Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 09:17 PM EDT

PDB ID	:	6DHO / pdb_00006dho
Title	:	RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.07 Angstrom resolution
Authors	:	Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on	:	2018-05-20
Resolution	:	2.07 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:

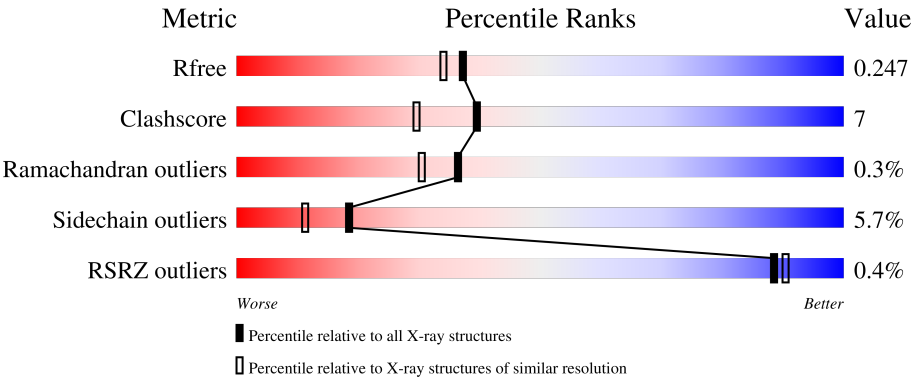
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	88% 11%

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Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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Mol	Chain	Length	Quality of chain
1	a	334	87% 10%
2	B	505	85% 14%
2	b	505	% 87% 13%
3	C	451	86% 12%
3	c	451	86% 13%
4	D	341	88% 11%
4	d	341	84% 16%
5	E	82	% 67% 28%
5	e	82	68% 30%
6	F	34	85% 12%
6	f	34	56% 41%
7	H	65	2% 83% 15%
7	h	65	69% 26%
8	I	36	78% 19%
8	i	36	3% 83% 17%
9	J	36	78% 19%
9	j	36	81% 11% 8%
10	K	37	70% 24% 5%
10	k	37	54% 43%
11	L	37	92% 8%
11	l	37	84% 11%
12	M	33	82% 15%
12	m	33	73% 21%
13	O	244	81% 17%
13	o	244	82% 15%

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Mol	Chain	Length	Quality of chain
14	T	30	83% 13%
14	t	30	3% 87% 13%
15	U	97	79% 19%
15	u	97	% 89% 10%
16	V	137	80% 19%
16	v	137	77% 22%
17	Y	30	10% 47% 27% 17% 10%
17	y	30	43% 53%
18	X	38	84% 16%
18	x	38	3% 53% 42% 5%
19	Z	62	3% 60% 27% 11%
19	z	62	3% 63% 31% 6%
20	R	34	3% 53% 41% 6%
20	r	34	3% 44% 44% 9%

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
36	HEC	V	201	X	-	-	-
36	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 105756 atoms, of which 52470 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	H	N	O	S	0	59	0
			6018	2010	2937	507	545	19			
1	a	334	Total	C	H	N	O	S	0	59	0
			6006	2007	2928	507	545	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	7	0
			6868	2282	3392	579	601	14			
3	c	451	Total	C	H	N	O	S	0	8	0
			7017	2324	3464	596	619	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			556	187	281	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	H	N	O	S	0	0	0
			1030	338	523	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			516	172	261	40	42	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	H	N	O	0	1	0
			620	209	318	46	47			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	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	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O		0	0	0
			600	197	304	47	52				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0	0
			525	171	269	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3730	1174	1850	317	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3718	1170	1844	317	383	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
14	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	Y	27	Total	C	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			
20	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

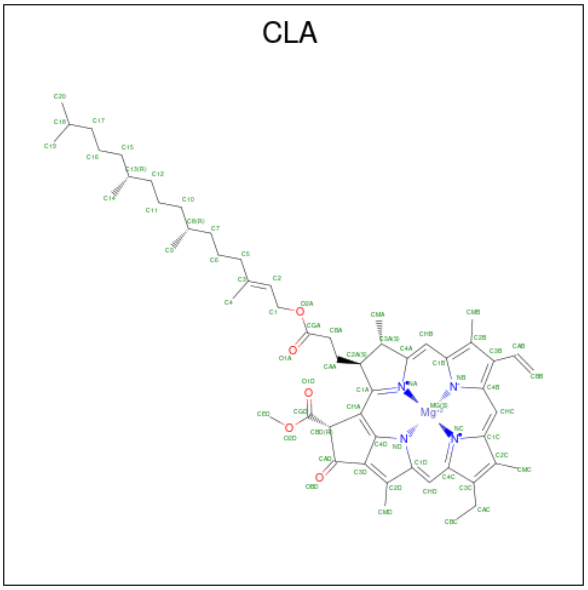
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	A	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	A	1	Total C H Mg N O 102 44 48 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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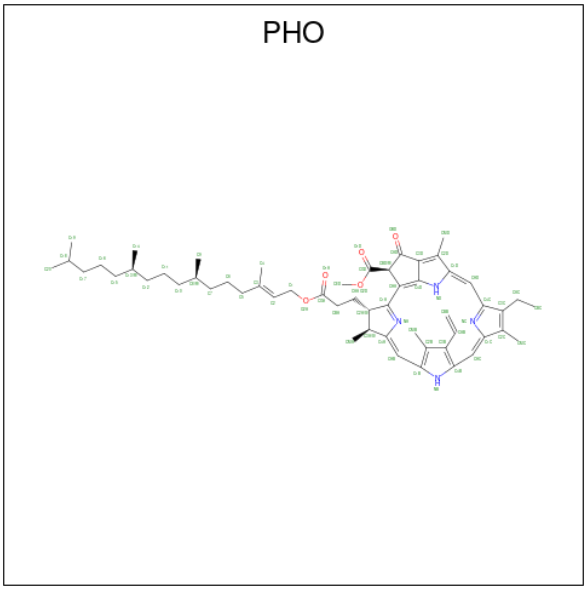
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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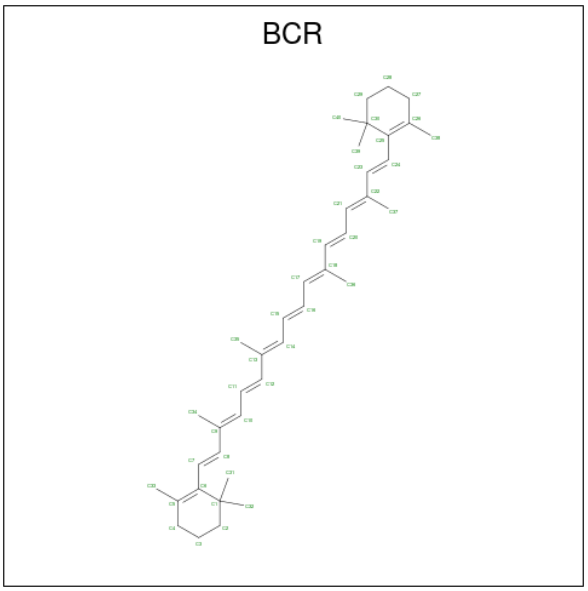
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	h	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

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



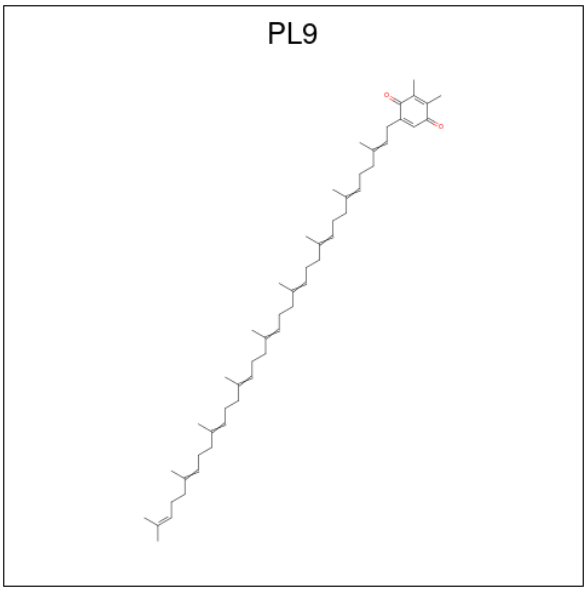
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	D	1	Total C H 96 40 56	0	0
25	H	1	Total C H 96 40 56	0	0
25	K	1	Total C H 96 40 56	0	0
25	K	1	Total C H 96 40 56	0	0
25	T	1	Total C H 96 40 56	0	0
25	Z	1	Total C H 96 40 56	0	0
25	a	1	Total C H 96 40 56	0	0
25	b	1	Total C H 96 40 56	0	0
25	b	1	Total C H 96 40 56	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	d	1	Total C H 96 40 56	0	0
25	k	1	Total C H 96 40 56	0	0
25	k	1	Total C H 96 40 56	0	0
25	t	1	Total C H 96 40 56	0	0
25	x	1	Total C H 96 40 56	0	0

- Molecule 26 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: $C_{53}H_{80}O_2$).



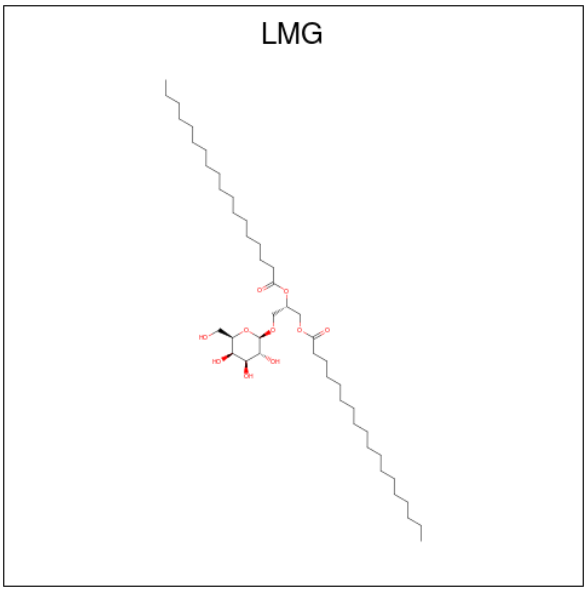
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C H O 135 53 80 2	0	0
26	D	1	Total C H O 135 53 80 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



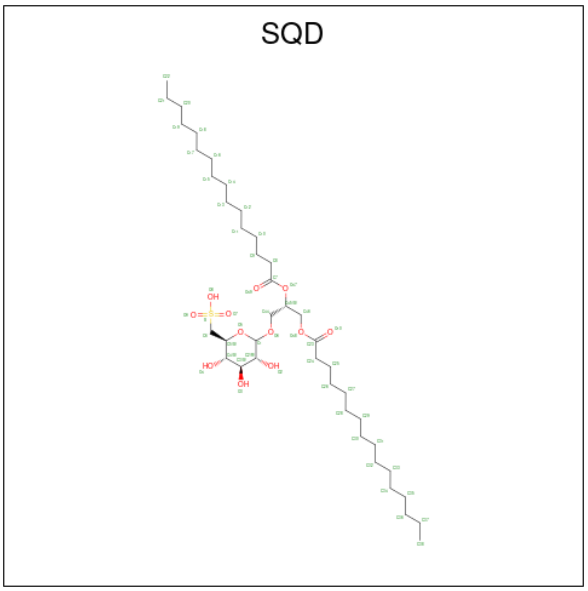
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			57	21	34	2		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C H O 117 38 69 10	0	0
27	c	1	Total C H O 117 39 68 10	0	0
27	d	1	Total C H O 102 34 58 10	0	0
27	m	1	Total C H O 123 41 72 10	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: $C_{41}H_{78}O_{12}S$).



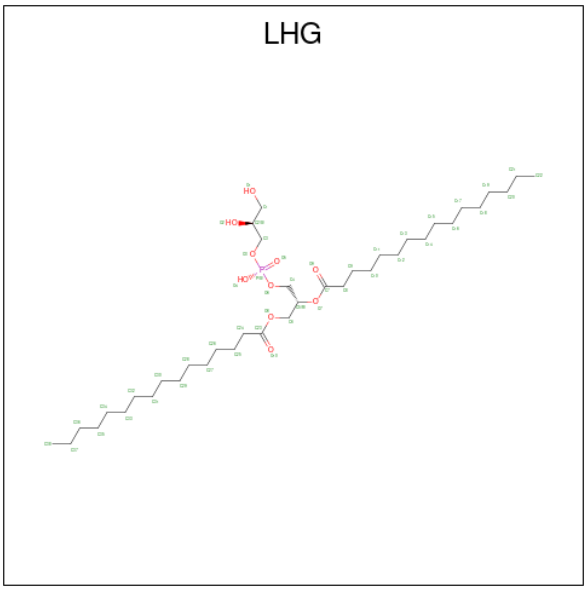
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H O S 122 39 70 12 1	0	0
28	A	1	Total C H O 104 35 65 4	0	0
28	B	1	Total C H O S 132 41 78 12 1	0	0
28	F	1	Total C H O S 81 25 45 10 1	0	0
28	a	1	Total C H O S 132 41 78 12 1	0	0
28	a	1	Total C H O 92 31 56 5	0	0
28	b	1	Total C H O S 114 36 65 12 1	0	0

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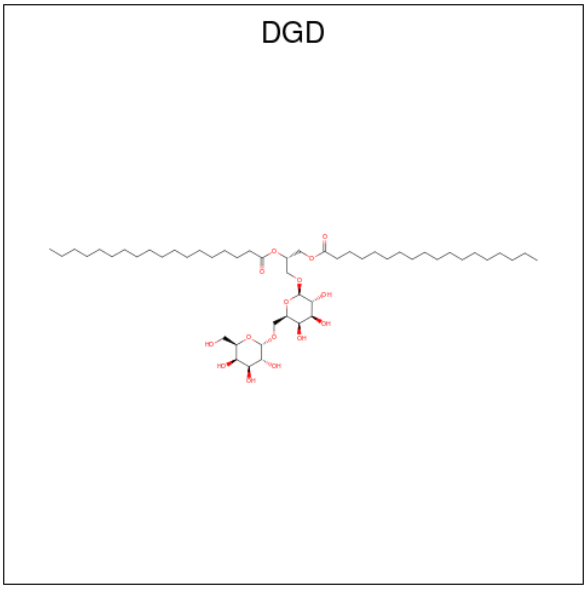
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



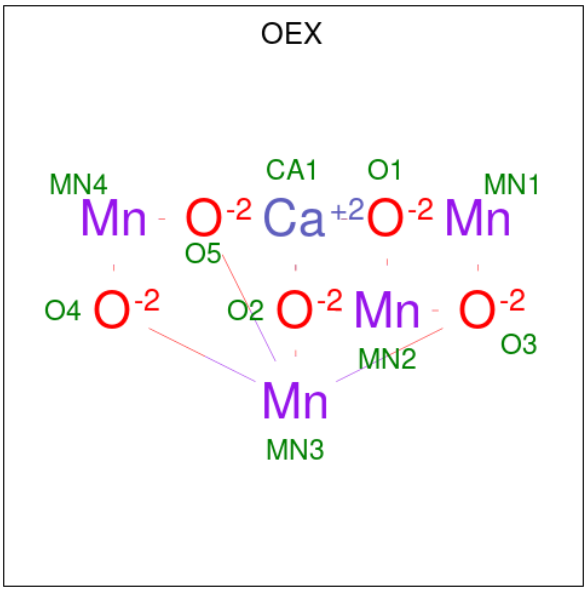
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
29	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
29	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



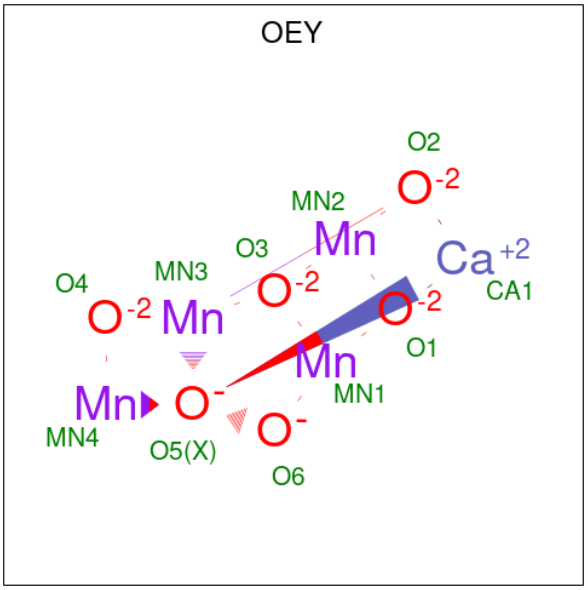
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	a	1	Total	C	H	O	0	0
			119	39	75	5		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



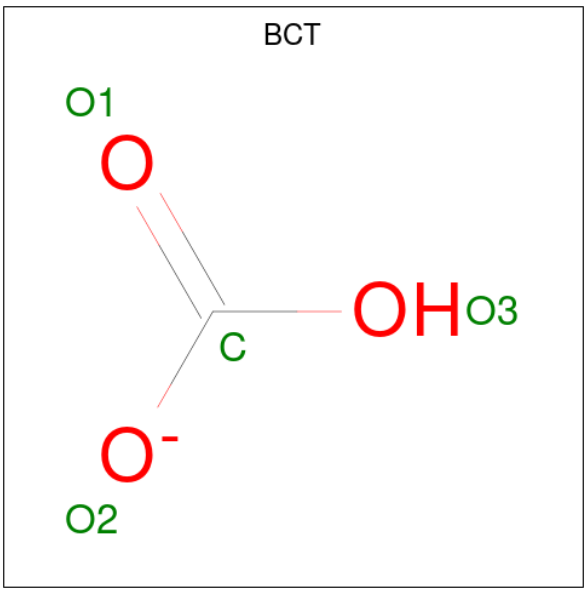
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: $CaMn_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
32	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C H O 5 1 1 3	0	0
33	a	1	Total C H O 5 1 1 3	0	0

- Molecule 34 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

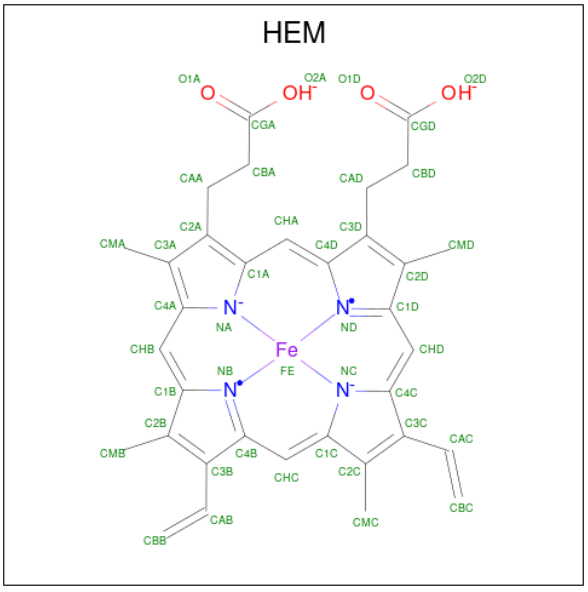
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	5	Total C H O 192 67 117 8	0	0
34	C	3	Total C H O 103 36 63 4	0	0
34	E	1	Total C H O 28 10 16 2	0	0
34	H	1	Total C H 53 18 35	0	0
34	I	1	Total C H 41 15 26	0	0
34	J	1	Total C H O 28 10 16 2	0	0
34	M	2	Total C H O 63 23 38 2	0	0
34	X	1	Total C H O 55 18 35 2	0	0
34	a	1	Total C H O 28 10 16 2	0	0

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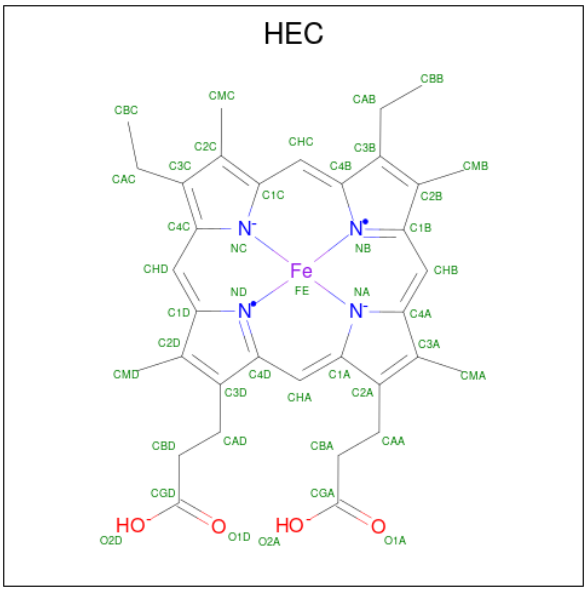
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	b	6	Total C H O 267 91 170 6	0	0
34	c	2	Total C H O 83 28 51 4	0	0
34	d	2	Total C H O 98 33 61 4	0	0
34	j	1	Total C H O 28 10 16 2	0	0
34	l	1	Total C H 53 18 35	0	0
34	m	1	Total C H O 28 10 16 2	0	0
34	t	2	Total C H O 60 22 36 2	0	0

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	E	1	Total C Fe H N O 73 34 1 30 4 4	0	0
35	e	1	Total C Fe H N O 73 34 1 30 4 4	0	0

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
36	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
36	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	146	Total	O	0	8
			146	146		
37	B	213	Total	O	0	0
			213	213		
37	C	193	Total	O	0	0
			193	193		
37	D	129	Total	O	0	0
			129	129		
37	E	29	Total	O	0	0
			29	29		
37	F	14	Total	O	0	0
			14	14		
37	H	29	Total	O	0	0
			29	29		
37	I	14	Total	O	0	0
			14	14		
37	J	12	Total	O	0	0
			12	12		
37	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	L	8	Total O 8 8	0	0
37	M	7	Total O 7 7	0	0
37	O	123	Total O 123 123	0	0
37	T	14	Total O 14 14	0	0
37	U	49	Total O 49 49	0	0
37	V	73	Total O 73 73	0	0
37	Y	3	Total O 3 3	0	0
37	X	8	Total O 8 8	0	0
37	Z	4	Total O 4 4	0	0
37	R	3	Total O 3 3	0	0
37	a	125	Total O 125 125	0	8
37	b	188	Total O 188 188	0	0
37	c	159	Total O 159 159	0	0
37	d	123	Total O 123 123	0	0
37	e	22	Total O 22 22	0	0
37	f	5	Total O 5 5	0	0
37	h	20	Total O 20 20	0	0
37	i	12	Total O 12 12	0	0
37	j	8	Total O 8 8	0	0
37	k	4	Total O 4 4	0	0
37	l	10	Total O 10 10	0	0

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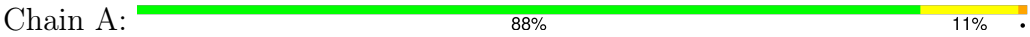
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	m	6	Total O 6 6	0	0
37	o	120	Total O 120 120	0	0
37	t	12	Total O 12 12	0	0
37	u	50	Total O 50 50	0	0
37	v	68	Total O 68 68	0	0
37	y	4	Total O 4 4	0	0
37	x	11	Total O 11 11	0	0
37	z	1	Total O 1 1	0	0
37	r	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1 1

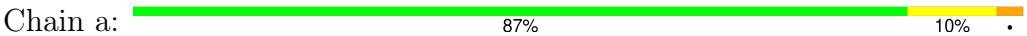
Chain A:

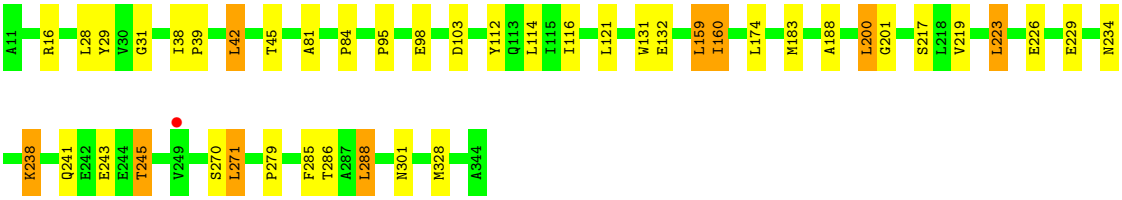




• Molecule 1: Photosystem II protein D1 1

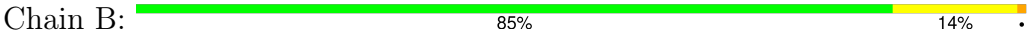
Chain a:

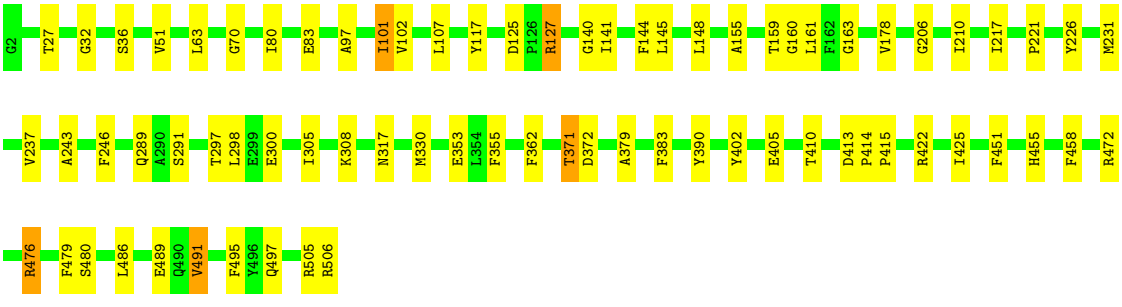




• Molecule 2: Photosystem II CP47 reaction center protein

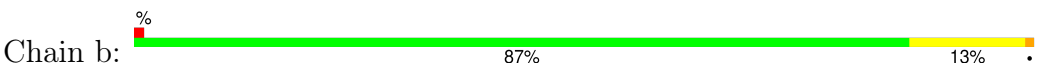
Chain B:





• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

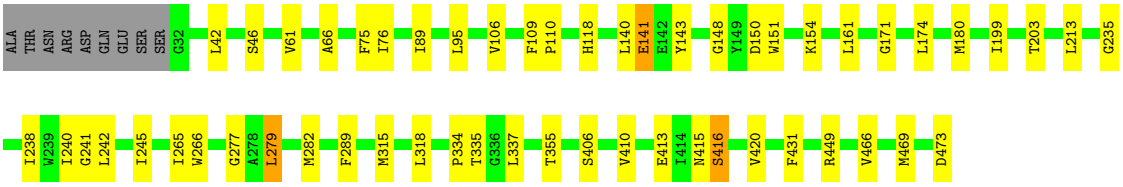




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

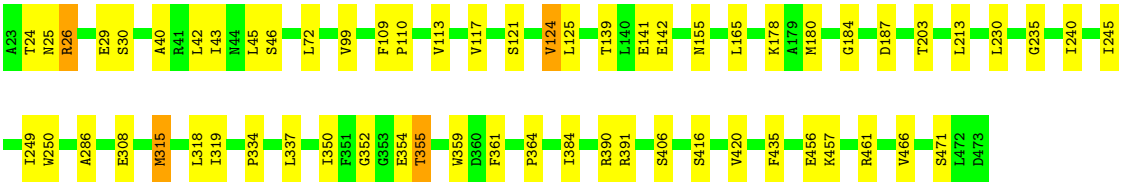




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

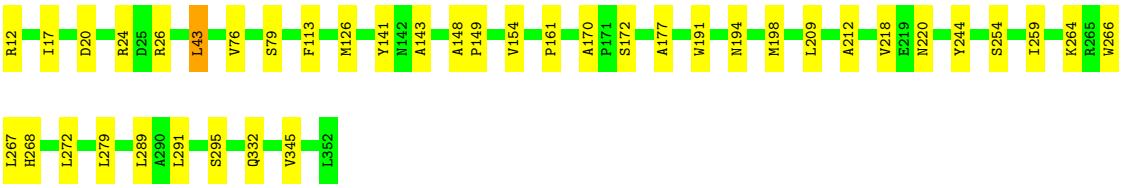




• Molecule 4: Photosystem II D2 protein

Chain D:

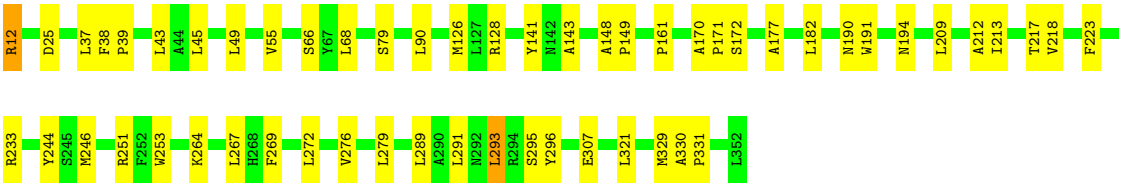




• Molecule 4: Photosystem II D2 protein

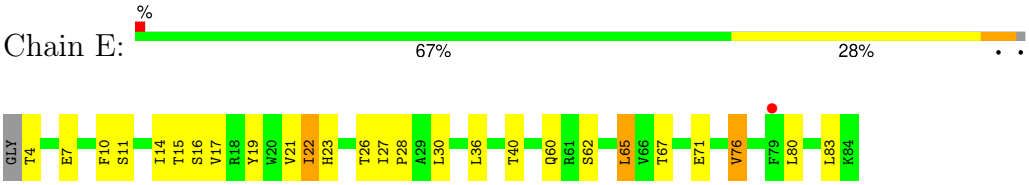
Chain d:





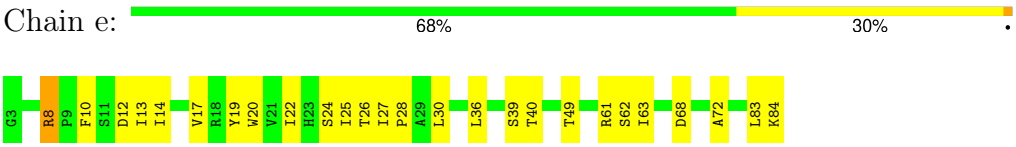
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



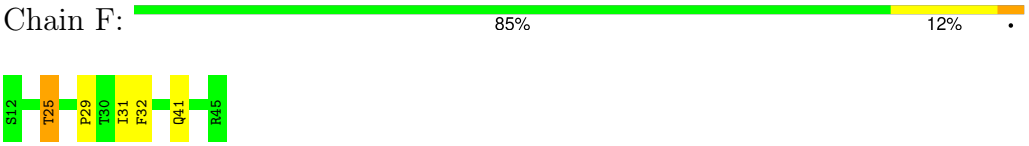
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



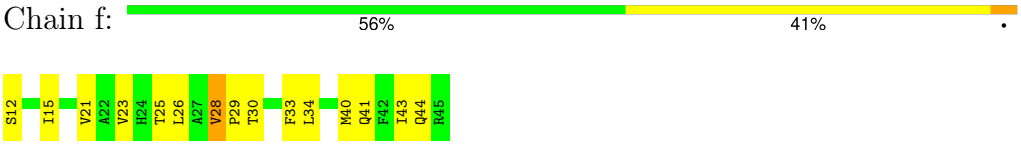
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



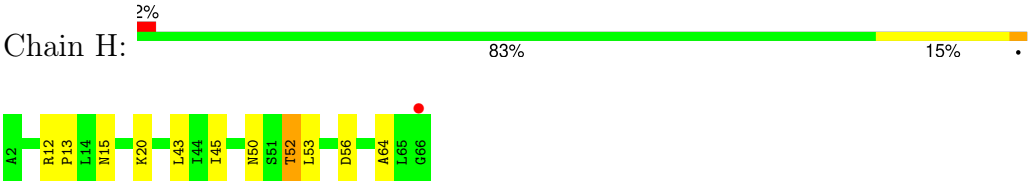
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



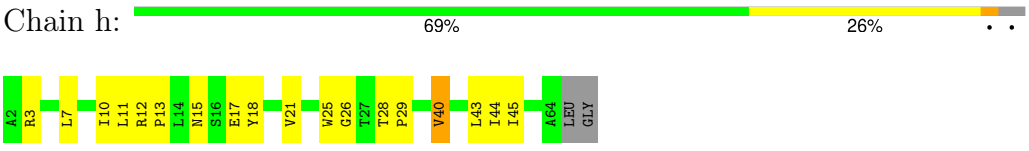
• Molecule 7: Photosystem II reaction center protein H

Chain H:



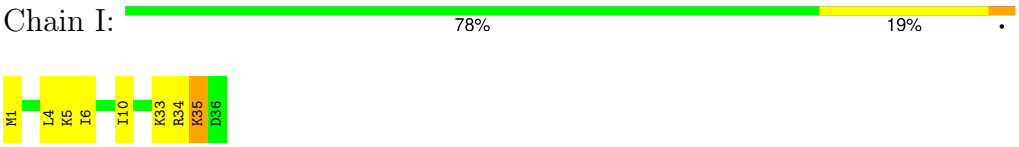
• Molecule 7: Photosystem II reaction center protein H

Chain h:



• Molecule 8: Photosystem II reaction center protein I

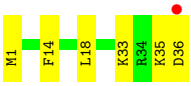
Chain I:



• 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:

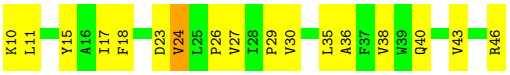




• Molecule 10: Photosystem II reaction center protein K

Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:

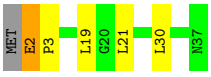




• Molecule 11: Photosystem II reaction center protein L

Chain l:

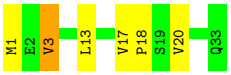




• Molecule 12: Photosystem II reaction center protein M

Chain M:

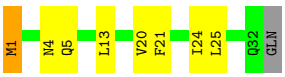




• Molecule 12: Photosystem II reaction center protein M

Chain m:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

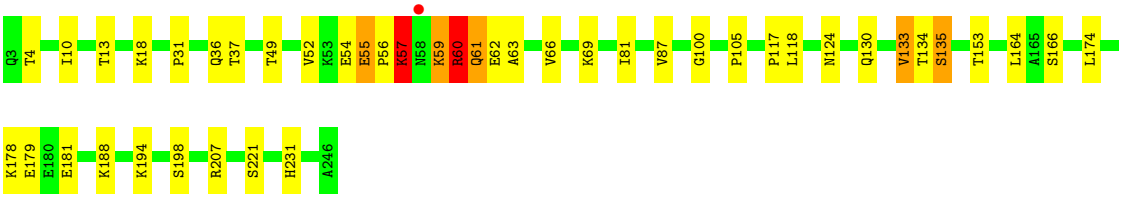




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:





• Molecule 14: Photosystem II reaction center protein T

Chain T:





• Molecule 14: Photosystem II reaction center protein T

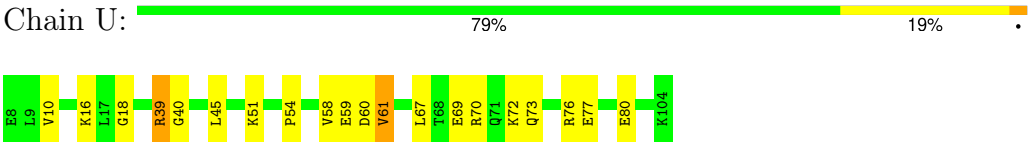
Chain t:





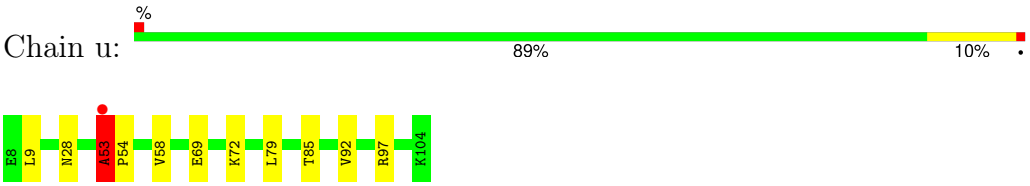
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



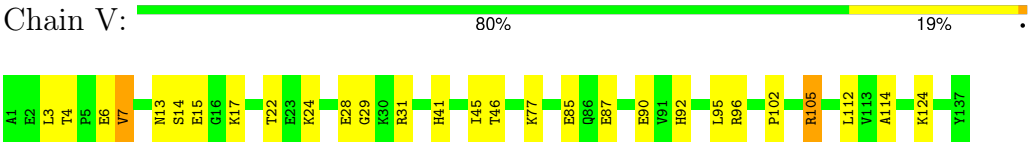
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



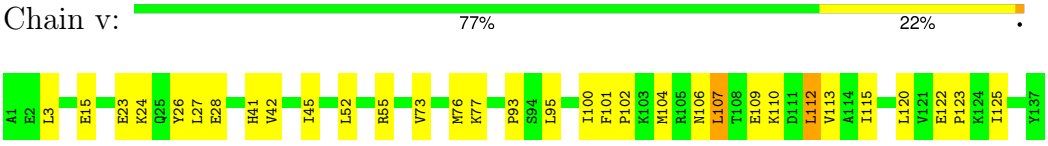
• Molecule 16: Cytochrome c-550

Chain V:



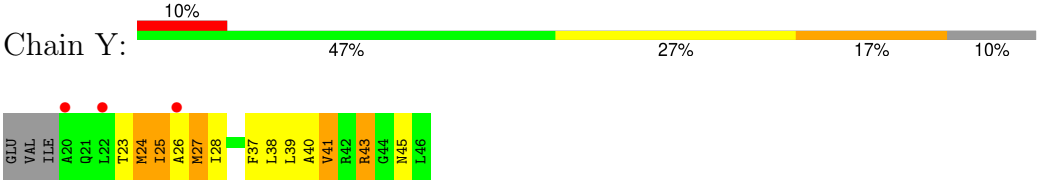
• Molecule 16: Cytochrome c-550

Chain v:



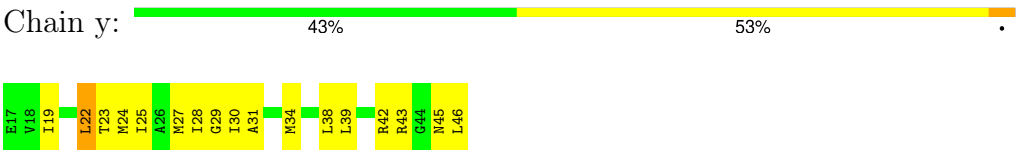
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



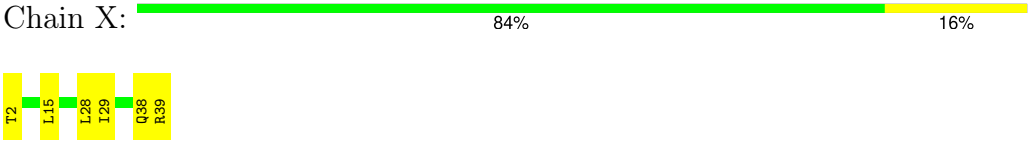
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



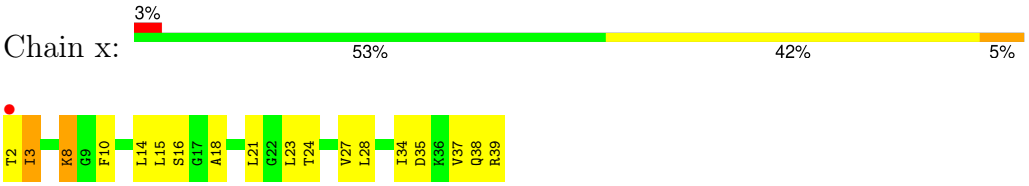
• Molecule 18: Photosystem II reaction center X protein

Chain X:



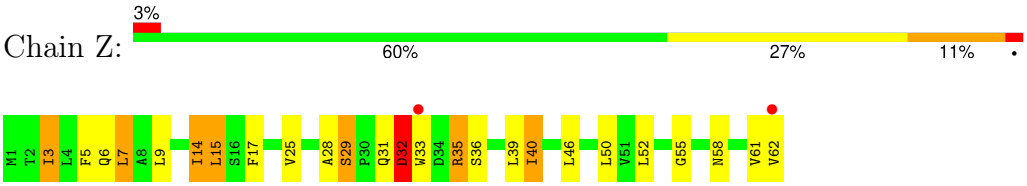
• Molecule 18: Photosystem II reaction center X protein

Chain x:



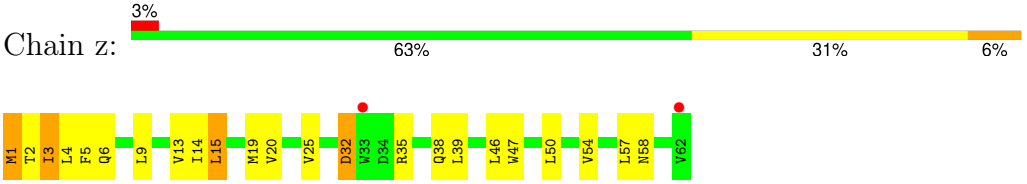
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



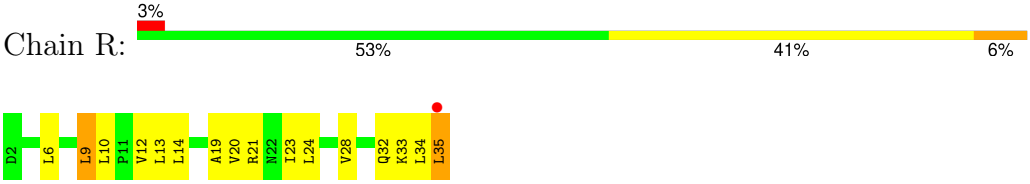
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



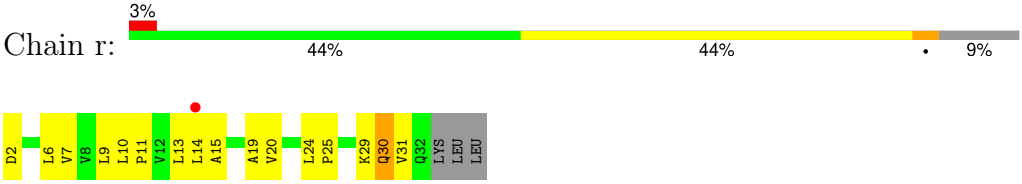
• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y

Chain r:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.01Å 221.54Å 308.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.58 – 2.07 30.58 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.58-2.07) 87.0 (30.58-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.54 (at 2.06Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.184 , 0.247 0.184 , 0.247	Depositor DCC
R_{free} test set	4294 reflections (0.73%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	105756	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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

5.1 Standard geometry

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

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	0.56	0/3179	0.66	0/4331
1	a	0.52	0/3176	0.63	0/4327
2	B	0.59	1/4160 (0.0%)	0.66	1/5668 (0.0%)
2	b	0.55	0/4118	0.65	0/5611
3	C	0.58	1/3593 (0.0%)	0.63	0/4891
3	c	0.51	0/3673	0.64	0/4998
4	D	0.60	0/2820	0.66	0/3840
4	d	0.57	0/2829	0.65	0/3852
5	E	0.44	0/684	0.62	0/935
5	e	0.42	0/683	0.57	0/932
6	F	0.43	0/284	0.62	0/387
6	f	0.38	0/284	0.65	0/387
7	H	0.55	0/520	0.66	0/709
7	h	0.49	0/511	0.61	0/697
8	I	0.59	0/293	0.61	0/396
8	i	0.60	0/293	0.74	0/396
9	J	0.48	0/263	0.61	0/356
9	j	0.40	0/261	0.52	0/353
10	K	0.43	0/314	0.52	0/427
10	k	0.39	0/303	0.50	0/416
11	L	0.57	0/311	0.69	0/422
11	l	0.59	0/303	0.65	0/412
12	M	0.56	0/249	0.61	0/341
12	m	0.57	0/244	0.66	0/334
13	O	0.55	0/1914	0.65	0/2596
13	o	0.53	0/1905	0.65	0/2583
14	T	0.60	0/257	0.71	0/349
14	t	0.57	0/255	0.62	0/346
15	U	0.47	0/785	0.60	0/1064
15	u	0.54	0/785	0.68	0/1064
16	V	0.52	0/1085	0.61	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.48	0/1085	0.60	0/1473
17	Y	0.37	0/197	0.67	0/264
17	y	0.32	0/219	0.49	0/294
18	X	0.46	0/284	0.54	0/384
18	x	0.34	0/284	0.46	0/384
19	Z	0.40	0/490	0.55	0/669
19	z	0.35	0/488	0.53	0/666
20	R	0.36	0/277	0.55	0/380
20	r	0.27	0/233	0.47	0/323
All	All	0.54	2/43891 (0.0%)	0.64	1/59730 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	u	0	1
19	Z	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	ILE	CA-CB	-11.60	1.48	1.54
2	B	221	PRO	CA-C	-8.10	1.47	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	221	PRO	O-C-N	-5.70	118.69	121.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	Z	32	ASP	Peptide
15	u	53	ALA	Peptide

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	3081	2937	2950	29	0
1	a	3078	2928	2941	28	0
2	B	4004	3845	3864	43	0
2	b	3978	3811	3836	48	0
3	C	3476	3392	3405	35	0
3	c	3553	3464	3477	37	0
4	D	2726	2624	2632	29	0
4	d	2732	2630	2638	40	0
5	E	662	647	648	17	0
5	e	664	647	648	21	0
6	F	275	281	282	4	0
6	f	275	281	282	8	0
7	H	507	523	523	7	0
7	h	498	518	518	8	0
8	I	296	311	311	3	0
8	i	296	311	311	3	0
9	J	257	268	268	8	0
9	j	255	261	261	7	0
10	K	302	318	318	12	0
10	k	293	305	305	14	0
11	L	304	316	316	3	0
11	l	296	304	304	2	0
12	M	256	269	269	6	0
12	m	251	267	267	7	0
13	O	1880	1850	1852	33	0
13	o	1874	1844	1846	23	0
14	T	258	261	261	2	0
14	t	256	256	256	2	0
15	U	774	772	773	12	0
15	u	774	772	773	7	0
16	V	1064	1070	1073	16	0
16	v	1064	1070	1073	22	0
17	Y	196	208	217	11	0
17	y	218	241	241	10	0
18	X	281	312	312	2	0
18	x	281	312	312	15	0
19	Z	479	509	516	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	477	509	509	25	0
20	R	271	298	298	7	0
20	r	227	234	224	11	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	184	192	192	4	0
23	B	1035	1139	1139	20	0
23	C	839	922	922	11	0
23	D	195	216	216	3	0
23	a	260	288	288	5	0
23	b	970	1067	1067	28	0
23	c	839	919	919	8	0
23	d	130	144	144	1	0
23	h	65	72	72	3	0
24	A	128	148	148	1	0
24	a	64	74	74	0	0
24	d	64	74	74	2	0
25	A	40	56	56	2	0
25	B	120	168	168	8	0
25	C	40	56	56	1	0
25	D	40	56	56	5	0
25	H	40	56	56	2	0
25	K	80	112	112	3	0
25	T	40	56	56	3	0
25	Z	40	56	56	4	0
25	a	40	56	56	2	0
25	b	120	168	168	8	0
25	c	80	112	112	2	0
25	d	40	56	56	3	0
25	k	80	112	112	4	0
25	t	40	56	56	6	0
25	x	40	56	56	2	0
26	A	55	80	80	6	0
26	D	55	80	80	0	0
26	a	55	80	80	6	0
26	d	55	80	80	2	0
27	A	48	66	66	1	0
27	B	28	40	40	0	0
27	C	48	66	66	0	0
27	D	84	117	117	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	M	51	72	72	0	0
27	b	78	120	120	2	0
27	c	134	181	181	4	0
27	d	44	58	58	1	0
27	m	51	72	72	1	0
28	A	91	135	134	2	0
28	B	54	78	78	1	0
28	F	36	45	46	0	0
28	a	90	134	132	4	0
28	b	49	65	65	1	0
28	f	41	49	49	2	0
29	A	49	74	74	4	0
29	B	98	148	148	2	0
29	D	96	141	141	3	0
29	d	137	199	199	9	0
29	e	42	57	57	2	0
29	l	49	74	74	1	0
30	A	66	96	96	3	0
30	C	186	246	244	0	0
30	H	62	82	82	1	0
30	a	44	75	75	3	0
30	c	186	246	243	0	0
30	h	62	82	82	1	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	A	11	0	0	2	0
32	a	11	0	0	1	0
33	A	4	1	1	0	0
33	a	4	1	1	0	0
34	B	75	117	0	0	0
34	C	40	63	0	0	0
34	E	12	16	0	0	0
34	H	18	35	0	0	0
34	I	15	26	0	0	0
34	J	12	16	0	0	0
34	M	25	38	0	0	0
34	X	20	35	0	0	0
34	a	12	16	0	0	0
34	b	97	170	0	0	0
34	c	32	51	0	0	0
34	d	37	61	0	0	0
34	j	12	16	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	l	18	35	0	0	0
34	m	12	16	0	0	0
34	t	24	36	0	0	0
35	E	43	30	30	5	0
35	e	43	30	30	3	0
36	V	43	30	30	1	0
36	v	43	30	30	0	0
37	A	146	0	0	4	0
37	B	213	0	0	8	0
37	C	193	0	0	0	0
37	D	129	0	0	4	0
37	E	29	0	0	2	0
37	F	14	0	0	0	0
37	H	29	0	0	0	0
37	I	14	0	0	1	0
37	J	12	0	0	2	0
37	K	6	0	0	0	0
37	L	8	0	0	0	0
37	M	7	0	0	0	0
37	O	123	0	0	8	0
37	R	3	0	0	0	0
37	T	14	0	0	0	0
37	U	49	0	0	7	0
37	V	73	0	0	2	0
37	X	8	0	0	0	0
37	Y	3	0	0	0	0
37	Z	4	0	0	0	0
37	a	125	0	0	1	0
37	b	188	0	0	6	0
37	c	159	0	0	6	0
37	d	123	0	0	3	0
37	e	22	0	0	0	0
37	f	5	0	0	0	0
37	h	20	0	0	2	0
37	i	12	0	0	0	0
37	j	8	0	0	1	0
37	k	4	0	0	0	0
37	l	10	0	0	0	0
37	m	6	0	0	1	0
37	o	120	0	0	4	0
37	r	6	0	0	2	0
37	t	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	u	50	0	0	2	0
37	v	68	0	0	2	0
37	x	11	0	0	2	0
37	y	4	0	0	0	0
37	z	1	0	0	0	0
All	All	53286	52470	51850	688	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 7.

