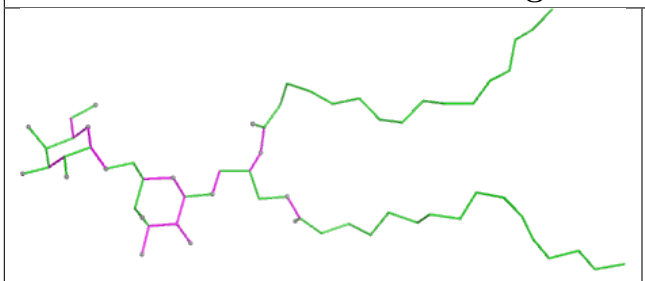


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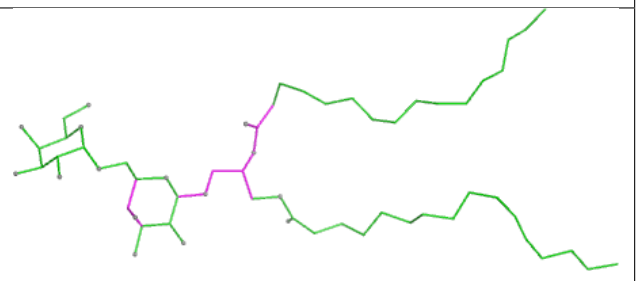


Rings

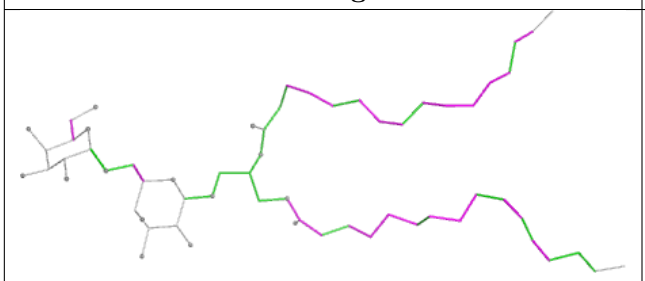
Ligand DGD c 518



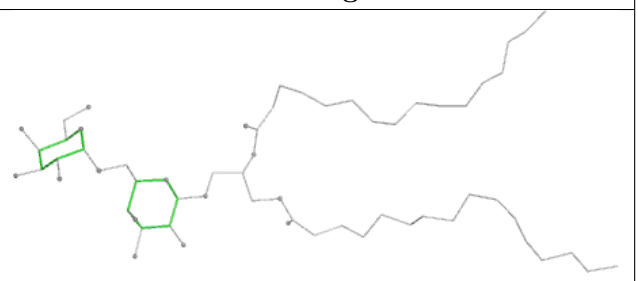
Bond lengths



Bond angles

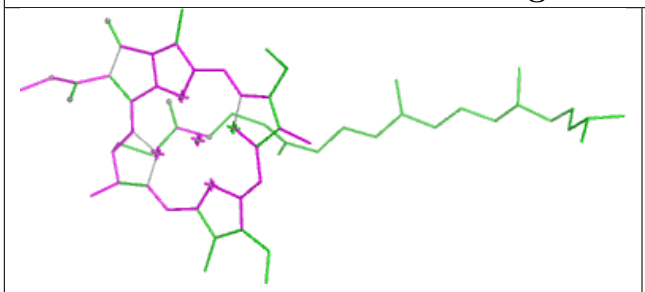


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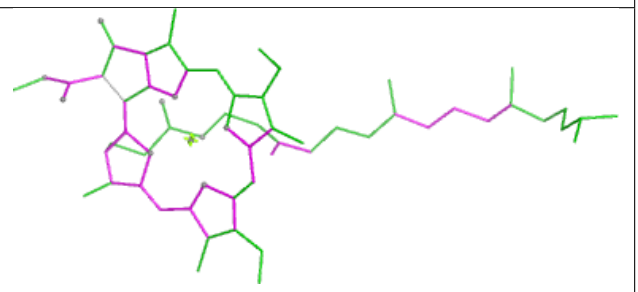


Rings

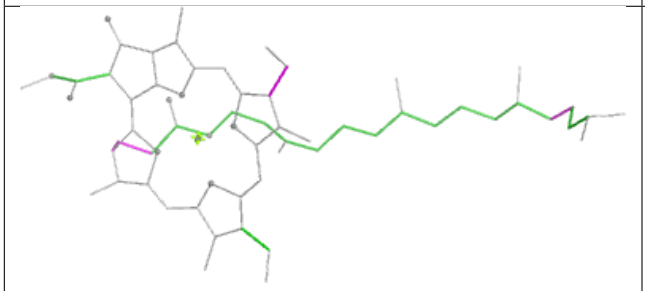
Ligand CLA b 610



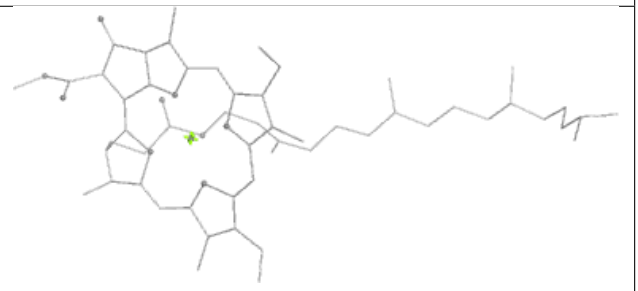
Bond lengths



Bond angles

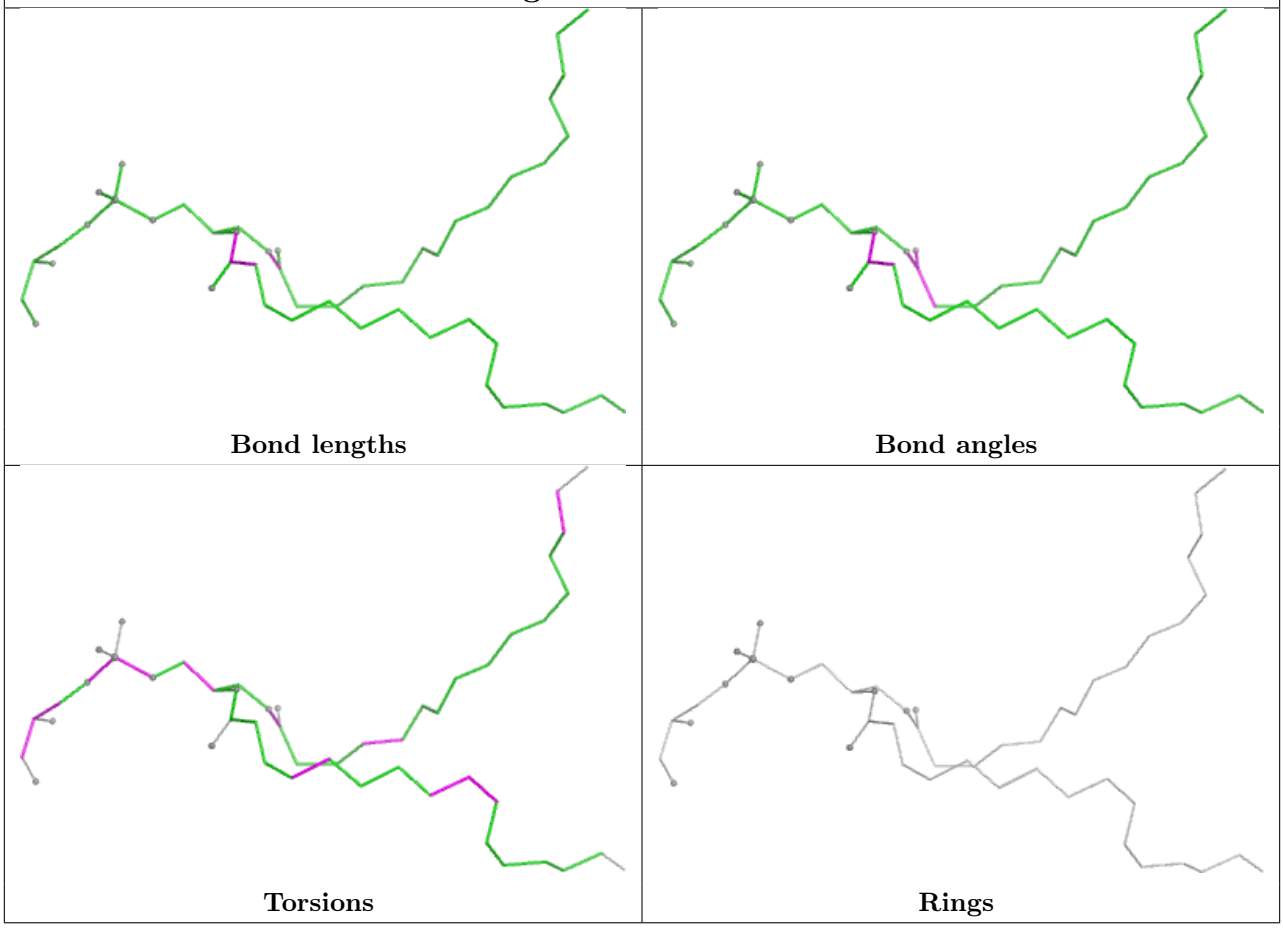


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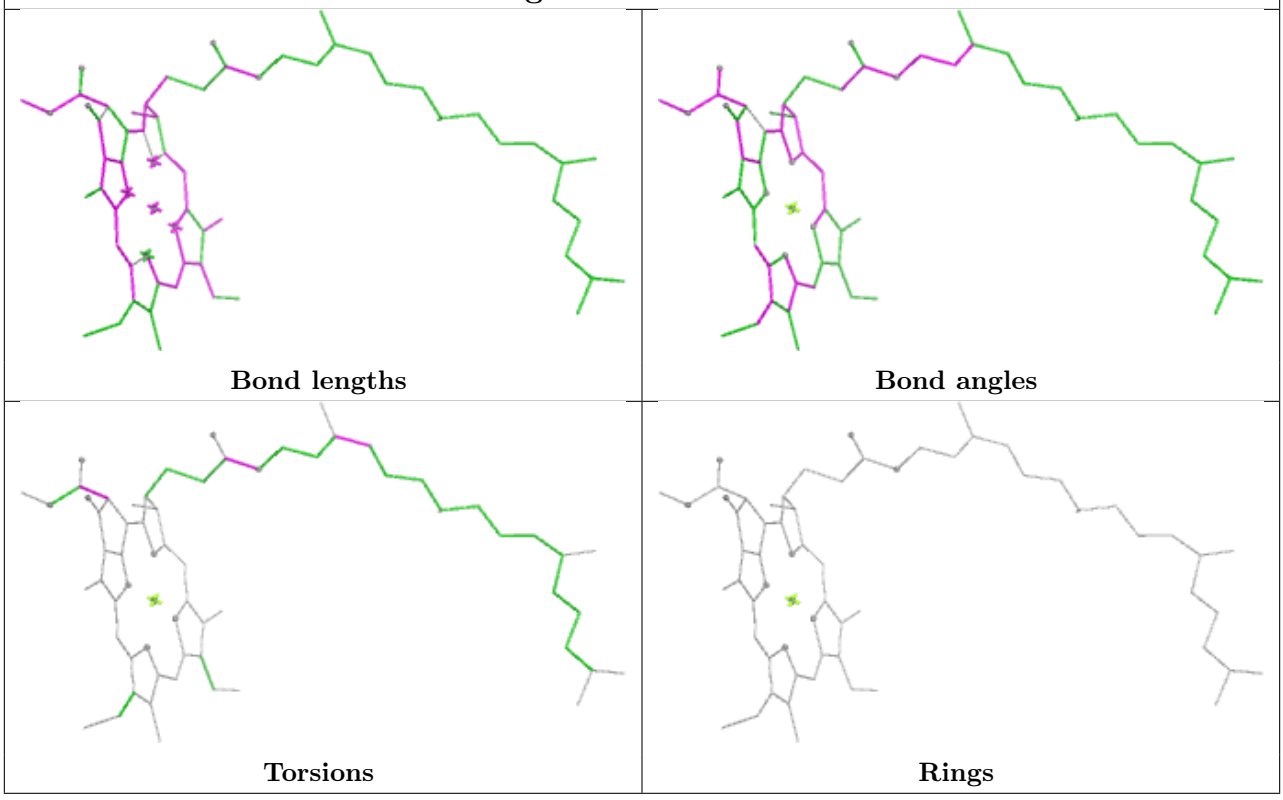


Rings

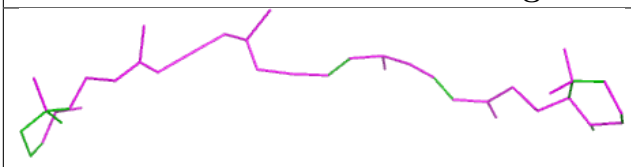
Ligand LHG D 407



Ligand CLA B 610



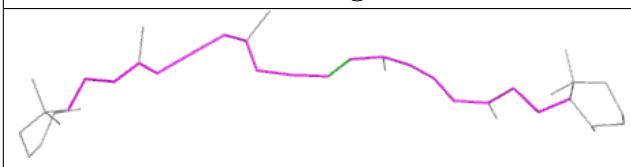
Ligand BCR T 101



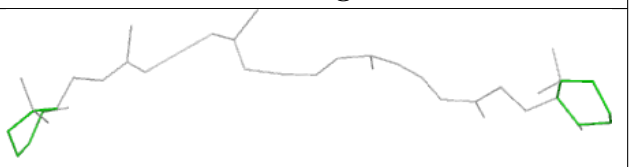
Bond lengths



Bond angles

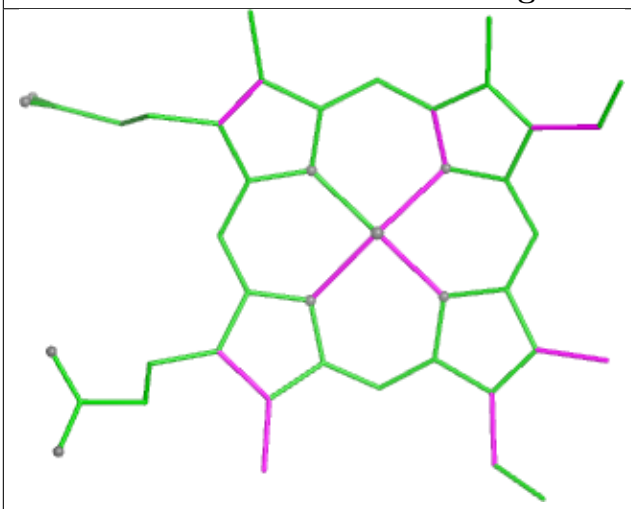


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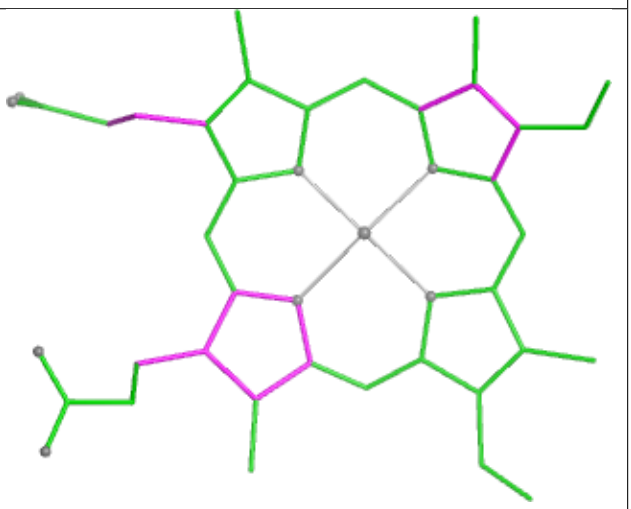


Rings

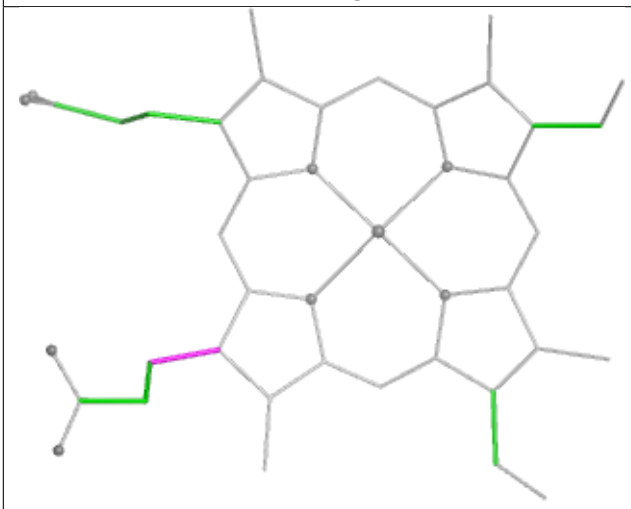
Ligand HEM V 201



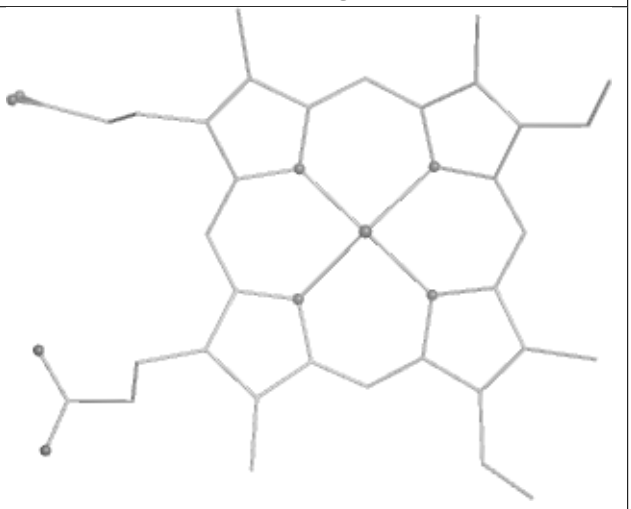
Bond lengths



Bond angles

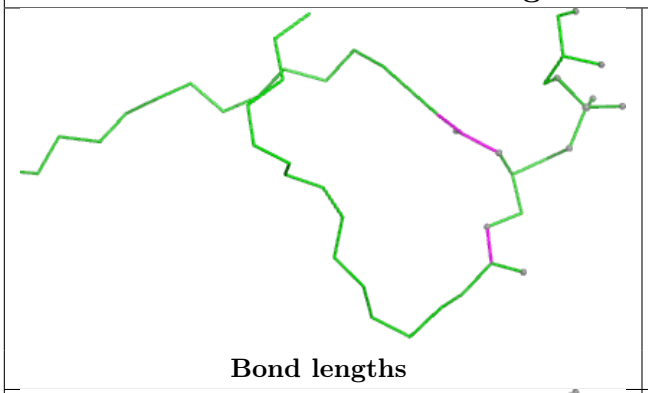


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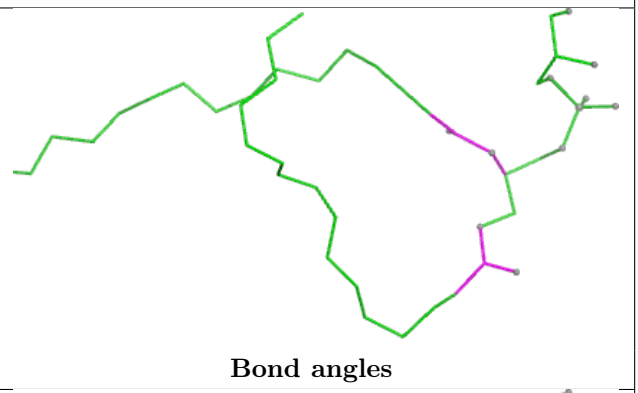


Rings

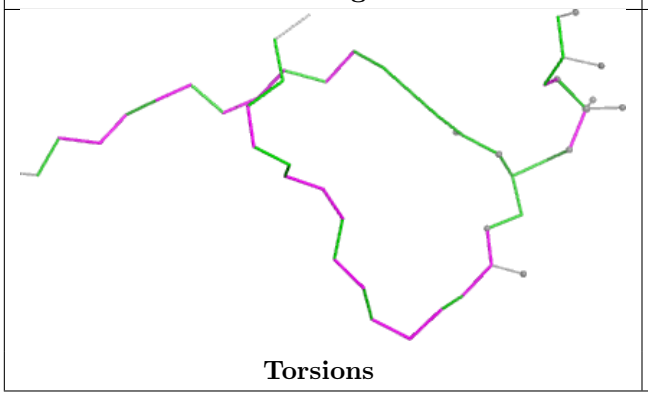
Ligand LHG A 615



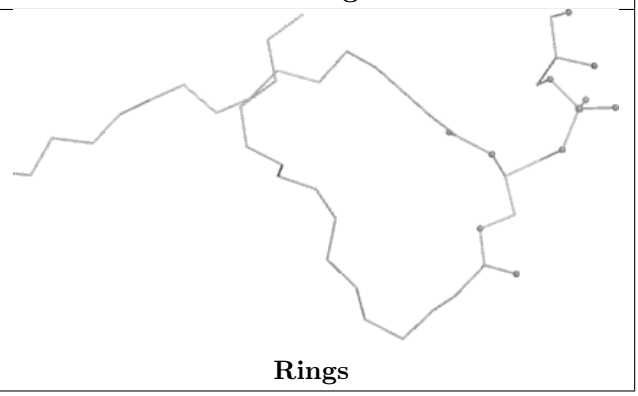
Bond lengths



Bond angles

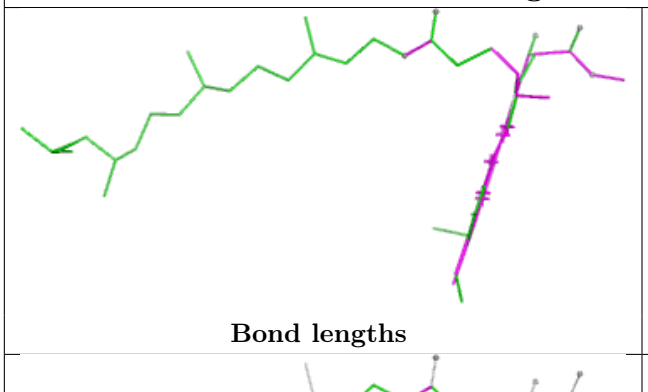


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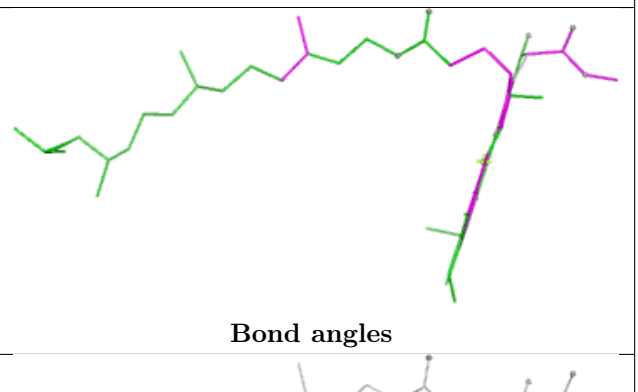


Rings

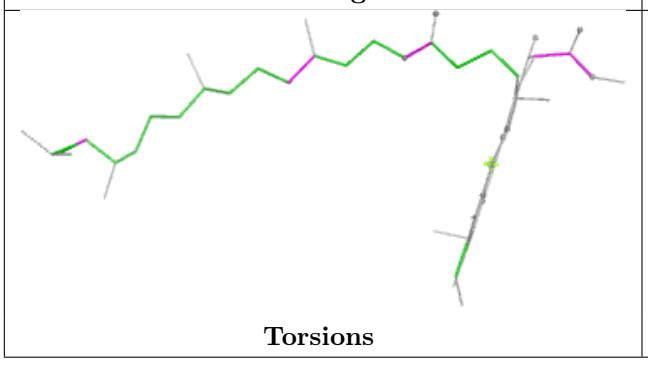
Ligand CLA B 606



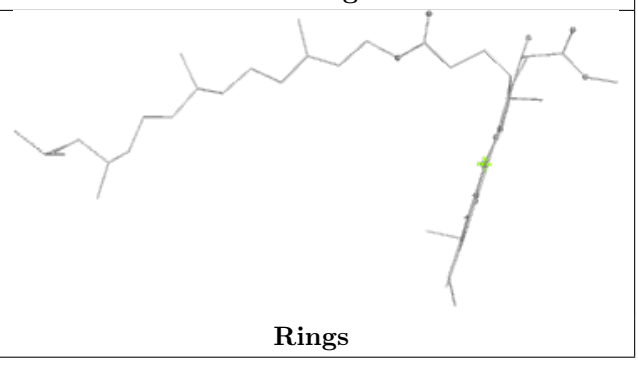
Bond lengths



Bond angles

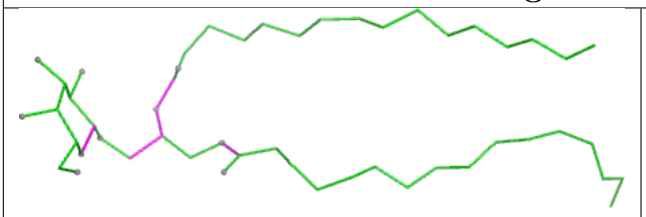


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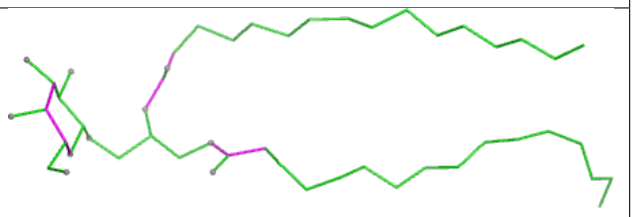


Rings

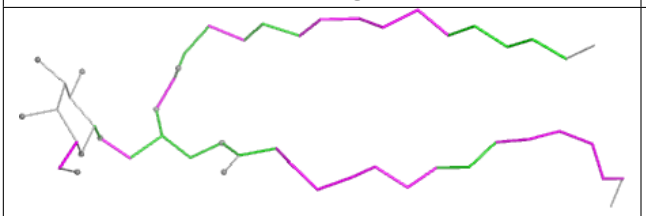
Ligand LMG c 520



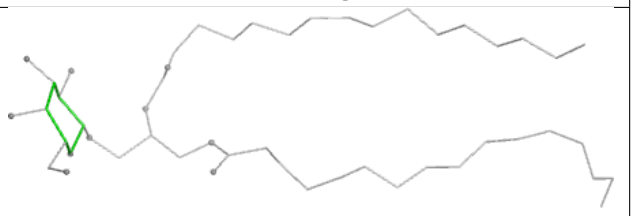
Bond lengths



Bond angles

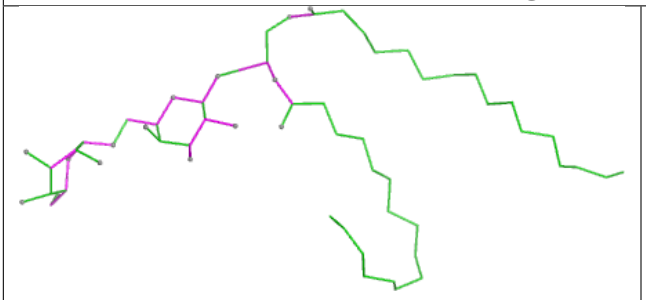


Torsions



Rings

Ligand DGD d 405



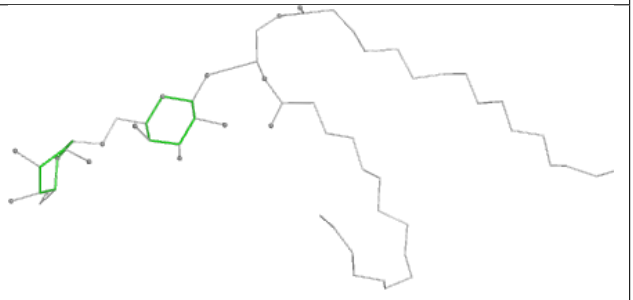
Bond lengths



Bond angles

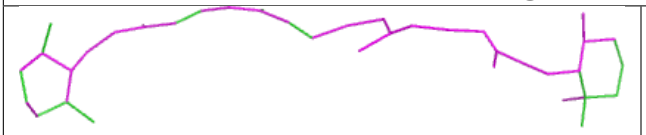


Torsions

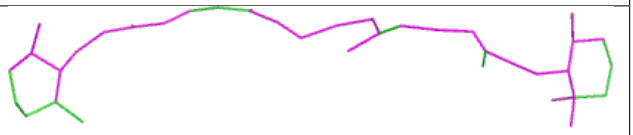


Rings

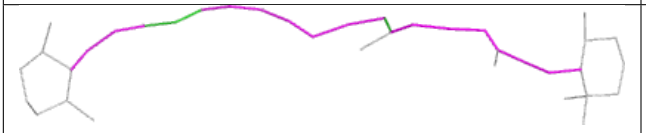
Ligand BCR K 102



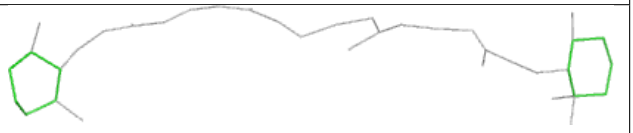
Bond lengths



Bond angles

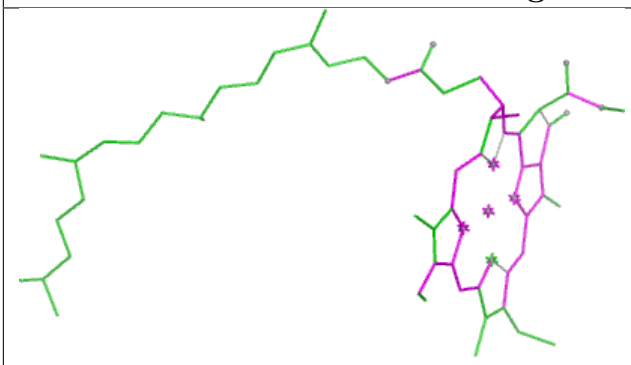


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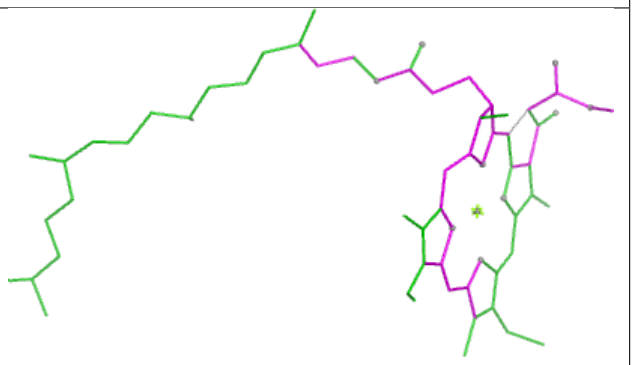


Rings

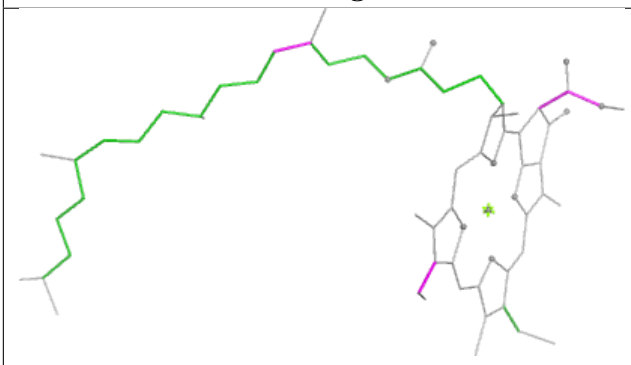
Ligand CLA b 611



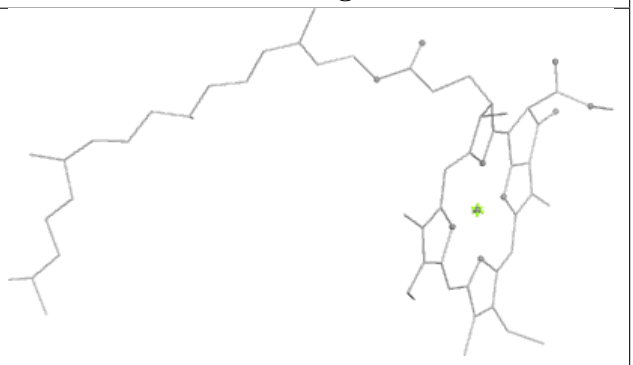
Bond lengths



Bond angles

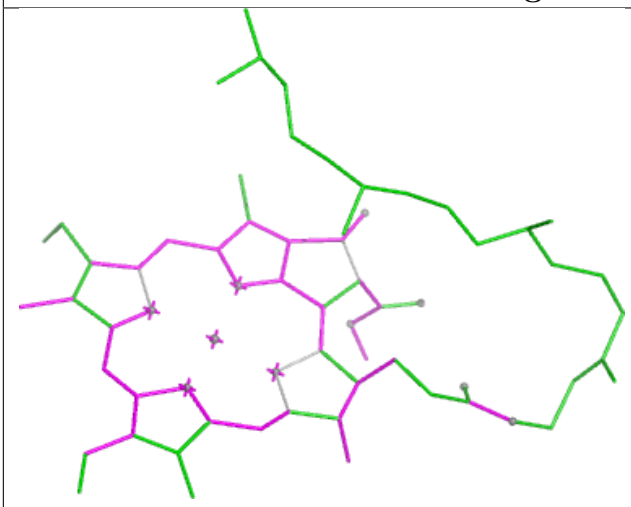


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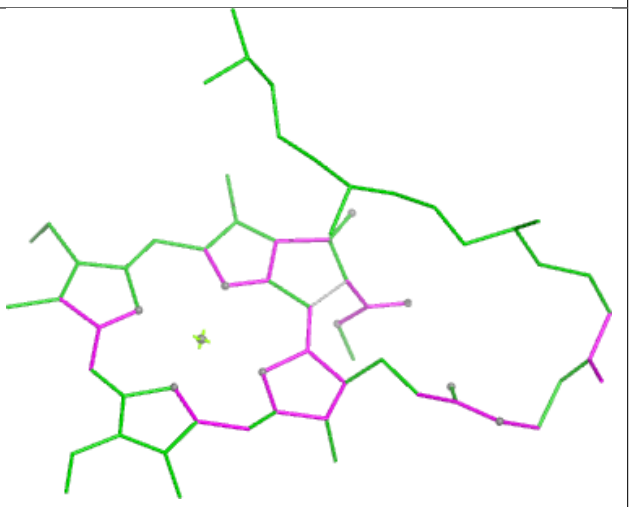


Rings

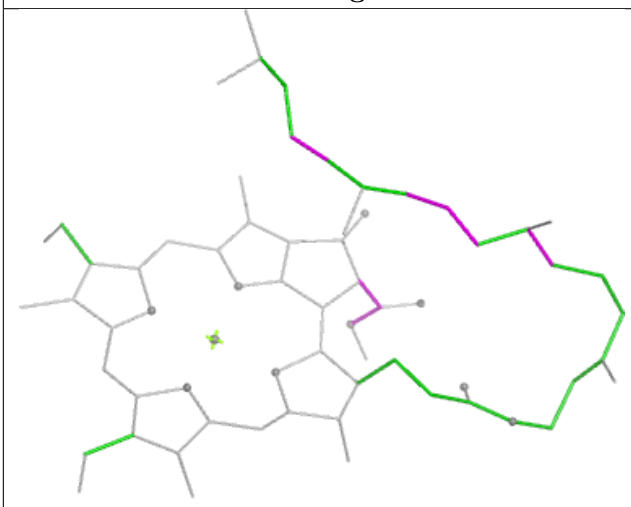
Ligand CLA C 509



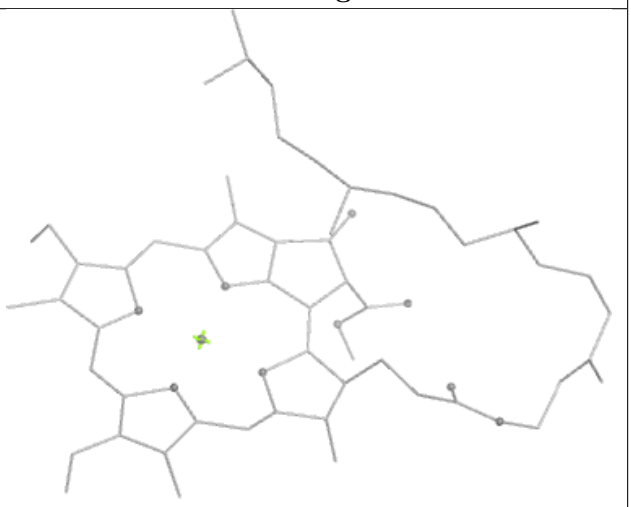
Bond lengths



Bond angles

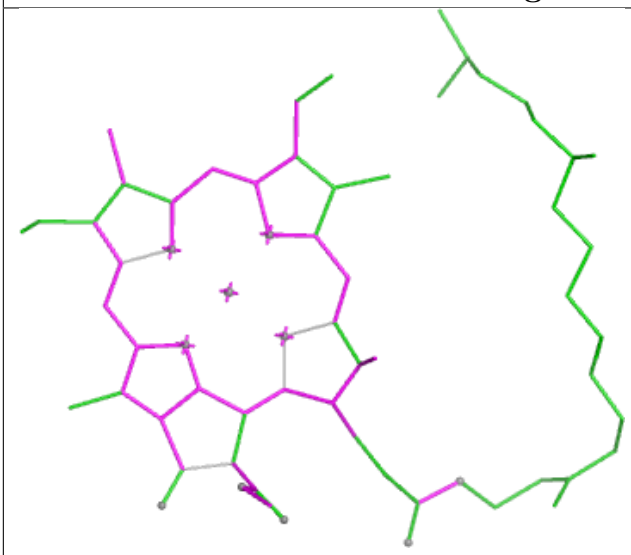


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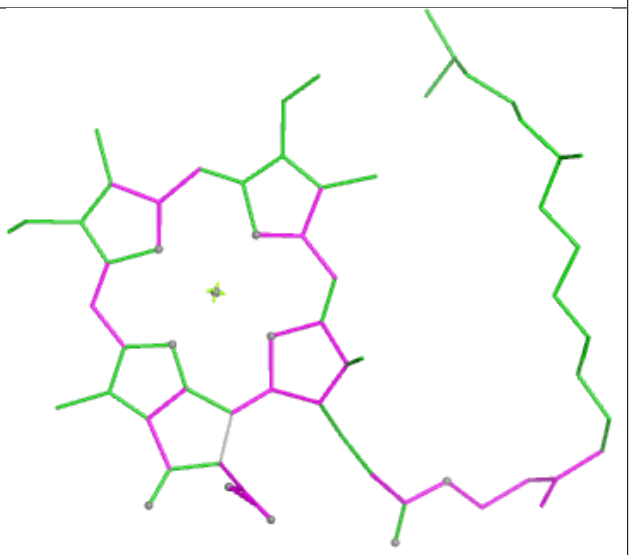


Rings

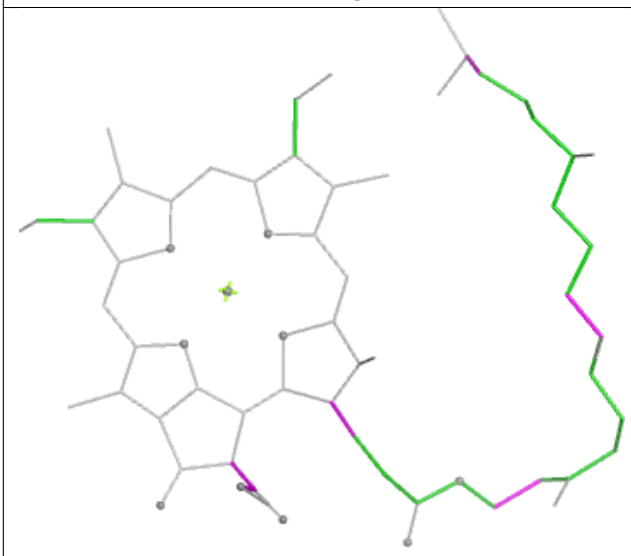
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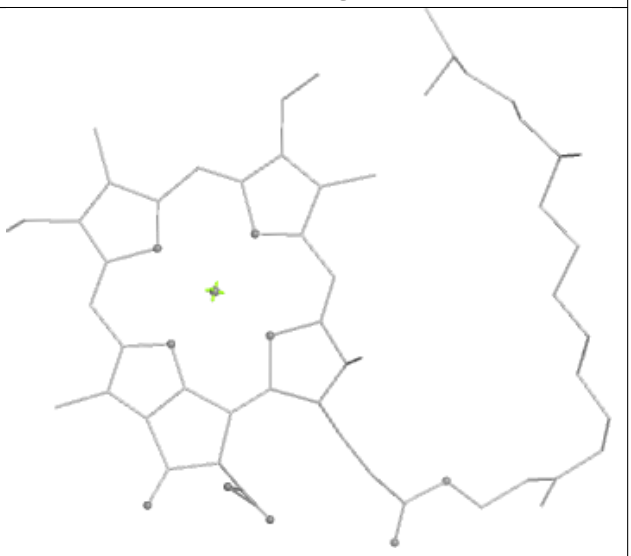
Bond lengths



Bond angles

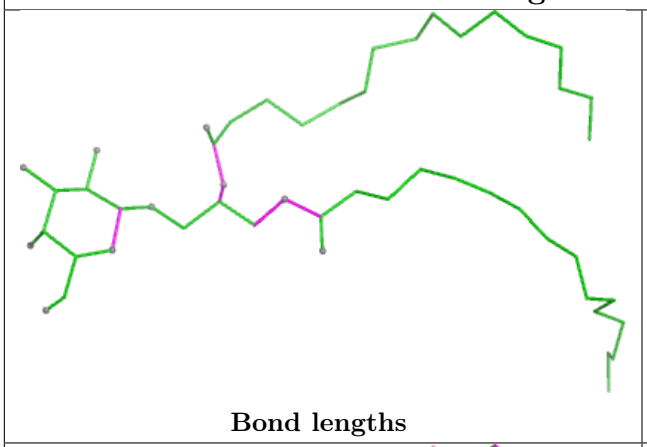


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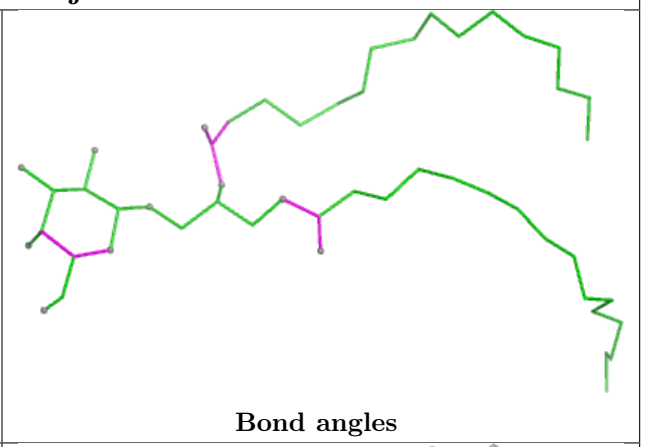


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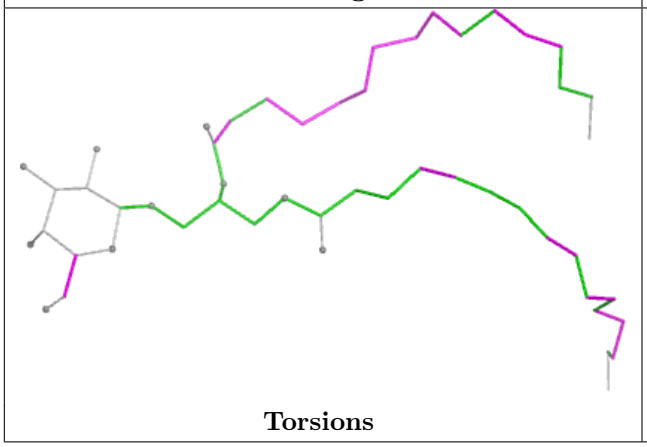
Ligand LMG j 101



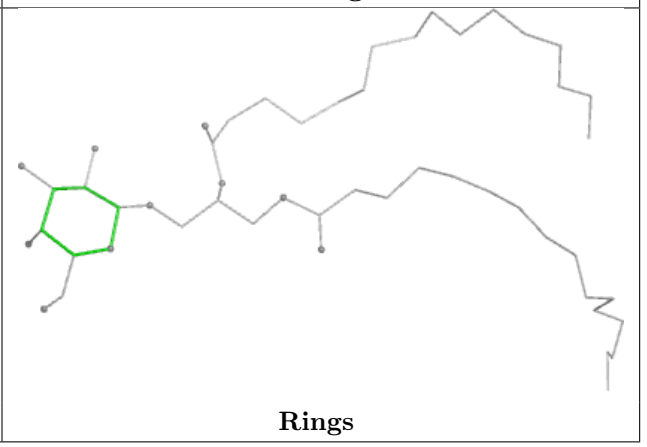
Bond lengths



Bond angles

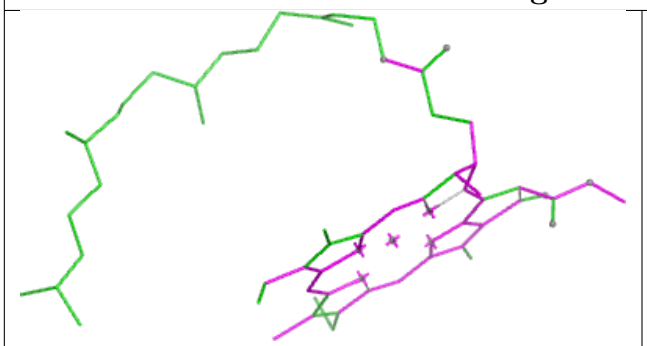


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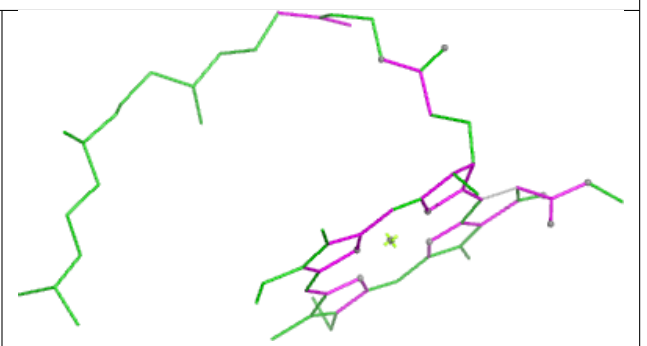


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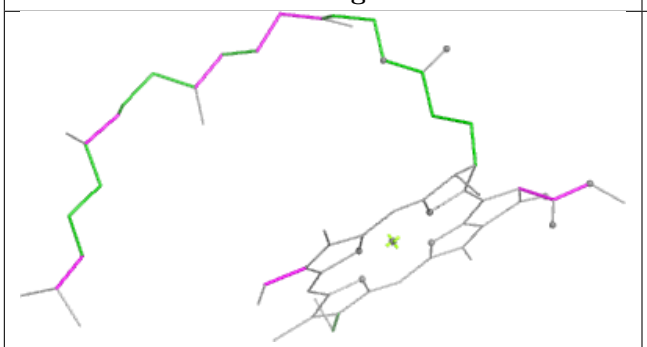
Ligand CLA c 513



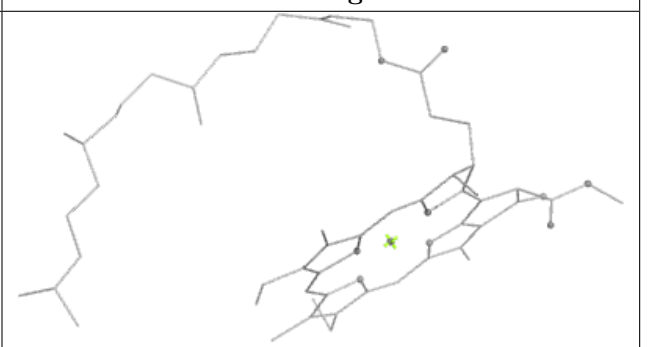
Bond lengths



Bond angles

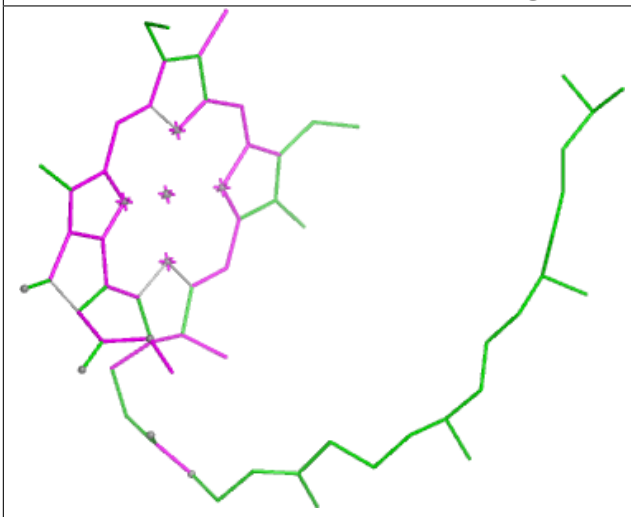


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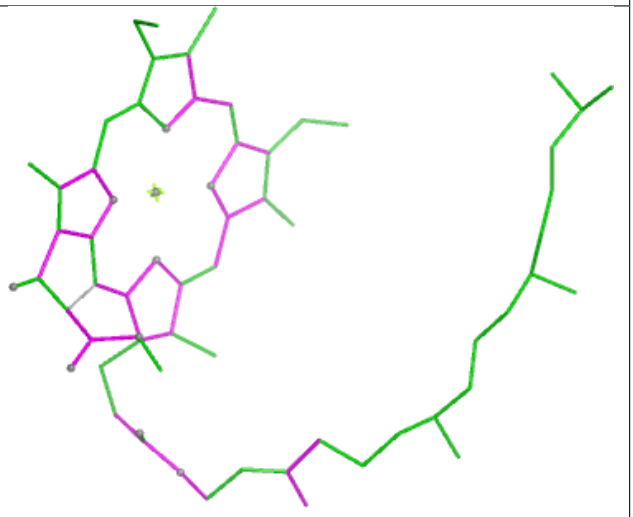


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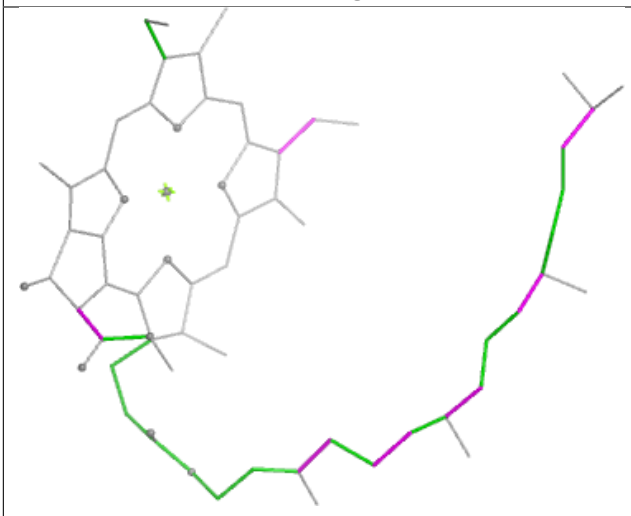
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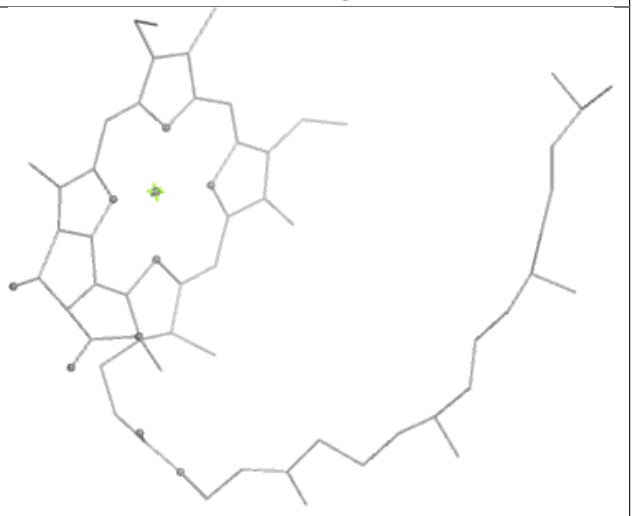
Bond lengths



Bond angles

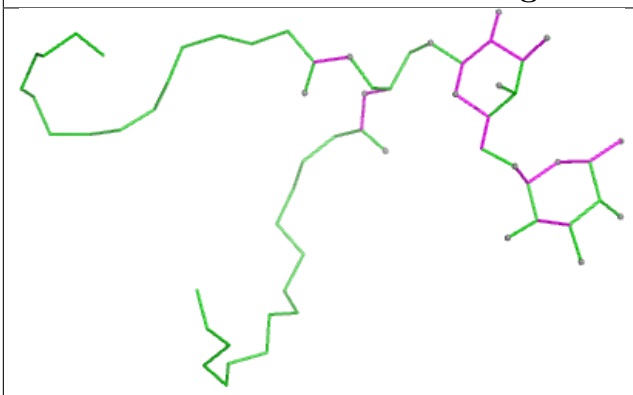


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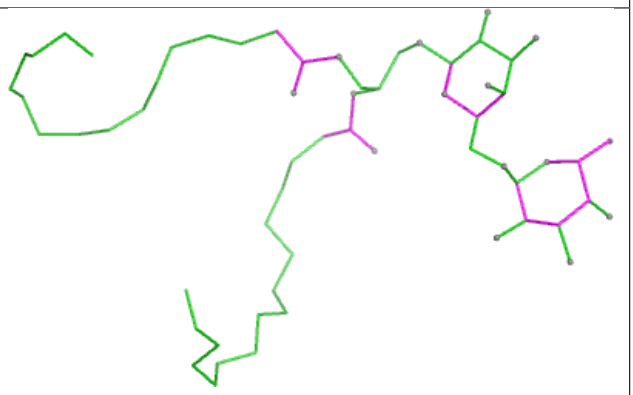


Rings

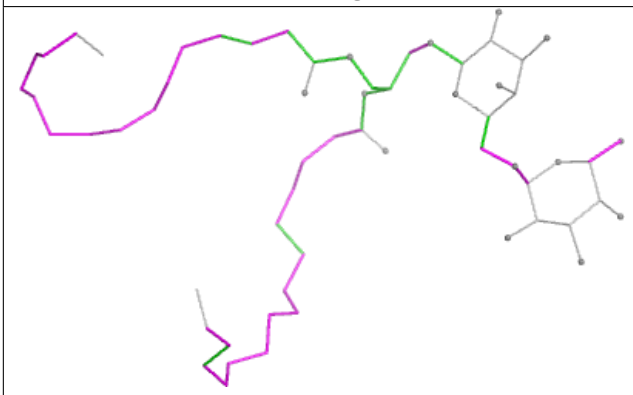
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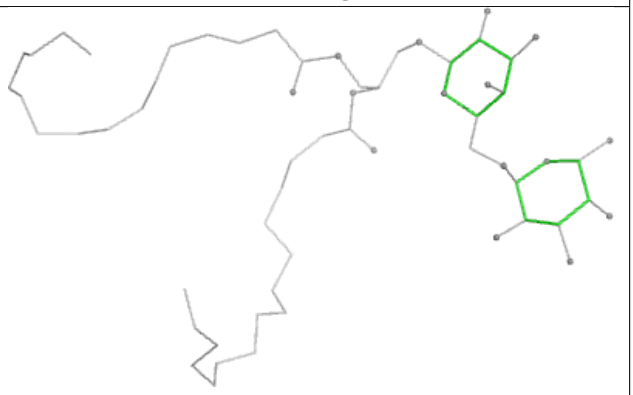
Bond lengths



Bond angles

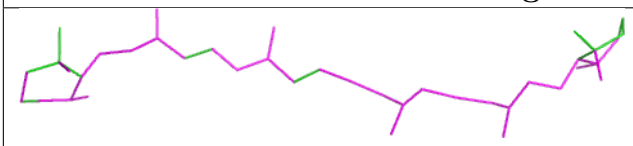


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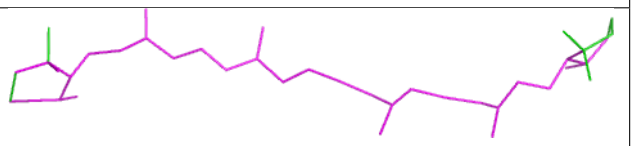


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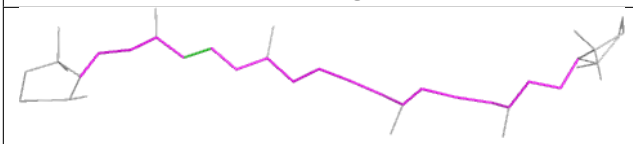
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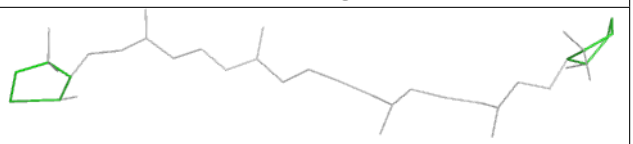
Bond lengths



Bond angles

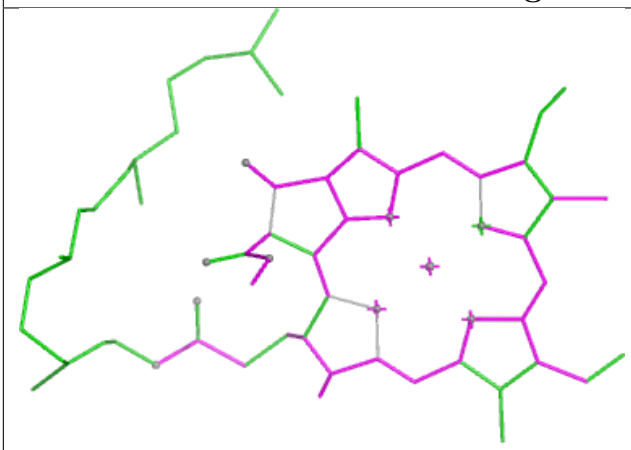


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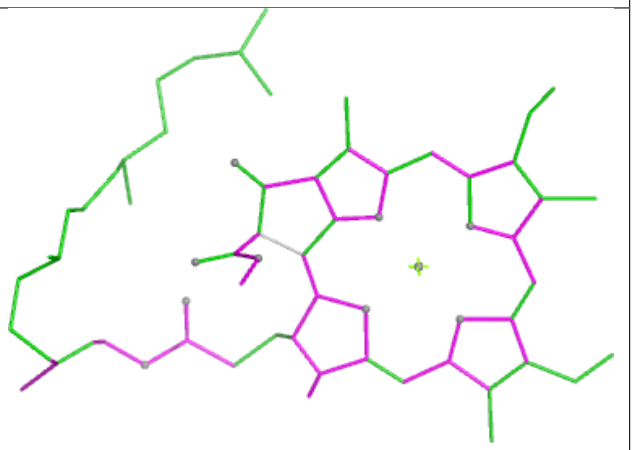


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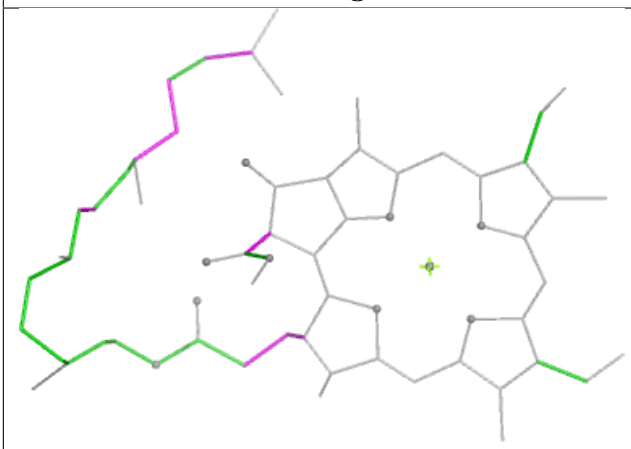
Ligand CLA B 611



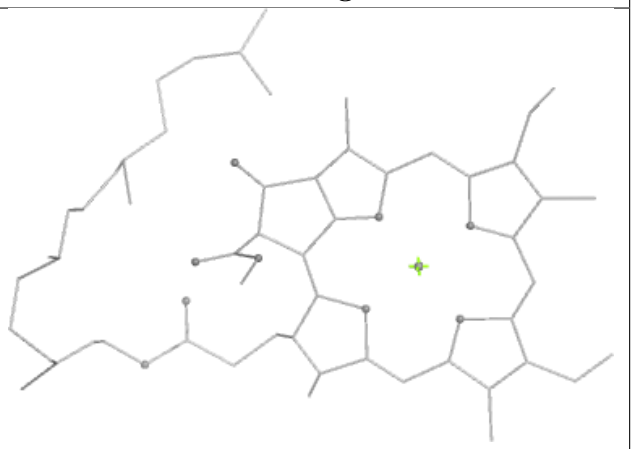
Bond lengths



Bond angles

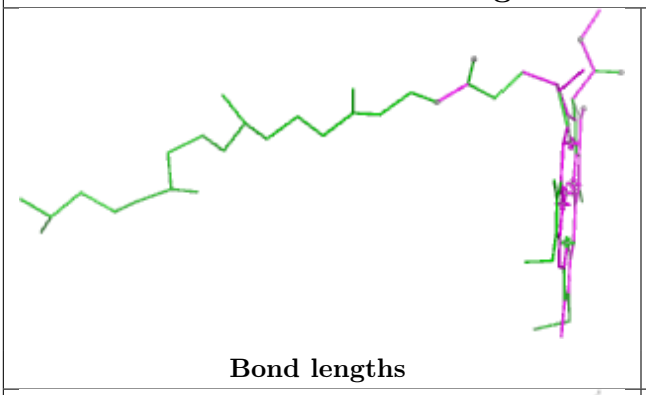


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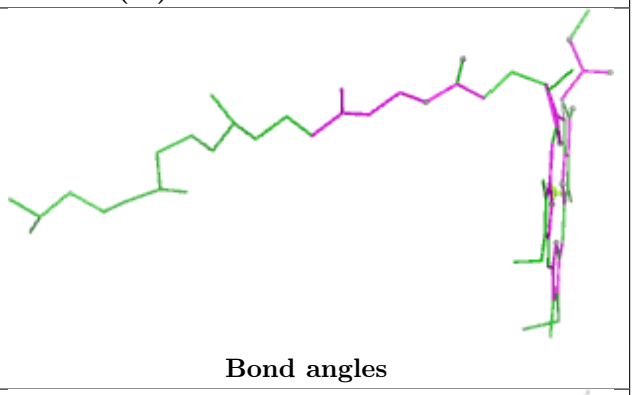


Rings

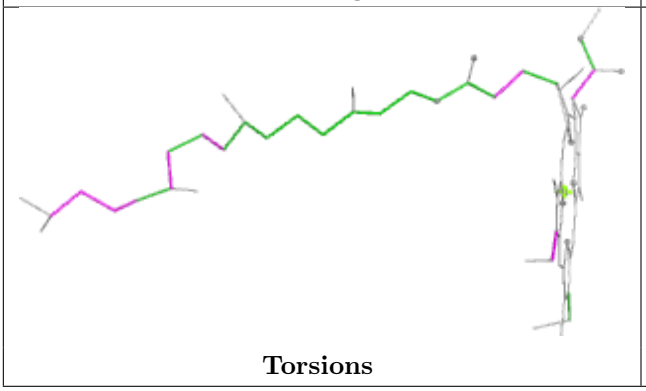
Ligand CLA b 608 (A)



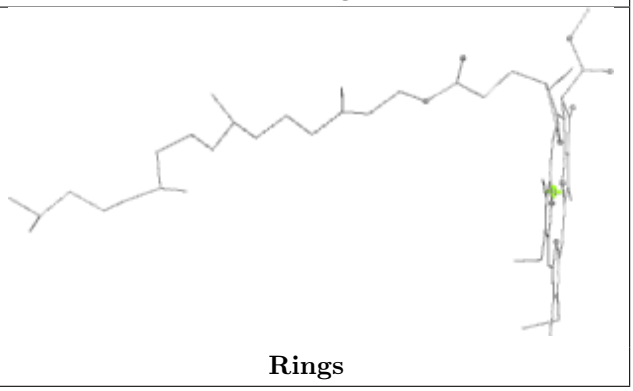
Bond lengths



Bond angles

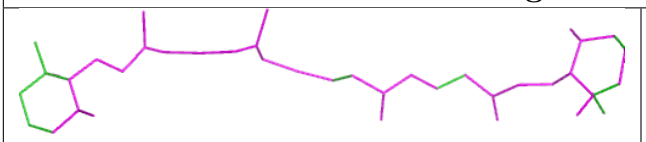


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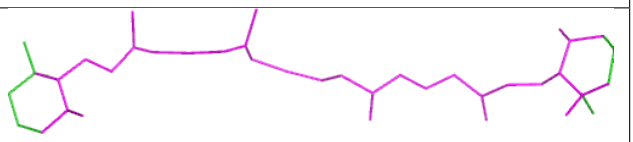


Rings

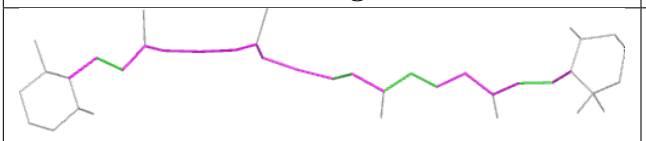
Ligand BCR b 621



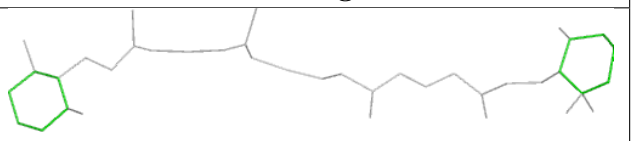
Bond lengths



Bond angles

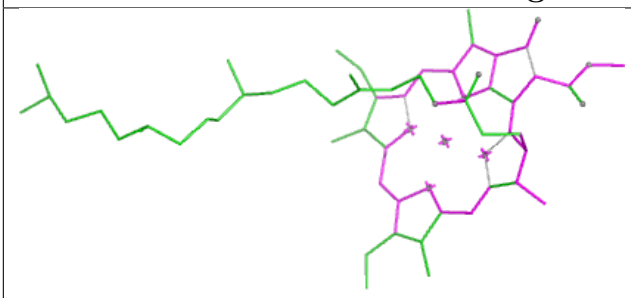


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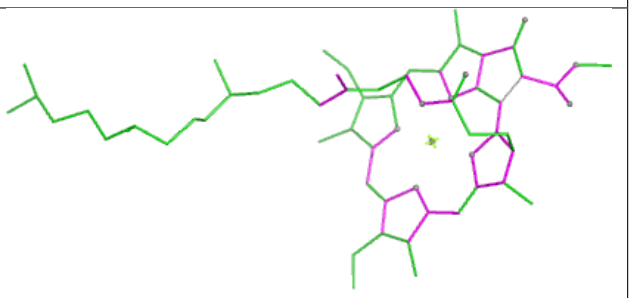


Rings

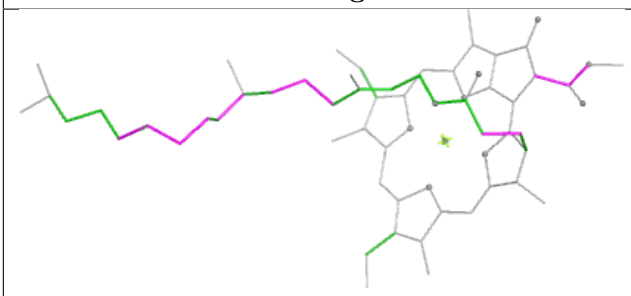
Ligand CLA b 616



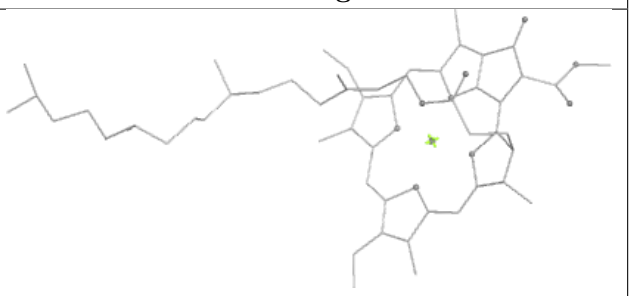
Bond lengths



Bond angles

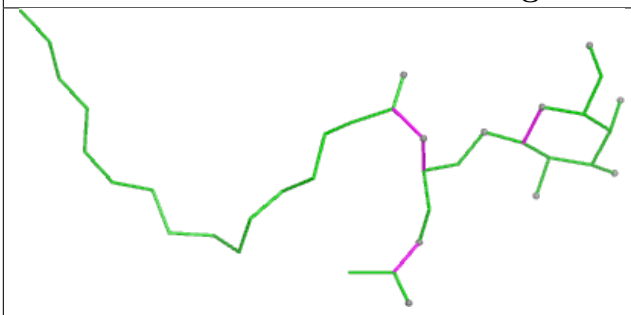


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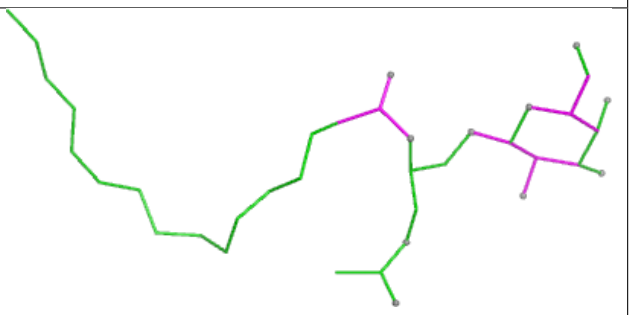


Rings

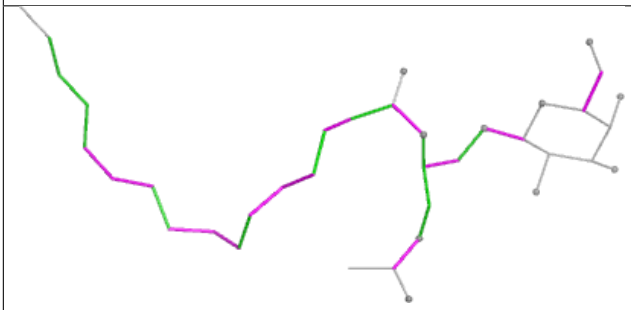
Ligand LMG Z 101



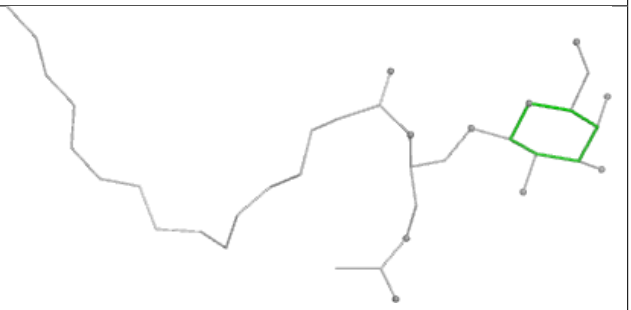
Bond lengths



Bond angles

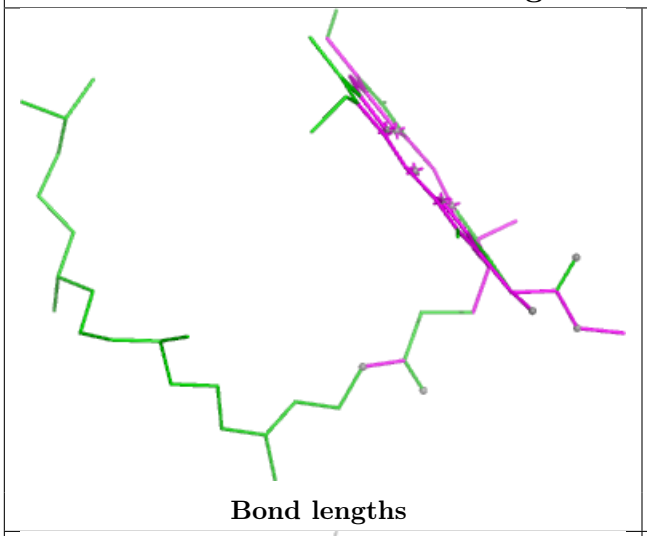


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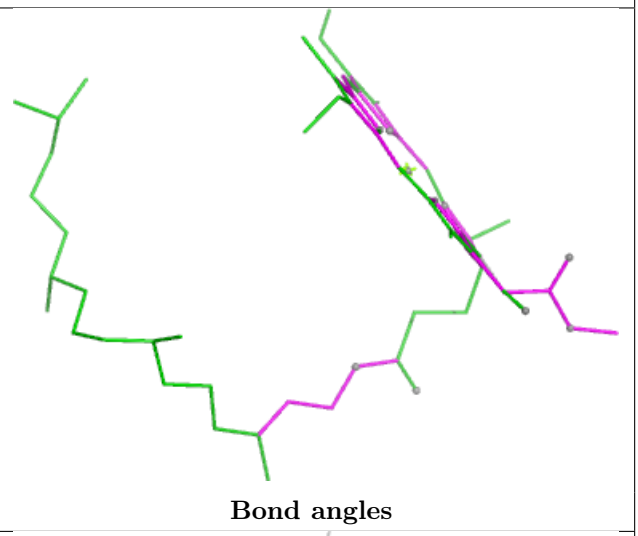


Rings

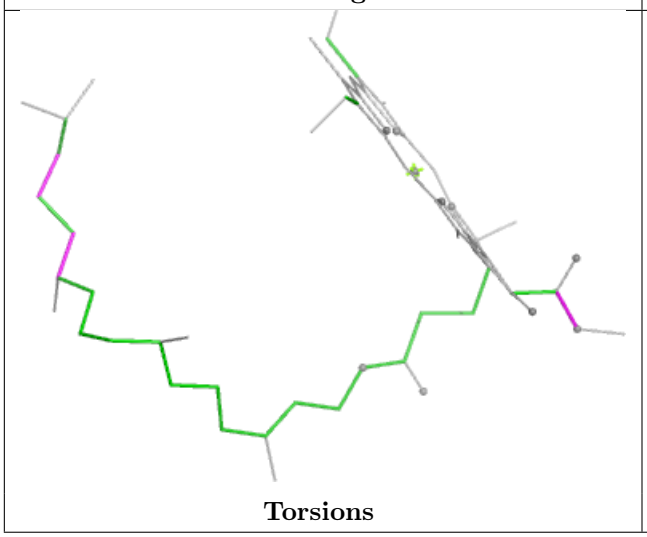
Ligand CLA B 612



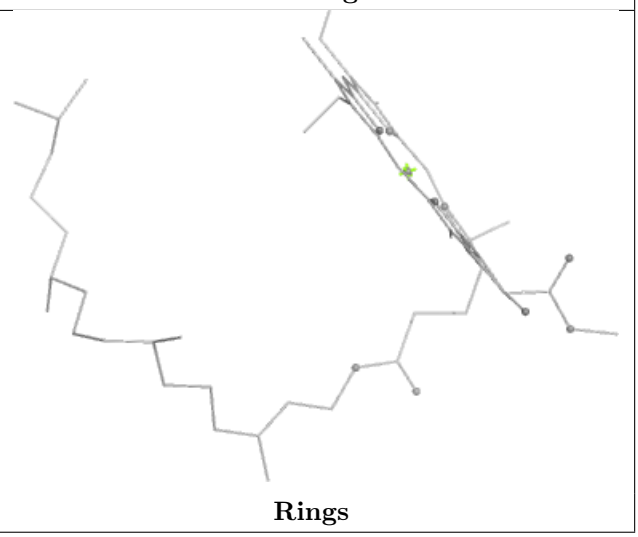
Bond lengths



Bond angles

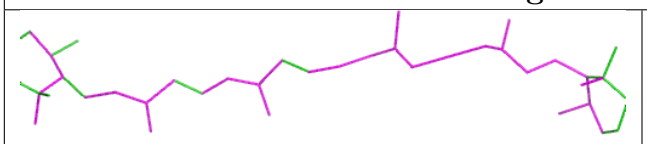


Torsions

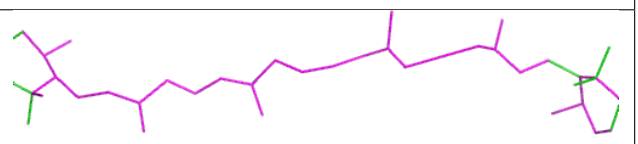


Rings

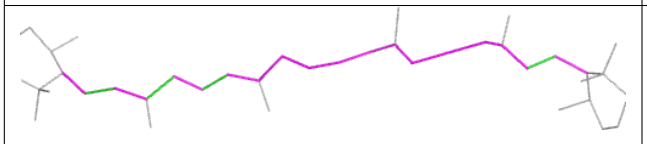
Ligand BCR b 620



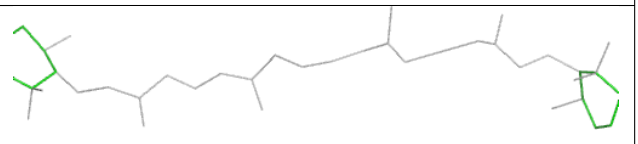
Bond lengths



Bond angles

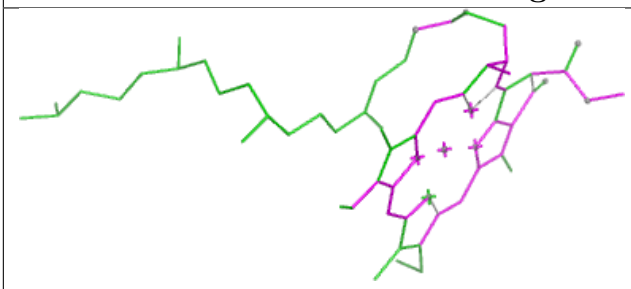


Torsions

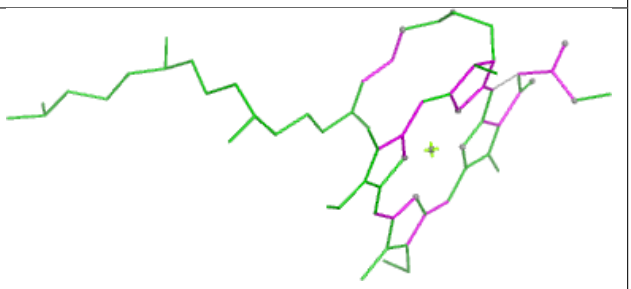


Rings

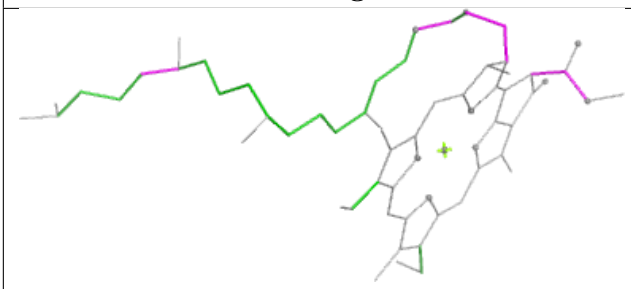
Ligand CLA c 505



Bond lengths



Bond angles

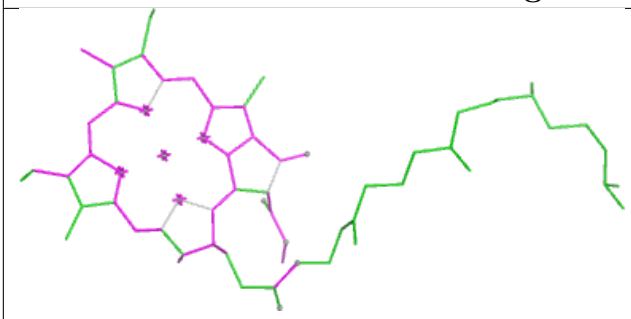


Torsions

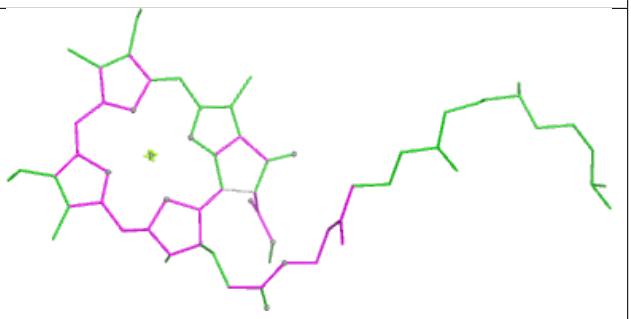


Rings

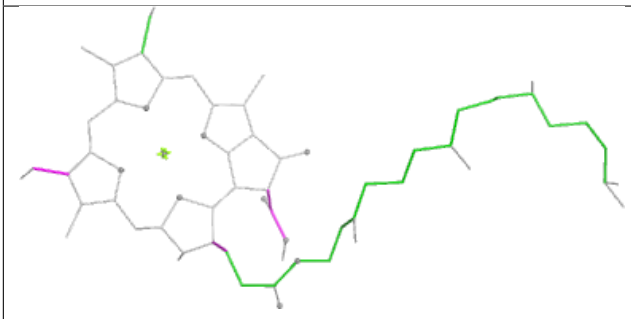
Ligand CLA B 603



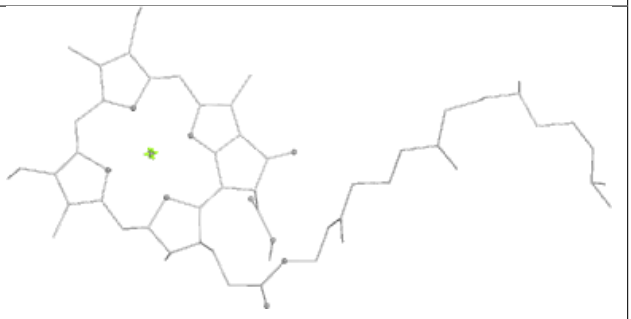
Bond lengths



Bond angles

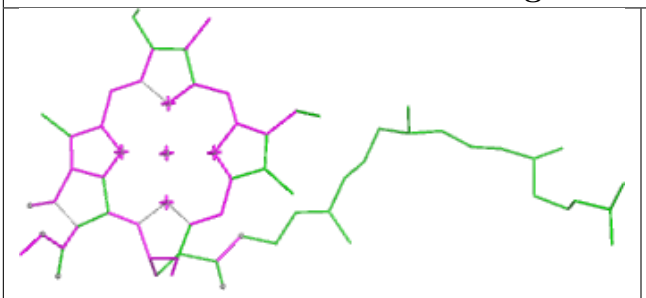


Torsions

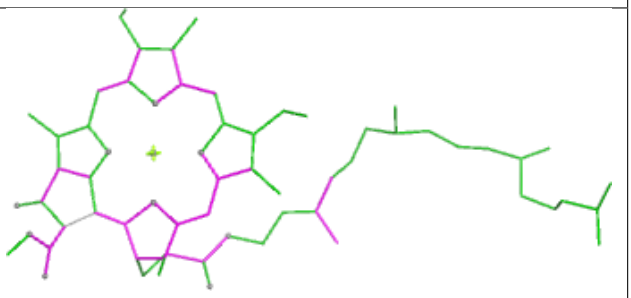


Rings

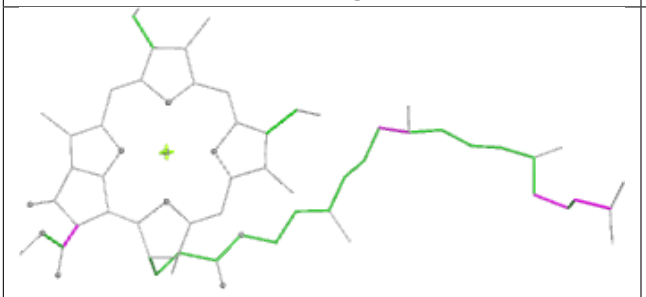
Ligand CLA B 604



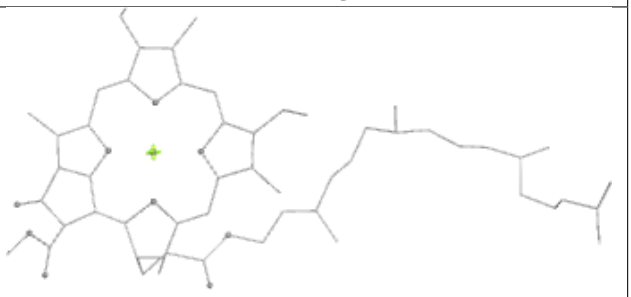
Bond lengths



Bond angles

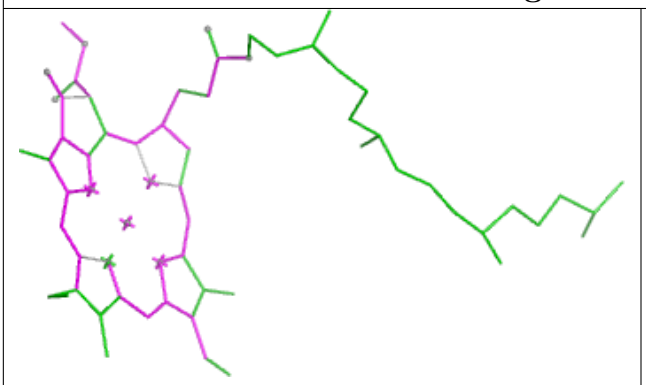


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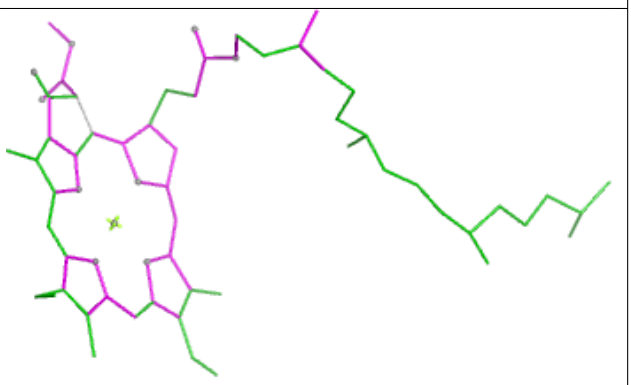


Rings

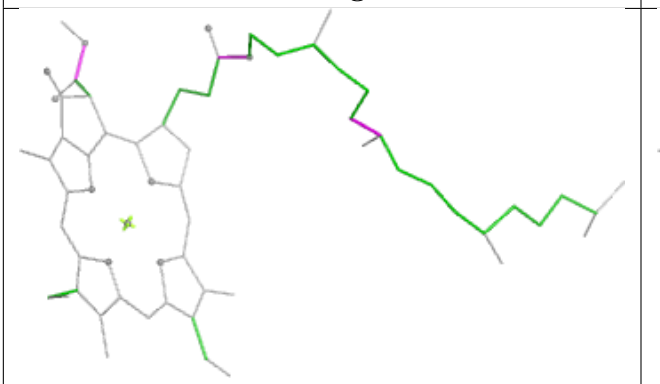
Ligand CLA C 511



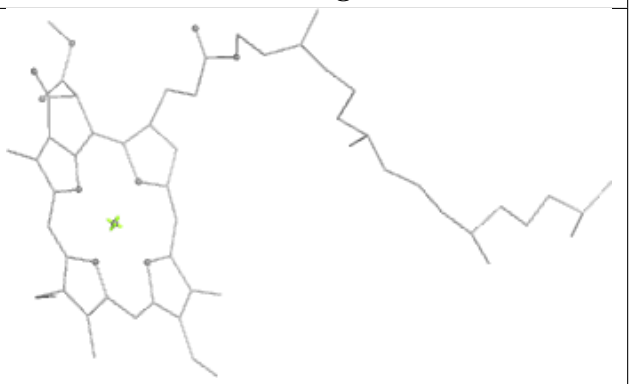
Bond lengths



Bond angles

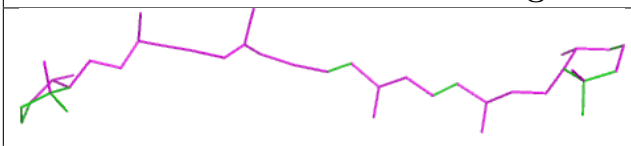


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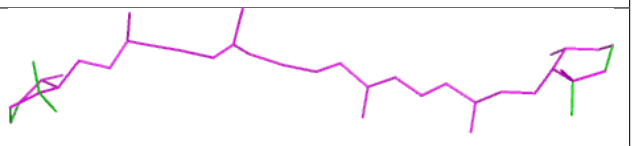


Rings

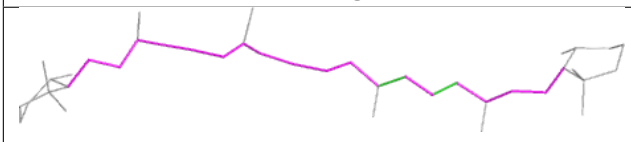
Ligand BCR c 514



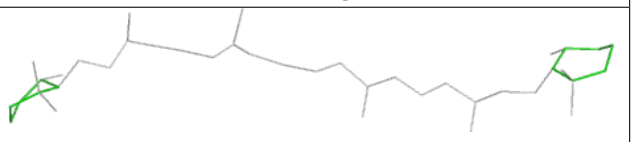
Bond lengths



Bond angles

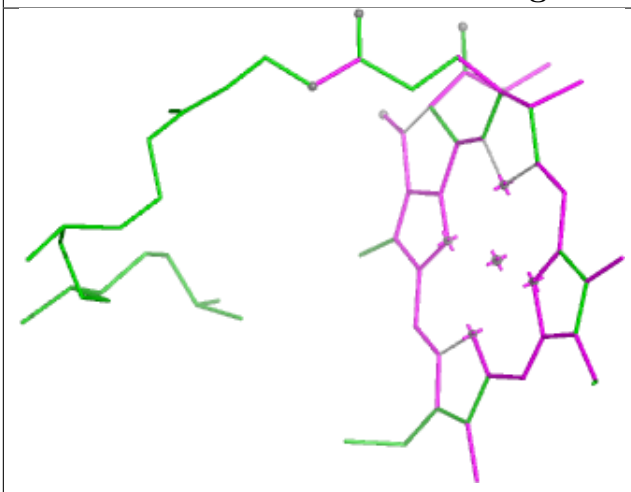


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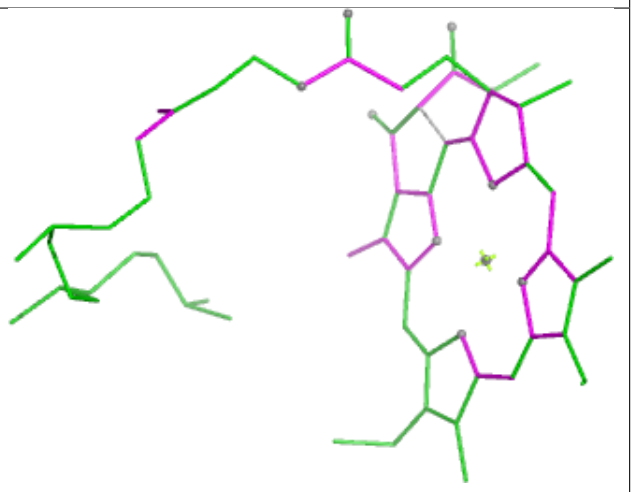


Rings

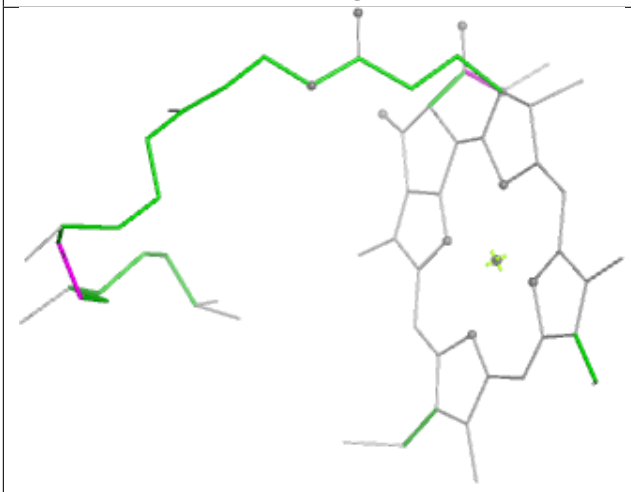
Ligand CLA c 503



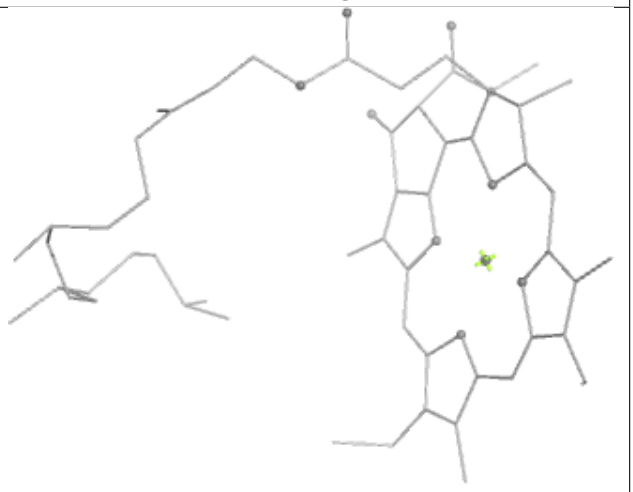
Bond lengths



Bond angles

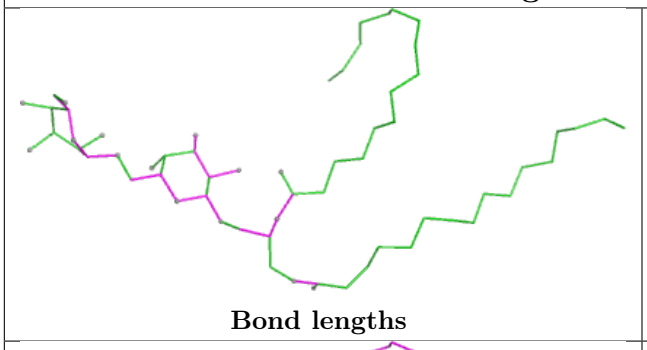


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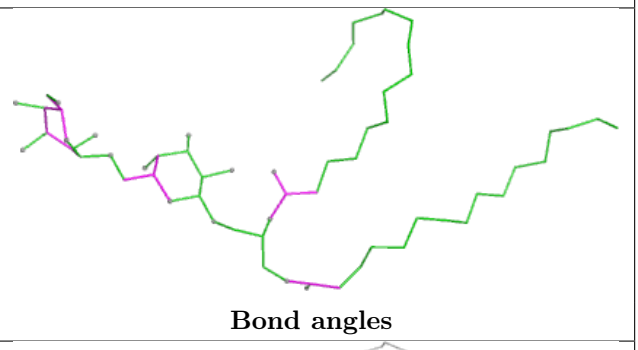


Rings

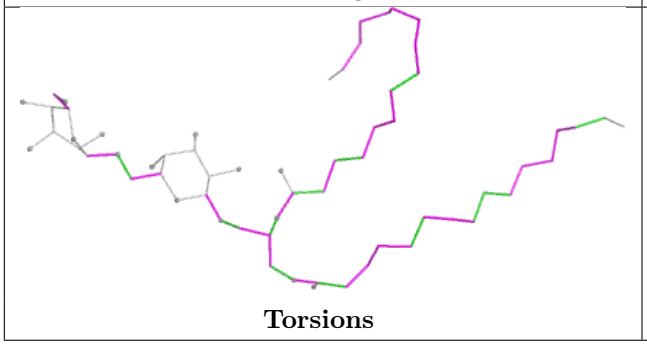
Ligand DGD E 101



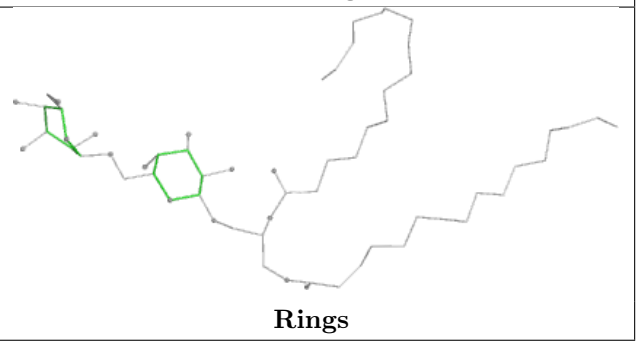
Bond lengths



Bond angles

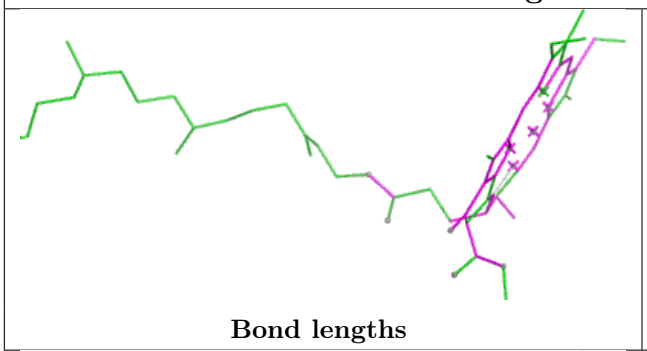


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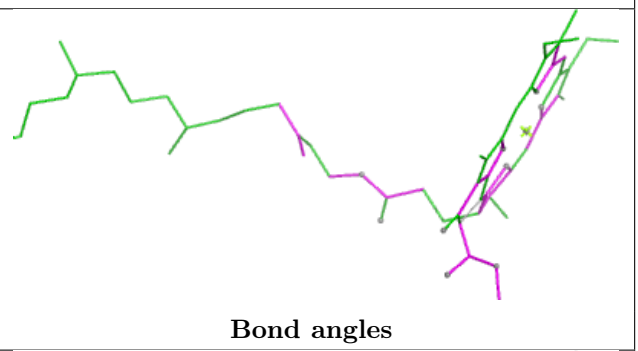


Rings

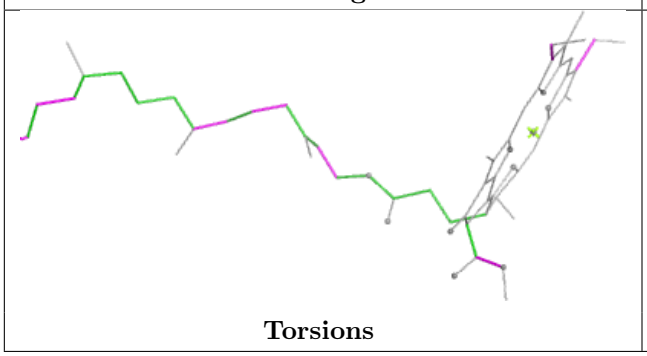
Ligand CLA B 605



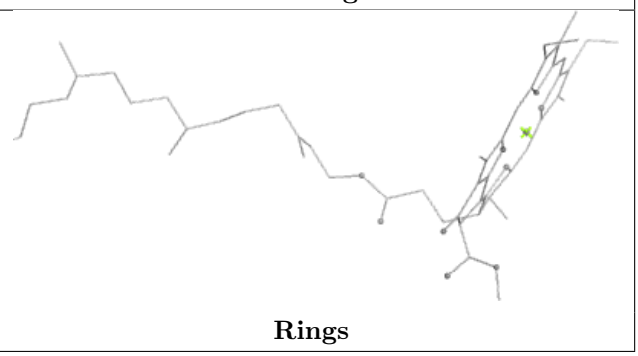
Bond lengths



Bond angles

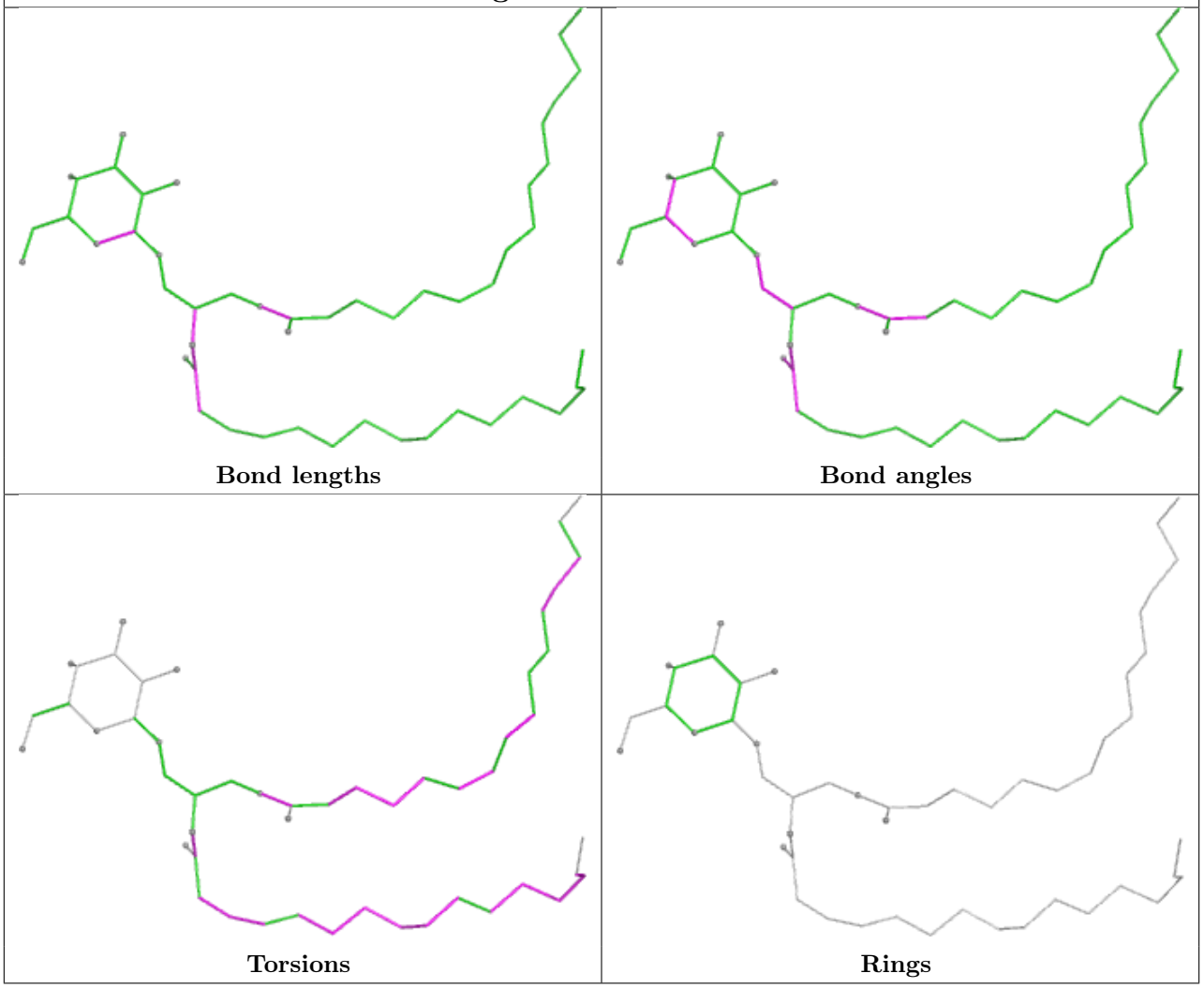


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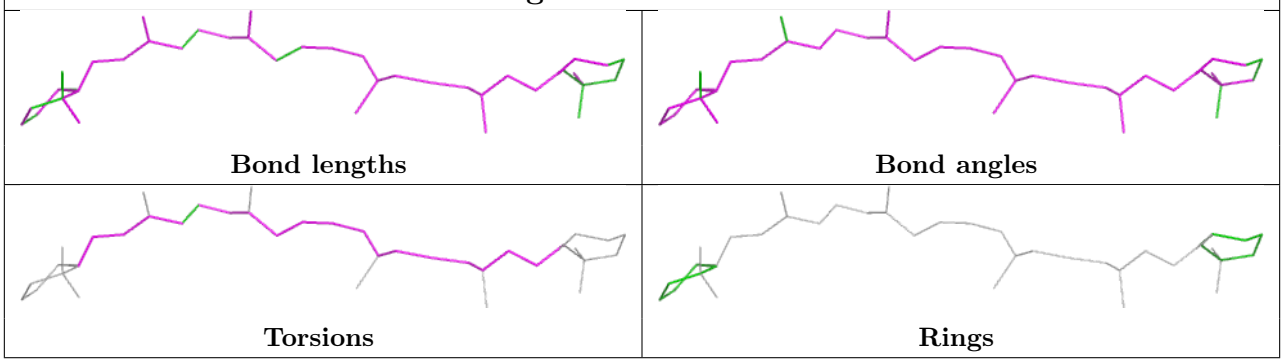


Rings

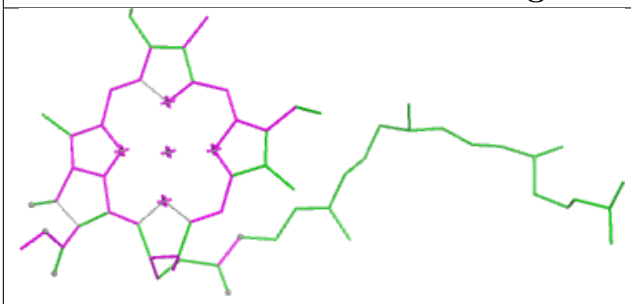
Ligand LMG c 519



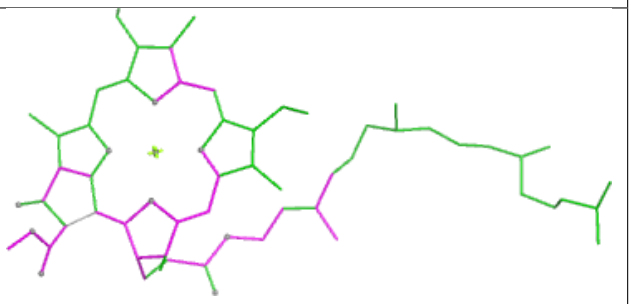
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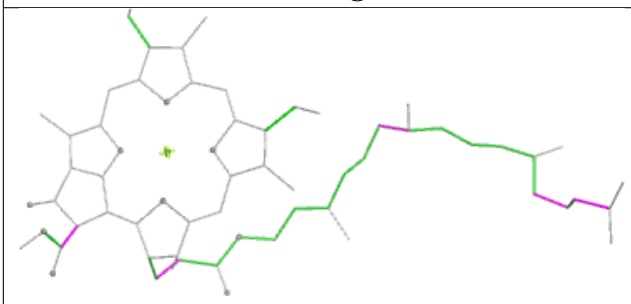
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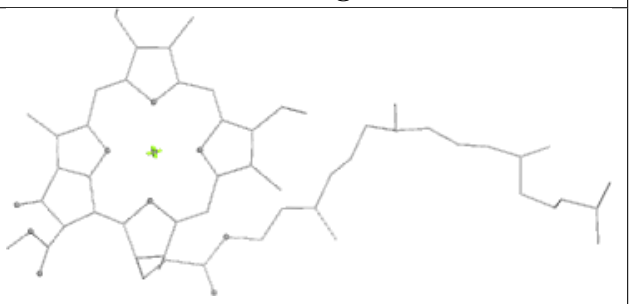
Bond lengths



Bond angles

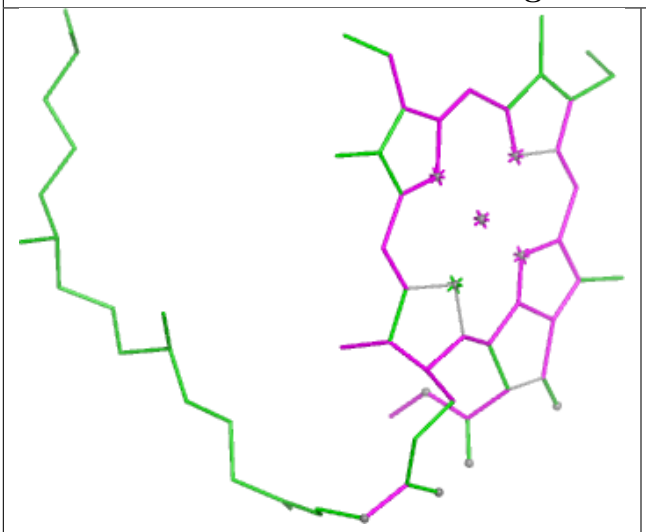


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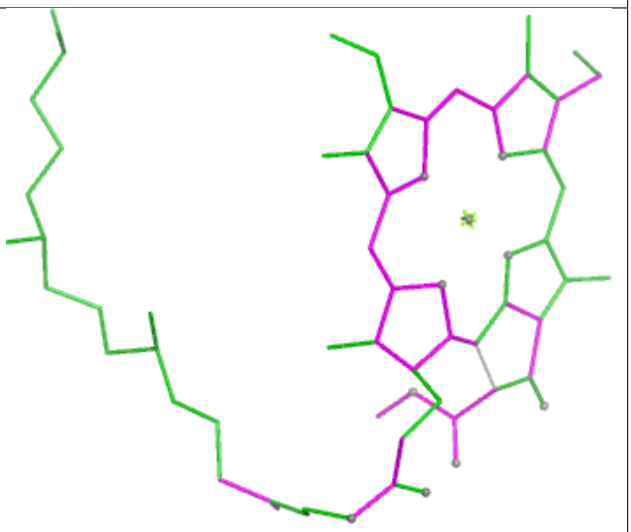


Rings

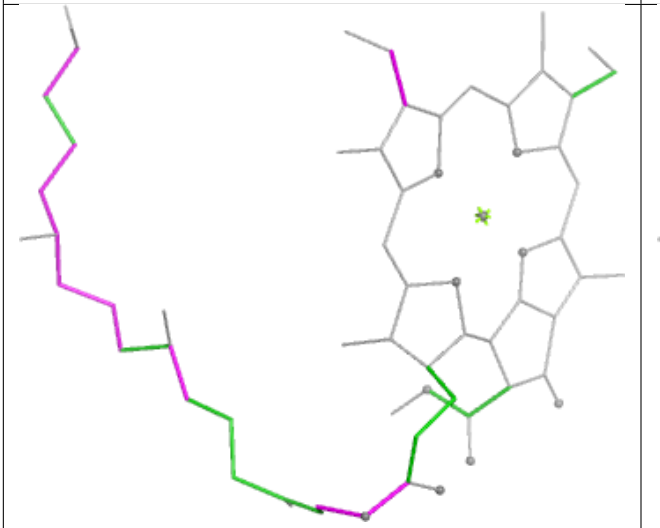
Ligand CLA B 617



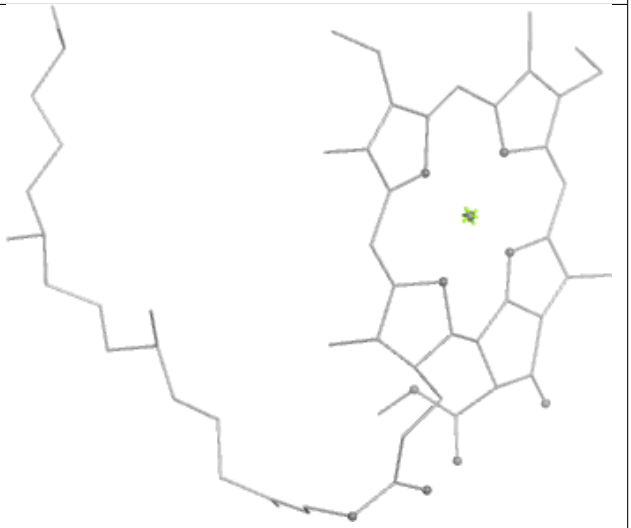
Bond lengths



Bond angles

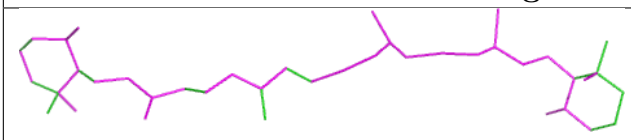


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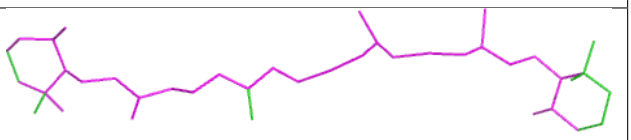


Rings

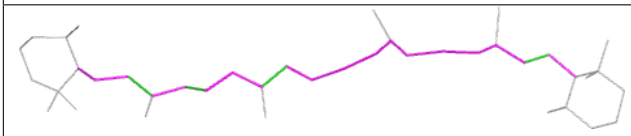
Ligand BCR B 620



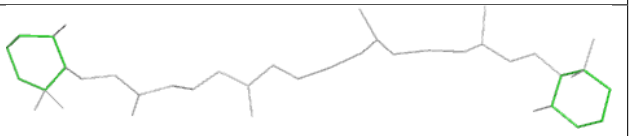
Bond lengths



Bond angles

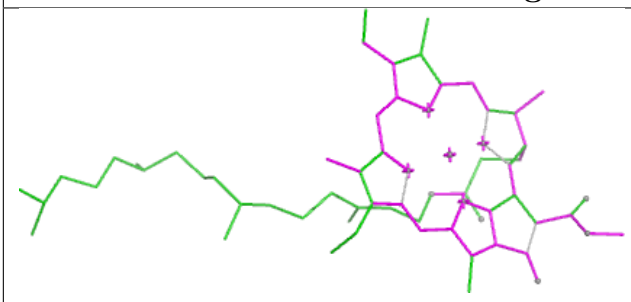


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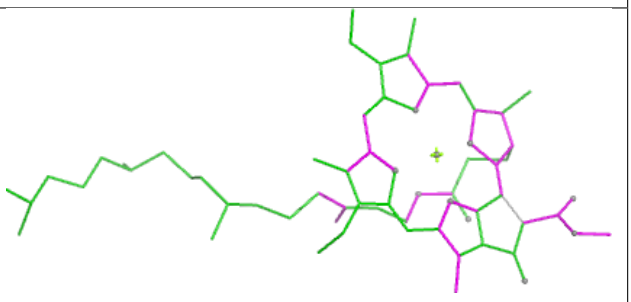


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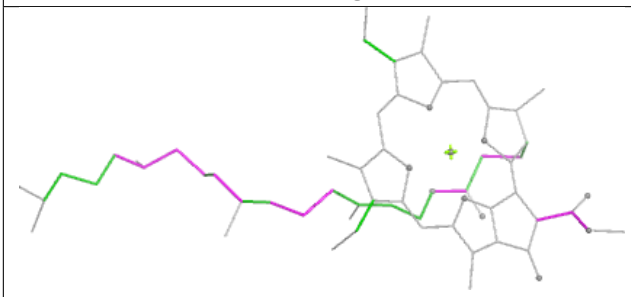
Ligand CLA B 615



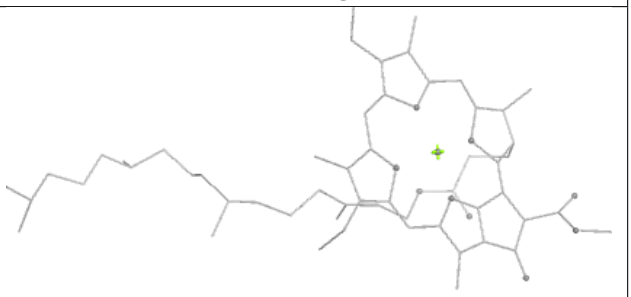
Bond lengths



Bond angles



Torsions



Rings

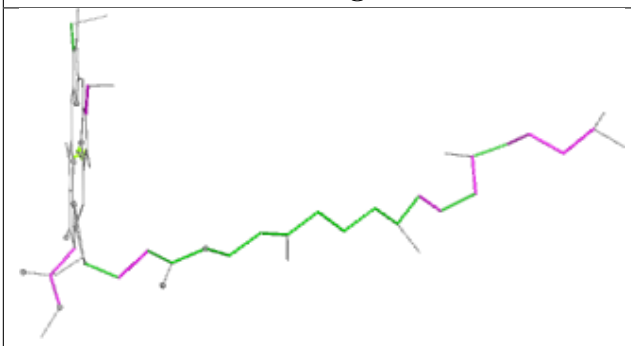
Ligand CLA B 607 (A)



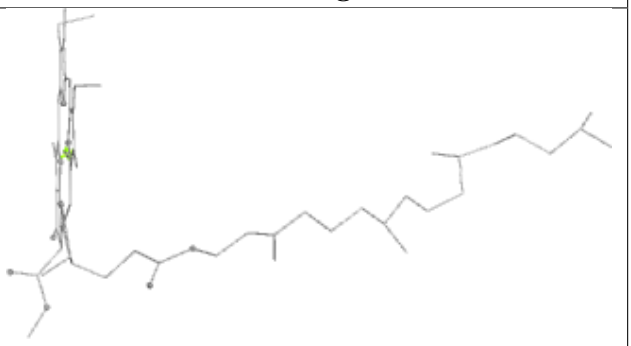
Bond lengths



Bond angles

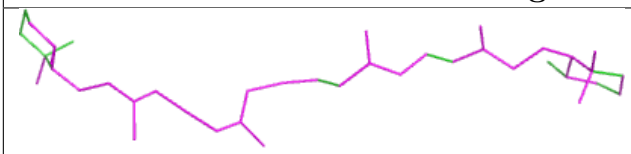


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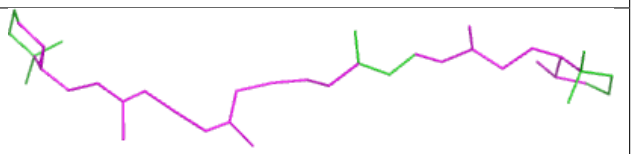


Rings

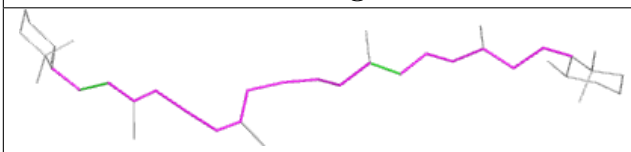
Ligand BCR I 101



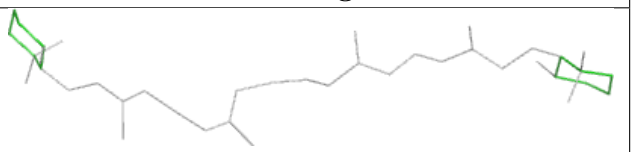
Bond lengths



Bond angles

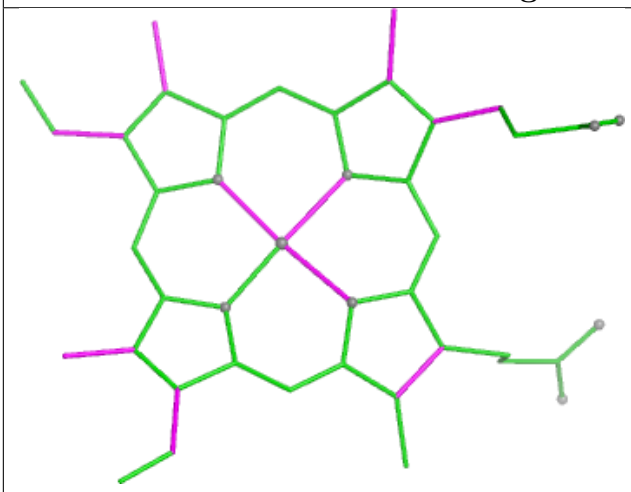


Torsions

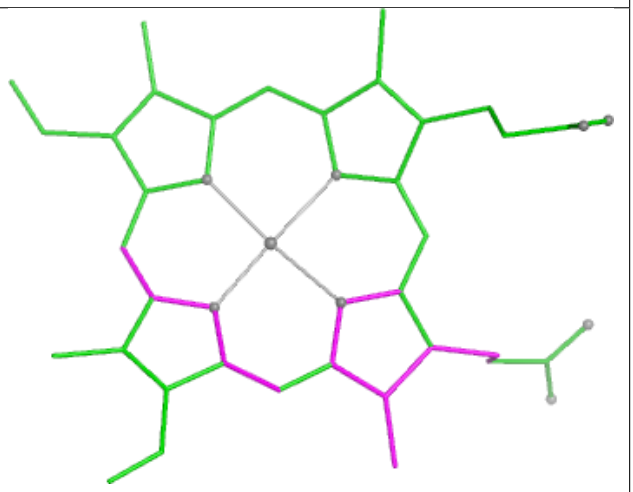


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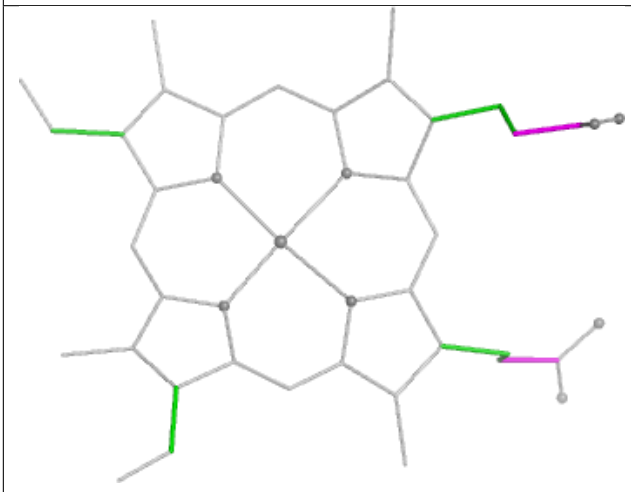
Ligand HEM E 103



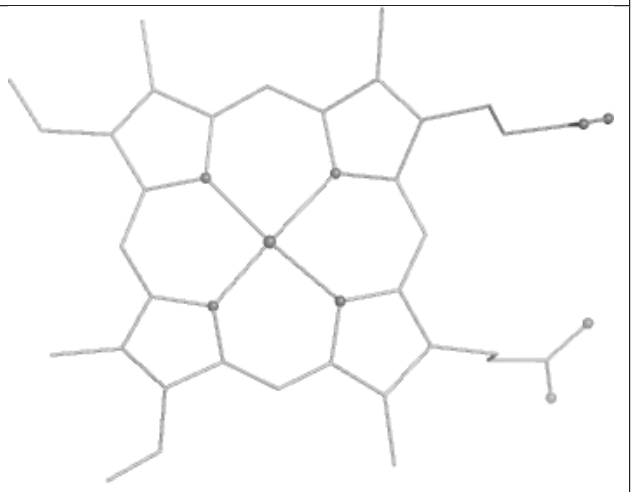
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Bond angles

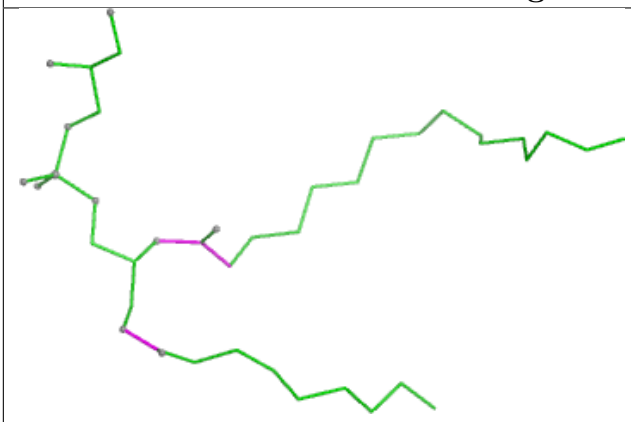


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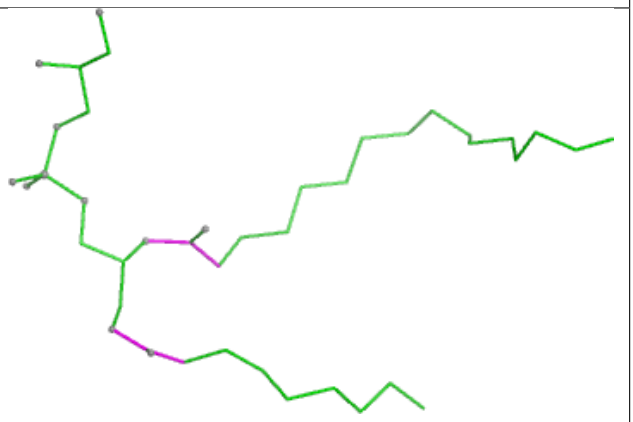


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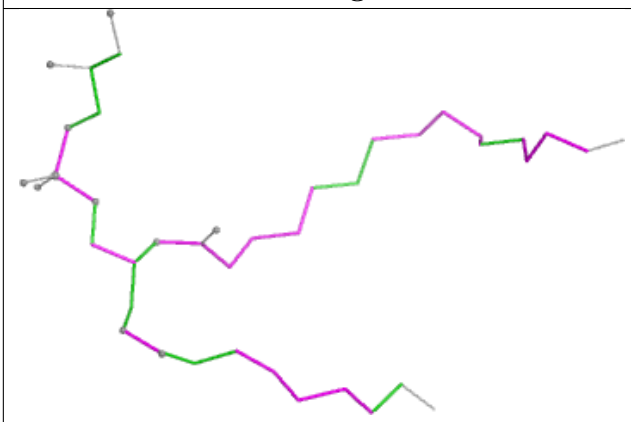
Ligand LHG e 101



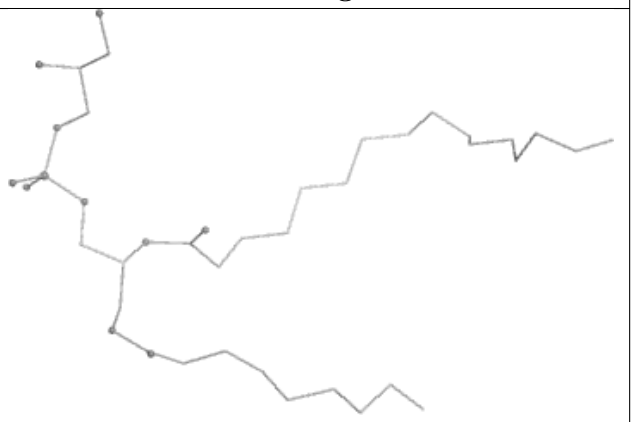
Bond lengths



Bond angles

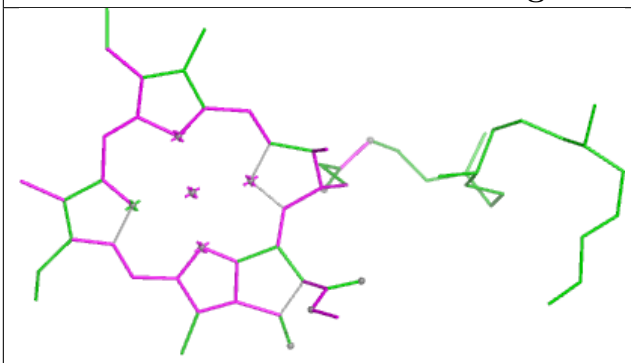


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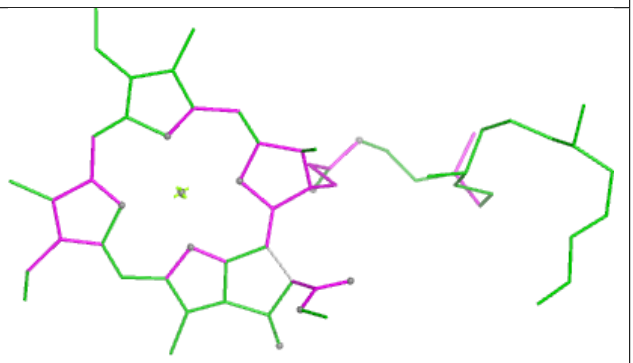


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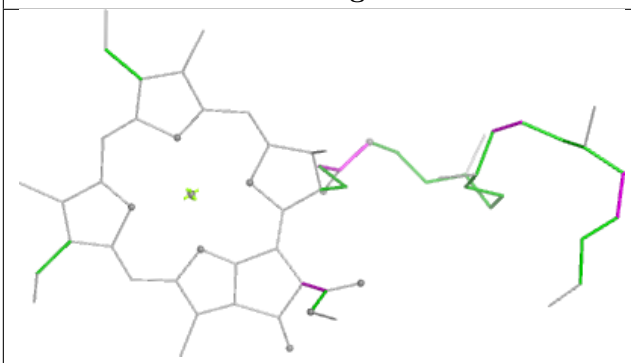
Ligand CLA b 614



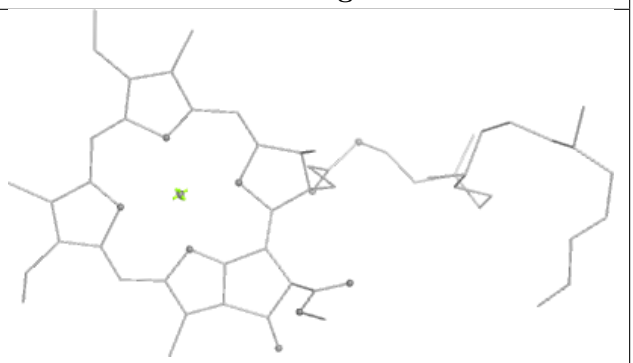
Bond lengths



Bond angles

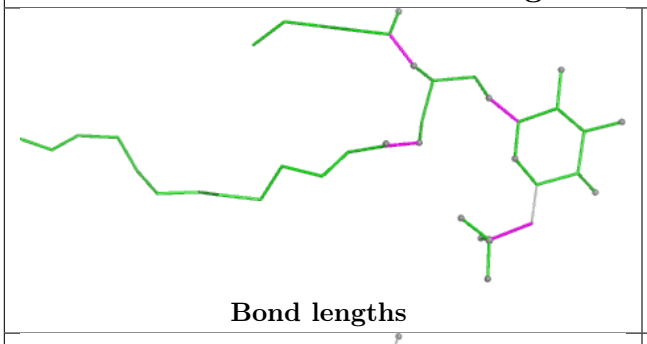


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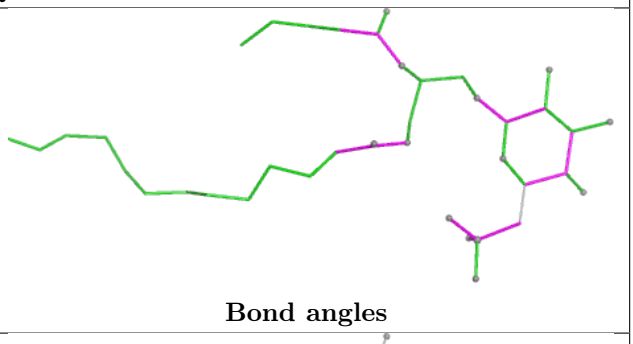


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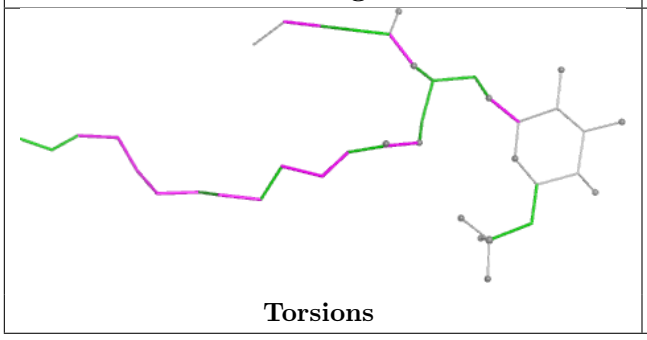
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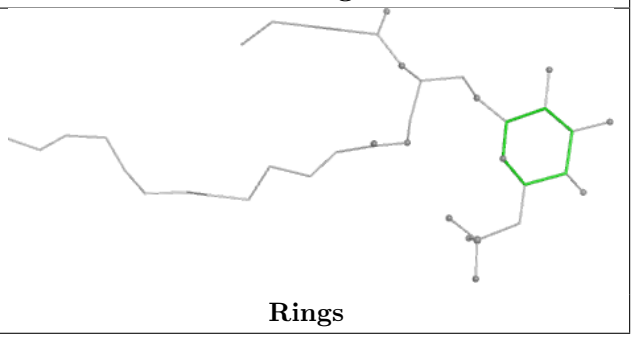
Bond lengths



Bond angles

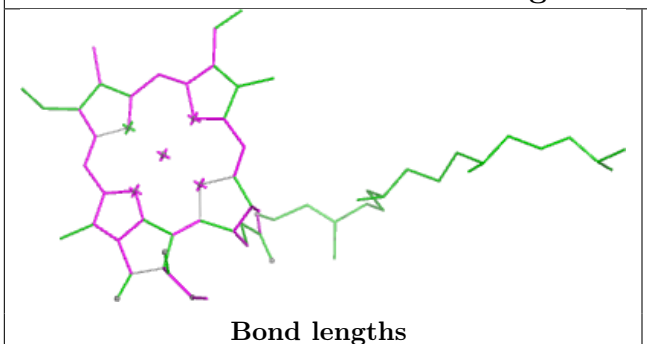


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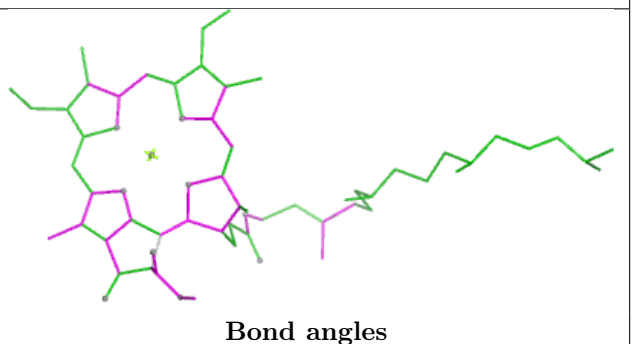


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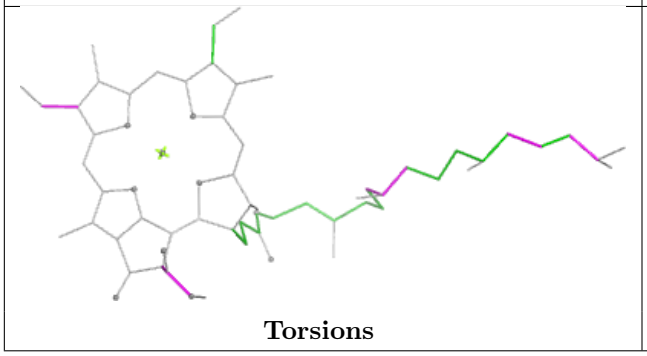
Ligand CLA a 607



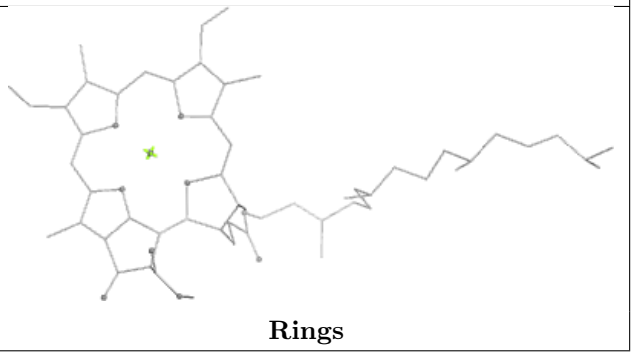
Bond lengths



Bond angles

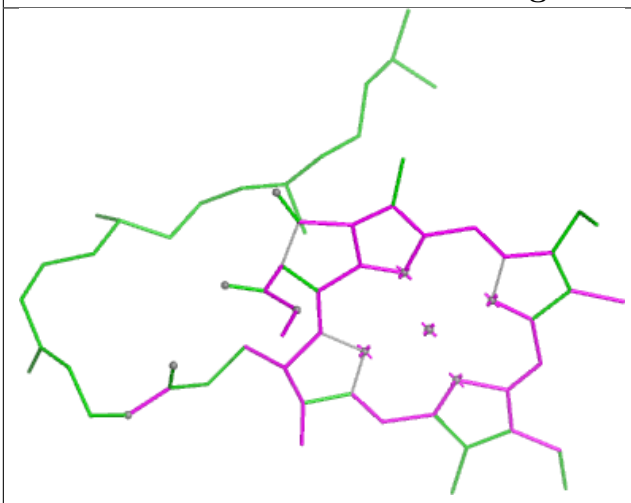


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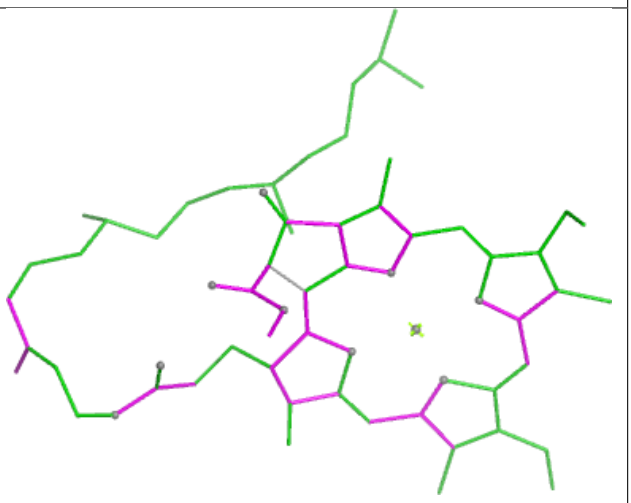


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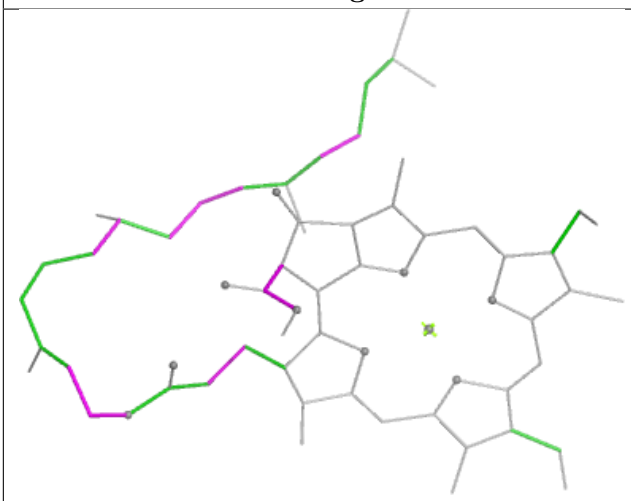
Ligand CLA c 509



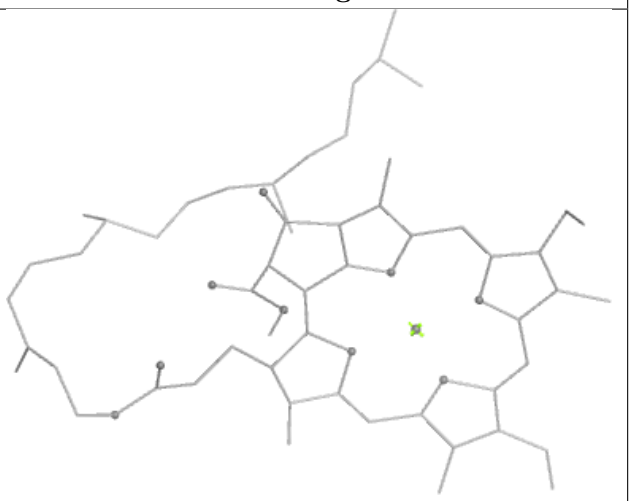
Bond lengths



Bond angles

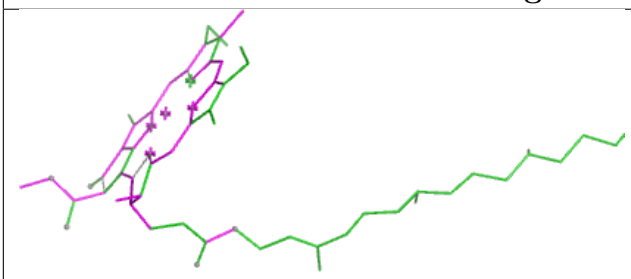


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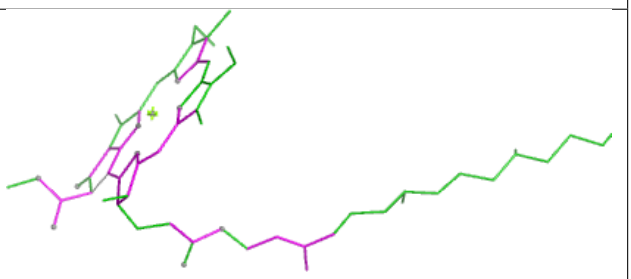


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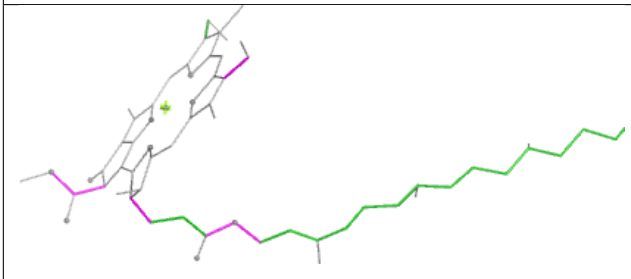
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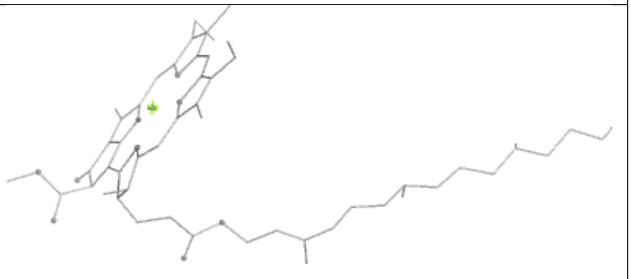
Bond lengths



Bond angles

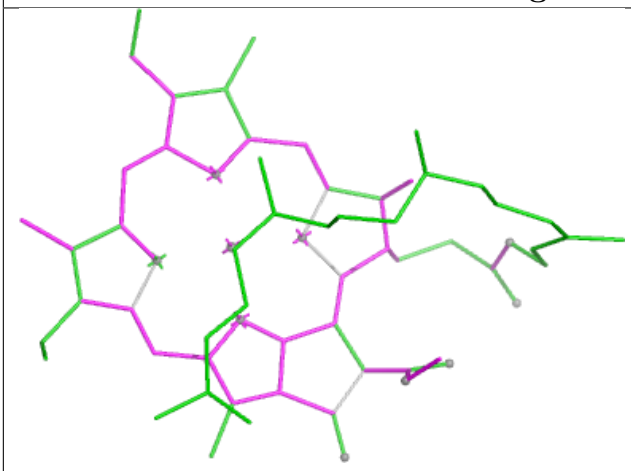


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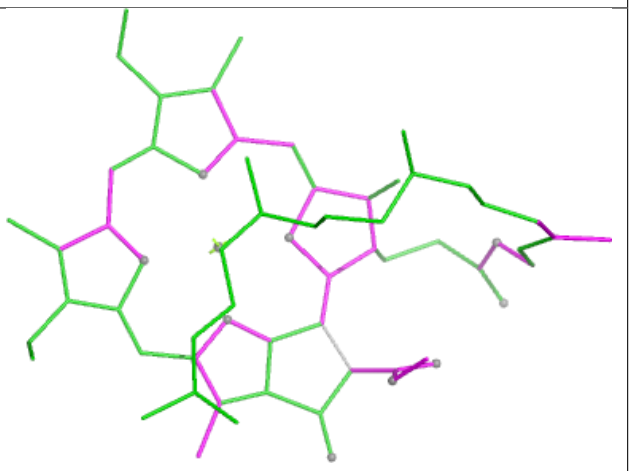


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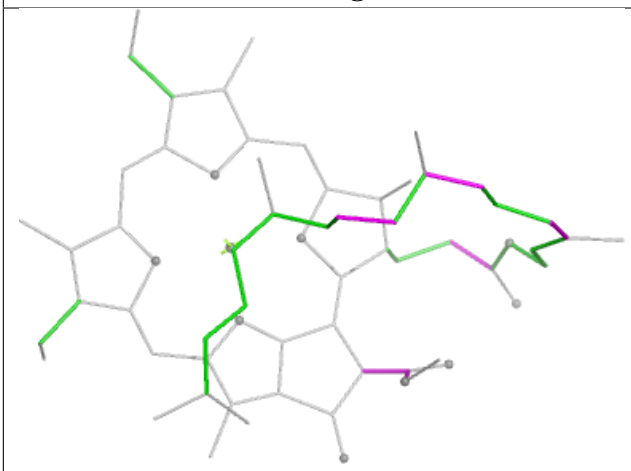
Ligand CLA c 510



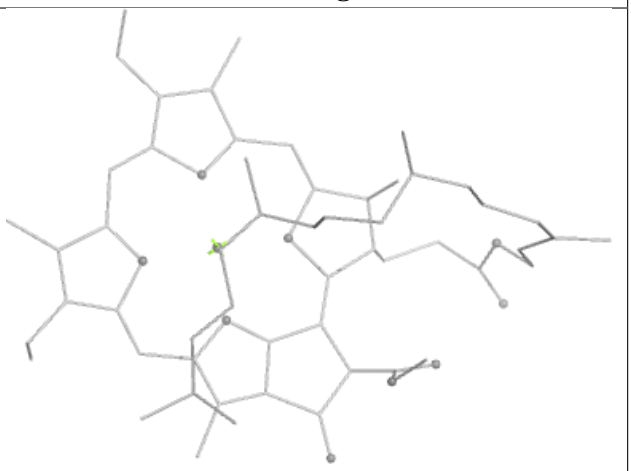
Bond lengths



Bond angles

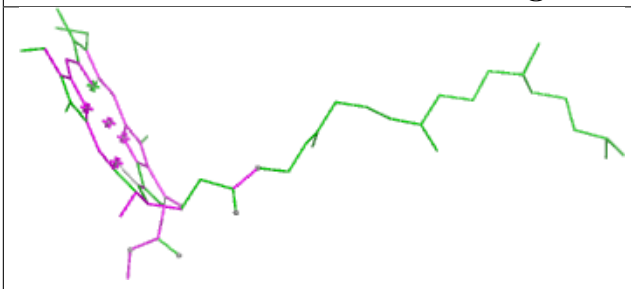


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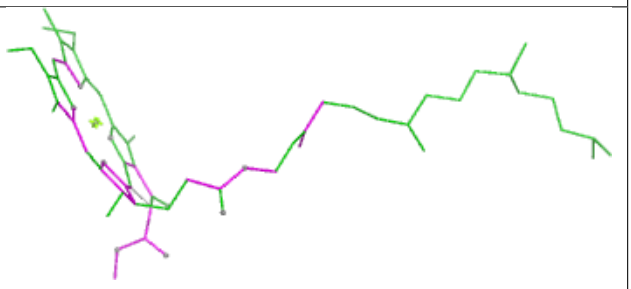


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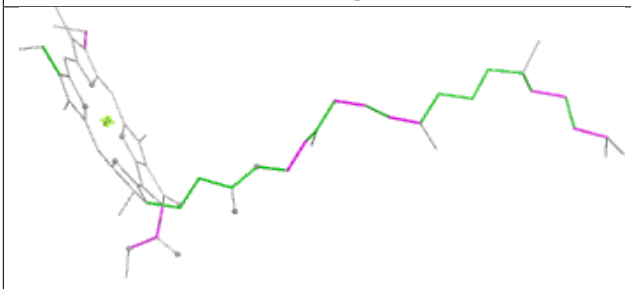
Ligand CLA b 606



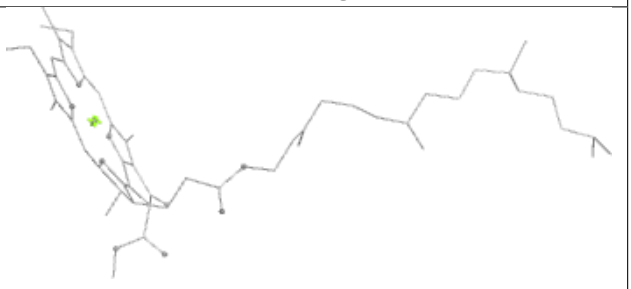
Bond lengths



Bond angles

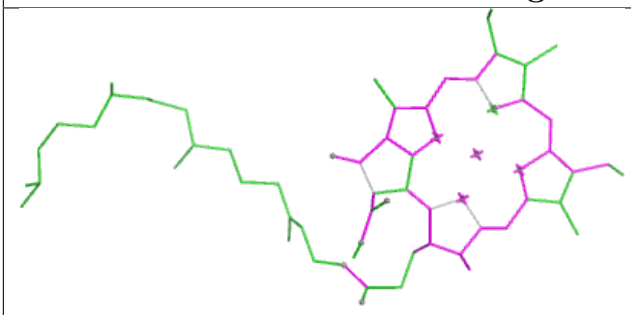


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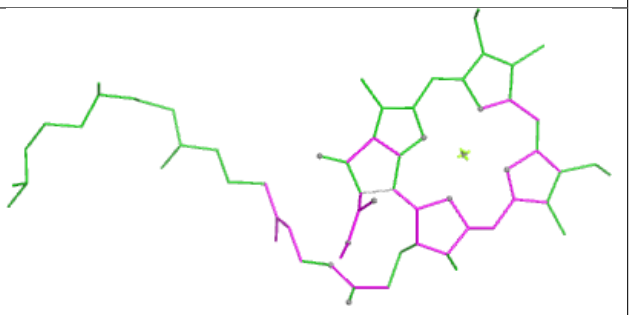


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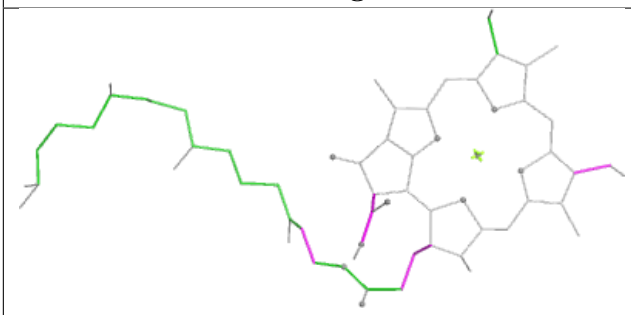
Ligand CLA b 604



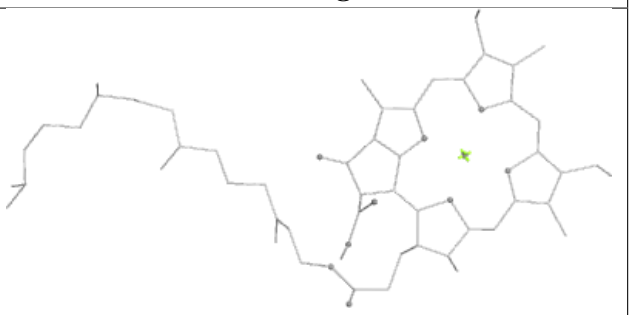
Bond lengths



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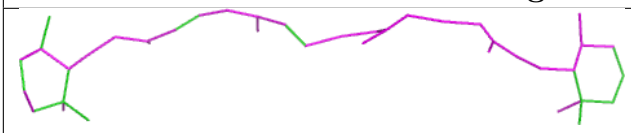


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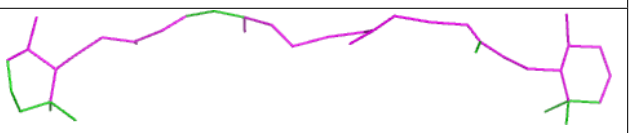


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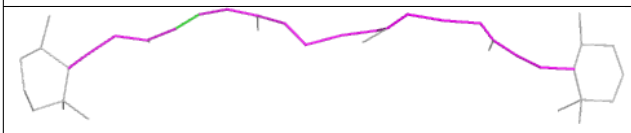
Ligand BCR c 521



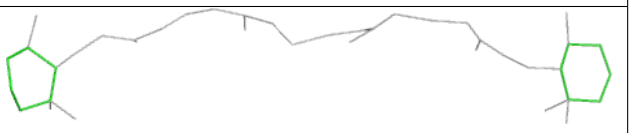
Bond lengths



Bond angles

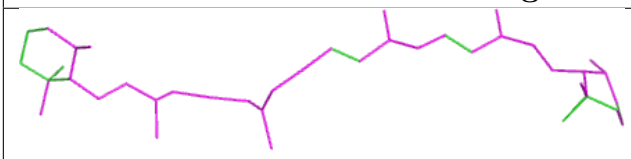


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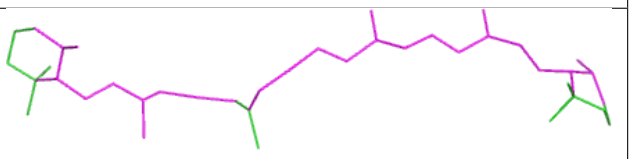


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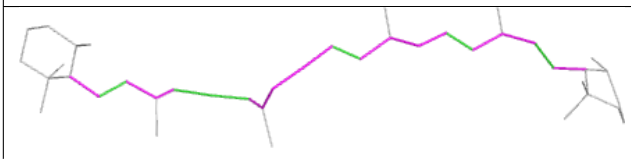
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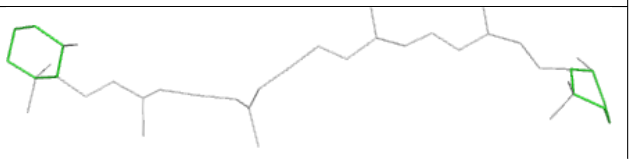
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Bond angles

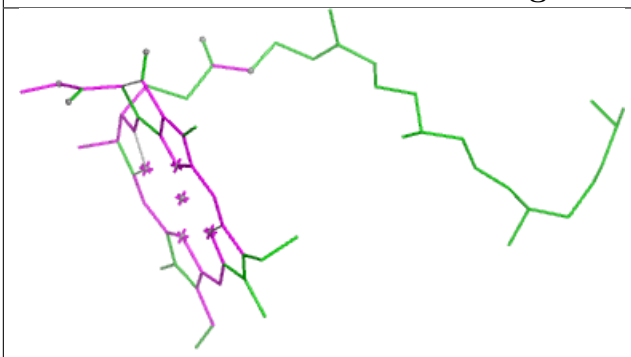


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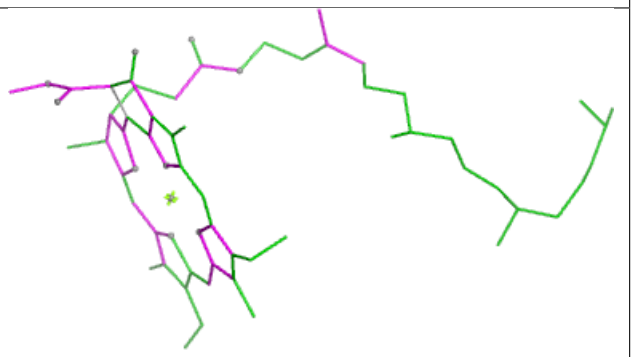


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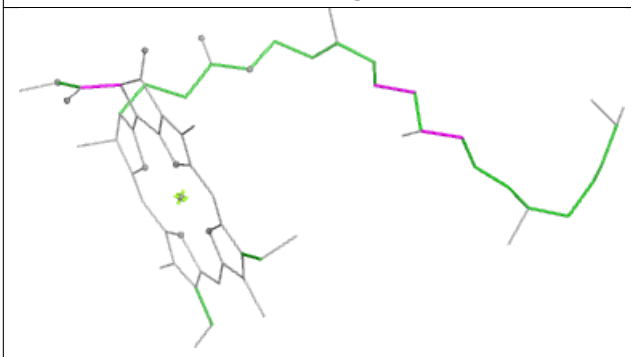
Ligand CLA c 508



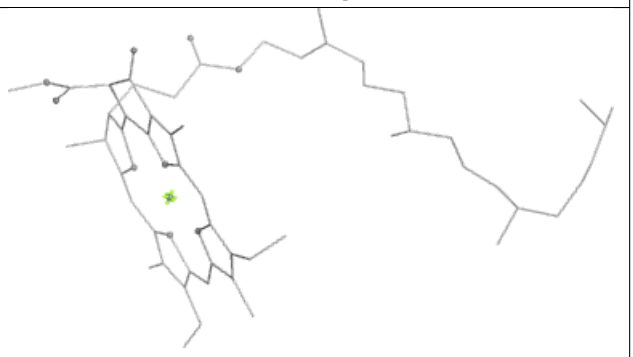
Bond lengths



Bond angles

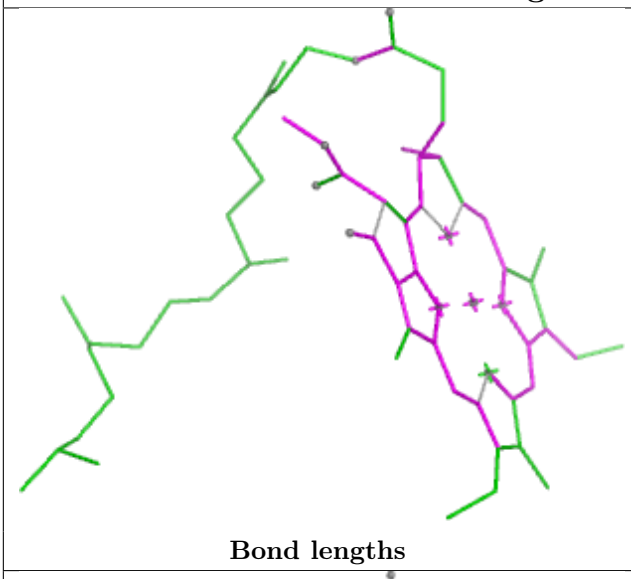


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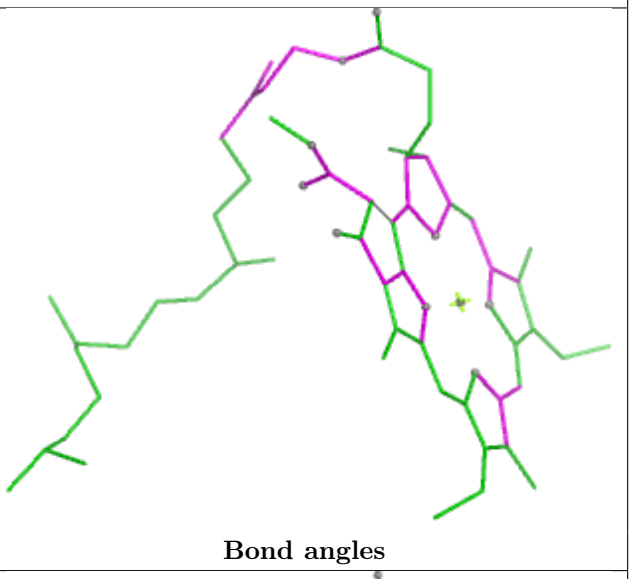


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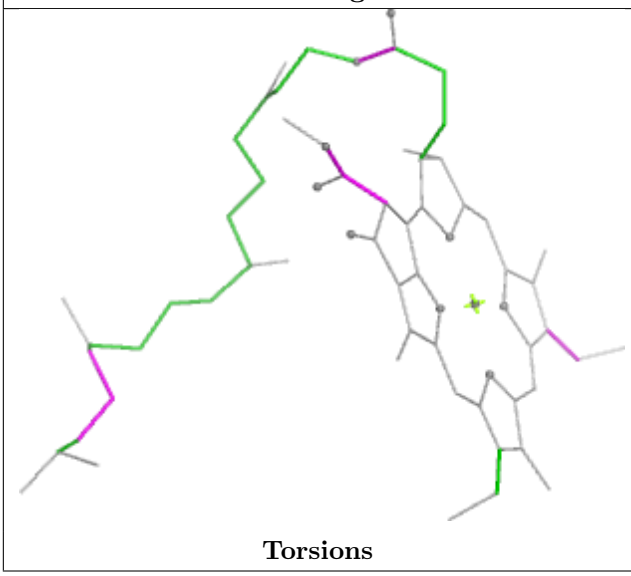
Ligand CLA b 615