All (688) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:THR:O	37:B:701:HOH:O	1.74	1.04
3:c:391[A]:ARG:NH1	37:c:601:HOH:O	1.98	0.96
13:O:90:ASP:OD1	37:O:301:HOH:O	1.82	0.95
12:m:5:GLN:O	37:m:201:HOH:O	1.87	0.92
2:b:505:ARG:HG3	2:b:506:ARG:HG3	1.49	0.92
7:H:56:ASP:OD1	18:X:2:THR:N	2.07	0.87
15:U:80:GLU:O	37:U:201:HOH:O	1.94	0.84
2:B:413:ASP:OD1	37:B:702:HOH:O	1.95	0.83
1:a:243:GLU:OE1	37:a:501:HOH:O	1.95	0.83
15:U:54:PRO:O	37:U:202:HOH:O	1.97	0.82
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.61	0.80
2:B:506:ARG:HD3	37:B:879:HOH:O	1.82	0.80
3:C:171:GLY:HA2	3:C:174:LEU:HD12	1.64	0.79
13:O:24:ASP:OD2	37:O:302:HOH:O	2.01	0.79
16:v:120:LEU:O	37:v:301:HOH:O	2.00	0.79
13:O:92:SER:N	37:O:301:HOH:O	2.12	0.78
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.65	0.78
18:x:39:ARG:O	37:x:201:HOH:O	2.03	0.77
13:O:156:PHE:O	37:O:303:HOH:O	2.04	0.76
4:d:12:ARG:N	37:d:502:HOH:O	2.20	0.75
2:B:497:GLN:OE1	37:B:703:HOH:O	2.04	0.74
23:b:611:CLA:H202	23:b:613:CLA:HMD3	1.67	0.74
20:r:2:ASP:N	37:r:101:HOH:O	2.19	0.74
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.69	0.73
2:b:292:LEU:O	37:b:701:HOH:O	2.06	0.73
20:r:29:LYS:O	20:r:31:VAL:N	2.21	0.73
2:b:489:GLU:OE2	2:b:505:ARG:NH1	2.22	0.73
15:U:60:ASP:OD1	37:U:203:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:40:ALA:O	3:c:43:ILE:HD12	1.88	0.72
15:U:76:ARG:NH1	37:U:204:HOH:O	2.22	0.72
12:m:4:ASN:ND2	27:m:101:LMG:O10	2.22	0.72
2:B:371:THR:HG23	2:B:372:ASP:O	1.89	0.72
23:C:504:CLA:H143	23:C:508:CLA:C14	2.21	0.71
32:a:417[B]:OEY:O6	32:a:417[B]:OEY:O5	2.07	0.71
3:c:384:ILE:O	37:c:602:HOH:O	2.09	0.71
17:y:23:THR:HG23	17:y:24:MET:HE2	1.71	0.71
4:d:25:ASP:OD1	37:d:501:HOH:O	2.08	0.71
35:e:102:HEM:HHC	35:e:102:HEM:HBB2	1.72	0.71
4:d:246:MET:HE3	4:d:264:LYS:CG	2.20	0.71
23:a:405:CLA:HMB3	23:a:405:CLA:HBB1	1.73	0.70
2:b:283:GLU:OE2	37:b:702:HOH:O	2.09	0.70
3:c:113:VAL:O	3:c:117:VAL:HG23	1.92	0.70
23:b:614:CLA:H192	29:d:406:LHG:H222	1.74	0.70
5:E:7:GLU:OE2	37:E:201:HOH:O	2.10	0.69
1:A:16:ARG:NH2	37:A:501:HOH:O	2.26	0.69
35:E:101:HEM:HBC2	35:E:101:HEM:HHD	1.75	0.69
3:c:391[B]:ARG:NE	37:c:605:HOH:O	2.25	0.69
25:t:101:BCR:H321	25:t:101:BCR:HC8	1.75	0.69
1:a:103:ASP:OD2	13:o:69:LYS:NZ	2.23	0.69
13:O:19:CYS:O	37:O:304:HOH:O	2.11	0.69
32:A:417[B]:OEY:O5	32:A:417[B]:OEY:O6	2.10	0.68
19:z:1:MET:HB2	19:z:4:LEU:HD23	1.75	0.68
9:J:36:LEU:O	37:J:201:HOH:O	2.12	0.67
5:e:61:ARG:NH2	16:v:125:ILE:O	2.27	0.67
9:j:19:MET:O	9:j:23:VAL:HG23	1.94	0.67
5:E:36:LEU:O	5:E:40:THR:HG23	1.94	0.67
15:U:16:LYS:NZ	37:U:205:HOH:O	2.26	0.67
25:D:404:BCR:H331	25:D:404:BCR:C8	2.24	0.66
6:f:40:MET:HA	6:f:43:ILE:HD13	1.78	0.66
5:e:20:TRP:O	5:e:24:SER:OG	2.07	0.66
20:R:9:LEU:O	20:R:12:VAL:HG22	1.95	0.66
23:b:604:CLA:H2	23:b:606:CLA:H91	1.76	0.66
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.31	0.66
2:B:305:ILE:O	37:B:704:HOH:O	2.12	0.66
16:V:4:THR:OG1	16:V:6:GLU:OE1	2.10	0.65
2:b:99:ALA:HB1	23:b:607:CLA:H72	1.77	0.65
20:R:24:LEU:O	20:R:28:VAL:HG23	1.97	0.65
3:C:66:ALA:HB1	10:K:25:LEU:HB3	1.79	0.65
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:267:LEU:C	4:d:267:LEU:HD23	2.21	0.64
28:f:101:SQD:H312	18:x:27:VAL:HG11	1.79	0.64
9:j:36:LEU:O	37:j:201:HOH:O	2.15	0.64
23:h:101:CLA:HMB3	23:h:101:CLA:H193	1.79	0.64
9:J:5:GLY:N	37:J:202:HOH:O	2.30	0.64
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.31	0.64
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.78	0.64
1:a:234:ASN:ND2	29:d:406:LHG:O1	2.31	0.64
23:c:501:CLA:H192	23:c:507:CLA:HBB1	1.79	0.64
19:z:32:ASP:OD1	19:z:32:ASP:N	2.27	0.64
13:O:56:PRO:O	13:O:58:ASN:N	2.30	0.63
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.81	0.63
1:A:334[A]:ARG:NH2	37:A:503:HOH:O	2.31	0.63
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.82	0.62
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.34	0.62
17:Y:23:THR:O	17:Y:27:MET:HE1	2.00	0.61
18:x:3:ILE:H	18:x:3:ILE:HD12	1.66	0.61
25:C:514:BCR:H331	25:C:514:BCR:C8	2.29	0.61
37:A:547:HOH:O	13:O:107:THR:HG21	2.00	0.61
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.82	0.61
23:b:614:CLA:H192	29:d:406:LHG:C22	2.30	0.61
19:z:1:MET:CB	19:z:4:LEU:HD23	2.31	0.61
13:o:164:LEU:HD13	13:o:188:LYS:O	2.01	0.61
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.81	0.60
4:D:332:GLN:NE2	37:D:501:HOH:O	2.33	0.60
23:d:403:CLA:H92	18:x:18:ALA:HB2	1.83	0.60
35:E:101:HEM:O2A	37:E:202:HOH:O	2.16	0.60
8:i:14:PHE:CZ	8:i:18:LEU:HD11	2.36	0.60
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.84	0.60
3:c:245:ILE:HD13	27:c:521:LMG:H371	1.83	0.60
13:o:179:GLU:OE2	37:o:301:HOH:O	2.17	0.60
25:K:101:BCR:H322	19:Z:17:PHE:CE1	2.37	0.60
4:D:291:LEU:HD21	30:H:102:DGD:CGB	2.32	0.59
3:c:45:LEU:HA	3:c:139:THR:HG22	1.84	0.59
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.84	0.59
19:Z:36:SER:O	19:Z:39:LEU:N	2.36	0.59
23:B:604:CLA:H43	23:B:605:CLA:H2	1.84	0.59
23:c:509:CLA:H43	23:c:509:CLA:O1A	2.03	0.59
25:d:404:BCR:H381	27:d:409:LMG:H162	1.84	0.59
10:k:17:ILE:HD11	19:z:6:GLN:HG2	1.84	0.59
5:e:10:PHE:N	29:e:101:LHG:O4	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:H:101:BCR:H331	25:H:101:BCR:C8	2.32	0.58
1:A:303:ASN:O	3:C:415:ASN:ND2	2.30	0.58
30:a:414:DGD:O1G	30:a:414:DGD:O1B	2.21	0.58
25:d:404:BCR:H331	25:d:404:BCR:C8	2.33	0.58
2:b:317:ASN:HA	2:b:330:MET:HE1	1.85	0.58
9:J:15:THR:HG22	9:J:19:MET:CE	2.34	0.58
11:L:36:PHE:HB3	12:M:3:VAL:HG22	1.86	0.58
10:K:18:PHE:CE2	19:Z:9:LEU:HD21	2.38	0.57
10:K:22:VAL:HA	10:K:25:LEU:HD22	1.86	0.57
13:o:194:LYS:NZ	37:o:306:HOH:O	2.36	0.57
16:v:41:HIS:HA	16:v:45:ILE:O	2.05	0.57
4:d:141:TYR:OH	29:d:406:LHG:O4	2.16	0.57
17:Y:39:LEU:HD21	19:Z:28:ALA:HB3	1.85	0.57
3:C:213:LEU:HG	23:C:506:CLA:H193	1.85	0.57
13:O:35:SER:OG	13:O:36:GLN:N	2.38	0.57
23:a:411:CLA:O1A	23:a:411:CLA:H43	2.05	0.57
35:e:102:HEM:HMC1	35:e:102:HEM:HBC2	1.87	0.57
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.86	0.57
2:b:125:ASP:HB2	2:b:132:ALA:HB3	1.86	0.57
3:c:406:SER:HA	3:c:420:VAL:HG23	1.86	0.57
4:d:49:LEU:HD13	25:d:404:BCR:C15	2.35	0.57
1:a:114:LEU:C	1:a:114:LEU:HD23	2.30	0.57
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.86	0.57
2:b:324:LEU:HA	4:d:293:LEU:HD13	1.86	0.56
3:C:337:LEU:HD23	13:O:105:PRO:CG	2.35	0.56
3:C:277:GLY:C	23:C:505:CLA:HBC2	2.30	0.56
23:C:504:CLA:H143	23:C:508:CLA:H143	1.87	0.56
4:D:254:SER:OG	14:T:24:ARG:NH2	2.39	0.56
23:b:615:CLA:H92	25:b:618:BCR:H362	1.86	0.56
15:u:53:ALA:O	15:u:54:PRO:C	2.48	0.56
27:b:622:LMG:O8	27:b:622:LMG:C10	2.53	0.56
23:c:506:CLA:O1A	23:c:506:CLA:C2	2.52	0.56
29:d:407:LHG:H321	14:t:21:ILE:HD11	1.86	0.56
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.56
4:d:246:MET:HE3	4:d:264:LYS:HG3	1.86	0.56
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.88	0.56
23:B:606:CLA:H72	25:B:619:BCR:H311	1.87	0.56
16:V:102:PRO:HA	16:V:105:ARG:HD3	1.87	0.56
5:e:63:ILE:HD12	5:e:63:ILE:N	2.20	0.56
25:t:101:BCR:C8	25:t:101:BCR:H311	2.35	0.56
26:a:410:PL9:H303	4:d:45:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:126:MET:HE3	4:d:143:ALA:O	2.06	0.56
4:d:209:LEU:HD23	4:d:209:LEU:C	2.31	0.55
25:t:101:BCR:HC8	25:t:101:BCR:H311	1.88	0.55
2:B:298:LEU:HD23	2:B:402:TYR:CE1	2.41	0.55
25:b:619:BCR:H331	25:b:619:BCR:C8	2.36	0.55
13:O:44:CYS:C	13:O:45:LEU:HD12	2.31	0.55
10:k:24:VAL:O	10:k:27:VAL:HG22	2.07	0.55
15:U:69:GLU:OE1	15:U:72:LYS:NZ	2.39	0.55
13:O:107:THR:HG22	37:O:342:HOH:O	2.05	0.55
5:e:8:ARG:NH2	5:e:12:ASP:OD2	2.39	0.55
5:e:68:ASP:O	5:e:72:ALA:HB2	2.07	0.55
13:O:58:ASN:HB3	37:b:703:HOH:O	2.05	0.55
5:e:17:VAL:H	9:j:7:ARG:HD2	1.71	0.55
10:k:18:PHE:HE1	19:z:13:VAL:HG21	1.72	0.55
23:B:606:CLA:H91	28:a:413:SQD:H211	1.88	0.55
29:B:623:LHG:O4	4:D:141:TYR:OH	2.15	0.55
10:k:35:LEU:HD13	10:k:35:LEU:O	2.06	0.54
25:x:101:BCR:H331	25:x:101:BCR:C8	2.37	0.54
26:A:410:PL9:H361	6:F:25:THR:HG21	1.88	0.54
23:D:401:CLA:HBB1	23:D:401:CLA:HMB3	1.89	0.54
17:Y:40:ALA:O	17:Y:41:VAL:HB	2.08	0.54
4:D:272:LEU:C	4:D:272:LEU:HD23	2.32	0.54
28:f:101:SQD:H351	18:x:27:VAL:HG21	1.90	0.54
25:B:618:BCR:H331	25:B:618:BCR:C8	2.37	0.54
2:B:317:ASN:HA	2:B:330:MET:HE1	1.90	0.54
2:b:480:SER:N	37:b:710:HOH:O	2.39	0.53
10:K:17:ILE:N	10:K:17:ILE:HD12	2.23	0.53
3:c:26:ARG:O	10:k:46:ARG:HD2	2.08	0.53
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.90	0.53
23:A:405:CLA:H92	27:D:406:LMG:C25	2.38	0.53
20:R:33:LYS:O	20:R:35:LEU:N	2.41	0.53
13:o:56:PRO:HD3	13:o:63:ALA:HB2	1.90	0.53
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.91	0.53
13:O:33:ASP:OD2	13:O:35:SER:OG	2.20	0.53
2:b:125:ASP:OD2	2:b:127:ARG:HB2	2.09	0.53
10:k:26:PRO:O	10:k:29:PRO:HD2	2.09	0.53
1:A:290:ILE:CG1	23:A:404:CLA:HED2	2.39	0.52
2:B:36:SER:OG	25:B:618:BCR:H362	2.08	0.52
2:b:458:PHE:HB3	23:b:605:CLA:HBC2	1.89	0.52
19:Z:32:ASP:OD2	19:Z:35:ARG:NE	2.38	0.52
2:b:36:SER:OG	25:b:619:BCR:H362	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:145:LEU:HD11	23:b:616:CLA:CMB	2.39	0.52
16:v:26:TYR:CD2	16:v:27:LEU:HD23	2.44	0.52
25:T:101:BCR:H382	25:T:101:BCR:H23C	1.92	0.52
8:i:33:LYS:O	8:i:35:LYS:NZ	2.43	0.52
23:b:611:CLA:H202	23:b:613:CLA:CMD	2.39	0.52
5:E:30:LEU:HD23	20:R:12:VAL:HG12	1.90	0.52
25:D:404:BCR:H392	25:D:404:BCR:H23C	1.92	0.52
2:b:62:VAL:HB	23:b:606:CLA:HED3	1.92	0.51
23:b:608:CLA:C10	23:b:614:CLA:H202	2.40	0.51
23:A:404:CLA:HBB1	23:A:404:CLA:HMB1	1.93	0.51
3:c:46:SER:OG	3:c:141:GLU:OE1	2.27	0.51
16:v:55:ARG:NH2	37:v:304:HOH:O	2.43	0.51
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.92	0.51
4:D:26:ARG:NH1	37:D:504:HOH:O	2.41	0.51
7:h:3:ARG:NH1	37:h:201:HOH:O	2.35	0.51
10:k:35:LEU:HD13	10:k:35:LEU:C	2.36	0.51
16:v:100:ILE:C	16:v:102:PRO:HD3	2.35	0.51
5:E:22[A]:ILE:HD12	20:R:19:ALA:HB1	1.92	0.51
4:d:272:LEU:C	4:d:272:LEU:HD23	2.35	0.51
5:e:30:LEU:HD11	6:f:28:VAL:HB	1.91	0.51
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.93	0.51
23:B:615:CLA:H201	23:B:615:CLA:C1B	2.40	0.51
2:b:145:LEU:HD11	23:b:616:CLA:HMB1	1.92	0.51
4:d:68:LEU:HD23	5:e:49:THR:HG21	1.92	0.51
16:v:23:GLU:O	16:v:27:LEU:HG	2.11	0.51
16:V:95:LEU:HD11	16:V:112:LEU:HD11	1.92	0.51
6:f:26:LEU:O	6:f:29:PRO:HD2	2.09	0.51
2:B:476:ARG:NH1	37:B:714:HOH:O	2.44	0.50
5:e:36:LEU:O	5:e:40:THR:HG23	2.10	0.50
25:D:404:BCR:H352	6:F:29:PRO:HG2	1.94	0.50
7:H:12:ARG:HB3	7:H:13:PRO:HD3	1.93	0.50
9:J:15:THR:HG22	9:J:19:MET:HE3	1.94	0.50
15:U:39:ARG:HG2	37:U:234:HOH:O	2.11	0.50
3:c:315:MET:HE3	3:c:319:ILE:HD11	1.93	0.50
8:I:6:ILE:HG22	8:I:10:ILE:HD12	1.92	0.50
11:L:36:PHE:HB3	12:M:3:VAL:CG2	2.42	0.50
2:B:237:VAL:HG12	23:B:612:CLA:HMD1	1.93	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.50
5:e:17:VAL:HG23	9:j:7:ARG:HB2	1.92	0.50
6:f:21:VAL:O	6:f:25:THR:HG23	2.12	0.50
24:A:407:PHO:HBC3	4:D:279:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:41:HIS:HA	16:V:45:ILE:O	2.11	0.50
13:o:178:LYS:NZ	37:o:303:HOH:O	2.26	0.50
16:v:26:TYR:OH	16:v:122:GLU:OE2	2.26	0.50
7:h:12:ARG:NH2	7:h:15:ASN:O	2.45	0.50
1:A:290:ILE:HG13	23:A:404:CLA:HED2	1.93	0.50
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.12	0.49
17:Y:25:ILE:O	17:Y:28:ILE:N	2.43	0.49
2:B:102:VAL:HA	25:B:618:BCR:C40	2.42	0.49
2:b:451:PHE:CE1	2:b:455:HIS:CE1	3.00	0.49
4:D:194:ASN:HA	4:D:295:SER:OG	2.12	0.49
19:z:14:ILE:N	19:z:14:ILE:HD12	2.27	0.49
19:Z:32:ASP:O	19:Z:36:SER:OG	2.30	0.49
2:b:249:ALA:HB3	2:b:459:ALA:HB2	1.94	0.49
18:x:8:LYS:NZ	37:x:203:HOH:O	2.45	0.49
10:k:18:PHE:CE2	19:z:9:LEU:HD23	2.47	0.49
15:U:70:ARG:NH2	16:V:85:GLU:OE1	2.36	0.49
17:y:23:THR:CG2	17:y:24:MET:HE2	2.40	0.49
29:A:413:LHG:H271	29:A:413:LHG:H311	1.93	0.49
23:B:609:CLA:NC	25:H:101:BCR:H332	2.27	0.49
1:A:189[B]:GLU:CD	32:A:417[B]:OEY:O6	2.51	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.49
5:E:22[A]:ILE:HD12	20:R:19:ALA:CB	2.43	0.49
20:r:6:LEU:O	20:r:10:LEU:HG	2.14	0.48
23:B:601:CLA:H151	23:B:601:CLA:H192	1.94	0.48
7:h:25:TRP:O	7:h:26:GLY:C	2.56	0.48
2:B:472:ARG:HG3	2:B:479[B]:PHE:CE1	2.48	0.48
8:I:35:LYS:HD2	8:I:35:LYS:N	2.27	0.48
3:C:318:LEU:C	3:C:318:LEU:HD23	2.38	0.48
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.48
19:z:15:LEU:HD11	19:z:19:MET:HE2	1.96	0.48
2:B:155:ALA:O	2:B:159:THR:OG1	2.29	0.48
2:b:249:ALA:HB2	23:b:605:CLA:HBC3	1.96	0.48
11:l:2:GLU:N	11:l:3:PRO:CD	2.76	0.48
26:a:410:PL9:H402	4:d:38:PHE:CD1	2.48	0.48
4:d:39:PRO:O	4:d:43:LEU:HG	2.13	0.48
5:e:14:ILE:O	5:e:20:TRP:NE1	2.44	0.48
16:V:87:GLU:HB3	37:V:336:HOH:O	2.14	0.48
17:Y:37:PHE:O	17:Y:40:ALA:O	2.31	0.48
18:X:38:GLN:O	18:X:39:ARG:HB2	2.14	0.48
5:e:26:THR:HA	20:r:15:ALA:HB1	1.96	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:407:LHG:H242	11:l:19:LEU:HD23	1.95	0.48
19:z:32:ASP:CB	19:z:35:ARG:HB3	2.44	0.48
3:C:410:VAL:HG22	3:C:413[B]:GLU:CG	2.44	0.48
25:D:404:BCR:H331	25:D:404:BCR:HC8	1.96	0.48
7:H:50:ASN:OD1	7:H:52:THR:CG2	2.62	0.48
2:b:414:PRO:N	2:b:415:PRO:HD2	2.29	0.48
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.14	0.48
17:y:23:THR:O	17:y:27:MET:HE2	2.14	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.13	0.47
5:e:22:ILE:HG23	20:r:19:ALA:HB2	1.95	0.47
28:B:624:SQD:H442	14:t:23:PHE:CD1	2.49	0.47
1:a:200:LEU:HD23	1:a:285:PHE:CG	2.48	0.47
26:a:410:PL9:H252	24:d:401:PHO:HBA2	1.96	0.47
13:o:124:ASN:HA	37:o:327:HOH:O	2.14	0.47
13:o:133:VAL:HG12	13:o:133:VAL:O	2.13	0.47
19:z:32:ASP:HB2	19:z:35:ARG:HB3	1.95	0.47
20:r:7:VAL:HA	20:r:10:LEU:HD12	1.96	0.47
23:B:602:CLA:H43	7:H:45:ILE:HG22	1.95	0.47
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.96	0.47
4:d:170:ALA:HB1	4:d:171:PRO:CD	2.44	0.47
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.96	0.47
19:Z:5:PHE:C	19:Z:7:LEU:H	2.22	0.47
16:v:104:MET:HA	16:v:107:LEU:HD22	1.96	0.47
23:B:602:CLA:HBB1	23:B:602:CLA:HMB1	1.96	0.47
3:C:473:ASP:OD2	14:T:24:ARG:HD3	2.15	0.47
10:K:26:PRO:O	10:K:29:PRO:HD2	2.15	0.47
15:U:58:VAL:O	15:U:61:VAL:HG22	2.15	0.47
17:y:39:LEU:HD21	19:z:25:VAL:HA	1.96	0.47
29:B:623:LHG:H222	12:M:18:PRO:HG3	1.97	0.47
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.96	0.47
30:A:415:DGD:HD5	2:b:75:TRP:HB3	1.96	0.47
23:b:608:CLA:H101	23:b:614:CLA:H202	1.96	0.47
4:D:79:SER:HA	4:D:172:SER:HB3	1.97	0.47
5:E:22[A]:ILE:HD11	35:E:101:HEM:CHB	2.45	0.47
3:c:334:PRO:HA	13:o:153:THR:OG1	2.15	0.47
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.97	0.46
23:b:604:CLA:C4B	23:b:606:CLA:H93	2.45	0.46
23:B:604:CLA:H172	23:B:604:CLA:H141	1.97	0.46
3:C:141:GLU:HA	3:C:148:GLY:HA3	1.96	0.46
3:C:337:LEU:HD23	13:O:105:PRO:HG2	1.97	0.46
16:v:76:MET:HE1	16:v:115:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.96	0.46
1:A:214:MET:O	1:A:218:LEU:HG	2.15	0.46
1:a:112:TYR:CE2	1:a:116:ILE:HD13	2.51	0.46
2:b:144:PHE:CE2	2:b:148:LEU:HD11	2.50	0.46
3:c:456:GLU:OE1	3:c:457:LYS:NZ	2.29	0.46
13:o:57:LYS:O	13:o:60:ARG:N	2.43	0.46
30:a:414:DGD:O1B	30:a:414:DGD:C1A	2.64	0.46
37:d:519:HOH:O	9:j:36:LEU:HD21	2.14	0.46
1:A:218:LEU:HD12	26:A:410:PL9:C3	2.45	0.46
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.46
12:M:20:VAL:HG13	12:m:20:VAL:HG13	1.97	0.46
17:Y:41:VAL:O	17:Y:41:VAL:CG1	2.64	0.46
19:z:2:THR:HG23	19:z:3:ILE:HG23	1.98	0.46
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.51	0.46
37:A:604:HOH:O	4:D:264:LYS:HE3	2.16	0.46
3:C:109:PHE:N	3:C:110:PRO:CD	2.78	0.46
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.04	0.46
3:c:391[B]:ARG:CZ	37:c:605:HOH:O	2.63	0.46
25:t:101:BCR:H321	25:t:101:BCR:C8	2.44	0.46
7:H:12:ARG:NH1	7:H:15:ASN:O	2.48	0.46
13:O:189:ARG:NE	37:O:309:HOH:O	2.36	0.46
3:c:203:THR:O	3:c:235:GLY:HA3	2.16	0.46
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.97	0.46
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.97	0.46
5:E:60:GLN:NE2	5:E:62:SER:O	2.49	0.46
18:x:34:ILE:HG22	18:x:35:ASP:N	2.31	0.46
4:D:17:ILE:O	4:D:20:ASP:HB2	2.16	0.46
13:O:98:GLU:CG	37:O:355:HOH:O	2.64	0.46
16:V:13:ASN:OD1	16:V:15:GLU:HB2	2.16	0.46
29:l:101:LHG:H241	29:l:101:LHG:H101	1.98	0.46
25:t:101:BCR:H23C	25:t:101:BCR:H382	1.98	0.46
16:v:26:TYR:HD2	16:v:27:LEU:HD23	1.80	0.46
25:Z:101:BCR:C8	25:Z:101:BCR:H331	2.44	0.45
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.98	0.45
35:e:102:HEM:HBC2	35:e:102:HEM:CMC	2.45	0.45
1:A:291:SER:HB3	3:C:431:PHE:CE2	2.52	0.45
23:B:602:CLA:OBD	23:B:603:CLA:H43	2.16	0.45
25:K:101:BCR:H361	25:K:101:BCR:H20C	1.78	0.45
12:M:17:VAL:HB	12:M:18:PRO:HD3	1.97	0.45
7:h:17:GLU:O	7:h:18:TYR:C	2.56	0.45
29:A:413:LHG:HC92	5:E:10:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:264:LYS:NZ	37:D:510:HOH:O	2.50	0.45
2:b:150:CYS:HB2	23:b:604:CLA:CMC	2.46	0.45
13:o:52:VAL:O	13:o:66:VAL:HG22	2.16	0.45
10:K:15:TYR:OH	19:Z:58:ASN:OD1	2.12	0.45
2:b:442:ILE:HD11	13:o:174:LEU:HD23	1.98	0.45
16:V:29:GLY:HA3	16:V:114:ALA:O	2.16	0.45
23:b:606:CLA:H41	23:b:606:CLA:H61	1.67	0.45
13:o:60:ARG:O	13:o:61:GLN:HB2	2.17	0.45
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.52	0.45
2:B:243:ALA:HA	2:B:246:PHE:CE1	2.51	0.45
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.52	0.45
3:c:178:LYS:NZ	3:c:184:GLY:O	2.46	0.45
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.52	0.45
2:B:297:THR:HG23	2:B:300:GLU:OE1	2.16	0.45
3:c:187:ASP:HB2	3:c:230:LEU:HD12	1.99	0.45
25:c:514:BCR:H24C	25:c:514:BCR:H371	1.80	0.45
4:d:279:LEU:HD22	24:d:401:PHO:HBC3	1.98	0.45
25:a:409:BCR:H331	25:a:409:BCR:C8	2.47	0.45
23:b:611:CLA:H192	23:b:616:CLA:HMD2	1.98	0.45
4:d:55:VAL:O	4:d:66:SER:HB3	2.17	0.45
10:k:18:PHE:CE1	19:z:13:VAL:HG21	2.51	0.45
16:v:122:GLU:N	16:v:123:PRO:HD2	2.32	0.45
20:r:20:VAL:O	20:r:24:LEU:HB2	2.16	0.45
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.98	0.45
3:C:466:VAL:HA	3:C:469:MET:HG3	1.99	0.45
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.52	0.45
27:c:523:LMG:H301	27:c:523:LMG:HC91	1.98	0.45
2:B:32:GLY:HA3	25:B:618:BCR:H17C	1.99	0.45
5:E:76:VAL:O	5:E:80:LEU:HG	2.17	0.45
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.17	0.45
2:b:181:VAL:HG12	2:b:199:VAL:HG21	1.99	0.45
23:b:606:CLA:HMA1	23:b:607:CLA:H3A	1.99	0.45
4:d:37:LEU:CD2	4:d:128:ARG:HD2	2.47	0.45
10:k:40:GLN:HA	10:k:43:VAL:HG22	1.99	0.45
13:o:55:GLU:OE1	13:o:231:HIS:CD2	2.70	0.45
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	1.99	0.44
25:B:619:BCR:C8	25:B:619:BCR:H331	2.48	0.44
3:C:95:LEU:HD21	23:C:501:CLA:OBD	2.17	0.44
15:u:69:GLU:OE2	15:u:72:LYS:NZ	2.45	0.44
19:z:19:MET:HE1	19:z:47:TRP:HB2	2.00	0.44
20:r:29:LYS:O	20:r:30:GLN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.52	0.44
3:C:143:TYR:CE1	23:C:513:CLA:HED3	2.53	0.44
5:E:17:VAL:O	5:E:21:VAL:HG23	2.17	0.44
6:F:31:ILE:O	6:F:32:PHE:C	2.59	0.44
10:K:15:TYR:O	10:K:16:ALA:C	2.59	0.44
1:a:45:THR:HG23	23:a:411:CLA:H201	1.98	0.44
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.99	0.44
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.99	0.44
20:r:2:ASP:N	37:r:102:HOH:O	2.50	0.44
3:C:180:MET:HG2	3:C:199:ILE:O	2.17	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.44
2:b:433:ASP:OD1	2:b:433:ASP:C	2.60	0.44
3:C:150:ASP:OD1	3:C:150:ASP:C	2.59	0.44
1:a:42:LEU:CD1	28:a:413:SQD:H322	2.47	0.44
10:K:15:TYR:C	10:K:17:ILE:N	2.74	0.44
13:o:59:LYS:C	13:o:60:ARG:HG3	2.43	0.44
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.47	0.44
13:O:84:GLU:OE1	13:O:86:LYS:NZ	2.45	0.44
15:U:18:GLY:HA3	37:U:241:HOH:O	2.17	0.44
23:h:101:CLA:CHA	23:h:101:CLA:HBA2	2.48	0.44
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.00	0.44
3:C:61:VAL:HG12	3:C:118:HIS:O	2.17	0.44
13:O:189:ARG:CZ	13:O:226:GLY:HA3	2.48	0.44
19:Z:33:TRP:CZ3	19:Z:40:ILE:HD11	2.53	0.44
10:k:36:ALA:HB2	25:k:102:BCR:H391	1.99	0.44
18:x:14:LEU:HD12	18:x:14:LEU:HA	1.88	0.44
13:O:33:ASP:O	13:O:35:SER:N	2.51	0.44
2:b:213:GLY:O	2:b:217:ILE:HG13	2.17	0.44
23:c:510:CLA:H93	23:c:510:CLA:H112	1.91	0.44
7:h:28:THR:N	7:h:29:PRO:HD2	2.32	0.44
1:A:249:VAL:HG12	2:B:491:VAL:HG11	2.00	0.44
25:D:404:BCR:H20C	25:D:404:BCR:H361	1.81	0.44
15:U:40:GLY:O	15:U:45:LEU:HD12	2.18	0.44
17:Y:23:THR:O	17:Y:23:THR:HG22	2.18	0.44
17:Y:25:ILE:O	17:Y:26:ALA:C	2.59	0.44
19:Z:25:VAL:O	19:Z:29:SER:HB2	2.18	0.44
3:c:26:ARG:HD3	10:k:46:ARG:NH2	2.33	0.44
3:c:350:ILE:HG21	3:c:359:TRP:HB2	1.99	0.44
25:k:101:BCR:H16C	17:y:29:GLY:O	2.18	0.44
2:B:141:ILE:O	2:B:145:LEU:HG	2.17	0.43
23:C:513:CLA:H143	25:Z:101:BCR:H392	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:90:ASP:OD1	13:O:90:ASP:N	2.45	0.43
1:a:217:SER:HA	4:d:272:LEU:HD12	1.99	0.43
25:a:409:BCR:H15C	25:a:409:BCR:H351	1.84	0.43
3:c:121:SER:O	3:c:124:VAL:HG13	2.18	0.43
2:B:414:PRO:N	2:B:415:PRO:HD2	2.33	0.43
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	2.00	0.43
16:V:28:GLU:OE2	16:V:31:ARG:NH2	2.47	0.43
3:c:213:LEU:HD21	25:c:515:BCR:C20	2.48	0.43
4:d:45:LEU:HD12	4:d:45:LEU:HA	1.80	0.43
16:v:28:GLU:HA	16:v:28:GLU:OE1	2.18	0.43
16:v:73:VAL:HG21	16:v:113:VAL:HG12	2.00	0.43
2:B:353:GLU:HG2	2:B:355:PHE:CZ	2.53	0.43
3:C:238:ILE:O	3:C:242:LEU:HG	2.18	0.43
16:V:7:VAL:HA	16:V:124:LYS:HE2	2.01	0.43
1:a:95:PRO:HG2	1:a:98:GLU:HG2	2.00	0.43
2:b:504:THR:CG2	18:x:37:VAL:HG11	2.48	0.43
29:d:408:LHG:H242	29:d:408:LHG:H272	1.90	0.43
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.53	0.43
19:z:5:PHE:HA	19:z:57:LEU:HD13	1.98	0.43
19:z:57:LEU:O	19:z:58:ASN:C	2.61	0.43
1:A:249:VAL:O	2:B:491:VAL:HG11	2.19	0.43
4:D:209:LEU:HD23	4:D:209:LEU:C	2.43	0.43
4:D:266:TRP:CD1	29:D:407:LHG:HC31	2.53	0.43
5:E:23:HIS:HA	5:E:26:THR:OG1	2.18	0.43
9:J:10:LEU:HD12	9:J:13:VAL:HB	2.01	0.43
19:Z:62:VAL:O	19:Z:62:VAL:HG12	2.18	0.43
2:b:475:PHE:O	2:b:476:ARG:C	2.62	0.43
2:b:506:ARG:HG2	37:b:857:HOH:O	2.17	0.43
3:c:286:ALA:HB2	23:c:502:CLA:HMD2	1.99	0.43
3:c:337:LEU:HD23	13:o:105:PRO:HG3	2.00	0.43
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.54	0.43
4:d:330:ALA:N	4:d:331:PRO:CD	2.81	0.43
10:k:38:VAL:HG23	25:k:101:BCR:H21C	2.00	0.43
13:o:54:GLU:O	13:o:56:PRO:HD3	2.18	0.43
19:z:14:ILE:O	19:z:15:LEU:HB2	2.19	0.43
2:B:97:ALA:O	2:B:101:ILE:HD12	2.19	0.43
23:B:614:CLA:H61	23:B:614:CLA:H41	1.67	0.43
2:b:154:GLY:O	2:b:159:THR:HG23	2.19	0.43
5:e:13:ILE:HG22	5:e:19:TYR:CD2	2.53	0.43
26:a:410:PL9:H261	29:e:101:LHG:H201	2.01	0.43
2:B:206:GLY:O	2:B:210:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	2.01	0.43
5:E:65:LEU:O	5:E:67:THR:HG23	2.19	0.43
5:e:25:ILE:HD12	5:e:25:ILE:N	2.34	0.43
17:y:19:ILE:O	17:y:23:THR:HG22	2.18	0.43
23:B:601:CLA:H192	23:B:601:CLA:C15	2.48	0.43
3:c:391[B]:ARG:NH1	37:c:605:HOH:O	2.52	0.43
6:f:29:PRO:O	6:f:33:PHE:HD2	2.02	0.43
12:m:21:PHE:CZ	12:m:25:LEU:HD11	2.54	0.43
13:O:61:GLN:O	13:O:62:GLU:O	2.36	0.43
16:V:17:LYS:HG3	37:V:348:HOH:O	2.18	0.43
16:V:28:GLU:OE2	16:V:31:ARG:NH1	2.47	0.43
19:Z:36:SER:HA	19:Z:39:LEU:HD12	2.01	0.43
1:a:279:PRO:HG2	4:d:212:ALA:HB2	2.01	0.43
2:b:30:VAL:HG12	23:b:606:CLA:HHD	2.00	0.43
2:b:414:PRO:N	2:b:415:PRO:CD	2.82	0.43
2:b:504:THR:HG22	18:x:37:VAL:HG11	2.01	0.43
8:i:35:LYS:O	8:i:36:ASP:C	2.62	0.43
12:m:20:VAL:HG12	12:m:24:ILE:HD12	2.00	0.43
1:A:161[B]:TYR:HB3	1:A:162[B]:PRO:HD3	2.00	0.42
23:B:613:CLA:C10	23:B:613:CLA:H142	2.49	0.42
1:A:161[A]:TYR:HB3	1:A:162[A]:PRO:HD3	2.01	0.42
37:B:860:HOH:O	7:H:64:ALA:HB1	2.18	0.42
3:C:46:SER:HG	3:C:140:LEU:H	1.67	0.42
1:a:183[B]:MET:HG2	23:a:411:CLA:HBC1	2.01	0.42
2:b:159:THR:O	2:b:180:PRO:HB3	2.19	0.42
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.00	0.42
19:z:14:ILE:O	19:z:14:ILE:HG22	2.18	0.42
2:B:117:TYR:HA	11:L:1:MET:HE1	2.01	0.42
4:D:20:ASP:O	4:D:24:ARG:HG2	2.19	0.42
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.01	0.42
19:Z:55:GLY:HA2	25:Z:101:BCR:H323	2.01	0.42
28:a:413:SQD:H292	29:d:407:LHG:H383	2.01	0.42
7:h:11:LEU:C	7:h:13:PRO:HD2	2.44	0.42
30:A:415:DGD:C2B	23:b:607:CLA:H201	2.50	0.42
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.54	0.42
2:b:505:ARG:O	2:b:506:ARG:HB2	2.20	0.42
25:b:619:BCR:H24C	25:b:619:BCR:H371	1.89	0.42
3:c:109:PHE:N	3:c:110:PRO:CD	2.82	0.42
19:z:1:MET:HB2	19:z:4:LEU:CD2	2.46	0.42
19:z:3:ILE:HG12	19:z:4:LEU:HD22	2.01	0.42
19:z:14:ILE:O	19:z:15:LEU:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:r:24:LEU:N	20:r:25:PRO:HD2	2.34	0.42
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.02	0.42
3:C:337:LEU:HD23	13:O:105:PRO:HG3	2.01	0.42
16:V:77:LYS:O	16:V:96:ARG:HB2	2.19	0.42
17:Y:24:MET:HE3	17:Y:27:MET:SD	2.60	0.42
1:a:29:TYR:CE2	1:a:31:GLY:HA3	2.55	0.42
2:b:413:ASP:O	2:b:417:VAL:HG23	2.19	0.42
23:h:101:CLA:H91	23:h:101:CLA:H111	1.83	0.42
25:t:101:BCR:H371	25:t:101:BCR:H24C	1.81	0.42
18:x:37:VAL:HG12	18:x:38:GLN:N	2.34	0.42
25:K:102:BCR:H20C	25:K:102:BCR:H361	1.85	0.42
1:A:217:SER:HB3	4:D:272:LEU:HD12	2.02	0.42
26:A:410:PL9:H523	26:A:410:PL9:H531	1.88	0.42
30:A:415:DGD:HB22	23:b:607:CLA:H201	2.02	0.42
2:B:125:ASP:OD2	2:B:127:ARG:HD3	2.20	0.42
2:B:451:PHE:CD2	2:B:451:PHE:C	2.97	0.42
4:D:218:VAL:HG13	4:D:244:TYR:CD2	2.54	0.42
29:D:408:LHG:H341	29:D:408:LHG:H141	2.00	0.42
12:M:20:VAL:HG11	12:m:20:VAL:HG22	2.01	0.42
1:a:238:LYS:HG2	1:a:241:GLN:HB3	2.02	0.42
2:b:347:ARG:O	2:b:397:VAL:HA	2.19	0.42
25:b:618:BCR:H341	25:b:618:BCR:H11C	1.76	0.42
19:z:15:LEU:CD2	19:z:50:LEU:HD12	2.49	0.42
4:D:43:LEU:HG	4:D:113:PHE:HZ	1.85	0.42
5:E:15:THR:HB	9:J:8:ILE:O	2.19	0.42
9:J:15:THR:HG22	9:J:19:MET:HE2	2.01	0.42
10:K:18:PHE:HE2	19:Z:9:LEU:HD21	1.81	0.42
1:a:219:VAL:O	1:a:223:LEU:HD13	2.19	0.42
1:a:271:LEU:HD21	26:a:410:PL9:HC71	2.02	0.42
2:b:298:LEU:HD23	2:b:298:LEU:HA	1.89	0.42
5:e:36:LEU:HA	5:e:39:SER:OG	2.20	0.42
3:c:180:MET:HE1	27:c:521:LMG:HC72	2.02	0.42
5:e:30:LEU:HD23	5:e:30:LEU:HA	1.87	0.42
18:x:23:LEU:O	18:x:27:VAL:HG23	2.19	0.42
18:x:24:THR:HG22	18:x:28:LEU:HD12	2.01	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.42
10:K:15:TYR:O	10:K:17:ILE:N	2.53	0.42
13:O:83:GLY:HA3	13:O:96:VAL:O	2.20	0.42
19:Z:55:GLY:HA2	19:Z:58:ASN:HB3	2.01	0.42
2:b:10:THR:HB	2:b:13:ILE:HD12	2.02	0.42
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:523:LMG:C9	27:c:523:LMG:C30	2.98	0.42
1:A:265:PHE:O	26:A:410:PL9:H532	2.20	0.41
3:C:141:GLU:CD	3:C:141:GLU:H	2.28	0.41
25:T:101:BCR:H20C	25:T:101:BCR:H361	1.78	0.41
23:b:603:CLA:H43	7:h:45:ILE:HG22	2.02	0.41
3:c:352:GLY:O	3:c:355[B]:THR:HG22	2.20	0.41
4:d:148:ALA:HB2	4:d:276:VAL:HG13	2.01	0.41
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.55	0.41
4:d:194:ASN:HA	4:d:295:SER:OG	2.20	0.41
13:o:31:PRO:HA	13:o:135:SER:OG	2.19	0.41
15:u:85:THR:HG22	37:u:246:HOH:O	2.19	0.41
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.54	0.41
1:A:102:LEU:O	1:A:106:LEU:HG	2.20	0.41
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.56	0.41
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.73	0.41
3:C:466:VAL:HG23	37:D:546:HOH:O	2.19	0.41
16:V:41:HIS:CE1	16:V:46:THR:OG1	2.73	0.41
7:h:40:VAL:O	7:h:44:ILE:HG13	2.21	0.41
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.51	0.41
28:A:414:SQD:H383	23:b:607:CLA:H93	2.01	0.41
5:E:22[A]:ILE:HD11	35:E:101:HEM:C4A	2.56	0.41
13:O:31:PRO:HA	13:O:135:SER:HA	2.03	0.41
13:O:33:ASP:O	13:O:34:SER:C	2.62	0.41
15:U:73:GLN:O	15:U:77:GLU:HG3	2.20	0.41
4:d:217:THR:HG21	26:d:405:PL9:C1	2.51	0.41
16:v:3:LEU:HD12	16:v:3:LEU:HA	1.90	0.41
26:A:410:PL9:H152	29:A:413:LHG:H381	2.03	0.41
3:C:75:PHE:C	3:C:76:ILE:HD12	2.45	0.41
13:O:54:GLU:O	13:O:63:ALA:HB3	2.20	0.41
26:a:410:PL9:H303	4:d:45:LEU:CD2	2.51	0.41
2:b:222:PRO:HD3	37:h:204:HOH:O	2.19	0.41
23:c:504:CLA:H91	23:c:508:CLA:C18	2.51	0.41
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.39	0.41
12:m:1:FME:O1	12:m:1:FME:C	2.68	0.41
17:y:28:ILE:O	17:y:31:ALA:HB3	2.21	0.41
1:A:161[A]:TYR:N	1:A:162[A]:PRO:CD	2.84	0.41
16:V:92:HIS:CD2	36:V:201:HEC:ND	2.88	0.41
2:b:506:ARG:CG	37:b:857:HOH:O	2.68	0.41
25:b:620:BCR:C8	25:b:620:BCR:H331	2.48	0.41
3:c:364:PRO:HD2	37:c:645:HOH:O	2.21	0.41
23:B:608:CLA:H43	23:B:609:CLA:H101	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:MET:SD	23:D:401:CLA:HED2	2.61	0.41
17:Y:41:VAL:O	17:Y:41:VAL:HG12	2.18	0.41
19:Z:31:GLN:CG	19:Z:32:ASP:H	2.34	0.41
23:b:615:CLA:H191	25:b:618:BCR:H331	2.03	0.41
4:d:218:VAL:HG22	4:d:244:TYR:CE1	2.56	0.41
19:z:1:MET:HB2	19:z:4:LEU:HB2	2.01	0.41
2:B:506:ARG:HB3	37:B:890:HOH:O	2.20	0.41
4:D:126:MET:HE3	4:D:143:ALA:O	2.20	0.41
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.45	0.41
1:a:81:ALA:HA	1:a:174[A]:LEU:O	2.21	0.41
1:a:183[A]:MET:HG2	23:a:411:CLA:HBC1	2.03	0.41
2:b:226:TYR:HA	2:b:231:MET:HG3	2.01	0.41
25:b:618:BCR:H20C	25:b:618:BCR:H361	1.93	0.41
17:y:42:ARG:O	17:y:43:ARG:C	2.64	0.41
1:A:84:PRO:HA	1:A:112:TYR:CG	2.56	0.41
25:B:618:BCR:H371	25:B:618:BCR:H24C	1.84	0.41
23:D:403:CLA:H42	7:H:43:LEU:HD11	2.02	0.41
5:E:30:LEU:HD12	35:E:101:HEM:HMC1	2.02	0.41
10:K:17:ILE:H	10:K:17:ILE:CD1	2.34	0.41
13:O:33:ASP:C	13:O:35:SER:N	2.77	0.41
16:V:22:THR:OG1	16:V:24:LYS:HB3	2.21	0.41
1:a:159:LEU:HB3	1:a:160[A]:ILE:HD13	2.03	0.41
1:a:201:GLY:HA3	1:a:286:THR:HB	2.03	0.41
30:a:414:DGD:O1G	30:a:414:DGD:C1B	2.69	0.41
27:b:622:LMG:H211	27:b:622:LMG:H372	2.03	0.41
25:k:102:BCR:H24C	25:k:102:BCR:H371	1.87	0.41
16:v:41:HIS:O	16:v:42:VAL:C	2.63	0.41
16:v:77:LYS:HG2	16:v:95:LEU:HD12	2.02	0.41
17:y:34:MET:HE3	17:y:34:MET:HB2	1.97	0.41
27:A:411:LMG:O10	27:A:411:LMG:C31	2.68	0.41
23:B:605:CLA:HMC3	23:B:615:CLA:H43	2.01	0.41
3:C:150:ASP:OD1	3:C:151:TRP:N	2.54	0.41
3:C:241:GLY:O	3:C:245:ILE:HG13	2.21	0.41
3:C:279:LEU:CD2	3:C:282:MET:HE3	2.51	0.41
2:b:503:THR:O	18:x:39:ARG:HG2	2.21	0.41
3:c:318:LEU:C	3:c:318:LEU:HD23	2.46	0.41
4:d:79:SER:HA	4:d:172:SER:HB3	2.03	0.41
5:e:62:SER:C	5:e:63:ILE:HD12	2.46	0.41
13:o:36:GLN:HG3	13:o:37:THR:N	2.36	0.41
15:u:9:LEU:HA	37:u:218:HOH:O	2.21	0.41
1:A:173[A]:PRO:HB2	1:A:178[A]:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:GLY:HA3	2:B:217:ILE:HG13	2.03	0.40
25:B:619:BCR:H383	25:B:619:BCR:C23	2.51	0.40
4:D:267:LEU:C	4:D:267:LEU:HD23	2.46	0.40
23:b:603:CLA:H203	30:h:102:DGD:HBT1	2.03	0.40
3:c:461:ARG:HG2	4:d:223:PHE:CD1	2.56	0.40
6:f:30:THR:O	6:f:34:LEU:HG	2.21	0.40
13:o:117:PRO:O	13:o:221:SER:HB2	2.20	0.40
25:x:101:BCR:H24C	25:x:101:BCR:H371	1.89	0.40
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.10	0.40
4:d:269:PHE:CG	29:d:406:LHG:HC11	2.56	0.40
26:d:405:PL9:H421	26:d:405:PL9:H401	1.88	0.40
5:e:8:ARG:HG2	5:e:13:ILE:HG13	2.04	0.40
2:B:422:ARG:O	2:B:425:ILE:HG12	2.21	0.40
10:K:17:ILE:N	10:K:17:ILE:CD1	2.83	0.40
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.85	0.40
1:a:301:ASN:C	1:a:301:ASN:OD1	2.64	0.40
2:b:383:PHE:O	13:o:166:SER:HA	2.22	0.40
28:b:601:SQD:H121	23:b:615:CLA:C4	2.51	0.40
3:c:350:ILE:CG2	3:c:359:TRP:HB2	2.52	0.40
3:c:466:VAL:HG13	4:d:251:ARG:HD2	2.04	0.40
20:r:10:LEU:HB2	20:r:11:PRO:CD	2.51	0.40
28:A:412:SQD:H262	29:D:408:LHG:H151	2.04	0.40
2:B:160:GLY:HA2	2:B:163:GLY:O	2.21	0.40
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.56	0.40
23:C:505:CLA:CMB	23:C:505:CLA:HBB1	2.51	0.40
23:C:513:CLA:HMC2	25:Z:101:BCR:H372	2.03	0.40
13:O:57:LYS:HE2	2:b:338:GLN:O	2.21	0.40
19:Z:14:ILE:O	19:Z:15:LEU:C	2.62	0.40
20:R:19:ALA:O	20:R:23:ILE:HG22	2.22	0.40
1:a:288:LEU:HD11	3:c:435:PHE:CD2	2.56	0.40
23:b:611:CLA:H203	23:b:611:CLA:H162	1.88	0.40
15:u:28:ASN:OD1	15:u:54:PRO:HA	2.22	0.40
16:v:76:MET:HE1	16:v:115:ILE:CD1	2.51	0.40
25:A:409:BCR:H11C	25:A:409:BCR:H341	1.91	0.40
26:A:410:PL9:H28	29:A:413:LHG:H212	2.02	0.40
2:B:102:VAL:CG1	23:B:606:CLA:H111	2.51	0.40
8:I:5:LYS:NZ	37:I:201:HOH:O	2.53	0.40
17:Y:25:ILE:O	17:Y:27:MET:N	2.54	0.40
1:a:270:SER:OG	28:a:412:SQD:H3	2.21	0.40
3:c:249:ILE:O	3:c:250:TRP:C	2.64	0.40
23:c:510:CLA:H2A	23:c:510:CLA:O2A	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:10:LEU:O	9:j:13:VAL:HG22	2.20	0.40
13:o:10:ILE:O	13:o:13:THR:HG23	2.22	0.40
16:v:110:LYS:O	16:v:113:VAL:HG22	2.21	0.40
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.57	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	390/334 (117%)	381 (98%)	9 (2%)	0	100	100
1	a	390/334 (117%)	382 (98%)	8 (2%)	0	100	100
2	B	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
2	b	503/505 (100%)	495 (98%)	7 (1%)	1 (0%)	43	38
3	C	447/451 (99%)	435 (97%)	11 (2%)	1 (0%)	43	38
3	c	457/451 (101%)	442 (97%)	14 (3%)	1 (0%)	43	38
4	D	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
4	d	340/341 (100%)	329 (97%)	11 (3%)	0	100	100
5	E	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
5	e	80/82 (98%)	78 (98%)	2 (2%)	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	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	55 (90%)	6 (10%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	j	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	0	1 (3%)	3	0
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	226 (93%)	16 (7%)	1 (0%)	30	23
13	o	242/244 (99%)	230 (95%)	8 (3%)	4 (2%)	7	2
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
15	u	95/97 (98%)	90 (95%)	4 (4%)	1 (1%)	11	4
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	19 (76%)	4 (16%)	2 (8%)	1	0
17	y	28/30 (93%)	24 (86%)	4 (14%)	0	100	100
18	X	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	50 (83%)	7 (12%)	3 (5%)	1	0
19	z	60/62 (97%)	50 (83%)	9 (15%)	1 (2%)	7	2
20	R	32/34 (94%)	30 (94%)	1 (3%)	1 (3%)	3	0
20	r	29/34 (85%)	22 (76%)	6 (21%)	1 (3%)	3	0
All	All	5365/5326 (101%)	5164 (96%)	183 (3%)	18 (0%)	36	30

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	62	GLU
3	c	416	SER
13	o	60	ARG
13	o	61	GLN

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Mol	Chain	Res	Type
15	u	53	ALA
19	z	15	LEU
20	r	30	GLN
10	K	16	ALA
17	Y	41	VAL
17	Y	43	ARG
20	R	34	LEU
19	Z	3	ILE
13	o	57	LYS
19	Z	6	GLN
2	b	127	ARG
13	o	62	GLU
19	Z	14	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	319/270 (118%)	311 (98%)	8 (2%)	42 38
1	a	318/270 (118%)	303 (95%)	15 (5%)	23 16
2	B	407/403 (101%)	388 (95%)	19 (5%)	23 16
2	b	402/403 (100%)	389 (97%)	13 (3%)	34 29
3	C	351/352 (100%)	341 (97%)	10 (3%)	38 34
3	c	360/352 (102%)	341 (95%)	19 (5%)	20 13
4	D	277/276 (100%)	271 (98%)	6 (2%)	45 43
4	d	278/276 (101%)	269 (97%)	9 (3%)	34 29
5	E	72/72 (100%)	62 (86%)	10 (14%)	3 1
5	e	71/72 (99%)	68 (96%)	3 (4%)	26 20
6	F	28/28 (100%)	27 (96%)	1 (4%)	31 25
6	f	28/28 (100%)	23 (82%)	5 (18%)	2 0
7	H	53/54 (98%)	50 (94%)	3 (6%)	18 11
7	h	53/54 (98%)	48 (91%)	5 (9%)	8 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	I	32/32 (100%)	28 (88%)	4 (12%)	4 1
8	i	32/32 (100%)	32 (100%)	0	100 100
9	J	24/24 (100%)	23 (96%)	1 (4%)	26 20
9	j	23/24 (96%)	20 (87%)	3 (13%)	4 1
10	K	31/30 (103%)	26 (84%)	5 (16%)	2 0
10	k	30/30 (100%)	25 (83%)	5 (17%)	2 0
11	L	35/35 (100%)	34 (97%)	1 (3%)	37 33
11	l	34/35 (97%)	31 (91%)	3 (9%)	9 4
12	M	28/29 (97%)	26 (93%)	2 (7%)	13 7
12	m	28/29 (97%)	27 (96%)	1 (4%)	31 25
13	O	208/207 (100%)	194 (93%)	14 (7%)	15 8
13	o	207/207 (100%)	191 (92%)	16 (8%)	12 5
14	T	26/26 (100%)	22 (85%)	4 (15%)	2 0
14	t	25/26 (96%)	24 (96%)	1 (4%)	28 22
15	U	84/84 (100%)	78 (93%)	6 (7%)	13 7
15	u	84/84 (100%)	84 (100%)	0	100 100
16	V	117/117 (100%)	112 (96%)	5 (4%)	26 20
16	v	117/117 (100%)	110 (94%)	7 (6%)	17 10
17	Y	19/23 (83%)	13 (68%)	6 (32%)	0 0
17	y	22/23 (96%)	17 (77%)	5 (23%)	1 0
18	X	31/31 (100%)	28 (90%)	3 (10%)	8 3
18	x	31/31 (100%)	25 (81%)	6 (19%)	1 0
19	Z	52/52 (100%)	41 (79%)	11 (21%)	1 0
19	z	51/52 (98%)	44 (86%)	7 (14%)	3 1
20	R	28/29 (97%)	19 (68%)	9 (32%)	0 0
20	r	19/29 (66%)	16 (84%)	3 (16%)	2 0
All	All	4435/4348 (102%)	4181 (94%)	254 (6%)	18 11

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	15	GLU

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Mol	Chain	Res	Type
1	A	16	ARG
1	A	102	LEU
1	A	229	GLU
1	A	243	GLU
1	A	248	ILE
1	A	286	THR
2	B	63	LEU
2	B	80	ILE
2	B	83	GLU
2	B	101	ILE
2	B	127	ARG
2	B	161	LEU
2	B	289	GLN
2	B	291	SER
2	B	362	PHE
2	B	371	THR
2	B	405	GLU
2	B	476	ARG
2	B	480[A]	SER
2	B	480[B]	SER
2	B	486	LEU
2	B	489	GLU
2	B	491	VAL
2	B	495	PHE
2	B	505	ARG
3	C	106	VAL
3	C	141	GLU
3	C	161	LEU
3	C	240	ILE
3	C	279	LEU
3	C	289	PHE
3	C	315	MET
3	C	355[A]	THR
3	C	355[B]	THR
3	C	416	SER
4	D	12	ARG
4	D	43	LEU
4	D	76	VAL
4	D	154	VAL
4	D	259	ILE
4	D	345	VAL
5	E	4	THR

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Mol	Chain	Res	Type
5	E	11	SER
5	E	14	ILE
5	E	16	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	65	LEU
5	E	71	GLU
5	E	76	VAL
5	E	83	LEU
6	F	25	THR
7	H	20	LYS
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	33	LYS
8	I	34	ARG
8	I	35	LYS
9	J	8	ILE
10	K	10	LYS
10	K	25	LEU
10	K	43	VAL
10	K	46[A]	ARG
10	K	46[B]	ARG
11	L	2	GLU
12	M	3	VAL
12	M	13	LEU
13	O	3	GLN
13	O	23	ASP
13	O	25	THR
13	O	39	ARG
13	O	40	ILE
13	O	55	GLU
13	O	57	LYS
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	214	THR
13	O	234	LYS
14	T	2	GLU
14	T	24	ARG

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Mol	Chain	Res	Type
14	T	25	GLU
14	T	29	ILE
15	U	10	VAL
15	U	39	ARG
15	U	51	LYS
15	U	59	GLU
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	14	SER
16	V	90	GLU
16	V	105	ARG
17	Y	24	MET
17	Y	25	ILE
17	Y	27	MET
17	Y	38	LEU
17	Y	43	ARG
17	Y	45	ASN
18	X	15	LEU
18	X	28	LEU
18	X	29	ILE
19	Z	3	ILE
19	Z	7	LEU
19	Z	15	LEU
19	Z	29	SER
19	Z	32	ASP
19	Z	35	ARG
19	Z	40	ILE
19	Z	46	LEU
19	Z	50	LEU
19	Z	52	LEU
19	Z	61	VAL
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	13	LEU
20	R	14	LEU
20	R	20	VAL
20	R	21	ARG
20	R	32	GLN
20	R	35	LEU

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Mol	Chain	Res	Type
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159	LEU
1	a	160[A]	ILE
1	a	160[B]	ILE
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	238	LYS
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	13	ILE
2	b	86	ILE
2	b	128	THR
2	b	137	LYS
2	b	149	LEU
2	b	207	ILE
2	b	219	VAL
2	b	236	THR
2	b	252	VAL
2	b	362	PHE
2	b	397	VAL
2	b	467	ILE
2	b	490	GLN
3	c	24	THR
3	c	25	ASN
3	c	26	ARG
3	c	29	GLU
3	c	30	SER
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	142	GLU
3	c	155	ASN
3	c	165	LEU
3	c	240	ILE
3	c	315	MET

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Mol	Chain	Res	Type
3	c	354[A]	GLU
3	c	354[B]	GLU
3	c	355[A]	THR
3	c	355[B]	THR
3	c	471	SER
4	d	12	ARG
4	d	90	LEU
4	d	182	LEU
4	d	233	ARG
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	8	ARG
5	e	83	LEU
5	e	84	LYS
6	f	12	SER
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
6	f	44	GLN
7	h	7	LEU
7	h	10	ILE
7	h	21	VAL
7	h	40	VAL
7	h	43	LEU
9	j	7	ARG
9	j	13	VAL
9	j	36	LEU
10	k	10	LYS
10	k	11	LEU
10	k	23	ASP
10	k	24	VAL
10	k	30	VAL
11	l	2	GLU
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	4	THR
13	o	18	LYS
13	o	49	THR

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Mol	Chain	Res	Type
13	o	55	GLU
13	o	57	LYS
13	o	59	LYS
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	133	VAL
13	o	134	THR
13	o	135	SER
13	o	181	GLU
13	o	198	SER
13	o	207	ARG
14	t	25	GLU
16	v	15	GLU
16	v	24	LYS
16	v	52	LEU
16	v	106	ASN
16	v	107	LEU
16	v	109	GLU
16	v	112	LEU
17	y	22	LEU
17	y	30	ILE
17	y	38	LEU
17	y	45	ASN
17	y	46	LEU
18	x	2	THR
18	x	3	ILE
18	x	8	LYS
18	x	15	LEU
18	x	16	SER
18	x	21	LEU
19	z	1	MET
19	z	3	ILE
19	z	20	VAL
19	z	32	ASP
19	z	38	GLN
19	z	39	LEU
19	z	46	LEU
20	r	9	LEU
20	r	13	LEU
20	r	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	247	ASN
1	A	261	GLN
2	B	490	GLN
4	D	61	HIS
4	D	186	GLN
4	D	334	GLN
4	D	336	HIS
13	O	82	GLN
13	O	124	ASN
13	O	147	ASN
13	O	231	HIS
17	Y	45	ASN
18	X	33	GLN
2	b	338	GLN
2	b	409	GLN
2	b	497	GLN
3	c	25	ASN
3	c	201	ASN
13	o	58	ASN
13	o	124	ASN
16	v	34	GLN
19	z	38	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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	FME	M	1	12	8,9,10	0.96	1 (12%)	8,9,11	1.01	0
14	FME	T	1	14	8,9,10	1.13	1 (12%)	8,9,11	1.73	3 (37%)
8	FME	i	1	8	8,9,10	1.02	0	8,9,11	1.11	1 (12%)
8	FME	I	1	8	8,9,10	0.90	1 (12%)	8,9,11	1.61	3 (37%)
14	FME	t	1	14	8,9,10	1.10	1 (12%)	8,9,11	1.97	1 (12%)
12	FME	m	1	12	8,9,10	1.06	1 (12%)	8,9,11	0.97	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.79	1.42	1.46
14	T	1	FME	CA-N	-2.43	1.43	1.46
12	m	1	FME	CA-N	-2.19	1.43	1.46
8	I	1	FME	CA-N	-2.03	1.43	1.46
12	M	1	FME	CA-N	-2.02	1.43	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-4.32	116.18	122.82
8	I	1	FME	CA-N-CN	-3.12	118.02	122.82
14	T	1	FME	CA-N-CN	-2.62	118.79	122.82
14	T	1	FME	CB-CA-N	2.45	114.97	110.52
8	I	1	FME	CB-CA-N	2.40	114.88	110.52
8	i	1	FME	C-CA-N	2.37	114.07	109.50
14	T	1	FME	O1-CN-N	-2.18	119.68	125.32
12	m	1	FME	CB-CA-N	2.17	114.46	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1	FME	O1-CN-N	-2.07	119.96	125.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 188 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 151 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	$\#\|Z\| > 2$
25	BCR	d	404	-	41,41,41	1.21	3 (7%)	56,56,56	1.22	6 (10%)
23	CLA	b	610	2	69,73,73	1.34	10 (14%)	82,113,113	1.13	4 (4%)
30	DGD	c	518	-	63,63,67	1.11	6 (9%)	77,77,81	1.46	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	HEM	E	101	6,5	50,50,50	1.43	8 (16%)	67,82,82	1.13	4 (5%)
23	CLA	c	506	3	69,73,73	1.88	9 (13%)	82,113,113	1.34	15 (18%)
25	BCR	A	409	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	8 (14%)
33	BCT	A	418	21	3,3,3	1.03	0	2,3,3	3.51	2 (100%)
29	LHG	D	407	-	48,48,48	1.02	3 (6%)	51,54,54	1.33	7 (13%)
23	CLA	B	612	2	69,73,73	1.23	8 (11%)	82,113,113	1.39	8 (9%)
25	BCR	B	617	-	41,41,41	1.23	4 (9%)	56,56,56	1.37	6 (10%)
23	CLA	B	610	37	69,73,73	1.35	9 (13%)	82,113,113	1.40	10 (12%)
23	CLA	h	101	37	69,73,73	1.49	10 (14%)	82,113,113	1.39	10 (12%)
23	CLA	c	507	37	69,73,73	1.26	9 (13%)	82,113,113	1.34	8 (9%)
23	CLA	D	402	4	69,73,73	1.15	9 (13%)	82,113,113	1.26	6 (7%)
24	PHO	A	407	-	58,69,69	1.96	10 (17%)	55,99,99	1.43	9 (16%)
24	PHO	d	401	-	58,69,69	2.14	13 (22%)	55,99,99	1.73	10 (18%)
28	SQD	a	413	-	35,35,54	1.13	2 (5%)	37,37,65	1.40	5 (13%)
25	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.44	10 (17%)
29	LHG	B	623	-	48,48,48	0.90	2 (4%)	51,54,54	1.45	6 (11%)
25	BCR	k	102	-	41,41,41	0.93	1 (2%)	56,56,56	1.18	4 (7%)
25	BCR	x	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	6 (10%)
23	CLA	b	614	2	69,73,73	1.43	10 (14%)	82,113,113	1.35	12 (14%)
23	CLA	C	505	3	69,73,73	1.24	6 (8%)	82,113,113	1.14	5 (6%)
23	CLA	b	615	2	69,73,73	1.26	7 (10%)	82,113,113	1.43	9 (10%)
33	BCT	a	404	21	3,3,3	1.24	0	2,3,3	3.17	2 (100%)
31	OEX	A	416[A]	3,37,1	0,14,14	-	-	-		
28	SQD	B	624	-	52,54,54	0.93	2 (3%)	62,65,65	1.78	12 (19%)
25	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	12 (21%)
27	LMG	M	101	-	51,51,55	0.99	3 (5%)	59,59,63	1.50	11 (18%)
28	SQD	f	101	-	39,41,54	1.16	4 (10%)	49,52,65	1.66	8 (16%)
23	CLA	c	501	3	69,73,73	1.41	11 (15%)	82,113,113	1.56	10 (12%)
23	CLA	a	406	37	69,73,73	1.51	10 (14%)	82,113,113	1.41	7 (8%)
23	CLA	B	607	37	69,73,73	1.34	9 (13%)	82,113,113	1.35	8 (9%)
23	CLA	B	601	37	69,73,73	1.39	8 (11%)	82,113,113	1.69	10 (12%)
29	LHG	l	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.24	5 (9%)
27	LMG	c	519	-	37,37,55	1.14	4 (10%)	45,45,63	1.27	6 (13%)
23	CLA	b	608	37	69,73,73	1.43	9 (13%)	82,113,113	1.24	8 (9%)
28	SQD	A	414	-	38,38,54	1.05	3 (7%)	40,40,65	1.26	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LHG	d	406	-	48,48,48	0.74	1 (2%)	51,54,54	1.31	6 (11%)
23	CLA	c	502	3	69,73,73	1.40	10 (14%)	82,113,113	1.35	8 (9%)
29	LHG	A	413	-	48,48,48	1.01	4 (8%)	51,54,54	1.23	4 (7%)
23	CLA	B	606	2	69,73,73	1.58	10 (14%)	82,113,113	1.57	13 (15%)
23	CLA	C	501	3	69,73,73	1.48	12 (17%)	82,113,113	1.38	8 (9%)
29	LHG	e	101	-	41,41,48	0.93	3 (7%)	44,47,54	1.40	5 (11%)
24	PHO	a	407	-	58,69,69	2.26	13 (22%)	55,99,99	1.34	6 (10%)
25	BCR	B	619	-	41,41,41	1.27	4 (9%)	56,56,56	1.34	9 (16%)
27	LMG	D	409	-	31,31,55	1.02	3 (9%)	33,33,63	1.26	3 (9%)
23	CLA	B	603	2	69,73,73	1.27	10 (14%)	82,113,113	1.27	10 (12%)
23	CLA	C	510	3	69,73,73	1.34	10 (14%)	82,113,113	1.31	7 (8%)
32	OEY	A	417[B]	3,37,1	0,16,16	-	-	-		
23	CLA	b	604	2	69,73,73	1.19	6 (8%)	82,113,113	1.45	12 (14%)
25	BCR	H	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.42	6 (10%)
29	LHG	D	408	-	46,46,48	1.10	4 (8%)	49,52,54	1.33	5 (10%)
23	CLA	C	508	3	69,73,73	1.20	8 (11%)	82,113,113	1.34	11 (13%)
25	BCR	b	618	-	41,41,41	1.19	3 (7%)	56,56,56	1.43	10 (17%)
30	DGD	H	102	-	63,63,67	1.33	8 (12%)	77,77,81	1.45	10 (12%)
35	HEM	e	102	6,5	50,50,50	1.51	7 (14%)	67,82,82	1.19	6 (8%)
23	CLA	C	507	37	69,73,73	1.30	8 (11%)	82,113,113	1.42	8 (9%)
29	LHG	d	407	-	48,48,48	0.82	1 (2%)	51,54,54	1.31	6 (11%)
27	LMG	b	623	-	21,21,55	0.88	1 (4%)	20,20,63	0.96	1 (5%)
23	CLA	b	606	2	69,73,73	1.16	10 (14%)	82,113,113	1.48	15 (18%)
23	CLA	b	607	2	69,73,73	1.43	7 (10%)	82,113,113	1.57	8 (9%)
23	CLA	c	505	3	69,73,73	1.21	8 (11%)	82,113,113	1.38	10 (12%)
27	LMG	d	409	-	44,44,55	1.04	3 (6%)	52,52,63	1.33	7 (13%)
23	CLA	c	508	3	68,72,73	1.43	9 (13%)	80,111,113	1.34	8 (10%)
23	CLA	b	603	2	69,73,73	1.19	8 (11%)	82,113,113	1.35	8 (9%)
27	LMG	C	518	-	48,48,55	1.04	3 (6%)	56,56,63	1.34	8 (14%)
23	CLA	D	401	37	69,73,73	1.15	7 (10%)	82,113,113	1.25	8 (9%)
25	BCR	b	619	-	41,41,41	1.25	2 (4%)	56,56,56	1.23	6 (10%)
23	CLA	b	613	2	69,73,73	1.34	8 (11%)	82,113,113	1.34	13 (15%)
23	CLA	B	611	2	69,73,73	1.17	6 (8%)	82,113,113	1.39	10 (12%)
23	CLA	C	512	3	69,73,73	1.42	9 (13%)	82,113,113	1.31	11 (13%)
25	BCR	T	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.54	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	614	2	69,73,73	1.13	9 (13%)	82,113,113	1.39	10 (12%)
30	DGD	C	516	-	63,63,67	1.08	4 (6%)	77,77,81	1.44	11 (14%)
23	CLA	b	616	2	69,73,73	1.42	12 (17%)	82,113,113	1.27	4 (4%)
27	LMG	B	621	-	26,26,55	0.79	0	26,26,63	1.12	2 (7%)
23	CLA	C	513	3	69,73,73	1.38	10 (14%)	82,113,113	1.40	6 (7%)
25	BCR	K	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	6 (10%)
23	CLA	C	506	3	69,73,73	1.76	11 (15%)	82,113,113	1.24	7 (8%)
32	OEY	a	417[B]	3,37,1	0,16,16	-	-	-		
25	BCR	k	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.26	6 (10%)
23	CLA	c	509	3	69,73,73	1.28	8 (11%)	82,113,113	1.40	9 (10%)
28	SQD	F	101	-	34,36,54	1.01	3 (8%)	42,45,65	1.68	9 (21%)
25	BCR	t	101	-	41,41,41	1.02	3 (7%)	56,56,56	1.43	9 (16%)
23	CLA	B	616	2	64,68,73	1.36	7 (10%)	76,107,113	1.45	12 (15%)
23	CLA	a	411	37	69,73,73	1.54	9 (13%)	82,113,113	1.65	9 (10%)
27	LMG	D	406	-	51,51,55	1.00	2 (3%)	59,59,63	1.28	8 (13%)
23	CLA	B	608	2	69,73,73	1.18	7 (10%)	82,113,113	1.29	8 (9%)
23	CLA	d	403	4	69,73,73	1.23	9 (13%)	82,113,113	1.23	9 (10%)
23	CLA	c	503	3	69,73,73	1.43	10 (14%)	82,113,113	1.55	9 (10%)
23	CLA	B	605	2	69,73,73	1.30	8 (11%)	82,113,113	1.39	15 (18%)
25	BCR	c	515	-	41,41,41	1.33	3 (7%)	56,56,56	1.41	9 (16%)
23	CLA	B	604	2	69,73,73	1.30	6 (8%)	82,113,113	1.45	12 (14%)
25	BCR	C	514	-	41,41,41	1.21	4 (9%)	56,56,56	1.32	6 (10%)
27	LMG	A	411	-	48,48,55	0.95	2 (4%)	56,56,63	1.40	9 (16%)
23	CLA	C	502	3	69,73,73	1.19	7 (10%)	82,113,113	1.31	10 (12%)
24	PHO	A	406	-	58,69,69	1.66	8 (13%)	55,99,99	1.50	8 (14%)
23	CLA	A	405	37	69,73,73	1.39	8 (11%)	82,113,113	1.32	10 (12%)
23	CLA	C	504	37	63,67,73	1.25	9 (14%)	74,105,113	1.21	7 (9%)
30	DGD	C	517	-	63,63,67	1.14	7 (11%)	77,77,81	1.36	8 (10%)
23	CLA	B	615	2	69,73,73	1.42	12 (17%)	82,113,113	1.25	7 (8%)
29	LHG	d	408	-	38,38,48	0.89	1 (2%)	41,44,54	1.23	3 (7%)
26	PL9	A	410	-	55,55,55	1.08	2 (3%)	68,69,69	1.66	13 (19%)
36	HEC	v	201	16	50,50,50	1.44	5 (10%)	68,82,82	1.23	7 (10%)
30	DGD	h	102	-	63,63,67	1.02	5 (7%)	77,77,81	1.54	14 (18%)
25	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	9 (16%)
23	CLA	c	512	3	69,73,73	1.25	10 (14%)	82,113,113	1.34	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	511	3	69,73,73	1.48	10 (14%)	82,113,113	1.54	5 (6%)
28	SQD	a	412	-	52,54,54	0.97	4 (7%)	62,65,65	1.87	11 (17%)
36	HEC	V	201	16	50,50,50	1.45	5 (10%)	68,82,82	1.20	6 (8%)
25	BCR	D	404	-	41,41,41	1.21	2 (4%)	56,56,56	1.28	5 (8%)
23	CLA	c	511	3	69,73,73	1.50	9 (13%)	82,113,113	1.34	7 (8%)
23	CLA	B	613	2	69,73,73	1.31	8 (11%)	82,113,113	1.34	5 (6%)
23	CLA	b	612	2	69,73,73	1.29	8 (11%)	82,113,113	1.37	12 (14%)
30	DGD	C	515	-	63,63,67	1.41	9 (14%)	77,77,81	1.33	9 (11%)
30	DGD	c	516	-	63,63,67	1.29	6 (9%)	77,77,81	1.38	11 (14%)
30	DGD	c	517	-	63,63,67	1.10	6 (9%)	77,77,81	1.41	9 (11%)
23	CLA	A	404	1	69,73,73	1.49	12 (17%)	82,113,113	1.37	11 (13%)
23	CLA	c	504	37	64,68,73	1.21	10 (15%)	76,107,113	1.35	11 (14%)
23	CLA	d	402	4	69,73,73	1.34	9 (13%)	82,113,113	1.58	7 (8%)
27	LMG	c	521	-	48,48,55	1.12	6 (12%)	56,56,63	1.37	9 (16%)
28	SQD	b	601	-	47,49,54	0.94	3 (6%)	57,60,65	1.92	13 (22%)
31	OEX	a	416[A]	3,37,1	0,14,14	-	-	-		
28	SQD	A	412	-	50,52,54	1.06	3 (6%)	60,63,65	2.21	15 (25%)
23	CLA	C	503	3	69,73,73	1.61	11 (15%)	82,113,113	1.76	14 (17%)
23	CLA	C	509	3	69,73,73	1.33	9 (13%)	82,113,113	1.20	6 (7%)
27	LMG	m	101	-	51,51,55	0.83	2 (3%)	59,59,63	1.56	12 (20%)
23	CLA	a	405	1	69,73,73	1.33	6 (8%)	82,113,113	1.45	8 (9%)
23	CLA	D	403	4	69,73,73	1.62	10 (14%)	82,113,113	1.14	7 (8%)
23	CLA	b	617	2	64,68,73	1.05	6 (9%)	76,107,113	1.39	11 (14%)
23	CLA	B	609	2	69,73,73	1.40	12 (17%)	82,113,113	1.43	12 (14%)
25	BCR	b	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	8 (14%)
27	LMG	c	523	-	49,49,55	0.90	2 (4%)	57,57,63	1.31	7 (12%)
25	BCR	Z	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	8 (14%)
26	PL9	a	410	-	55,55,55	1.12	4 (7%)	68,69,69	1.72	11 (16%)
26	PL9	d	405	-	55,55,55	1.40	9 (16%)	68,69,69	1.74	18 (26%)
30	DGD	A	415	-	67,67,67	1.25	8 (11%)	81,81,81	1.48	9 (11%)
25	BCR	a	409	-	41,41,41	1.02	2 (4%)	56,56,56	1.33	10 (17%)
23	CLA	c	513	3	69,73,73	1.21	9 (13%)	82,113,113	1.18	7 (8%)
23	CLA	b	611	37	69,73,73	1.20	7 (10%)	82,113,113	1.28	8 (9%)
29	LHG	B	622	-	48,48,48	0.71	1 (2%)	51,54,54	1.13	4 (7%)
23	CLA	a	408	1	69,73,73	1.48	11 (15%)	82,113,113	1.32	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	605	2	69,73,73	1.23	7 (10%)	82,113,113	1.46	10 (12%)
23	CLA	B	602	2	69,73,73	1.55	11 (15%)	82,113,113	1.35	9 (10%)
27	LMG	b	622	-	55,55,55	1.05	3 (5%)	63,63,63	1.46	7 (11%)
23	CLA	b	609	2	69,73,73	1.34	9 (13%)	82,113,113	1.49	14 (17%)
26	PL9	D	405	-	55,55,55	1.61	10 (18%)	68,69,69	1.44	11 (16%)
23	CLA	c	510	3	69,73,73	1.26	9 (13%)	82,113,113	1.42	8 (9%)
23	CLA	A	408	1	58,62,73	1.66	9 (15%)	68,99,113	1.39	12 (17%)
30	DGD	a	414	-	43,43,67	1.49	6 (13%)	45,45,81	1.51	7 (15%)