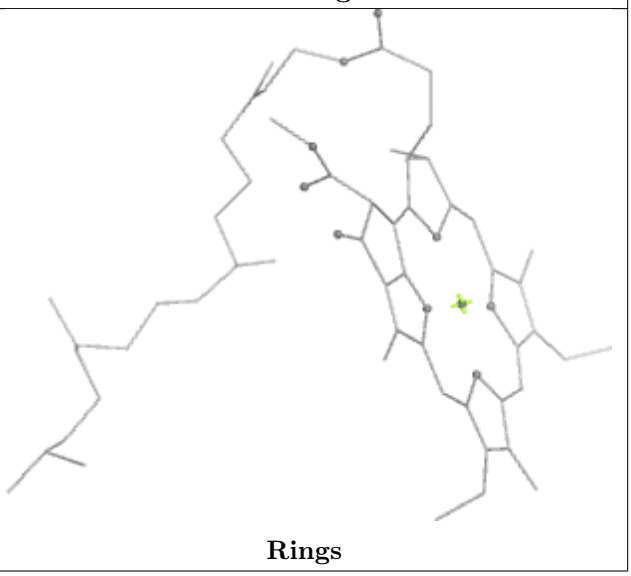
Bond lengths



Bond angles

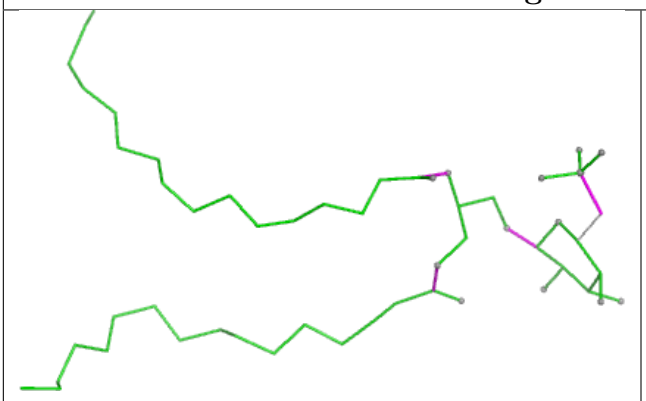


Torsions

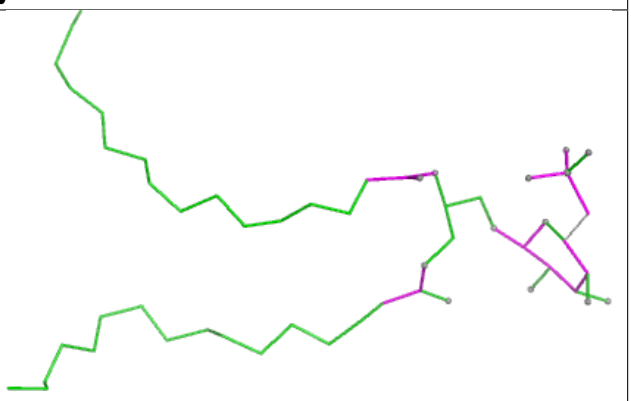


Rings

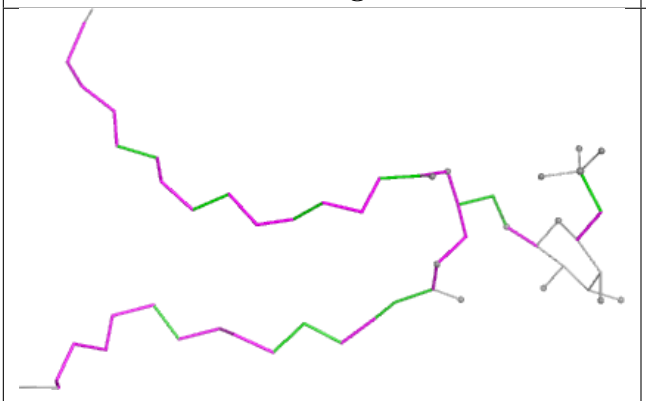
Ligand SQD B 622



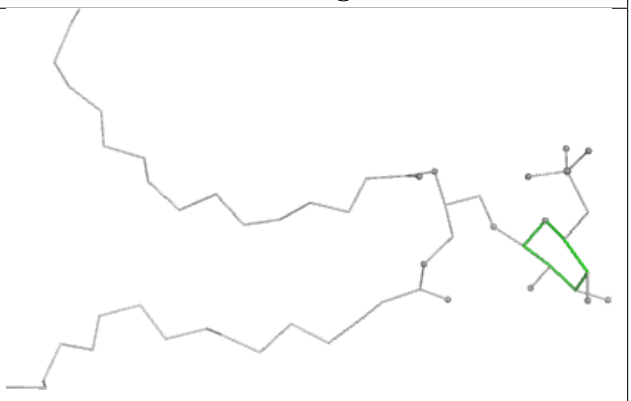
Bond lengths



Bond angles

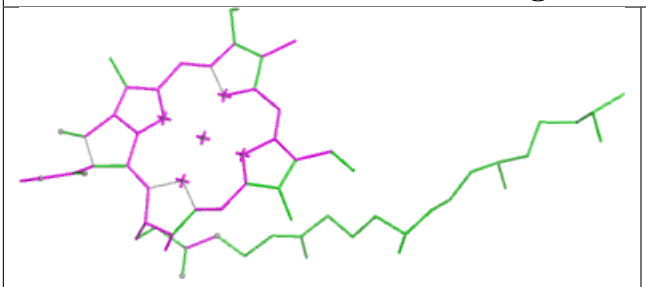


Torsions

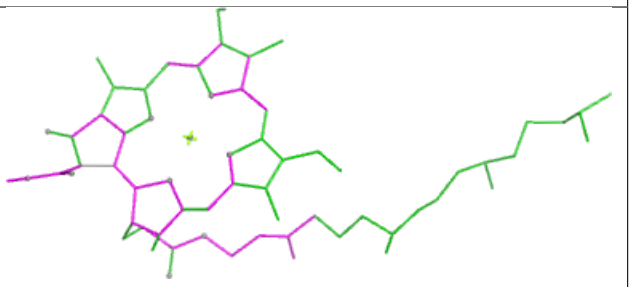


Rings

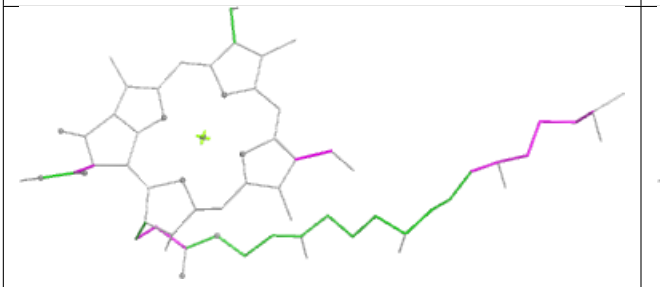
Ligand CLA c 501



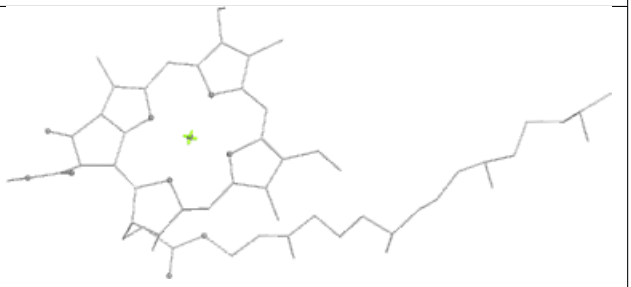
Bond lengths



Bond angles

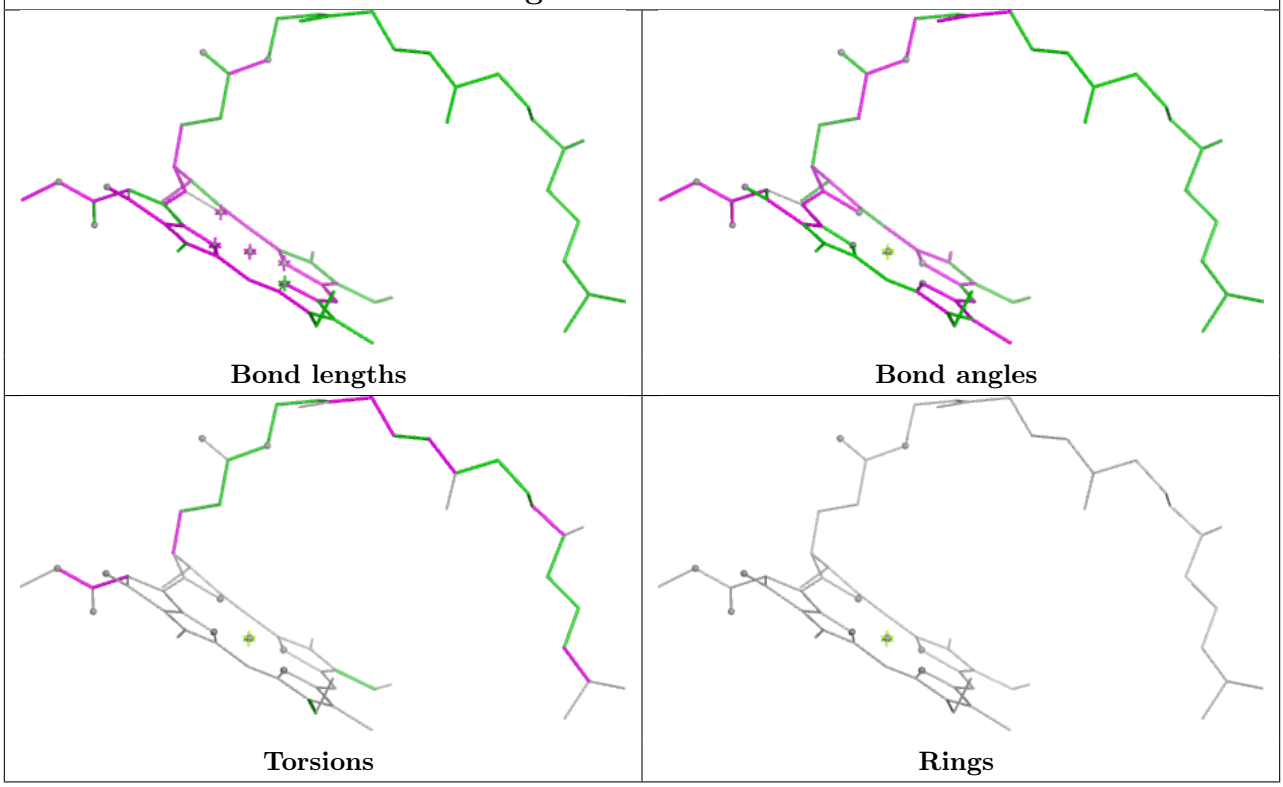


Torsions

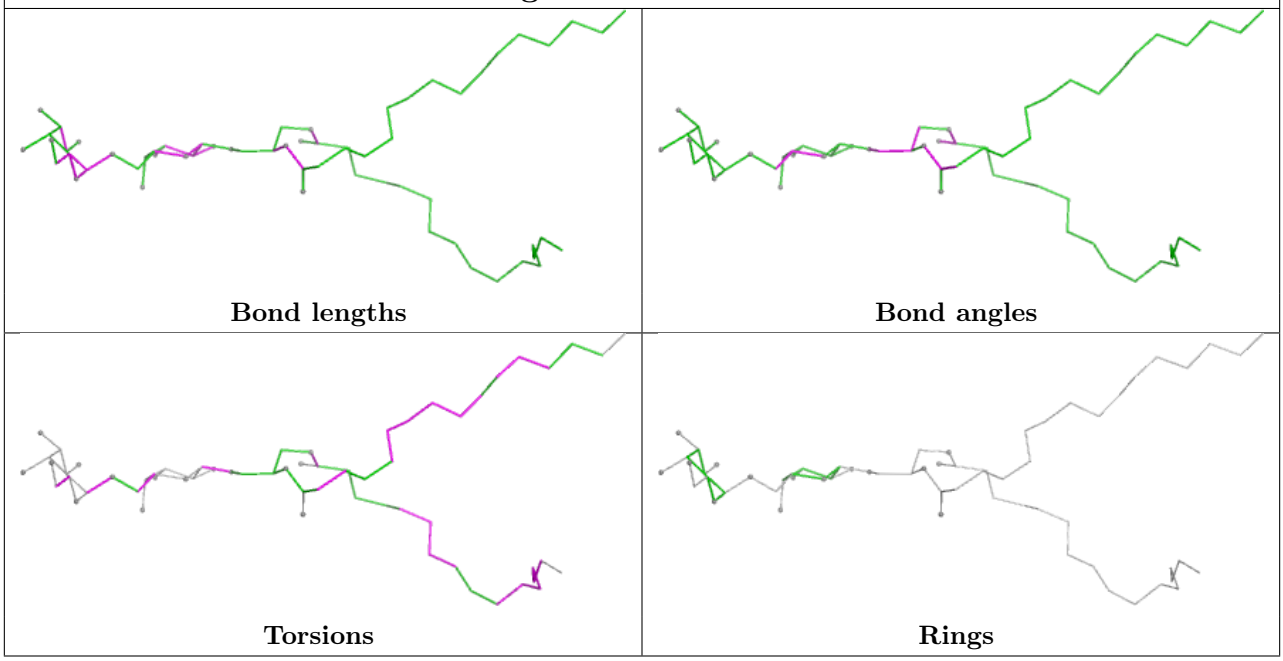


Rings

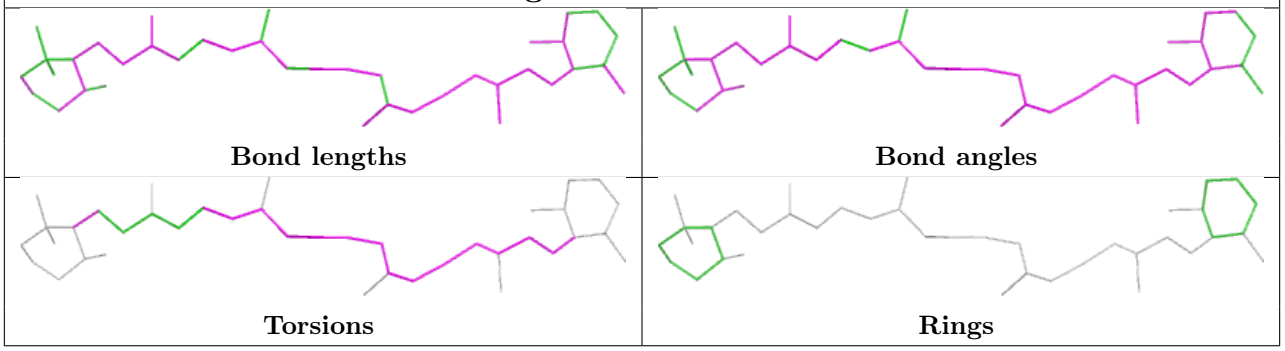
Ligand CLA C 513



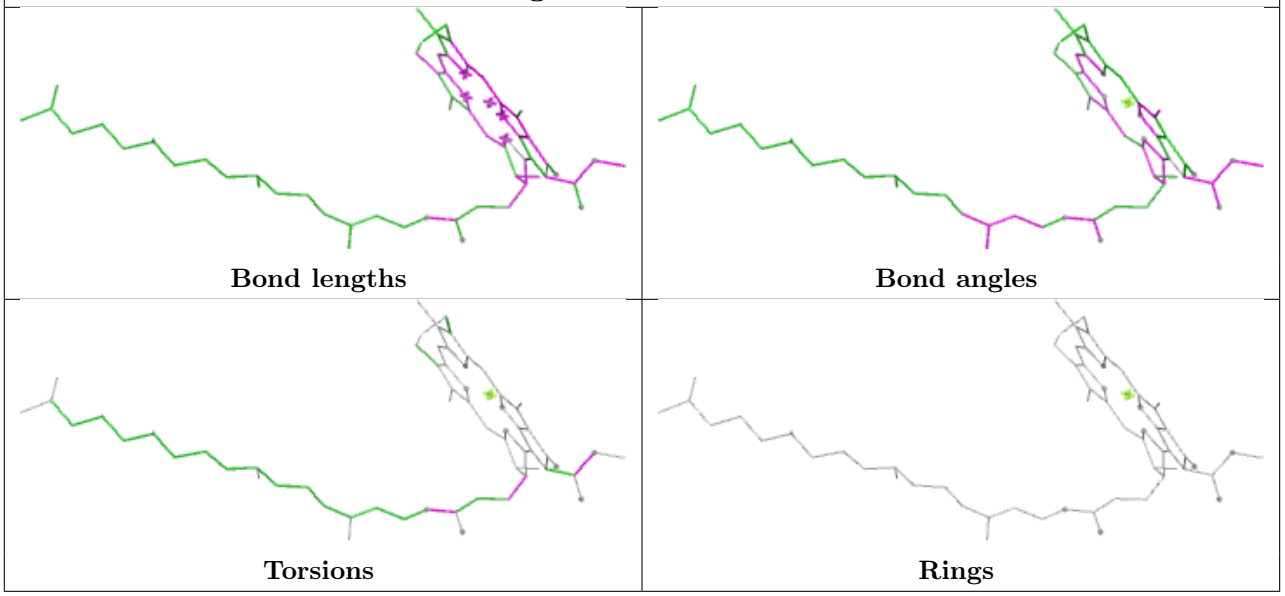
Ligand DGD C 515



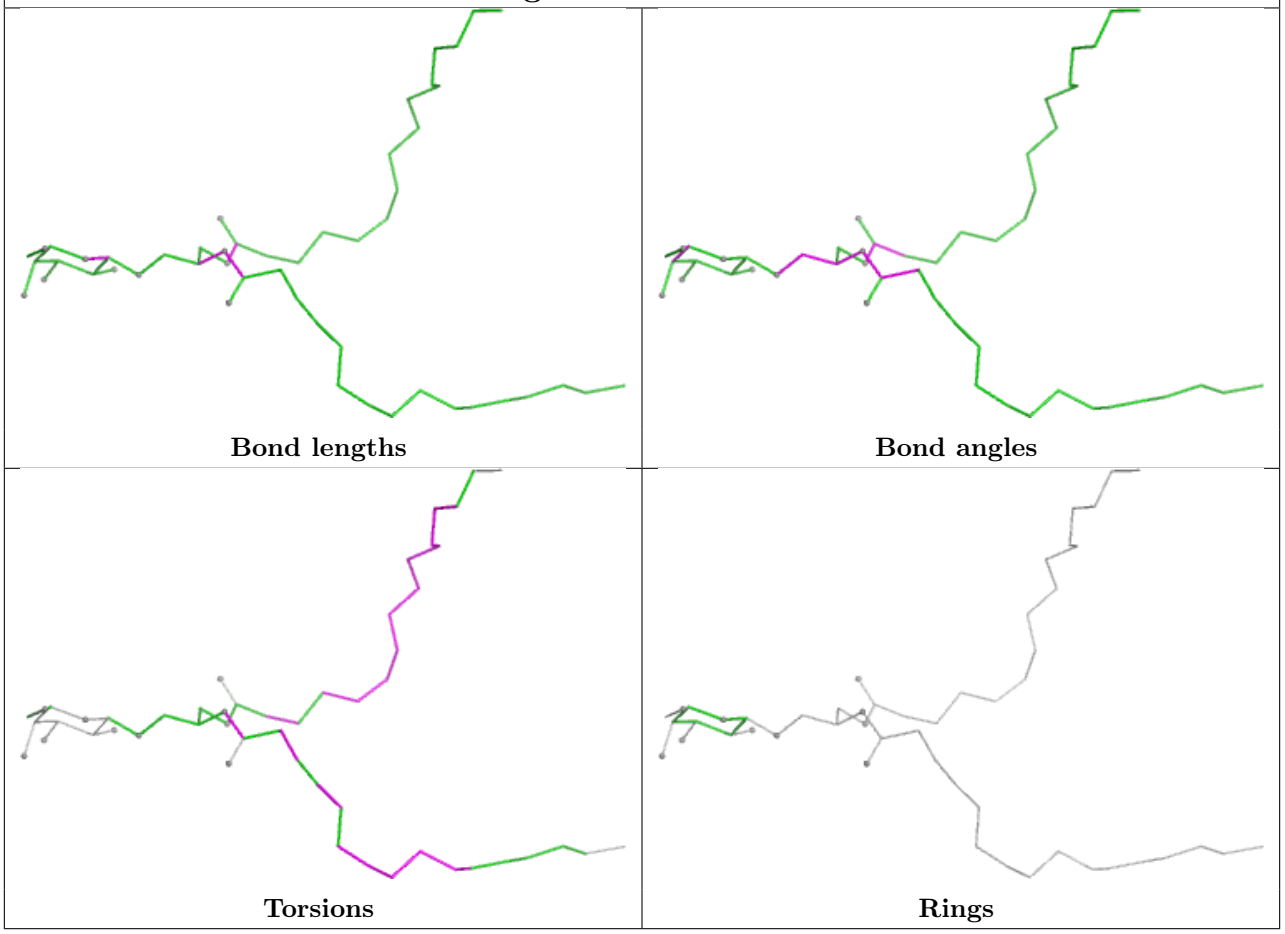
Ligand BCR F 101



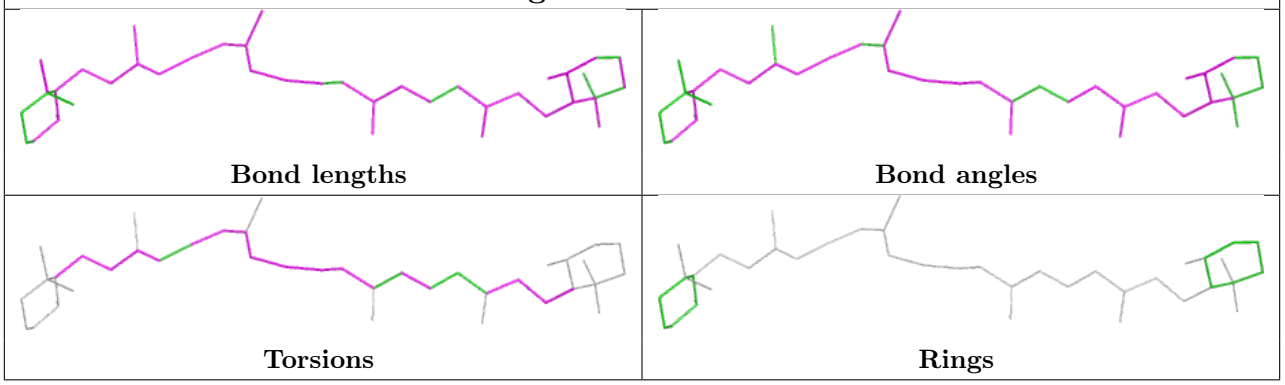
Ligand CLA b 609



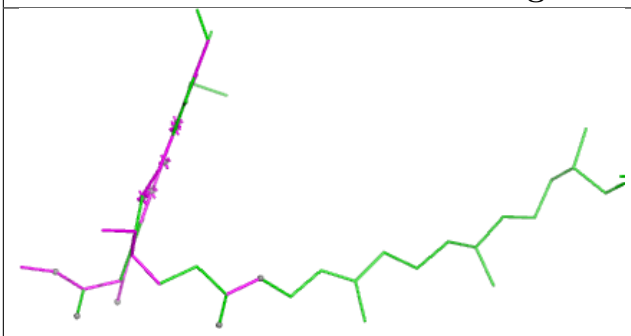
Ligand LMG b 622



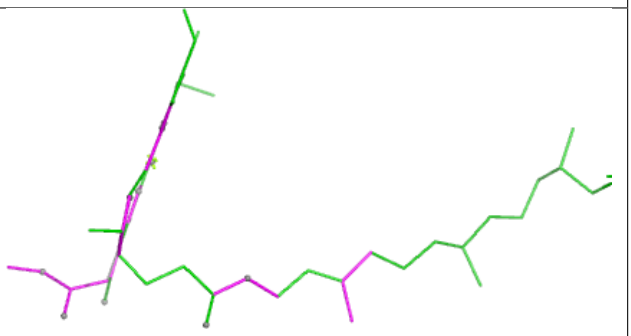
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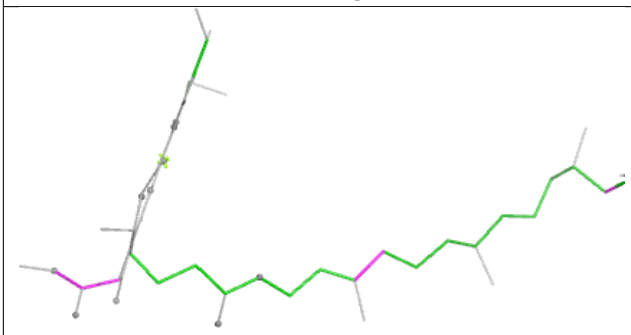
Ligand CLA b 607



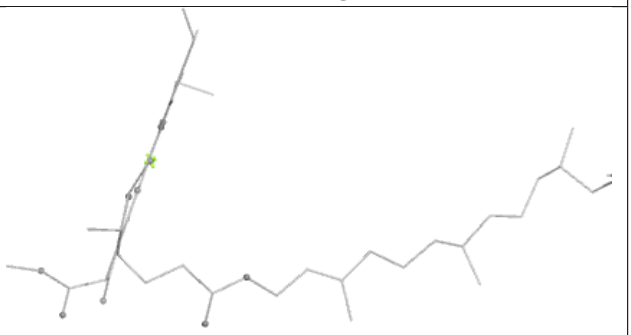
Bond lengths



Bond angles

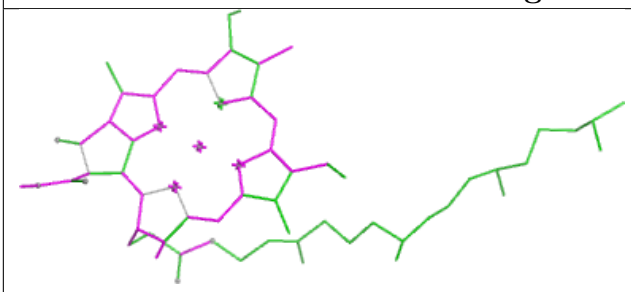


Torsions

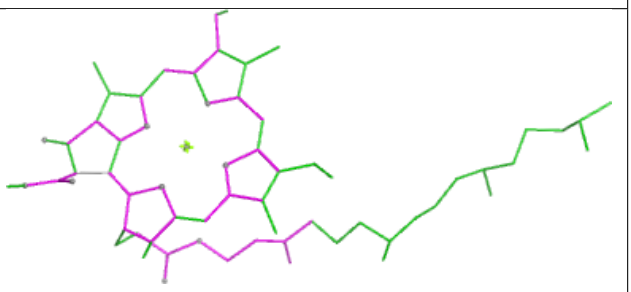


Rings

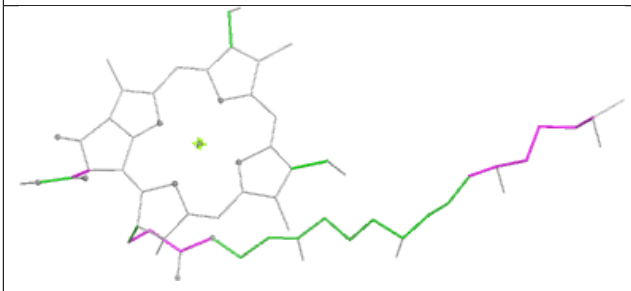
Ligand CLA C 501



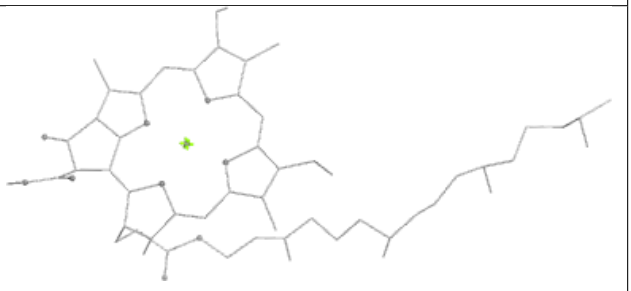
Bond lengths



Bond angles

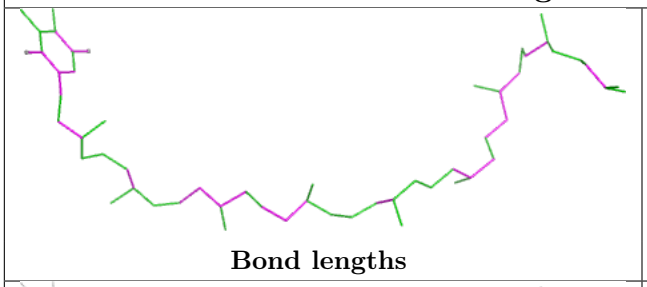


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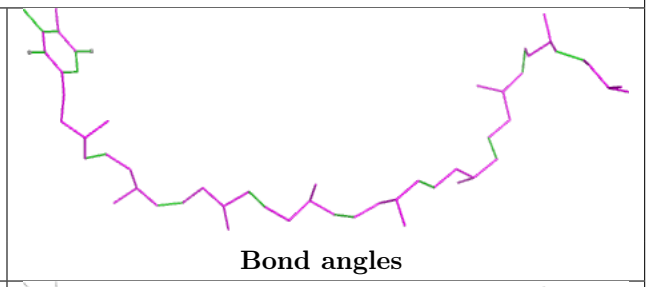


Rings

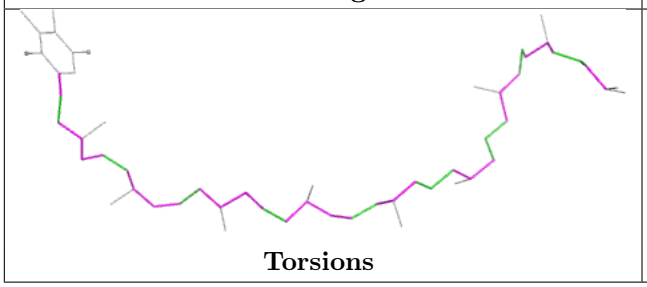
Ligand PL9 a 611



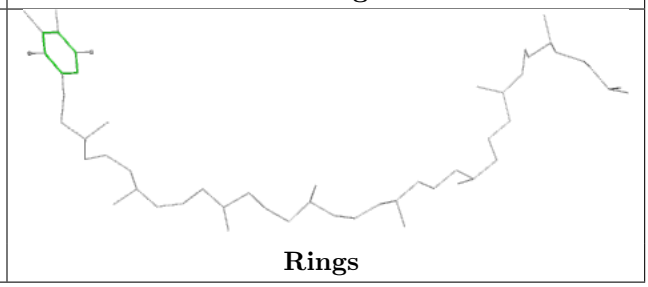
Bond lengths



Bond angles

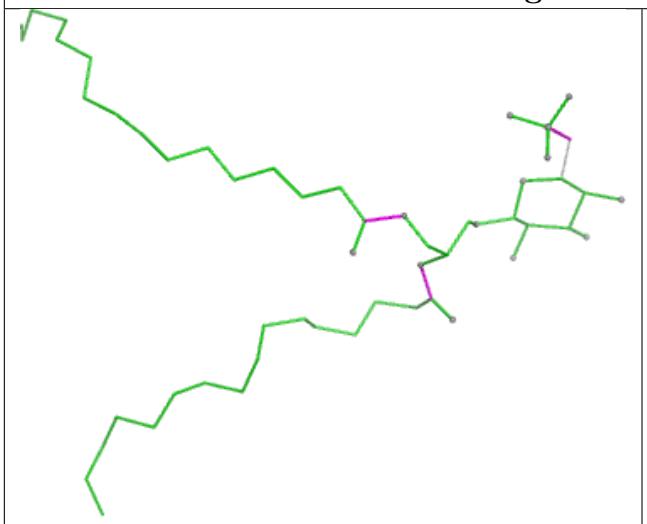


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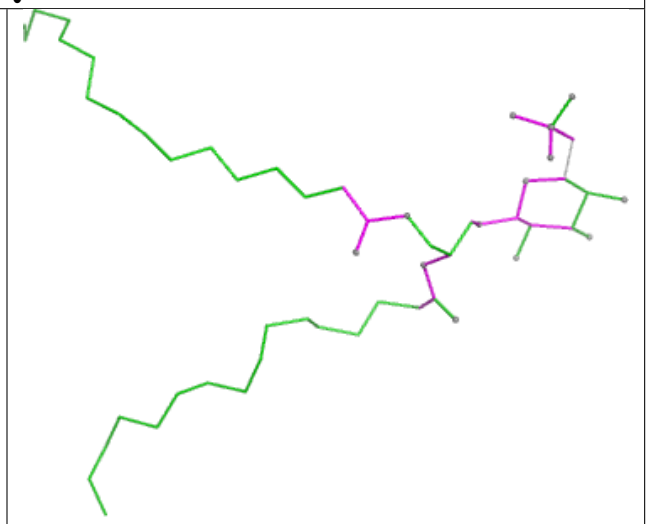


Rings

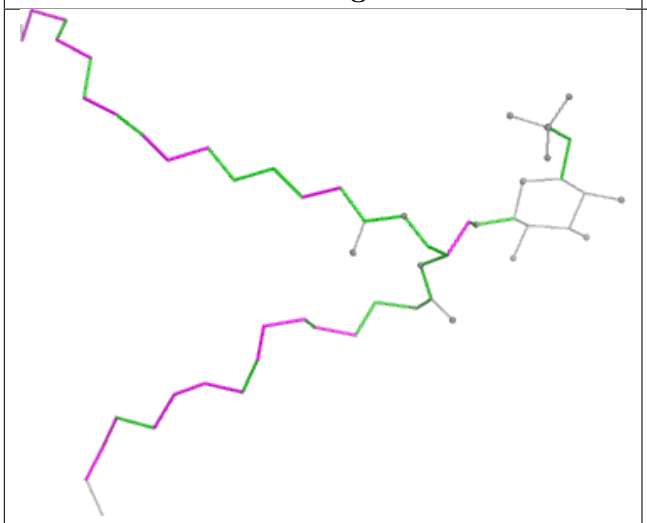
Ligand SQD A 612



Bond lengths



Bond angles

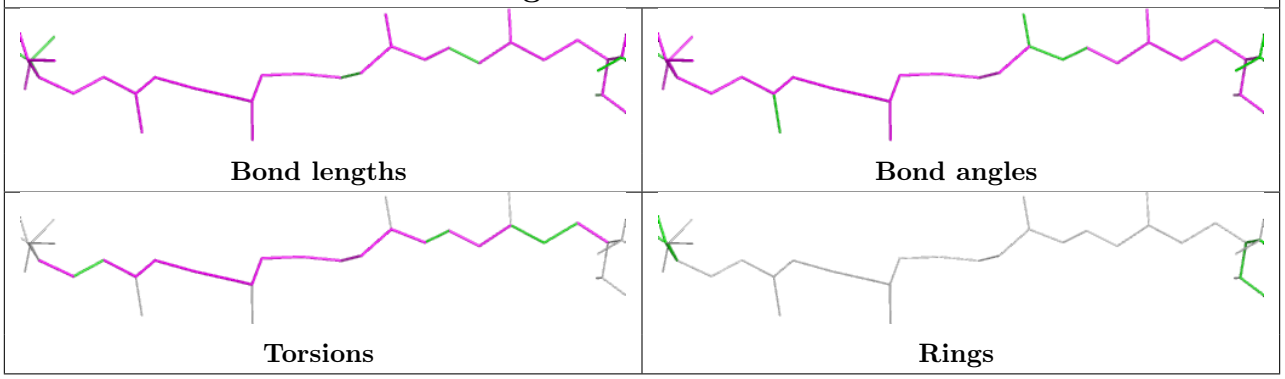


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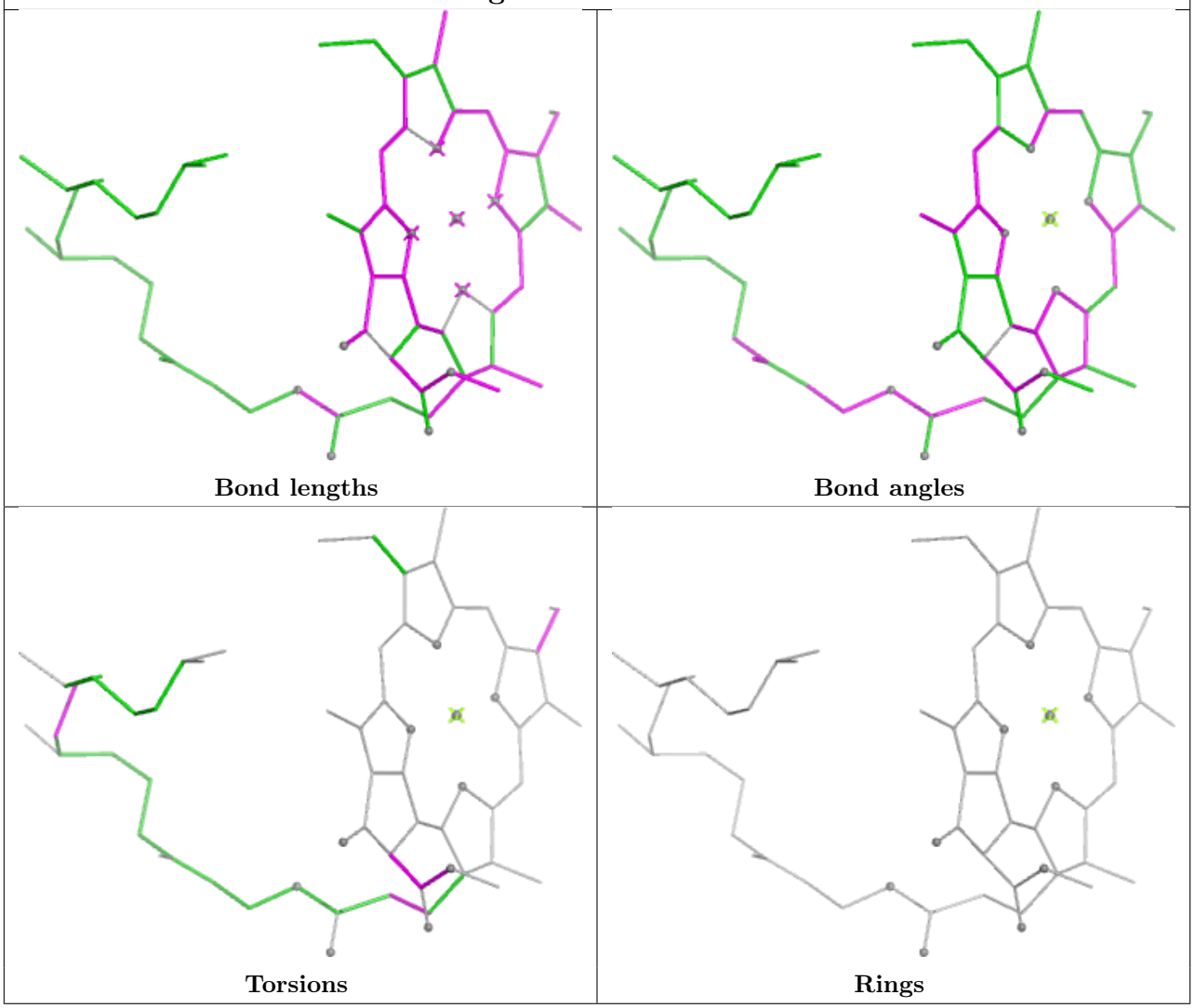


Rings

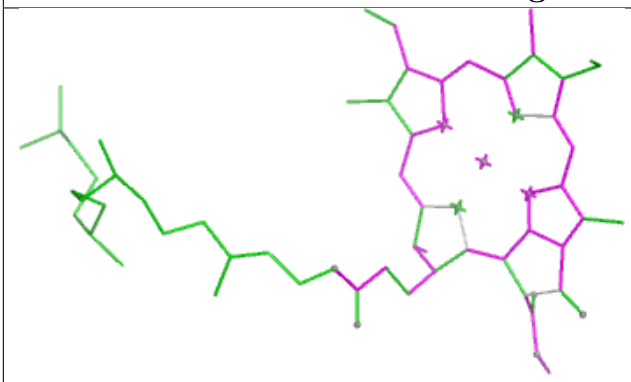
Ligand BCR A 610



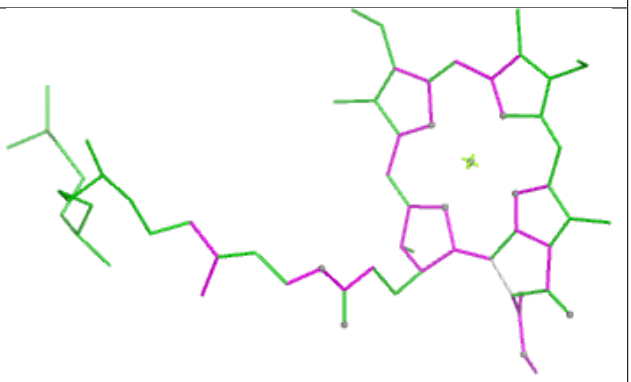
Ligand CLA C 503



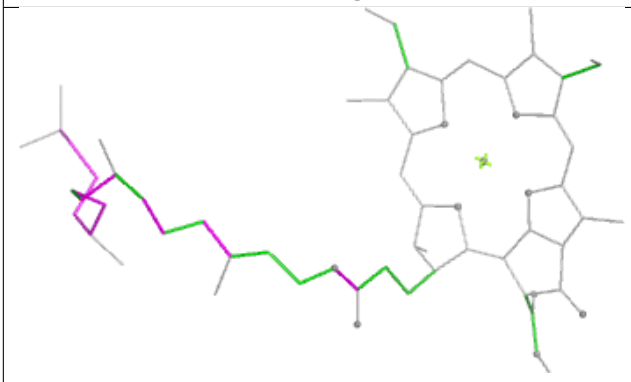
Ligand CLA a 609



Bond lengths



Bond angles

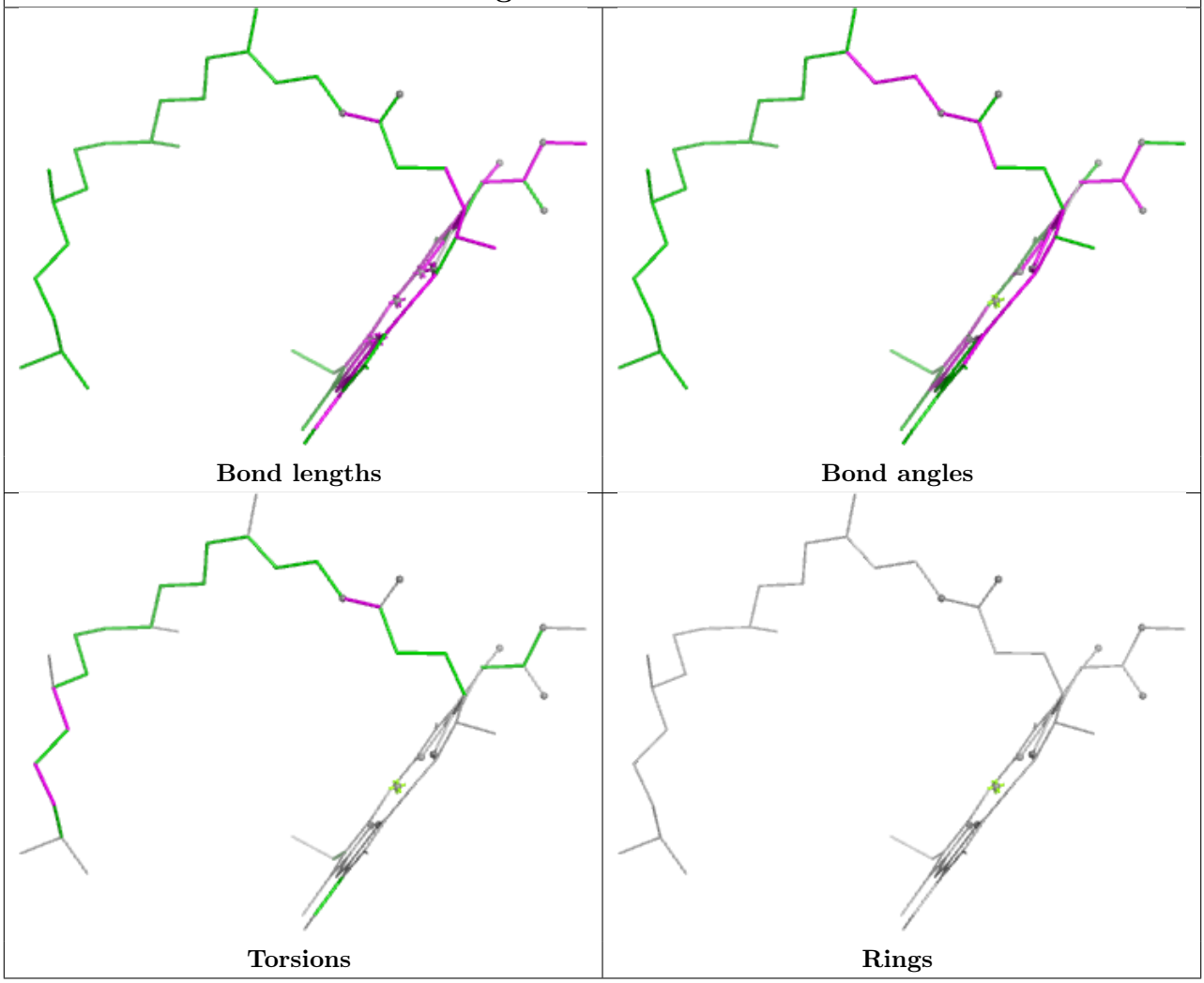


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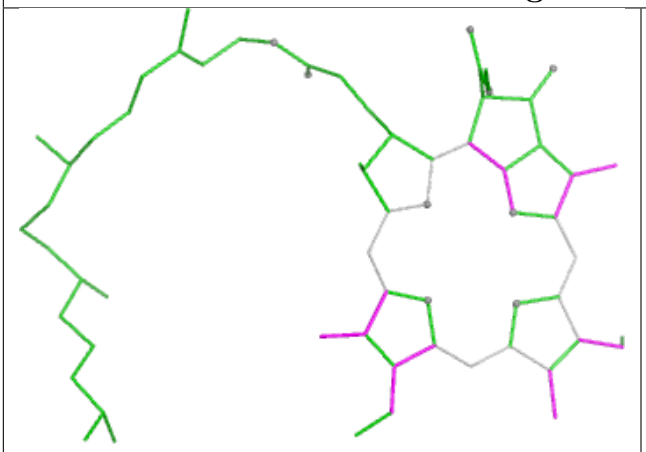


Rings

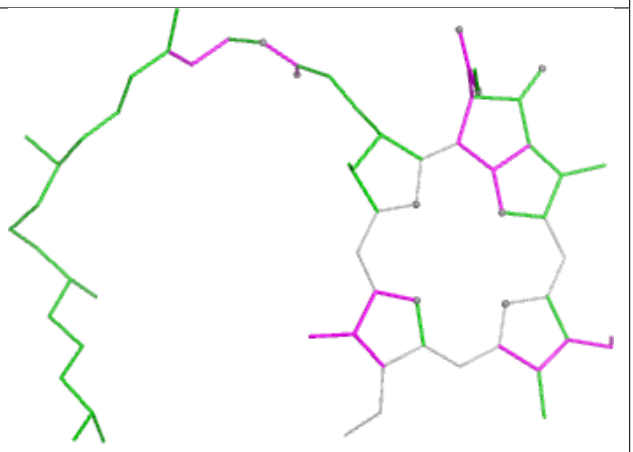
Ligand CLA b 613



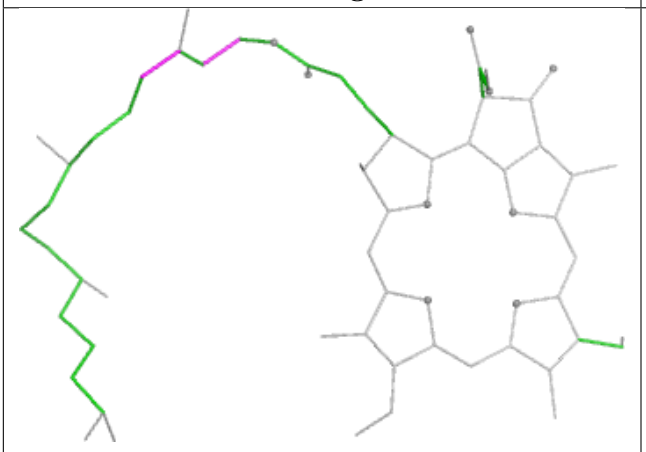
Ligand PHO a 608



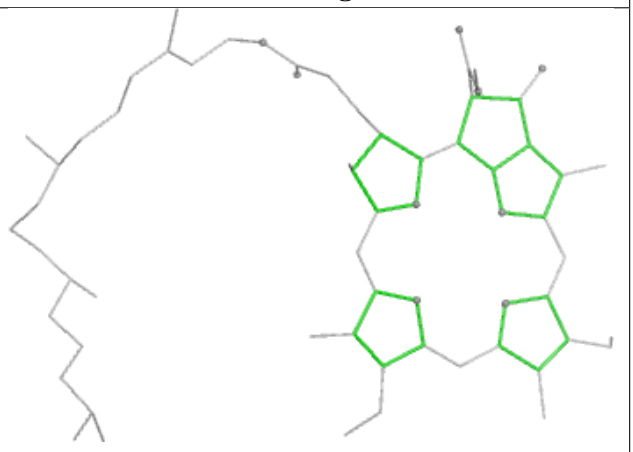
Bond lengths



Bond angles

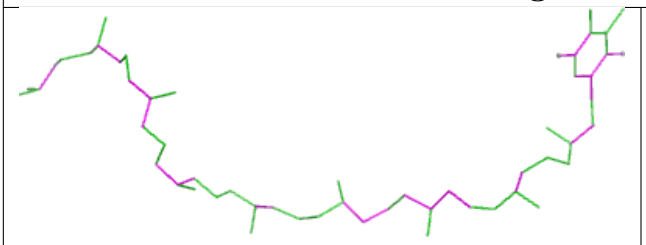


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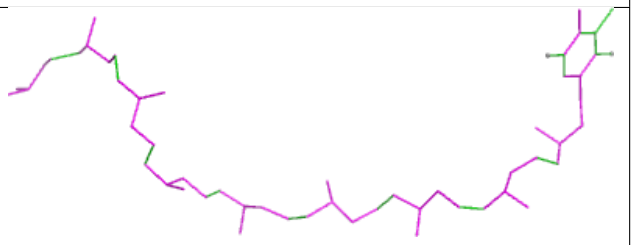


Rings

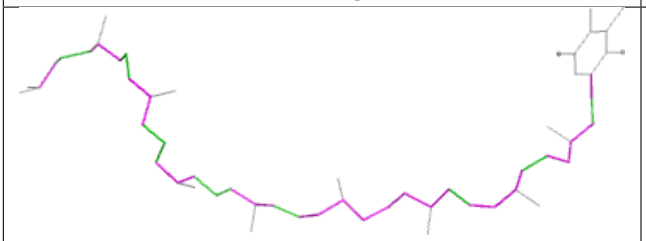
Ligand PL9 A 611



Bond lengths



Bond angles

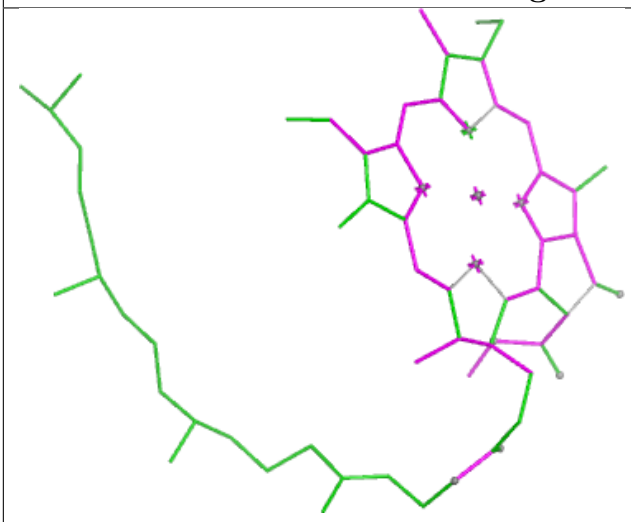


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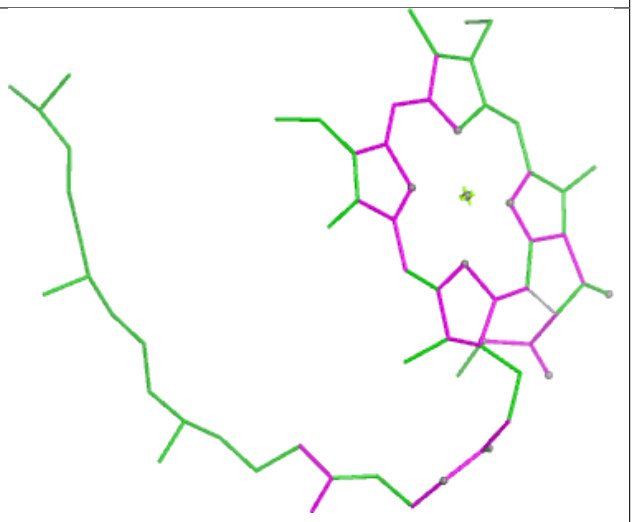


Rings

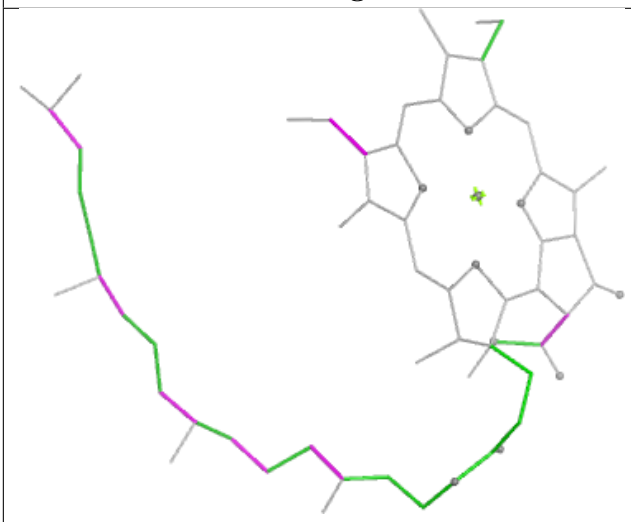
Ligand CLA c 507



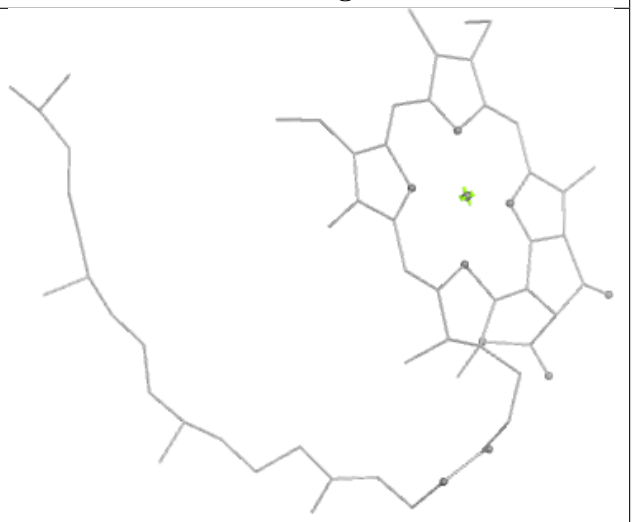
Bond lengths



Bond angles

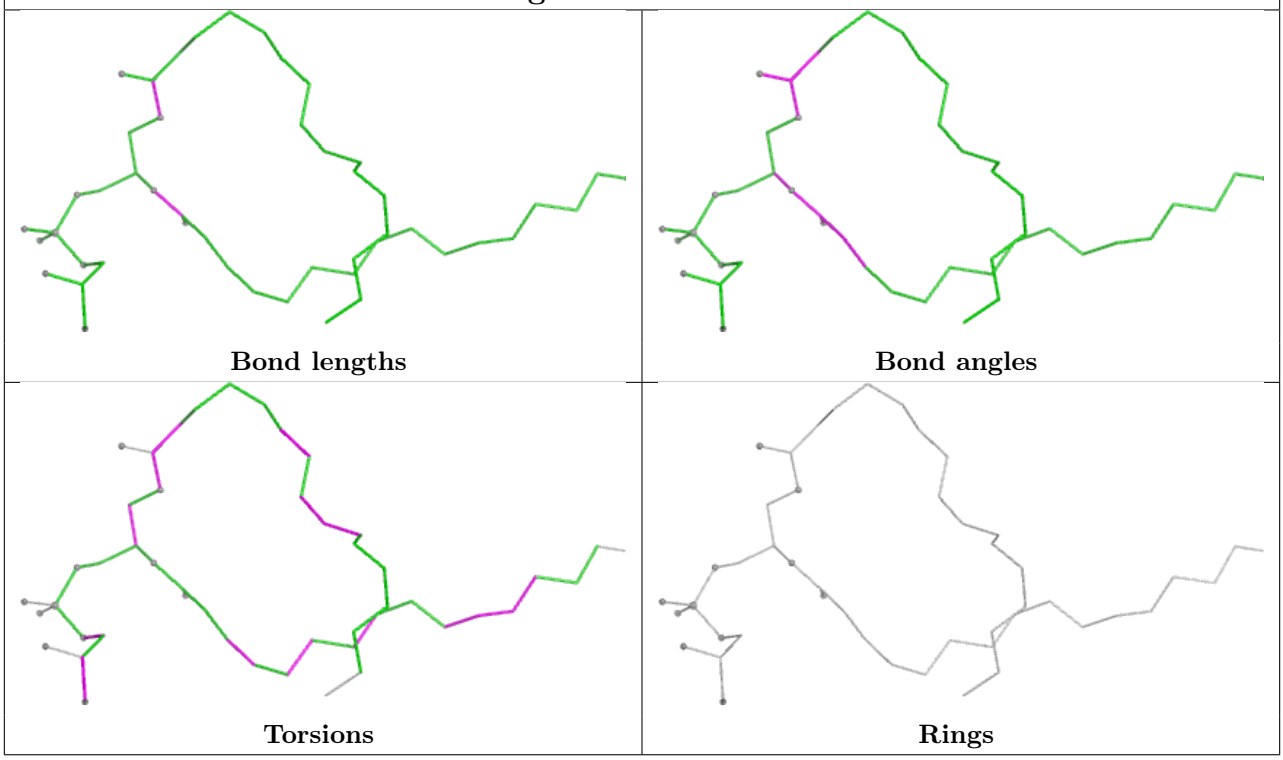


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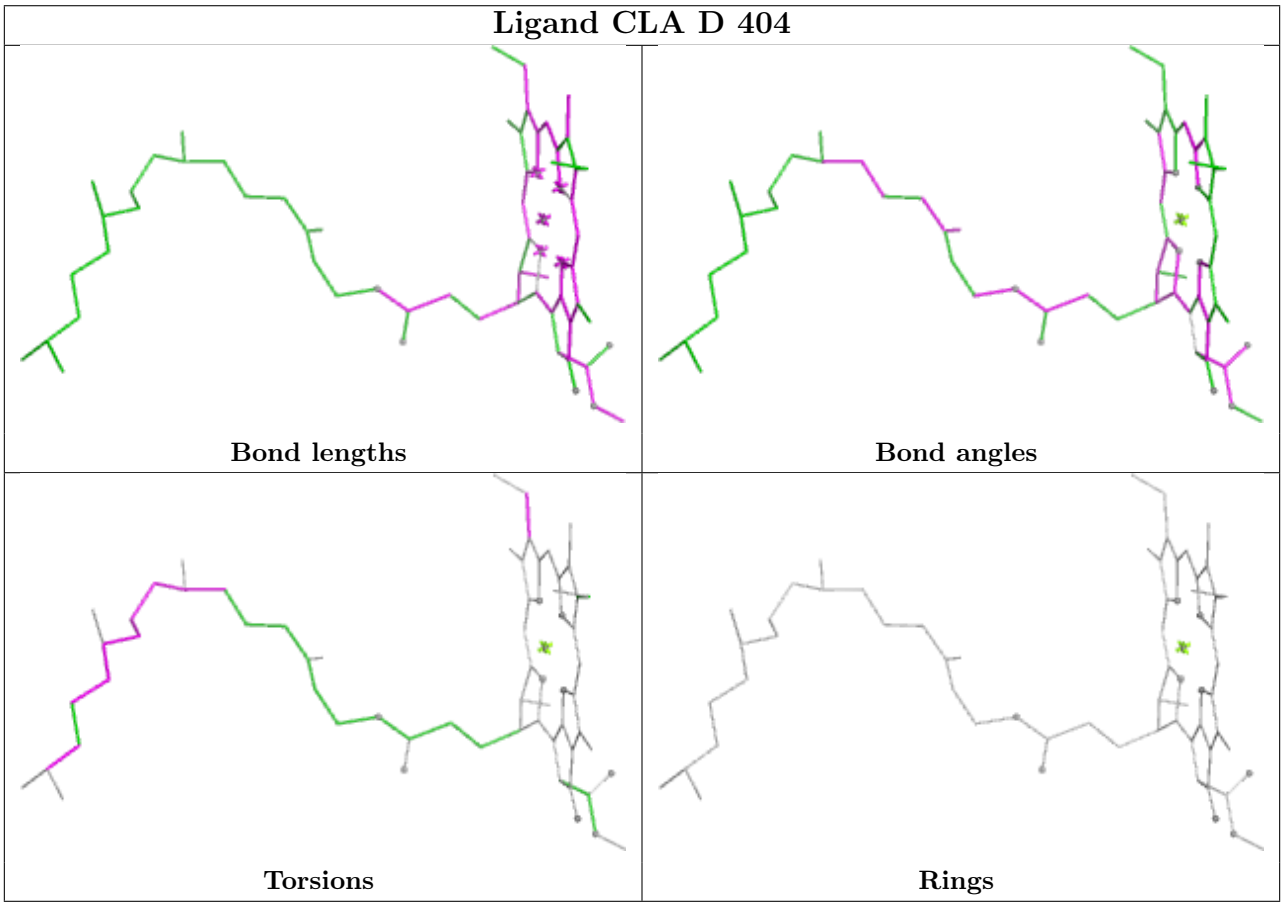


Rings

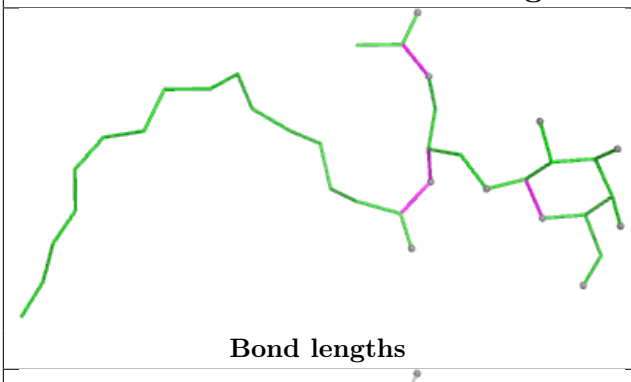
Ligand LHG a 616



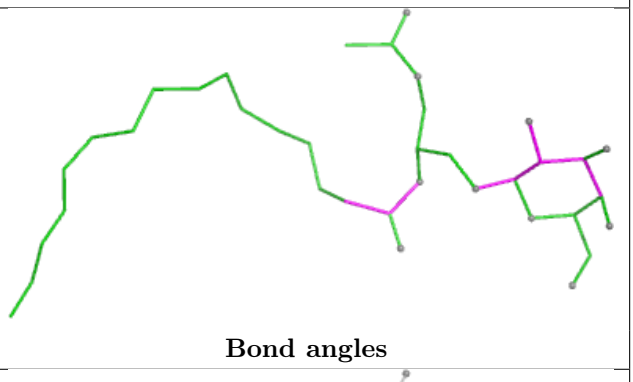
Ligand CLA D 404



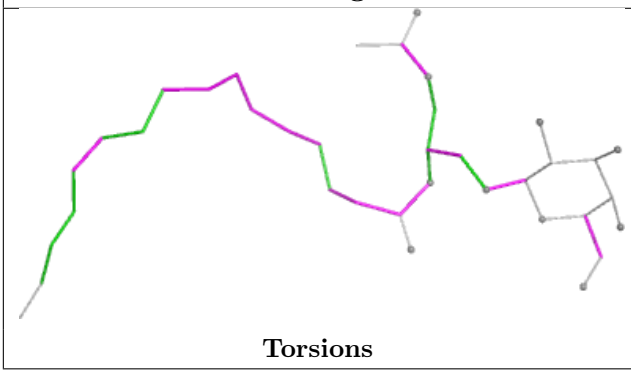
Ligand LMG z 101



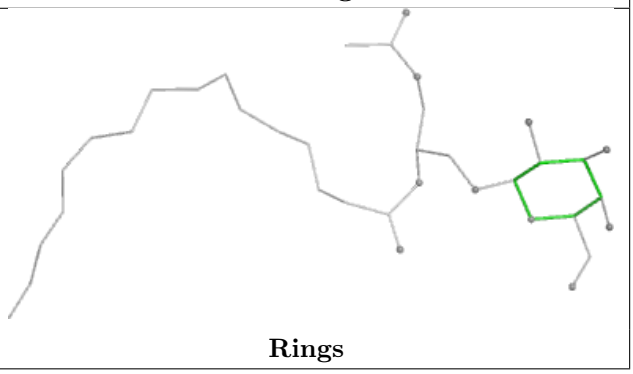
Bond lengths



Bond angles

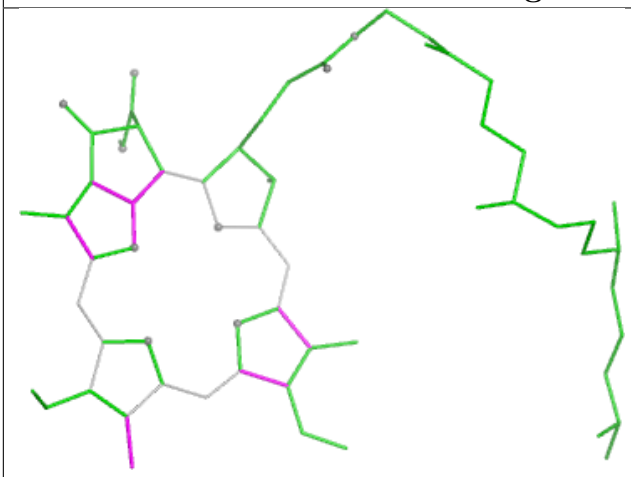


Torsions

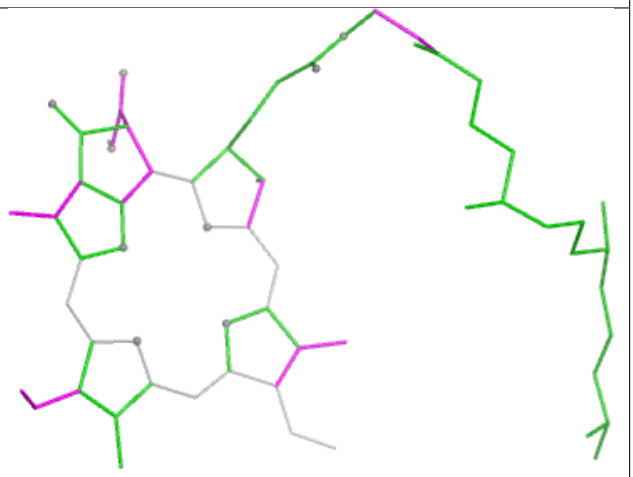


Rings

Ligand PHO d 401



Bond lengths



Bond angles

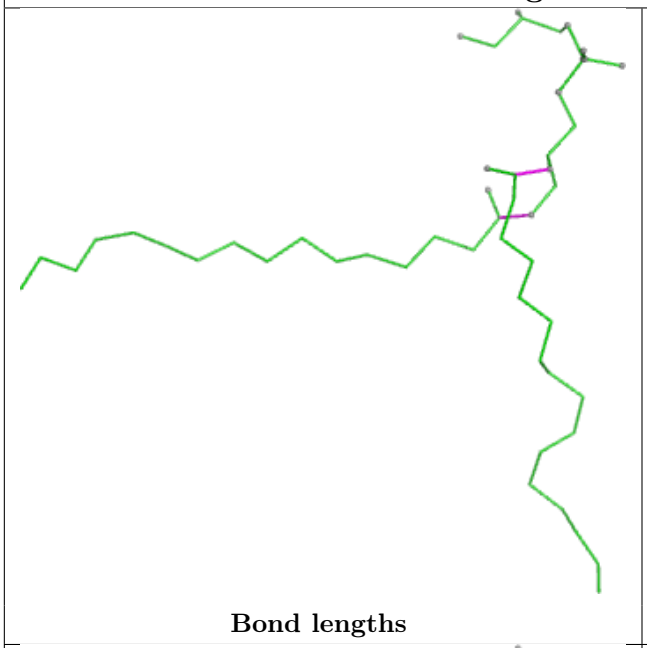


Torsions

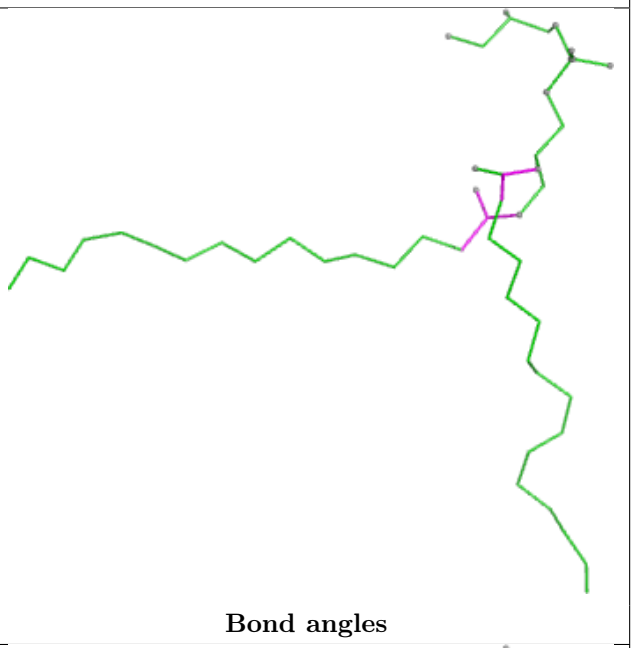


Rings

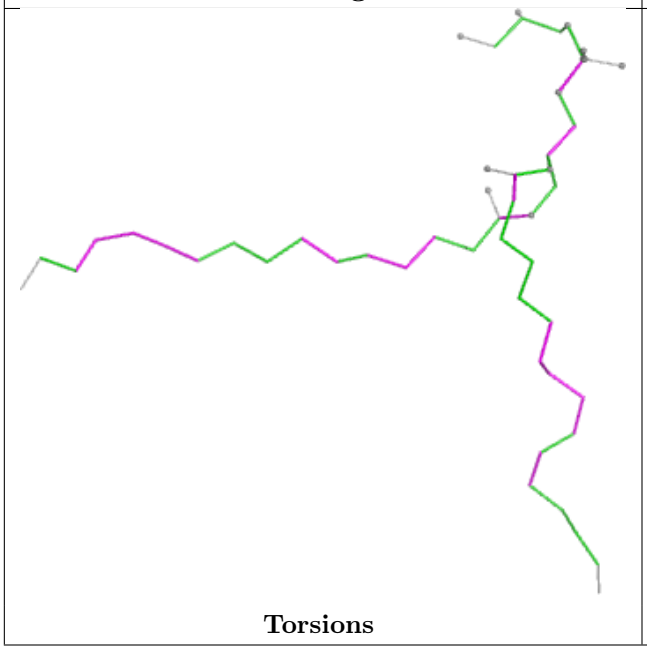
Ligand LHG L 101



Bond lengths



Bond angles

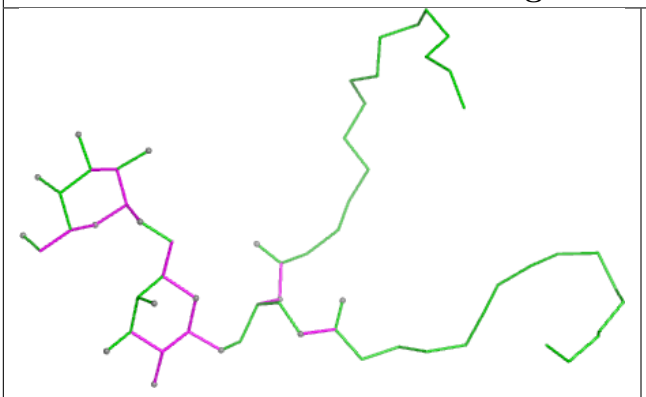


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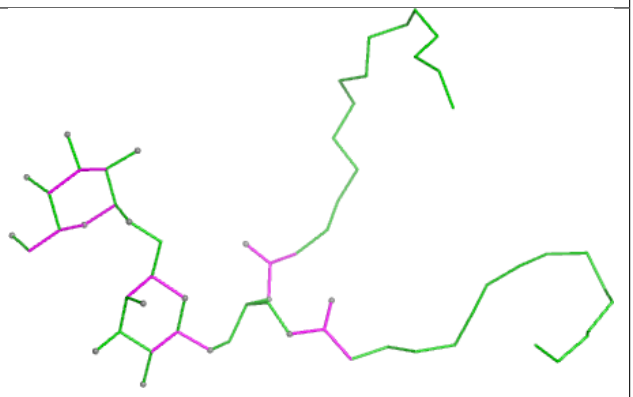


Rings

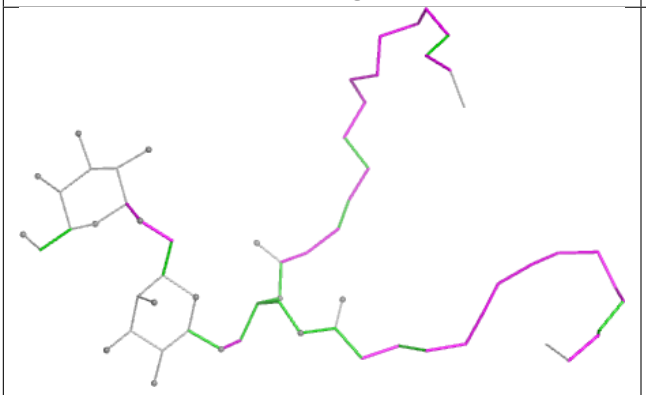
Ligand DGD c 517



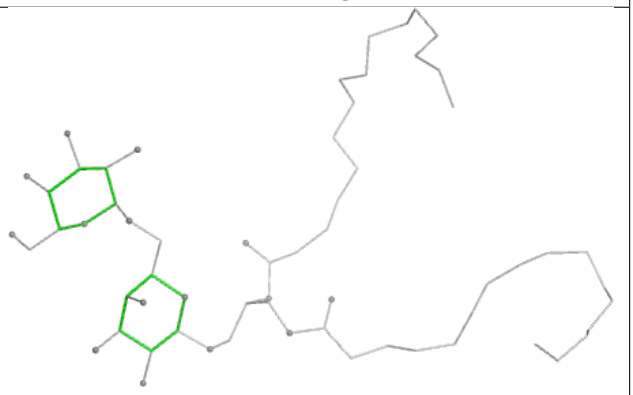
Bond lengths



Bond angles

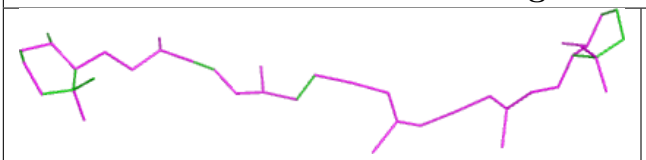


Torsions



Rings

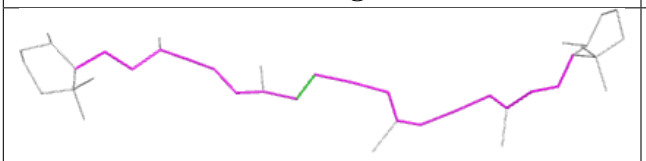
Ligand BCR t 101



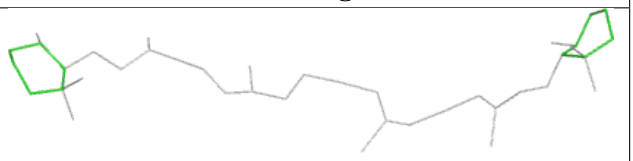
Bond lengths



Bond angles

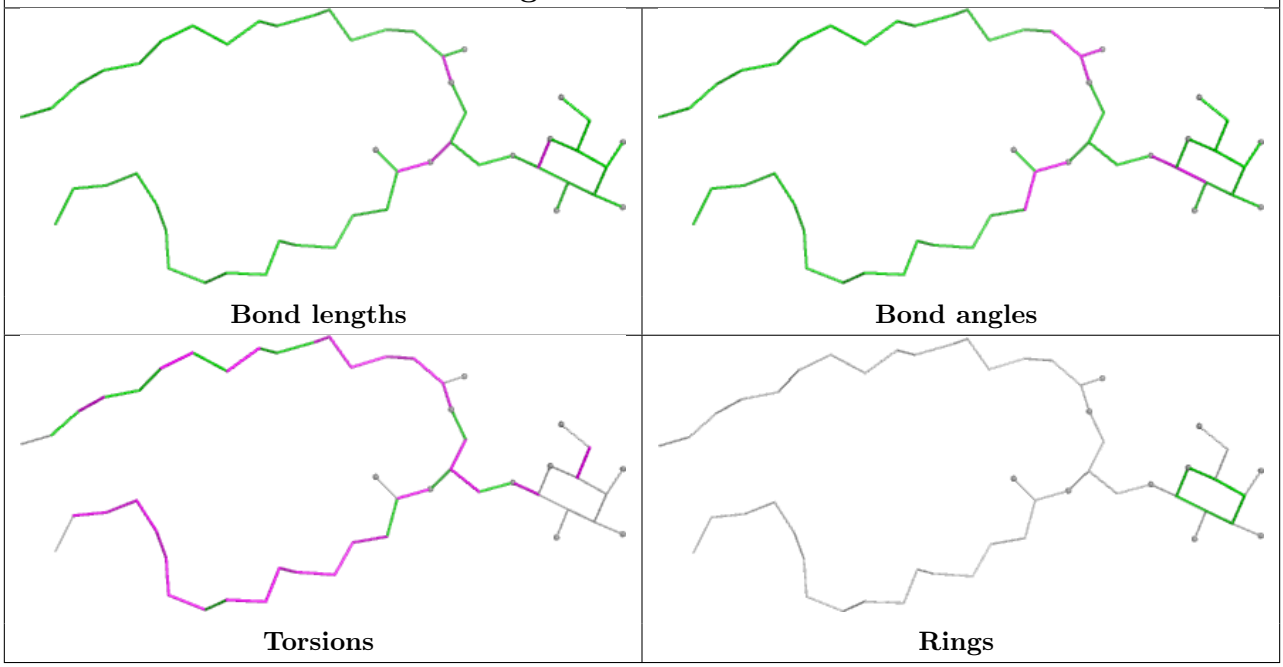


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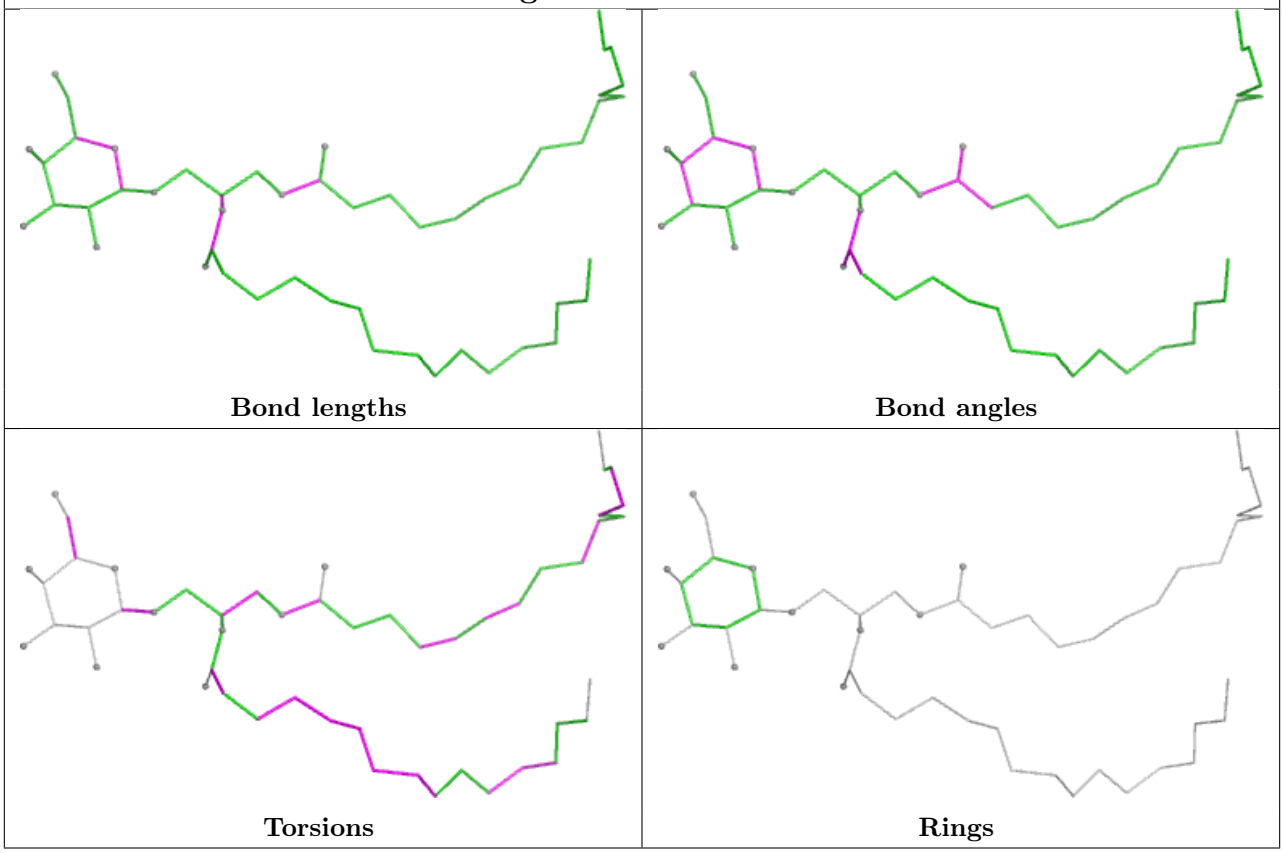


Rings

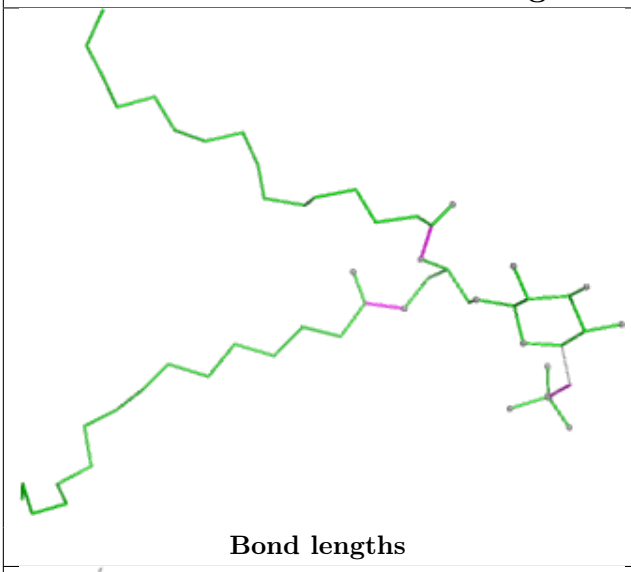
Ligand LMG A 613



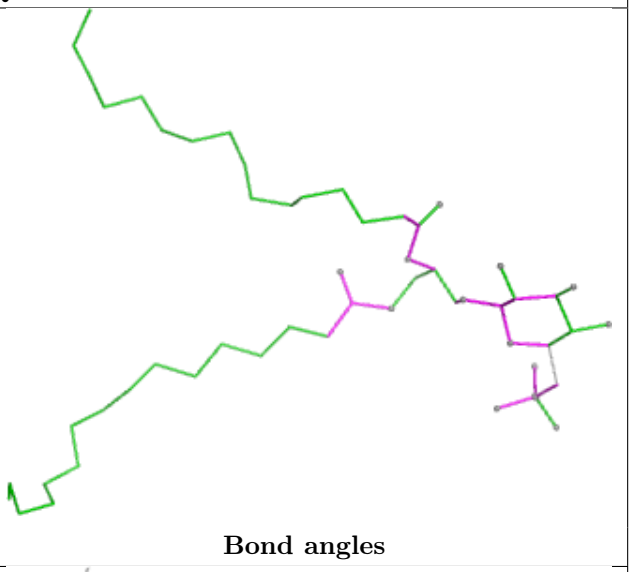
Ligand LMG D 408



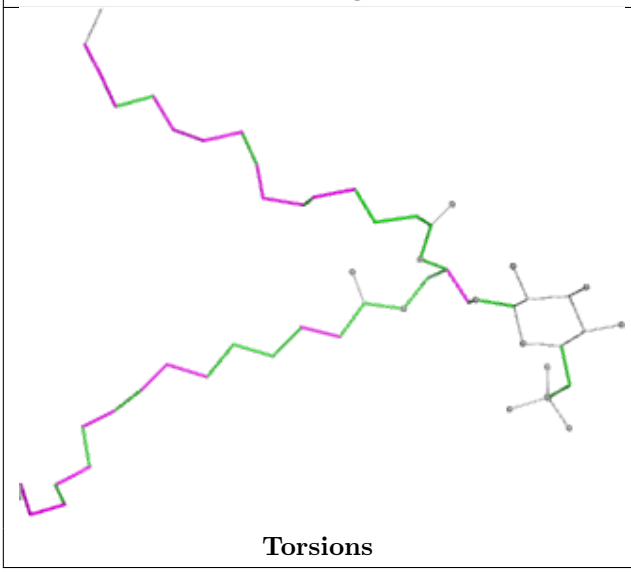
Ligand SQD a 612



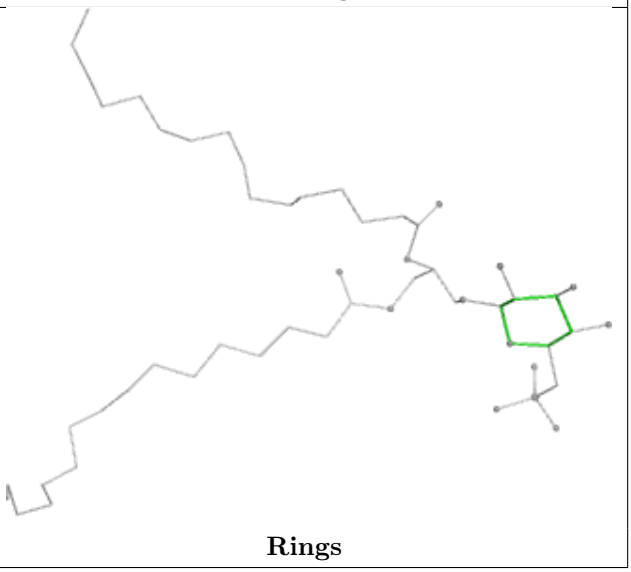
Bond lengths



Bond angles

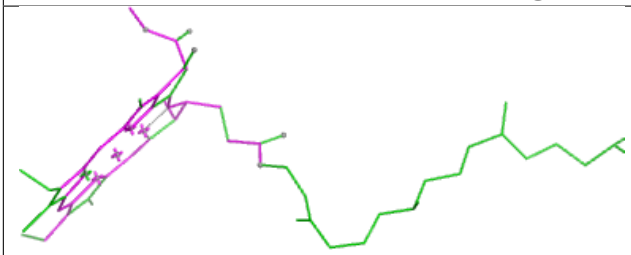


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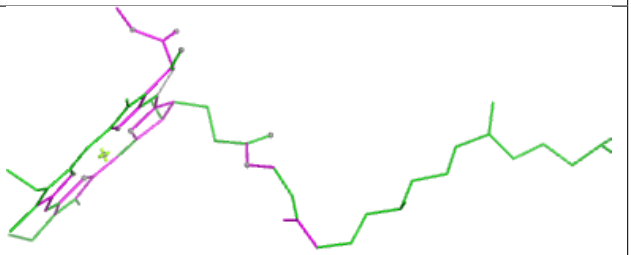