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
25	BCR	d	404	-	-	7/29/63/63	0/2/2/2
23	CLA	b	610	2	-	10/39/115/115	-
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
35	HEM	E	101	6,5	-	3/14/54/54	-
23	CLA	c	506	3	-	14/39/115/115	-
25	BCR	A	409	-	-	11/29/63/63	0/2/2/2
29	LHG	D	407	-	-	25/53/53/53	-
23	CLA	B	612	2	-	4/39/115/115	-
25	BCR	B	617	-	-	11/29/63/63	0/2/2/2
23	CLA	B	610	37	-	6/39/115/115	-
23	CLA	h	101	37	-	19/39/115/115	-
23	CLA	c	507	37	-	12/39/115/115	-
23	CLA	D	402	4	-	7/39/115/115	-
24	PHO	A	407	-	-	1/37/103/103	0/5/6/6
24	PHO	d	401	-	-	5/37/103/103	0/5/6/6
28	SQD	a	413	-	-	19/37/37/69	-
25	BCR	K	101	-	-	5/29/63/63	0/2/2/2
29	LHG	B	623	-	-	21/53/53/53	-
25	BCR	k	102	-	-	4/29/63/63	0/2/2/2
25	BCR	x	101	-	-	5/29/63/63	0/2/2/2
23	CLA	b	614	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	505	3	-	12/39/115/115	-
23	CLA	b	615	2	-	14/39/115/115	-
28	SQD	B	624	-	-	24/49/69/69	0/1/1/1
25	BCR	c	514	-	-	16/29/63/63	0/2/2/2
27	LMG	M	101	-	-	19/46/66/70	0/1/1/1
28	SQD	f	101	-	-	13/36/56/69	0/1/1/1
23	CLA	c	501	3	-	5/39/115/115	-
23	CLA	a	406	37	-	11/39/115/115	-
23	CLA	B	607	37	-	11/39/115/115	-
23	CLA	B	601	37	-	16/39/115/115	-
29	LHG	l	101	-	-	18/53/53/53	-
27	LMG	c	519	-	-	12/31/51/70	0/1/1/1
23	CLA	b	608	37	-	11/39/115/115	-
28	SQD	A	414	-	-	18/39/39/69	-
29	LHG	d	406	-	-	22/53/53/53	-
23	CLA	c	502	3	-	4/39/115/115	-
29	LHG	A	413	-	-	27/53/53/53	-
23	CLA	B	606	2	-	11/39/115/115	-
23	CLA	C	501	3	-	6/39/115/115	-
29	LHG	e	101	-	-	27/46/46/53	-
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
25	BCR	B	619	-	-	7/29/63/63	0/2/2/2
27	LMG	D	409	-	-	13/33/33/70	-
23	CLA	B	603	2	-	16/39/115/115	-
23	CLA	C	510	3	-	10/39/115/115	-
23	CLA	b	604	2	-	9/39/115/115	-
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
29	LHG	D	408	-	-	20/51/51/53	-
23	CLA	C	508	3	-	3/39/115/115	-
25	BCR	b	618	-	-	6/29/63/63	0/2/2/2
30	DGD	H	102	-	-	13/51/91/95	0/2/2/2
35	HEM	e	102	6,5	-	5/14/54/54	-
23	CLA	C	507	37	-	8/39/115/115	-
29	LHG	d	407	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	b	623	-	-	9/17/17/70	-
23	CLA	b	606	2	-	8/39/115/115	-
23	CLA	b	607	2	-	10/39/115/115	-
23	CLA	c	505	3	-	12/39/115/115	-
27	LMG	d	409	-	-	13/39/59/70	0/1/1/1
23	CLA	c	508	3	-	10/38/114/115	-
23	CLA	b	603	2	-	8/39/115/115	-
27	LMG	C	518	-	-	15/43/63/70	0/1/1/1
23	CLA	D	401	37	-	3/39/115/115	-
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	b	613	2	-	9/39/115/115	-
23	CLA	B	611	2	-	8/39/115/115	-
23	CLA	C	512	3	-	10/39/115/115	-
25	BCR	T	101	-	-	6/29/63/63	0/2/2/2
23	CLA	B	614	2	-	12/39/115/115	-
30	DGD	C	516	-	-	21/51/91/95	0/2/2/2
23	CLA	b	616	2	-	6/39/115/115	-
27	LMG	B	621	-	-	11/22/22/70	-
23	CLA	C	513	3	-	9/39/115/115	-
25	BCR	K	102	-	-	10/29/63/63	0/2/2/2
23	CLA	C	506	3	-	10/39/115/115	-
25	BCR	k	101	-	-	11/29/63/63	0/2/2/2
23	CLA	c	509	3	-	12/39/115/115	-
28	SQD	F	101	-	-	16/28/48/69	0/1/1/1
25	BCR	t	101	-	-	5/29/63/63	0/2/2/2
23	CLA	B	616	2	-	8/33/109/115	-
23	CLA	a	411	37	-	3/39/115/115	-
27	LMG	D	406	-	-	14/46/66/70	0/1/1/1
23	CLA	B	608	2	-	0/39/115/115	-
23	CLA	d	403	4	-	6/39/115/115	-
23	CLA	c	503	3	-	7/39/115/115	-
23	CLA	B	605	2	-	11/39/115/115	-
25	BCR	c	515	-	-	9/29/63/63	0/2/2/2
23	CLA	B	604	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	514	-	-	2/29/63/63	0/2/2/2
27	LMG	A	411	-	-	20/43/63/70	0/1/1/1
23	CLA	C	502	3	-	8/39/115/115	-
24	PHO	A	406	-	-	5/37/103/103	0/5/6/6
23	CLA	A	405	37	-	5/39/115/115	-
23	CLA	C	504	37	-	8/32/108/115	-
30	DGD	C	517	-	-	15/51/91/95	0/2/2/2
23	CLA	B	615	2	-	10/39/115/115	-
29	LHG	d	408	-	-	12/43/43/53	-
26	PL9	A	410	-	-	27/53/73/73	0/1/1/1
36	HEC	v	201	16	1/1/7/7	2/14/54/54	-
30	DGD	h	102	-	-	17/51/91/95	0/2/2/2
25	BCR	B	618	-	-	4/29/63/63	0/2/2/2
23	CLA	c	512	3	-	19/39/115/115	-
23	CLA	C	511	3	-	3/39/115/115	-
28	SQD	a	412	-	-	24/49/69/69	0/1/1/1
36	HEC	V	201	16	1/1/7/7	6/14/54/54	-
25	BCR	D	404	-	-	5/29/63/63	0/2/2/2
23	CLA	c	511	3	-	9/39/115/115	-
23	CLA	B	613	2	-	8/39/115/115	-
23	CLA	b	612	2	-	8/39/115/115	-
30	DGD	C	515	-	-	21/51/91/95	0/2/2/2
30	DGD	c	516	-	-	26/51/91/95	0/2/2/2
30	DGD	c	517	-	-	18/51/91/95	0/2/2/2
23	CLA	A	404	1	-	5/39/115/115	-
23	CLA	c	504	37	-	5/33/109/115	-
23	CLA	d	402	4	-	10/39/115/115	-
27	LMG	c	521	-	-	20/43/63/70	0/1/1/1
28	SQD	b	601	-	-	18/44/64/69	0/1/1/1
28	SQD	A	412	-	-	20/47/67/69	0/1/1/1
23	CLA	C	503	3	-	6/39/115/115	-
23	CLA	C	509	3	-	10/39/115/115	-
27	LMG	m	101	-	-	18/46/66/70	0/1/1/1
23	CLA	a	405	1	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	403	4	-	12/39/115/115	-
23	CLA	b	617	2	-	9/33/109/115	-
23	CLA	B	609	2	-	3/39/115/115	-
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
27	LMG	c	523	-	-	27/44/64/70	0/1/1/1
25	BCR	Z	101	-	-	9/29/63/63	0/2/2/2
26	PL9	a	410	-	-	24/53/73/73	0/1/1/1
26	PL9	d	405	-	-	17/53/73/73	0/1/1/1
30	DGD	A	415	-	-	25/55/95/95	0/2/2/2
25	BCR	a	409	-	-	6/29/63/63	0/2/2/2
23	CLA	c	513	3	-	7/39/115/115	-
23	CLA	b	611	37	-	11/39/115/115	-
29	LHG	B	622	-	-	20/53/53/53	-
23	CLA	a	408	1	-	12/39/115/115	-
23	CLA	b	605	2	-	11/39/115/115	-
23	CLA	B	602	2	-	4/39/115/115	-
27	LMG	b	622	-	-	25/50/70/70	0/1/1/1
23	CLA	b	609	2	-	6/39/115/115	-
26	PL9	D	405	-	-	11/53/73/73	0/1/1/1
23	CLA	c	510	3	-	14/39/115/115	-
23	CLA	A	408	1	-	3/26/102/115	-
30	DGD	a	414	-	-	24/45/45/95	-