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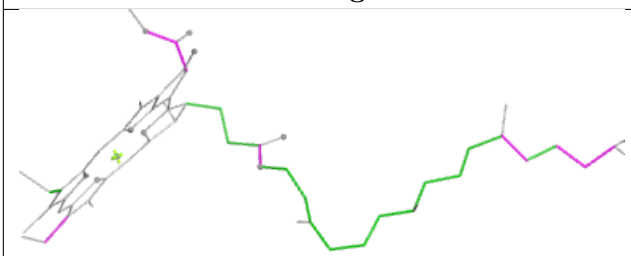
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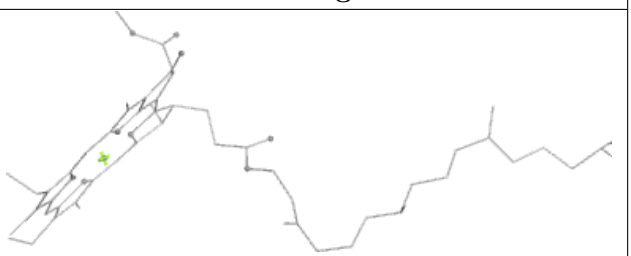
Bond lengths



Bond angles

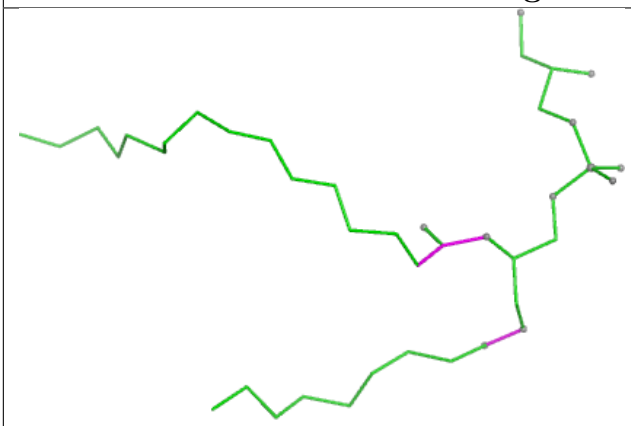


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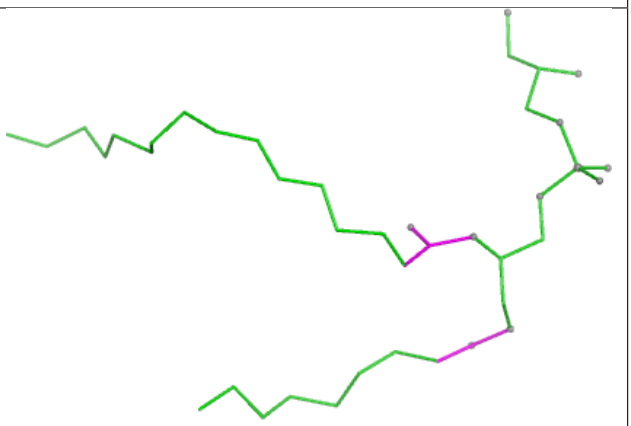


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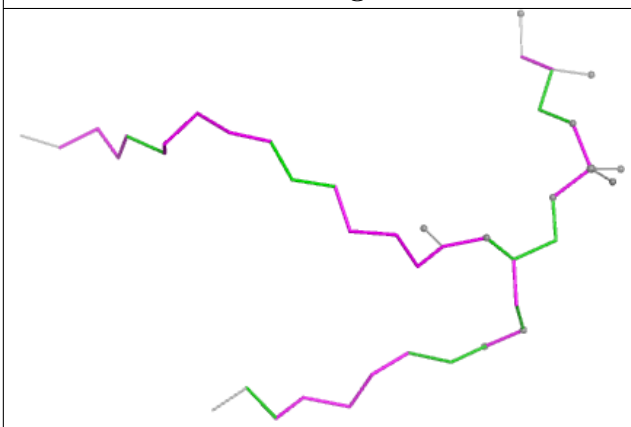
Ligand LHG E 102



Bond lengths



Bond angles

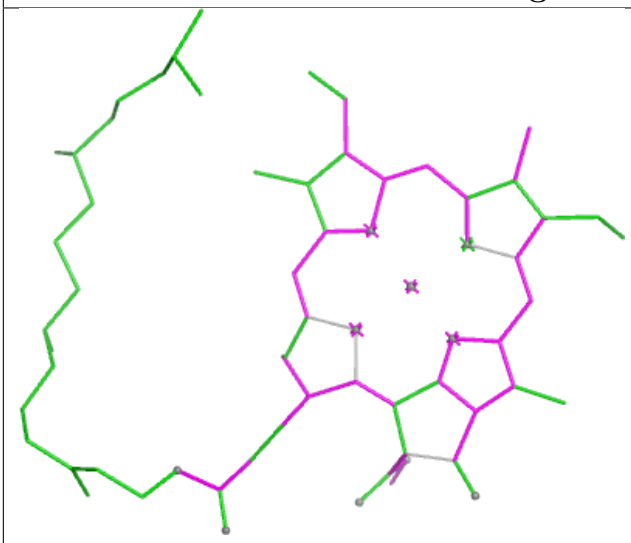


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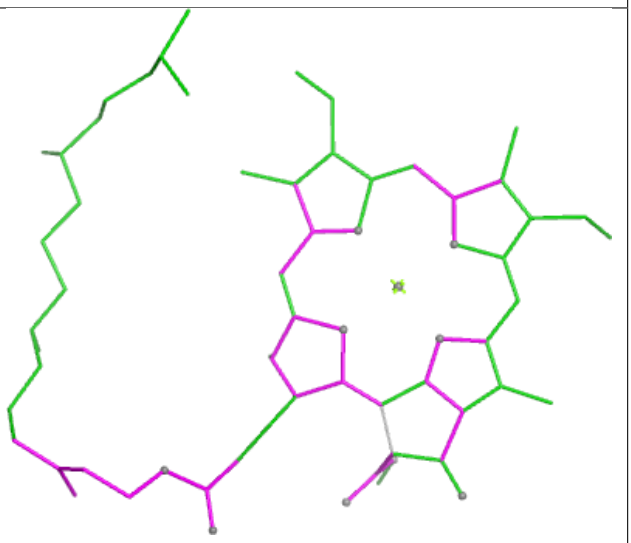


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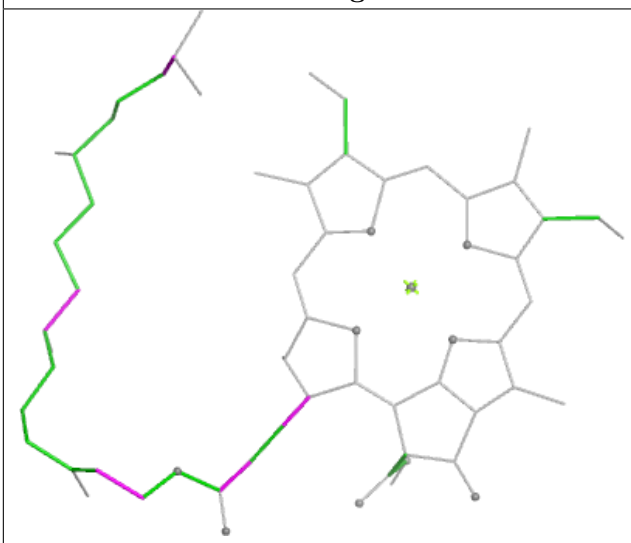
Ligand CLA c 512



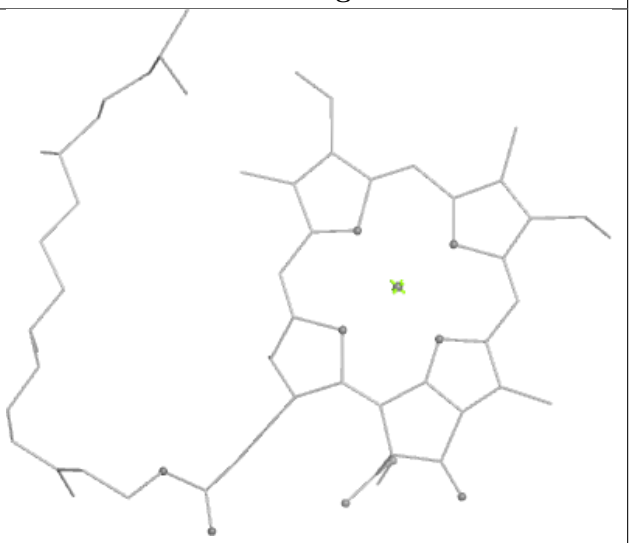
Bond lengths



Bond angles

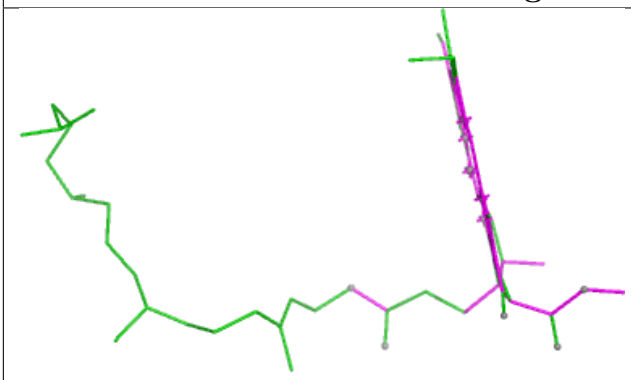


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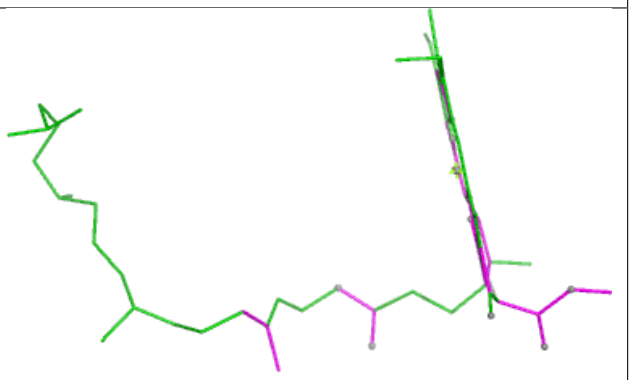


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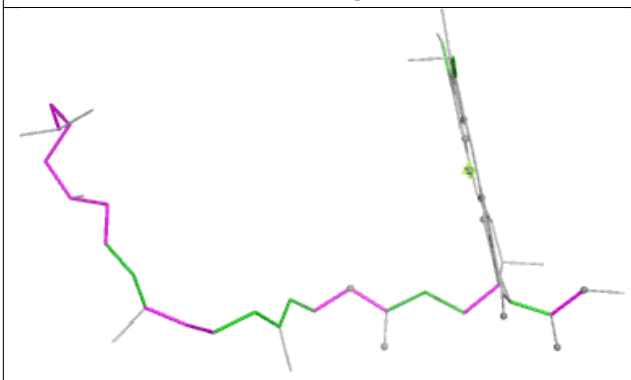
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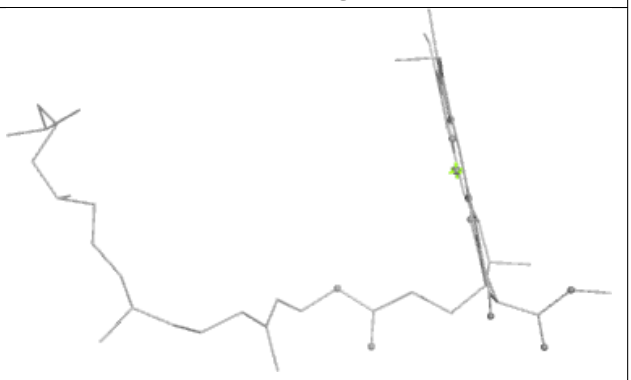
Bond lengths



Bond angles

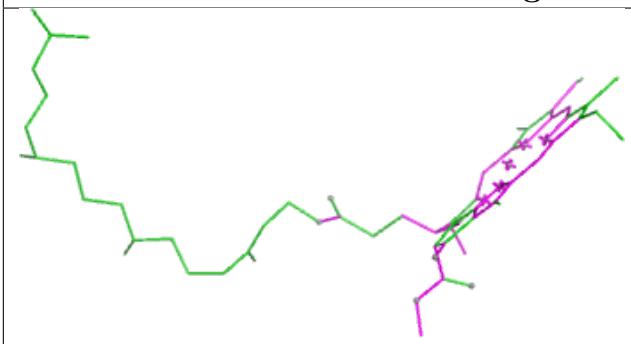


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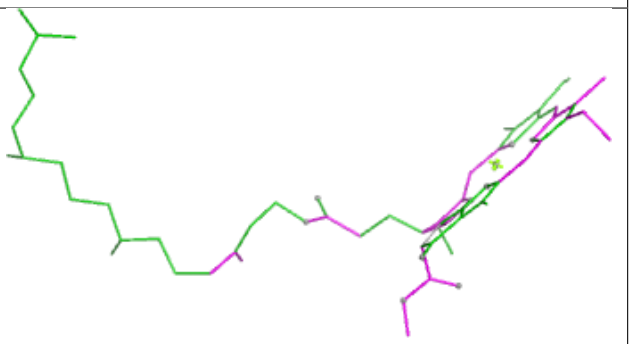


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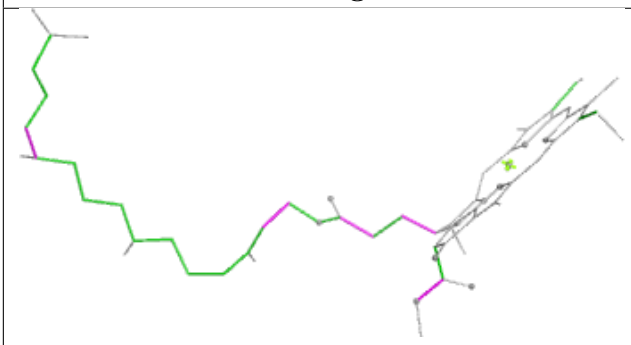
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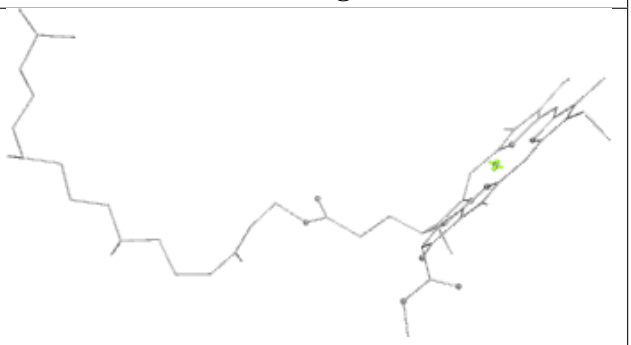
Bond lengths



Bond angles

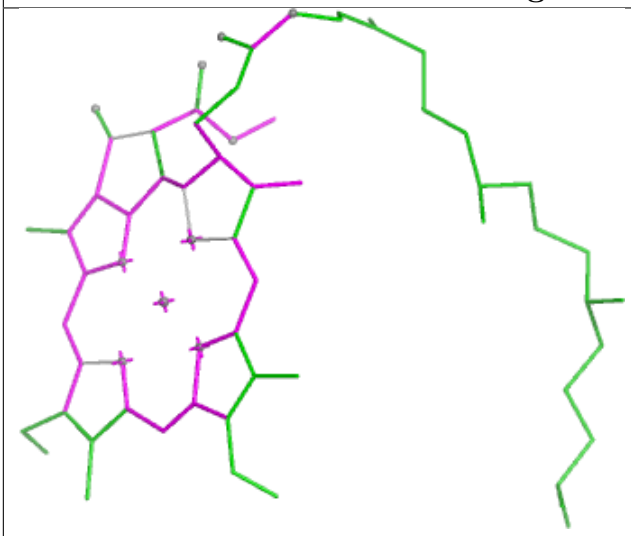


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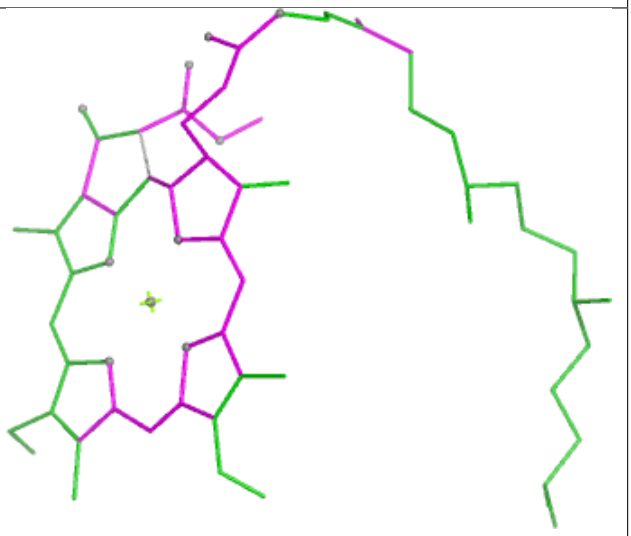


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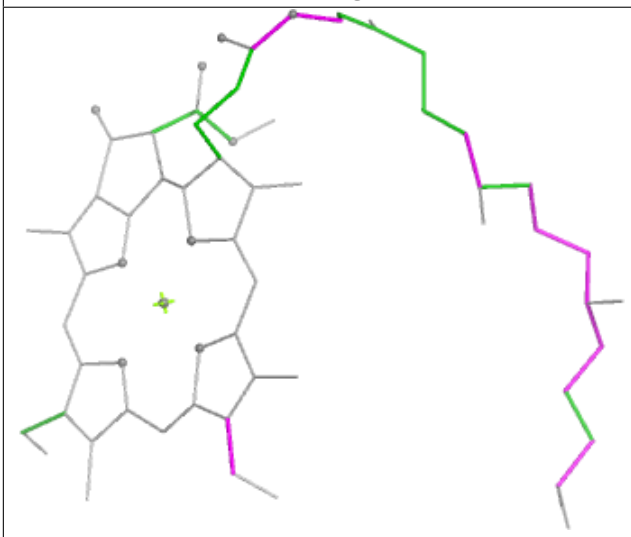
Ligand CLA b 618



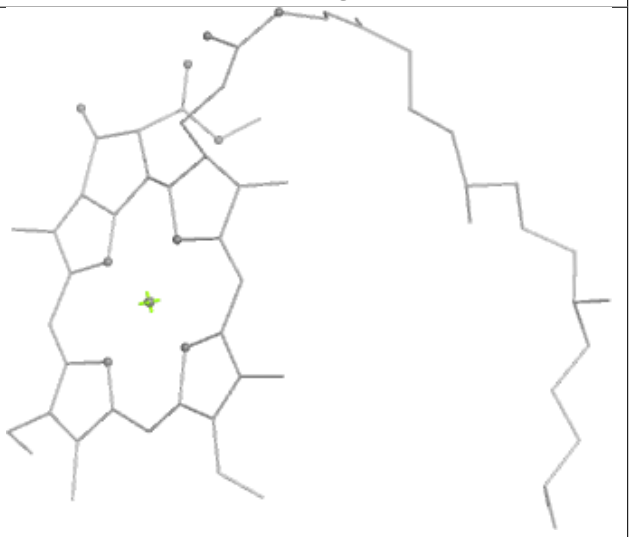
Bond lengths



Bond angles

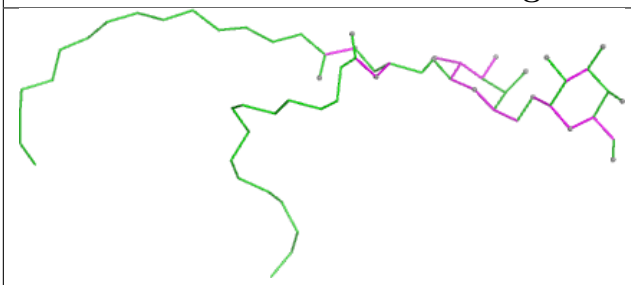


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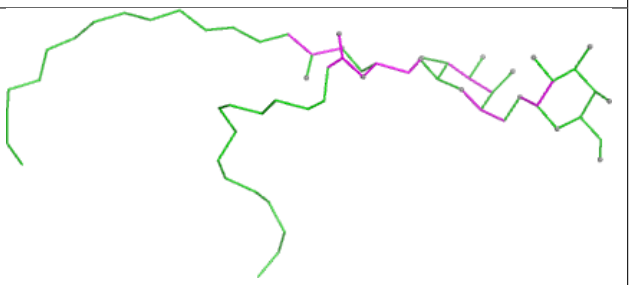


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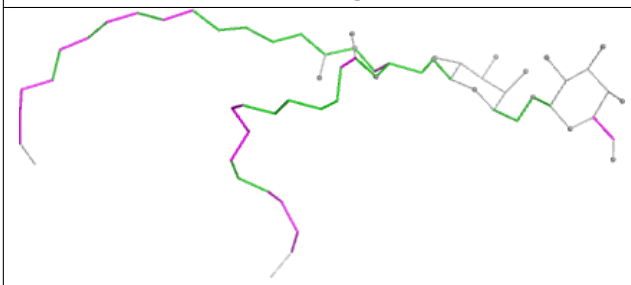
Ligand DGD h 102



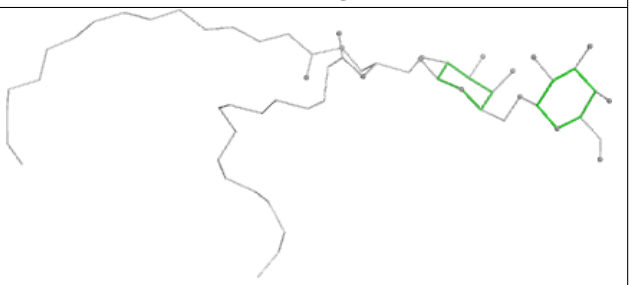
Bond lengths



Bond angles

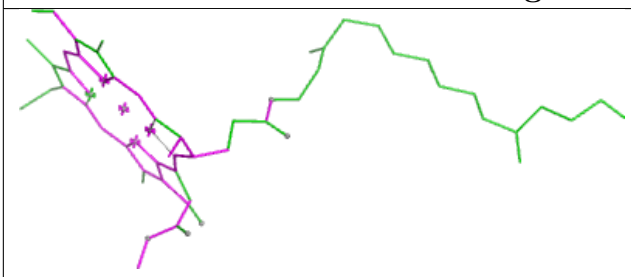


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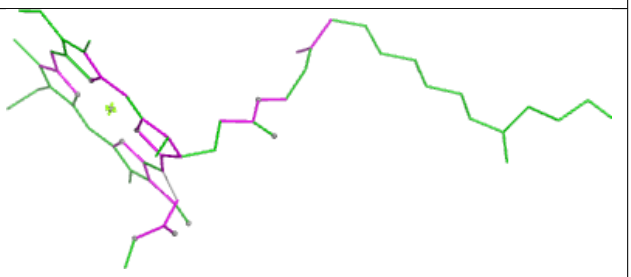


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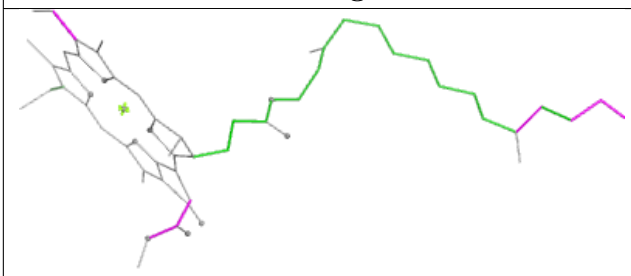
Ligand CLA C 502



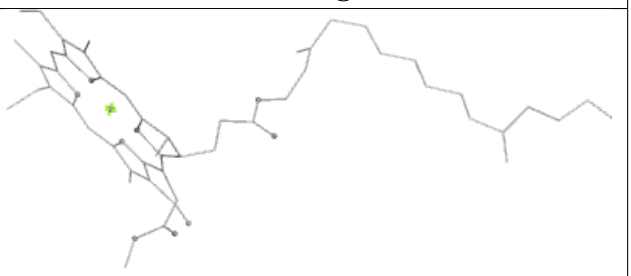
Bond lengths



Bond angles

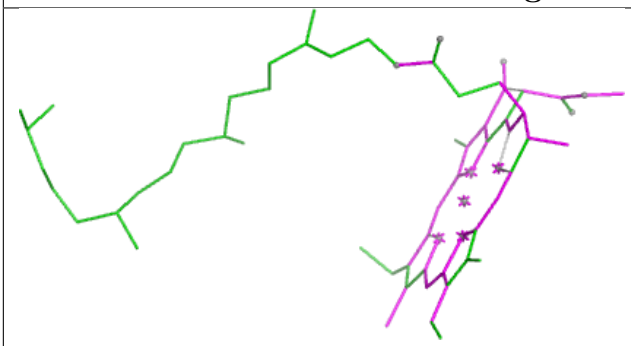


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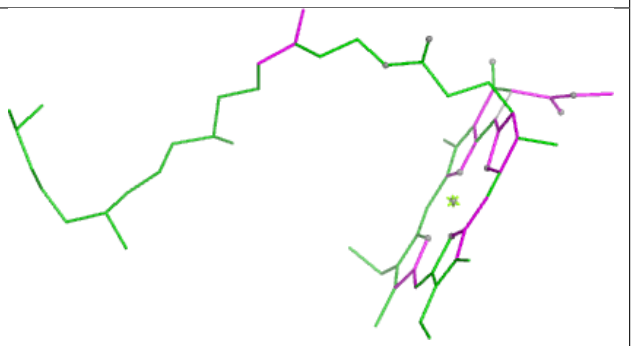


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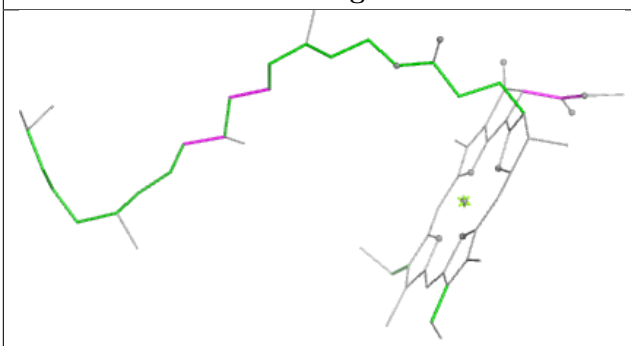
Ligand CLA C 508



Bond lengths



Bond angles



Torsions



Rings

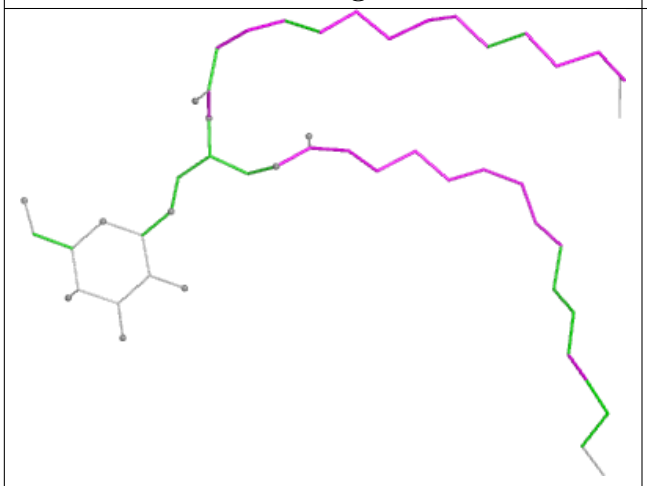
Ligand LMG C 518



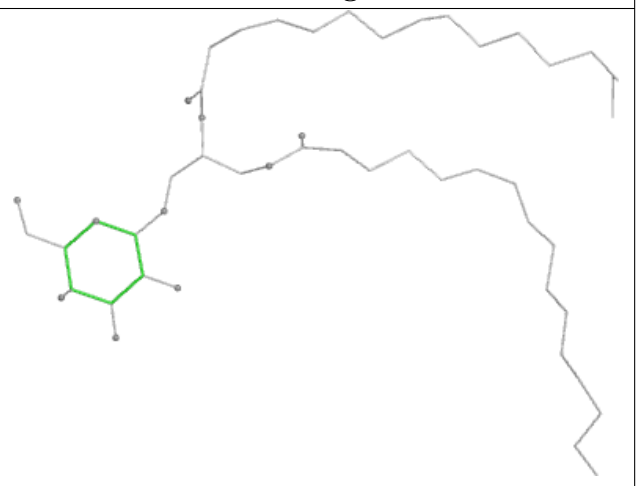
Bond lengths



Bond angles

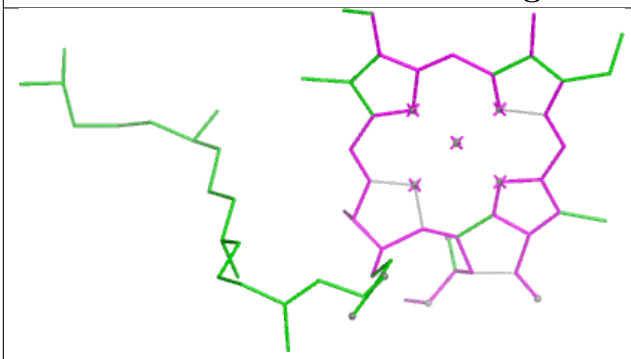


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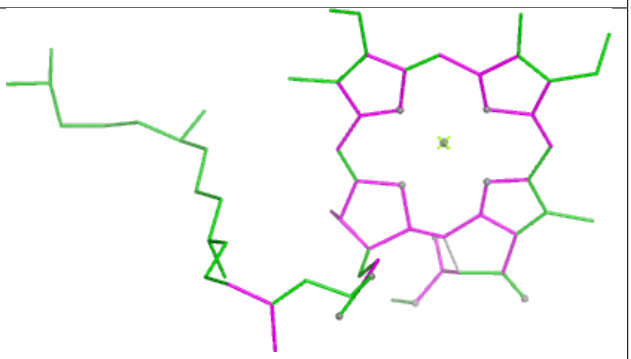


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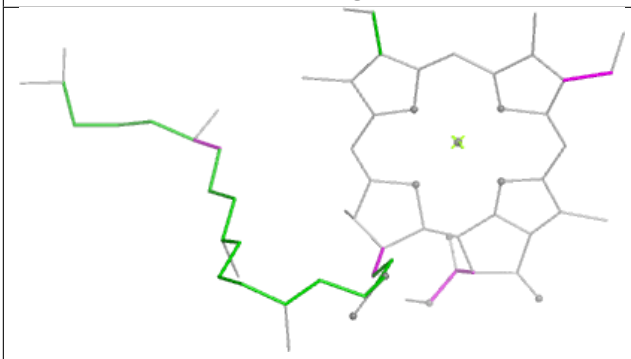
Ligand CLA D 402



Bond lengths



Bond angles

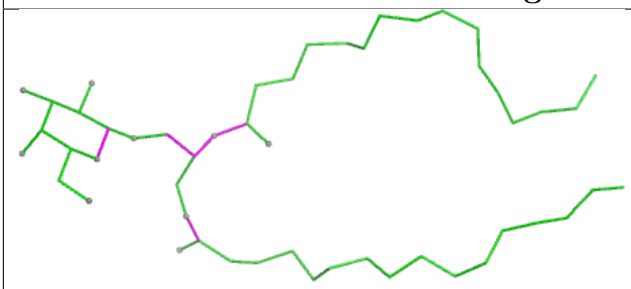


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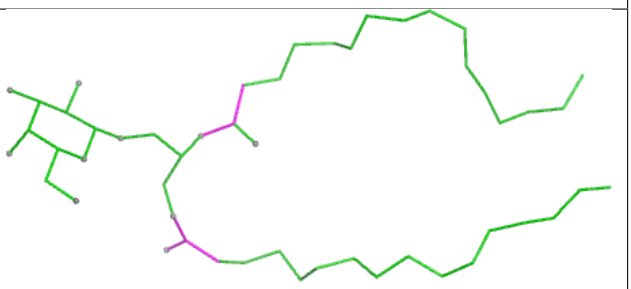


Rings

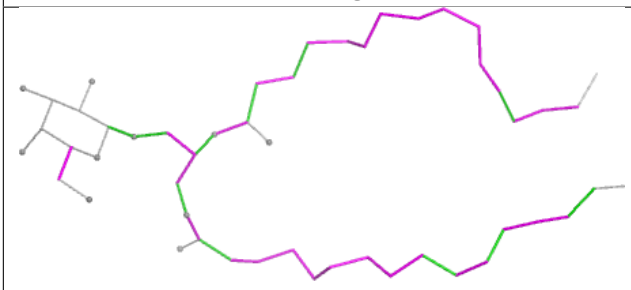
Ligand LMG a 613



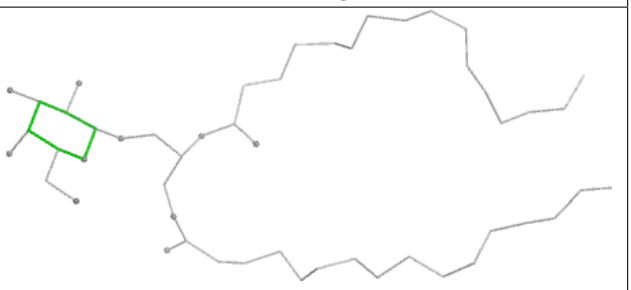
Bond lengths



Bond angles

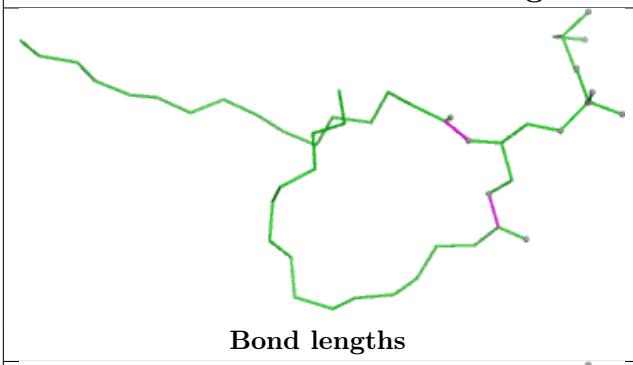


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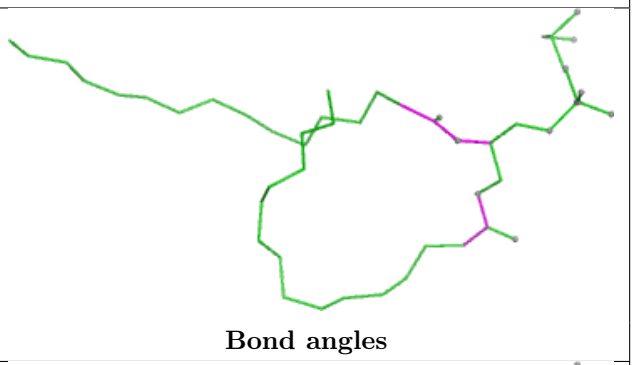


Rings

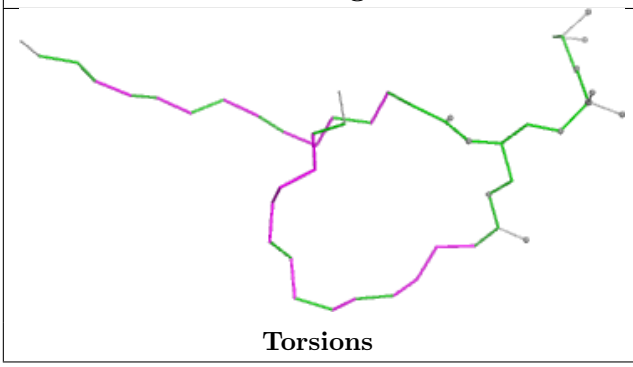
Ligand LHG d 406



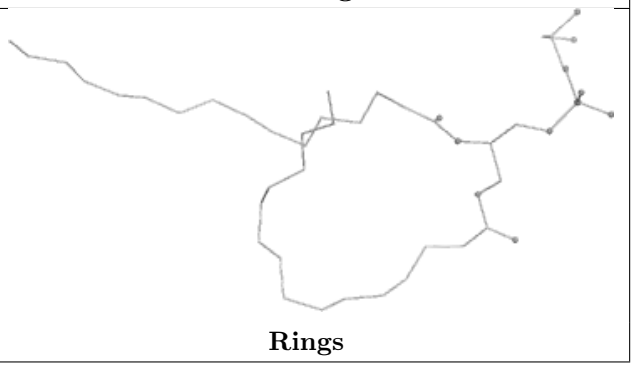
Bond lengths



Bond angles

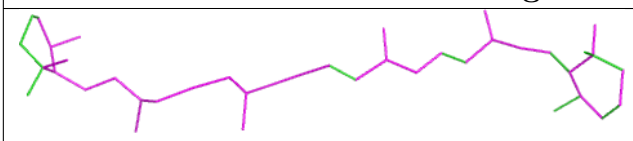


Torsions

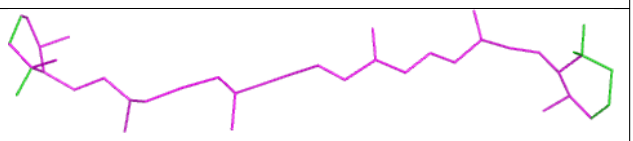


Rings

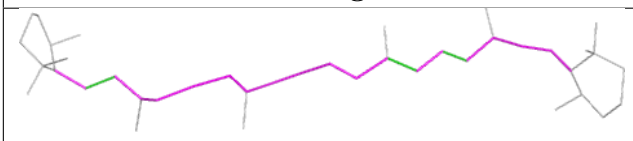
Ligand BCR B 619



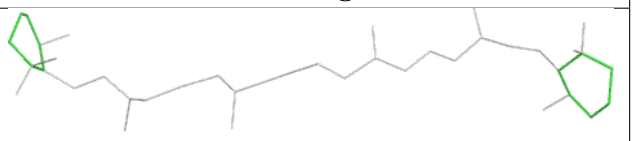
Bond lengths



Bond angles

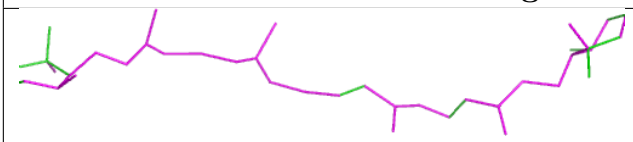


Torsions



Rings

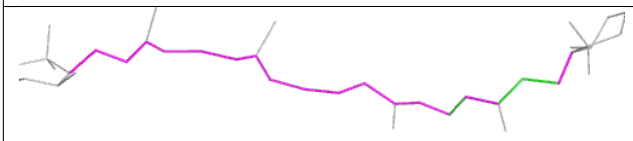
Ligand BCR H 101



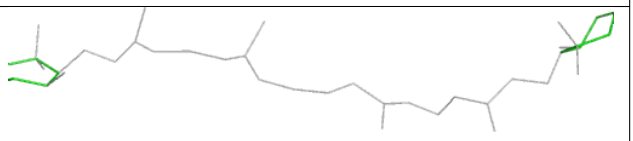
Bond lengths



Bond angles

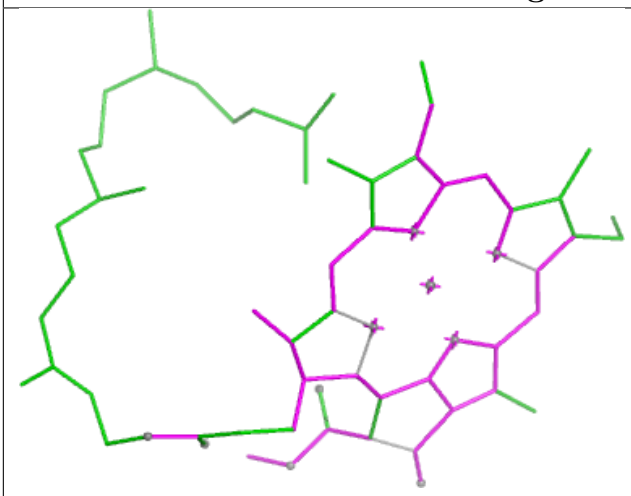


Torsions

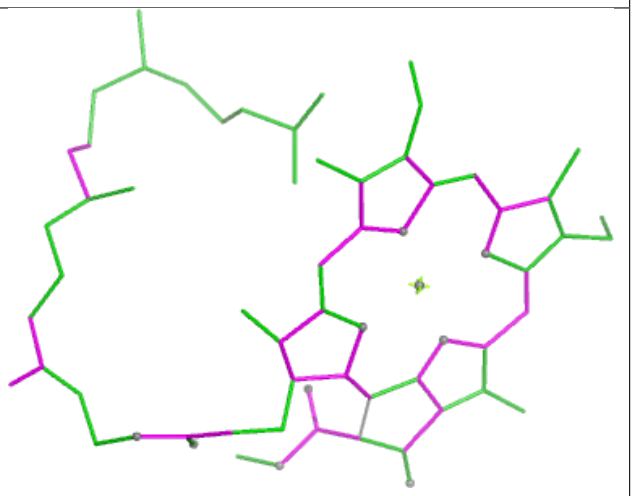


Rings

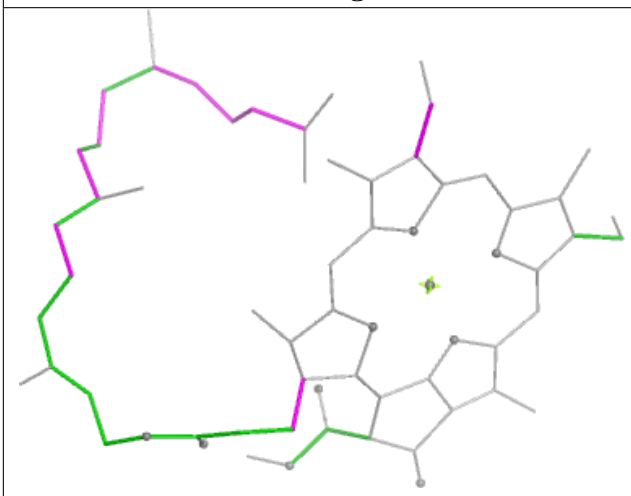
Ligand CLA b 617



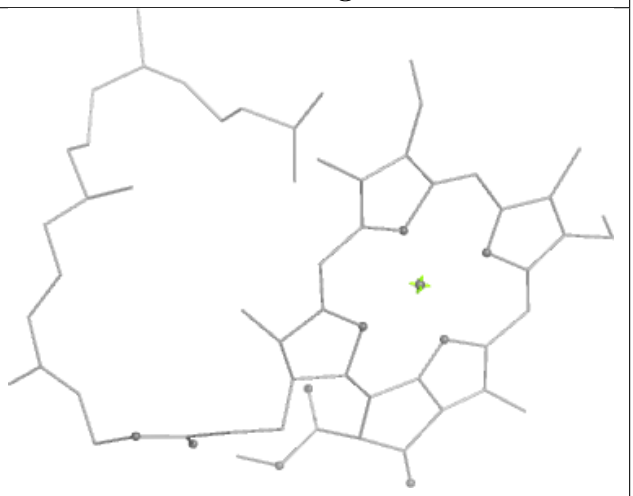
Bond lengths



Bond angles

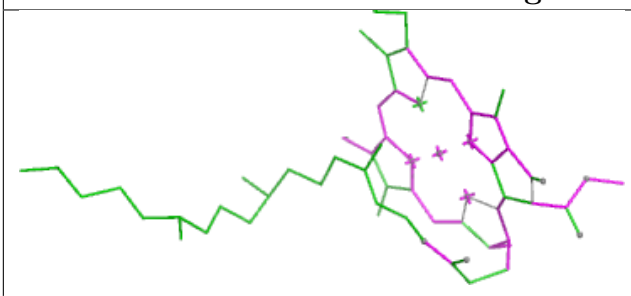


Torsions

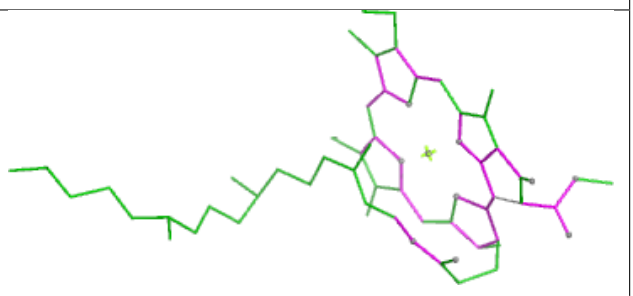


Rings

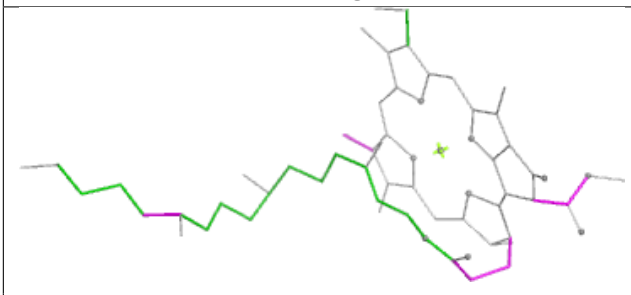
Ligand CLA C 505



Bond lengths



Bond angles

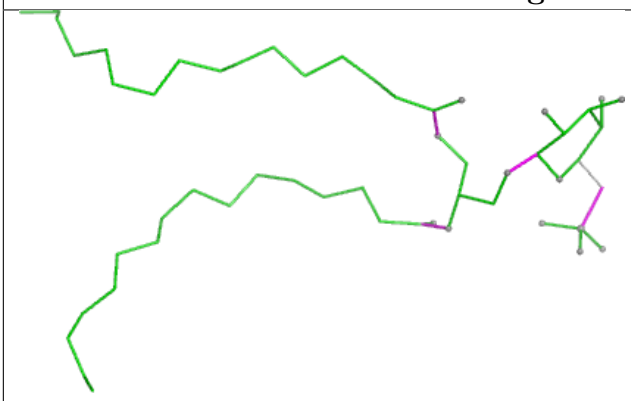


Torsions

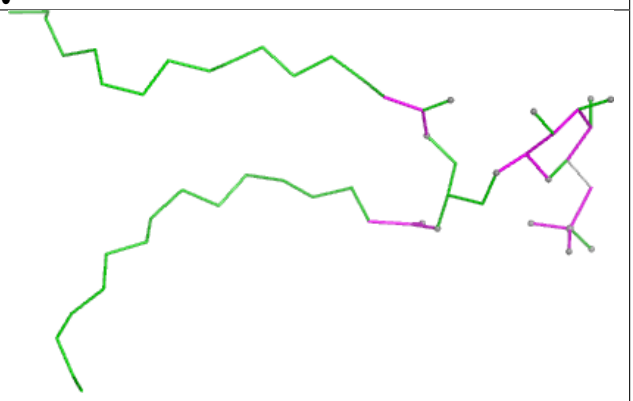


Rings

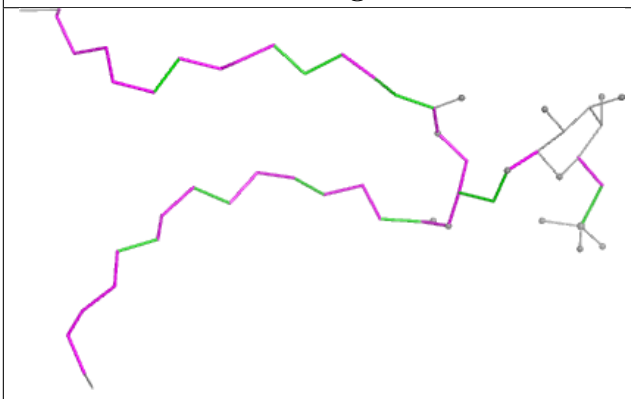
Ligand SQD b 601



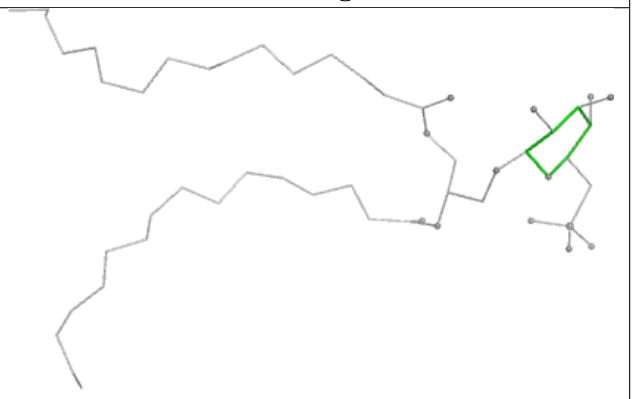
Bond lengths



Bond angles

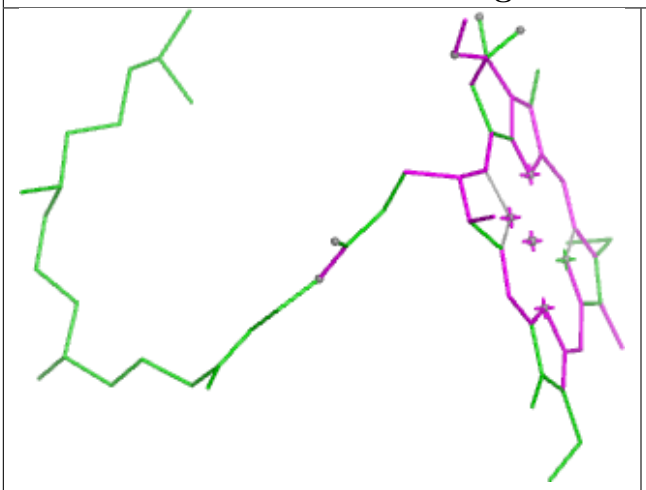


Torsions

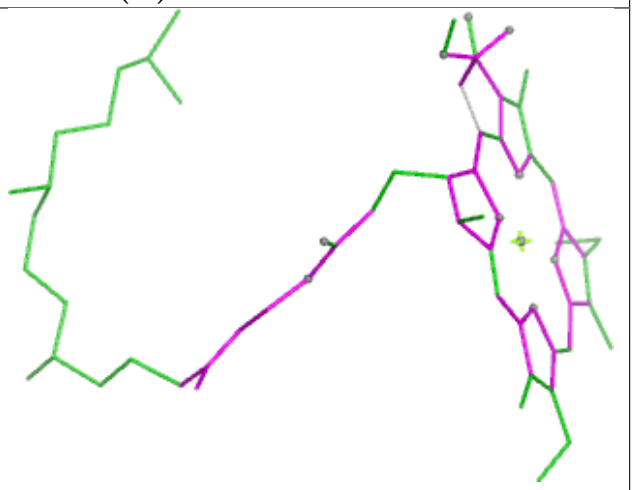


Rings

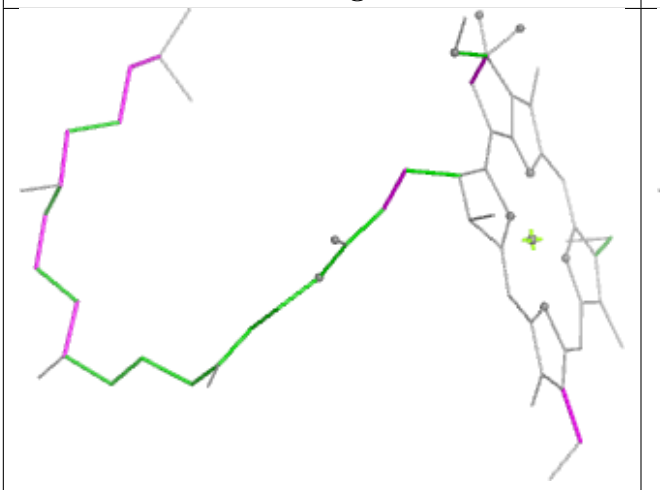
Ligand CLA b 608 (B)



Bond lengths



Bond angles

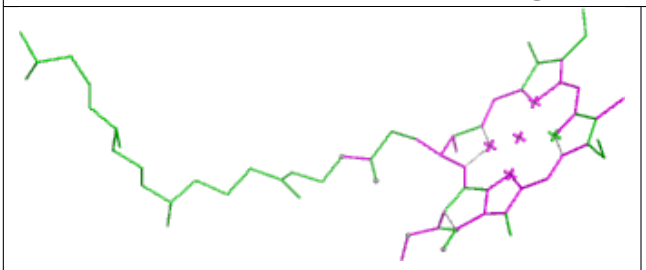


Torsions

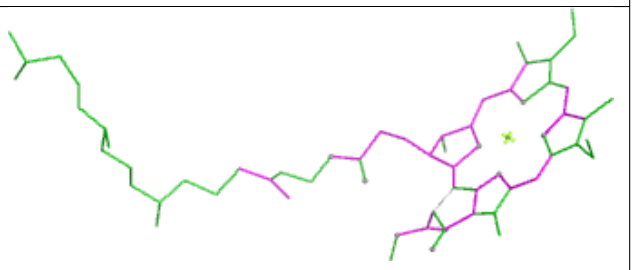


Rings

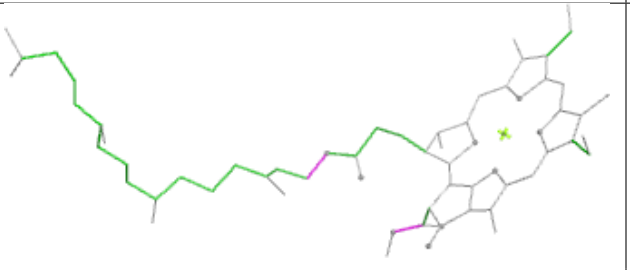
Ligand CLA a 606



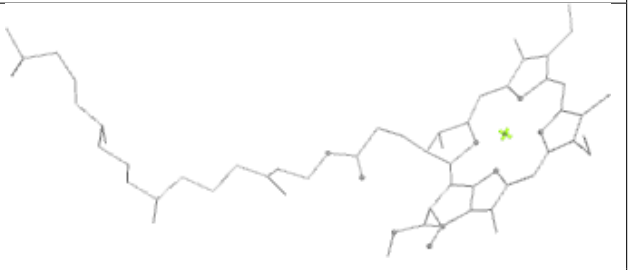
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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, 95^{th} 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	334/334 (100%)	1.45	69 (20%)	2 3	39, 63, 84, 93	4 (1%)
1	a	334/334 (100%)	1.74	110 (32%)	1 1	52, 84, 104, 114	4 (1%)
2	B	504/504 (100%)	1.29	96 (19%)	3 3	41, 68, 89, 111	10 (1%)
2	b	504/504 (100%)	1.73	160 (31%)	1 1	53, 88, 110, 131	10 (1%)
3	C	451/451 (100%)	1.31	89 (19%)	3 3	43, 72, 84, 97	5 (1%)
3	c	451/451 (100%)	1.74	154 (34%)	1 1	57, 92, 105, 118	5 (1%)
4	D	342/342 (100%)	1.32	71 (20%)	2 3	57, 64, 80, 102	0
4	d	342/342 (100%)	1.72	111 (32%)	1 1	78, 85, 101, 123	0
5	E	81/81 (100%)	1.53	20 (24%)	2 2	47, 80, 98, 104	2 (2%)
5	e	81/81 (100%)	1.93	37 (45%)	0 1	61, 101, 119, 125	2 (2%)
6	F	34/34 (100%)	1.39	6 (17%)	4 4	68, 74, 99, 102	0
6	f	34/34 (100%)	1.62	11 (32%)	1 1	89, 95, 120, 122	0
7	H	65/65 (100%)	1.43	16 (24%)	2 2	43, 74, 81, 99	2 (3%)
7	h	65/65 (100%)	1.99	25 (38%)	1 1	55, 95, 101, 120	2 (3%)
8	I	38/38 (100%)	1.76	13 (34%)	1 1	36, 74, 105, 109	1 (2%)
8	i	38/38 (100%)	2.13	16 (42%)	0 1	45, 95, 126, 130	1 (2%)
9	J	38/38 (100%)	1.65	9 (23%)	2 2	66, 78, 109, 112	0
9	j	38/38 (100%)	1.83	14 (36%)	1 1	87, 99, 129, 133	0
10	K	37/37 (100%)	1.06	3 (8%)	18 12	74, 79, 86, 88	0
10	k	37/37 (100%)	1.87	11 (29%)	1 1	94, 100, 107, 108	0
11	L	37/37 (100%)	1.34	8 (21%)	2 3	37, 62, 90, 99	1 (2%)
11	l	37/37 (100%)	1.76	12 (32%)	1 1	49, 83, 111, 120	1 (2%)
12	M	34/34 (100%)	1.66	10 (29%)	1 1	39, 64, 77, 93	1 (2%)
12	m	34/34 (100%)	2.36	12 (35%)	1 1	51, 84, 98, 114	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/243 (100%)	1.42	56 (23%) 2 2	40, 73, 95, 111	4 (1%)
13	o	243/243 (100%)	1.98	95 (39%) 1 1	53, 94, 116, 132	4 (1%)
14	T	30/30 (100%)	1.08	4 (13%) 7 6	32, 64, 85, 93	2 (6%)
14	t	30/30 (100%)	1.72	7 (23%) 2 2	43, 84, 105, 114	2 (6%)
15	U	97/97 (100%)	1.17	15 (15%) 5 5	64, 71, 89, 90	0
15	u	97/97 (100%)	1.64	30 (30%) 1 1	84, 92, 110, 111	0
16	V	137/137 (100%)	1.24	28 (20%) 3 3	39, 69, 80, 88	1 (0%)
16	v	137/137 (100%)	1.53	36 (26%) 1 2	51, 89, 101, 109	1 (0%)
17	Y	29/29 (100%)	1.43	7 (24%) 2 2	82, 89, 115, 118	0
17	y	29/29 (100%)	1.95	11 (37%) 1 1	103, 110, 136, 138	0
18	X	39/39 (100%)	1.32	6 (15%) 5 5	48, 80, 107, 108	1 (2%)
18	x	39/39 (100%)	1.71	11 (28%) 1 1	61, 101, 127, 129	1 (2%)
19	Z	62/62 (100%)	1.50	18 (29%) 1 1	80, 89, 109, 112	0
19	z	62/62 (100%)	2.04	29 (46%) 0 1	101, 110, 129, 133	0
All	All	5264/5264 (100%)	1.57	1436 (27%) 1 2	32, 83, 107, 138	68 (1%)

All (1436) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	11	GLU	12.1
12	m	5	GLN	11.3
8	i	38	GLU	10.2
2	b	485	GLU	10.0
9	j	3	SER	8.4
9	J	4	GLU	8.2
2	b	492	GLU	8.1
13	O	207	ARG	8.1
3	c	23	ALA	7.9
12	M	5	GLN	7.8
2	B	505	ARG	7.7
12	m	33	GLN	7.7
6	f	12	SER	7.6
13	o	55	GLU	7.6
18	x	40	SER	7.4
11	l	1	MET	7.3
3	c	201	ASN	7.3
1	A	13	LEU	7.2

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Mol	Chain	Res	Type	RSRZ
2	b	121	GLU	7.2
3	C	454	GLY	7.1
12	M	33	GLN	7.0
14	t	28	ARG	6.9
13	o	163	GLY	6.9
3	c	183	GLY	6.9
1	a	296	ASN	6.9
12	m	2	GLU	6.8
11	l	2	GLU	6.5
4	d	98	GLN	6.5
19	Z	35	ARG	6.4
3	c	135	ARG	6.3
15	u	101	GLY	6.3
7	H	2	ALA	6.3
4	D	11	GLU	6.2
9	j	7	ARG	6.2
3	c	293	ASN	6.2
3	c	44	ASN	6.2
10	k	46	ARG	6.2
9	J	3	SER	6.1
2	b	505	ARG	6.1
13	o	57	LYS	6.1
3	C	135	ARG	6.0
1	a	138	GLY	6.0
7	h	63[A]	LYS	5.9
12	m	30	GLU	5.9
3	C	266	TRP	5.9
2	b	83	GLU	5.9
3	c	153	ASP	5.9
13	o	62	GLU	5.7
13	o	98	GLU	5.7
10	k	10	LYS	5.7
13	o	64	GLU	5.7
7	h	26	GLY	5.5
2	b	387	GLU	5.5
18	x	38	GLN	5.5
17	y	42	ARG	5.5
6	F	12	SER	5.5
1	a	12	ASN	5.4
12	M	34	LYS	5.4
5	e	82	GLN	5.4
18	X	38	GLN	5.4

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Mol	Chain	Res	Type	RSRZ
11	L	2	GLU	5.4
7	h	66	GLY	5.4
1	A	19	ASN	5.3
19	z	2	THR	5.3
5	E	60	GLN	5.3
8	I	34	ARG	5.3
13	o	60	ARG	5.3
4	d	217	THR	5.3
15	u	70	ARG	5.2
3	C	267	SER	5.2
4	D	251	ARG	5.2
2	B	497	GLN	5.1
1	A	170	ASP	5.1
19	Z	34	ASP	5.1
13	O	163	GLY	5.1
2	b	130[A]	GLU	5.1
3	c	262	ARG	5.1
3	c	184	GLY	5.0
7	H	26	GLY	5.0
7	H	65	LEU	5.0
4	D	172	SER	5.0
5	e	54[A]	SER	5.0
3	c	338	GLY	4.9
1	a	337	HIS	4.9
8	i	27	ASP	4.9
16	v	77	LYS	4.9
19	z	30	PRO	4.9
2	b	124	ARG	4.9
17	y	41	VAL	4.9
4	d	141	TYR	4.9
3	C	417	VAL	4.8
5	E	12	ASP	4.8
2	b	490	GLN	4.8
13	O	64	GLU	4.8
2	b	443	PHE	4.8
12	m	32	GLN	4.8
3	C	201	ASN	4.8
2	b	70	GLY	4.8
1	A	242	GLU	4.8
18	x	39	ARG	4.7
4	D	227	GLU	4.7
16	v	6	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
10	K	10	LYS	4.7
13	o	4	THR	4.7
2	B	14	ASN	4.7
3	c	129	GLY	4.7
3	c	200	THR	4.7
3	c	128	GLY	4.7
1	A	266	ASN	4.7
17	y	19	ILE	4.7
5	e	61	ARG	4.6
4	d	318	ASN	4.6
1	a	229	GLU	4.6
2	b	226	TYR	4.6
16	V	34	GLN	4.6
13	o	161	GLY	4.6
3	C	23	ALA	4.6
3	c	458	GLY	4.6
13	o	222	ASP	4.6
1	a	19	ASN	4.6
1	a	266	ASN	4.6
12	m	31	SER	4.6
13	o	173	ALA	4.6
13	o	58	ASN	4.6
2	B	259	GLY	4.6
13	o	56	PRO	4.6
1	a	139	MET	4.6
13	o	54	GLU	4.5
1	a	105	TRP	4.5
2	b	322	GLY	4.5
5	e	6	GLY	4.5
19	z	3	ILE	4.5
8	i	35	LYS	4.5
4	d	234	ALA	4.5
4	d	332	GLN	4.5
2	b	129	GLY	4.5
3	C	131	TYR	4.5
2	B	387	GLU	4.5
13	O	57	LYS	4.5
11	l	7	ARG	4.5
2	B	328	GLY	4.4
1	A	243	GLU	4.4
2	B	495	PHE	4.4
2	b	167	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
2	b	224	ARG	4.4
2	b	302	TRP	4.4
15	u	37	GLN	4.4
3	c	74	HIS	4.4
5	e	41	GLY	4.4
9	J	5	GLY	4.4
1	A	191	ASN	4.4
19	Z	27	TYR	4.4
4	d	12	ARG	4.4
2	B	188	ASP	4.4
1	a	262	TYR	4.3
4	d	337	GLU	4.3
1	A	12	ASN	4.3
3	C	145[A]	SER	4.3
13	O	59	LYS	4.3
3	c	159	THR	4.3
1	a	243	GLU	4.3
7	h	57	GLY	4.3
3	c	53	HIS	4.3
2	B	485	GLU	4.3
8	i	2	GLU	4.3
1	a	140	ARG	4.3
6	F	44	GLN	4.2
2	B	127	ARG	4.2
14	T	28	ARG	4.2
3	c	102	GLY	4.2
2	b	476	ARG	4.2
13	o	207	ARG	4.2
4	D	71	CYS	4.2
4	d	295	SER	4.2
8	I	25	SER	4.2
2	b	87	ASP	4.2
11	l	4	ASN	4.2
19	z	34	ASP	4.2
13	o	84	GLU	4.2
9	j	4	GLU	4.2
2	B	393	GLU	4.2
2	b	497	GLN	4.2
3	c	302	TYR	4.2
16	V	6	GLU	4.2
1	a	221[A]	SER	4.1
3	C	451	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	b	171	PRO	4.1
3	c	292	PHE	4.1
11	L	1	MET	4.1
3	c	24	THR	4.1
13	o	39	ARG	4.1
1	a	302	PHE	4.1
10	k	43	VAL	4.1
13	o	139	SER	4.1
1	a	11	ALA	4.1
2	b	493	TRP	4.1
5	e	77	GLU	4.1
8	I	2	GLU	4.1
4	d	174	GLY	4.1
4	D	95	PRO	4.1
11	l	3	PRO	4.1
2	b	268	PHE	4.0
2	b	489	GLU	4.0
13	O	55	GLU	4.0
15	u	77	GLU	4.0
16	v	85	GLU	4.0
7	H	66	GLY	4.0
7	h	65	LEU	4.0
4	D	19	ASP	4.0
13	o	25	THR	4.0
13	o	132	ASN	4.0
5	E	18	ARG	4.0
7	h	4	ARG	4.0
4	d	54	PHE	4.0
4	d	71	CYS	4.0
7	h	2	ALA	4.0
13	O	29	ALA	4.0
13	o	27	ARG	4.0
1	a	236	GLY	3.9
1	A	296	ASN	3.9
3	c	163	PHE	3.9
3	c	194	GLY	3.9
5	e	59	GLU	3.9
16	v	90	GLU	3.9
2	b	386	ALA	3.9
4	d	27	PHE	3.9
4	d	172	SER	3.9
15	U	15	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
13	O	241	ALA	3.9
15	u	102	LEU	3.9
13	O	74[A]	GLU	3.9
5	e	84	LYS	3.9
7	H	63[A]	LYS	3.9
5	e	83	LEU	3.9
7	h	15	ASN	3.9
9	J	7	ARG	3.8
8	I	28	PRO	3.8
1	a	90	GLY	3.8
1	a	230	THR	3.8
3	c	297	TYR	3.8
8	I	38	GLU	3.8
1	A	61	ASP	3.8
2	b	59	GLY	3.8
3	c	261	ARG	3.8
1	a	190	HIS	3.8
3	c	342	MET	3.8
2	b	435[A]	GLU	3.8
3	c	473	ASP	3.8
15	u	8	GLU	3.8
2	b	218	LEU	3.8
3	c	373	ASN	3.8
13	o	155	ASN	3.8
2	B	357	ARG	3.8
17	y	43	ARG	3.8
19	z	35	ARG	3.8
2	B	134	ASP	3.8
4	D	131	GLU	3.8
13	o	86	LYS	3.8
5	e	18	ARG	3.8
13	o	189	ARG	3.8
2	b	330	MET	3.8
1	a	170	ASP	3.8
2	b	190	PHE	3.7
2	b	405[A]	GLU	3.7
8	I	32	PRO	3.7
16	v	118	HIS	3.7
2	b	137	LYS	3.7
2	b	373	LYS	3.7
13	o	53	LYS	3.7
14	t	30	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	492	GLU	3.7
9	j	9	PRO	3.7
4	d	323	GLU	3.7
15	u	24	LYS	3.7
3	c	25	ASN	3.7
3	c	192	GLY	3.7
9	j	6	GLY	3.7
13	o	184	ARG	3.7
4	D	255	GLN	3.7
13	o	202	ALA	3.7
3	c	347	GLY	3.7
2	b	144	PHE	3.7
3	c	456	GLU	3.7
3	C	200	THR	3.6
13	o	21	THR	3.6
12	m	1	MET	3.6
19	z	4	LEU	3.6
3	c	417	VAL	3.6
4	d	233	ARG	3.6
16	V	31	ARG	3.6
13	o	69	LYS	3.6
2	B	282	GLN	3.6
3	c	34	ALA	3.6
4	d	64	ALA	3.6
4	d	297	ASP	3.6
13	o	191	SER	3.6
1	A	171	GLY	3.6
3	c	85	GLY	3.6
12	m	34	LYS	3.6
3	c	415	ASN	3.6
1	a	235	TYR	3.6
2	b	494	GLY	3.6
17	Y	19	ILE	3.6
2	B	226	TYR	3.6
5	E	55	TYR	3.6
13	o	181	GLU	3.6
8	I	24	LEU	3.6
2	b	232	GLY	3.6
13	O	213	GLY	3.6
5	e	60	GLN	3.5
13	o	59	LYS	3.5
1	a	242	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
13	o	97	GLU	3.5
13	o	151	TYR	3.5
15	U	86	GLU	3.5
2	b	333	GLY	3.5
1	A	304	HIS	3.5
3	C	229	ASN	3.5
7	h	20	LYS	3.5
1	A	262	TYR	3.5
3	c	186	TYR	3.5
4	D	59	TYR	3.5
19	z	26	ALA	3.5
4	d	206	GLY	3.5
1	A	108	ASN	3.5
16	v	24	LYS	3.5
4	d	186	GLN	3.5
3	c	193	GLY	3.5
4	d	237	PRO	3.5
3	C	70	PHE	3.5
2	b	111	ALA	3.5
2	b	279	TYR	3.5
7	H	64	ALA	3.5
2	B	2	GLY	3.5
2	B	396	GLY	3.5
4	d	338	ASN	3.5
1	A	17	PHE	3.5
3	C	29	GLU	3.5
2	b	480	SER	3.5
5	e	74	GLN	3.5
11	l	14	ARG	3.5
3	C	44	ASN	3.5
4	d	336	HIS	3.5
3	c	269	GLU	3.4
1	a	109	GLY	3.4
2	b	169	SER	3.4
13	O	209	GLY	3.4
2	B	7	ARG	3.4
3	c	357	ARG	3.4
1	a	335	ASN	3.4
4	d	223	PHE	3.4
17	Y	45	ASN	3.4
7	H	18	TYR	3.4
16	V	75	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
13	o	114	GLU	3.4
1	A	74	GLY	3.4
1	a	234	ASN	3.4
12	M	4	ASN	3.4
16	v	106	ASN	3.4
16	v	60	ALA	3.4
3	c	26	ARG	3.4
7	H	56	ASP	3.4
15	U	37	GLN	3.4
2	b	77	GLY	3.4
4	d	226	GLY	3.4
4	d	258	GLY	3.4
9	J	6	GLY	3.4
13	o	190	PHE	3.4
13	o	244	GLU	3.4
16	v	132	GLY	3.4
3	c	188	THR	3.4
3	c	294	ASN	3.4
14	t	22	PHE	3.4
1	A	240	GLY	3.3
2	b	350	GLU	3.3
13	o	46	GLN	3.3
13	o	61	GLN	3.3
4	D	252	PHE	3.3
7	h	51	SER	3.3
13	O	203	LYS	3.3
2	b	500	GLY	3.3
5	E	84	LYS	3.3
13	o	65	PHE	3.3
16	V	24	LYS	3.3
1	a	222	SER	3.3
3	c	155	ASN	3.3
5	E	61	ARG	3.3
2	b	441	GLY	3.3
2	B	83	GLU	3.3
1	a	61	ASP	3.3
2	b	212	ALA	3.3
1	a	320	ILE	3.3
16	v	100	ILE	3.3
2	b	193	TYR	3.3
5	e	55	TYR	3.3
3	C	300	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
19	z	1	MET	3.3
2	b	349	LYS	3.3
1	a	141	PRO	3.3
1	a	294	ALA	3.3
1	a	314	ILE	3.3
16	v	66	ARG	3.3
4	d	65	SER	3.3
1	A	166	GLY	3.3
13	O	237	GLY	3.3
13	o	112	GLY	3.3
2	B	114	HIS	3.3
3	c	359	TRP	3.3
7	h	21	VAL	3.3
13	O	61	GLN	3.3
16	v	34	GLN	3.3
17	Y	21	GLN	3.3
9	j	38	SER	3.2
13	o	34	SER	3.2
2	b	14	ASN	3.2
1	a	15	GLU	3.2
5	e	7	GLU	3.2
13	o	179	GLU	3.2
5	e	42	LEU	3.2
19	z	29	SER	3.2
3	c	126	GLY	3.2
18	X	2	THR	3.2
2	b	40	TYR	3.2
2	b	123	PHE	3.2
1	a	304	HIS	3.2
16	v	1	ALA	3.2
1	A	246	TYR	3.2
13	O	54	GLU	3.2
19	Z	4	LEU	3.2
4	D	70	GLY	3.2
2	b	363	PHE	3.2
3	C	87	ILE	3.2
13	o	186	ASN	3.2
1	A	257	ARG	3.2
3	C	271	TYR	3.2
3	c	138	GLU	3.2
5	E	17	VAL	3.2
10	k	42	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
13	O	139	SER	3.2
4	D	189	HIS	3.2
19	z	57	LEU	3.2
2	B	426	PHE	3.2
4	d	31	GLY	3.2
5	e	81	GLU	3.2
13	o	18	LYS	3.2
4	D	27	PHE	3.1
6	F	16	PHE	3.1
2	b	262	THR	3.1
17	y	45	ASN	3.1
3	c	215	LYS	3.1
16	v	110	LYS	3.1
2	B	266	GLU	3.1
4	d	25	ASP	3.1
7	h	64	ALA	3.1
19	z	8	ALA	3.1
5	E	9	PRO	3.1
1	A	182	PHE	3.1
3	C	134	ILE	3.1
3	c	132	HIS	3.1
8	i	30	ARG	3.1
13	O	82	GLN	3.1
3	C	418	ASN	3.1
16	V	26	TYR	3.1
19	Z	62	VAL	3.1
1	a	103	ASP	3.1
19	Z	32	ASP	3.1
2	b	425	ILE	3.1
4	D	24	ARG	3.1
15	u	76	ARG	3.1
13	o	130	GLN	3.1
17	y	21	GLN	3.1
1	a	317	TRP	3.1
2	B	493	TRP	3.1
1	A	11	ALA	3.1
3	C	142	GLU	3.1
2	b	46	ASP	3.1
3	c	288	CYS	3.1
13	o	8	ASP	3.1
19	z	14	ILE	3.1
2	b	264	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	73	PHE	3.1
1	a	74	GLY	3.1
19	Z	31	GLN	3.1
13	o	35	SER	3.1
2	b	64	PRO	3.1
5	e	12	ASP	3.1
8	i	34	ARG	3.1
10	k	19	ASP	3.1
3	c	398	HIS	3.1
1	a	306	VAL	3.1
4	D	292	ASN	3.1
2	B	130[A]	GLU	3.1
16	v	15	GLU	3.1
16	v	70	GLU	3.1
2	b	422	ARG	3.1
3	c	180	MET	3.1
19	z	52	LEU	3.1
1	A	190	HIS	3.1
2	b	282	GLN	3.0
1	A	222	SER	3.0
4	d	165	SER	3.0
13	o	221	SER	3.0
16	V	121	VAL	3.0
3	c	411	ALA	3.0
2	b	496	TYR	3.0
4	d	142	ASN	3.0
16	v	17	LYS	3.0
4	d	219	GLU	3.0
4	d	304	ARG	3.0
4	D	309	PRO	3.0
2	B	70	GLY	3.0
7	H	57	GLY	3.0
13	O	4	THR	3.0
4	d	87	HIS	3.0
1	A	87	ASN	3.0
1	a	191	ASN	3.0
2	b	18	ARG	3.0
13	O	60	ARG	3.0
4	d	242	GLU	3.0
6	F	14	PRO	3.0
1	A	256	GLY	3.0
1	A	299	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	c	360	ASP	3.0
19	Z	2	THR	3.0
1	a	257	ARG	3.0
2	B	476	ARG	3.0
1	a	254	TYR	3.0
7	h	18	TYR	3.0
1	a	65	GLU	3.0
8	i	33	LYS	3.0
1	a	13	LEU	3.0
3	C	263	ALA	3.0
3	C	26	ARG	3.0
1	a	247	ASN	3.0
3	C	186	TYR	3.0
4	d	59	TYR	3.0
4	d	350	ASN	3.0
13	o	200	ASN	3.0
3	C	389	GLU	3.0
4	d	312	GLU	3.0
14	t	2	GLU	3.0
4	D	140	PRO	3.0
4	d	171	PRO	3.0
8	i	28	PRO	3.0
2	B	341	LYS	3.0
14	t	29	ILE	3.0
10	k	44	GLY	3.0
2	b	483	ASP	3.0
3	c	107	ASP	3.0
3	C	151	TRP	3.0
13	o	178	LYS	3.0
17	y	25	ILE	3.0
3	C	268	GLY	3.0
2	b	84	THR	3.0
15	u	39	ARG	3.0
1	a	319	ASP	3.0
1	a	108	ASN	2.9
13	o	88	ASN	2.9
5	e	52	PRO	2.9
16	V	15	GLU	2.9
16	v	57	GLU	2.9
3	c	63	TRP	2.9
4	D	328	TRP	2.9
3	C	146	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	c	109	PHE	2.9
4	D	56	THR	2.9
13	o	166	SER	2.9
4	d	20	ASP	2.9
8	i	36	ASP	2.9
4	d	184	PHE	2.9
1	A	312	ASN	2.9
1	a	339	PHE	2.9
2	B	183	PRO	2.9
3	c	127	PHE	2.9
3	c	221	GLU	2.9
4	D	69	GLU	2.9
5	e	10	PHE	2.9
3	c	449	ARG	2.9
7	H	3	ARG	2.9
6	f	44	GLN	2.9
3	C	52	ALA	2.9
2	B	325	PHE	2.9
2	b	93	PHE	2.9
4	D	314	PHE	2.9
2	b	191	ASN	2.9
13	O	62	GLU	2.9
1	a	16	ARG	2.9
13	O	27	ARG	2.9
2	B	499	VAL	2.9
4	D	295	SER	2.9
13	o	11	VAL	2.9
13	O	26	ALA	2.9
1	A	125	CYS	2.9
2	b	267	LEU	2.9
1	a	303	ASN	2.9
2	B	488	PRO	2.9
3	c	149	TYR	2.9
9	J	9	PRO	2.9
11	L	5	PRO	2.9
2	b	307	GLU	2.9
4	D	241	GLU	2.9
4	d	307	GLU	2.9
16	v	31	ARG	2.9
1	A	86	SER	2.9
1	a	240	GLY	2.9
3	C	215	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	6	GLY	2.9
18	X	36	LYS	2.9
2	B	167	TRP	2.9
2	b	503	THR	2.9
1	A	344	ALA	2.9
1	A	16	ARG	2.9
19	z	27	TYR	2.9
15	u	63	ASN	2.9
3	C	347	GLY	2.8
18	X	33	GLN	2.8
2	b	5	TRP	2.8
13	O	127	ALA	2.8
3	C	149	TYR	2.8
4	d	42	TYR	2.8
1	a	241	GLN	2.8
3	c	306	GLY	2.8
13	o	28	GLY	2.8
15	u	18	GLY	2.8
16	v	84	GLY	2.8
4	D	234	ALA	2.8
3	C	423	ARG	2.8
3	c	340	TYR	2.8
15	u	54	PRO	2.8
2	B	121	GLU	2.8
3	c	353	GLY	2.8
4	d	40	CYS	2.8
16	V	86	GLN	2.8
1	a	233	ALA	2.8
8	I	36	ASP	2.8
1	a	274	PHE	2.8
2	b	392	PHE	2.8
4	d	314	PHE	2.8
2	b	357	ARG	2.8
13	o	172	ILE	2.8
3	c	296	VAL	2.8
1	a	199	GLN	2.8
2	b	323	GLY	2.8
4	d	86	GLY	2.8
12	m	4	ASN	2.8
1	a	212	CYS	2.8
1	a	293	MET	2.8
2	B	443	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	396	MET	2.8
13	o	203	LYS	2.8
8	I	30	ARG	2.8
13	o	152	ARG	2.8
2	b	12	LEU	2.8
2	b	52	LEU	2.8
3	c	253	LEU	2.8
4	D	135	LEU	2.8
3	C	25	ASN	2.8
3	c	29	GLU	2.8
19	Z	38	GLN	2.8
3	C	342	MET	2.8
2	B	227	LYS	2.8
11	L	7	ARG	2.8
3	c	46	SER	2.8
2	B	117	TYR	2.8
1	a	261	GLN	2.8
3	c	229	ASN	2.8
3	c	300	GLU	2.8
4	d	203	GLY	2.8
4	D	338	ASN	2.8
13	o	41	ALA	2.8
1	a	269	ARG	2.7
16	V	55[A]	ARG	2.7
1	A	25	ASP	2.7
4	d	218	VAL	2.7
3	c	381	LYS	2.7
11	l	8	GLN	2.7
15	u	47	LYS	2.7
3	c	409	GLY	2.7
1	a	344	ALA	2.7
5	E	77	GLU	2.7
13	O	210	GLU	2.7
2	B	255	THR	2.7
7	h	12[A]	ARG	2.7
3	c	266	TRP	2.7
13	o	135	SER	2.7
2	B	93	PHE	2.7
2	B	432	PHE	2.7
2	b	139	PHE	2.7
4	d	246	MET	2.7
17	y	27	MET	2.7