All (917) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	MG-ND	-11.97	1.82	2.05
24	a	407	PHO	C1B-C2B	10.42	1.50	1.39
24	d	401	PHO	C1B-C2B	9.72	1.50	1.39
23	D	403	CLA	MG-NB	-9.15	1.87	2.05
24	a	407	PHO	C3B-C4B	8.51	1.50	1.41
24	d	401	PHO	C3B-C4B	8.29	1.49	1.41
23	C	506	CLA	MG-NB	7.91	2.21	2.05
24	A	407	PHO	C1B-C2B	7.90	1.48	1.39
23	b	607	CLA	MG-NA	7.60	2.24	2.06
23	C	506	CLA	MG-ND	-7.53	1.90	2.05
24	A	407	PHO	C3B-C4B	7.37	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	MG-NA	7.33	2.23	2.06
23	C	503	CLA	MG-NA	7.18	2.23	2.06
23	a	406	CLA	MG-NC	6.79	2.22	2.06
23	A	405	CLA	MG-NB	-6.57	1.92	2.05
23	A	408	CLA	MG-ND	-6.52	1.92	2.05
23	c	511	CLA	MG-NA	6.36	2.21	2.06
23	h	101	CLA	MG-NA	6.19	2.21	2.06
23	b	613	CLA	MG-ND	-6.16	1.93	2.05
23	b	616	CLA	MG-NA	6.10	2.20	2.06
24	A	406	PHO	C1B-C2B	6.09	1.46	1.39
23	b	614	CLA	MG-NB	-6.06	1.93	2.05
23	c	508	CLA	MG-NB	6.04	2.17	2.05
24	A	406	PHO	C3B-C4B	6.03	1.47	1.41
23	B	604	CLA	MG-NA	5.96	2.20	2.06
35	e	102	HEM	FE-NA	5.92	2.14	1.95
23	C	511	CLA	MG-NA	5.86	2.20	2.06
23	c	502	CLA	MG-NA	5.84	2.20	2.06
23	b	608	CLA	MG-NB	-5.83	1.94	2.05
23	a	411	CLA	MG-ND	5.82	2.17	2.05
23	A	408	CLA	MG-NC	-5.76	1.92	2.06
23	C	513	CLA	MG-NB	-5.66	1.94	2.05
23	C	512	CLA	MG-NB	5.60	2.16	2.05
23	c	501	CLA	MG-NB	-5.59	1.94	2.05
23	C	507	CLA	MG-NA	5.53	2.19	2.06
23	a	411	CLA	MG-NA	5.52	2.19	2.06
23	B	607	CLA	MG-NB	-5.48	1.94	2.05
23	B	601	CLA	MG-NA	5.42	2.19	2.06
23	B	616	CLA	MG-NA	5.35	2.19	2.06
23	A	404	CLA	MG-NA	5.32	2.18	2.06
30	a	414	DGD	O2G-C1B	5.27	1.49	1.34
23	a	408	CLA	MG-NB	-5.24	1.95	2.05
23	B	602	CLA	MG-ND	-5.23	1.95	2.05
23	a	408	CLA	MG-ND	-5.23	1.95	2.05
23	C	505	CLA	MG-NB	-5.13	1.95	2.05
23	c	503	CLA	MG-NC	5.06	2.18	2.06
26	D	405	PL9	C11-C9	-4.93	1.41	1.51
23	C	501	CLA	MG-NA	4.88	2.17	2.06
23	C	501	CLA	MG-ND	-4.85	1.96	2.05
30	A	415	DGD	C4D-C5D	4.80	1.63	1.53
25	c	515	BCR	C1-C6	-4.78	1.47	1.53
30	C	515	DGD	C4E-C3E	4.75	1.64	1.52
23	a	405	CLA	MG-NB	4.73	2.15	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C4B-NB	4.73	1.44	1.37
26	D	405	PL9	C6-C1	-4.72	1.40	1.48
23	d	402	CLA	MG-NA	4.66	2.17	2.06
23	c	503	CLA	MG-NB	4.64	2.15	2.05
23	c	510	CLA	MG-NA	4.62	2.17	2.06
23	B	609	CLA	MG-NA	4.58	2.17	2.06
23	b	614	CLA	C4B-NB	4.58	1.43	1.37
23	A	404	CLA	MG-NC	-4.58	1.95	2.06
26	d	405	PL9	C6-C1	-4.53	1.41	1.48
25	A	409	BCR	C1-C6	-4.49	1.48	1.53
23	B	613	CLA	C1D-ND	4.47	1.43	1.37
23	b	609	CLA	MG-NA	4.44	2.16	2.06
23	c	509	CLA	C1D-ND	4.43	1.43	1.37
23	b	610	CLA	MG-NA	4.38	2.16	2.06
25	x	101	BCR	C30-C25	-4.38	1.48	1.53
25	D	404	BCR	C30-C25	-4.37	1.48	1.53
23	B	605	CLA	MG-NB	4.33	2.14	2.05
23	C	512	CLA	MG-ND	-4.32	1.97	2.05
23	a	408	CLA	C1D-ND	4.32	1.43	1.37
30	c	516	DGD	O2G-C2G	-4.24	1.36	1.46
25	B	619	BCR	C1-C6	-4.22	1.48	1.53
29	D	407	LHG	O7-C5	-4.22	1.36	1.46
23	B	615	CLA	MG-NC	4.20	2.16	2.06
23	C	509	CLA	MG-ND	4.17	2.14	2.05
25	K	101	BCR	C1-C6	-4.14	1.48	1.53
23	B	610	CLA	MG-ND	-4.13	1.97	2.05
27	d	409	LMG	O7-C8	-4.11	1.36	1.46
23	b	609	CLA	MG-ND	-4.08	1.97	2.05
23	c	511	CLA	MG-NC	4.07	2.15	2.06
23	C	509	CLA	MG-NB	-4.06	1.97	2.05
25	d	404	BCR	C1-C6	-4.05	1.48	1.53
23	b	605	CLA	MG-NB	4.05	2.13	2.05
25	H	101	BCR	C30-C25	-4.05	1.48	1.53
23	C	503	CLA	MG-NB	4.04	2.13	2.05
23	B	610	CLA	MG-NC	-4.04	1.96	2.06
23	d	403	CLA	MG-NB	-4.00	1.97	2.05
23	B	602	CLA	C1B-C2B	3.99	1.52	1.43
29	D	408	LHG	P-O6	3.98	1.75	1.59
23	C	513	CLA	MG-ND	3.98	2.13	2.05
25	b	619	BCR	C1-C6	-3.94	1.48	1.53
23	B	612	CLA	MG-NB	3.94	2.13	2.05
23	a	405	CLA	C1D-ND	3.91	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	v	201	HEC	CBC-CAC	-3.91	1.34	1.51
23	B	602	CLA	C1D-ND	3.88	1.43	1.37
23	B	601	CLA	C4B-NB	3.87	1.42	1.37
23	C	502	CLA	MG-NC	3.86	2.15	2.06
23	b	605	CLA	MG-NA	3.85	2.15	2.06
36	V	201	HEC	CBB-CAB	-3.85	1.35	1.51
25	C	514	BCR	C1-C6	-3.84	1.48	1.53
23	C	508	CLA	MG-NA	3.83	2.15	2.06
23	C	511	CLA	C1B-C2B	3.83	1.52	1.43
36	v	201	HEC	FE-NA	3.83	2.07	1.95
25	K	102	BCR	C30-C25	-3.83	1.48	1.53
23	b	612	CLA	MG-NA	3.81	2.15	2.06
23	B	606	CLA	MG-ND	3.81	2.13	2.05
25	K	101	BCR	C30-C25	-3.81	1.48	1.53
28	a	413	SQD	O47-C7	3.80	1.45	1.34
23	a	405	CLA	C1B-C2B	3.79	1.52	1.43
25	B	617	BCR	C1-C6	-3.79	1.48	1.53
30	h	102	DGD	C4D-C3D	3.78	1.62	1.52
26	A	410	PL9	C7-C3	-3.73	1.46	1.51
23	A	404	CLA	C1B-C2B	3.73	1.51	1.43
23	C	501	CLA	C4B-NB	3.72	1.42	1.37
23	d	402	CLA	MG-ND	-3.72	1.98	2.05
23	a	406	CLA	C1D-ND	3.71	1.42	1.37
36	V	201	HEC	FE-ND	3.71	2.06	1.94
23	B	616	CLA	C1D-ND	3.71	1.42	1.37
23	c	509	CLA	MG-NB	-3.71	1.98	2.05
25	Z	101	BCR	C30-C25	-3.70	1.49	1.53
25	k	101	BCR	C1-C6	-3.69	1.49	1.53
23	C	511	CLA	C1D-ND	3.69	1.42	1.37
23	c	508	CLA	C1D-ND	3.69	1.42	1.37
30	c	516	DGD	O2E-C2E	-3.68	1.33	1.43
25	b	618	BCR	C1-C6	-3.68	1.49	1.53
25	c	515	BCR	C30-C25	-3.67	1.49	1.53
23	c	501	CLA	C1D-ND	3.66	1.42	1.37
24	a	407	PHO	C1D-C2D	3.65	1.43	1.39
23	C	501	CLA	C1D-ND	3.65	1.42	1.37
30	A	415	DGD	C4D-C3D	3.64	1.61	1.52
23	c	507	CLA	MG-NC	-3.63	1.97	2.06
23	C	510	CLA	C1D-ND	3.61	1.42	1.37
23	C	509	CLA	C1D-ND	3.61	1.42	1.37
25	x	101	BCR	C1-C6	-3.61	1.49	1.53
36	v	201	HEC	CBB-CAB	-3.60	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	521	LMG	O1-C1	3.60	1.46	1.40
23	B	611	CLA	MG-NC	-3.59	1.97	2.06
25	B	619	BCR	C30-C25	-3.58	1.49	1.53
24	A	407	PHO	C1D-C2D	3.57	1.43	1.39
25	b	618	BCR	C30-C25	-3.56	1.49	1.53
23	A	405	CLA	C1D-ND	3.56	1.42	1.37
24	d	401	PHO	C1D-C2D	3.55	1.43	1.39
25	b	619	BCR	C30-C25	-3.55	1.49	1.53
23	b	610	CLA	MG-ND	-3.55	1.98	2.05
28	f	101	SQD	O47-C7	3.53	1.44	1.34
26	d	405	PL9	C3-C4	-3.52	1.44	1.49
23	b	615	CLA	C4B-NB	3.52	1.42	1.37
23	C	510	CLA	C1B-C2B	3.52	1.51	1.43
23	b	608	CLA	MG-NC	3.51	2.14	2.06
30	A	415	DGD	C1E-C2E	3.51	1.62	1.52
23	c	506	CLA	C1D-ND	3.50	1.42	1.37
23	b	607	CLA	C1D-ND	3.49	1.42	1.37
24	A	406	PHO	C4D-ND	-3.49	1.33	1.38
28	A	414	SQD	O48-C23	3.49	1.43	1.33
28	a	412	SQD	O48-C23	3.48	1.43	1.33
30	C	517	DGD	O1G-C1G	-3.48	1.37	1.45
30	a	414	DGD	C3G-C2G	3.48	1.59	1.51
23	B	609	CLA	C1D-ND	3.47	1.42	1.37
23	c	512	CLA	C1D-ND	3.47	1.42	1.37
23	c	507	CLA	MG-NB	-3.47	1.98	2.05
36	V	201	HEC	CBC-CAC	-3.47	1.36	1.51
26	D	405	PL9	C41-C39	-3.45	1.44	1.51
28	a	413	SQD	O48-C23	3.45	1.43	1.33
23	b	610	CLA	C4B-NB	3.44	1.42	1.37
25	c	514	BCR	C1-C6	-3.43	1.49	1.53
26	d	405	PL9	C46-C44	-3.43	1.44	1.51
24	d	401	PHO	CMC-C2C	-3.43	1.45	1.50
23	D	403	CLA	C1D-ND	3.43	1.42	1.37
23	B	612	CLA	C1D-ND	3.43	1.42	1.37
30	c	516	DGD	C4D-C3D	3.43	1.61	1.52
23	c	502	CLA	MG-NB	-3.42	1.99	2.05
27	C	518	LMG	O7-C8	-3.40	1.38	1.46
30	C	515	DGD	O5D-C1E	3.39	1.45	1.40
24	A	407	PHO	C4D-ND	-3.39	1.33	1.38
23	B	603	CLA	MG-NA	3.38	2.14	2.06
25	d	404	BCR	C30-C25	-3.38	1.49	1.53
23	C	506	CLA	C1D-ND	3.37	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	101	HEM	FE-NA	3.36	2.06	1.95
23	C	511	CLA	C4B-NB	3.35	1.42	1.37
23	B	602	CLA	MG-NA	3.32	2.14	2.06
28	A	414	SQD	O47-C7	3.31	1.43	1.34
28	F	101	SQD	O48-C23	3.31	1.43	1.33
23	b	604	CLA	MG-ND	-3.31	1.99	2.05
23	B	606	CLA	MG-NC	-3.31	1.98	2.06
23	c	503	CLA	C1D-ND	3.30	1.42	1.37
23	a	405	CLA	C1B-NB	-3.29	1.33	1.37
23	A	404	CLA	MG-NB	3.29	2.12	2.05
23	b	616	CLA	C4B-NB	3.28	1.42	1.37
23	b	614	CLA	MG-NA	3.28	2.14	2.06
23	B	612	CLA	MG-NA	3.27	2.14	2.06
28	b	601	SQD	O48-C23	3.27	1.42	1.33
23	C	510	CLA	MG-NB	3.26	2.12	2.05
23	b	603	CLA	C1B-C2B	3.26	1.50	1.43
23	a	406	CLA	C4B-NB	3.26	1.42	1.37
23	C	504	CLA	MG-NA	3.25	2.14	2.06
30	c	517	DGD	O2G-C2G	-3.24	1.39	1.46
23	h	101	CLA	C1D-ND	3.24	1.42	1.37
23	b	604	CLA	C1B-NB	-3.24	1.33	1.37
25	a	409	BCR	C1-C6	-3.23	1.49	1.53
28	B	624	SQD	O47-C7	3.23	1.43	1.34
30	C	517	DGD	O3G-C3G	-3.23	1.38	1.43
23	c	505	CLA	CHC-C1C	3.22	1.44	1.38
29	d	408	LHG	P-O6	3.22	1.72	1.59
23	B	603	CLA	C1D-ND	3.22	1.42	1.37
23	b	603	CLA	C1D-ND	3.21	1.42	1.37
25	k	101	BCR	C30-C25	-3.20	1.49	1.53
23	c	513	CLA	C1B-C2B	3.19	1.50	1.43
23	B	601	CLA	C1D-ND	3.19	1.42	1.37
23	B	614	CLA	C4B-NB	3.19	1.42	1.37
23	C	503	CLA	C1B-C2B	3.19	1.50	1.43
28	A	412	SQD	O48-C23	3.18	1.42	1.33
23	B	601	CLA	C1B-C2B	3.17	1.50	1.43
25	Z	101	BCR	C1-C6	-3.17	1.49	1.53
23	c	501	CLA	C4B-NB	3.17	1.42	1.37
27	c	523	LMG	C4-C5	3.17	1.59	1.53
30	C	517	DGD	O2G-C2G	-3.17	1.39	1.46
23	B	608	CLA	C1D-ND	3.17	1.42	1.37
23	a	406	CLA	CHC-C1C	3.16	1.44	1.38
23	c	504	CLA	MG-ND	-3.16	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	MG-ND	3.16	2.12	2.05
30	H	102	DGD	C4D-C5D	3.16	1.59	1.53
23	b	608	CLA	C1D-ND	3.16	1.42	1.37
23	C	507	CLA	MG-NC	-3.15	1.98	2.06
23	c	510	CLA	C1D-ND	3.15	1.42	1.37
25	b	620	BCR	C30-C25	-3.15	1.49	1.53
23	d	402	CLA	C1D-ND	3.14	1.42	1.37
30	C	516	DGD	C4D-C3D	3.14	1.60	1.52
25	D	404	BCR	C1-C6	-3.14	1.49	1.53
23	B	606	CLA	C1D-ND	3.14	1.42	1.37
23	B	605	CLA	CHC-C1C	3.13	1.44	1.38
23	c	513	CLA	MG-NA	3.13	2.13	2.06
23	c	508	CLA	C1B-C2B	3.12	1.50	1.43
30	c	516	DGD	C3G-C2G	3.12	1.60	1.50
30	H	102	DGD	O5D-C1E	3.11	1.45	1.40
23	c	506	CLA	MG-NB	3.11	2.12	2.05
25	b	620	BCR	C1-C6	-3.11	1.49	1.53
23	c	501	CLA	MG-NC	3.11	2.13	2.06
23	h	101	CLA	C1B-C2B	3.11	1.50	1.43
30	a	414	DGD	O1G-C1A	3.11	1.42	1.33
23	b	610	CLA	C1D-ND	3.11	1.41	1.37
30	c	518	DGD	C6D-C5D	3.11	1.60	1.51
23	B	615	CLA	CMD-C2D	-3.10	1.44	1.50
23	B	609	CLA	CMD-C2D	-3.09	1.44	1.50
29	A	413	LHG	O8-C23	3.09	1.42	1.33
35	E	101	HEM	FE-NB	3.09	2.04	1.94
23	b	611	CLA	C1B-C2B	3.09	1.50	1.43
23	a	411	CLA	C1B-C2B	3.08	1.50	1.43
23	A	408	CLA	C1D-ND	3.08	1.41	1.37
25	T	101	BCR	C30-C25	-3.08	1.49	1.53
23	B	605	CLA	C1B-NB	-3.08	1.33	1.37
23	b	605	CLA	C1D-ND	3.08	1.41	1.37
23	c	511	CLA	C1D-ND	3.08	1.41	1.37
25	B	618	BCR	C1-C6	-3.08	1.49	1.53
23	C	502	CLA	C1D-ND	3.08	1.41	1.37
23	B	611	CLA	C1B-C2B	3.07	1.50	1.43
23	c	512	CLA	C4B-NB	3.07	1.41	1.37
23	B	607	CLA	C1B-C2B	3.06	1.50	1.43
28	A	412	SQD	O47-C7	3.06	1.42	1.34
27	M	101	LMG	C9-C8	3.05	1.60	1.50
23	h	101	CLA	MG-NB	-3.05	1.99	2.05
24	d	401	PHO	C4D-ND	-3.04	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C1D-ND	3.04	1.41	1.37
23	D	402	CLA	MG-NB	3.04	2.11	2.05
23	c	503	CLA	CHC-C1C	3.04	1.44	1.38
23	c	509	CLA	MG-NC	3.03	2.13	2.06
23	B	608	CLA	C1B-C2B	3.03	1.50	1.43
25	B	618	BCR	C30-C25	-3.03	1.49	1.53
23	d	402	CLA	CMB-C2B	-3.02	1.44	1.50
23	b	611	CLA	C1D-ND	3.02	1.41	1.37
30	c	516	DGD	O6D-C1D	3.02	1.49	1.41
23	B	610	CLA	C4B-NB	3.01	1.41	1.37
23	C	503	CLA	C4B-NB	3.01	1.41	1.37
23	B	610	CLA	C1B-C2B	3.01	1.50	1.43
23	b	615	CLA	MG-NB	-3.00	1.99	2.05
30	H	102	DGD	C4E-C5E	3.00	1.59	1.53
27	A	411	LMG	C1-C2	3.00	1.61	1.52
24	A	406	PHO	CMD-C2D	-2.99	1.45	1.51
27	b	622	LMG	C4-C3	2.99	1.60	1.52
23	b	615	CLA	CMC-C2C	-2.99	1.44	1.50
28	B	624	SQD	O48-C23	2.98	1.42	1.33
23	b	612	CLA	CMD-C2D	-2.98	1.44	1.50
25	K	102	BCR	C1-C6	-2.98	1.50	1.53
23	B	606	CLA	CHC-C1C	2.98	1.44	1.38
24	a	407	PHO	C4D-CHA	2.97	1.44	1.39
29	B	623	LHG	O7-C5	-2.97	1.39	1.46
23	B	613	CLA	MG-ND	-2.97	1.99	2.05
23	D	401	CLA	C1D-ND	2.97	1.41	1.37
23	a	408	CLA	C4B-NB	2.97	1.41	1.37
24	A	407	PHO	CAC-C3C	-2.97	1.46	1.51
23	B	607	CLA	C1D-ND	2.96	1.41	1.37
23	c	511	CLA	CHC-C1C	2.96	1.44	1.38
28	f	101	SQD	O48-C23	2.96	1.42	1.33
23	A	405	CLA	MG-NA	2.95	2.13	2.06
26	a	410	PL9	C53-C6	-2.95	1.44	1.50
23	h	101	CLA	C4B-NB	2.95	1.41	1.37
23	b	616	CLA	C1B-C2B	2.94	1.50	1.43
23	B	603	CLA	CMC-C2C	-2.94	1.44	1.50
23	C	508	CLA	C1B-C2B	2.94	1.50	1.43
28	b	601	SQD	O47-C7	2.94	1.42	1.34
23	a	406	CLA	MG-NB	2.94	2.11	2.05
23	b	604	CLA	C1D-ND	2.94	1.41	1.37
23	B	605	CLA	C3B-C4B	2.92	1.51	1.42
23	a	408	CLA	C1B-C2B	2.92	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	MG-NC	2.92	2.13	2.06
23	c	507	CLA	CMC-C2C	-2.91	1.44	1.50
23	B	609	CLA	C4B-NB	2.91	1.41	1.37
23	C	513	CLA	C1D-ND	2.90	1.41	1.37
25	B	617	BCR	C33-C5	-2.90	1.46	1.50
24	a	407	PHO	O2D-CGD	2.90	1.40	1.33
23	C	509	CLA	C1B-C2B	2.90	1.49	1.43
23	c	501	CLA	MG-NA	2.90	2.13	2.06
25	B	617	BCR	C30-C25	-2.89	1.50	1.53
23	c	505	CLA	MG-ND	2.89	2.11	2.05
23	d	403	CLA	MG-ND	-2.89	2.00	2.05
23	B	615	CLA	C1B-NB	-2.89	1.34	1.37
27	D	409	LMG	C7-C8	2.89	1.58	1.51
24	a	407	PHO	C3B-C2B	-2.88	1.36	1.40
23	b	603	CLA	C4B-NB	2.88	1.41	1.37
23	B	604	CLA	C1D-ND	2.86	1.41	1.37
23	b	608	CLA	C1B-C2B	2.86	1.49	1.43
28	a	412	SQD	O47-C7	2.85	1.42	1.34
23	C	507	CLA	C1B-NB	-2.85	1.34	1.37
30	C	517	DGD	C1D-C2D	2.85	1.60	1.52
27	b	622	LMG	C4-C5	2.84	1.59	1.53
23	C	503	CLA	CMB-C2B	-2.84	1.44	1.50
23	B	615	CLA	CMB-C2B	-2.84	1.44	1.50
23	b	609	CLA	CHC-C1C	2.84	1.44	1.38
36	V	201	HEC	CMB-C2B	2.84	1.56	1.50
27	M	101	LMG	C1-C2	2.84	1.60	1.52
23	b	605	CLA	CHC-C1C	2.83	1.44	1.38
23	B	615	CLA	C1B-C2B	2.83	1.49	1.43
23	b	615	CLA	CHC-C1C	2.83	1.44	1.38
23	D	402	CLA	CMD-C2D	-2.82	1.45	1.50
23	B	607	CLA	CAC-C3C	-2.82	1.43	1.51
23	c	502	CLA	C1D-ND	2.82	1.41	1.37
24	d	401	PHO	CMD-C2D	-2.82	1.46	1.51
23	C	506	CLA	C1B-C2B	2.81	1.49	1.43
23	C	503	CLA	MG-NC	2.81	2.12	2.06
23	c	503	CLA	C1B-C2B	2.81	1.49	1.43
23	b	606	CLA	C3B-C4B	2.81	1.50	1.42
23	c	505	CLA	C4B-NB	2.80	1.41	1.37
23	B	613	CLA	C1B-C2B	2.80	1.49	1.43
23	B	615	CLA	C4B-NB	2.80	1.41	1.37
23	b	615	CLA	MG-NA	2.80	2.12	2.06
23	C	512	CLA	MG-NA	2.79	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1D-ND	2.79	1.41	1.37
30	C	515	DGD	O4D-C4D	2.79	1.49	1.43
23	b	604	CLA	CMC-C2C	-2.79	1.45	1.50
23	c	513	CLA	C4B-NB	2.79	1.41	1.37
24	A	406	PHO	CMC-C2C	-2.78	1.46	1.50
23	b	617	CLA	C1D-ND	2.78	1.41	1.37
23	B	613	CLA	C4B-NB	2.78	1.41	1.37
23	c	512	CLA	C1B-C2B	2.78	1.49	1.43
23	b	610	CLA	C1B-C2B	2.77	1.49	1.43
26	a	410	PL9	C6-C1	-2.77	1.44	1.48
24	A	407	PHO	CMD-C2D	-2.77	1.46	1.51
24	d	401	PHO	CMB-C2B	-2.77	1.46	1.51
24	A	407	PHO	CMB-C2B	-2.76	1.46	1.51
23	c	511	CLA	C4B-NB	2.75	1.41	1.37
23	C	512	CLA	C3B-C4B	2.75	1.50	1.42
25	C	514	BCR	C30-C25	-2.75	1.50	1.53
23	a	411	CLA	C1B-NB	-2.75	1.34	1.37
23	a	408	CLA	CMD-C2D	-2.75	1.45	1.50
27	c	519	LMG	C7-C8	2.74	1.59	1.50
23	a	411	CLA	CMB-C2B	-2.74	1.45	1.50
23	C	505	CLA	C4B-NB	2.74	1.41	1.37
23	c	513	CLA	MG-ND	-2.74	2.00	2.05
23	A	408	CLA	C1B-C2B	2.74	1.49	1.43
29	B	623	LHG	C24-C23	2.73	1.58	1.50
25	a	409	BCR	C30-C25	-2.73	1.50	1.53
23	c	505	CLA	MG-NB	2.73	2.11	2.05
23	b	612	CLA	C1B-NB	-2.72	1.34	1.37
27	d	409	LMG	C4-C3	2.72	1.59	1.52
23	a	411	CLA	CHC-C1C	2.72	1.43	1.38
23	B	603	CLA	C1A-CHA	-2.72	1.31	1.43
23	c	504	CLA	C4B-NB	2.71	1.41	1.37
23	D	401	CLA	C1B-C2B	2.71	1.49	1.43
23	C	510	CLA	MG-NA	2.70	2.12	2.06
23	b	606	CLA	C1B-C2B	2.70	1.49	1.43
23	b	611	CLA	C3D-C4D	2.69	1.50	1.44
23	c	510	CLA	C4B-NB	2.69	1.41	1.37
30	c	518	DGD	C2A-C1A	-2.69	1.42	1.50
26	d	405	PL9	C46-C47	-2.68	1.44	1.53
30	c	517	DGD	C4D-C3D	2.68	1.59	1.52
23	b	612	CLA	C1B-C2B	2.67	1.49	1.43
23	d	402	CLA	C1B-C2B	2.67	1.49	1.43
23	b	608	CLA	MG-NA	2.67	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	MG-ND	-2.67	2.00	2.05
30	C	515	DGD	C6E-C5E	2.67	1.60	1.51
23	c	506	CLA	CAC-C3C	-2.66	1.44	1.51
23	c	507	CLA	MG-NA	2.66	2.12	2.06
23	b	608	CLA	CMD-C2D	-2.65	1.45	1.50
29	D	408	LHG	O3-C3	-2.65	1.34	1.44
23	c	508	CLA	C3B-C4B	2.65	1.50	1.42
23	a	411	CLA	CMD-C2D	-2.65	1.45	1.50
23	b	611	CLA	C3B-C4B	2.65	1.50	1.42
23	b	610	CLA	CMB-C2B	-2.64	1.45	1.50
23	B	610	CLA	CMB-C2B	-2.64	1.45	1.50
24	A	407	PHO	CMC-C2C	-2.64	1.46	1.50
23	C	510	CLA	C4B-NB	2.64	1.41	1.37
23	B	603	CLA	C1B-C2B	2.63	1.49	1.43
23	b	606	CLA	C1D-ND	2.63	1.41	1.37
23	b	603	CLA	C3B-C4B	2.63	1.50	1.42
23	C	510	CLA	CMD-C2D	-2.63	1.45	1.50
23	c	507	CLA	C1B-C2B	2.63	1.49	1.43
23	c	502	CLA	CMC-C2C	-2.62	1.45	1.50
30	H	102	DGD	C6E-C5E	2.62	1.60	1.51
23	A	404	CLA	CMC-C2C	-2.62	1.45	1.50
23	b	603	CLA	MG-NC	-2.62	2.00	2.06
28	A	414	SQD	O47-C45	-2.61	1.42	1.47
23	b	608	CLA	C4B-NB	2.61	1.41	1.37
30	C	515	DGD	C2A-C1A	-2.60	1.43	1.50
23	b	614	CLA	CMB-C2B	-2.60	1.45	1.50
23	C	510	CLA	CHC-C1C	2.60	1.43	1.38
23	B	615	CLA	CAC-C3C	-2.60	1.44	1.51
30	c	518	DGD	C1D-C2D	2.59	1.60	1.52
30	C	515	DGD	O1G-C1A	2.59	1.40	1.33
23	C	501	CLA	C1B-C2B	2.59	1.49	1.43
23	c	512	CLA	CMB-C2B	-2.58	1.45	1.50
29	e	101	LHG	C24-C23	2.58	1.58	1.50
29	l	101	LHG	O7-C5	-2.58	1.40	1.46
23	c	511	CLA	C3B-C4B	2.57	1.50	1.42
23	a	411	CLA	C3B-C4B	2.57	1.50	1.42
23	B	607	CLA	CMB-C2B	-2.57	1.45	1.50
23	d	403	CLA	MG-NA	2.57	2.12	2.06
23	B	609	CLA	CHC-C4B	-2.57	1.33	1.39
23	c	505	CLA	C3B-C4B	2.57	1.50	1.42
23	B	611	CLA	MG-NA	2.57	2.12	2.06
24	a	407	PHO	CBD-CGD	-2.56	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	CMC-C2C	-2.56	1.45	1.50
23	b	615	CLA	C3B-C4B	2.56	1.50	1.42
23	b	614	CLA	C1B-NB	-2.56	1.34	1.37
23	d	403	CLA	C4B-NB	2.55	1.41	1.37
24	d	401	PHO	CAC-C3C	-2.55	1.47	1.51
23	B	613	CLA	CMD-C2D	-2.55	1.45	1.50
23	D	403	CLA	CMD-C2D	-2.55	1.45	1.50
23	B	614	CLA	CMB-C2B	-2.55	1.45	1.50
23	b	613	CLA	C3B-C4B	2.55	1.50	1.42
23	h	101	CLA	O2A-CGA	2.55	1.40	1.33
23	b	607	CLA	C1B-C2B	2.55	1.49	1.43
23	c	511	CLA	C1B-C2B	2.54	1.49	1.43
23	A	404	CLA	CMD-C2D	-2.54	1.45	1.50
23	d	403	CLA	CMD-C2D	-2.54	1.45	1.50
24	a	407	PHO	CMD-C2D	-2.54	1.46	1.51
30	C	516	DGD	O3E-C3E	-2.54	1.36	1.43
23	B	605	CLA	MG-NC	-2.54	2.00	2.06
28	a	412	SQD	O3-C3	-2.54	1.36	1.43
23	B	611	CLA	CMD-C2D	-2.54	1.45	1.50
23	b	613	CLA	C1D-ND	2.54	1.41	1.37
23	B	614	CLA	CMC-C2C	-2.53	1.45	1.50
30	H	102	DGD	C1E-C2E	2.53	1.59	1.52
27	C	518	LMG	C1-C2	2.53	1.59	1.52
29	e	101	LHG	O8-C23	2.53	1.40	1.33
23	A	404	CLA	C5-C3	-2.52	1.46	1.51
23	c	507	CLA	CMB-C2B	-2.52	1.45	1.50
23	c	508	CLA	C1B-NB	-2.52	1.34	1.37
30	c	518	DGD	O4D-C4D	-2.52	1.36	1.43
23	B	606	CLA	C1B-C2B	2.52	1.49	1.43
23	d	402	CLA	MG-NC	2.52	2.12	2.06
23	B	604	CLA	C3B-C4B	2.52	1.50	1.42
23	a	406	CLA	C1B-C2B	2.52	1.49	1.43
23	A	404	CLA	C1D-ND	2.52	1.41	1.37
23	c	507	CLA	C1D-ND	2.52	1.41	1.37
23	c	508	CLA	CHC-C1C	2.52	1.43	1.38
23	B	605	CLA	C1D-ND	2.52	1.41	1.37
30	c	517	DGD	O3E-C3E	-2.52	1.36	1.43
23	c	503	CLA	C3B-C4B	2.52	1.50	1.42
23	B	612	CLA	C1B-C2B	2.51	1.49	1.43
23	b	613	CLA	CMC-C2C	-2.51	1.45	1.50
23	D	402	CLA	C1D-ND	2.51	1.41	1.37
23	B	609	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C4B-NB	2.50	1.41	1.37
23	C	504	CLA	CMB-C2B	-2.50	1.45	1.50
27	c	519	LMG	C3-C2	2.50	1.58	1.52
23	C	504	CLA	C3B-C4B	2.50	1.50	1.42
23	A	408	CLA	CMD-C2D	-2.50	1.45	1.50
23	b	613	CLA	C1B-C2B	2.50	1.49	1.43
23	b	609	CLA	CAB-C3B	-2.50	1.40	1.47
23	B	613	CLA	MG-NA	2.50	2.12	2.06
23	b	611	CLA	CMD-C2D	-2.50	1.45	1.50
27	D	406	LMG	C4-C3	2.50	1.58	1.52
35	e	102	HEM	CAC-C3C	2.49	1.54	1.47
23	A	408	CLA	C3D-C4D	2.49	1.49	1.44
30	c	516	DGD	C6D-C5D	2.49	1.59	1.51
23	a	405	CLA	C3B-C4B	2.49	1.50	1.42
23	B	616	CLA	C1B-C2B	2.49	1.49	1.43
35	E	101	HEM	CAB-C3B	2.49	1.54	1.47
23	B	603	CLA	C3B-C4B	2.49	1.50	1.42
29	D	407	LHG	C24-C23	2.49	1.57	1.50
27	b	622	LMG	C9-C8	2.49	1.58	1.50
23	h	101	CLA	CMC-C2C	-2.49	1.45	1.50
25	k	102	BCR	C1-C6	-2.49	1.50	1.53
23	c	501	CLA	MG-ND	-2.49	2.00	2.05
30	H	102	DGD	C3E-C2E	2.48	1.58	1.52
27	c	521	LMG	C7-C8	2.48	1.58	1.50
23	B	607	CLA	CMD-C2D	-2.48	1.45	1.50
23	C	503	CLA	CHC-C1C	2.48	1.43	1.38
23	a	406	CLA	CMD-C2D	-2.48	1.45	1.50
23	b	616	CLA	CMD-C2D	-2.48	1.45	1.50
23	b	616	CLA	C1D-ND	2.48	1.41	1.37
23	c	508	CLA	CMC-C2C	-2.48	1.45	1.50
23	c	506	CLA	C1B-C2B	2.48	1.48	1.43
35	e	102	HEM	CAB-C3B	2.48	1.54	1.47
23	b	610	CLA	CMD-C2D	-2.47	1.45	1.50
23	b	605	CLA	C4B-NB	2.47	1.41	1.37
28	A	412	SQD	O2-C2	-2.47	1.36	1.43
35	e	102	HEM	C3B-C2B	-2.47	1.32	1.37
25	c	514	BCR	C30-C25	-2.47	1.50	1.53
23	B	611	CLA	C1D-ND	2.47	1.41	1.37
23	b	604	CLA	C4B-NB	2.47	1.41	1.37
36	V	201	HEC	C4B-NB	-2.47	1.36	1.40
23	C	513	CLA	C4B-NB	2.47	1.41	1.37
29	A	413	LHG	O7-C5	-2.46	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C1D-C2D	2.46	1.50	1.45
23	b	609	CLA	C3B-C4B	2.46	1.49	1.42
23	A	408	CLA	C4B-NB	2.46	1.41	1.37
23	C	505	CLA	C1B-C2B	2.46	1.48	1.43
25	c	515	BCR	C33-C5	-2.46	1.47	1.50
23	C	506	CLA	C1B-NB	-2.46	1.34	1.37
23	c	509	CLA	C1B-C2B	2.45	1.48	1.43
23	C	503	CLA	CMD-C2D	-2.45	1.45	1.50
27	D	409	LMG	C9-C8	2.45	1.58	1.50
23	c	503	CLA	C4B-NB	2.45	1.41	1.37
23	b	611	CLA	MG-NB	-2.45	2.00	2.05
27	M	101	LMG	O3-C3	-2.44	1.36	1.43
23	b	609	CLA	CMB-C2B	-2.44	1.45	1.50
26	D	405	PL9	C27-C28	-2.44	1.43	1.50
23	B	609	CLA	C3B-C4B	2.44	1.49	1.42
27	d	409	LMG	O6-C5	-2.44	1.38	1.44
23	C	501	CLA	C1D-C2D	2.44	1.50	1.45
23	B	610	CLA	C3B-C4B	2.43	1.49	1.42
23	D	402	CLA	CHC-C1C	2.43	1.43	1.38
23	d	403	CLA	C1B-C2B	2.43	1.48	1.43
23	B	614	CLA	MG-NA	2.43	2.12	2.06
25	t	101	BCR	C30-C25	-2.43	1.50	1.53
23	C	509	CLA	C3B-C4B	2.42	1.49	1.42
23	C	508	CLA	C3B-C4B	2.42	1.49	1.42
23	C	503	CLA	C1D-C2D	2.42	1.50	1.45
23	D	401	CLA	MG-NB	2.42	2.10	2.05
23	C	502	CLA	C4B-NB	2.42	1.41	1.37
23	B	602	CLA	C3B-C4B	2.42	1.49	1.42
30	C	516	DGD	O2G-C2G	-2.41	1.40	1.46
23	a	406	CLA	CMB-C2B	-2.41	1.45	1.50
23	C	512	CLA	CHC-C1C	2.41	1.43	1.38
23	C	511	CLA	C3B-C4B	2.41	1.49	1.42
27	c	521	LMG	C4-C3	2.41	1.58	1.52
35	e	102	HEM	CMA-C3A	2.40	1.55	1.50
30	A	415	DGD	O1G-C1G	-2.40	1.39	1.45
28	f	101	SQD	O3-C3	-2.40	1.37	1.43
23	B	613	CLA	MG-NB	-2.40	2.01	2.05
23	C	511	CLA	MG-NC	2.40	2.12	2.06
23	c	502	CLA	CMD-C2D	-2.40	1.45	1.50
23	B	606	CLA	C4B-NB	2.40	1.41	1.37
23	b	607	CLA	CAC-C3C	-2.40	1.45	1.51
23	B	610	CLA	CMD-C2D	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	PHO	C4D-CHA	2.39	1.43	1.39
23	B	609	CLA	MG-ND	-2.39	2.01	2.05
23	c	509	CLA	CHC-C1C	2.39	1.43	1.38
35	E	101	HEM	CMA-C3A	2.39	1.55	1.50
23	b	614	CLA	C1B-C2B	2.39	1.48	1.43
23	c	504	CLA	C1D-ND	2.39	1.41	1.37
26	D	405	PL9	C45-C44	-2.38	1.44	1.50
23	b	603	CLA	MG-NA	2.38	2.11	2.06
23	b	607	CLA	MG-NC	2.38	2.11	2.06
23	d	403	CLA	C1D-ND	2.38	1.41	1.37
23	c	512	CLA	C3D-C4D	2.37	1.49	1.44
23	B	607	CLA	CHC-C4B	-2.37	1.34	1.39
29	D	408	LHG	O8-C6	2.37	1.50	1.45
23	d	402	CLA	C4B-NB	2.37	1.41	1.37
23	C	507	CLA	C1D-ND	2.37	1.41	1.37
24	a	407	PHO	C1A-C2A	2.37	1.54	1.51
23	C	504	CLA	C1B-NB	-2.37	1.34	1.37
24	d	401	PHO	CBD-CGD	-2.36	1.49	1.52
25	H	101	BCR	C1-C6	-2.36	1.50	1.53
30	C	515	DGD	O2G-C2G	-2.36	1.41	1.46
25	b	618	BCR	C33-C5	-2.36	1.47	1.50
23	C	502	CLA	C1B-C2B	2.36	1.48	1.43
23	B	612	CLA	C3B-C4B	2.36	1.49	1.42
23	A	405	CLA	CMC-C2C	-2.36	1.45	1.50
23	B	605	CLA	C1B-C2B	2.36	1.48	1.43
30	H	102	DGD	O2D-C2D	-2.36	1.37	1.43
23	C	510	CLA	C3B-C4B	2.35	1.49	1.42
25	C	514	BCR	C33-C5	-2.35	1.47	1.50
23	b	616	CLA	CMC-C2C	-2.35	1.45	1.50
23	B	607	CLA	MG-NA	2.35	2.11	2.06
23	C	513	CLA	CHC-C4B	-2.35	1.34	1.39
25	k	101	BCR	C33-C5	-2.35	1.47	1.50
23	b	614	CLA	C1D-ND	2.35	1.40	1.37
23	c	506	CLA	CMD-C2D	-2.35	1.46	1.50
23	C	507	CLA	CHC-C1C	2.35	1.43	1.38
23	C	507	CLA	C1B-C2B	2.35	1.48	1.43
23	h	101	CLA	CMD-C2D	-2.35	1.46	1.50
26	d	405	PL9	C53-C6	-2.35	1.46	1.50
30	c	517	DGD	C6E-C5E	2.35	1.59	1.51
30	a	414	DGD	C1G-C2G	2.34	1.58	1.50
23	B	614	CLA	CHC-C1C	2.34	1.43	1.38
23	c	512	CLA	C1B-NB	-2.34	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CMD-C2D	-2.34	1.46	1.50
23	C	513	CLA	C1B-C2B	2.33	1.48	1.43
23	b	614	CLA	CMC-C2C	-2.33	1.46	1.50
23	B	614	CLA	MG-ND	-2.32	2.01	2.05
23	c	501	CLA	CAC-C3C	-2.32	1.45	1.51
24	a	407	PHO	CMB-C2B	-2.32	1.47	1.51
30	C	516	DGD	C1E-C2E	2.32	1.59	1.52
23	A	408	CLA	CHC-C4B	-2.32	1.34	1.39
23	C	501	CLA	C3D-C4D	2.32	1.49	1.44
23	c	505	CLA	C1B-C2B	2.32	1.48	1.43
23	b	606	CLA	CHC-C1C	2.31	1.43	1.38
29	A	413	LHG	C24-C23	2.31	1.57	1.50
23	c	510	CLA	CMB-C2B	-2.31	1.46	1.50
30	c	517	DGD	C6D-C5D	2.31	1.58	1.51
23	B	601	CLA	CHC-C1C	2.31	1.43	1.38
23	D	402	CLA	C1B-C2B	2.31	1.48	1.43
23	C	511	CLA	MG-ND	2.31	2.10	2.05
23	b	608	CLA	C3B-C4B	2.30	1.49	1.42
24	a	407	PHO	CAC-C3C	-2.30	1.47	1.51
23	c	513	CLA	CMB-C2B	-2.30	1.46	1.50
23	b	610	CLA	O2D-CGD	2.30	1.38	1.33
36	v	201	HEC	CMA-C3A	2.30	1.55	1.50
23	B	608	CLA	MG-NA	2.30	2.11	2.06
23	A	408	CLA	C1B-NB	-2.29	1.34	1.37
23	b	616	CLA	CMB-C2B	-2.29	1.46	1.50
23	c	509	CLA	C4B-NB	2.29	1.40	1.37
23	b	616	CLA	CAC-C3C	-2.29	1.45	1.51
29	D	407	LHG	O8-C6	-2.29	1.40	1.45
23	B	614	CLA	C1A-CHA	-2.29	1.33	1.43
23	B	608	CLA	MG-NC	2.28	2.11	2.06
23	B	615	CLA	CMC-C2C	-2.28	1.46	1.50
35	E	101	HEM	FE-NC	2.28	2.02	1.95
23	D	401	CLA	CHC-C4B	-2.28	1.34	1.39
24	d	401	PHO	C4D-CHA	2.28	1.43	1.39
26	D	405	PL9	C5-C4	-2.28	1.39	1.47
23	a	408	CLA	CHC-C4B	-2.28	1.34	1.39
23	c	504	CLA	CMC-C2C	-2.28	1.46	1.50
23	b	617	CLA	CMB-C2B	-2.28	1.46	1.50
23	b	612	CLA	CMC-C2C	-2.27	1.46	1.50
23	C	511	CLA	CMC-C2C	-2.27	1.46	1.50
23	a	408	CLA	MG-NA	2.27	2.11	2.06
23	C	506	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e	101	LHG	P-O6	2.27	1.68	1.59
23	D	401	CLA	C3B-C4B	2.26	1.49	1.42
30	C	517	DGD	C4E-C3E	2.26	1.58	1.52
26	d	405	PL9	C31-C29	-2.26	1.46	1.51
23	B	601	CLA	CMC-C2C	-2.25	1.46	1.50
23	b	616	CLA	C3B-C4B	2.25	1.49	1.42
30	A	415	DGD	O2G-C1B	2.25	1.40	1.34
23	B	603	CLA	CMA-C3A	-2.25	1.48	1.53
23	B	605	CLA	C3D-C4D	2.25	1.49	1.44
23	B	608	CLA	CMC-C2C	-2.25	1.46	1.50
23	c	509	CLA	C3B-C4B	2.25	1.49	1.42
25	d	404	BCR	C33-C5	-2.25	1.47	1.50
23	C	505	CLA	C1D-ND	2.25	1.40	1.37
29	D	408	LHG	O7-C7	2.25	1.40	1.34
26	a	410	PL9	C52-C5	-2.25	1.46	1.50
23	B	616	CLA	O2D-CGD	2.25	1.38	1.33
23	C	501	CLA	CHC-C1C	2.25	1.43	1.38
23	c	502	CLA	CHC-C1C	2.24	1.43	1.38
23	c	504	CLA	C1B-C2B	2.24	1.48	1.43
23	b	604	CLA	C1A-CHA	-2.24	1.33	1.43
23	c	501	CLA	CMC-C2C	-2.24	1.46	1.50
23	C	508	CLA	MG-NB	2.24	2.10	2.05
23	C	504	CLA	C4B-NB	2.24	1.40	1.37
23	c	503	CLA	C1B-NB	-2.24	1.34	1.37
23	B	604	CLA	O2A-CGA	2.24	1.39	1.33
23	C	508	CLA	CMC-C2C	-2.23	1.46	1.50
23	c	510	CLA	C3B-C4B	2.23	1.49	1.42
23	C	504	CLA	MG-ND	2.23	2.10	2.05
23	c	510	CLA	CHC-C1C	2.23	1.43	1.38
26	d	405	PL9	C16-C14	-2.23	1.46	1.51
23	c	511	CLA	CMB-C2B	-2.23	1.46	1.50
28	F	101	SQD	O2-C2	-2.23	1.37	1.43
23	B	613	CLA	CMB-C2B	-2.23	1.46	1.50
35	E	101	HEM	C2A-C3A	-2.23	1.33	1.38
27	m	101	LMG	O6-C1	2.23	1.47	1.41
23	C	508	CLA	C1D-C2D	2.22	1.49	1.45
23	C	506	CLA	C3B-C4B	2.22	1.49	1.42
23	A	405	CLA	C3D-C4D	2.22	1.49	1.44
28	f	101	SQD	O2-C2	-2.22	1.37	1.43
23	b	617	CLA	C1B-C2B	2.22	1.48	1.43
23	B	611	CLA	CMB-C2B	-2.22	1.46	1.50
23	c	504	CLA	CMD-C2D	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	MG-NB	-2.22	2.01	2.05
23	A	405	CLA	CMD-C2D	-2.22	1.46	1.50
23	C	502	CLA	CMC-C2C	-2.22	1.46	1.50
23	A	404	CLA	C3B-C4B	2.22	1.49	1.42
23	D	402	CLA	CMC-C2C	-2.22	1.46	1.50
23	b	603	CLA	CMD-C2D	-2.22	1.46	1.50
25	C	514	BCR	C36-C18	-2.21	1.46	1.50
23	D	403	CLA	CMB-C2B	-2.21	1.46	1.50
23	b	613	CLA	CHD-C1D	-2.21	1.34	1.38
23	c	504	CLA	CHC-C1C	2.21	1.42	1.38
35	e	102	HEM	CMC-C2C	2.21	1.55	1.50
27	b	623	LMG	O7-C10	2.21	1.38	1.30
23	c	502	CLA	C1B-C2B	2.21	1.48	1.43
35	E	101	HEM	CMC-C2C	2.21	1.55	1.50
30	h	102	DGD	C6D-C5D	2.21	1.58	1.51
23	b	606	CLA	CMB-C2B	-2.21	1.46	1.50
23	c	510	CLA	CMD-C2D	-2.21	1.46	1.50
23	B	616	CLA	CMD-C2D	-2.20	1.46	1.50
23	B	604	CLA	C1B-C2B	2.20	1.48	1.43
23	c	509	CLA	C3C-C2C	2.20	1.41	1.36
23	c	505	CLA	CMB-C2B	-2.20	1.46	1.50
23	C	512	CLA	C1B-C2B	2.20	1.48	1.43
29	d	407	LHG	P-O3	2.20	1.68	1.59
26	D	405	PL9	C53-C6	-2.20	1.46	1.50
23	c	504	CLA	MG-NA	2.20	2.11	2.06
23	b	603	CLA	CHC-C1C	2.20	1.42	1.38
23	B	616	CLA	CMC-C2C	-2.20	1.46	1.50
23	b	609	CLA	C1D-ND	2.20	1.40	1.37
23	b	615	CLA	O2D-CGD	2.20	1.38	1.33
28	a	412	SQD	O2-C2	-2.20	1.37	1.43
30	c	518	DGD	O5D-C1E	2.20	1.43	1.40
23	b	617	CLA	C4B-NB	2.19	1.40	1.37
30	C	515	DGD	C2B-C1B	-2.19	1.44	1.50
23	B	612	CLA	C3D-C4D	2.19	1.49	1.44
23	D	403	CLA	CHC-C4B	-2.19	1.34	1.39
23	b	606	CLA	CMD-C2D	-2.19	1.46	1.50
26	a	410	PL9	C41-C39	2.19	1.55	1.51
23	C	504	CLA	O2D-CGD	2.19	1.38	1.33
23	C	513	CLA	CMB-C2B	-2.19	1.46	1.50
23	b	606	CLA	C3D-C4D	2.19	1.49	1.44
23	a	405	CLA	MG-NA	2.19	2.11	2.06
23	C	504	CLA	MG-NB	-2.19	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	CMD-C2D	-2.19	1.46	1.50
24	d	401	PHO	C3B-C2B	-2.18	1.37	1.40
23	c	511	CLA	C1D-C2D	2.18	1.49	1.45
23	D	401	CLA	MG-NA	2.18	2.11	2.06
23	c	513	CLA	CMD-C2D	-2.18	1.46	1.50
26	d	405	PL9	C16-C17	2.18	1.60	1.53
24	A	406	PHO	C3B-C2B	-2.18	1.37	1.40
30	h	102	DGD	C3G-C2G	2.18	1.57	1.50
23	A	405	CLA	C4B-NB	2.18	1.40	1.37
25	T	101	BCR	C1-C6	-2.18	1.51	1.53
23	C	503	CLA	C1B-NB	-2.18	1.35	1.37
23	c	501	CLA	CMD-C2D	-2.18	1.46	1.50
23	B	610	CLA	MG-NB	2.18	2.10	2.05
23	C	513	CLA	MG-NC	2.18	2.11	2.06
23	c	507	CLA	CHC-C4B	-2.17	1.34	1.39
23	a	408	CLA	C3B-C4B	2.17	1.49	1.42
23	c	502	CLA	O2D-CGD	2.17	1.38	1.33
23	d	402	CLA	CMD-C2D	-2.17	1.46	1.50
23	C	508	CLA	C1D-ND	2.17	1.40	1.37
23	a	406	CLA	C3B-C4B	2.17	1.49	1.42
25	t	101	BCR	C1-C6	-2.17	1.51	1.53
23	c	501	CLA	CMB-C2B	-2.16	1.46	1.50
35	E	101	HEM	CAC-C3C	2.16	1.53	1.47
23	D	403	CLA	C4B-NB	2.16	1.40	1.37
30	C	515	DGD	O2G-C1B	2.16	1.40	1.34
23	C	506	CLA	C4B-NB	2.16	1.40	1.37
23	B	606	CLA	C3B-C4B	2.16	1.49	1.42
23	C	510	CLA	C3D-C4D	2.16	1.49	1.44
29	B	622	LHG	O7-C5	-2.16	1.41	1.46
23	b	606	CLA	C4B-NB	2.16	1.40	1.37
23	A	404	CLA	MG-ND	-2.16	2.01	2.05
23	D	403	CLA	CMC-C2C	-2.16	1.46	1.50
23	b	609	CLA	C3C-C2C	2.16	1.41	1.36
23	b	612	CLA	C4B-NB	2.16	1.40	1.37
23	B	603	CLA	CMB-C2B	-2.16	1.46	1.50
23	b	605	CLA	CMC-C2C	-2.16	1.46	1.50
23	B	615	CLA	MG-NB	-2.16	2.01	2.05
23	D	403	CLA	C3B-C4B	2.15	1.49	1.42
28	F	101	SQD	O3-C3	-2.15	1.37	1.43
27	c	519	LMG	C4-C5	2.15	1.57	1.53
23	b	616	CLA	MG-NC	-2.15	2.01	2.06
23	C	513	CLA	MG-NA	2.15	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CHC-C1C	2.15	1.42	1.38
23	B	606	CLA	C4D-CHA	2.15	1.45	1.38
26	D	405	PL9	C7-C3	-2.14	1.48	1.51
30	A	415	DGD	C3G-C2G	2.14	1.57	1.50
23	C	509	CLA	MG-NC	-2.14	2.01	2.06
23	C	501	CLA	CMB-C2B	-2.14	1.46	1.50
23	C	501	CLA	CMD-C2D	-2.14	1.46	1.50
23	c	510	CLA	C1B-C2B	2.14	1.48	1.43
30	C	517	DGD	O4E-C4E	-2.14	1.37	1.43
23	c	510	CLA	CMC-C2C	-2.14	1.46	1.50
30	A	415	DGD	C6E-C5E	2.14	1.59	1.51
23	b	606	CLA	CHC-C4B	-2.13	1.34	1.39
23	a	406	CLA	C1B-NB	-2.13	1.35	1.37
23	a	411	CLA	C1D-ND	2.13	1.40	1.37
23	C	513	CLA	CMD-C2D	-2.13	1.46	1.50
27	A	411	LMG	O1-C1	2.13	1.43	1.40
30	C	517	DGD	C6D-C5D	2.13	1.58	1.51
23	C	507	CLA	CMC-C2C	-2.13	1.46	1.50
23	C	506	CLA	C3D-C4D	2.13	1.49	1.44
24	A	407	PHO	C3D-CAD	-2.13	1.43	1.47
27	C	518	LMG	O8-C28	2.13	1.39	1.33
23	c	501	CLA	C1B-C2B	2.13	1.48	1.43
23	c	504	CLA	C3B-C4B	2.13	1.48	1.42
23	b	616	CLA	CHC-C1C	2.12	1.42	1.38
23	c	512	CLA	C3B-C4B	2.12	1.48	1.42
23	b	611	CLA	CMB-C2B	-2.12	1.46	1.50
23	B	602	CLA	CHC-C1C	2.12	1.42	1.38
23	B	615	CLA	C5-C3	-2.12	1.46	1.51
23	c	513	CLA	C3B-C4B	2.12	1.48	1.42
23	B	612	CLA	CHC-C1C	2.12	1.42	1.38
23	C	511	CLA	C1D-C2D	2.12	1.49	1.45
23	c	502	CLA	C1B-NB	-2.12	1.35	1.37
23	B	615	CLA	CHC-C4B	-2.12	1.34	1.39
27	c	521	LMG	C4-C5	2.12	1.57	1.53
25	B	619	BCR	C33-C5	-2.11	1.47	1.50
23	d	403	CLA	CMC-C2C	-2.11	1.46	1.50
26	A	410	PL9	C7-C8	-2.11	1.47	1.50
23	B	612	CLA	CMC-C2C	-2.11	1.46	1.50
30	H	102	DGD	C4E-C3E	2.11	1.57	1.52
23	C	501	CLA	C3B-C4B	2.11	1.48	1.42
23	B	614	CLA	C1B-C2B	2.11	1.48	1.43
25	B	617	BCR	C36-C18	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CMD-C2D	-2.10	1.46	1.50
23	d	403	CLA	C1A-CHA	-2.10	1.34	1.43
23	C	506	CLA	MG-NA	2.10	2.11	2.06
23	C	505	CLA	C3B-C4B	2.10	1.48	1.42
23	B	609	CLA	O2D-CGD	2.10	1.38	1.33
23	c	512	CLA	CMC-C2C	-2.10	1.46	1.50
23	h	101	CLA	C3B-C4B	2.10	1.48	1.42
23	C	509	CLA	O2D-CGD	2.10	1.38	1.33
23	B	604	CLA	CHC-C1C	2.10	1.42	1.38
23	C	502	CLA	CMB-C2B	-2.10	1.46	1.50
23	B	616	CLA	C1B-NB	-2.10	1.35	1.37
25	A	409	BCR	C33-C5	-2.10	1.47	1.50
23	c	505	CLA	C1D-ND	2.10	1.40	1.37
23	b	614	CLA	C5-C3	-2.09	1.47	1.51
23	b	607	CLA	C3B-C4B	2.09	1.48	1.42
23	B	610	CLA	CHC-C1C	2.09	1.42	1.38
23	b	617	CLA	CAB-C3B	-2.09	1.41	1.47
23	c	513	CLA	CMC-C2C	-2.09	1.46	1.50
23	B	603	CLA	CAB-C3B	-2.09	1.41	1.47
23	b	614	CLA	CMD-C2D	-2.09	1.46	1.50
30	c	517	DGD	O1G-C1G	-2.09	1.40	1.45
23	B	601	CLA	C3B-C4B	2.09	1.48	1.42
23	B	602	CLA	CMB-C2B	-2.08	1.46	1.50
27	D	406	LMG	C6-C5	2.08	1.58	1.51
23	C	507	CLA	C3B-C4B	2.08	1.48	1.42
23	C	509	CLA	C4B-NB	2.08	1.40	1.37
23	c	503	CLA	CMC-C2C	-2.08	1.46	1.50
23	c	507	CLA	C4B-NB	2.08	1.40	1.37
23	C	510	CLA	MG-NC	2.08	2.11	2.06
23	D	401	CLA	CMD-C2D	-2.08	1.46	1.50
30	a	414	DGD	O2G-C2G	2.08	1.51	1.46
26	D	405	PL9	C3-C4	-2.08	1.46	1.49
28	b	601	SQD	O2-C2	-2.08	1.37	1.43
30	c	518	DGD	O1G-C1G	-2.07	1.40	1.45
23	B	608	CLA	C1B-NB	-2.07	1.35	1.37
24	A	407	PHO	C4D-CHA	2.07	1.42	1.39
26	d	405	PL9	C52-C5	-2.07	1.46	1.50
23	b	616	CLA	C3D-C4D	2.07	1.48	1.44
24	d	401	PHO	CMA-C3A	-2.07	1.49	1.53
23	D	402	CLA	C1A-CHA	-2.06	1.34	1.43
25	T	101	BCR	C27-C26	-2.06	1.47	1.51
30	a	414	DGD	C2B-C1B	2.06	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C1B-NB	-2.06	1.35	1.37
23	B	602	CLA	C1C-C2C	2.06	1.48	1.44
23	b	606	CLA	MG-ND	2.06	2.09	2.05
23	c	508	CLA	CMB-C2B	-2.06	1.46	1.50
24	d	401	PHO	C3D-C4D	2.06	1.44	1.41
23	A	404	CLA	CHC-C1C	2.05	1.42	1.38
23	C	503	CLA	C3D-C4D	2.05	1.48	1.44
23	c	503	CLA	C1D-C2D	2.05	1.49	1.45
23	C	506	CLA	CAC-C3C	-2.05	1.45	1.51
23	B	609	CLA	C3D-C4D	2.05	1.48	1.44
23	b	607	CLA	C4B-NB	2.05	1.40	1.37
23	b	610	CLA	CHC-C1C	2.05	1.42	1.38
29	A	413	LHG	P-O3	2.05	1.67	1.59
23	B	602	CLA	MG-NC	2.05	2.11	2.06
23	h	101	CLA	CHC-C1C	2.05	1.42	1.38
23	B	609	CLA	C2-C3	2.05	1.37	1.33
23	D	402	CLA	C1C-NC	-2.04	1.34	1.37
27	c	521	LMG	O7-C10	2.04	1.40	1.34
23	C	504	CLA	C1D-ND	2.04	1.40	1.37
30	h	102	DGD	C1E-C2E	2.04	1.58	1.52
30	h	102	DGD	C3D-C2D	2.04	1.57	1.52
23	a	408	CLA	CMB-C2B	-2.04	1.46	1.50
23	C	512	CLA	CMB-C2B	-2.04	1.46	1.50
23	D	403	CLA	C1A-CHA	-2.04	1.34	1.43
23	b	605	CLA	C1B-C2B	2.04	1.47	1.43
23	B	602	CLA	C1B-NB	-2.03	1.35	1.37
24	a	407	PHO	C3D-C4D	2.03	1.44	1.41
23	B	607	CLA	CBD-CGD	-2.03	1.46	1.52
27	m	101	LMG	O7-C8	-2.03	1.41	1.46
23	B	608	CLA	C3D-C4D	2.03	1.48	1.44
35	e	102	HEM	C2A-C3A	-2.03	1.33	1.38
27	D	409	LMG	O8-C28	2.03	1.39	1.33
23	c	504	CLA	CAC-C3C	-2.03	1.45	1.51
27	c	519	LMG	C4-C3	2.03	1.57	1.52
23	b	610	CLA	CMC-C2C	-2.03	1.46	1.50
26	D	405	PL9	C11-C12	-2.03	1.47	1.53
24	a	407	PHO	CMC-C2C	-2.03	1.47	1.50
23	B	606	CLA	CMC-C2C	-2.02	1.46	1.50
23	C	508	CLA	CHC-C1C	2.02	1.42	1.38
23	B	601	CLA	MG-NB	-2.02	2.01	2.05
23	a	408	CLA	CMC-C2C	-2.02	1.46	1.50
23	b	617	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	CMC-C2C	-2.02	1.46	1.50
23	A	404	CLA	C4B-NB	2.02	1.40	1.37
23	C	512	CLA	O2D-CED	-2.02	1.40	1.45
23	C	511	CLA	CMB-C2B	-2.02	1.46	1.50
23	d	402	CLA	C3B-C4B	2.02	1.48	1.42
36	v	201	HEC	FE-NB	2.02	2.01	1.94
23	c	502	CLA	C3B-C4B	2.01	1.48	1.42
27	c	523	LMG	O7-C8	-2.01	1.41	1.46
23	D	402	CLA	MG-NA	2.01	2.11	2.06
23	b	609	CLA	C1B-C2B	2.01	1.47	1.43
23	b	613	CLA	CMB-C2B	-2.01	1.46	1.50
25	B	619	BCR	C31-C1	-2.01	1.49	1.53
27	c	521	LMG	C1-C2	2.01	1.58	1.52
29	d	406	LHG	O7-C5	-2.01	1.41	1.46
23	b	613	CLA	O2D-CED	-2.01	1.40	1.45
23	B	614	CLA	C3B-C4B	2.01	1.48	1.42
30	A	415	DGD	C3E-C2E	2.01	1.57	1.52
23	c	506	CLA	CMC-C2C	-2.01	1.46	1.50
25	t	101	BCR	C27-C26	-2.01	1.47	1.51
23	A	405	CLA	CAC-C3C	-2.01	1.46	1.51
23	B	603	CLA	CMD-C2D	-2.00	1.46	1.50
23	C	505	CLA	CHC-C1C	2.00	1.42	1.38
23	b	608	CLA	C1D-C2D	2.00	1.49	1.45
24	A	406	PHO	C3D-C4D	2.00	1.44	1.41