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Mol	Chain	Res	Type	RSRZ
19	z	60	PHE	2.7
4	d	334	GLN	2.7
13	O	130	GLN	2.7
15	u	38	TYR	2.7
1	a	226	GLU	2.7
3	c	69	LEU	2.7
7	h	14	LEU	2.7
13	o	164	LEU	2.7
1	a	198	HIS	2.7
2	b	341	LYS	2.7
3	C	46	SER	2.7
13	O	242	SER	2.7
13	o	24	ASP	2.7
4	d	153	PHE	2.7
8	i	32	PRO	2.7
2	B	320	ALA	2.7
3	c	352	GLY	2.7
4	d	224	GLN	2.7
16	V	37	CYS	2.7
2	b	57	ARG	2.7
3	c	343	ARG	2.7
13	o	74[A]	GLU	2.7
4	D	83	ASN	2.7
3	c	468	SER	2.7
13	o	150	SER	2.7
16	v	83	ASP	2.7
2	b	161	LEU	2.7
4	d	309	PRO	2.7
2	b	448	ARG	2.7
3	c	131	TYR	2.7
6	f	13	TYR	2.7
9	j	5	GLY	2.7
3	c	78	GLU	2.7
13	o	49[A]	THR	2.7
15	u	11	ASN	2.7
2	B	8	VAL	2.7
2	B	490	GLN	2.7
2	b	49	ASP	2.7
16	v	74	ASP	2.7
17	Y	42	ARG	2.7
1	a	166	GLY	2.7
2	b	140	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	b	320	ALA	2.7
4	D	244	TYR	2.7
13	o	177	ALA	2.7
2	b	393	GLU	2.7
13	O	97	GLU	2.7
15	U	8	GLU	2.7
16	v	109	GLU	2.7
16	v	124	LYS	2.7
2	b	362	PHE	2.7
16	V	14	SER	2.7
16	v	94	SER	2.7
18	x	37	VAL	2.6
5	e	51	ARG	2.6
10	k	12	PRO	2.6
19	z	24	PRO	2.6
3	c	84	GLN	2.6
2	b	146	ALA	2.6
3	C	326	ALA	2.6
4	d	108	GLY	2.6
9	j	37	GLY	2.6
16	V	43	GLY	2.6
16	v	75	TYR	2.6
3	C	457	LYS	2.6
3	c	231	GLU	2.6
1	A	139	MET	2.6
1	A	293	MET	2.6
3	C	293	ASN	2.6
1	A	197	PHE	2.6
3	c	242	LEU	2.6
1	a	68	SER	2.6
16	v	55[A]	ARG	2.6
1	a	340	PRO	2.6
1	a	100	ALA	2.6
13	O	80	GLN	2.6
3	C	325	GLY	2.6
3	c	151	TRP	2.6
3	c	454	GLY	2.6
2	B	431[A]	GLU	2.6
3	c	462[A]	GLU	2.6
4	D	219	GLU	2.6
3	c	140	LEU	2.6
11	l	6	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
13	O	35	SER	2.6
3	c	390	ARG	2.6
2	B	484	PRO	2.6
3	c	339	LYS	2.6
13	o	194	LYS	2.6
4	D	206	GLY	2.6
4	d	216	ALA	2.6
4	d	56	THR	2.6
13	o	118	LEU	2.6
1	A	98	GLU	2.6
1	A	189	GLU	2.6
4	D	242	GLU	2.6
13	o	145	GLU	2.6
5	E	24	SER	2.6
5	e	24	SER	2.6
2	b	499	VAL	2.6
3	c	167	VAL	2.6
2	b	230	ARG	2.6
2	b	321	LYS	2.6
2	b	50	PRO	2.6
4	D	336	HIS	2.6
5	e	58	GLN	2.6
13	O	196	GLN	2.6
16	V	25	GLN	2.6
4	D	137	GLY	2.6
4	D	228	GLY	2.6
5	E	41	GLY	2.6
19	z	15	LEU	2.6
1	a	197	PHE	2.6
4	d	185	PHE	2.6
6	F	13	TYR	2.6
9	j	33	TYR	2.6
2	b	266	GLU	2.6
2	b	353	GLU	2.6
4	D	16	ASP	2.6
13	O	169	ASP	2.6
13	o	218	GLU	2.6
8	i	25	SER	2.6
13	O	186	ASN	2.6
15	u	28	ASN	2.6
3	c	41	ARG	2.6
10	K	46	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
13	O	18	LYS	2.6
3	c	465	PRO	2.6
1	a	208	GLY	2.6
2	B	6	TYR	2.6
3	c	94	THR	2.6
1	a	333	GLU	2.6
2	b	127	ARG	2.6
3	c	195	ASP	2.6
2	b	194	ASN	2.6
3	C	294	ASN	2.6
4	d	83	ASN	2.6
4	d	139	ARG	2.6
1	A	241	GLN	2.6
11	L	8	GLN	2.6
2	b	295	GLY	2.6
3	c	112	PHE	2.6
8	i	26	GLY	2.6
2	B	203	ILE	2.5
3	c	143	TYR	2.5
13	O	7	TYR	2.5
19	Z	33	TRP	2.5
1	a	86	SER	2.5
2	B	448	ARG	2.5
2	b	300	GLU	2.5
3	c	104	GLU	2.5
3	c	216	SER	2.5
4	d	69	GLU	2.5
4	d	310	GLU	2.5
5	e	11	SER	2.5
1	A	306	VAL	2.5
3	C	155	ASN	2.5
3	C	187	ASP	2.5
2	B	218	LEU	2.5
3	C	411	ALA	2.5
15	u	73	GLN	2.5
1	a	92	HIS	2.5
1	a	228	THR	2.5
8	I	6	ILE	2.5
16	V	82	TYR	2.5
16	v	26	TYR	2.5
16	v	47	LYS	2.5
1	a	142	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
16	V	39	SER	2.5
13	O	58	ASN	2.5
13	o	23	ASP	2.5
2	b	182	ALA	2.5
15	u	40	GLY	2.5
1	A	73	TYR	2.5
1	A	305	SER	2.5
1	a	161	TYR	2.5
3	C	357	ARG	2.5
3	c	212	TYR	2.5
1	A	229	GLU	2.5
1	A	317	TRP	2.5
2	b	168	VAL	2.5
3	c	337	LEU	2.5
3	c	365	TRP	2.5
4	d	241	GLU	2.5
12	M	30	GLU	2.5
6	f	16	PHE	2.5
6	f	42	PHE	2.5
2	B	131	PRO	2.5
1	a	110	GLY	2.5
2	b	82	GLY	2.5
5	e	32	ILE	2.5
15	u	94	GLY	2.5
17	Y	25	ILE	2.5
2	B	286	ARG	2.5
7	h	11	LEU	2.5
12	m	8	LEU	2.5
2	b	491	VAL	2.5
4	d	78	VAL	2.5
3	c	291	TRP	2.5
13	O	180	GLU	2.5
4	D	98	GLN	2.5
4	D	170	ALA	2.5
4	d	239	GLN	2.5
4	d	275	PRO	2.5
4	d	303	ILE	2.5
18	x	3	ILE	2.5
19	Z	6	GLN	2.5
19	z	28	ALA	2.5
19	z	31	GLN	2.5
5	e	28	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	b	2	GLY	2.5
16	V	44	GLY	2.5
1	a	137	LEU	2.5
3	c	68	THR	2.5
8	I	3	THR	2.5
8	i	24	LEU	2.5
2	b	48	SER	2.5
2	b	294	SER	2.5
3	c	421	SER	2.5
2	B	299	GLU	2.5
2	b	299	GLU	2.5
2	b	428	GLU	2.5
1	a	315	ASN	2.5
2	B	418	LYS	2.5
2	b	337	ALA	2.5
3	c	134	ILE	2.5
13	o	147	ASN	2.5
2	b	338	GLN	2.5
2	B	375	GLY	2.5
3	C	222	GLY	2.5
3	c	336	GLY	2.5
3	c	408	GLY	2.5
4	d	99	GLY	2.5
7	h	24	GLY	2.5
10	k	23	ASP	2.5
2	B	503	THR	2.5
7	h	52	THR	2.5
1	a	82	VAL	2.5
13	o	204	VAL	2.5
1	A	107	TYR	2.5
1	a	73	TYR	2.5
3	C	340	TYR	2.5
2	B	26	HIS	2.4
2	B	321	LYS	2.4
2	B	435[A]	GLU	2.4
2	b	389	LYS	2.4
13	O	84	GLU	2.4
15	u	29	ASN	2.4
1	a	150	PRO	2.4
2	b	484	PRO	2.4
1	a	299	GLY	2.4
2	B	322	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	408	GLY	2.4
3	C	371	GLY	2.4
4	D	118	GLY	2.4
2	B	48	SER	2.4
2	b	487	SER	2.4
5	E	49	THR	2.4
1	a	17	PHE	2.4
1	a	135	TYR	2.4
2	b	495	PHE	2.4
1	a	244	GLU	2.4
1	a	290	ILE	2.4
3	C	221	GLU	2.4
3	c	389	GLU	2.4
5	E	81	GLU	2.4
1	a	223	LEU	2.4
2	b	185	TRP	2.4
7	h	62	TRP	2.4
3	c	39	ASN	2.4
4	D	260	ALA	2.4
16	v	36	ALA	2.4
3	C	80	PRO	2.4
2	b	465	GLY	2.4
3	c	220	GLY	2.4
3	c	258	GLY	2.4
3	c	268	GLY	2.4
9	j	35	GLY	2.4
2	b	440	ASP	2.4
8	i	3	THR	2.4
15	U	24	LYS	2.4
16	v	35	TYR	2.4
13	O	114	GLU	2.4
13	o	16	ALA	2.4
17	y	31	ALA	2.4
4	D	263	ASN	2.4
19	Z	1	MET	2.4
3	C	65	GLY	2.4
3	C	336	GLY	2.4
4	d	137	GLY	2.4
1	a	79	THR	2.4
1	a	305	SER	2.4
18	x	36	LYS	2.4
1	A	280	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
17	y	18	VAL	2.4
2	B	477	ASP	2.4
15	u	103	TYR	2.4
4	D	211	CYS	2.4
2	b	114	HIS	2.4
5	e	71	GLU	2.4
7	H	47	GLU	2.4
11	l	11	GLU	2.4
3	c	197	ARG	2.4
2	B	58	GLN	2.4
6	f	39	ALA	2.4
3	c	228	ASN	2.4
4	d	194	ASN	2.4
5	e	20	TRP	2.4
5	e	50	PRO	2.4
11	l	5	PRO	2.4
16	V	13	ASN	2.4
2	B	308	LYS	2.4
15	U	66	GLY	2.4
2	b	278	SER	2.4
2	b	65	PHE	2.4
3	C	24	THR	2.4
3	c	70	PHE	2.4
13	O	208	THR	2.4
2	b	134	ASP	2.4
7	H	49	TYR	2.4
5	e	8	ARG	2.4
1	a	328	MET	2.4
2	b	261	ALA	2.4
2	b	275	TRP	2.4
2	b	374	ASN	2.4
3	C	415	ASN	2.4
3	c	304	PRO	2.4
4	D	258	GLY	2.4
3	c	301	PHE	2.4
4	d	245	SER	2.4
13	o	242	SER	2.4
1	a	50	ILE	2.4
3	c	439	VAL	2.4
13	o	208	THR	2.4
19	z	39	LEU	2.4
3	c	354	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	290	ALA	2.4
19	Z	26	ALA	2.4
2	b	58	GLN	2.3
3	C	98	GLY	2.3
4	d	38	PHE	2.3
5	e	9	PRO	2.3
3	C	344	SER	2.3
4	D	14	TRP	2.3
5	e	31	PHE	2.3
19	Z	55	GLY	2.3
19	z	47	TRP	2.3
5	e	4	THR	2.3
13	o	134	THR	2.3
1	a	136	ARG	2.3
2	B	390	TYR	2.3
3	C	82	TYR	2.3
2	B	119	ASP	2.3
1	A	65	GLU	2.3
1	a	231	GLU	2.3
3	C	83	GLU	2.3
9	j	8	ILE	2.3
11	L	3	PRO	2.3
13	o	220	LEU	2.3
15	U	91	LEU	2.3
16	v	41	HIS	2.3
1	A	181	ASN	2.3
2	B	323	GLY	2.3
3	c	51	GLY	2.3
3	c	226	SER	2.3
1	a	220	THR	2.3
6	f	18	VAL	2.3
18	x	4	THR	2.3
2	b	7	ARG	2.3
1	a	88	ALA	2.3
4	d	240	ALA	2.3
2	b	280	PHE	2.3
3	c	431	PHE	2.3
4	d	298	PHE	2.3
5	e	79	PHE	2.3
9	J	36	LEU	2.3
1	a	177	SER	2.3
2	b	73	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	b	88	PRO	2.3
3	c	136	GLY	2.3
3	c	424	SER	2.3
3	c	463	SER	2.3
4	d	55	VAL	2.3
13	O	96	VAL	2.3
13	O	37	THR	2.3
4	d	264	LYS	2.3
3	C	395	TYR	2.3
12	m	26	TYR	2.3
4	D	168	PHE	2.3
4	d	210	LEU	2.3
19	Z	3	ILE	2.3
4	d	16	ASP	2.3
2	B	126	PRO	2.3
4	d	335	PRO	2.3
13	O	175	PRO	2.3
13	o	206	GLY	2.3
16	v	65	PRO	2.3
19	Z	24	PRO	2.3
3	C	74	HIS	2.3
4	d	61	HIS	2.3
4	d	75	THR	2.3
4	d	190	ASN	2.3
4	d	243	THR	2.3
4	d	292	ASN	2.3
5	E	4	THR	2.3
7	H	15	ASN	2.3
3	c	323	LYS	2.3
19	z	37	LYS	2.3
3	C	230	LEU	2.3
4	d	211	CYS	2.3
2	B	496	TYR	2.3
3	c	37	ALA	2.3
4	d	296	TYR	2.3
10	k	45	PHE	2.3
16	V	1	ALA	2.3
1	a	130	GLN	2.3
4	D	20	ASP	2.3
4	d	175	VAL	2.3
15	u	66	GLY	2.3
19	z	62	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	b	498	LYS	2.3
13	o	188	LYS	2.3
19	Z	37	LYS	2.3
1	A	179	THR	2.3
2	b	53	ASN	2.3
2	b	285	ASN	2.3
2	b	286	ARG	2.3
4	D	80	THR	2.3
13	O	94	THR	2.3
2	b	56	TRP	2.3
3	C	365	TRP	2.3
16	v	27	LEU	2.3
1	a	206	PHE	2.3
1	a	265	PHE	2.3
9	j	22	ILE	2.3
1	A	235	TYR	2.3
2	b	110	ALA	2.3
2	b	204	ALA	2.3
4	D	332	GLN	2.3
13	o	176	GLN	2.3
4	d	227	GLU	2.3
4	d	230	SER	2.3
13	o	180	GLU	2.3
15	U	56	GLU	2.3
1	a	111	PRO	2.3
3	C	235	GLY	2.3
9	J	13	VAL	2.3
13	O	100	GLY	2.3
13	o	67	PRO	2.3
15	U	51	LYS	2.3
15	U	54	PRO	2.3
15	u	65	PRO	2.3
1	A	328	MET	2.3
2	B	272	ARG	2.3
2	b	188	ASP	2.3
2	b	385	ARG	2.3
13	O	42	ARG	2.3
1	A	72	LEU	2.2
7	h	53	LEU	2.2
4	d	32	TRP	2.2
3	C	147	PHE	2.2
11	l	36	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
12	m	21	PHE	2.2
19	z	59	PHE	2.2
1	a	263	ALA	2.2
8	I	5	LYS	2.2
12	M	31	SER	2.2
3	C	104	GLU	2.2
15	U	59	GLU	2.2
4	D	203	GLY	2.2
13	o	225	MET	2.2
4	D	25	ASP	2.2
4	D	75	THR	2.2
13	o	9	ASP	2.2
13	o	141	ASP	2.2
1	a	186	PHE	2.2
2	B	479	PHE	2.2
4	d	29	PHE	2.2
2	b	301	ALA	2.2
4	d	229	ALA	2.2
13	o	171	ALA	2.2
13	o	246	ALA	2.2
19	z	10	ALA	2.2
1	A	187	GLN	2.2
1	a	246	TYR	2.2
3	C	302	TYR	2.2
13	O	176	GLN	2.2
16	V	47	LYS	2.2
2	B	405[A]	GLU	2.2
1	a	164	GLY	2.2
3	c	423	ARG	2.2
3	c	461	ARG	2.2
4	D	76	VAL	2.2
4	d	265	ARG	2.2
19	z	18	VAL	2.2
2	B	128	THR	2.2
4	d	263	ASN	2.2
18	X	34	ILE	2.2
3	c	91	HIS	2.2
13	O	16	ALA	2.2
15	u	72	LYS	2.2
3	C	311	GLN	2.2
3	c	144	SER	2.2
3	C	261	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
16	V	135	VAL	2.2
1	A	62	GLY	2.2
2	b	206	GLY	2.2
3	c	100	GLY	2.2
10	k	20	PRO	2.2
13	O	12	GLY	2.2
4	D	132	ILE	2.2
17	y	35	ILE	2.2
2	b	469	HIS	2.2
4	d	317	LYS	2.2
1	a	251	ALA	2.2
2	b	379	ALA	2.2
4	d	14	TRP	2.2
6	f	20	TRP	2.2
2	b	409	GLN	2.2
3	C	299	SER	2.2
3	c	230	LEU	2.2
3	c	404	LEU	2.2
4	D	57	SER	2.2
5	e	16	SER	2.2
12	M	32	GLN	2.2
6	f	19	ARG	2.2
13	o	125	LEU	2.2
16	V	105	ARG	2.2
2	B	178	VAL	2.2
3	c	227	VAL	2.2
3	C	71	GLU	2.2
2	b	482	ILE	2.2
3	c	256	PRO	2.2
4	D	307	GLU	2.2
6	f	35	GLY	2.2
7	H	17	GLU	2.2
13	o	213	GLY	2.2
16	V	65	PRO	2.2
5	e	78	THR	2.2
18	x	10	PHE	2.2
2	B	349	LYS	2.2
16	V	110	LYS	2.2
1	a	338	ASN	2.2
3	c	378	ASN	2.2
4	D	72	ASN	2.2
4	d	220	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	380	ASP	2.2
3	C	195	ASP	2.2
3	c	392	ALA	2.2
9	j	32	ALA	2.2
1	A	14	TRP	2.2
1	a	268	SER	2.2
2	b	340	TRP	2.2
3	c	45	LEU	2.2
2	b	358	ARG	2.2
6	f	41	GLN	2.2
15	u	71	GLN	2.2
2	b	314	TYR	2.2
1	a	189	GLU	2.2
2	b	16	PRO	2.2
4	D	54	PHE	2.2
4	d	73	PHE	2.2
15	u	23	GLU	2.2
15	u	80	GLU	2.2
15	u	86	GLU	2.2
2	b	72	THR	2.2
3	C	346	THR	2.2
14	T	30	THR	2.2
2	b	138	MET	2.2
4	D	318	ASN	2.2
8	i	1[A]	MET	2.2
12	M	1	MET	2.2
1	A	54	ALA	2.1
15	u	46	ALA	2.1
16	V	38	ALA	2.1
2	B	100	HIS	2.1
2	B	384	ARG	2.1
4	D	79	SER	2.1
5	E	82	GLN	2.1
6	F	45	ARG	2.1
7	h	56	ASP	2.1
15	U	60	ASP	2.1
2	B	113	TRP	2.1
5	E	56	TYR	2.1
17	Y	18	VAL	2.1
1	A	155	PHE	2.1
3	C	247	GLY	2.1
3	c	77	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	331	PRO	2.1
13	O	53	LYS	2.1
13	O	69	LYS	2.1
13	O	112	GLY	2.1
3	c	346	THR	2.1
2	b	225	LEU	2.1
1	A	294	ALA	2.1
1	a	54	ALA	2.1
4	d	249	ALA	2.1
2	b	472	ARG	2.1
2	b	223[A]	GLN	2.1
1	a	25	ASP	2.1
2	B	491	VAL	2.1
19	z	48	ILE	2.1
3	C	97	TRP	2.1
3	C	259	TRP	2.1
1	a	237	TYR	2.1
1	A	340	PRO	2.1
3	C	458	GLY	2.1
3	c	137	PRO	2.1
4	D	174	GLY	2.1
4	D	200	GLY	2.1
13	O	28	GLY	2.1
15	U	22	GLY	2.1
2	B	428	GLU	2.1
7	h	17	GLU	2.1
2	b	55	MET	2.1
3	C	180	MET	2.1
3	c	185	LEU	2.1
7	h	30	LEU	2.1
9	j	40	LEU	2.1
1	a	286	ALA	2.1
2	B	194	ASN	2.1
4	D	77	ALA	2.1
4	D	294	ARG	2.1
7	H	12[A]	ARG	2.1
11	L	14	ARG	2.1
2	B	76[A]	SER	2.1
3	C	310	SER	2.1
4	D	166	SER	2.1
18	x	33	GLN	2.1
1	A	310	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	106	VAL	2.1
10	K	30	VAL	2.1
10	k	18	PHE	2.1
2	B	258	TYR	2.1
2	B	273	TYR	2.1
7	h	49	TYR	2.1
3	c	219	GLY	2.1
3	C	138	GLU	2.1
13	O	153	THR	2.1
3	C	370	ARG	2.1
14	t	24	ARG	2.1
4	D	119	ALA	2.1
14	T	20	ALA	2.1
11	L	6	ASN	2.1
19	z	6	GLN	2.1
3	C	62	PHE	2.1
14	t	10	PHE	2.1
3	C	237	HIS	2.1
2	B	232	GLY	2.1
3	c	103	GLY	2.1
4	d	58	TRP	2.1
16	v	44	GLY	2.1
2	B	330	MET	2.1
2	B	415	PRO	2.1
3	c	71	GLU	2.1
3	c	254	THR	2.1
16	v	80	THR	2.1
1	A	225	ARG	2.1
15	U	70	ARG	2.1
1	A	88	ALA	2.1
3	c	349	ILE	2.1
17	Y	20	ALA	2.1
2	b	36[A]	SER	2.1
2	B	247	PHE	2.1
2	B	392	PHE	2.1
2	b	438	ASN	2.1
5	E	74	GLN	2.1
16	V	49	ASN	2.1
3	C	439	VAL	2.1
1	A	252	HIS	2.1
2	B	4	PRO	2.1
2	b	313	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	225	ASP	2.1
4	d	167	TRP	2.1
1	a	227	THR	2.1
7	h	47	GLU	2.1
13	o	210	GLU	2.1
4	D	12	ARG	2.1
1	A	70	SER	2.1
2	B	228	ALA	2.1
2	b	310	ALA	2.1
3	c	299	SER	2.1
3	c	330	SER	2.1
4	d	84	SER	2.1
3	c	351	PHE	2.1
3	C	405	ASN	2.1
4	d	322	ASN	2.1
4	d	340	VAL	2.1
9	J	33	TYR	2.0
12	M	7	GLY	2.0
2	b	54	PRO	2.0
2	b	183	PRO	2.0
1	A	15	GLU	2.0
2	B	398	THR	2.0
3	C	150	ASP	2.0
4	d	53	THR	2.0
4	d	221	THR	2.0
13	O	86	LYS	2.0
13	o	232	GLU	2.0
15	u	69	GLU	2.0
18	x	31	ILE	2.0
1	A	324	ALA	2.0
3	c	471[A]	SER	2.0
19	Z	60	PHE	2.0
2	b	309	LEU	2.0
19	z	7	LEU	2.0
13	o	87	VAL	2.0
2	b	481	GLY	2.0
15	U	40	GLY	2.0
1	A	92	HIS	2.0
3	C	262	ARG	2.0
3	c	400	PRO	2.0
13	O	56	PRO	2.0
13	O	178	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
16	V	41	HIS	2.0
5	e	49	THR	2.0
14	T	4	ILE	2.0
3	c	141	GLU	2.0
4	d	302	GLU	2.0
1	A	167	SER	2.0
1	A	186	PHE	2.0
2	b	155	ALA	2.0
4	d	166	SER	2.0
4	d	261	PHE	2.0
4	d	341	PHE	2.0
8	i	17	LEU	2.0
16	V	12	LEU	2.0
18	x	32	SER	2.0
7	H	59	ASN	2.0
2	B	17	GLY	2.0
2	B	449	GLY	2.0
2	B	164	PRO	2.0
2	B	414	PRO	2.0
3	C	447	ARG	2.0
3	c	271	TYR	2.0
4	D	141	TYR	2.0
5	e	56	TYR	2.0
11	l	15	THR	2.0
4	D	257	PHE	2.0
5	E	59	GLU	2.0
12	M	2	GLU	2.0
5	E	16	SER	2.0
8	I	27	ASP	2.0
18	X	10	PHE	2.0
13	o	63	ALA	2.0
13	o	111	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} 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
22	CL	u	201	1/1	0.10	0.94	112,112,112,112	0
28	SQD	B	622	54/54	0.31	0.29	119,127,141,142	0
28	SQD	L	102	54/54	0.35	0.30	119,131,146,147	0
22	CL	U	201	1/1	0.36	0.58	91,91,91,91	0
28	SQD	b	601	54/54	0.36	0.27	99,107,121,121	0
31	CA	o	301	1/1	0.39	0.28	110,110,110,110	0
28	SQD	l	101	54/54	0.53	0.24	98,110,125,126	0
22	CL	a	604	1/1	0.65	0.43	83,83,83,83	0
31	CA	b	602	1/1	0.70	0.41	137,137,137,137	0
29	LMG	c	520	51/55	0.71	0.45	104,137,142,143	0
29	LMG	Z	101	37/55	0.72	0.41	96,124,129,129	0
28	SQD	x	101	43/54	0.72	0.39	128,136,140,140	0
31	CA	O	301	1/1	0.74	0.17	90,90,90,90	0
31	CA	F	102	1/1	0.75	0.20	97,97,97,97	0
28	SQD	a	614	54/54	0.75	0.39	111,124,129,130	0
32	DGD	d	405	62/66	0.75	0.38	138,151,164,165	0
30	LHG	E	102	42/49	0.76	0.41	110,124,127,127	0
28	SQD	X	101	43/54	0.76	0.34	108,115,119,119	0
28	SQD	a	612	54/54	0.76	0.35	110,119,128,128	0
32	DGD	E	101	62/66	0.77	0.38	118,130,143,144	0
29	LMG	C	519	51/55	0.78	0.35	83,117,122,123	0
24	CLA	c	513	65/65	0.78	0.32	101,106,125,126	0
27	PL9	a	611	55/55	0.79	0.41	113,130,139,140	0
29	LMG	c	519	51/55	0.79	0.39	92,118,134,135	0
29	LMG	C	518	51/55	0.80	0.35	72,98,113,114	0
28	SQD	A	614	54/54	0.80	0.32	91,103,109,109	0
30	LHG	e	101	42/49	0.80	0.35	131,145,147,148	0
27	PL9	A	611	55/55	0.81	0.38	93,109,118,119	0
26	BCR	f	101	40/40	0.82	0.32	87,91,109,110	0
32	DGD	c	516	62/66	0.82	0.30	84,94,122,124	0
29	LMG	b	622	51/55	0.82	0.34	91,100,112,116	0
24	CLA	B	602	65/65	0.83	0.27	73,82,107,107	0
29	LMG	j	101	51/55	0.83	0.31	87,96,126,129	0
29	LMG	z	101	37/55	0.83	0.30	117,145,149,150	0
26	BCR	H	101	40/40	0.83	0.31	67,74,83,83	0
24	CLA	b	603	65/65	0.83	0.28	94,102,127,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	k	101	40/40	0.83	0.29	95,99,100,100	0
24	CLA	C	513	65/65	0.84	0.26	80,85,105,105	0
26	BCR	h	101	40/40	0.84	0.30	87,94,103,104	0
26	BCR	B	619	40/40	0.84	0.28	62,69,81,81	0
29	LMG	a	613	51/55	0.84	0.32	114,121,126,126	0
24	CLA	c	512	65/65	0.84	0.27	99,102,124,124	0
26	BCR	I	101	40/40	0.84	0.29	71,78,81,82	0
26	BCR	T	101	40/40	0.84	0.29	65,78,85,86	0
26	BCR	c	515	40/40	0.84	0.31	92,98,102,102	0
29	LMG	A	613	51/55	0.84	0.28	94,100,105,105	0
24	CLA	c	506	65/65	0.85	0.26	93,100,136,136	0
24	CLA	b	608[A]	65/65	0.85	0.27	85,90,102,103	65
29	LMG	D	408	51/55	0.85	0.29	66,76,106,108	0
26	BCR	c	521	40/40	0.85	0.30	91,95,98,99	0
24	CLA	b	608[B]	65/65	0.85	0.27	83,87,93,95	65
30	LHG	a	616	49/49	0.85	0.31	87,94,124,125	0
28	SQD	A	612	54/54	0.85	0.33	90,98,107,108	0
29	LMG	B	621	51/55	0.86	0.29	70,80,92,95	0
24	CLA	B	617	65/65	0.86	0.23	63,69,118,119	0
24	CLA	c	501	65/65	0.86	0.25	90,93,106,108	0
23	BCT	A	605	4/4	0.86	0.38	79,80,81,82	0
26	BCR	b	620	40/40	0.86	0.29	83,89,101,101	0
26	BCR	t	101	40/40	0.86	0.34	86,99,106,106	0
26	BCR	C	514	40/40	0.86	0.28	78,84,87,88	0
27	PL9	d	404	55/55	0.87	0.26	80,84,91,93	0
30	LHG	D	407	49/49	0.87	0.27	64,69,78,81	0
26	BCR	b	621	40/40	0.87	0.26	89,94,100,101	0
26	BCR	c	514	40/40	0.87	0.28	99,105,108,108	0
24	CLA	b	609	65/65	0.87	0.24	79,82,94,95	0
26	BCR	B	620	40/40	0.87	0.24	68,74,80,80	0
24	CLA	B	607[A]	65/65	0.87	0.22	65,69,81,82	65
24	CLA	B	607[B]	65/65	0.87	0.22	63,67,72,75	65
24	CLA	c	509	65/65	0.87	0.24	91,93,108,108	0
26	BCR	K	102	40/40	0.87	0.27	70,74,78,78	0
24	CLA	B	606	65/65	0.87	0.23	59,64,75,76	0
24	CLA	C	506	65/65	0.87	0.24	72,79,115,115	0
26	BCR	K	101	40/40	0.88	0.26	75,78,79,80	0
24	CLA	c	503	65/65	0.88	0.22	89,93,96,97	0
24	CLA	C	501	65/65	0.88	0.22	69,73,85,87	0
24	CLA	c	508	65/65	0.88	0.22	87,90,115,119	0
31	CA	f	102	1/1	0.88	0.14	118,118,118,118	0
24	CLA	b	618	65/65	0.88	0.23	83,90,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	F	101	40/40	0.88	0.23	66,71,88,90	0
24	CLA	c	511	65/65	0.88	0.24	90,95,99,99	0
32	DGD	c	517	62/66	0.88	0.25	84,96,124,124	0
24	CLA	C	507	65/65	0.88	0.23	70,74,92,94	0
24	CLA	b	606	65/65	0.89	0.22	81,84,111,112	0
24	CLA	B	616	65/65	0.89	0.20	65,68,86,87	0
30	LHG	d	406	49/49	0.89	0.26	91,96,102,102	0
24	CLA	C	505	65/65	0.89	0.20	69,71,85,85	0
31	CA	B	601	1/1	0.89	0.25	117,117,117,117	0
24	CLA	a	607	65/65	0.89	0.23	80,83,124,126	0
24	CLA	c	510	65/65	0.89	0.22	86,90,96,99	0
24	CLA	b	610	65/65	0.89	0.21	82,86,92,93	0
24	CLA	b	617	65/65	0.89	0.22	86,89,107,108	0
24	CLA	a	609	65/65	0.89	0.21	83,85,133,133	0
32	DGD	C	515	62/66	0.89	0.23	64,73,102,103	0
32	DGD	C	516	62/66	0.89	0.25	63,75,103,104	0
26	BCR	b	619	40/40	0.89	0.29	84,88,90,90	0
25	PHO	d	401	64/64	0.89	0.21	80,84,90,94	0
30	LHG	D	406	49/49	0.89	0.23	70,75,81,82	0
32	DGD	c	518	62/66	0.89	0.24	83,93,113,117	0
24	CLA	B	609	65/65	0.89	0.19	61,65,71,72	0
24	CLA	C	504	65/65	0.90	0.21	66,68,95,95	0
24	CLA	b	607	65/65	0.90	0.21	80,84,95,97	0
26	BCR	a	610	40/40	0.90	0.25	83,89,93,94	0
24	CLA	d	402	65/65	0.90	0.21	75,80,95,96	0
30	LHG	l	102	49/49	0.90	0.27	84,92,104,106	0
32	DGD	H	102	62/66	0.90	0.23	66,72,79,81	0
24	CLA	d	403	65/65	0.90	0.20	86,89,126,128	0
24	CLA	b	605	65/65	0.90	0.20	79,84,92,96	0
26	BCR	A	610	40/40	0.90	0.23	63,68,73,73	0
26	BCR	B	618	40/40	0.90	0.25	63,68,69,70	0
32	DGD	h	102	62/66	0.90	0.25	87,93,99,101	0
22	CL	A	603	1/1	0.91	0.24	65,65,65,65	0
24	CLA	C	509	65/65	0.91	0.21	70,72,87,88	0
24	CLA	C	512	65/65	0.91	0.20	78,82,103,104	0
24	CLA	B	608	65/65	0.91	0.20	58,61,73,74	0
24	CLA	b	611	65/65	0.91	0.19	85,90,92,93	0
24	CLA	b	612	65/65	0.91	0.20	82,86,94,98	0
24	CLA	b	615	65/65	0.91	0.20	80,84,106,108	0
24	CLA	B	603	65/65	0.91	0.19	64,67,72,73	0
24	CLA	C	502	65/65	0.91	0.17	65,67,80,83	0
24	CLA	C	503	65/65	0.91	0.18	68,72,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	LHG	A	615	49/49	0.91	0.23	67,74,103,104	0
24	CLA	B	610	65/65	0.91	0.17	64,69,72,73	0
24	CLA	c	504	65/65	0.91	0.21	86,89,115,116	0
24	CLA	c	505	65/65	0.91	0.19	89,92,106,106	0
24	CLA	B	611	65/65	0.91	0.21	62,65,73,77	0
24	CLA	B	613	65/65	0.91	0.20	61,64,71,72	0
30	LHG	d	407	49/49	0.91	0.23	85,89,98,102	0
24	CLA	c	502	65/65	0.92	0.17	85,87,101,103	0
25	PHO	D	401	64/64	0.92	0.18	59,63,69,73	0
24	CLA	C	508	65/65	0.92	0.18	66,70,95,99	0
24	CLA	A	609	65/65	0.92	0.20	62,65,112,113	0
24	CLA	b	604	65/65	0.92	0.18	85,88,93,94	0
24	CLA	C	511	65/65	0.92	0.18	70,75,78,79	0
24	CLA	c	507	65/65	0.92	0.19	91,94,113,115	0
24	CLA	b	613	65/65	0.92	0.20	80,83,94,96	0
24	CLA	b	614	65/65	0.92	0.21	81,85,91,92	0
32	DGD	C	517	62/66	0.92	0.20	62,72,93,97	0
24	CLA	B	604	65/65	0.92	0.18	58,63,72,76	0
24	CLA	b	616	65/65	0.92	0.22	82,86,121,122	0
30	LHG	L	101	49/49	0.92	0.22	63,72,83,85	0
24	CLA	B	605	65/65	0.92	0.20	60,63,91,91	0
27	PL9	D	405	55/55	0.92	0.22	60,64,70,72	0
24	CLA	D	402	65/65	0.92	0.21	54,59,70,76	0
22	CL	a	603	1/1	0.92	0.26	86,86,86,86	0
24	CLA	C	510	65/65	0.93	0.17	65,69,76,78	0
24	CLA	D	403	65/65	0.93	0.20	54,59,75,76	0
24	CLA	D	404	65/65	0.93	0.18	65,68,106,107	0
25	PHO	A	608	64/64	0.93	0.18	57,62,65,67	0
24	CLA	a	606	65/65	0.93	0.20	77,80,87,95	0
24	CLA	B	615	65/65	0.93	0.18	61,65,101,102	0
24	CLA	A	607	65/65	0.93	0.19	60,62,104,106	0
24	CLA	B	614	65/65	0.93	0.18	60,63,85,87	0
34	MG	J	101	1/1	0.93	0.23	68,68,68,68	0
24	CLA	a	615	65/65	0.94	0.22	75,79,91,96	0
24	CLA	A	606	65/65	0.94	0.18	56,59,66,75	0
23	BCT	a	605	4/4	0.94	0.22	100,101,101,103	0
25	PHO	a	608	64/64	0.94	0.19	78,83,86,87	0
33	HEM	e	102	43/43	0.94	0.21	101,103,107,108	0
33	HEM	v	201	43/43	0.94	0.19	84,86,88,90	0
24	CLA	B	612	65/65	0.94	0.17	60,62,73,75	0
33	HEM	V	201	43/43	0.95	0.17	63,65,68,69	0
33	HEM	E	103	43/43	0.95	0.20	80,82,86,87	0

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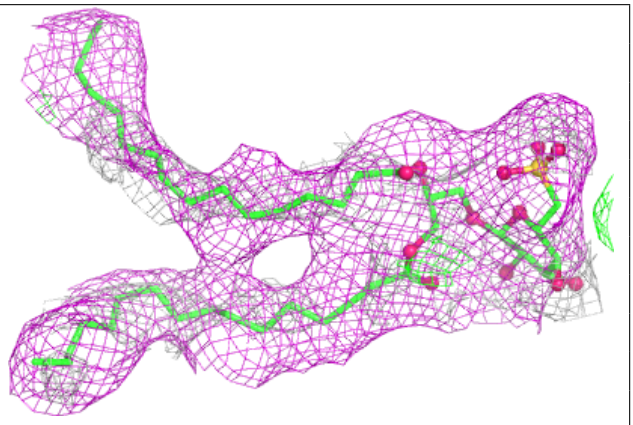
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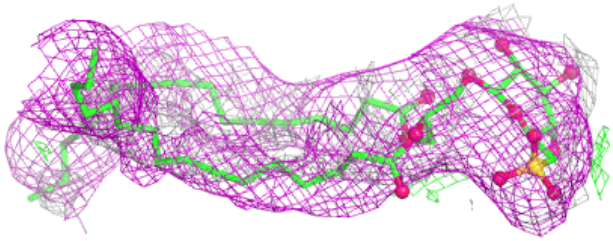
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CL	A	604	1/1	0.96	0.15	62,62,62,62	0
20	OEX	a	601	10/10	0.96	0.16	83,84,87,88	0
34	MG	j	102	1/1	0.96	0.11	89,89,89,89	0
20	OEX	A	601	10/10	0.98	0.14	63,64,67,67	0
21	FE2	A	602	1/1	0.98	0.07	67,67,67,67	0
21	FE2	a	602	1/1	0.99	0.10	88,88,88,88	0

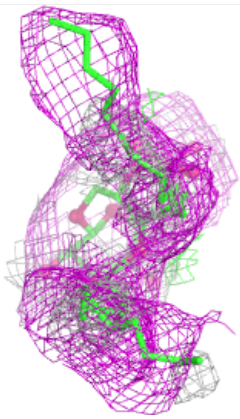
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SQD 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)

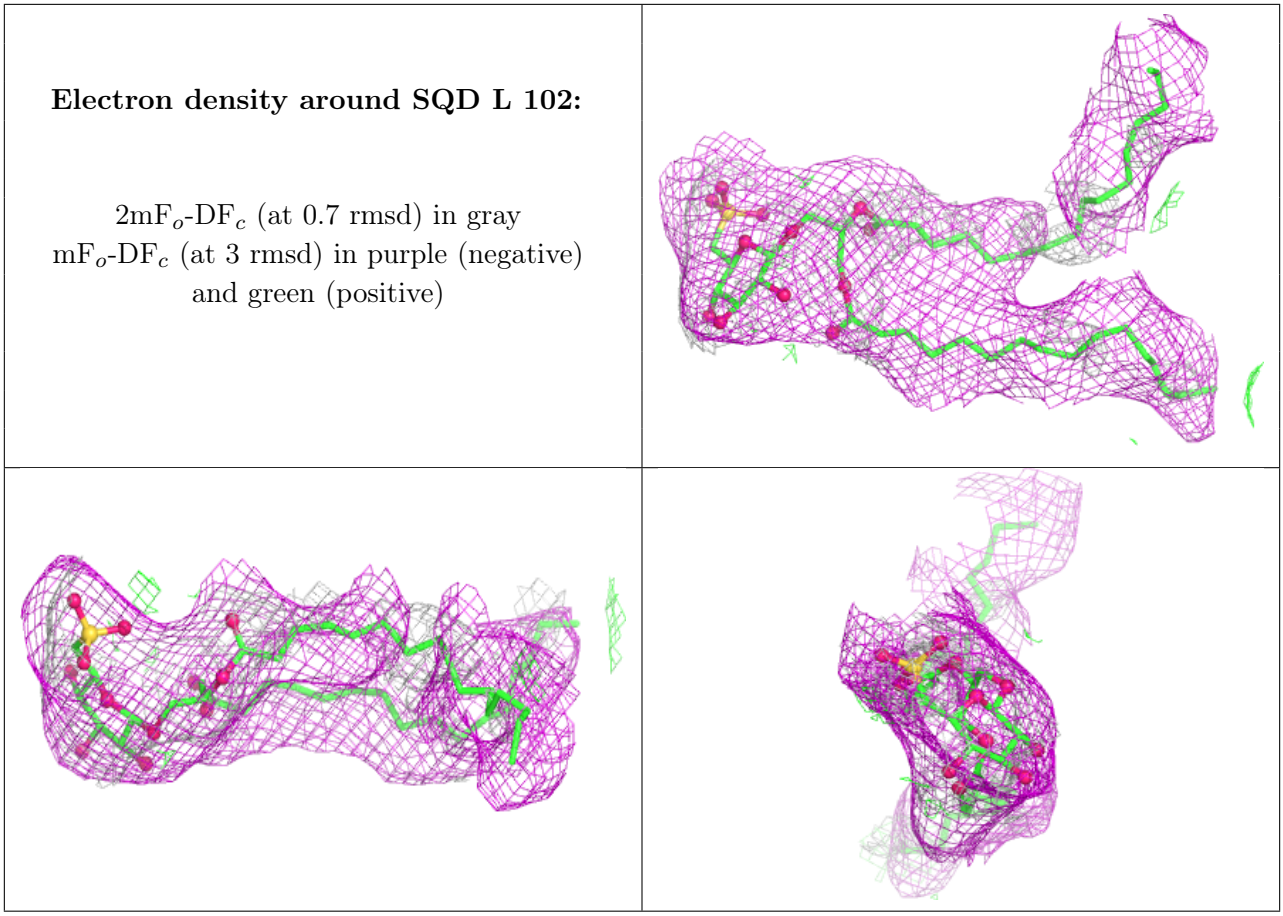






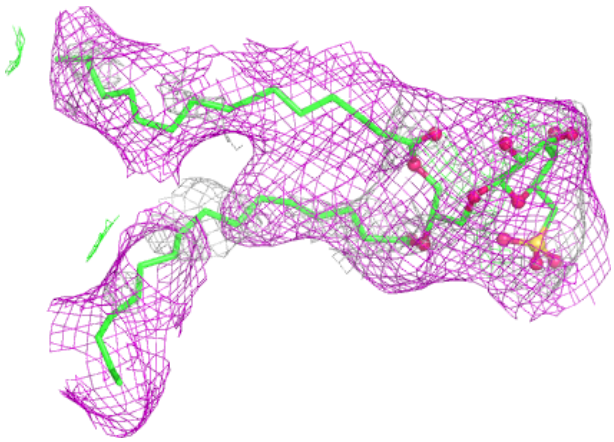
Electron density around SQD L 102:

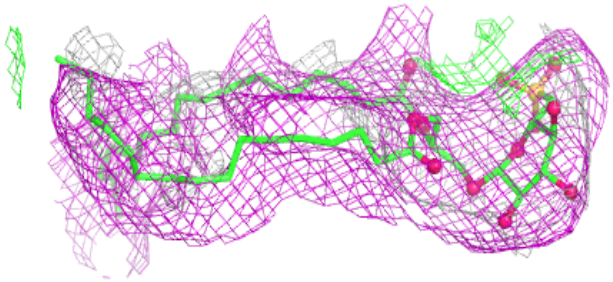
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

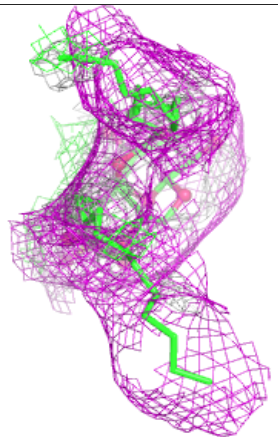


Electron density around SQD b 601:

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

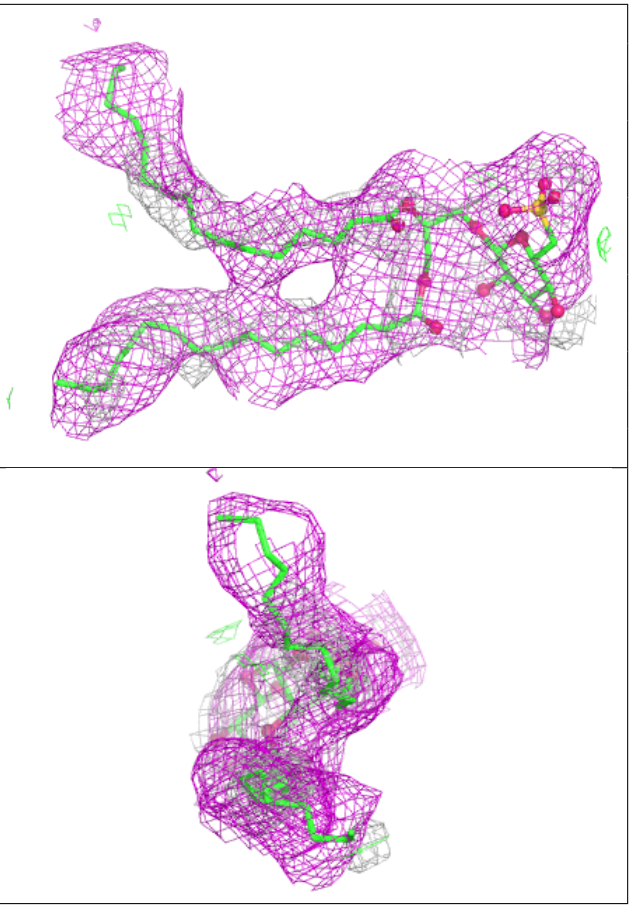






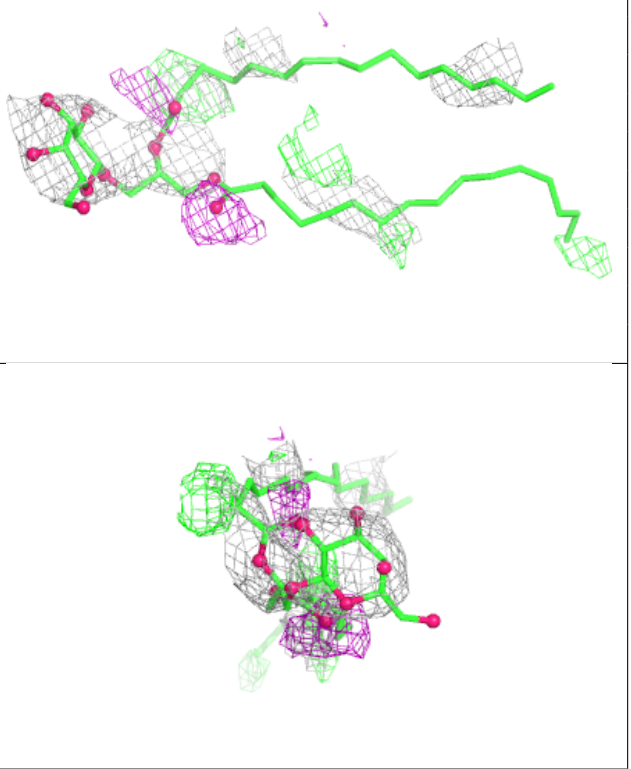
Electron density around SQD l 101:

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



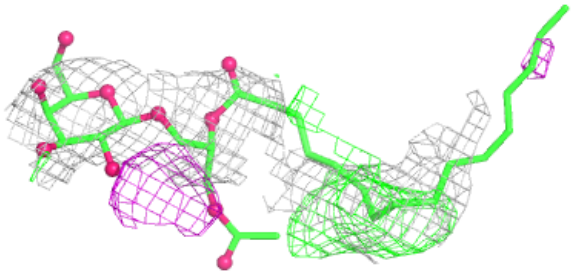
Electron density around LMG c 520:

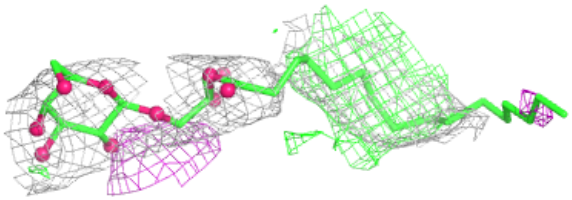
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

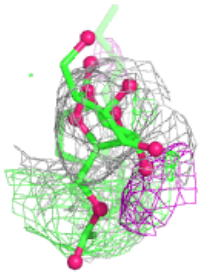


Electron density around LMG Z 101:

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

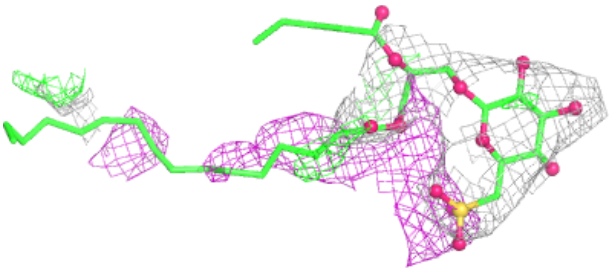


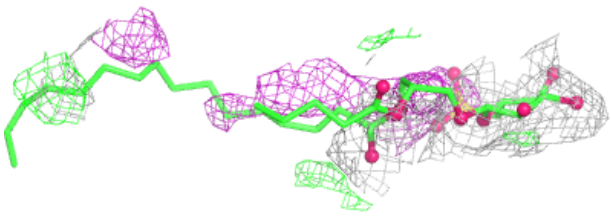


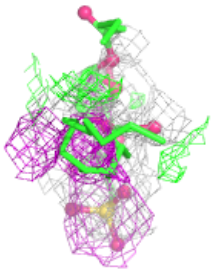


Electron density around SQD x 101:

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

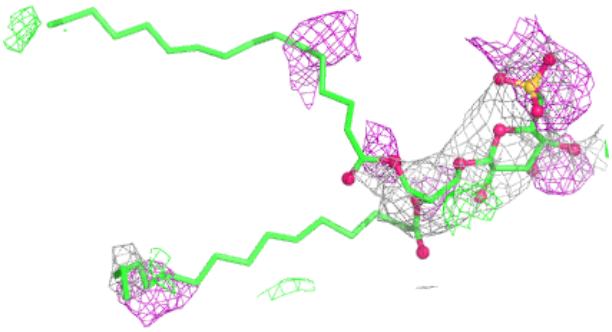


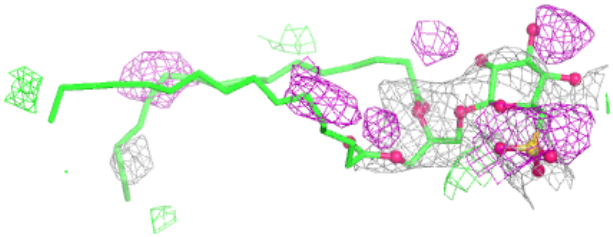




Electron density around SQD a 614:

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

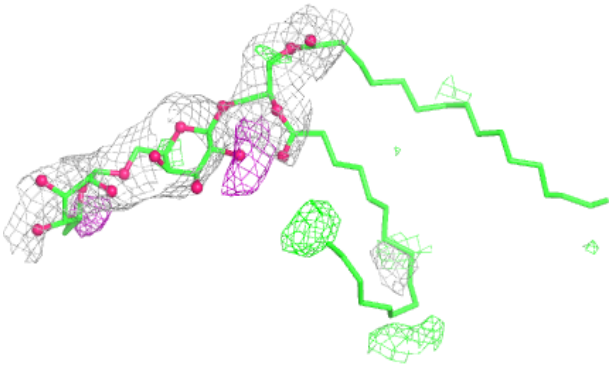


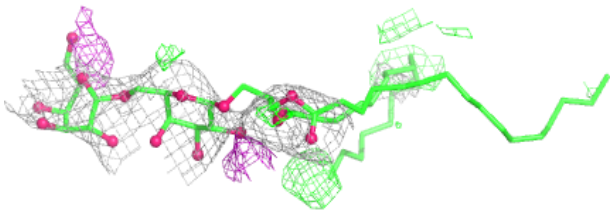




Electron density around DGD d 405:

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

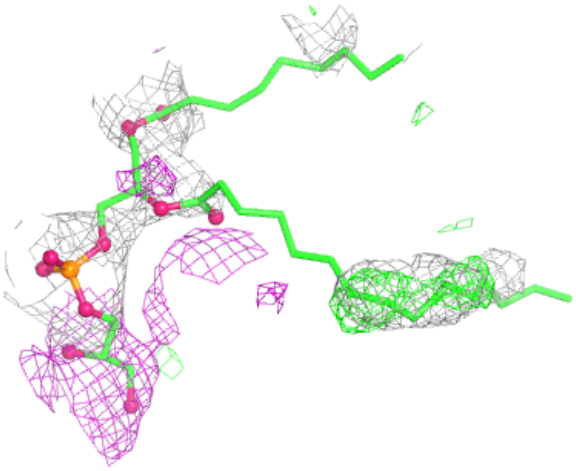


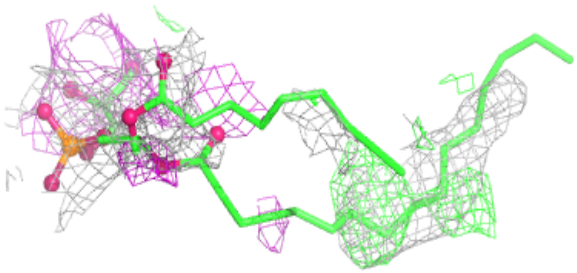


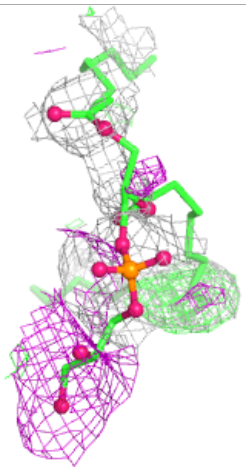


Electron density around LHG E 102:

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

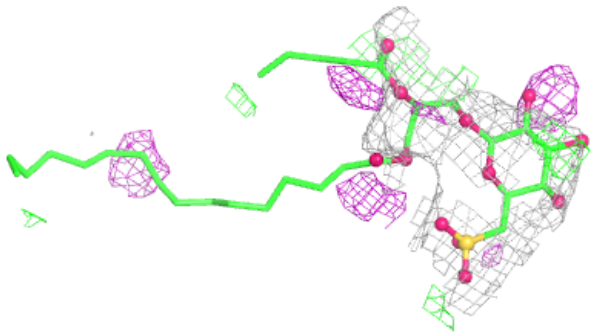


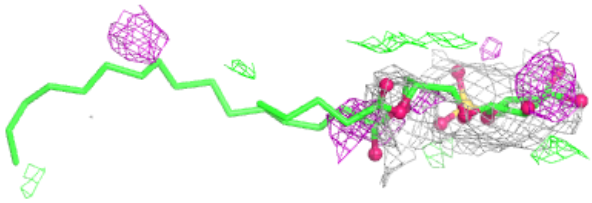




Electron density around SQD X 101:

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

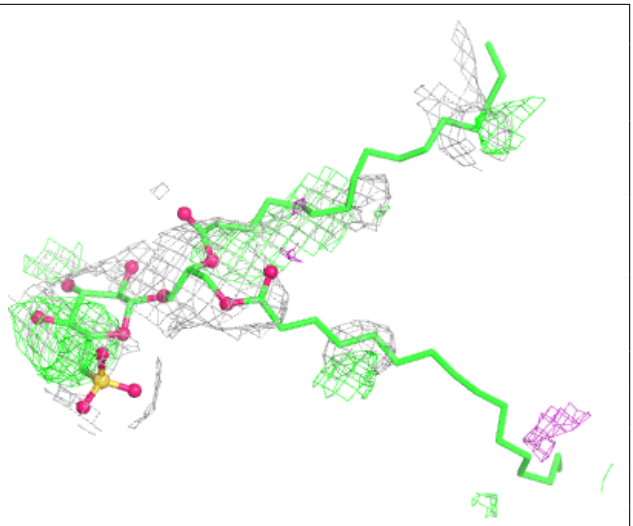


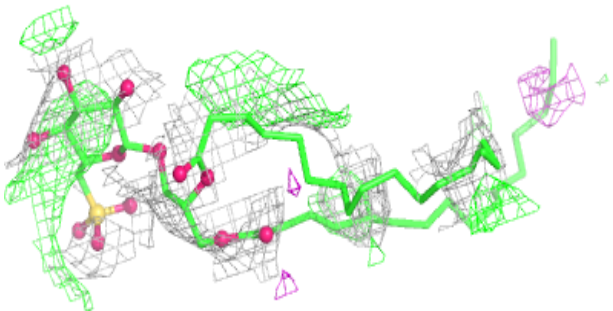




Electron density around SQD a 612:

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

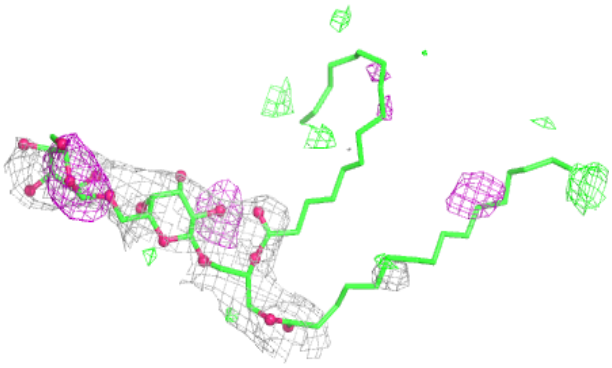


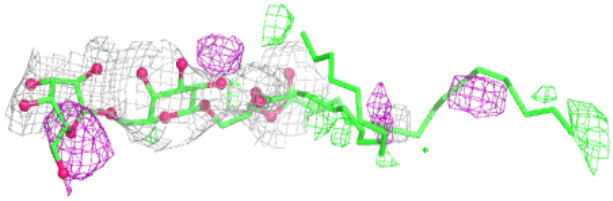


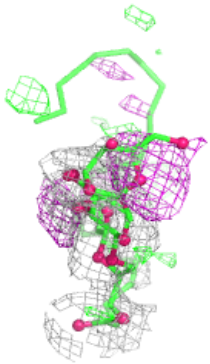


Electron density around DGD E 101:

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

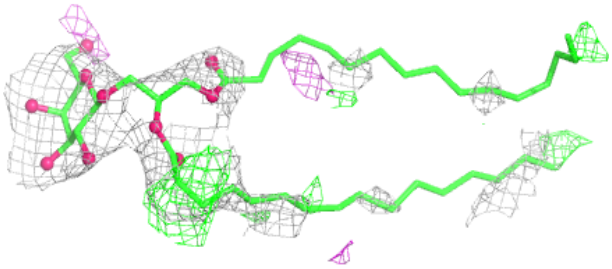


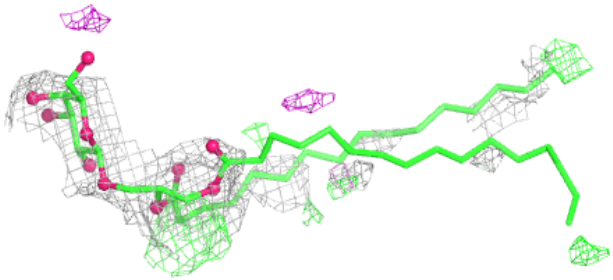


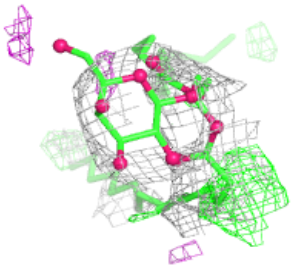


Electron density around LMG C 519:

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

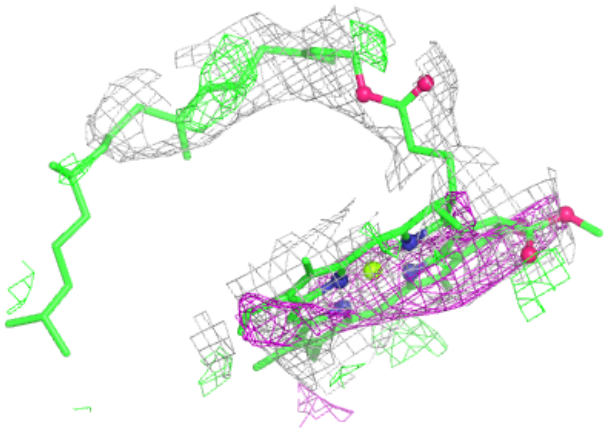


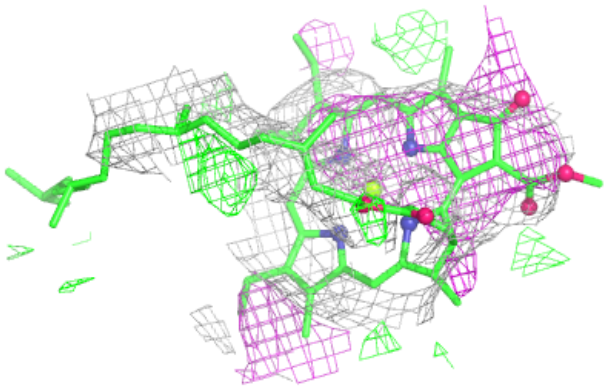


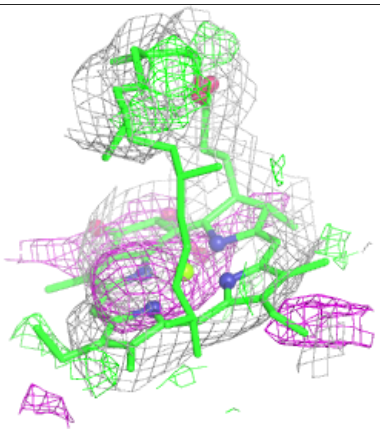


Electron density around CLA c 513:

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

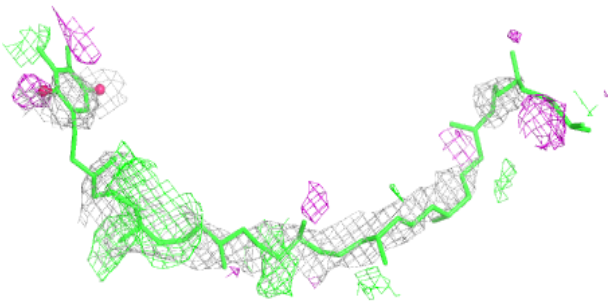


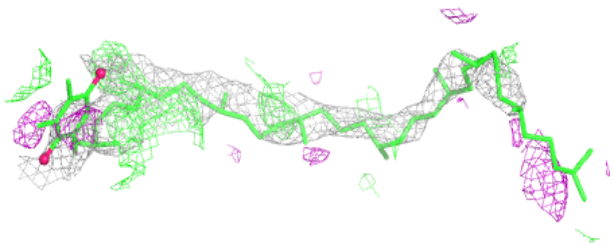


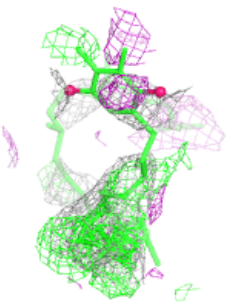


Electron density around PL9 a 611:

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

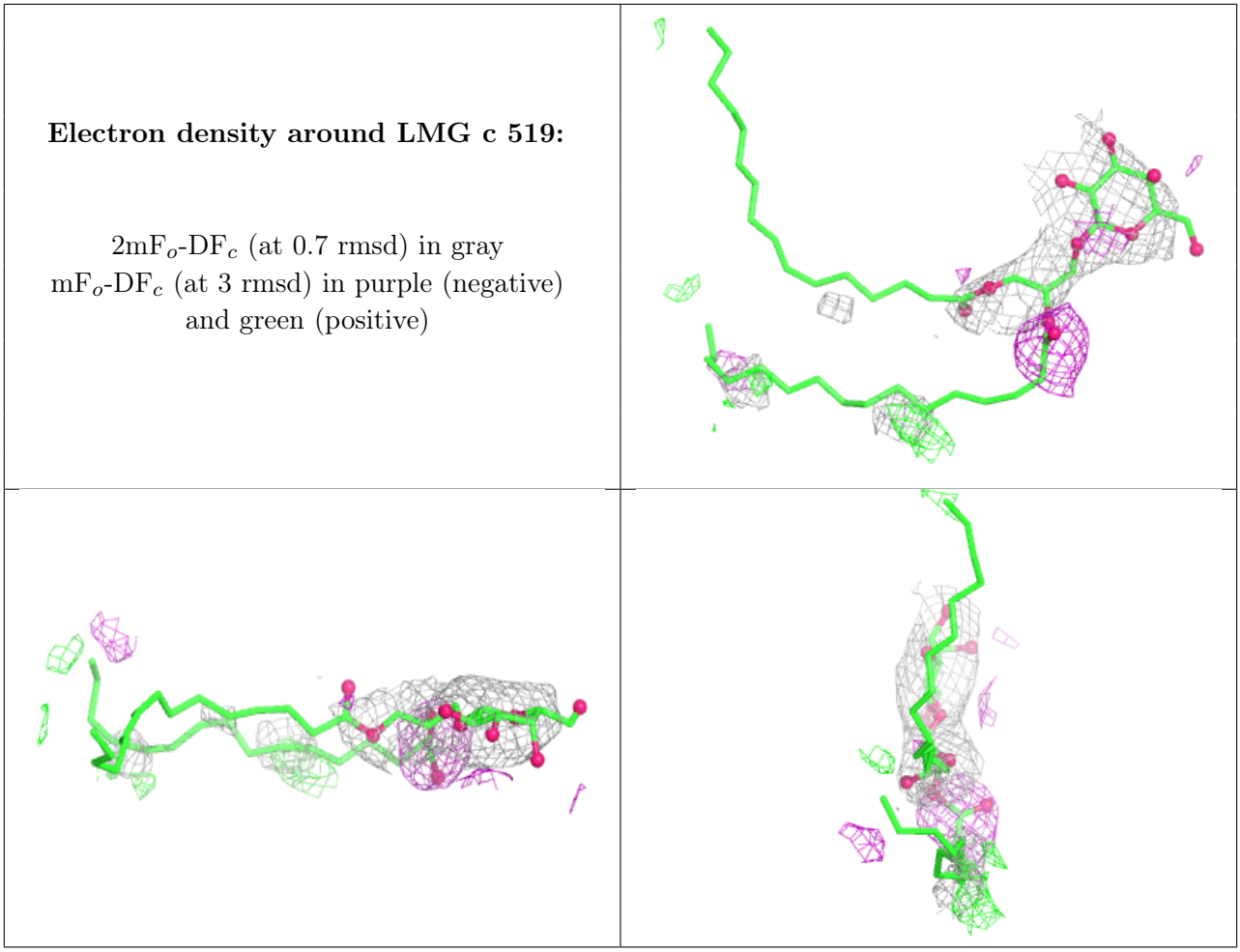






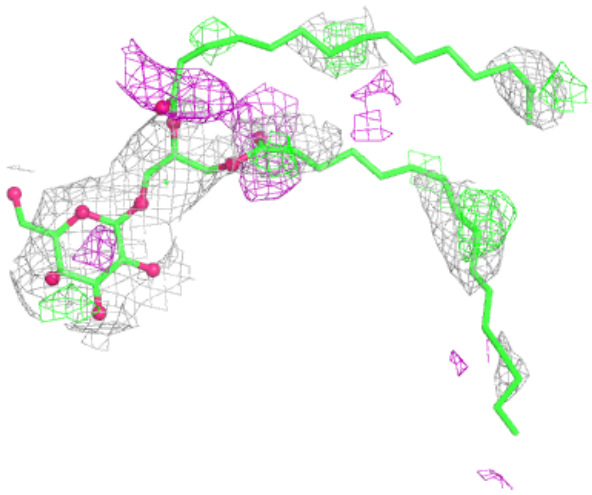
Electron density around LMG c 519:

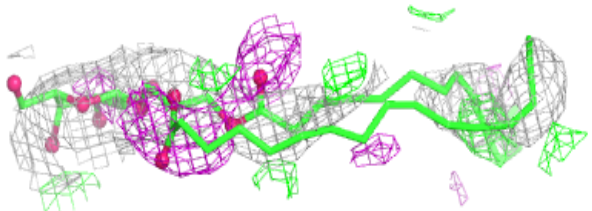
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG 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)

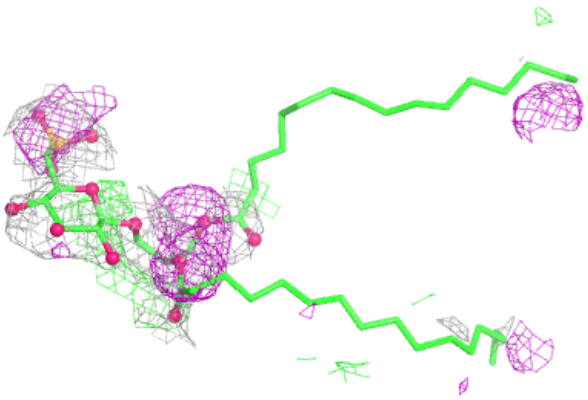


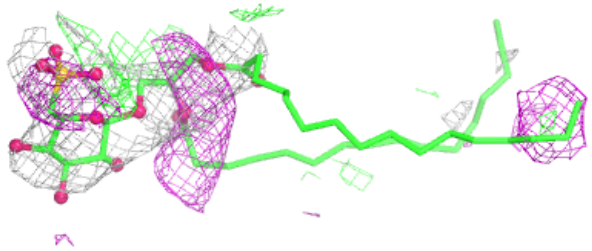


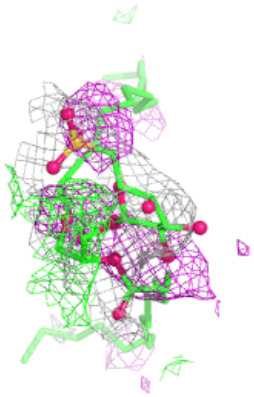


Electron density around SQD A 614:

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

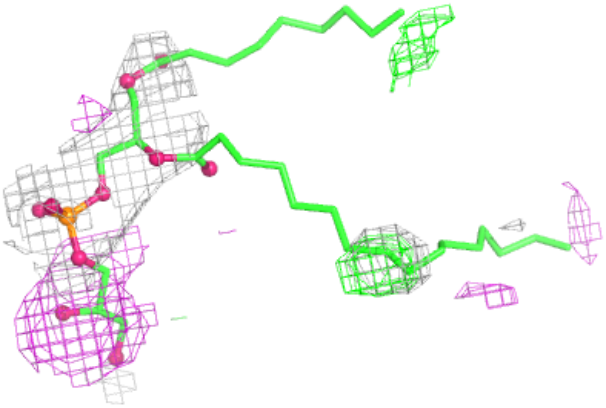


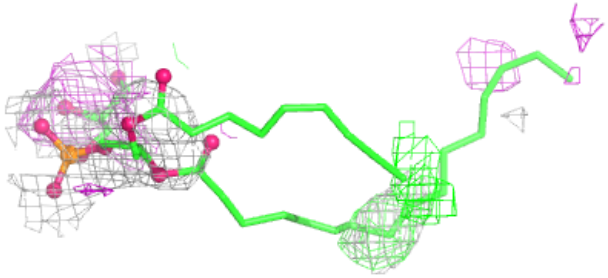




Electron density around LHG e 101:

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

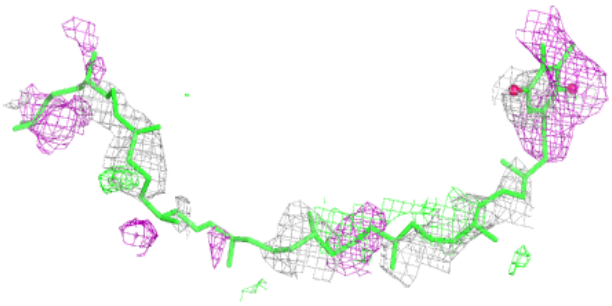


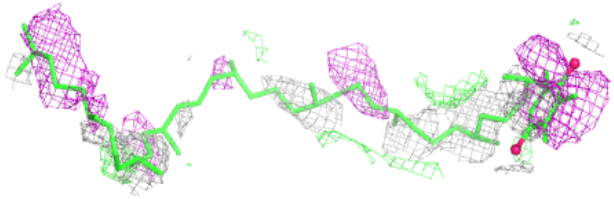


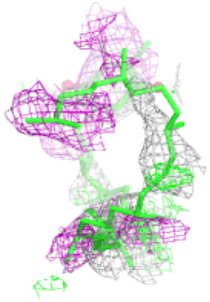


Electron density around PL9 A 611:

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

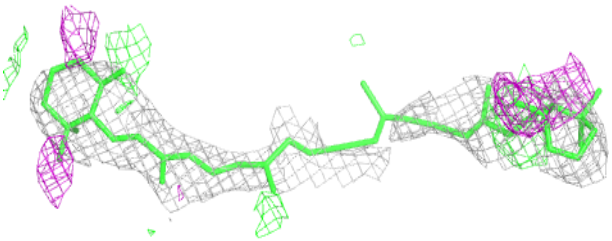


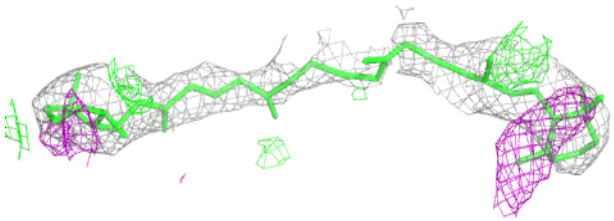


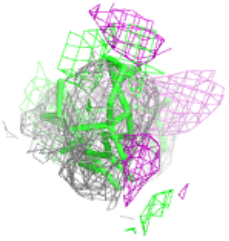


Electron density around BCR f 101:

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

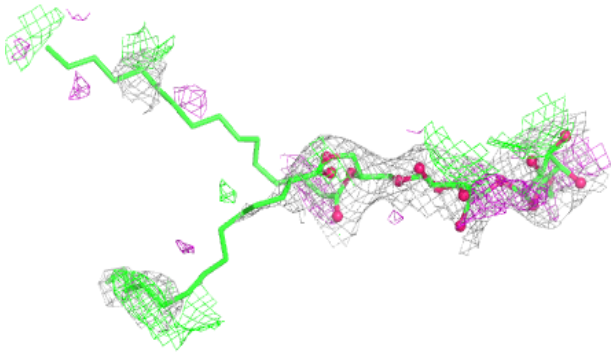


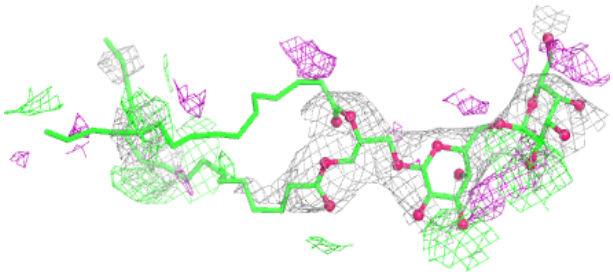


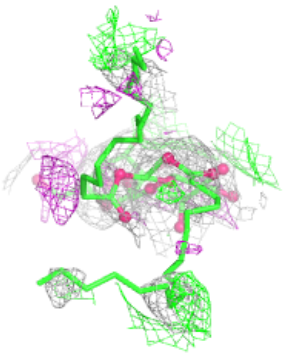


Electron density around DGD c 516:

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

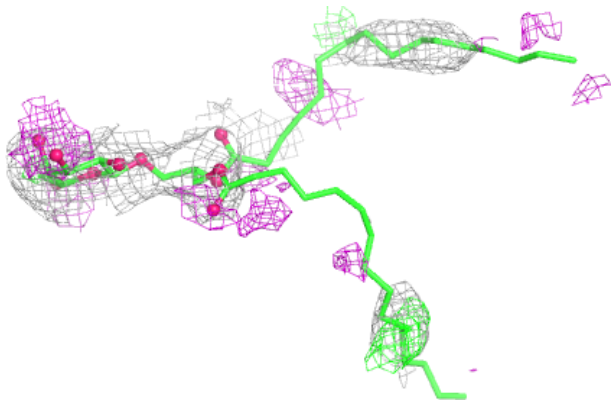


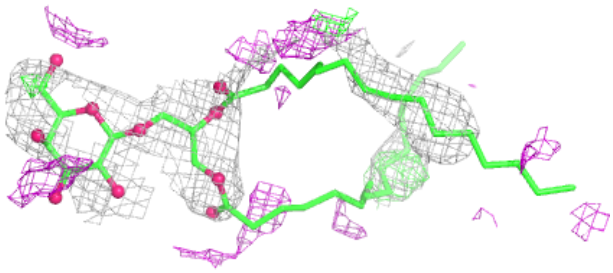


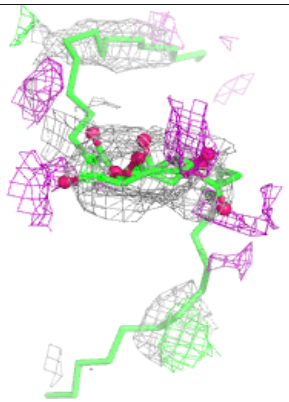


Electron density around LMG b 622:

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

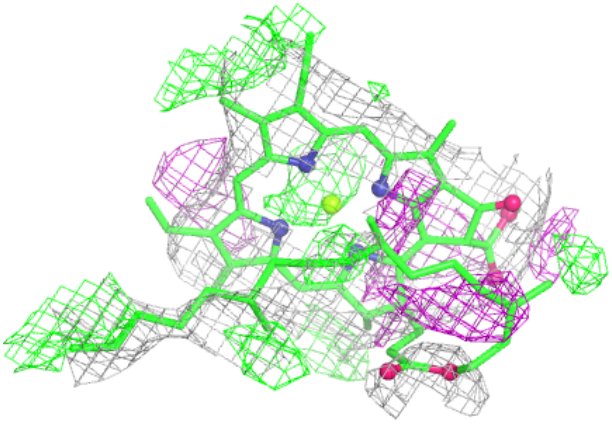


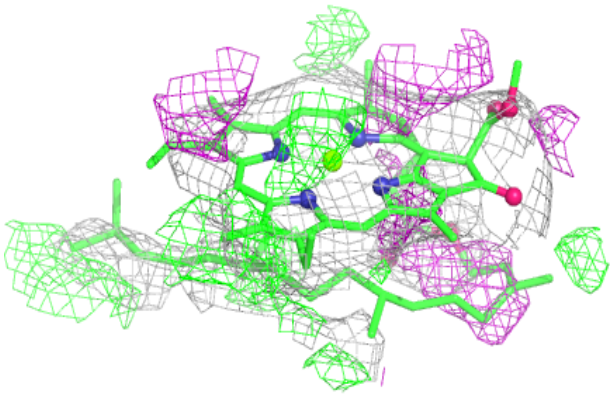


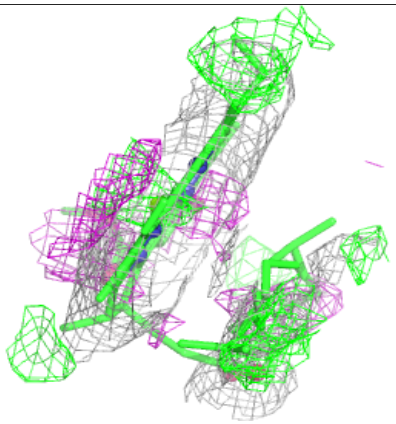


Electron density around CLA B 602:

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

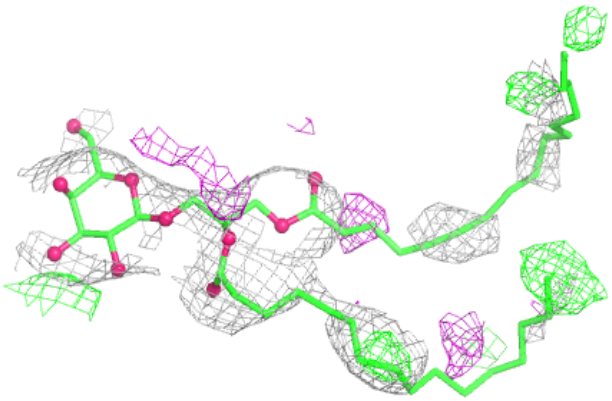


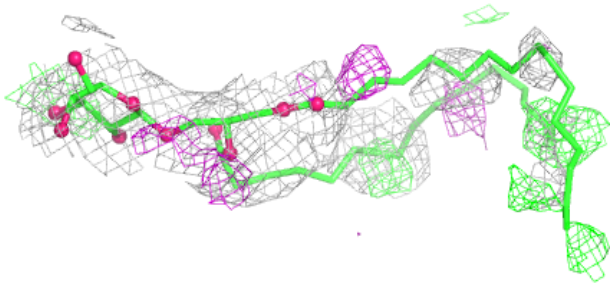


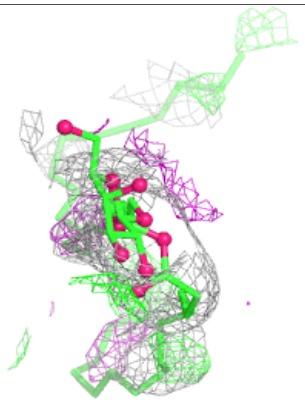


Electron density around LMG j 101:

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

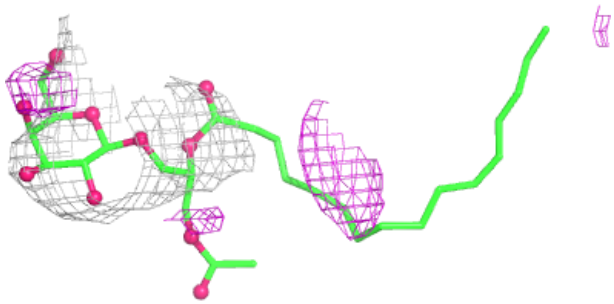


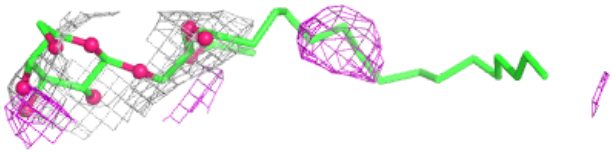


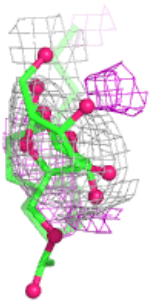


Electron density around LMG z 101:

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

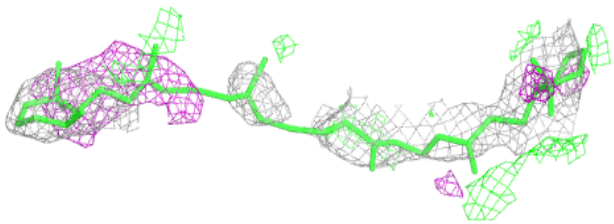


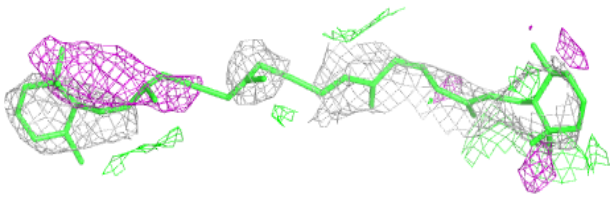


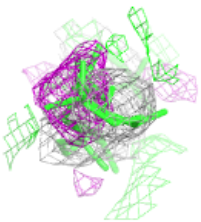


Electron density around BCR H 101:

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

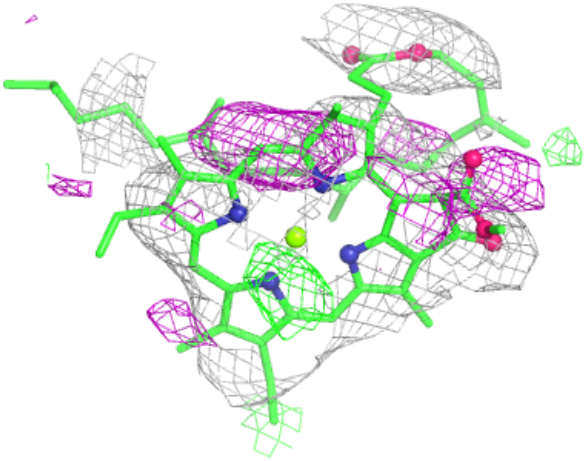


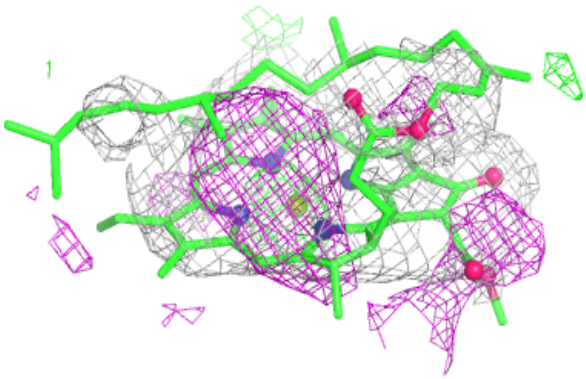


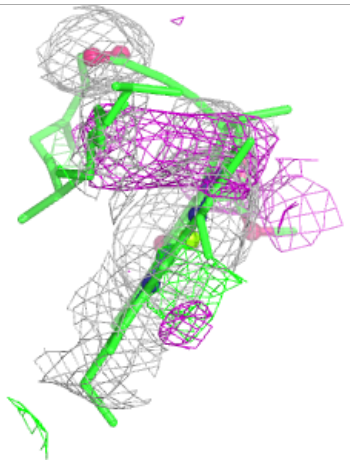


Electron density around CLA b 603:

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

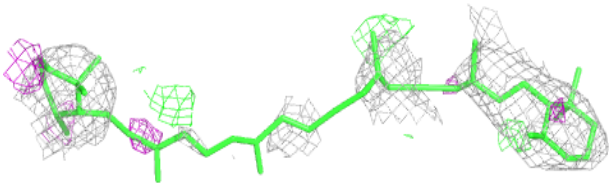


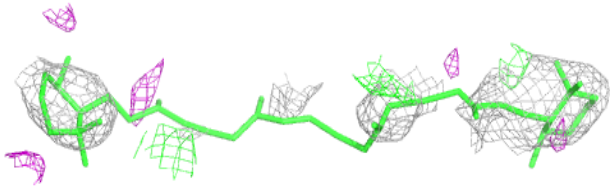


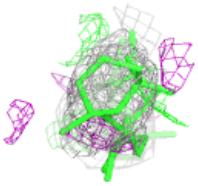


Electron density around BCR k 101:

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

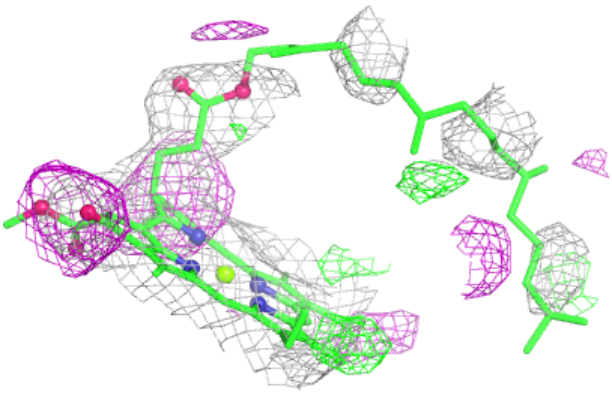


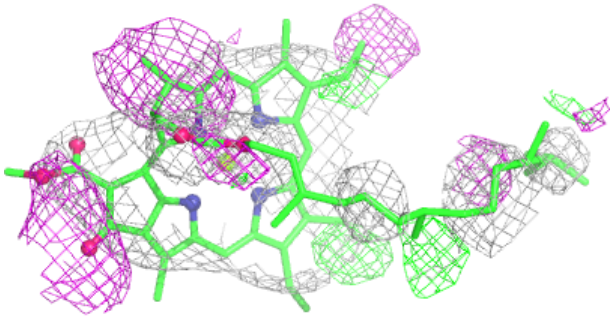


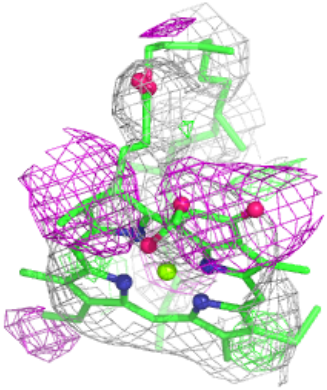


Electron density around CLA C 513:

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

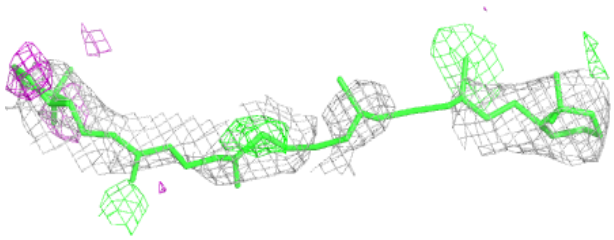


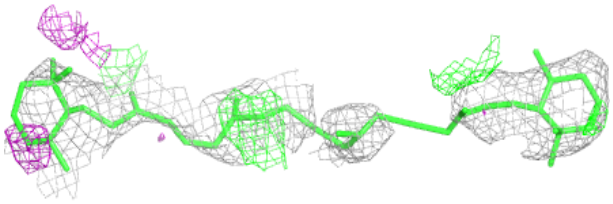


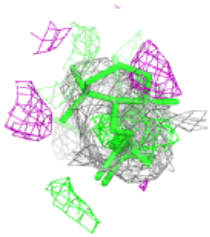


Electron density around BCR h 101:

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

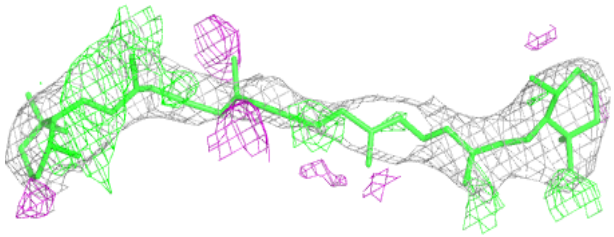


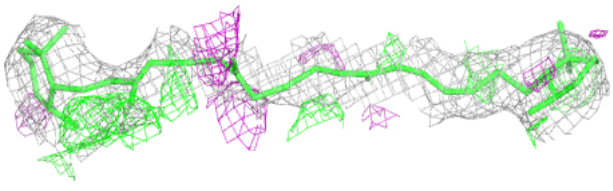


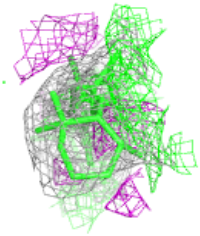


Electron density around BCR B 619:

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

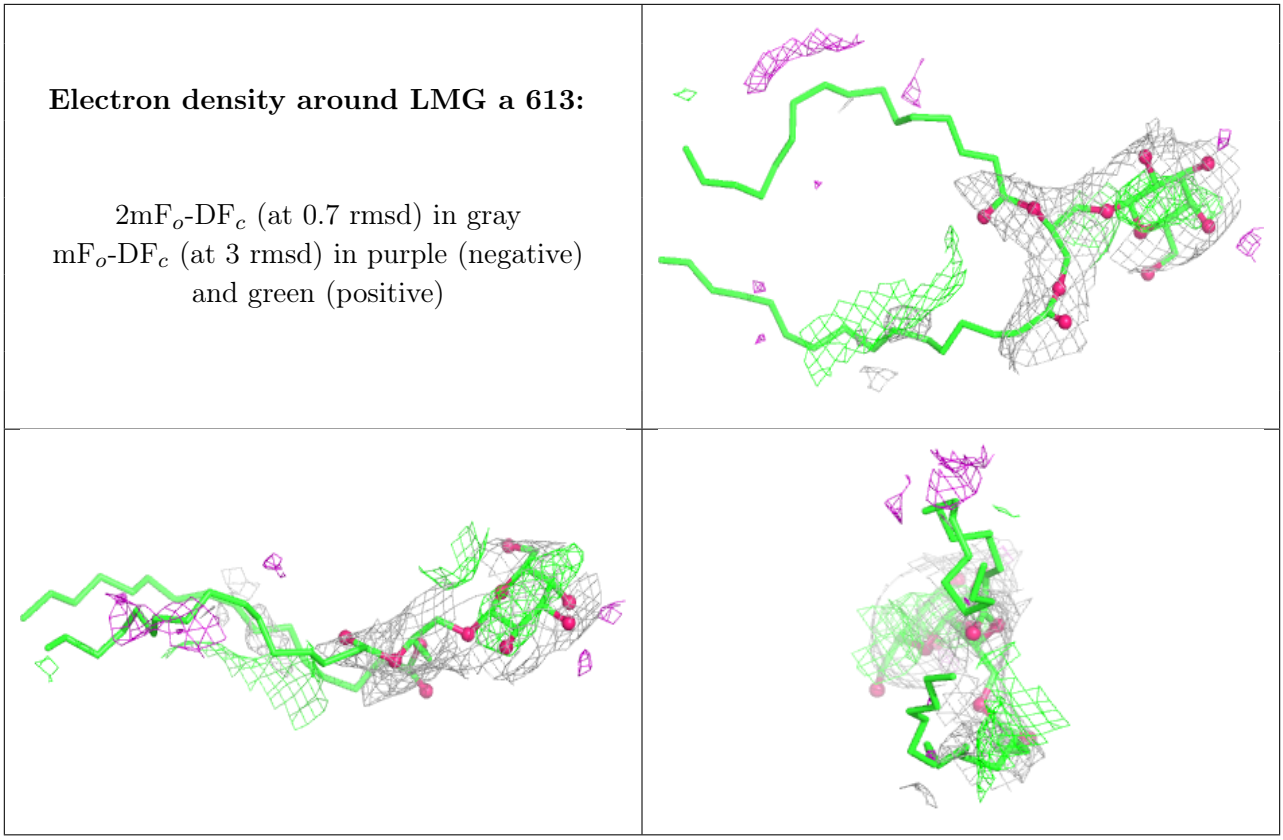






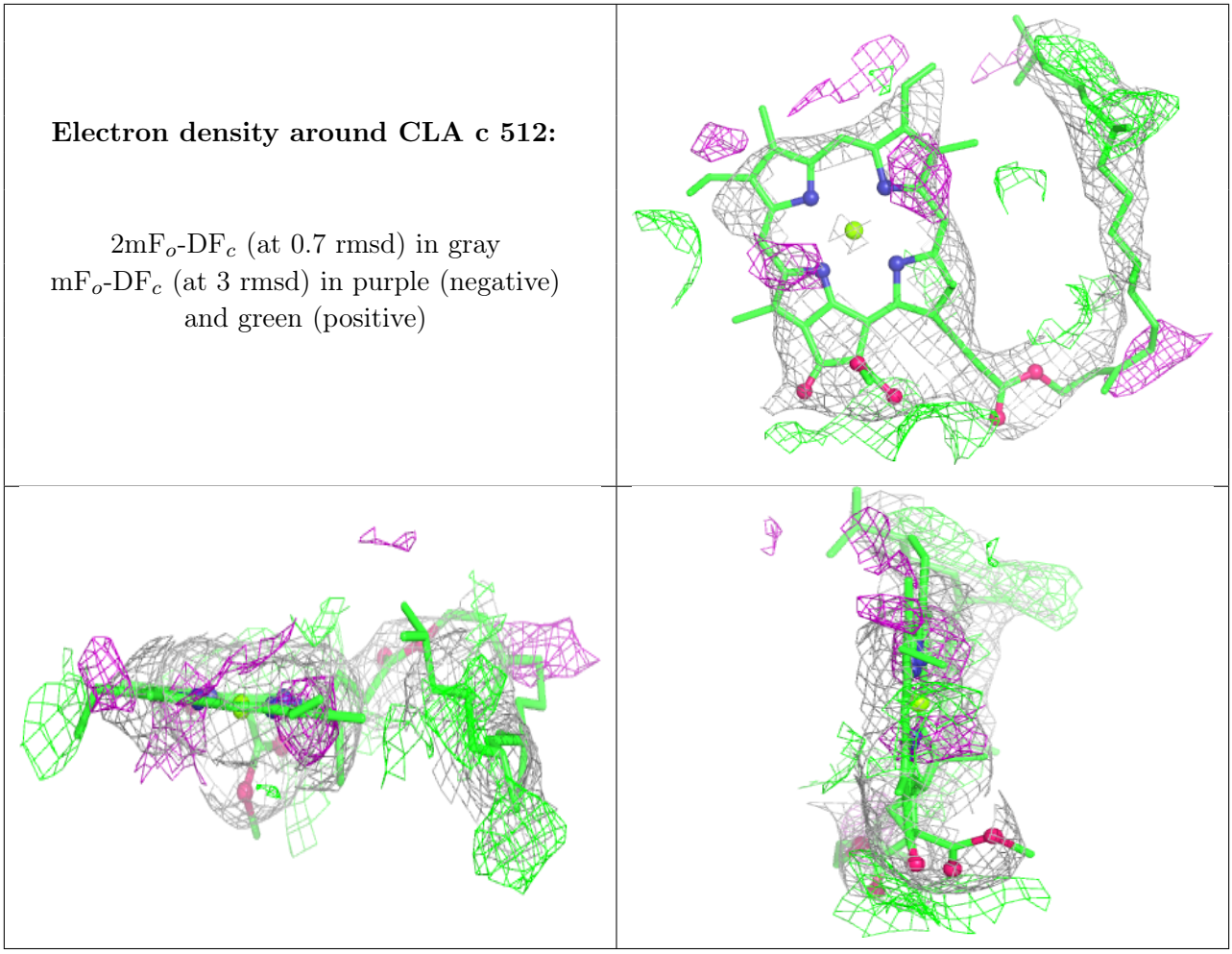
Electron density around LMG a 613:

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



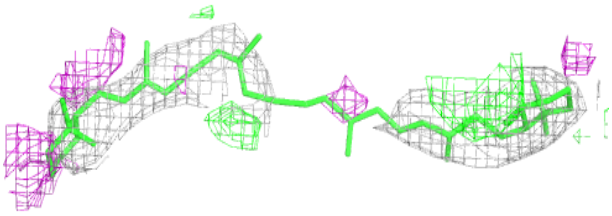
Electron density around CLA c 512:

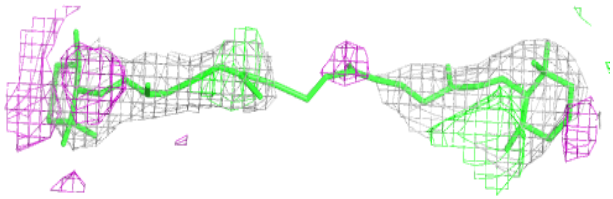
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

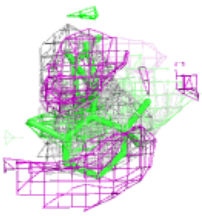


Electron density around BCR I 101:

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

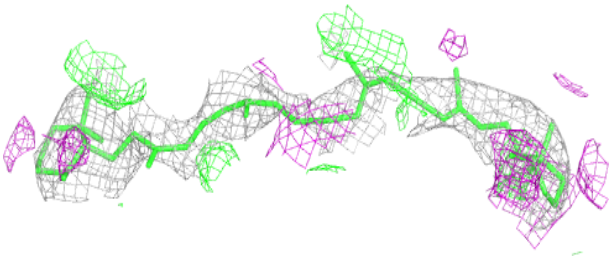


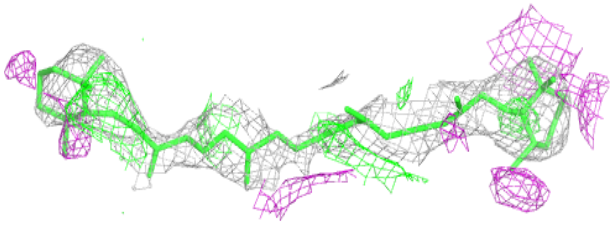


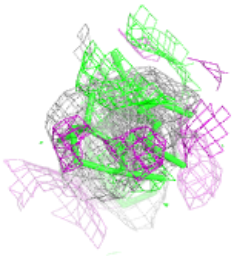


Electron density around BCR T 101:

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

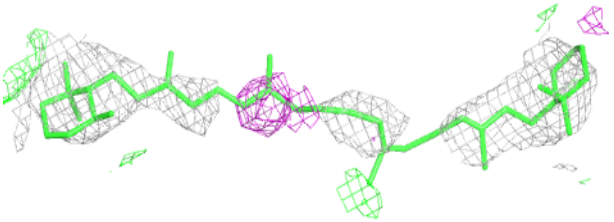


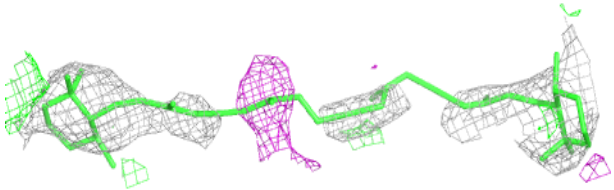


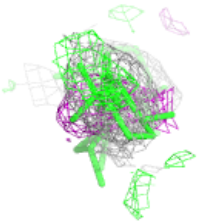


Electron density around BCR c 515:

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

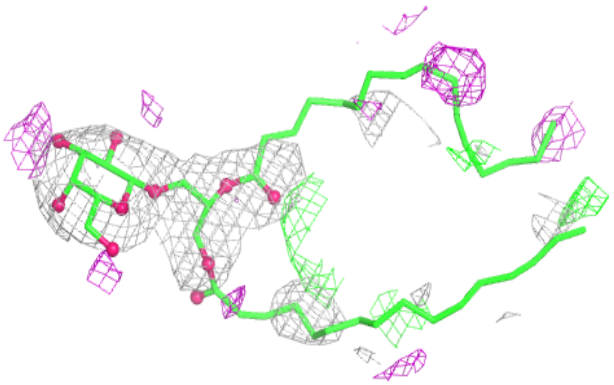


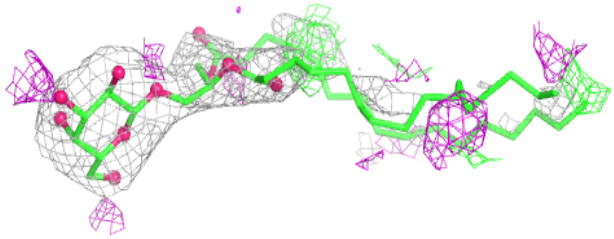


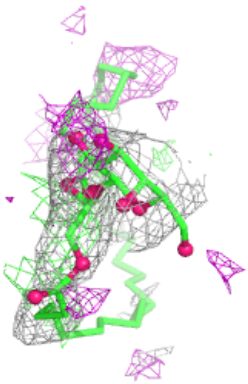


Electron density around LMG A 613:

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

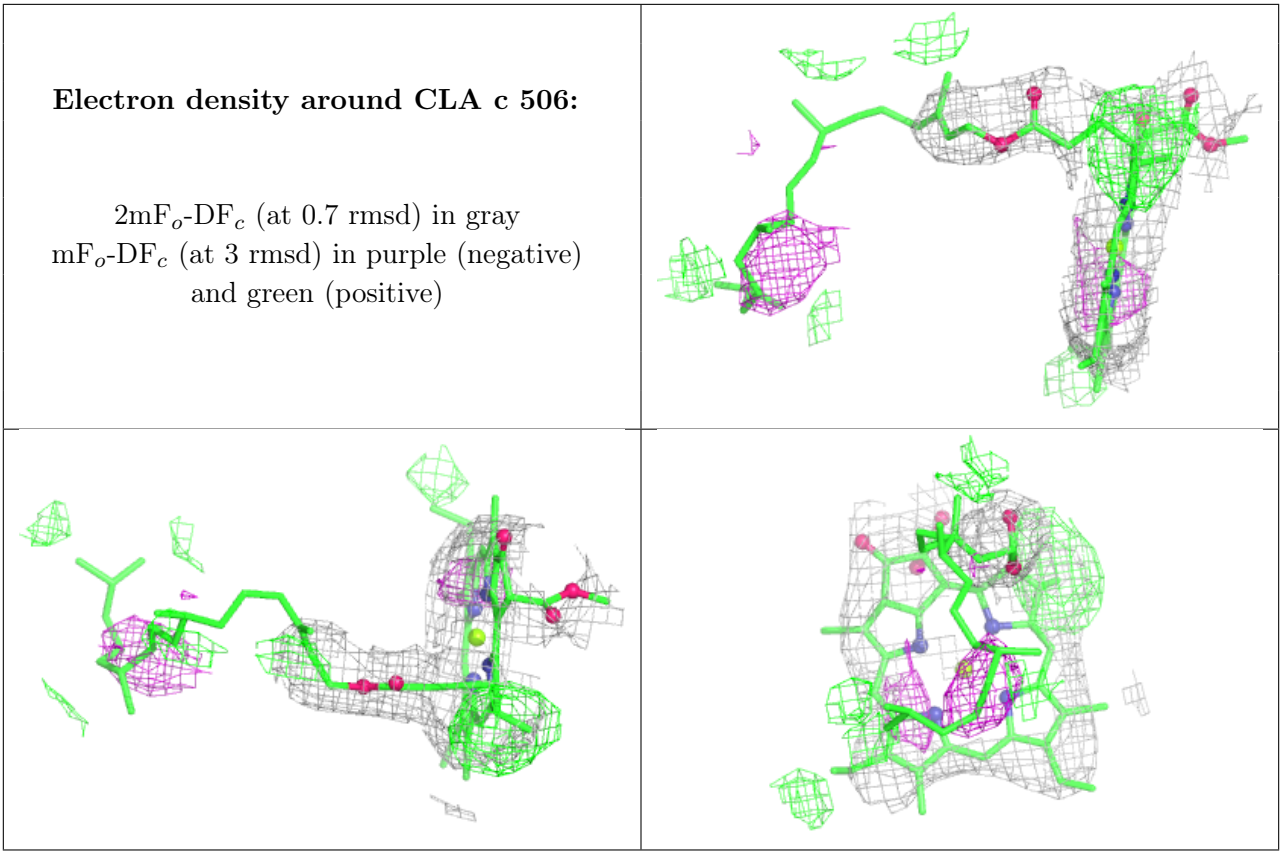






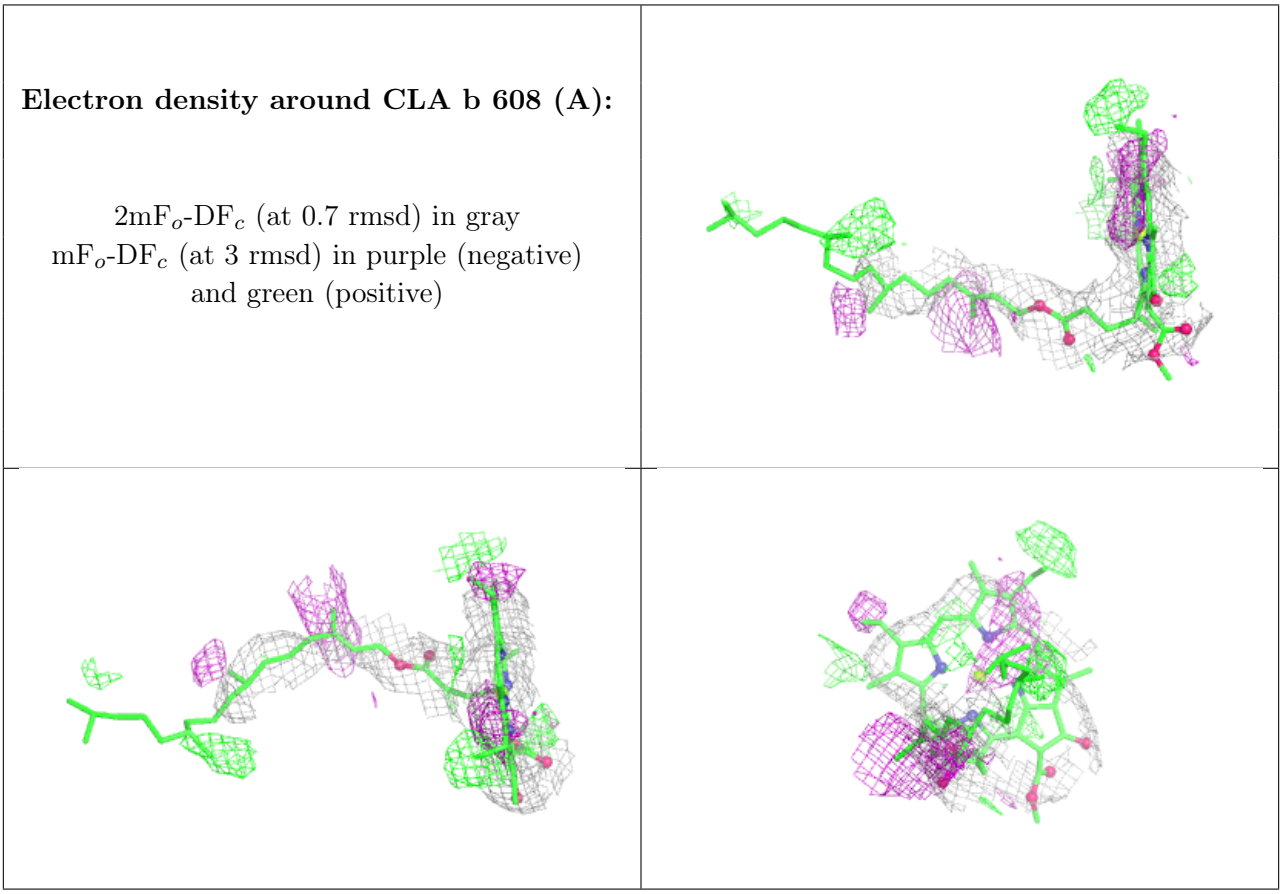
Electron density around CLA c 506:

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



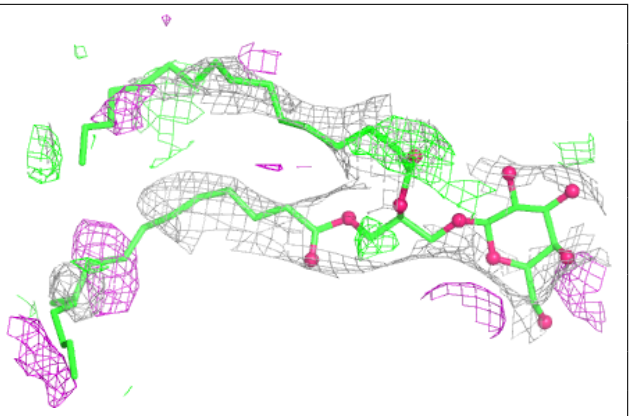
Electron density around CLA b 608 (A):

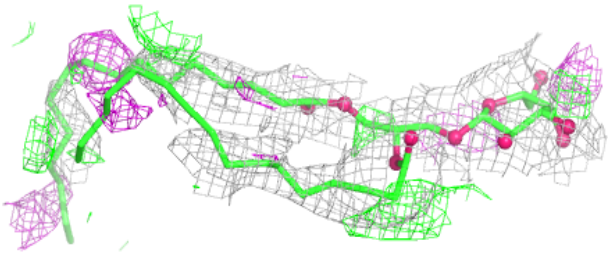
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

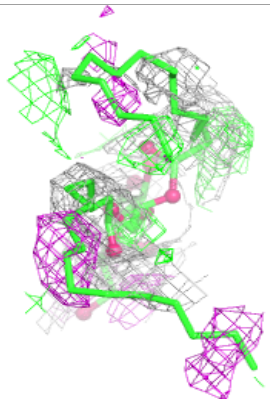


Electron density around LMG D 408:

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

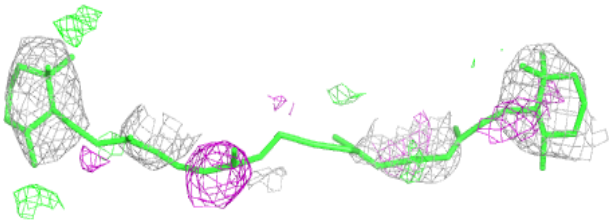


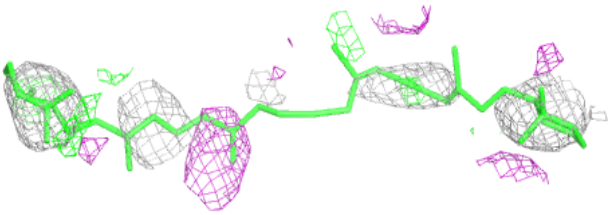


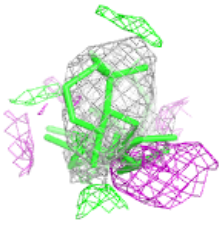


Electron density around BCR c 521:

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

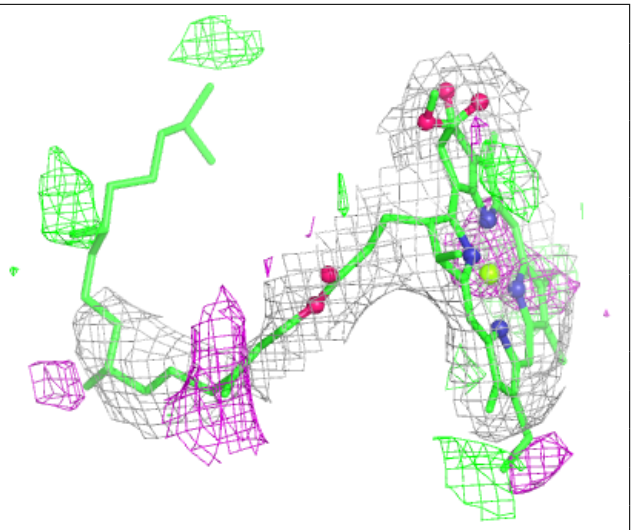


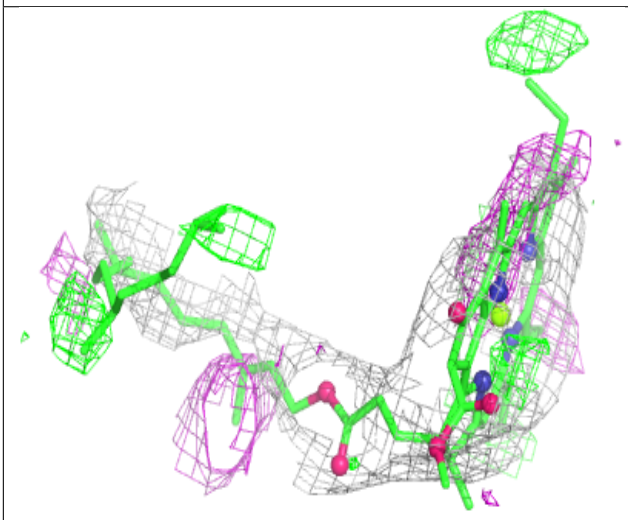


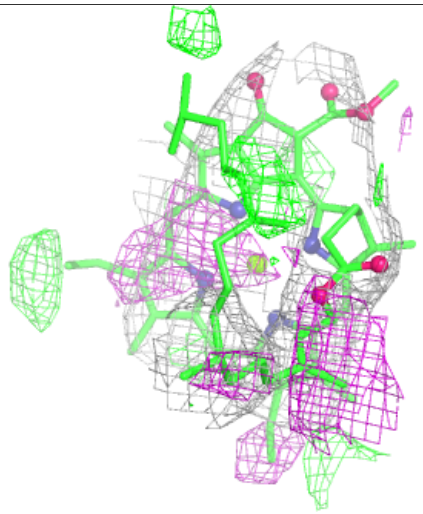


Electron density around CLA b 608 (B):

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

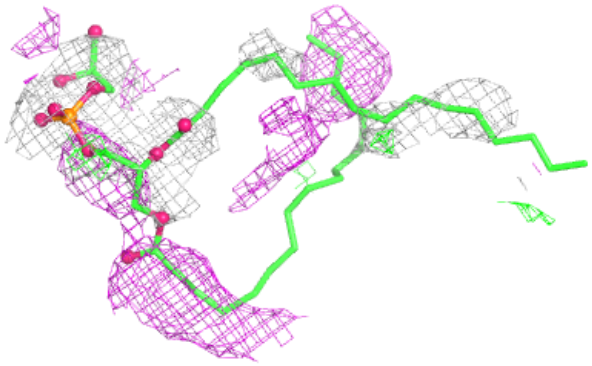


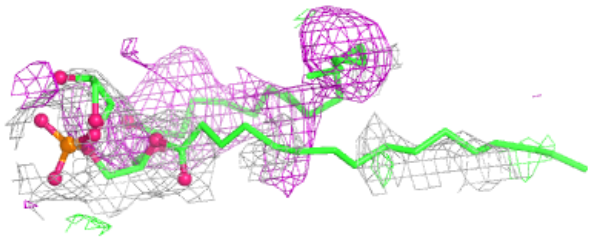


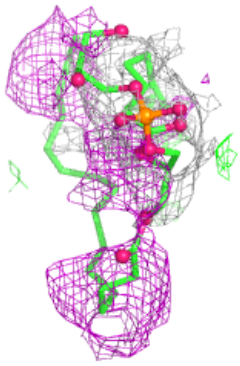


Electron density around LHG a 616:

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

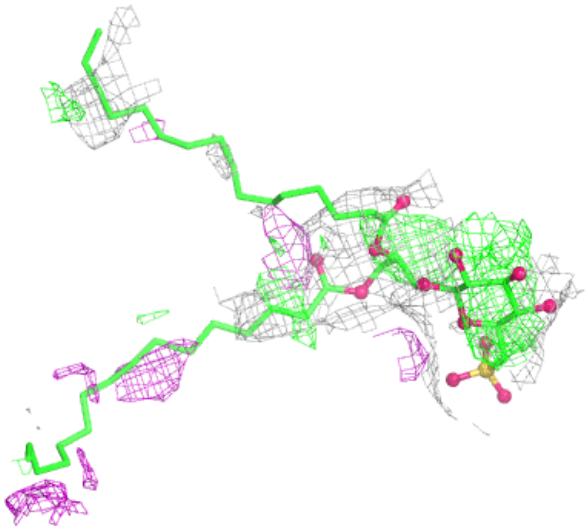


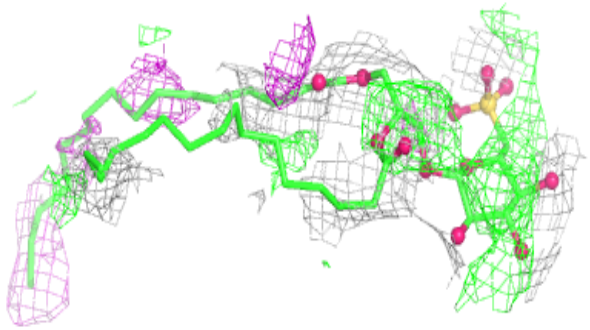


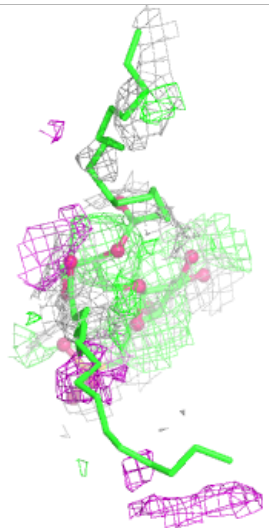


Electron density around SQD A 612:

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

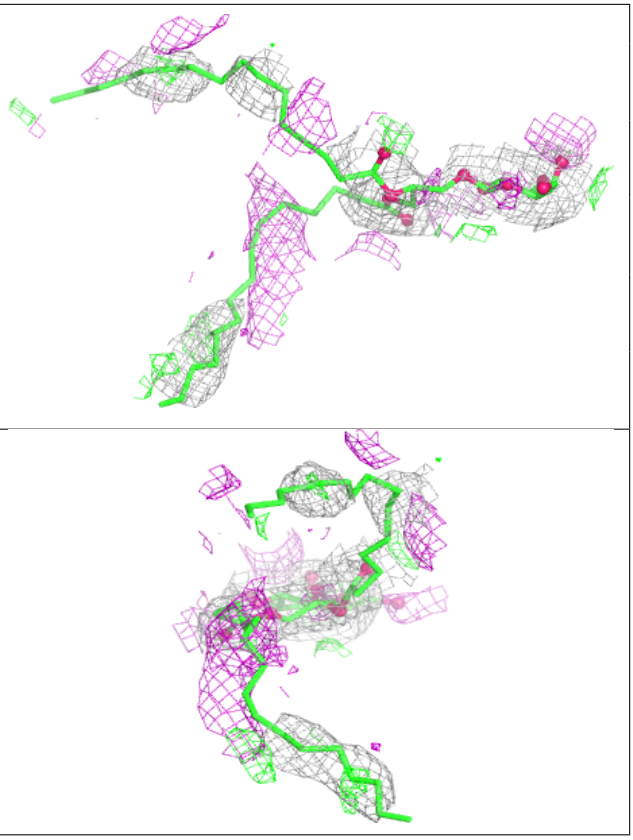


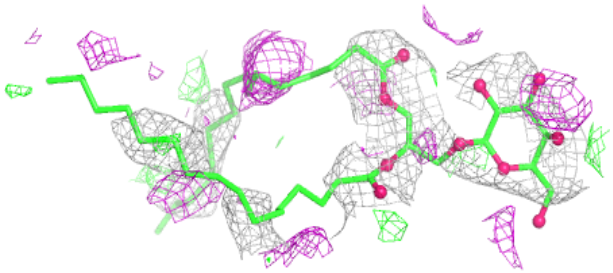




Electron density around LMG B 621:

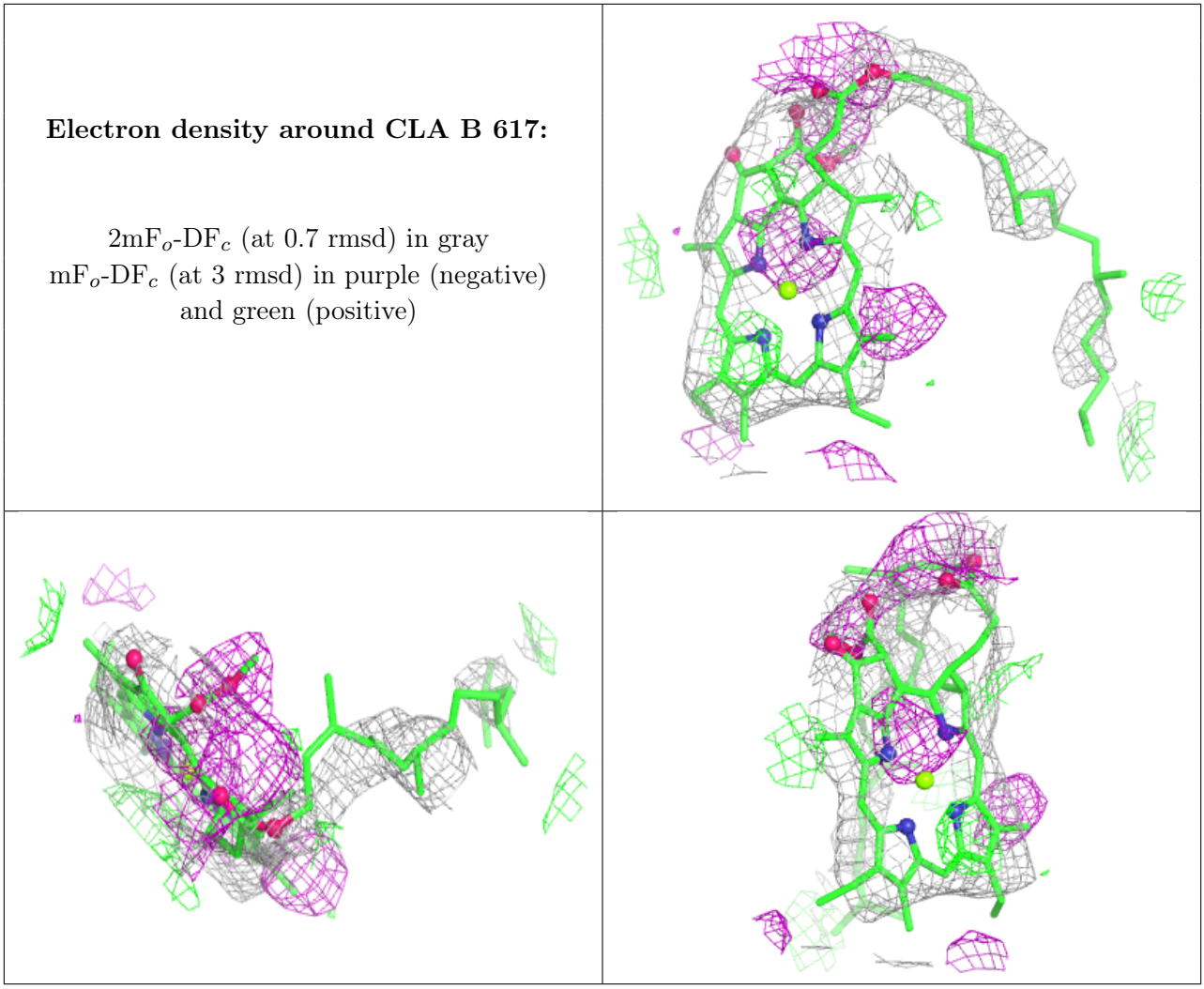
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





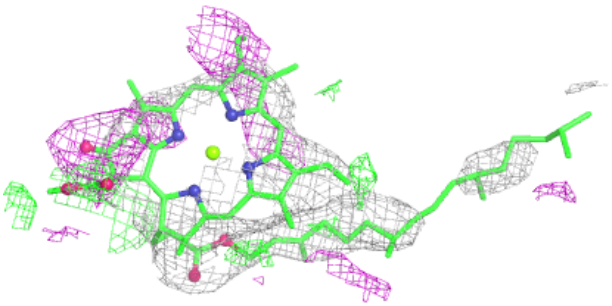
Electron density around CLA B 617:

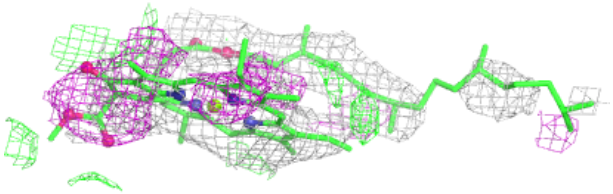
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

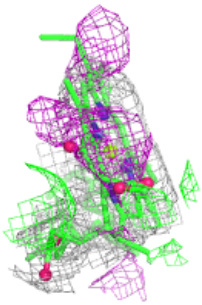


Electron density around CLA c 501:

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

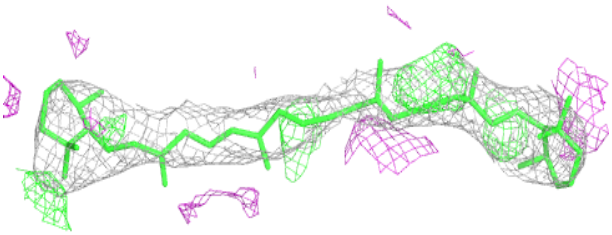


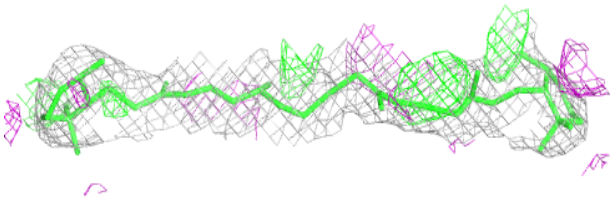


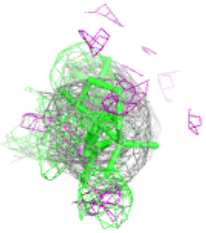


Electron density around BCR b 620:

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

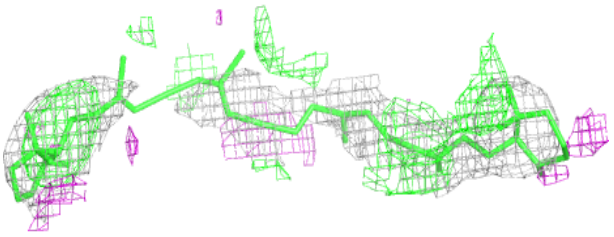


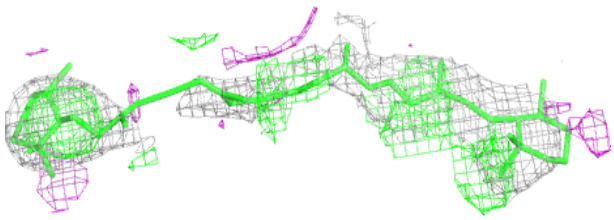


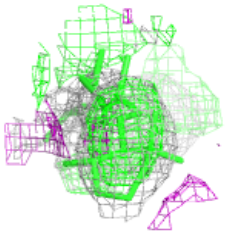


Electron density around BCR t 101:

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

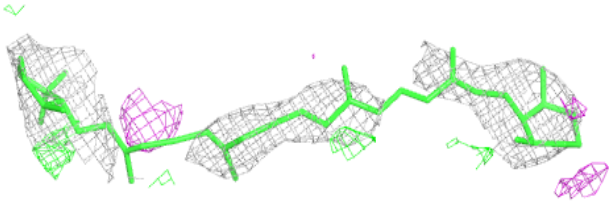


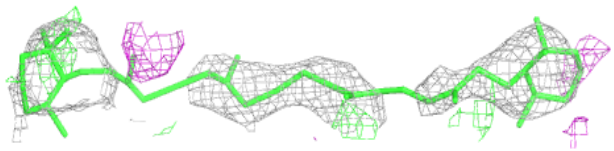


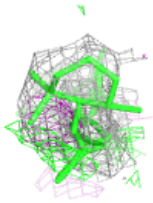


Electron density around BCR C 514:

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

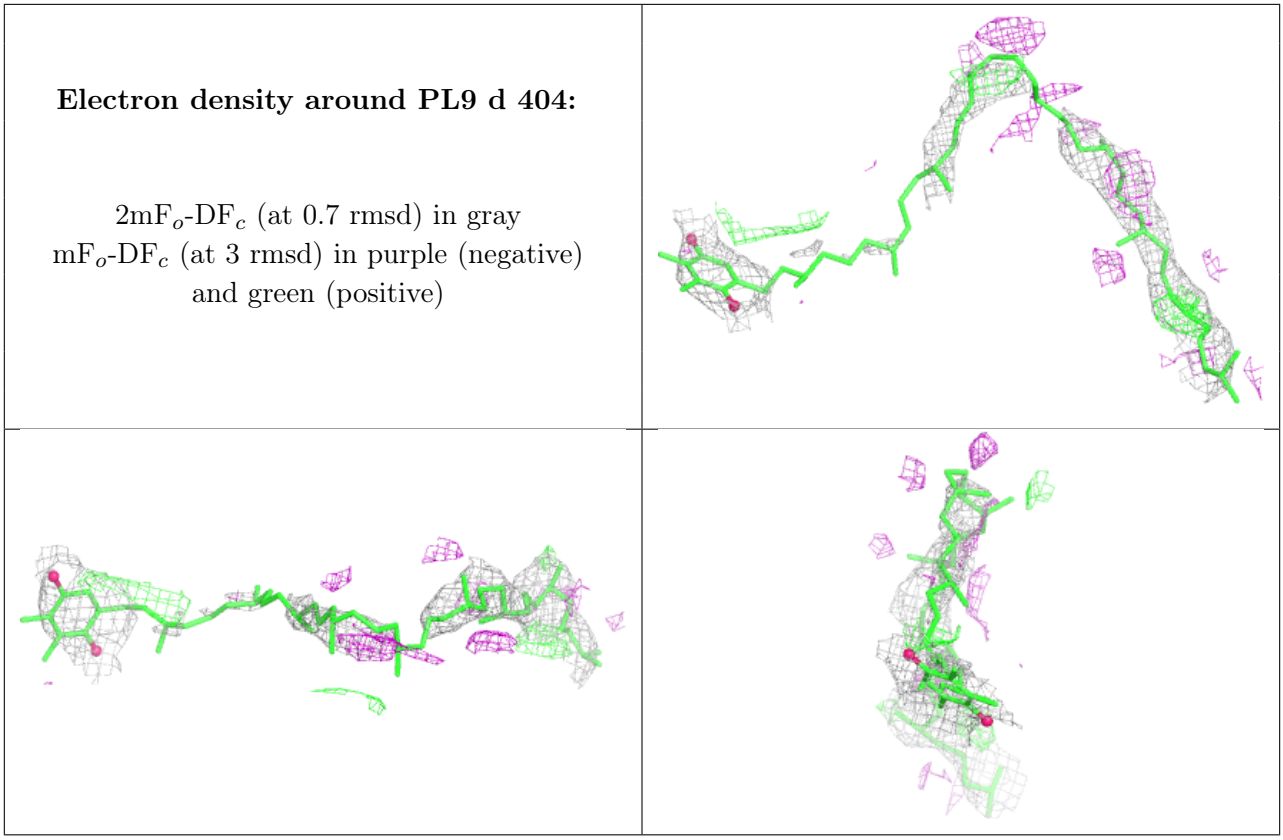






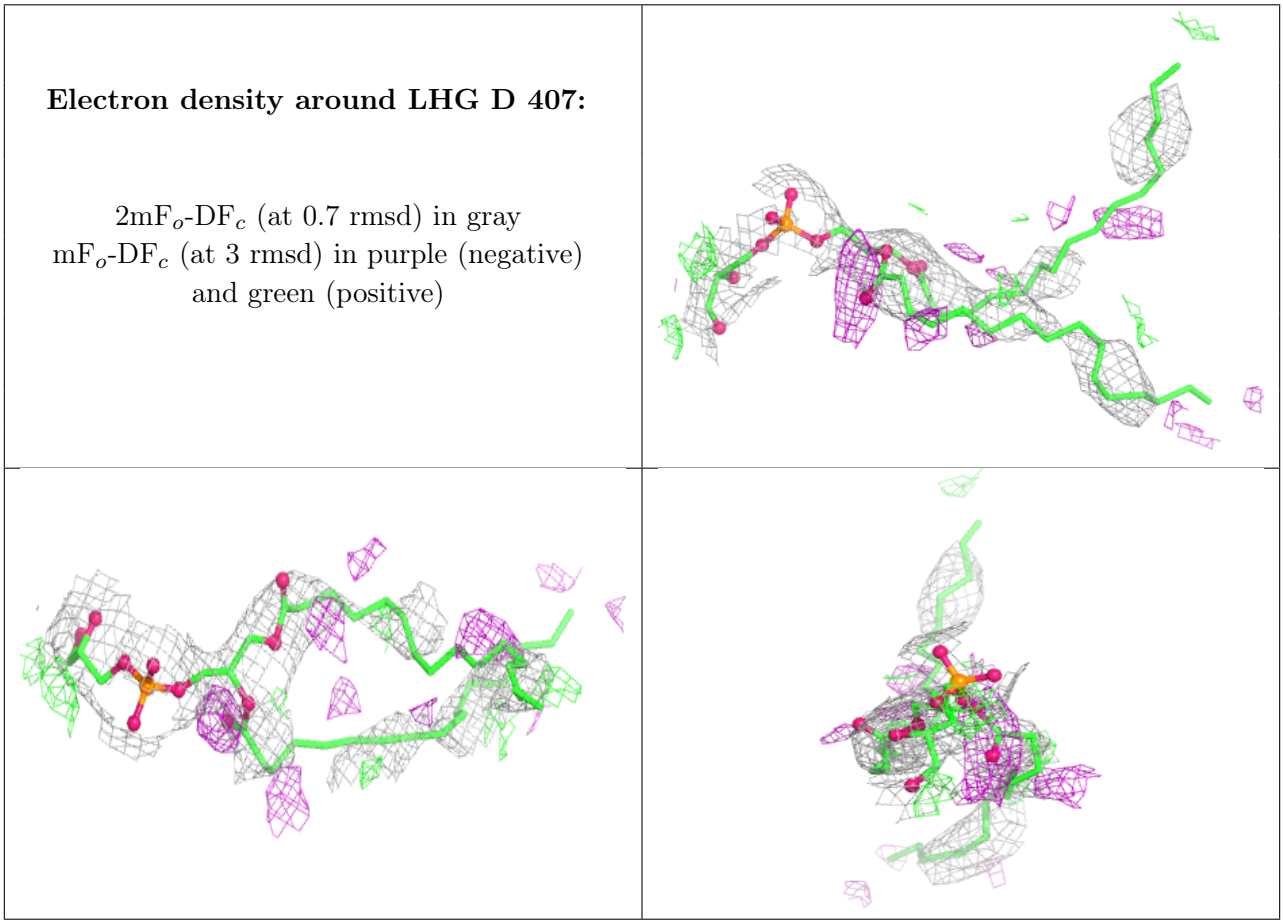
Electron density around PL9 d 404:

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



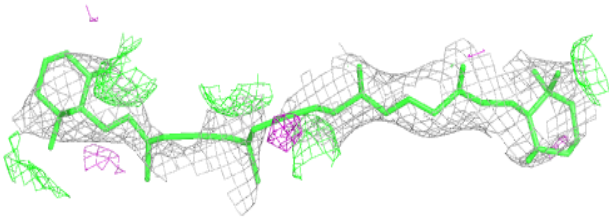
Electron density around LHG D 407:

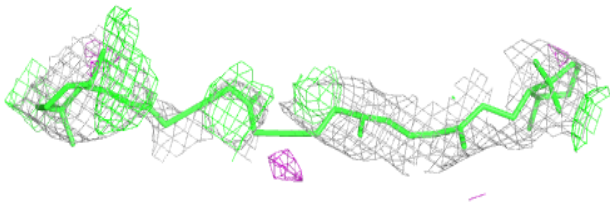
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

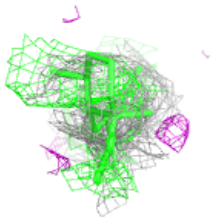


Electron density around BCR b 621:

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

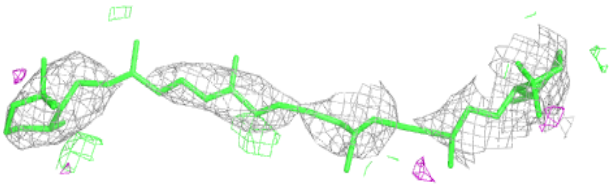


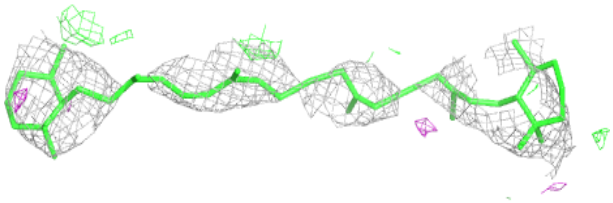


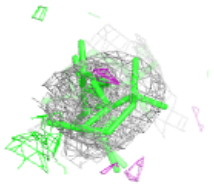


Electron density around BCR c 514:

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

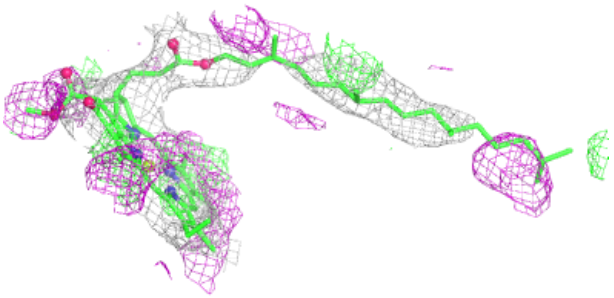


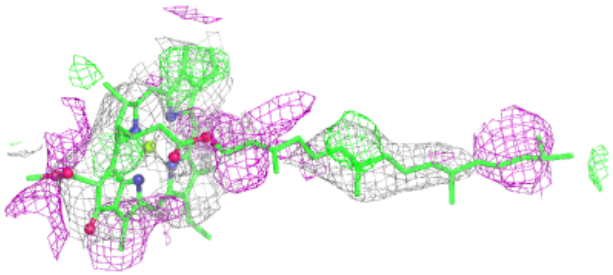


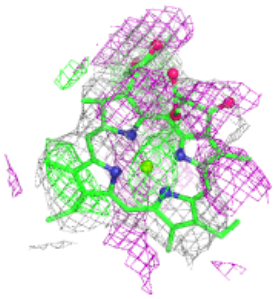


Electron density around CLA b 609:

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

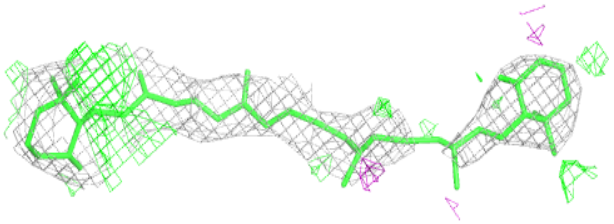


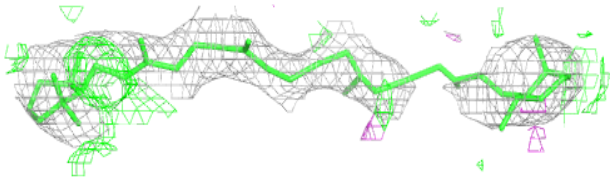


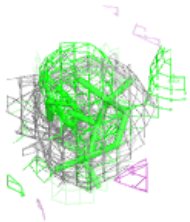


Electron density around BCR B 620:

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

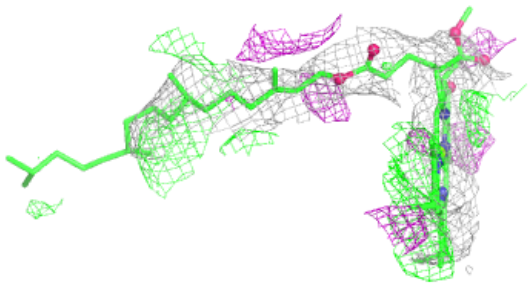


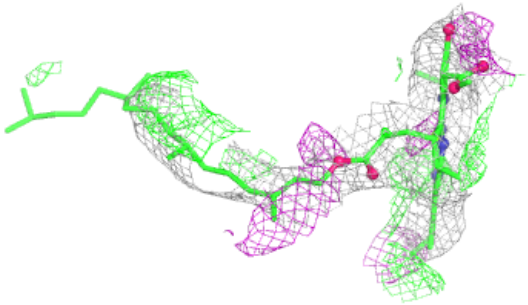


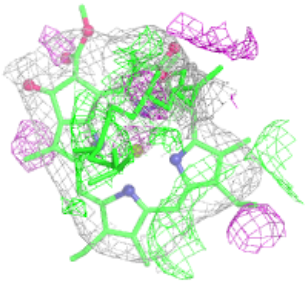


Electron density around CLA B 607 (A):

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

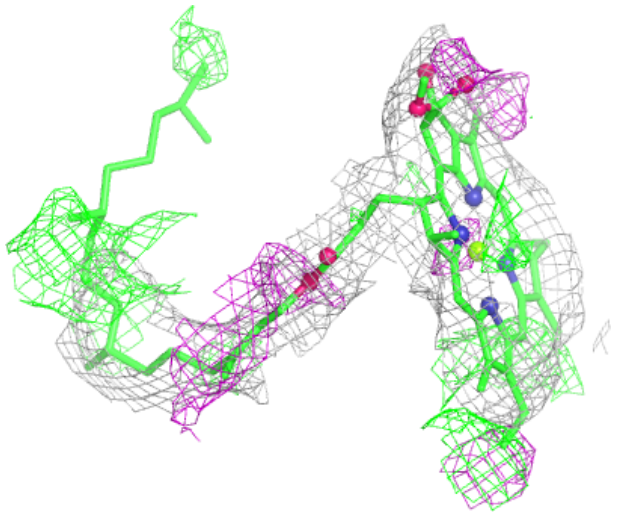


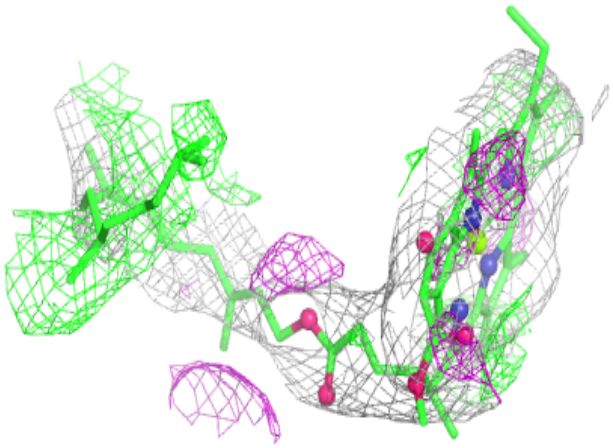


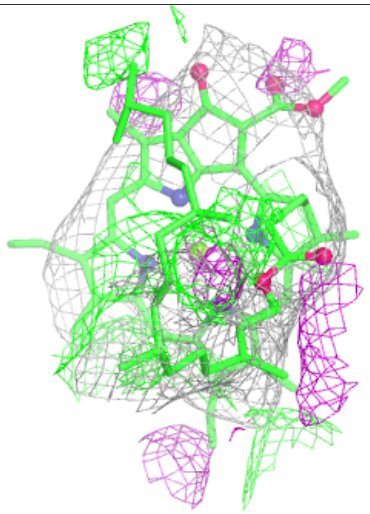


Electron density around CLA B 607 (B):

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

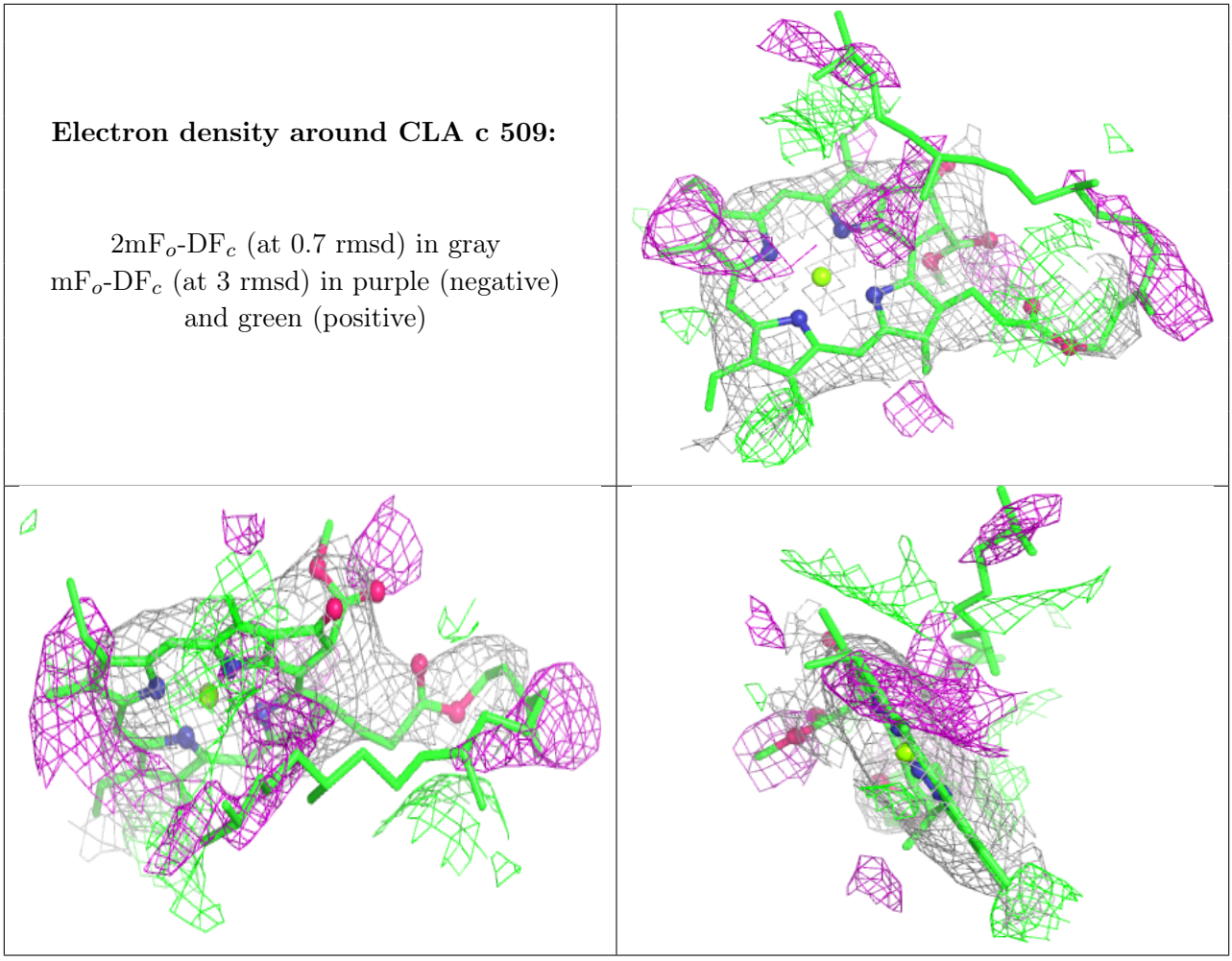






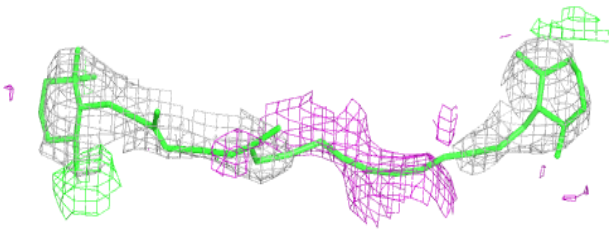
Electron density around CLA c 509:

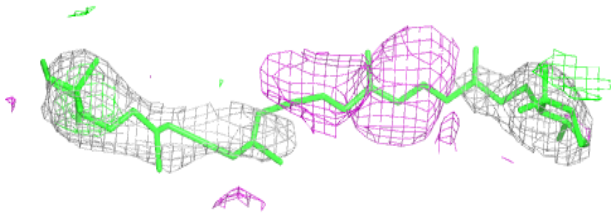
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

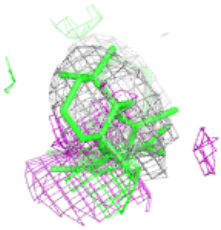


Electron density around BCR K 102:

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

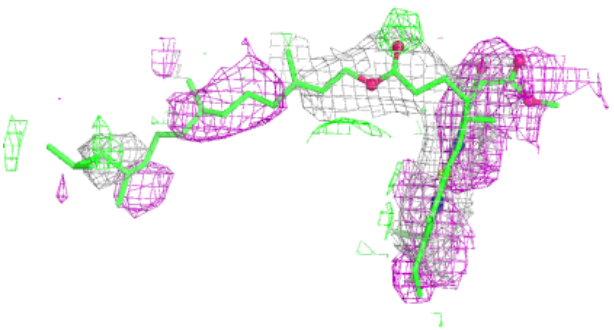


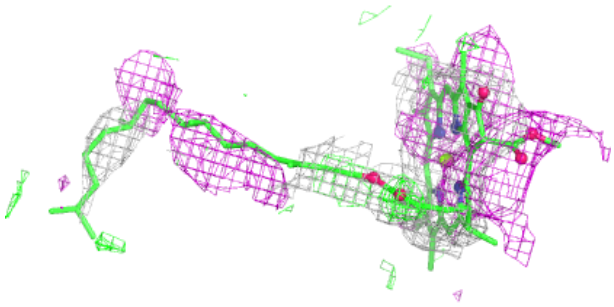


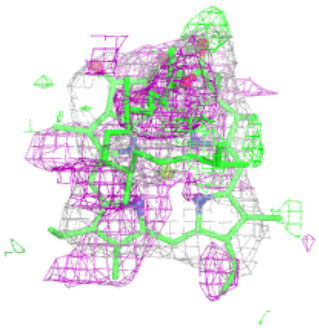


Electron density around CLA B 606:

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

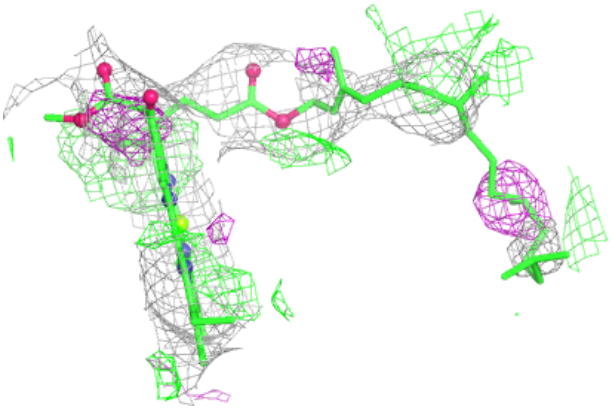


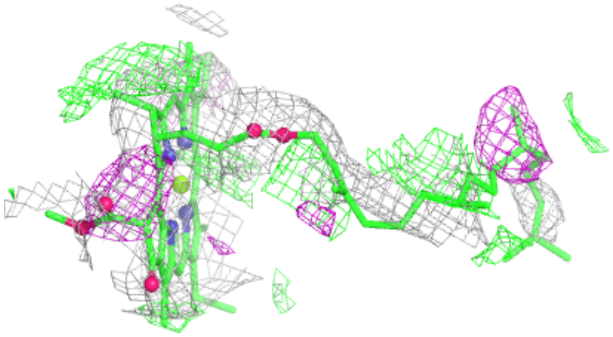


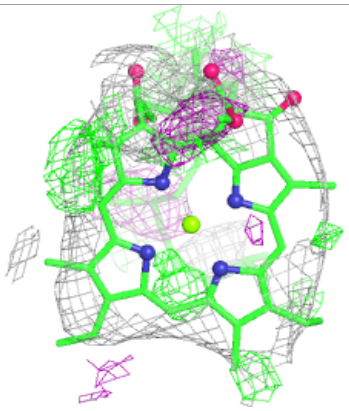


Electron density around CLA C 506:

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

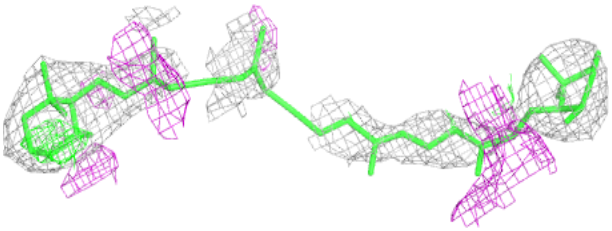


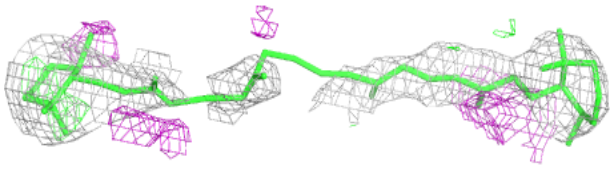


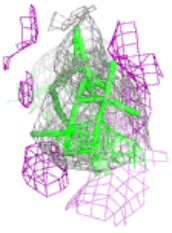


Electron density around BCR K 101:

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

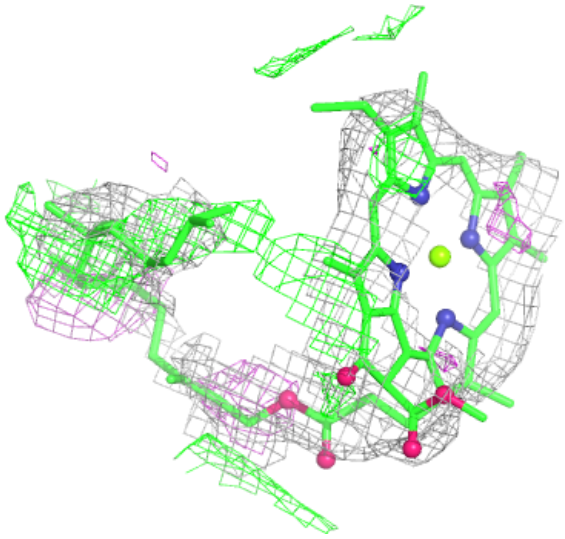


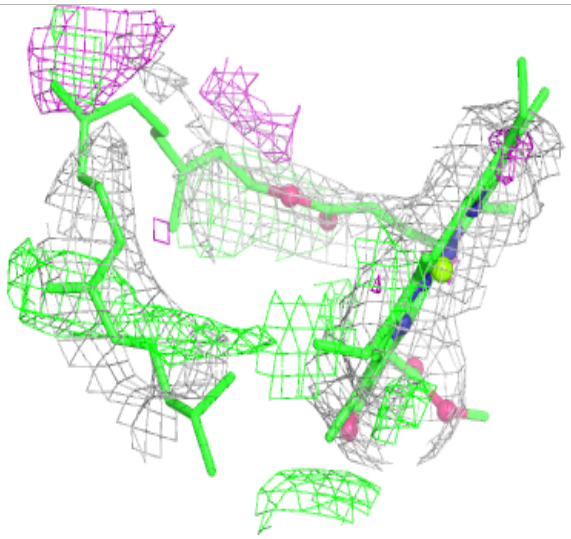


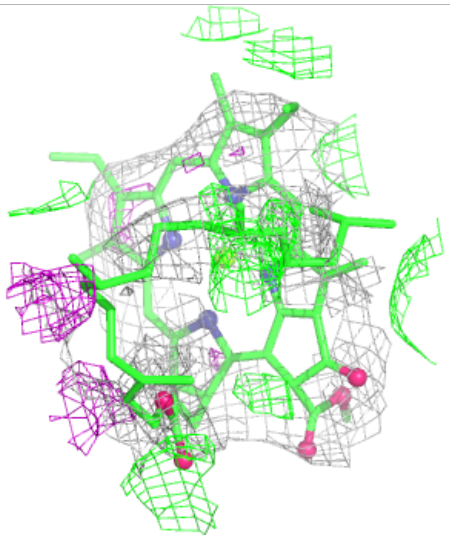


Electron density around CLA c 503:

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

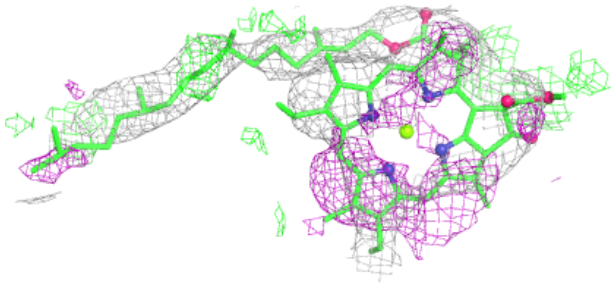


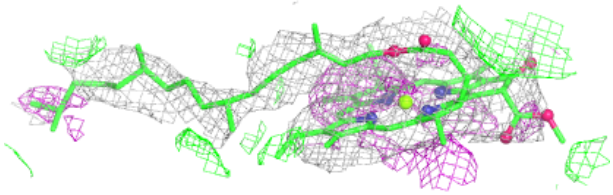


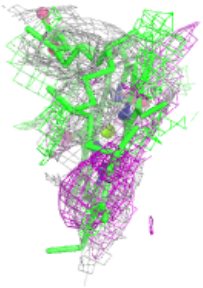


Electron density around CLA C 501:

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

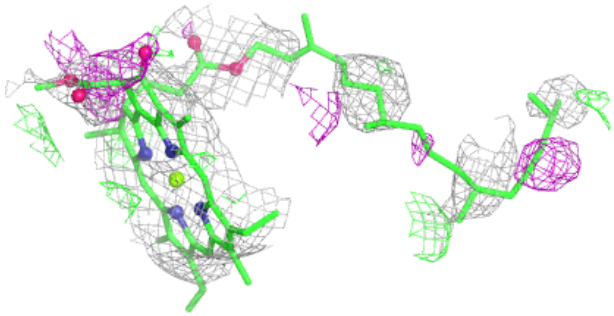


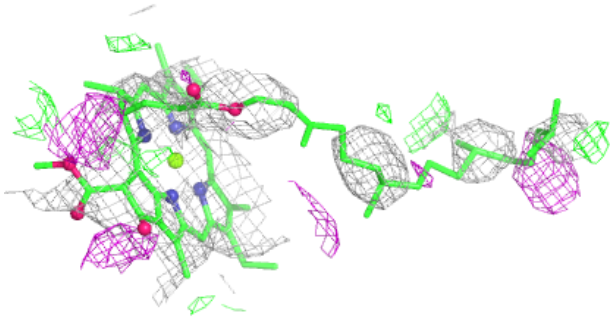


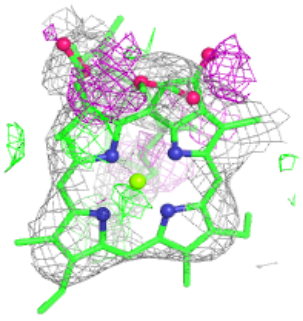


Electron density around CLA c 508:

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

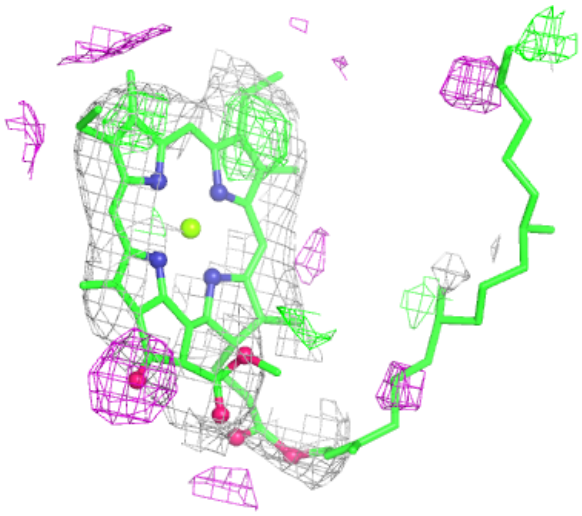


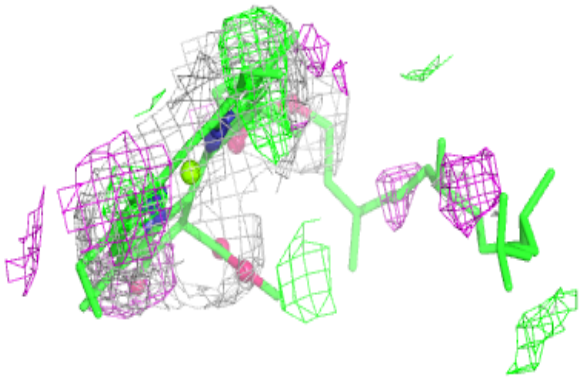


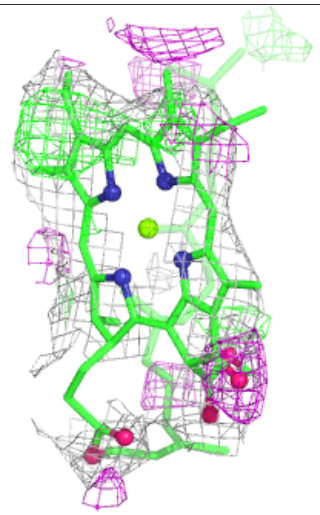


Electron density around CLA b 618:

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

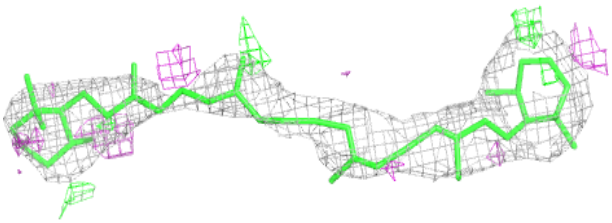


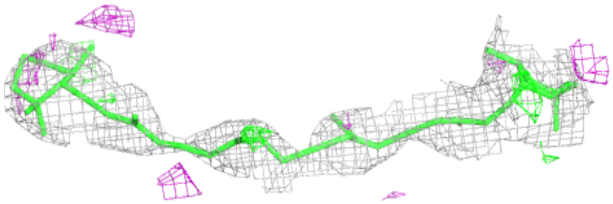


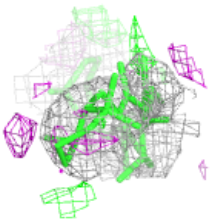


Electron density around BCR F 101:

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

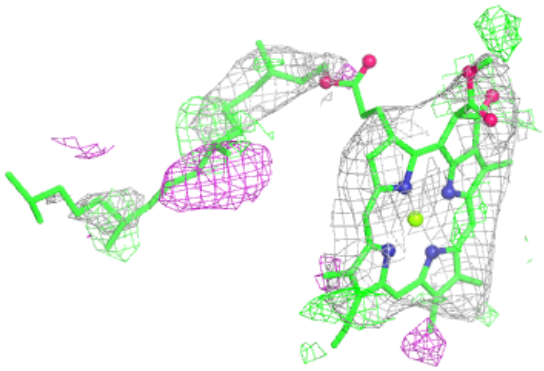


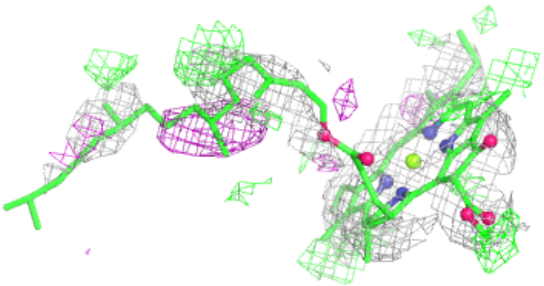


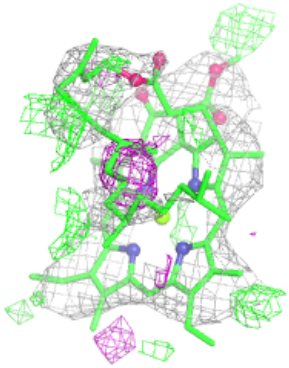


Electron density around CLA c 511:

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

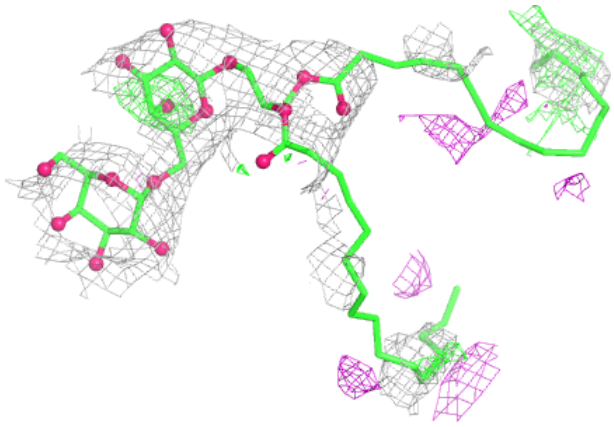


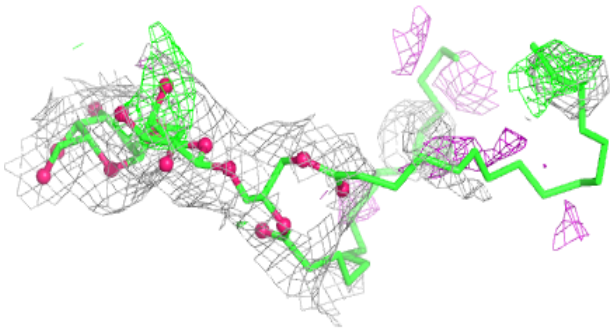


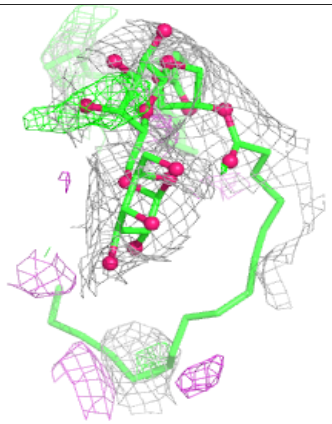


Electron density around DGD c 517:

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

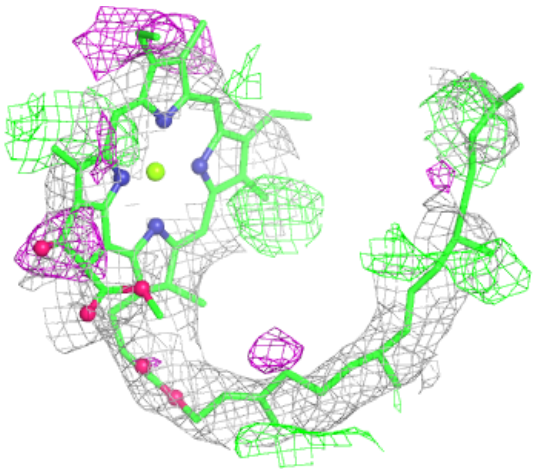


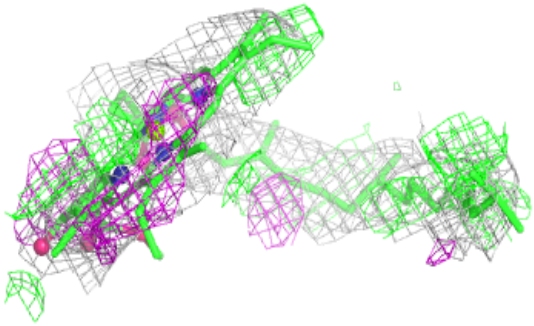


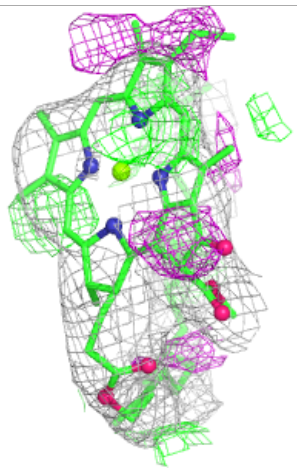


Electron density around CLA C 507:

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

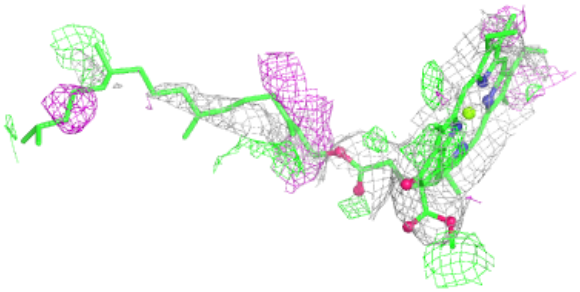


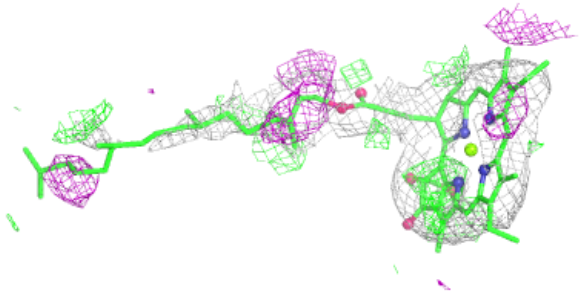


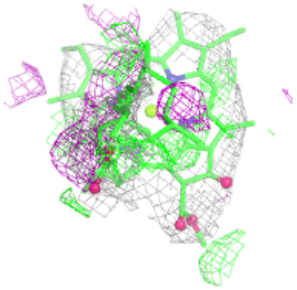


Electron density around CLA b 606:

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

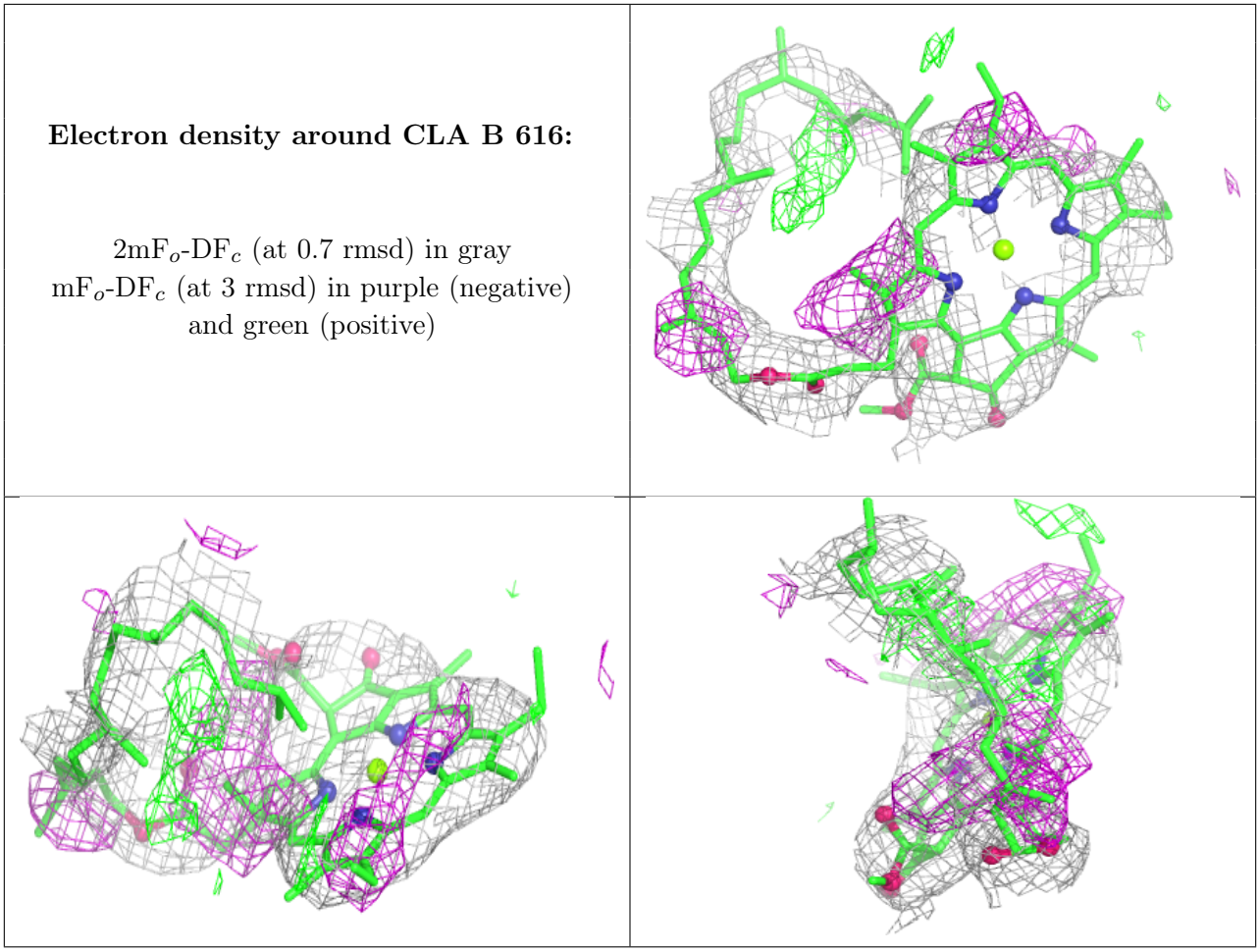






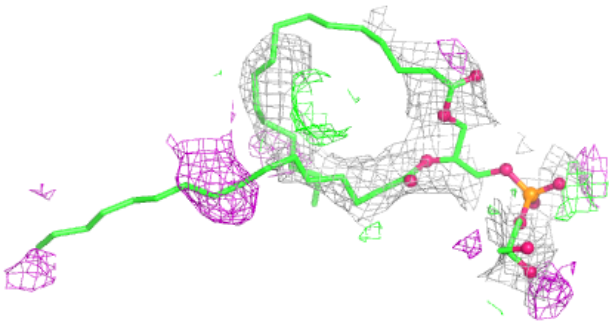
Electron density around CLA B 616:

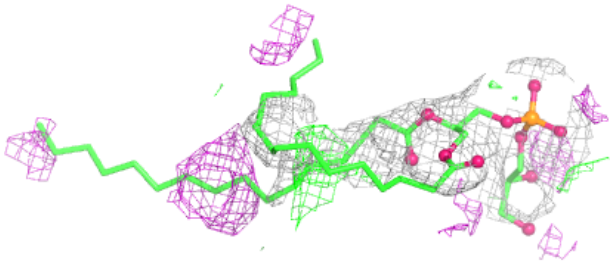
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

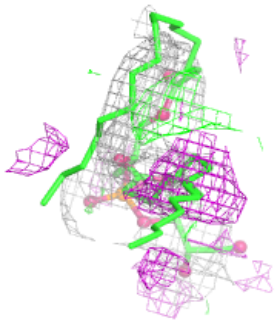


Electron density around LHG d 406:

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

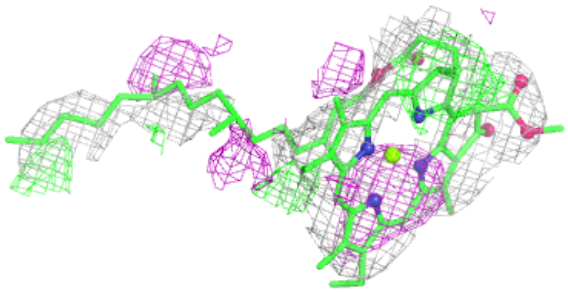


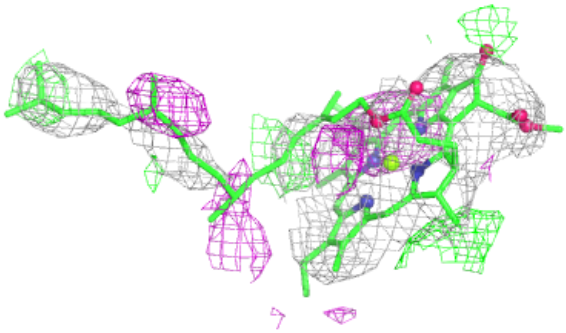


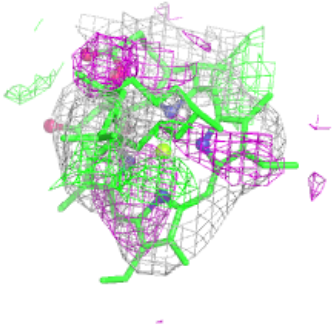


Electron density around CLA C 505:

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

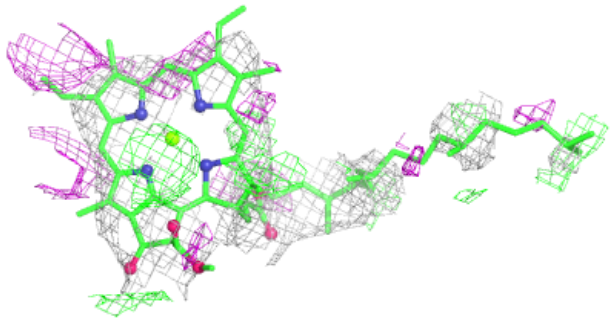


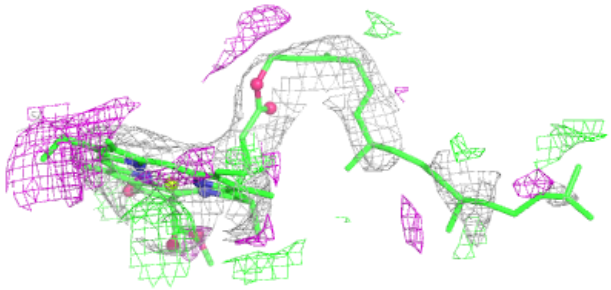


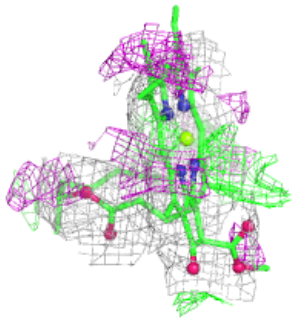


Electron density around CLA a 607:

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

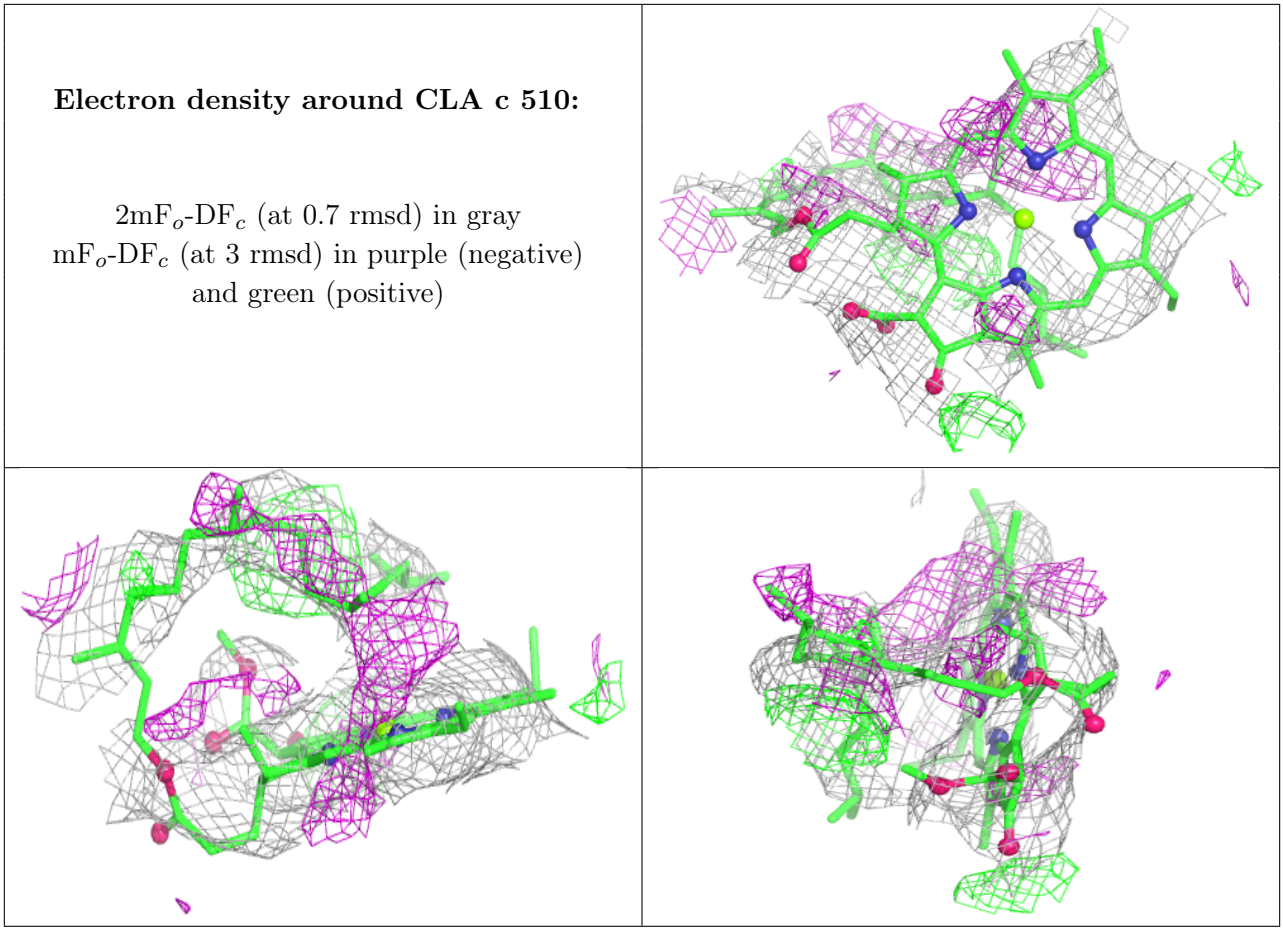






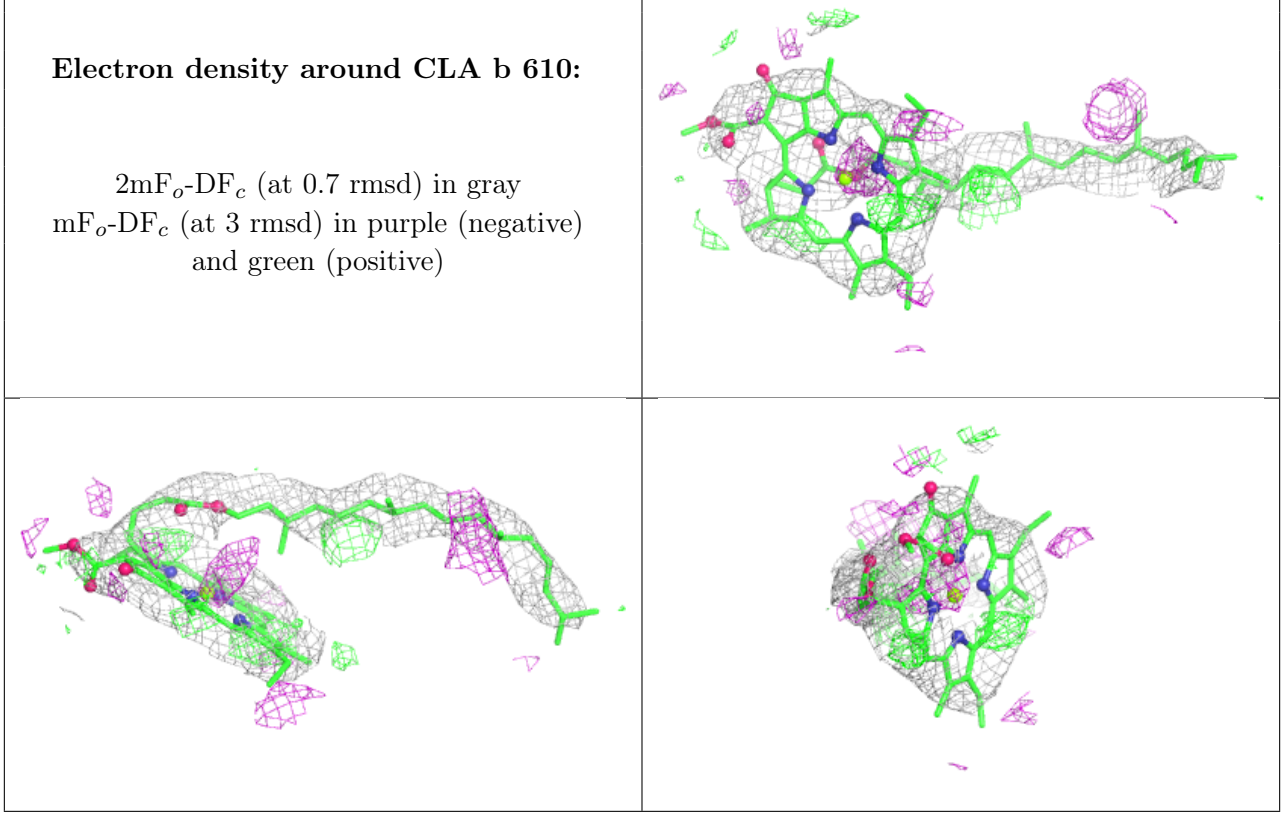
Electron density around CLA c 510:

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



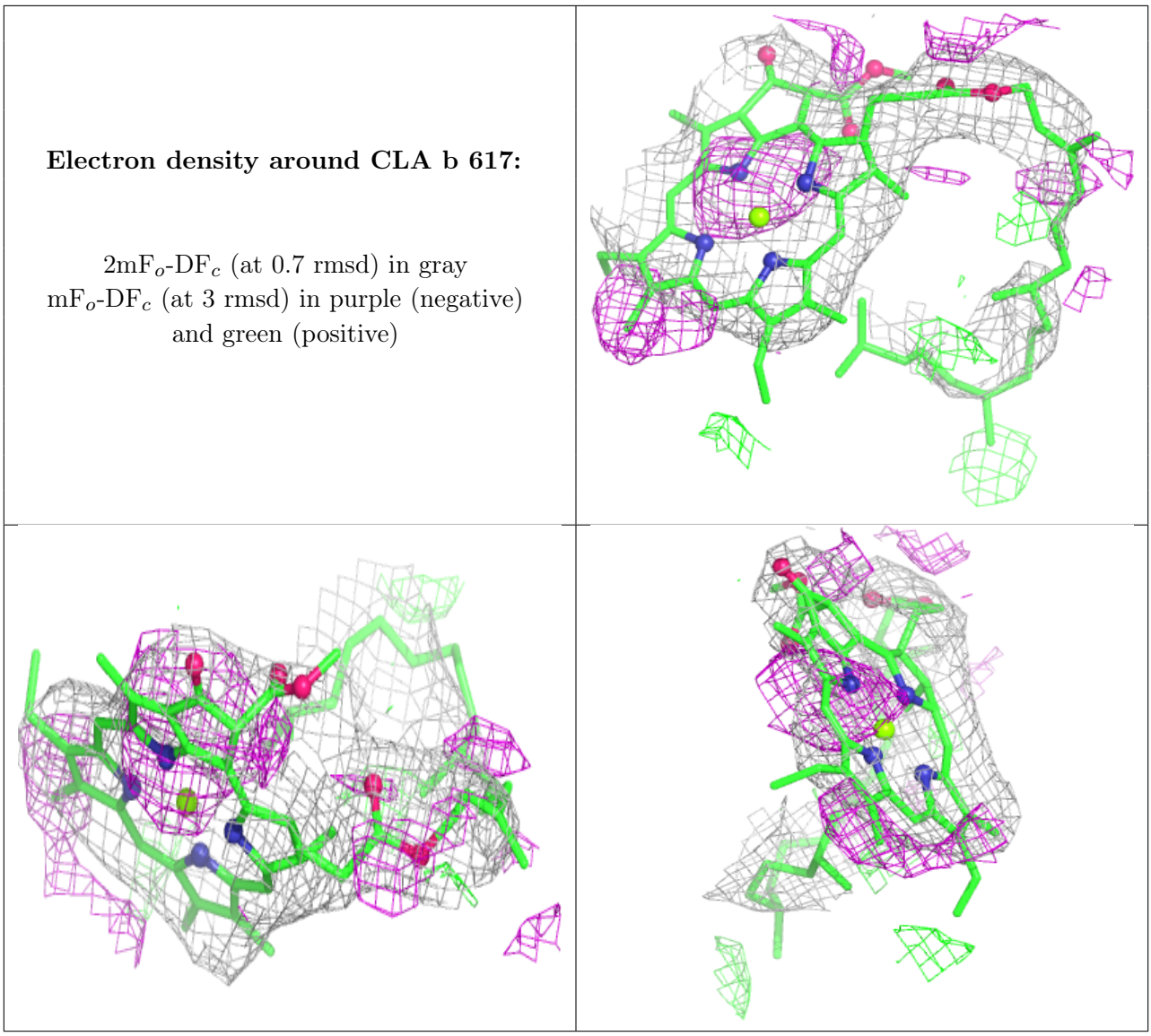
Electron density around CLA b 610:

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



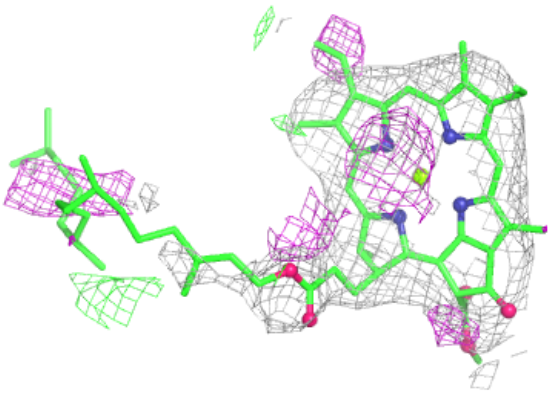
Electron density around CLA b 617:

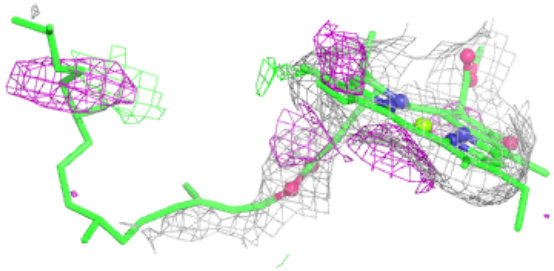
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

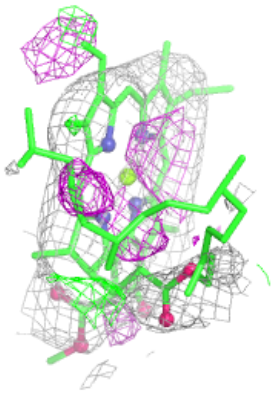


Electron density around CLA a 609:

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

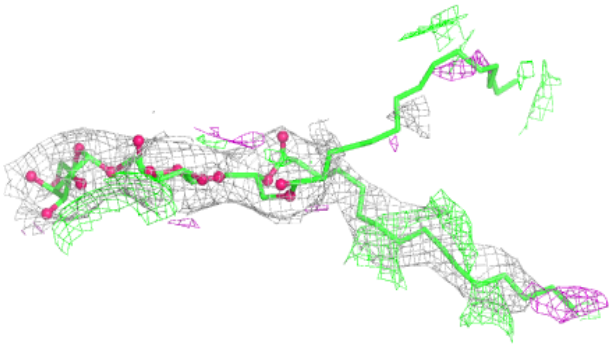


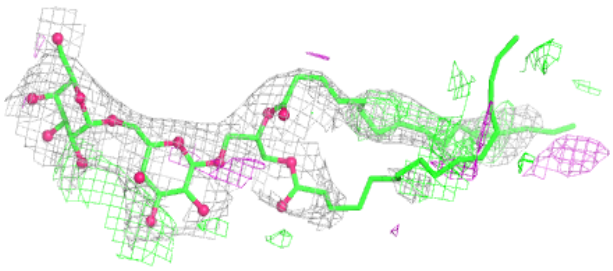


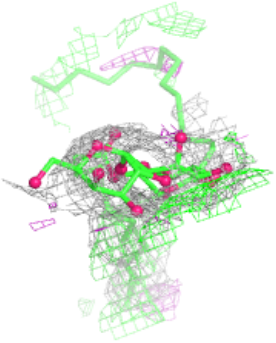


Electron density around DGD C 515:

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

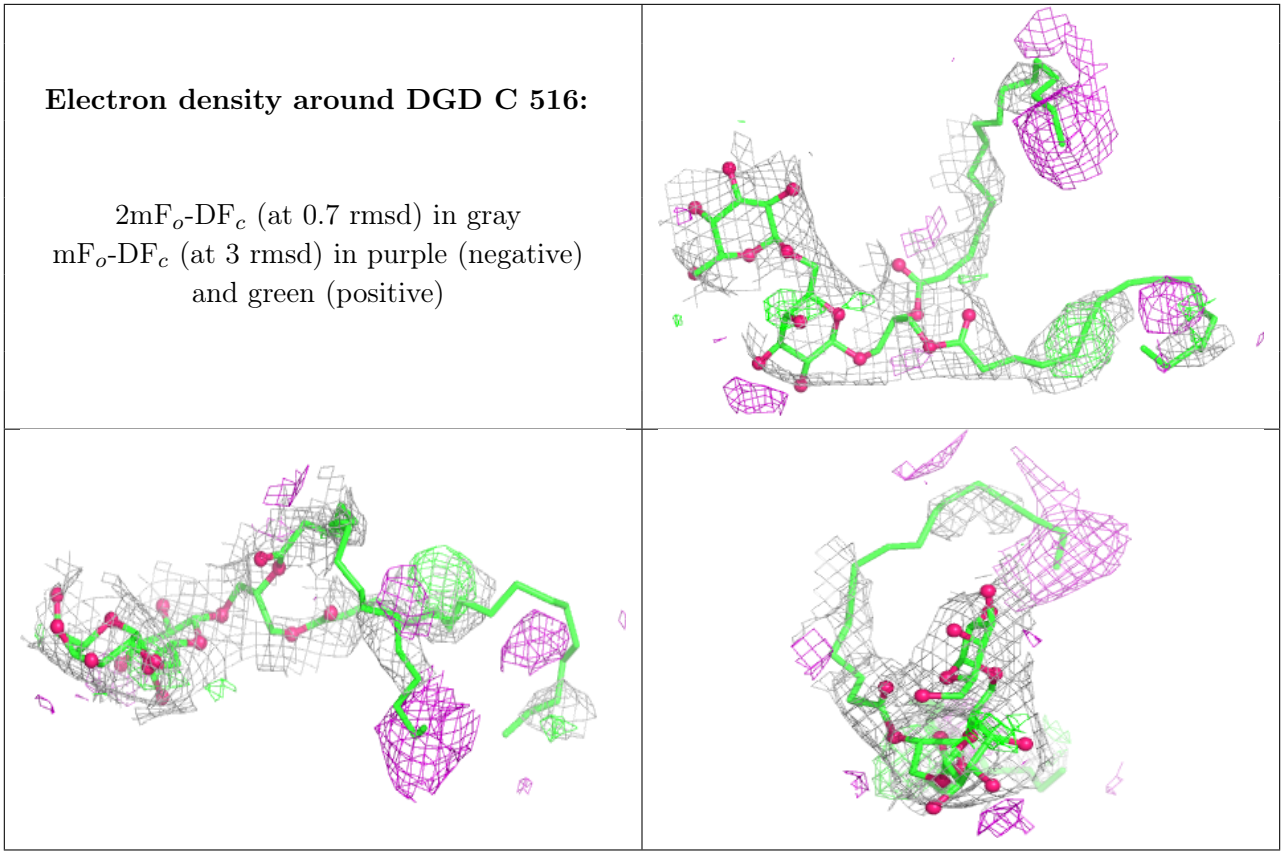






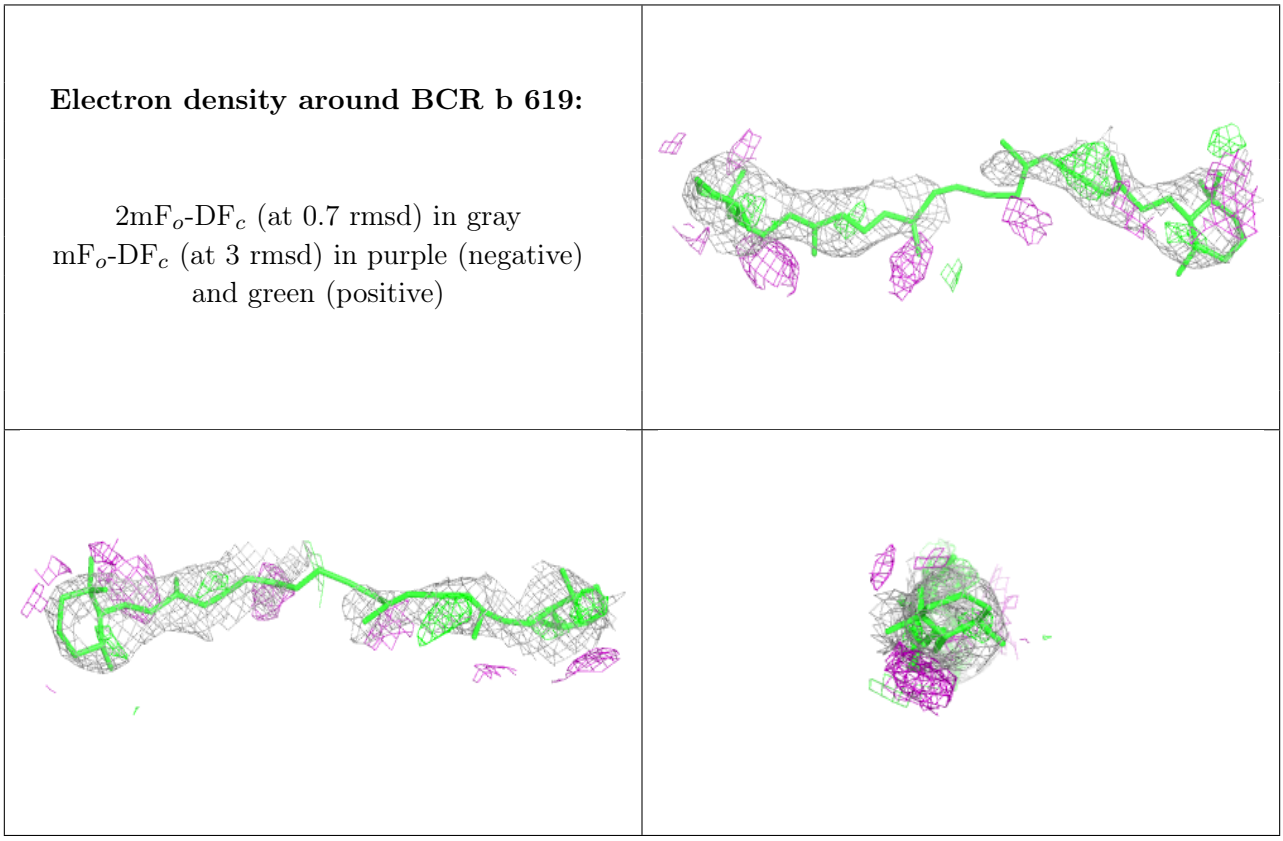
Electron density around DGD C 516:

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



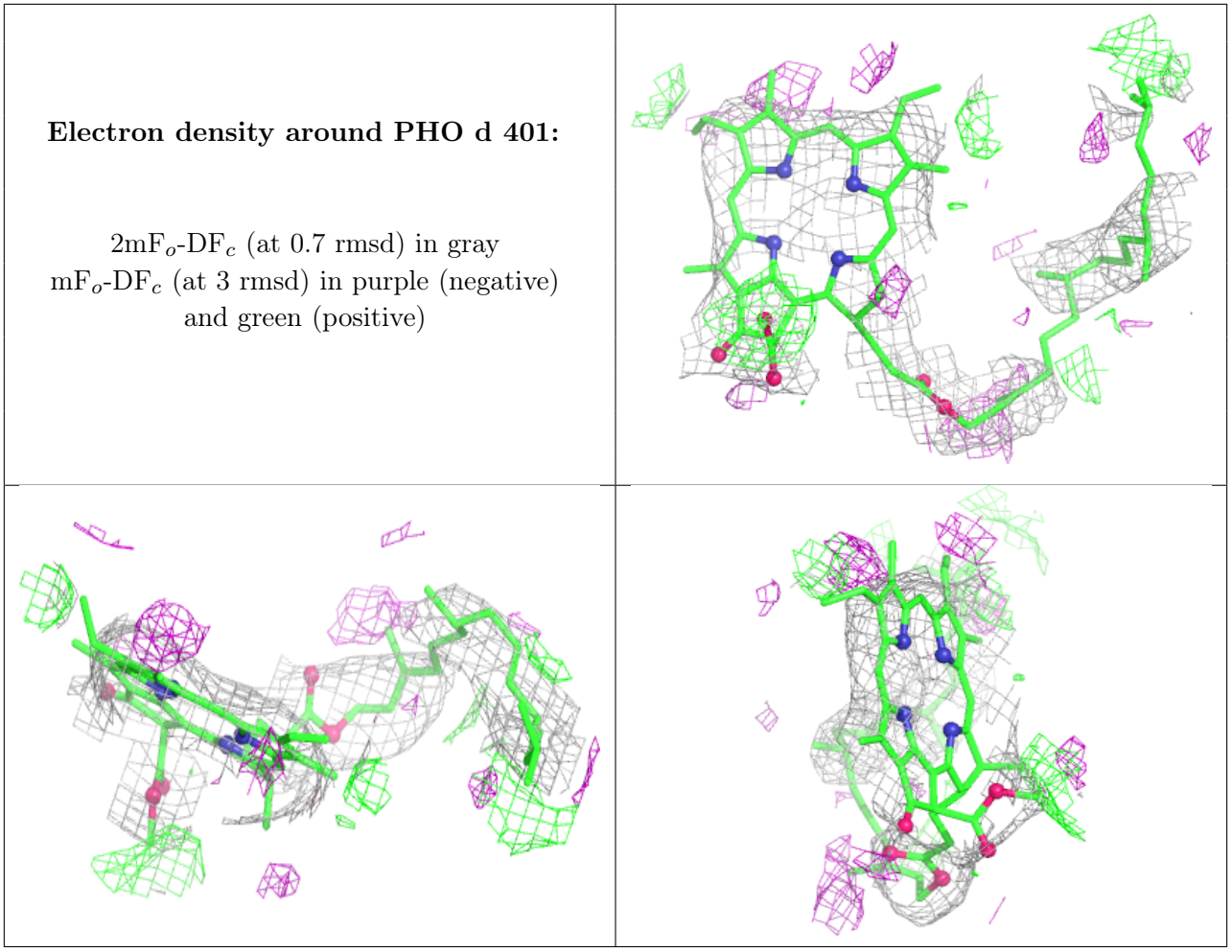
Electron density around BCR b 619:

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



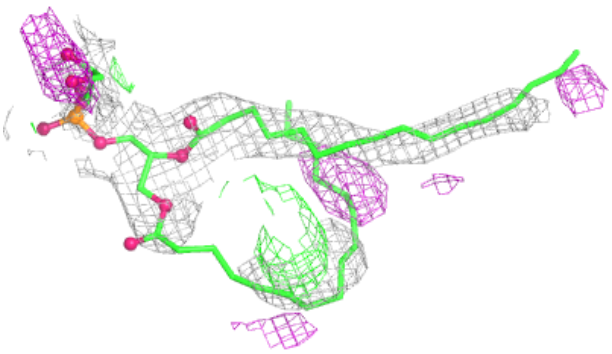
Electron density around PHO d 401:

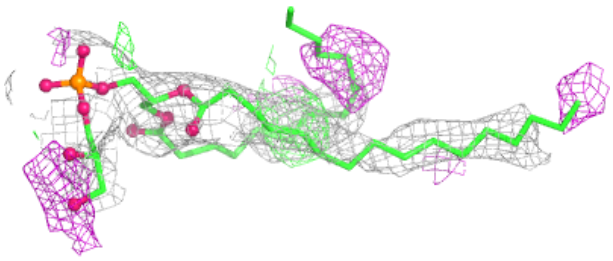
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

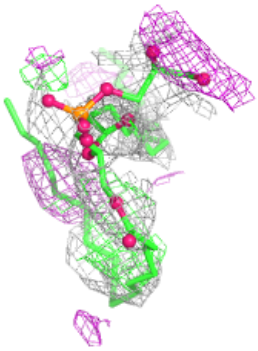


Electron density around LHG D 406:

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

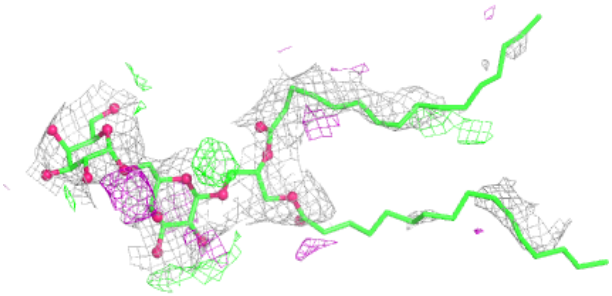


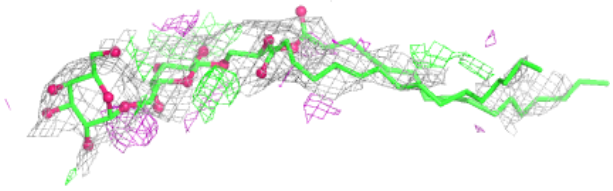


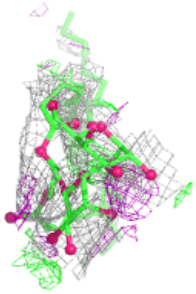


Electron density around DGD c 518:

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

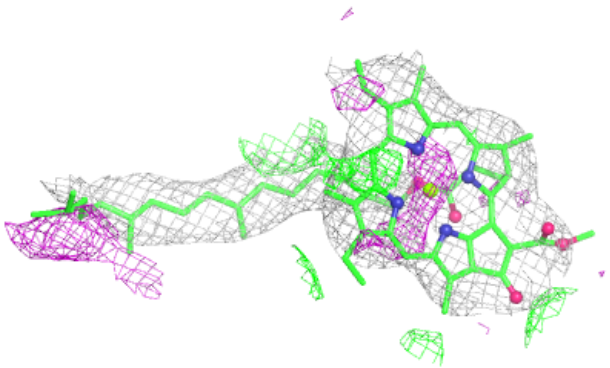


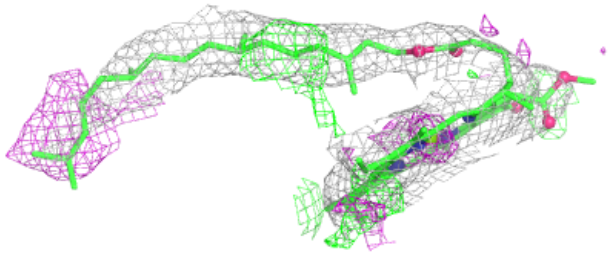


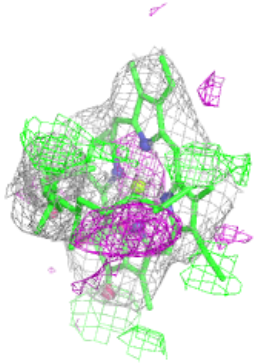


Electron density around CLA B 609:

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

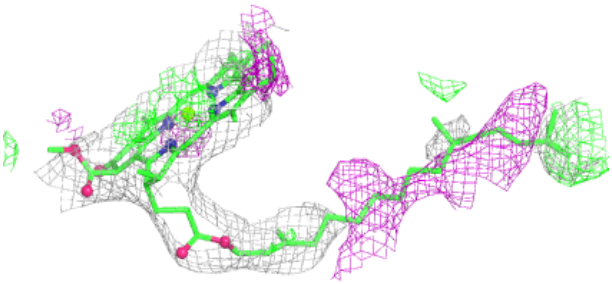


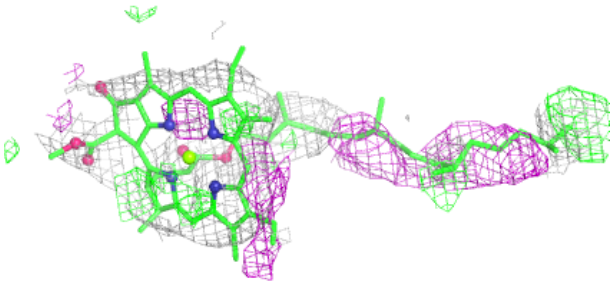


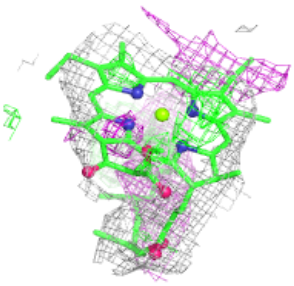


Electron density around CLA C 504:

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

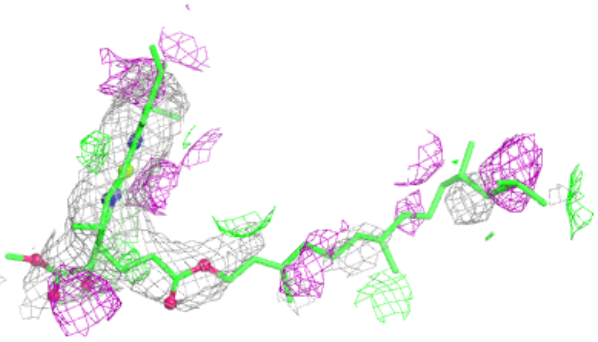


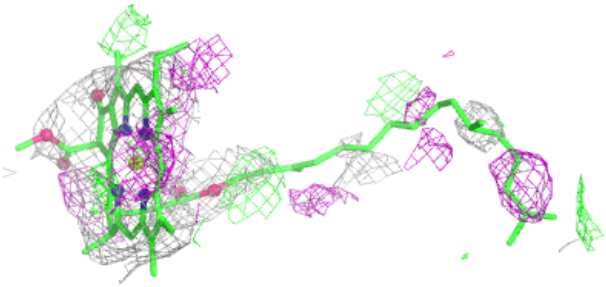


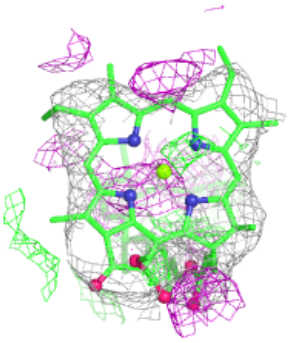


Electron density around CLA b 607:

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

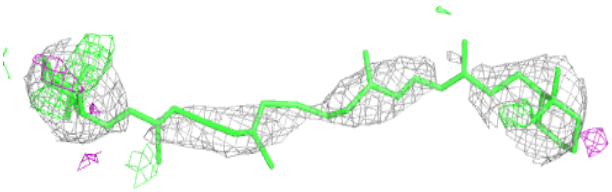


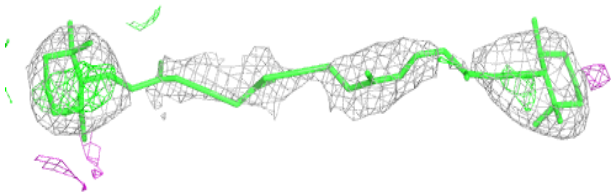


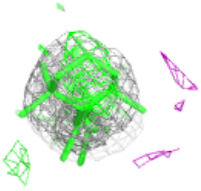


Electron density around BCR a 610:

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

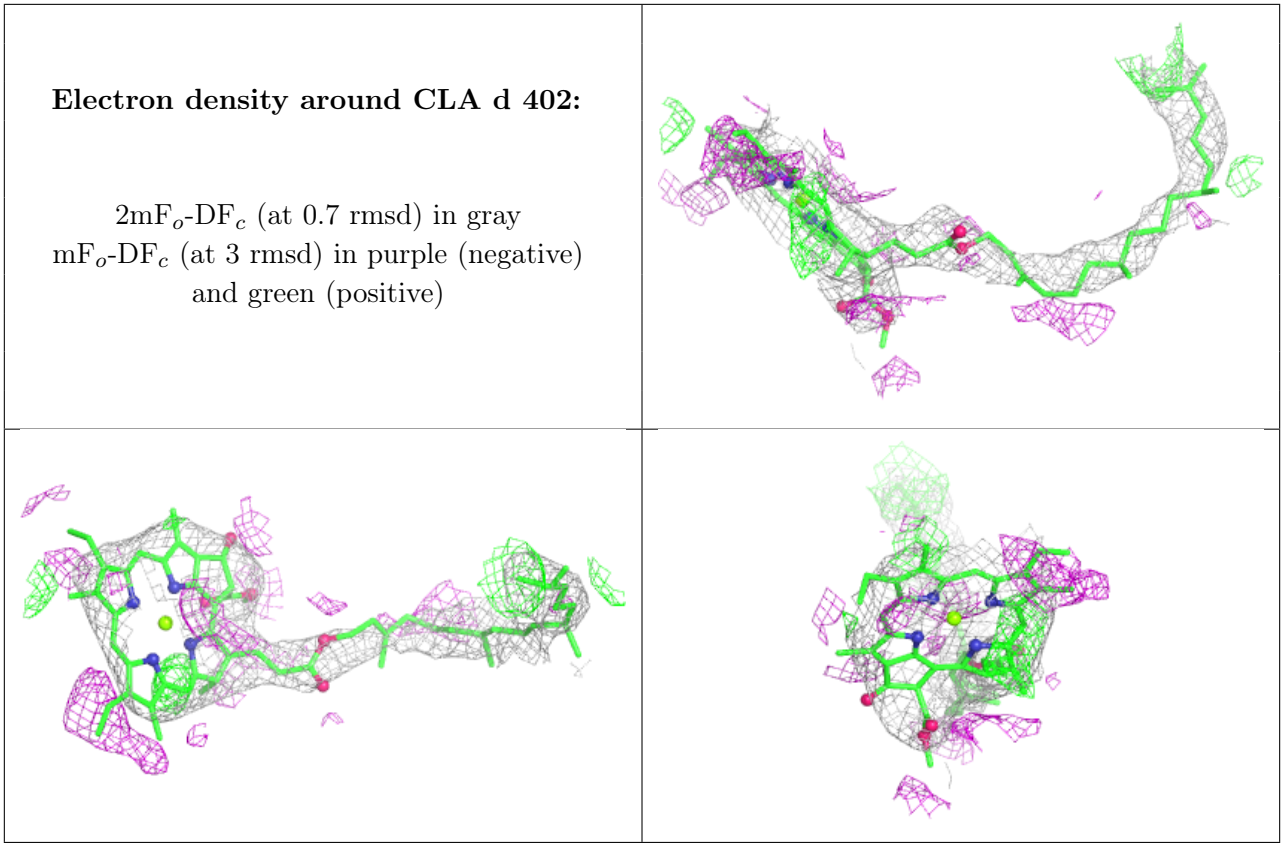






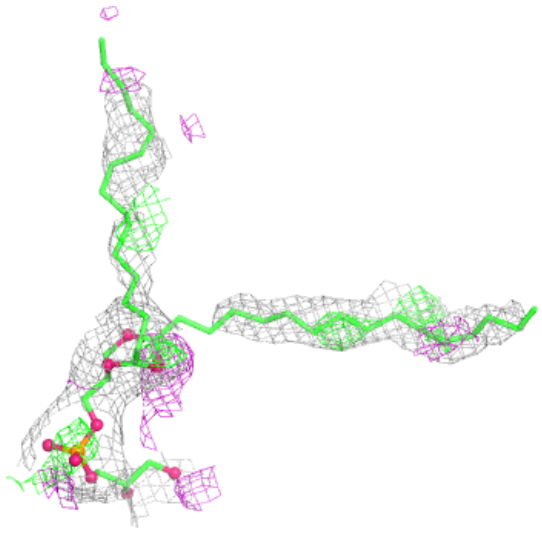
Electron density around CLA d 402:

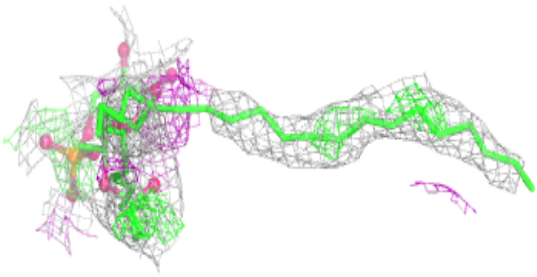
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

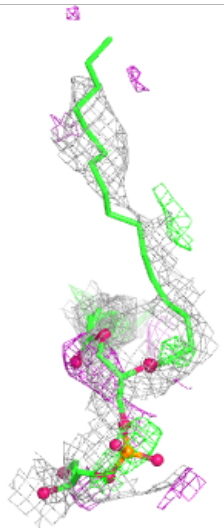


Electron density around LHG l 102:

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

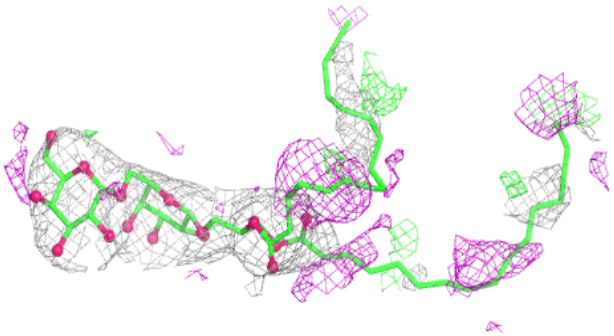


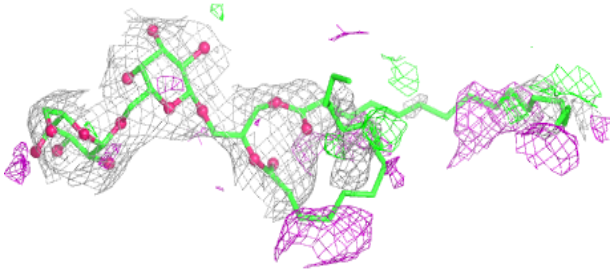


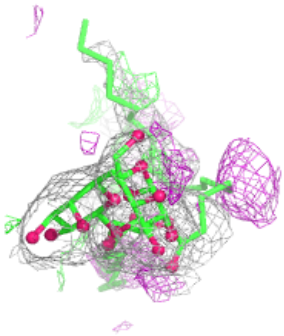


Electron density around DGD H 102:

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

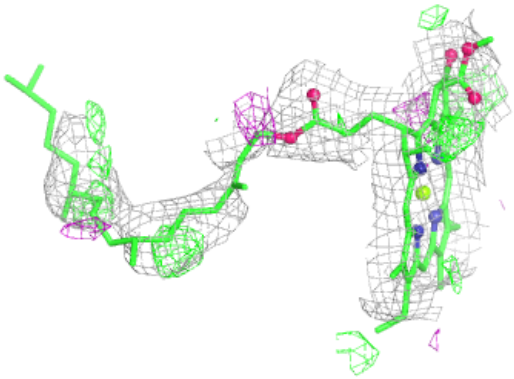


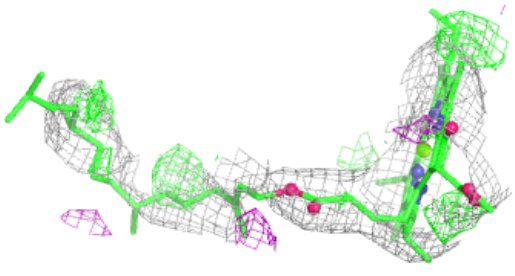


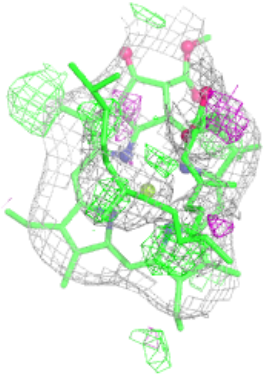


Electron density around CLA d 403:

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

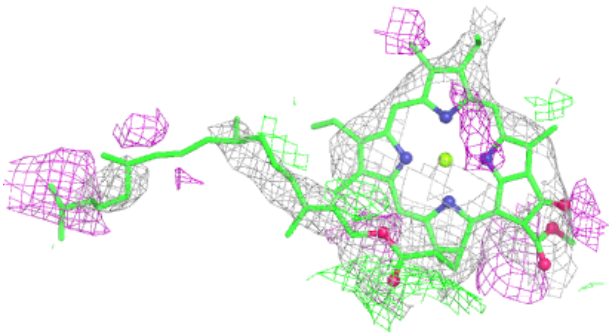


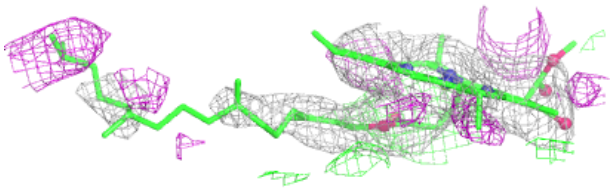


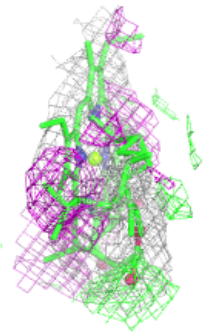


Electron density around CLA b 605:

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

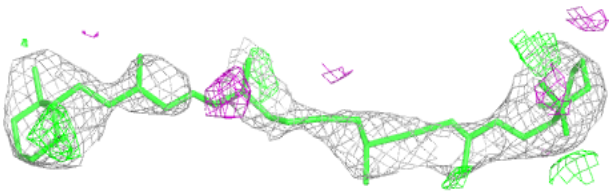


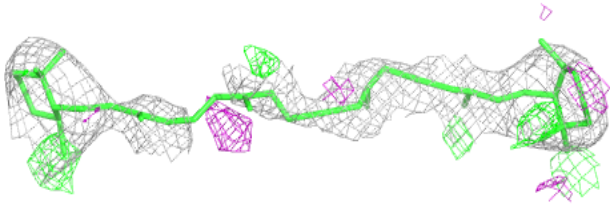


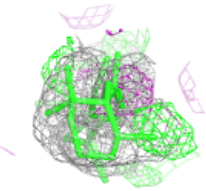


Electron density around BCR A 610:

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

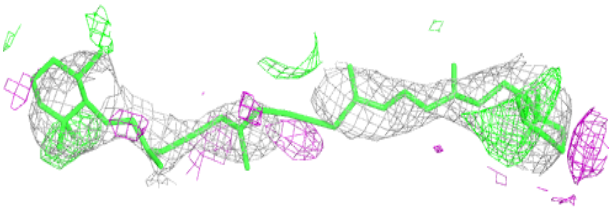


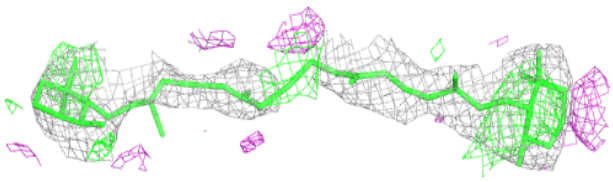


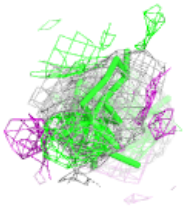


Electron density around BCR B 618:

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

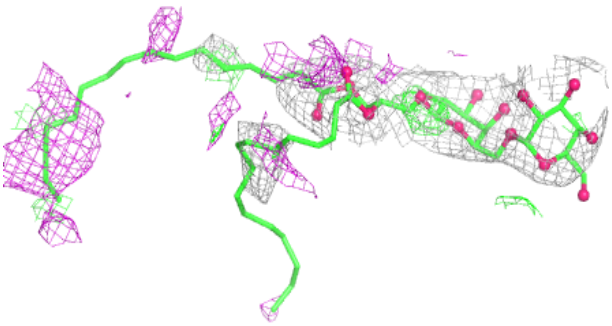


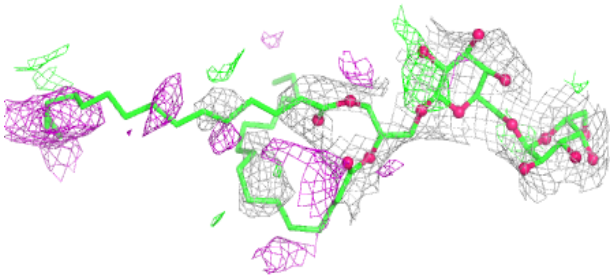


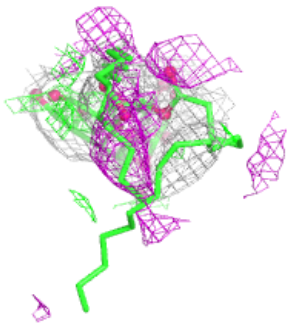


Electron density around DGD h 102:

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

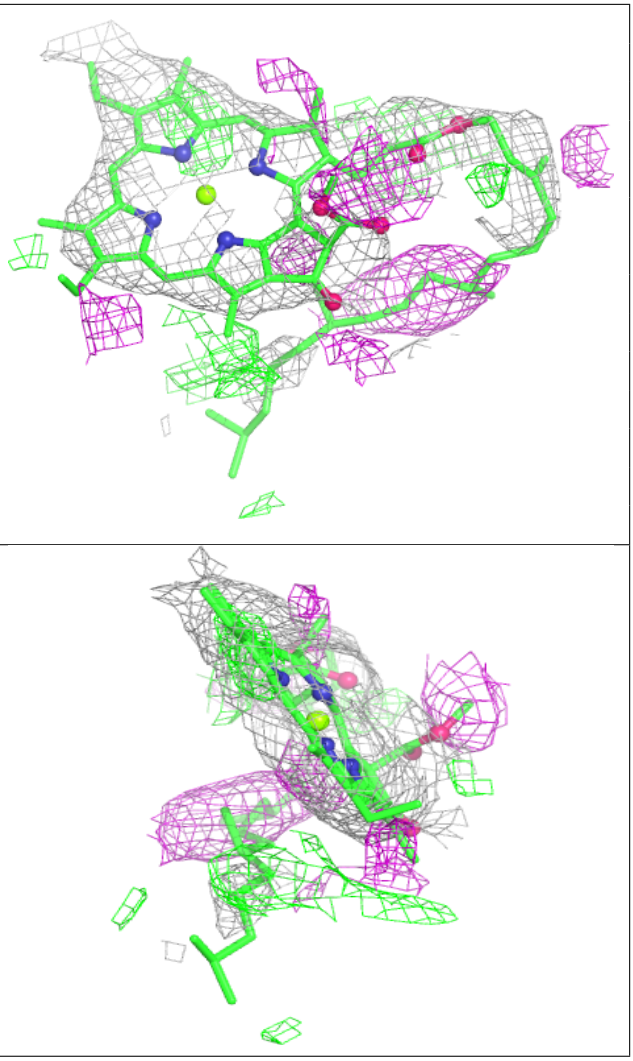


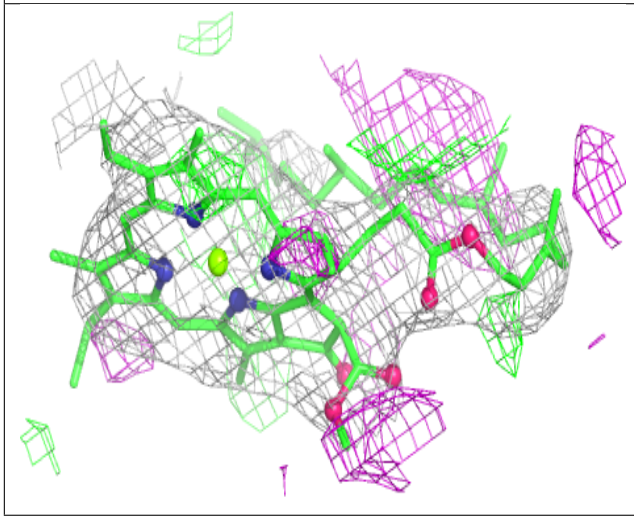




Electron density around CLA C 509:

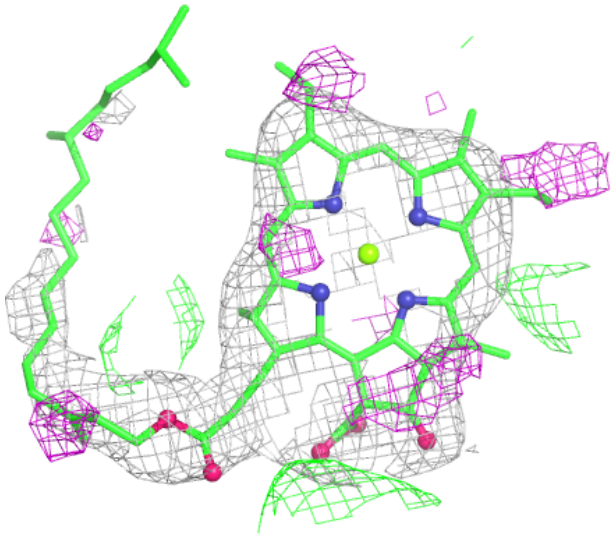
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

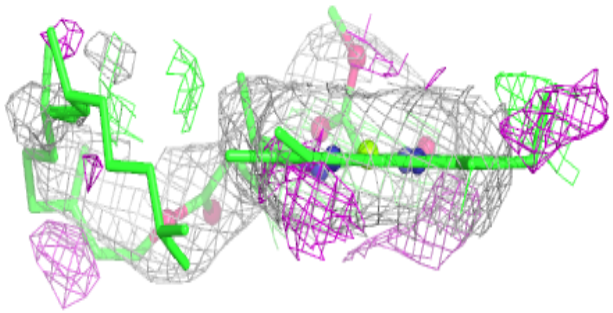


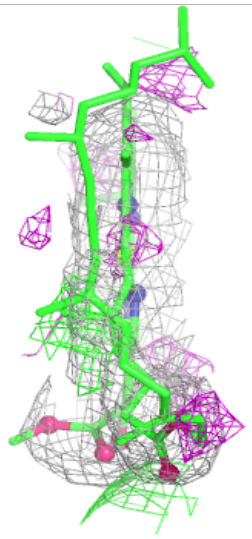


Electron density around CLA C 512:

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

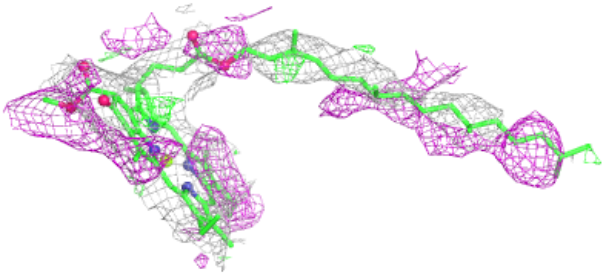


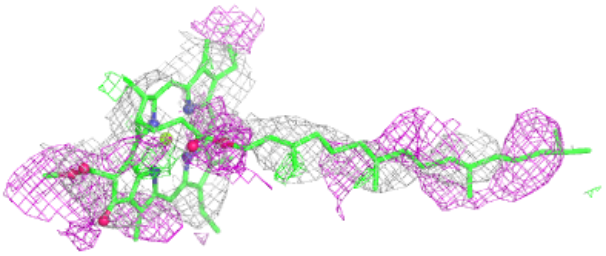


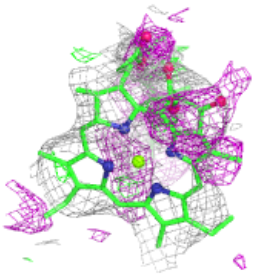


Electron density around CLA B 608:

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

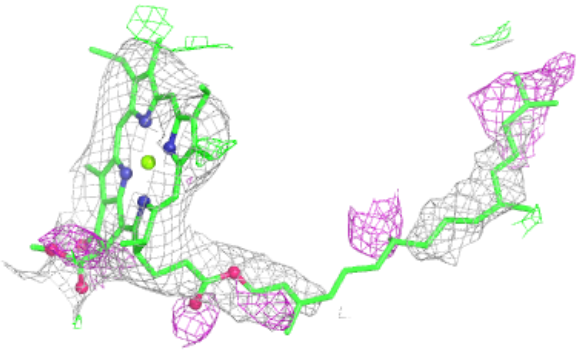


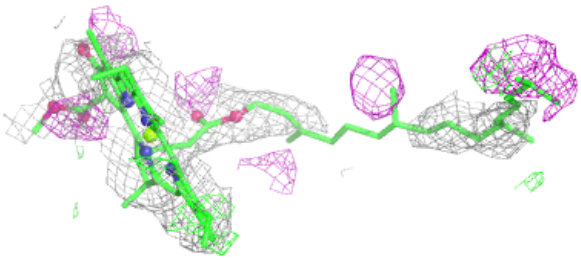


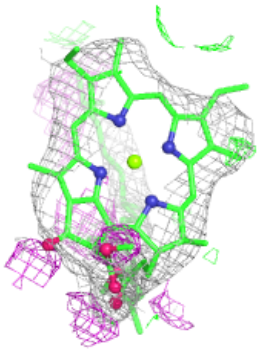


Electron density around CLA b 611:

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

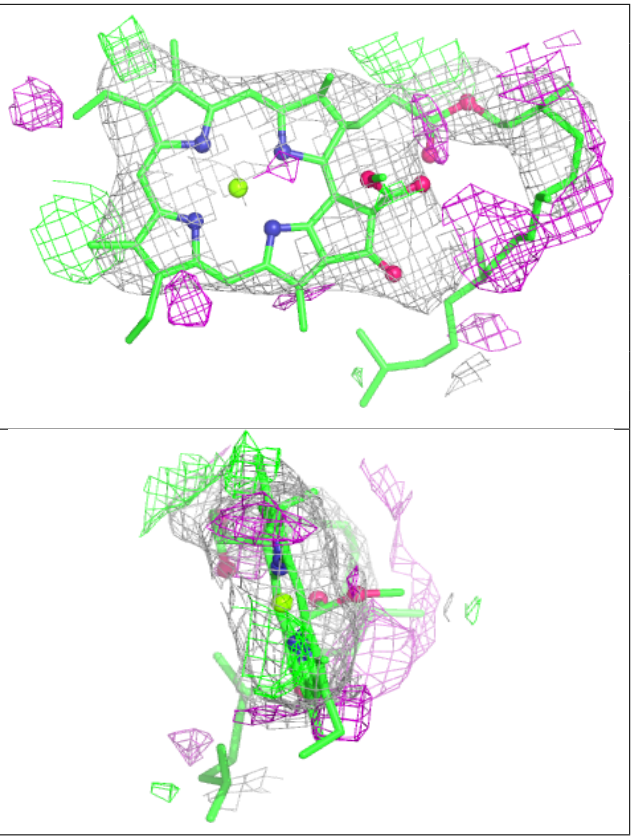


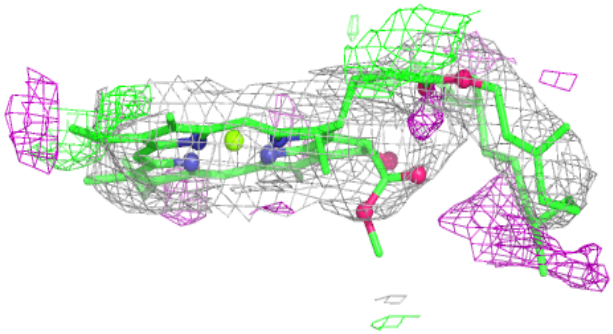




Electron density around CLA b 612:

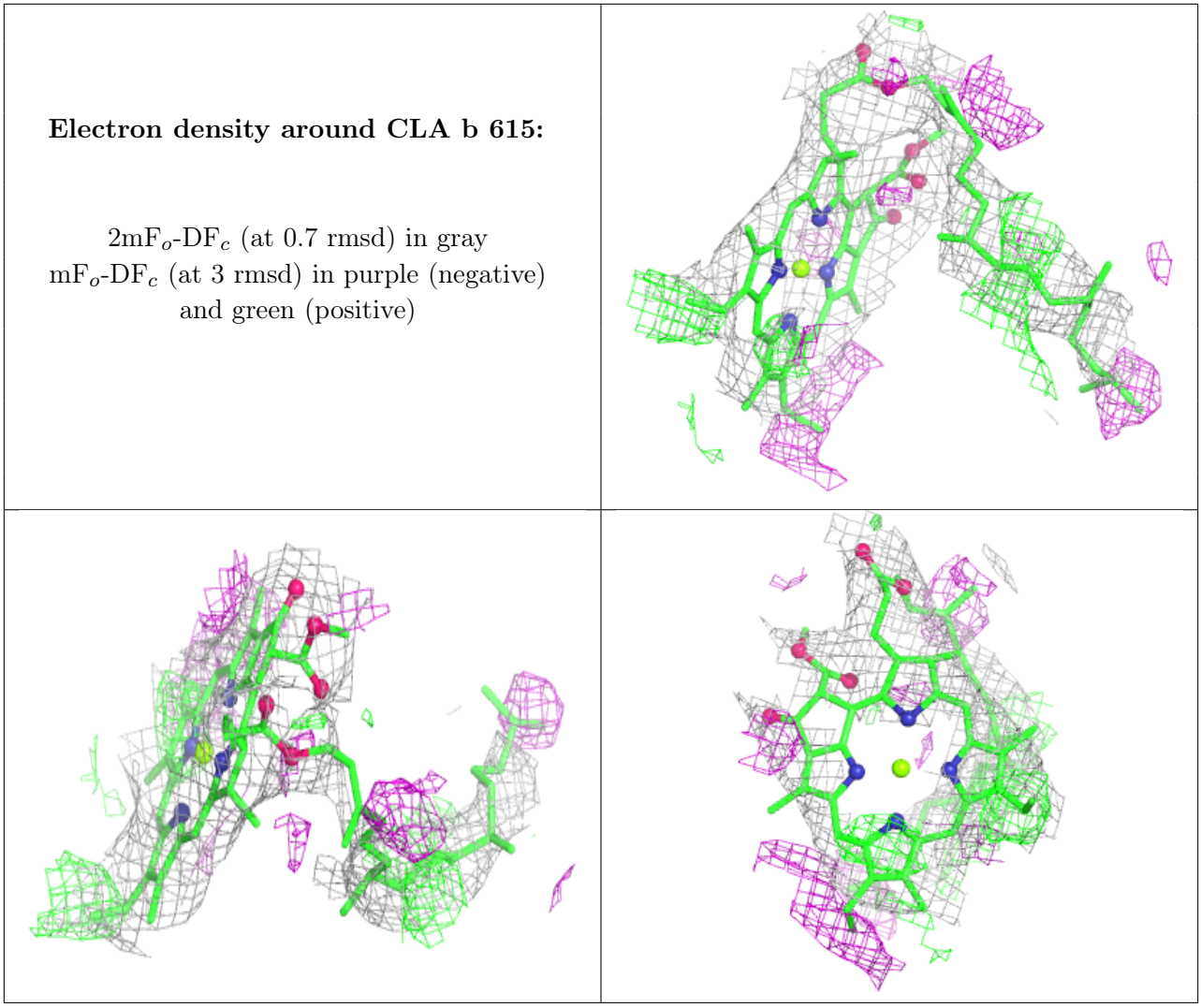
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





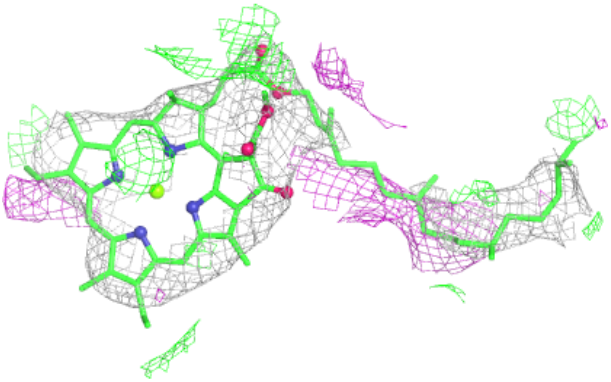
Electron density around CLA b 615:

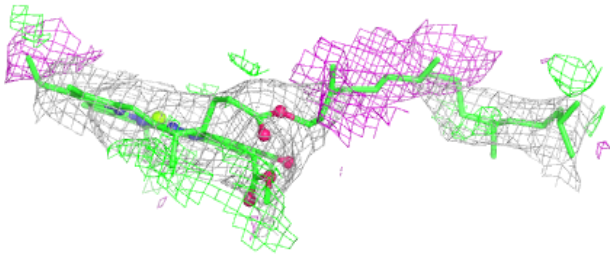
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

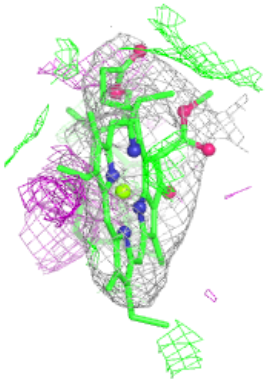


Electron density around CLA B 603:

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

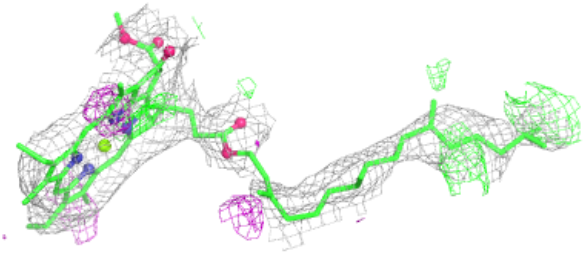


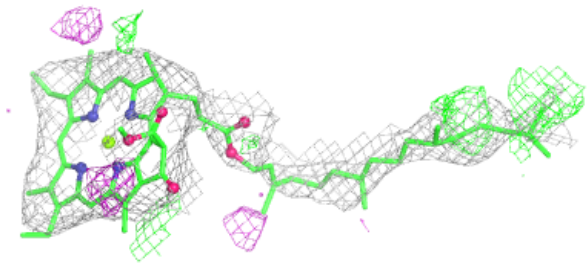


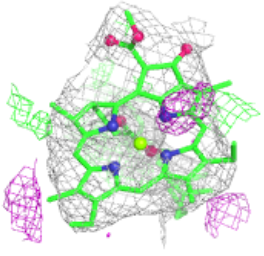


Electron density around CLA C 502:

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

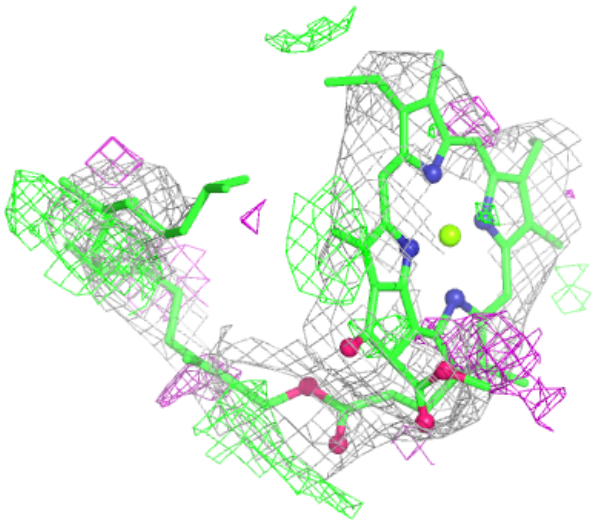


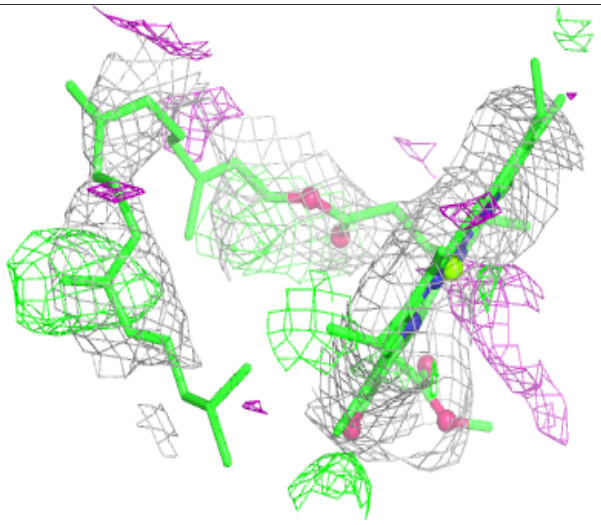


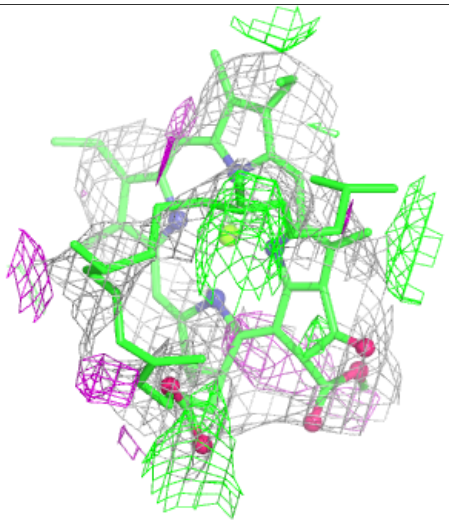


Electron density around CLA C 503:

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

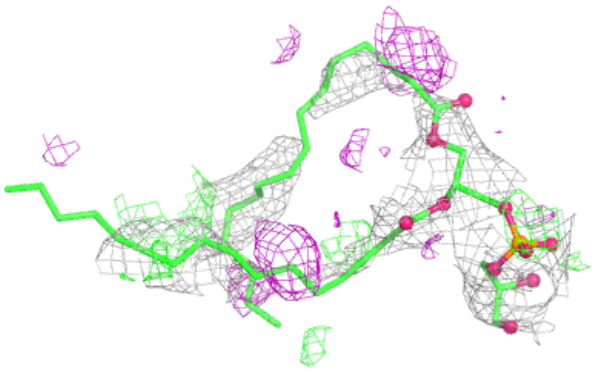


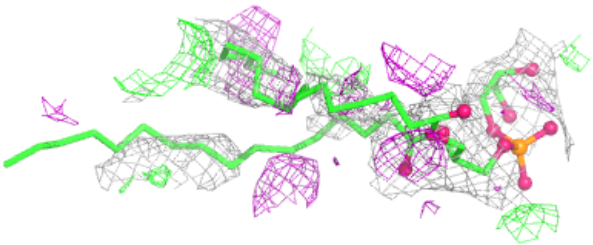


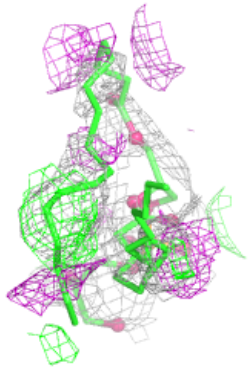


Electron density around LHG A 615:

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

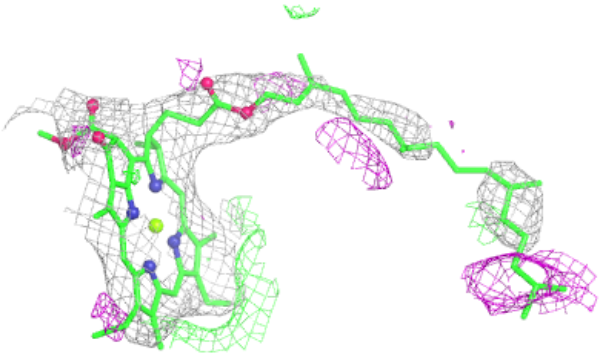


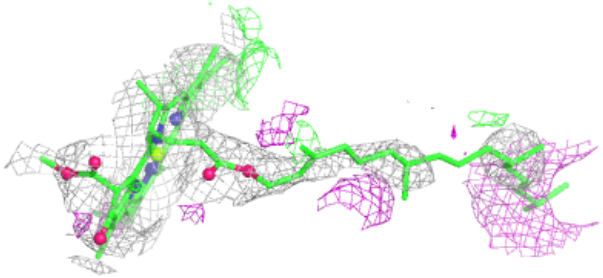


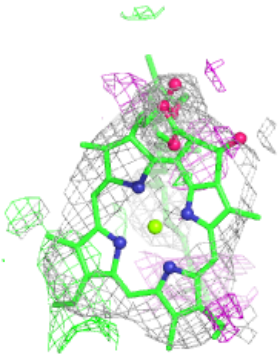


Electron density around CLA B 610:

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

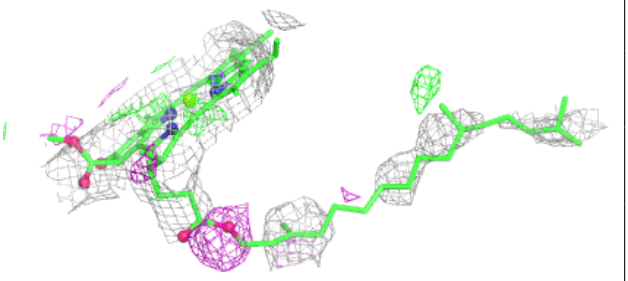


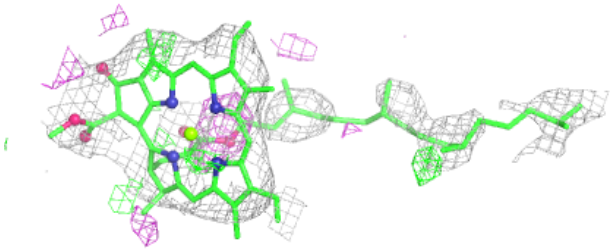


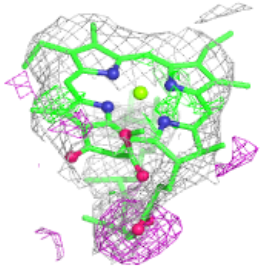


Electron density around CLA c 504:

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

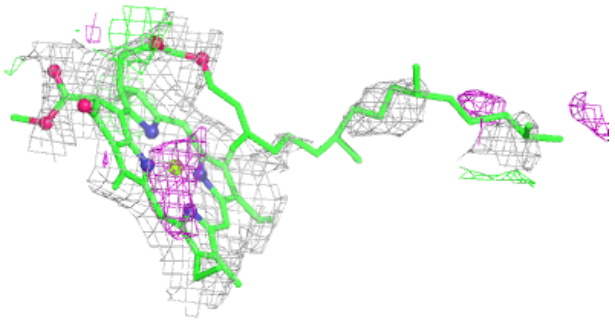


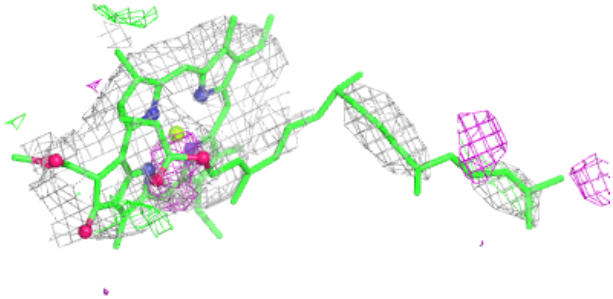


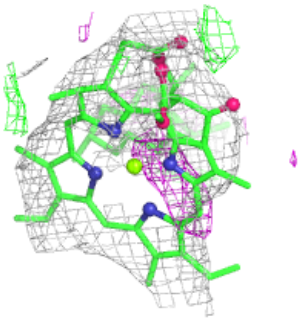


Electron density around CLA c 505:

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

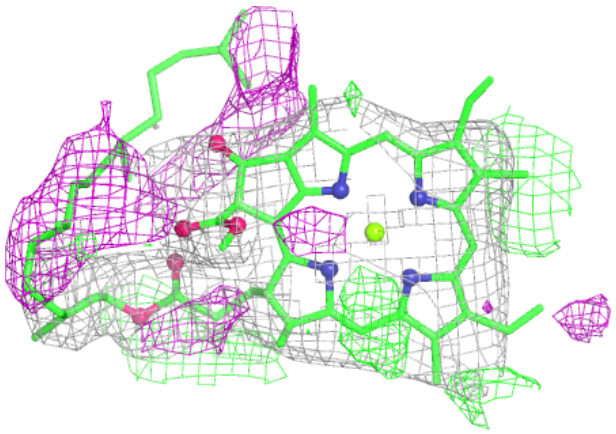


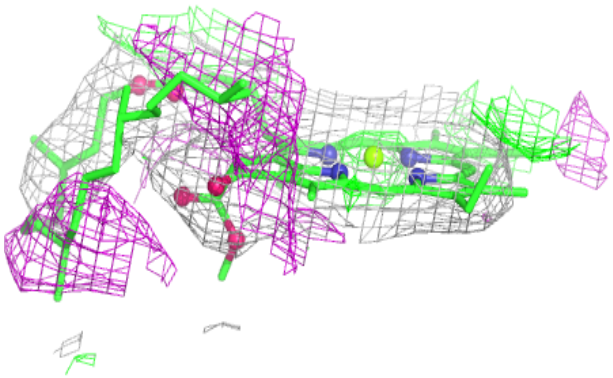


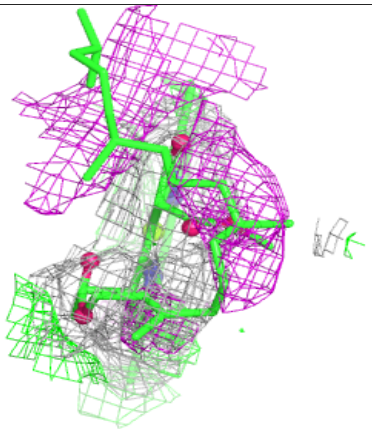


Electron density around CLA B 611:

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

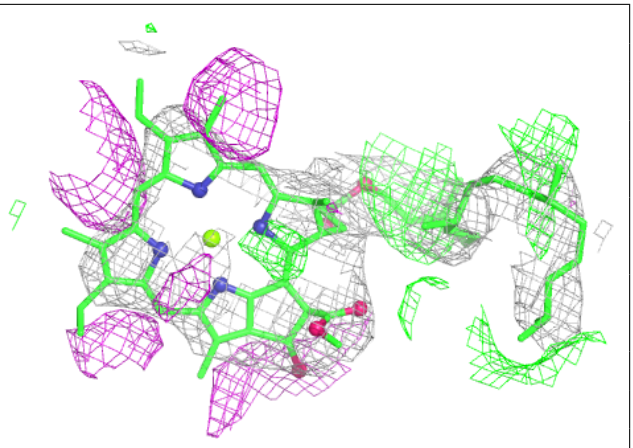


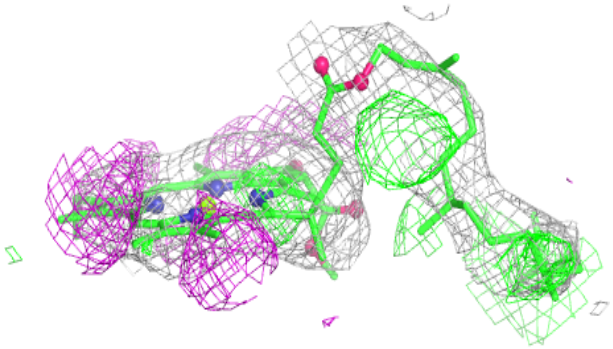


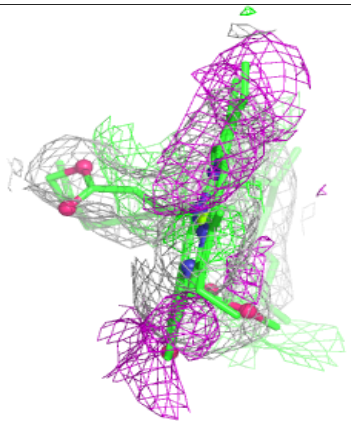


Electron density around CLA B 613:

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

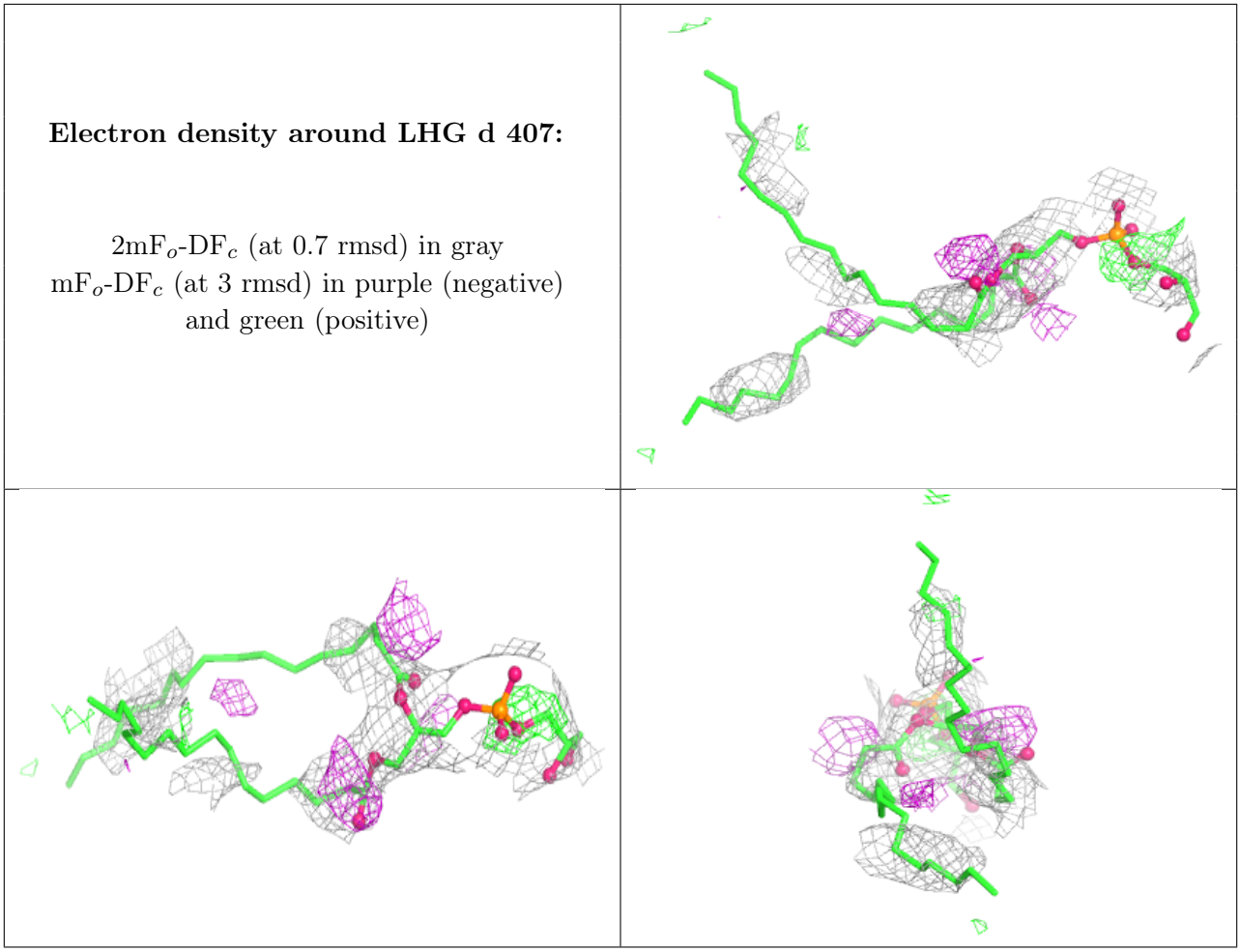






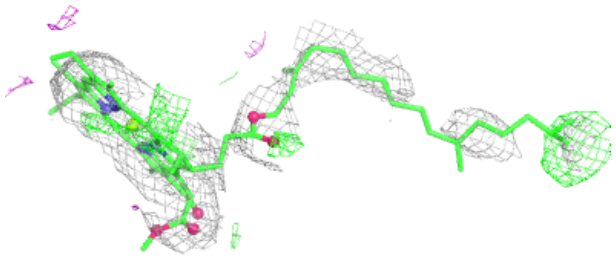
Electron density around LHG d 407:

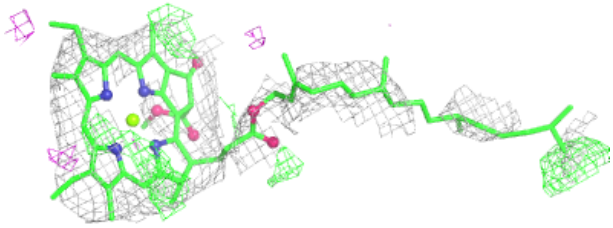
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

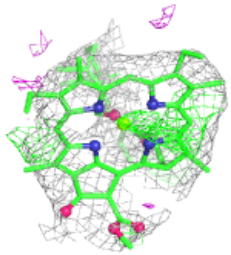


Electron density around CLA c 502:

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

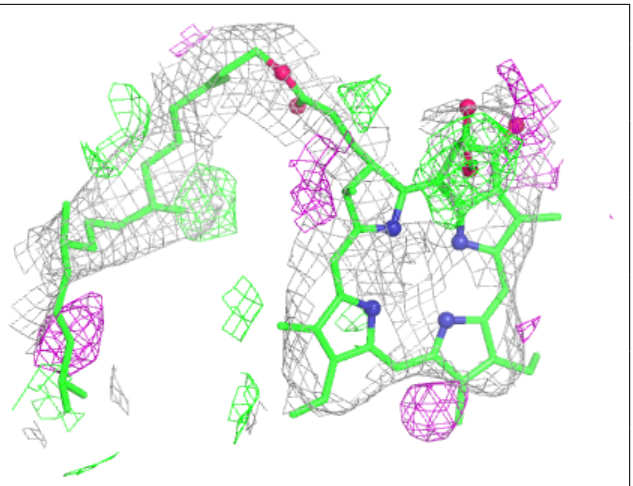


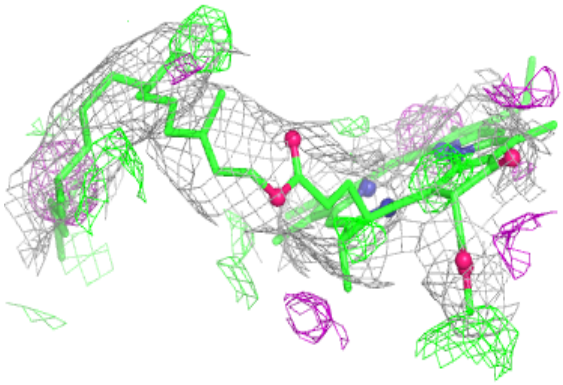


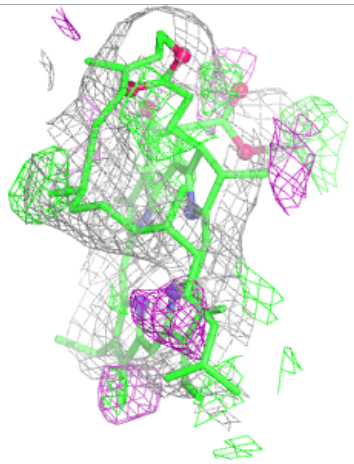


Electron density around PHO D 401:

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

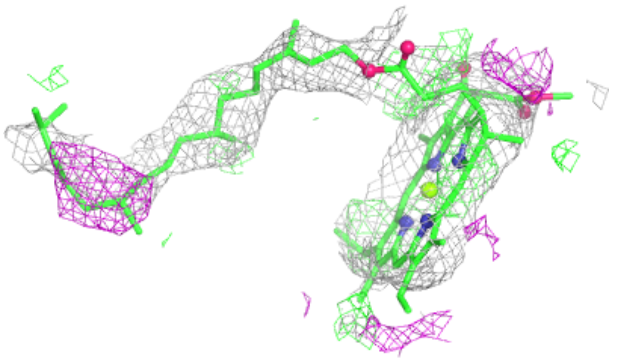


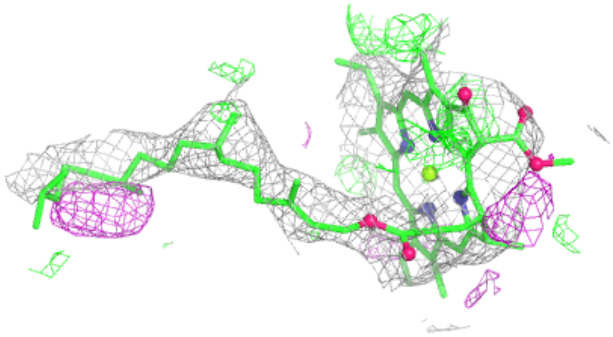


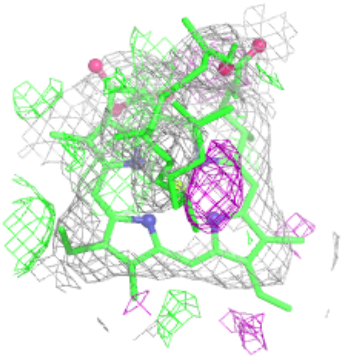


Electron density around CLA C 508:

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

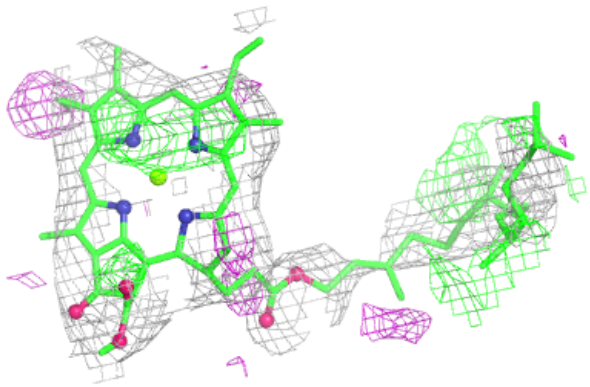


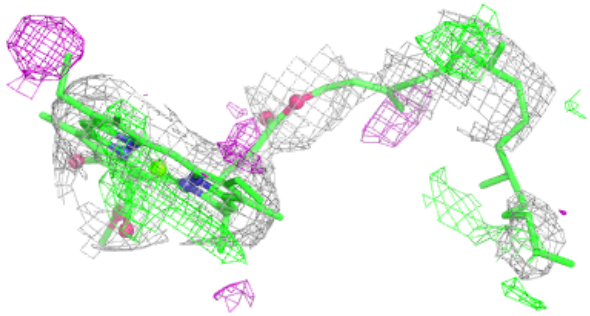


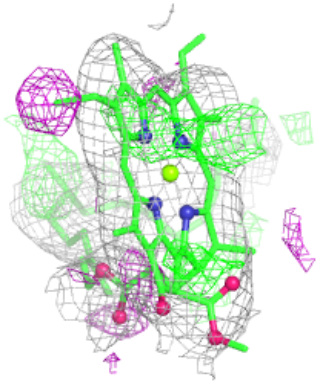


Electron density around CLA A 609:

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

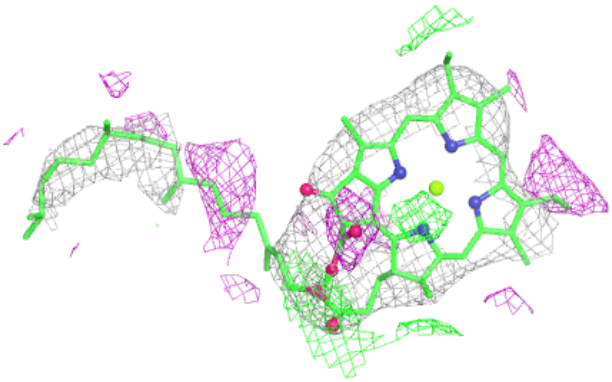


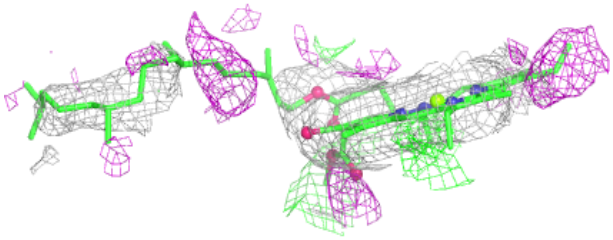


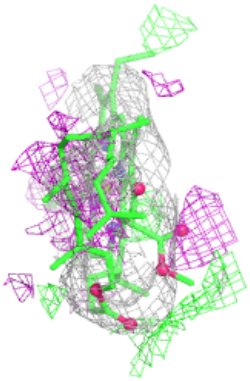


Electron density around CLA b 604:

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

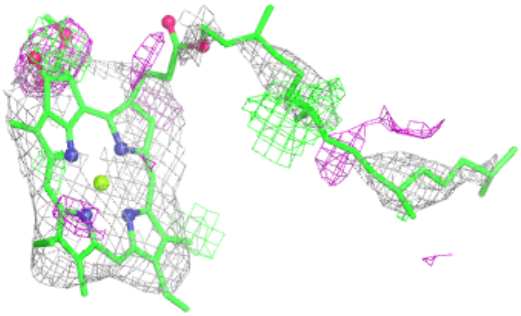


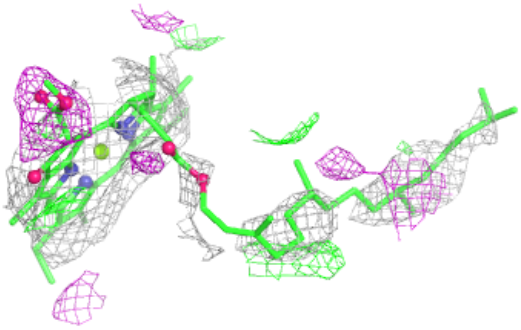


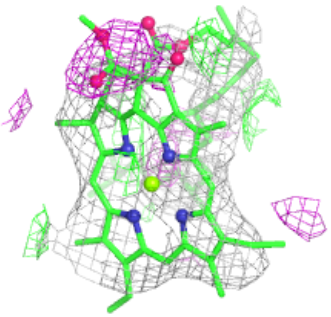


Electron density around CLA C 511:

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

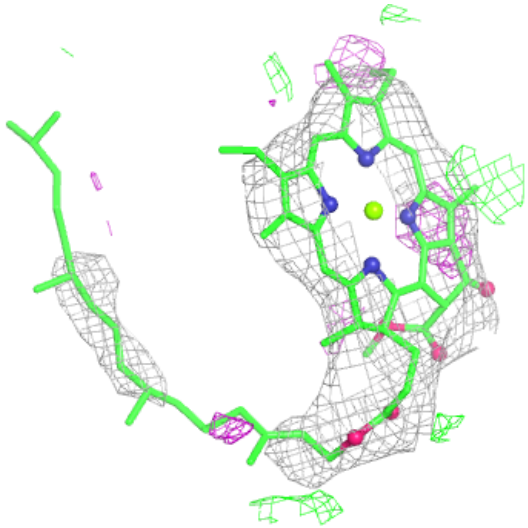


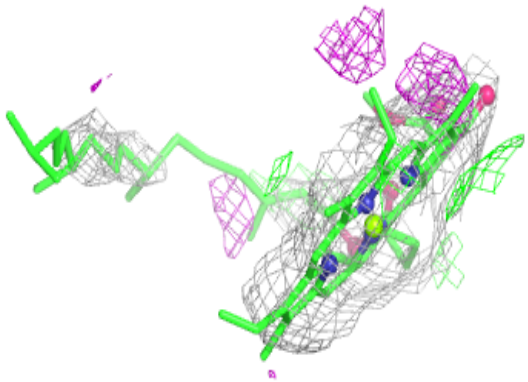


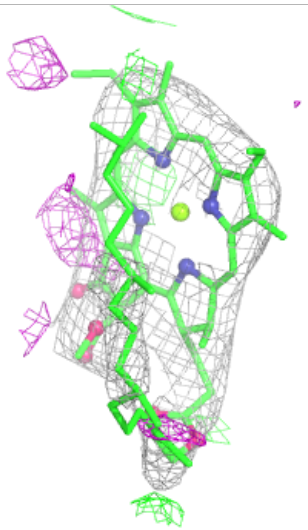


Electron density around CLA c 507:

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

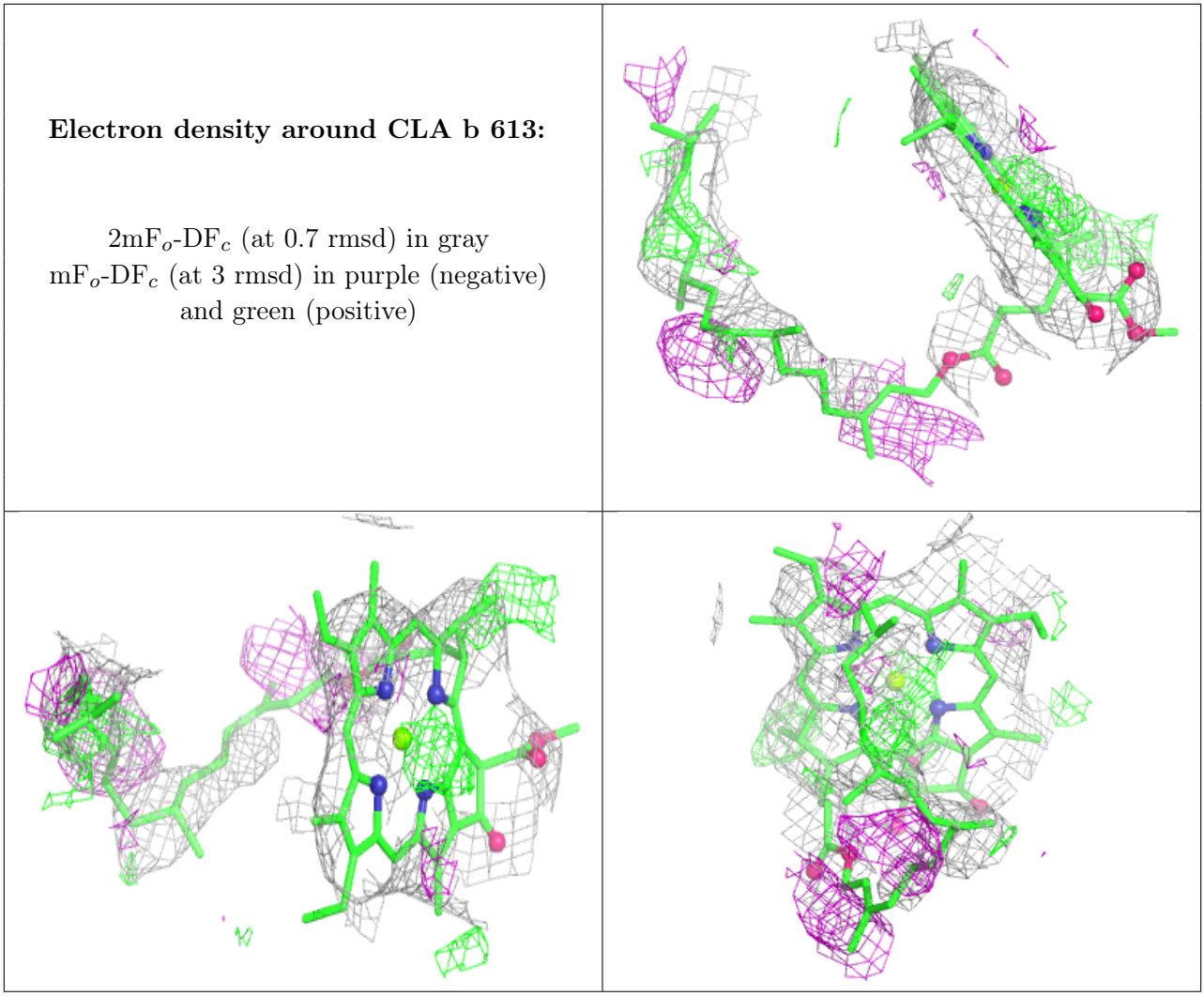






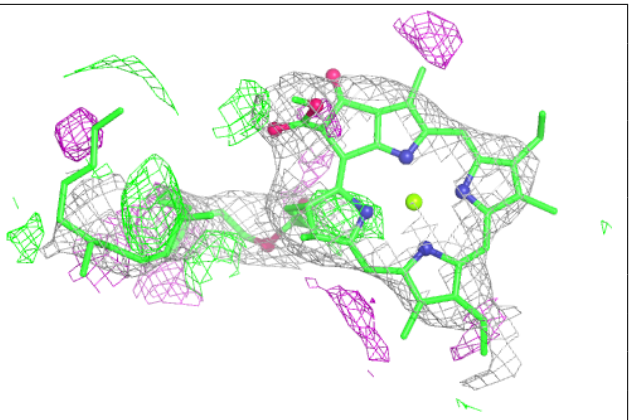
Electron density around CLA b 613:

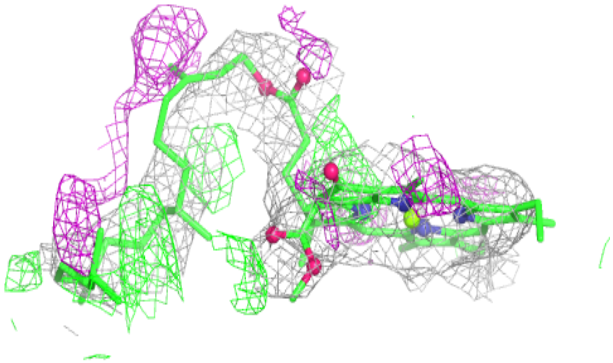
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

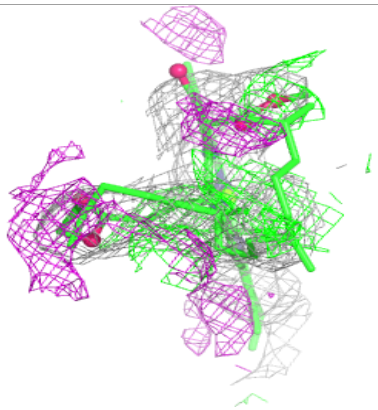


Electron density around CLA b 614:

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

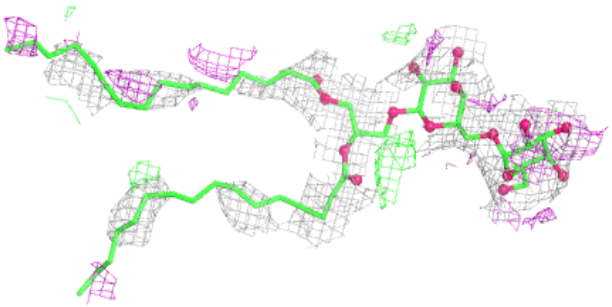


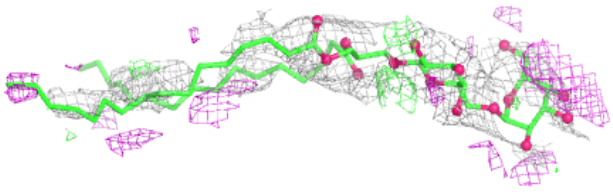


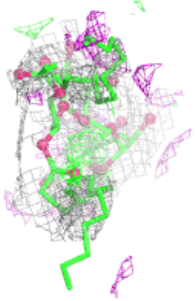


Electron density around DGD C 517:

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

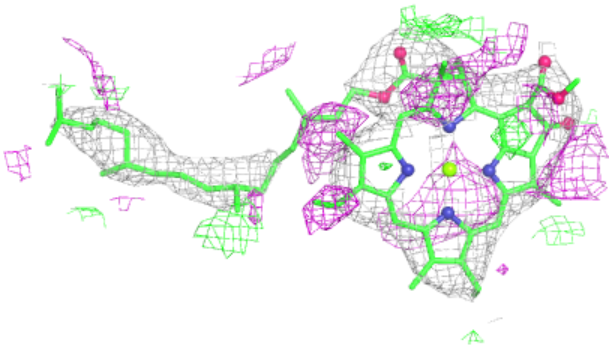


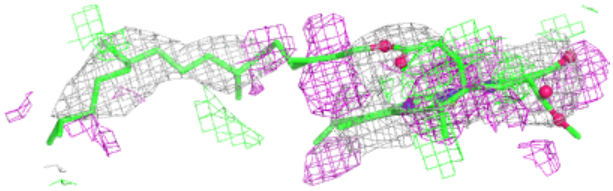


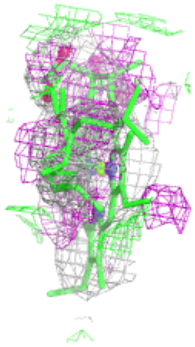


Electron density around CLA B 604:

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

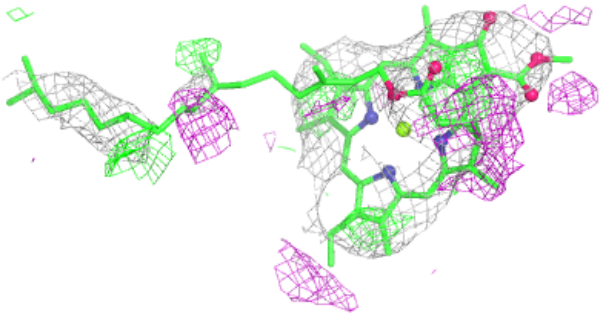


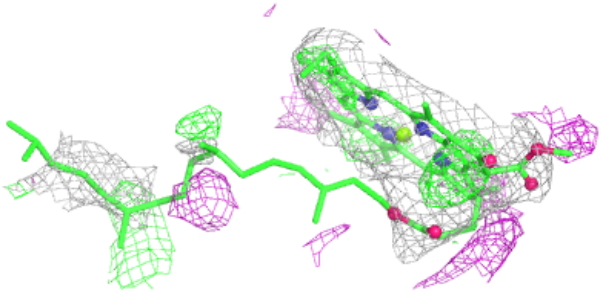


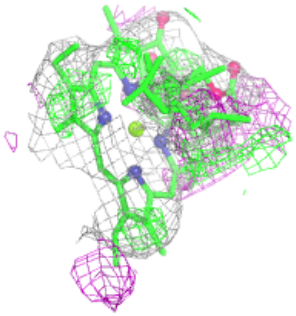


Electron density around CLA b 616:

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

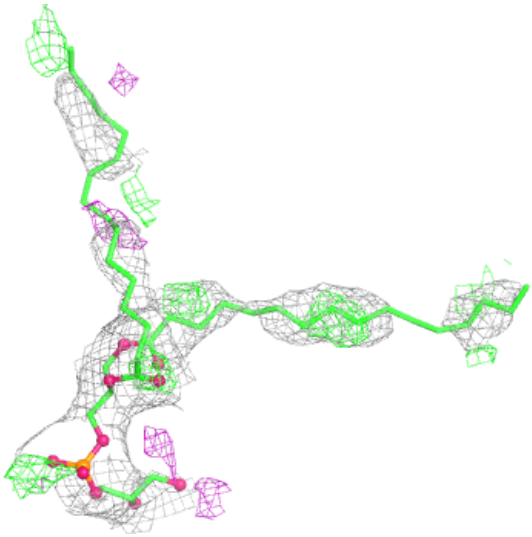


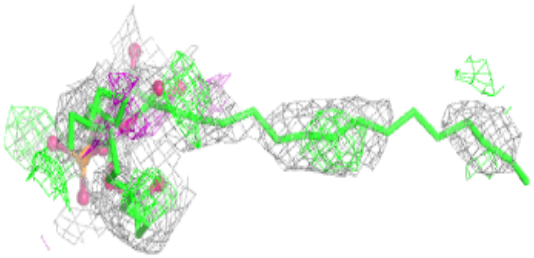


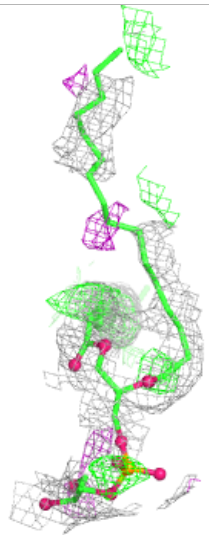


Electron density around LHG L 101:

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

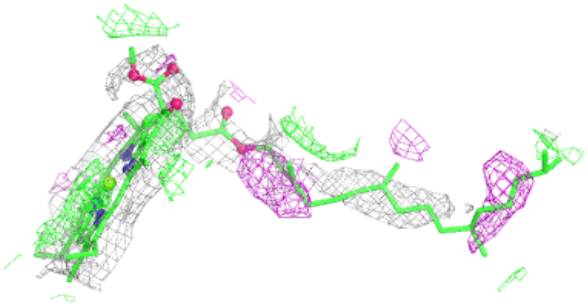


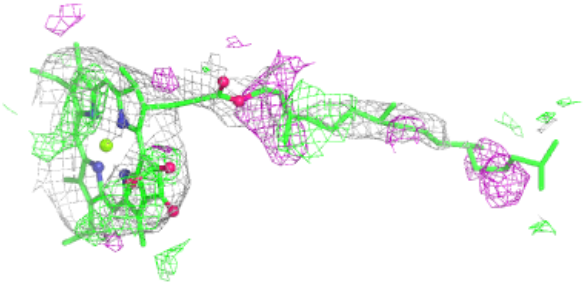


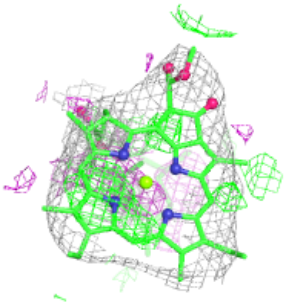


Electron density around CLA B 605:

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

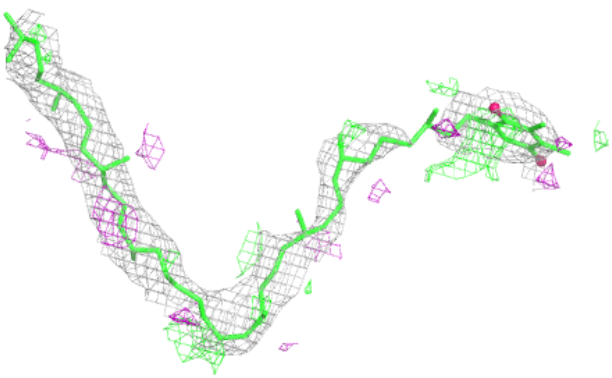


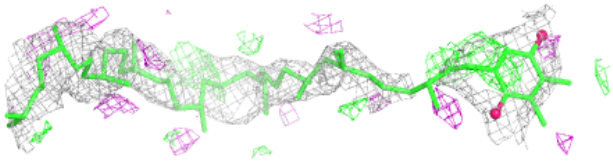


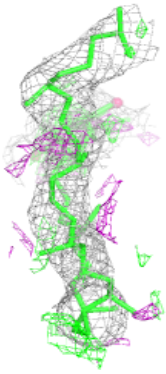


Electron density around PL9 D 405:

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

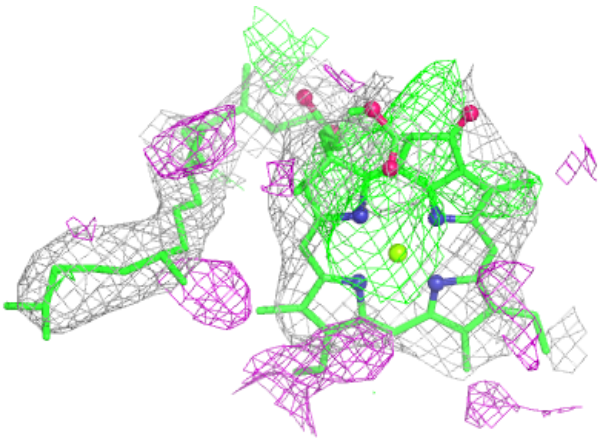


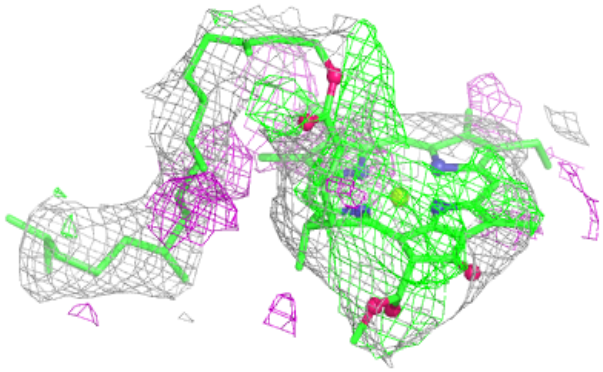


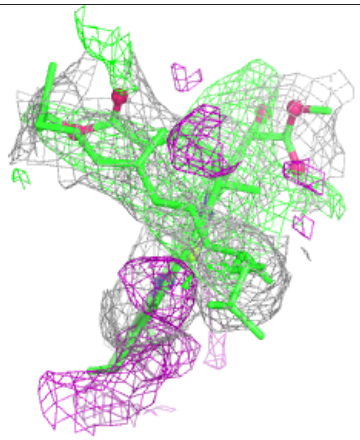


Electron density around CLA D 402:

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

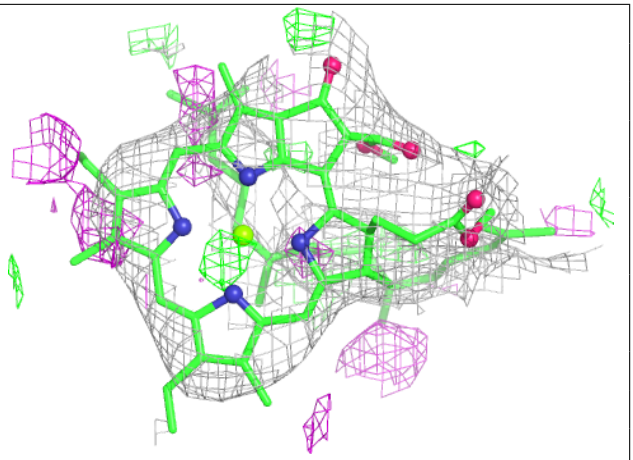


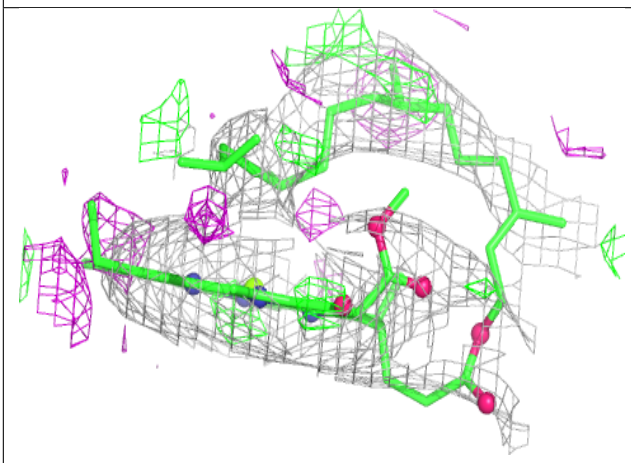


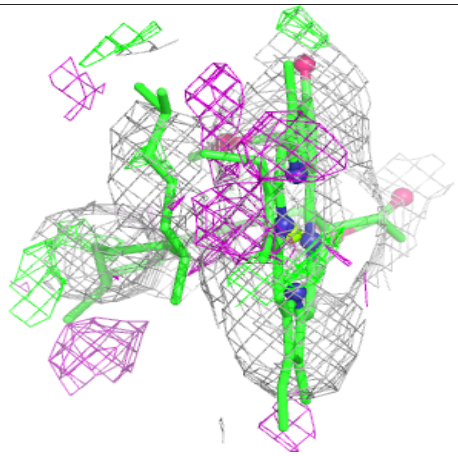


Electron density around CLA C 510:

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

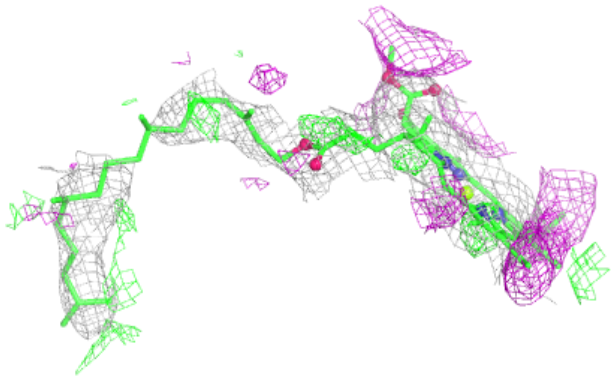


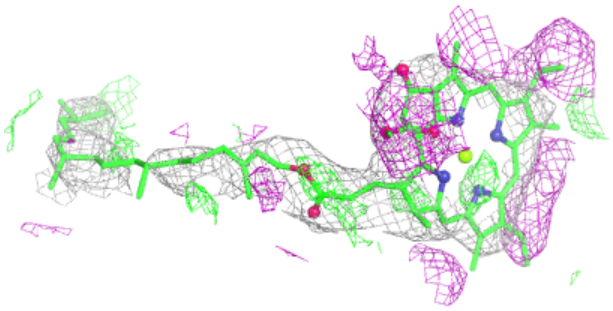




Electron density around CLA D 403:

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

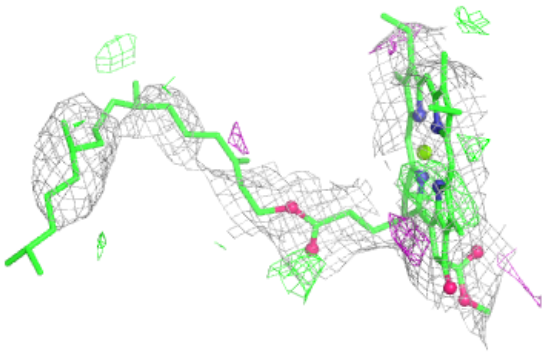


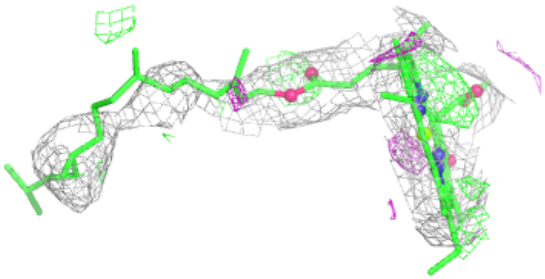


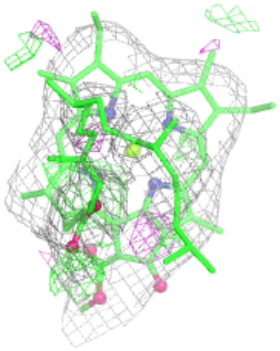


Electron density around CLA D 404:

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

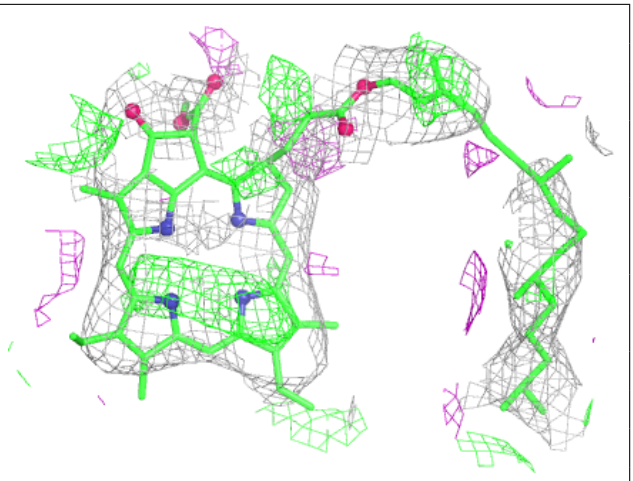


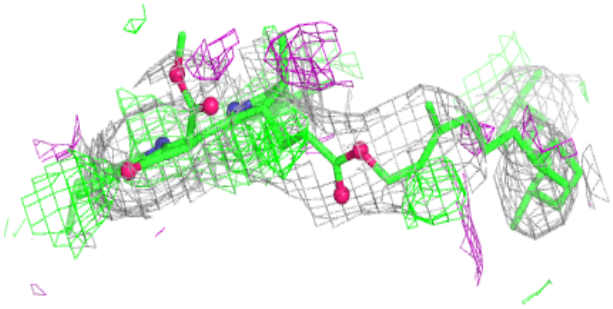


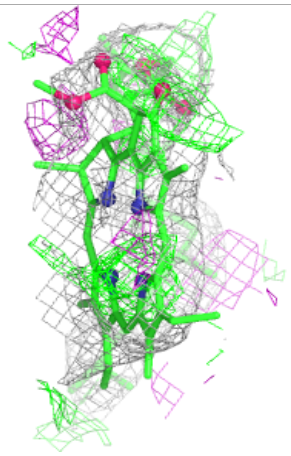


Electron density around PHO A 608:

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

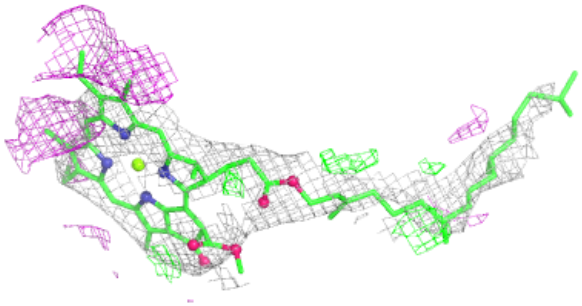


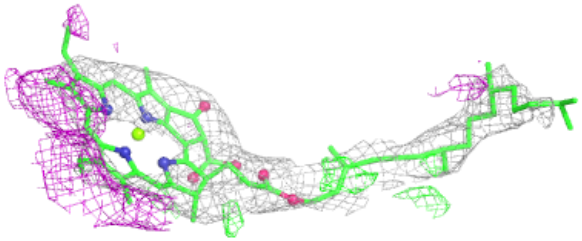


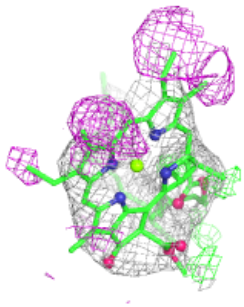


Electron density around CLA a 606:

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

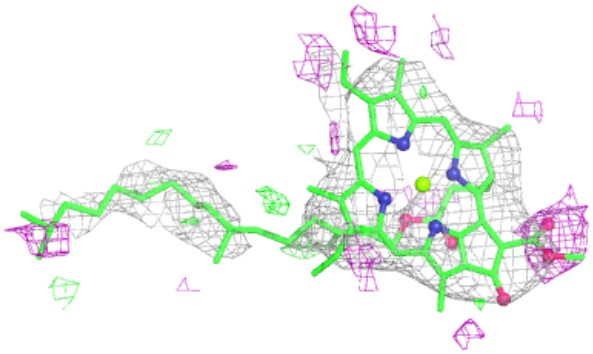


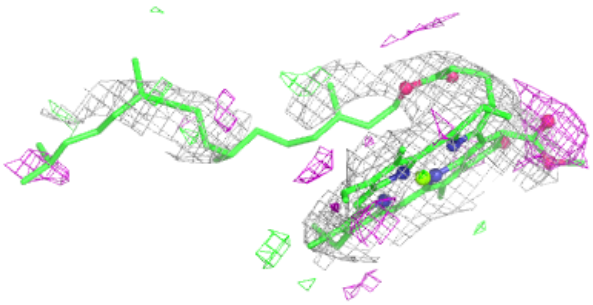


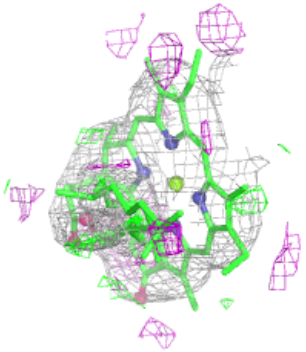


Electron density around CLA B 615:

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

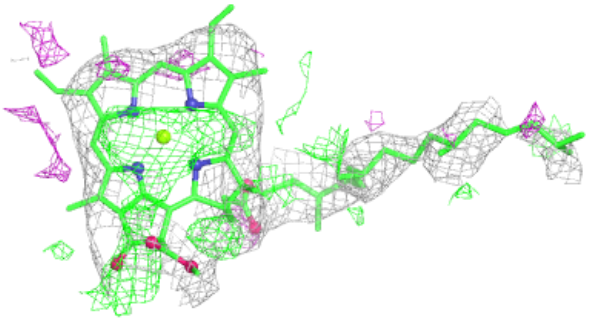


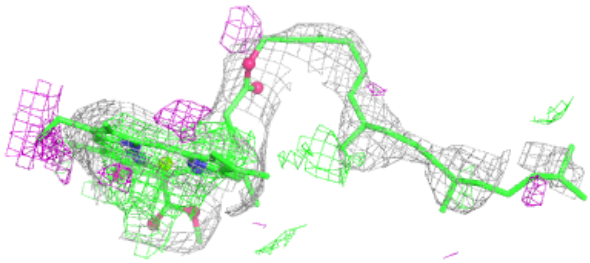


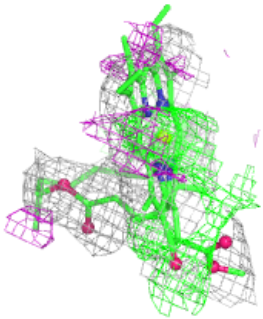


Electron density around CLA A 607:

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

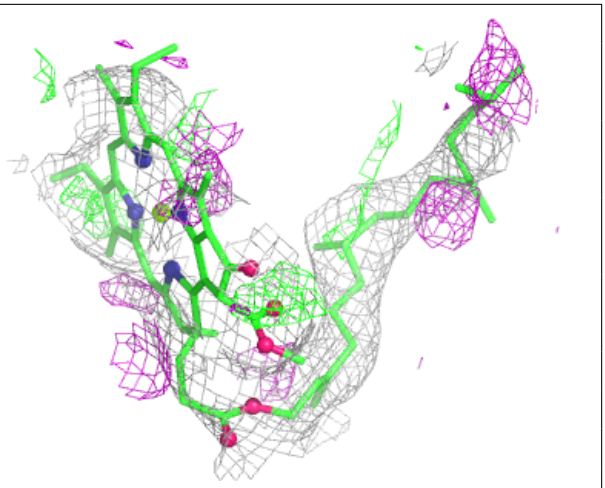


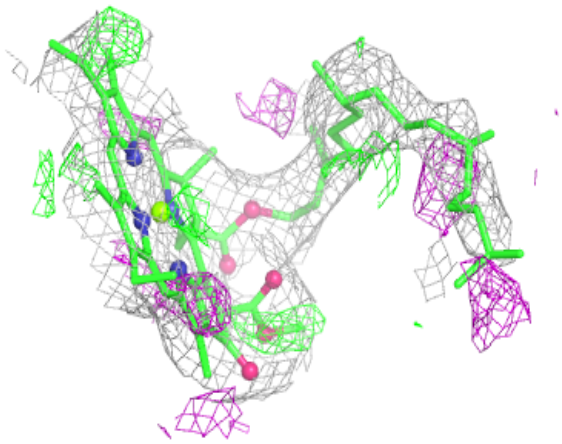


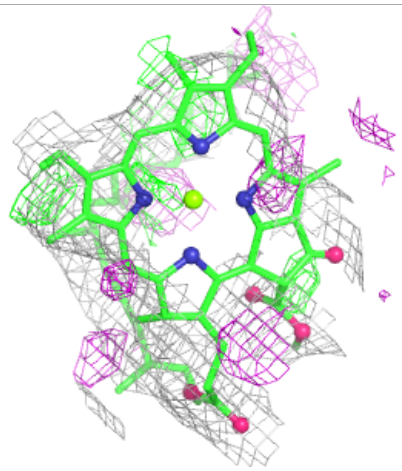


Electron density around CLA B 614:

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

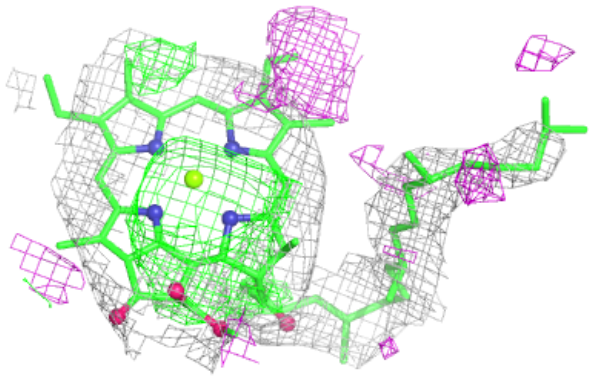


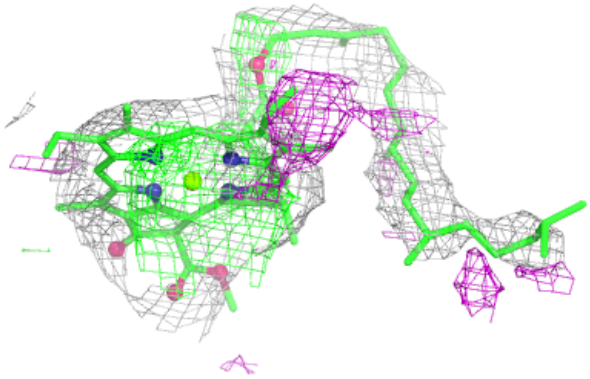


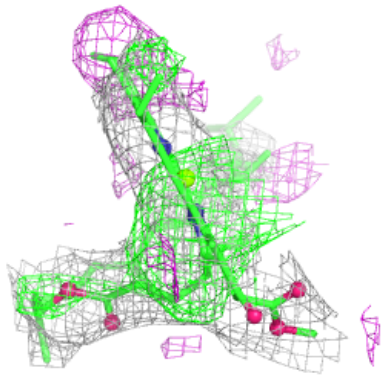


Electron density around CLA a 615:

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

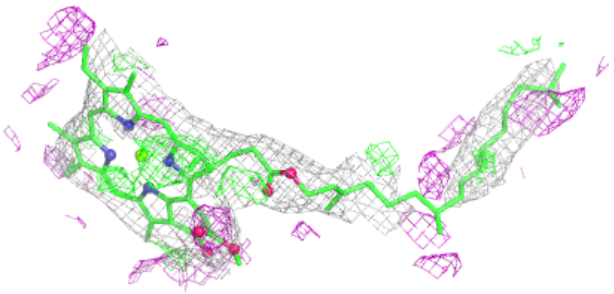


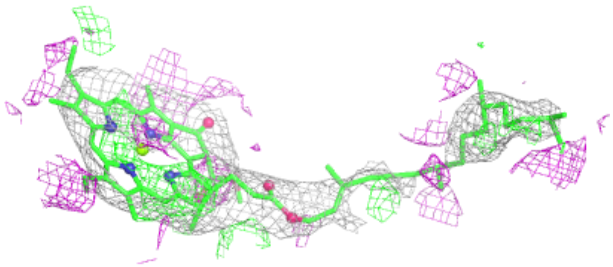


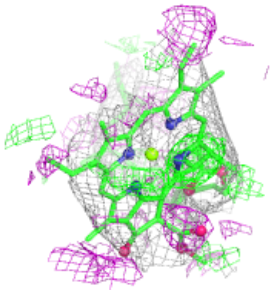


Electron density around CLA A 606:

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

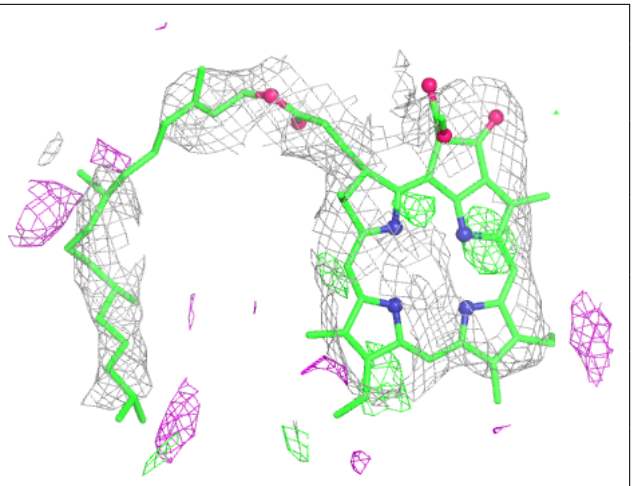


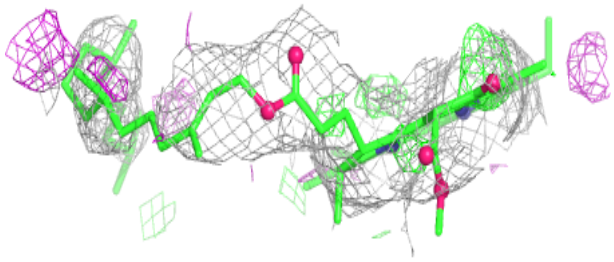


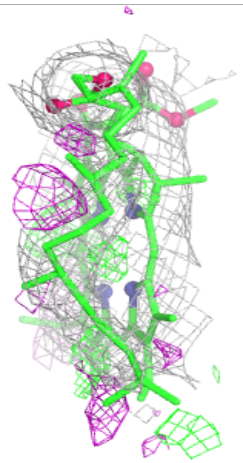


Electron density around PHO a 608:

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

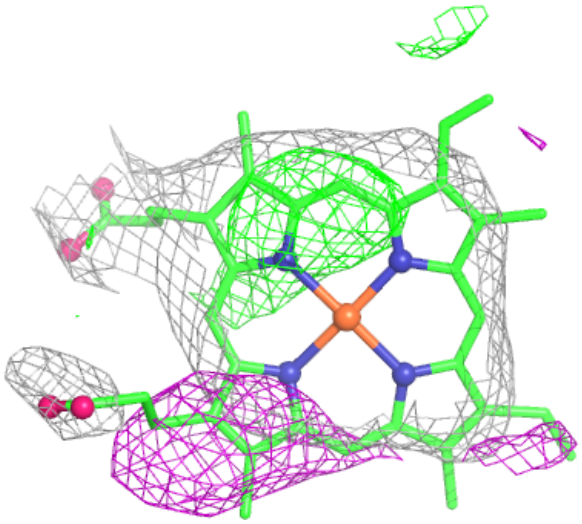


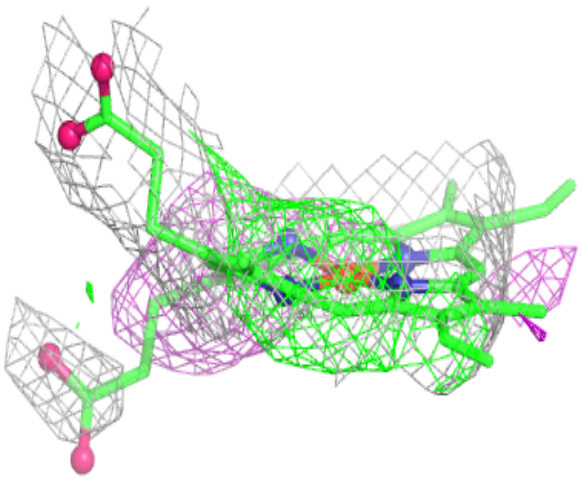


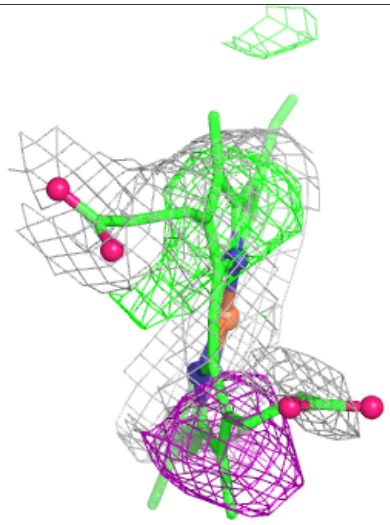


Electron density around HEM e 102:

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

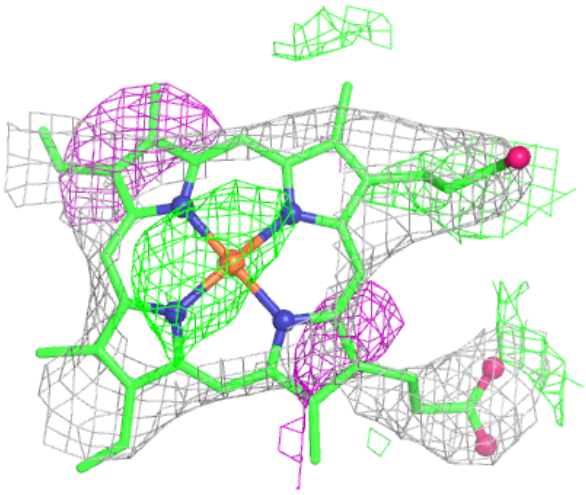


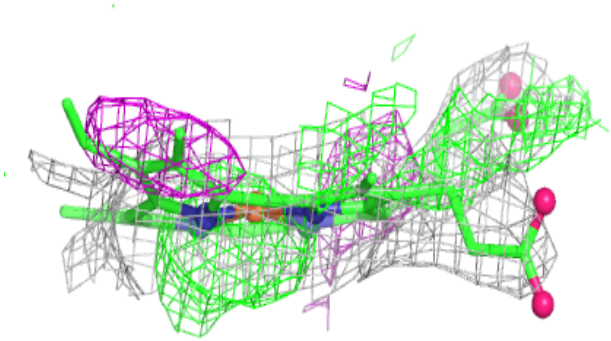


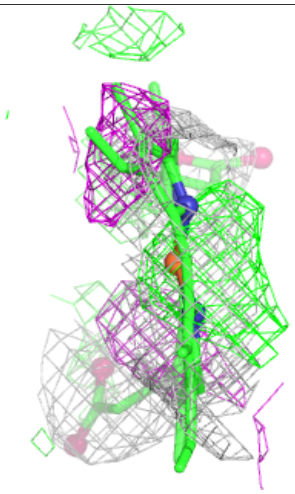


Electron density around HEM v 201:

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

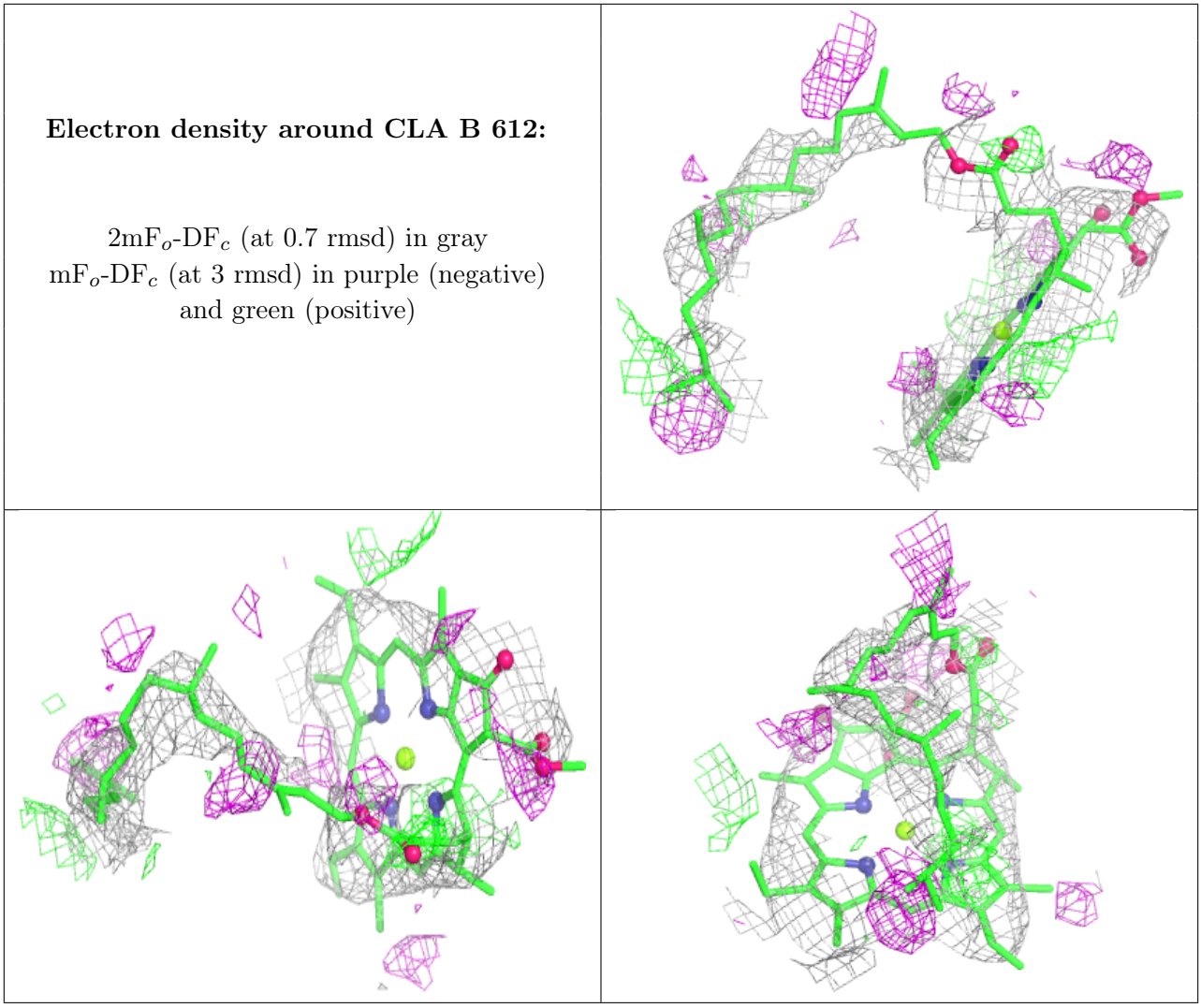






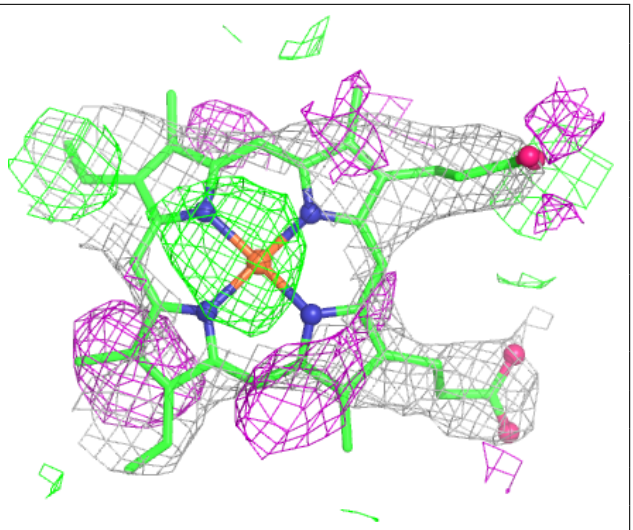
Electron density around CLA B 612:

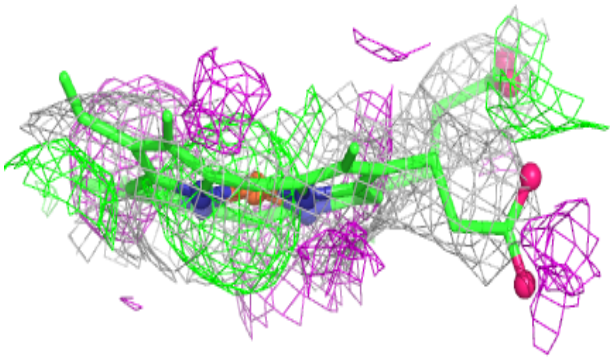
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

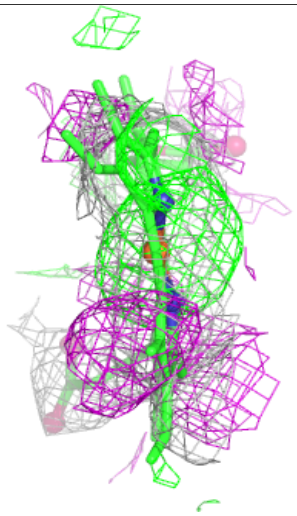


Electron density around HEM V 201:

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

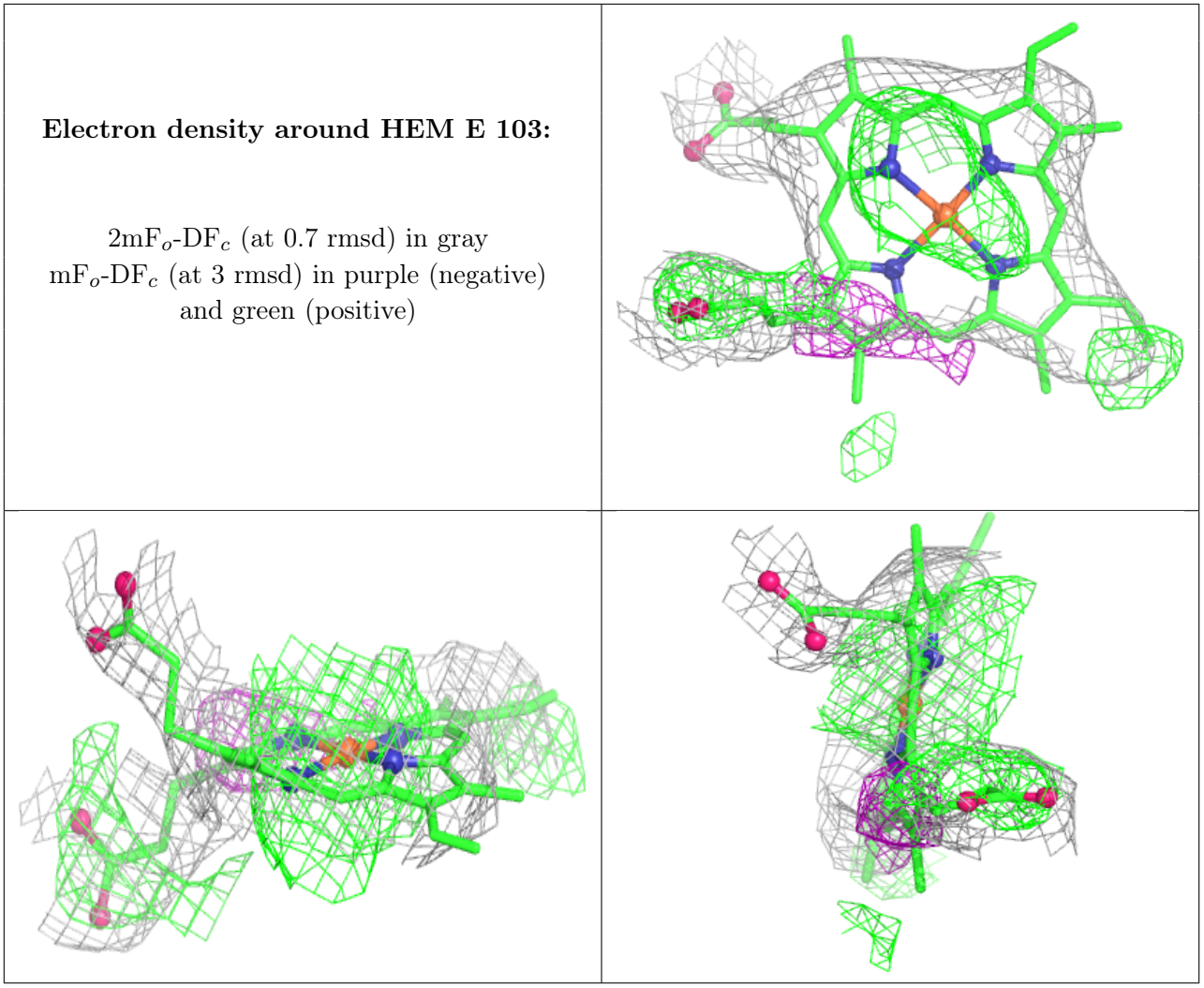






Electron density around HEM E 103:

$2mF_o$-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

There are no such residues in this entry.