All (1246) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	C4A-NA-C1A	9.80	111.15	106.68
23	C	511	CLA	C4A-NA-C1A	9.77	111.14	106.68
23	d	402	CLA	C4A-NA-C1A	9.76	111.13	106.68
23	C	503	CLA	C4A-NA-C1A	9.64	111.08	106.68
23	a	411	CLA	C4A-NA-C1A	9.54	111.03	106.68
28	A	412	SQD	O6-C1-C2	9.54	122.77	108.27
28	a	412	SQD	O6-C1-C2	8.57	121.29	108.27
23	b	607	CLA	C4A-NA-C1A	8.43	110.52	106.68
23	c	503	CLA	C4A-NA-C1A	8.43	110.52	106.68
23	C	513	CLA	C4A-NA-C1A	7.74	110.21	106.68
26	a	410	PL9	C7-C3-C4	7.71	123.26	116.91
23	B	606	CLA	C4A-NA-C1A	7.63	110.16	106.68
23	c	501	CLA	C4A-NA-C1A	7.45	110.08	106.68
28	b	601	SQD	O6-C1-C2	7.33	119.41	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	412	SQD	O7-S-C6	7.24	117.56	106.76
23	c	511	CLA	C4A-NA-C1A	7.18	109.95	106.68
23	B	607	CLA	C4A-NA-C1A	7.04	109.89	106.68
23	B	604	CLA	C4A-NA-C1A	7.03	109.88	106.68
23	b	615	CLA	C4A-NA-C1A	7.01	109.88	106.68
23	c	509	CLA	C4A-NA-C1A	6.76	109.76	106.68
23	c	508	CLA	C4A-NA-C1A	6.69	109.73	106.68
23	C	501	CLA	C4A-NA-C1A	6.67	109.72	106.68
23	B	613	CLA	C4A-NA-C1A	6.56	109.67	106.68
23	C	507	CLA	C4A-NA-C1A	6.56	109.67	106.68
23	C	510	CLA	C4A-NA-C1A	6.54	109.66	106.68
28	B	624	SQD	O6-C1-C2	6.33	117.88	108.27
23	a	405	CLA	C4A-NA-C1A	6.30	109.56	106.68
23	B	612	CLA	C4A-NA-C1A	6.23	109.52	106.68
23	B	609	CLA	C4A-NA-C1A	6.18	109.50	106.68
23	c	510	CLA	C4A-NA-C1A	6.17	109.49	106.68
23	b	605	CLA	C4A-NA-C1A	6.05	109.44	106.68
26	A	410	PL9	C7-C3-C4	5.97	121.83	116.91
23	c	502	CLA	C4A-NA-C1A	5.91	109.37	106.68
23	C	506	CLA	C4A-NA-C1A	5.88	109.36	106.68
23	c	507	CLA	C4A-NA-C1A	5.83	109.34	106.68
23	c	513	CLA	C4A-NA-C1A	5.78	109.31	106.68
23	B	614	CLA	O2D-CGD-O1D	-5.56	113.03	123.85
23	c	505	CLA	C4A-NA-C1A	5.55	109.21	106.68
24	d	401	PHO	C4D-CHA-CBD	-5.54	105.80	108.45
23	D	401	CLA	C4A-NA-C1A	5.50	109.19	106.68
23	B	608	CLA	C4A-NA-C1A	5.43	109.16	106.68
23	a	408	CLA	C4A-NA-C1A	5.43	109.16	106.68
23	D	402	CLA	C3B-C4B-NB	-5.35	105.75	110.53
23	b	606	CLA	C4A-NA-C1A	5.32	109.11	106.68
23	c	501	CLA	O2D-CGD-O1D	-5.29	113.54	123.85
26	a	410	PL9	C7-C3-C2	-5.29	117.16	123.39
23	B	616	CLA	C4A-NA-C1A	5.28	109.09	106.68
23	C	508	CLA	C4A-NA-C1A	5.28	109.09	106.68
23	b	609	CLA	C3B-C4B-NB	-5.26	105.83	110.53
23	B	602	CLA	C4A-NA-C1A	5.20	109.05	106.68
23	c	504	CLA	C4A-NA-C1A	5.19	109.05	106.68
23	A	404	CLA	C4A-NA-C1A	5.17	109.04	106.68
23	C	502	CLA	C4A-NA-C1A	5.12	109.02	106.68
23	b	616	CLA	C4A-NA-C1A	5.09	109.00	106.68
28	B	624	SQD	O47-C7-C8	5.02	122.34	111.48
23	c	505	CLA	C3B-C4B-NB	-5.00	106.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F	101	SQD	O6-C1-C2	4.96	115.81	108.27
23	c	512	CLA	C4A-NA-C1A	4.95	108.94	106.68
28	A	412	SQD	O9-S-O7	-4.95	97.73	113.82
23	a	406	CLA	C4A-NA-C1A	4.94	108.93	106.68
28	f	101	SQD	O9-S-C6	4.93	114.11	106.76
27	b	622	LMG	O1-C1-C2	-4.91	100.81	108.27
30	H	102	DGD	O3G-C3G-C2G	-4.91	98.87	110.82
23	B	601	CLA	O2D-CGD-O1D	-4.91	114.29	123.85
23	h	101	CLA	O2D-CGD-O1D	-4.87	114.37	123.85
28	a	413	SQD	O47-C7-C8	4.86	121.99	111.48
23	b	614	CLA	C4A-NA-C1A	4.82	108.88	106.68
28	f	101	SQD	O6-C1-C2	4.81	115.58	108.27
28	F	101	SQD	O8-S-C6	4.75	115.14	105.97
30	a	414	DGD	C2G-O2G-C1B	4.65	128.92	117.80
24	a	407	PHO	C4D-CHA-CBD	-4.63	106.23	108.45
23	a	406	CLA	O2D-CGD-CBD	4.59	119.25	111.23
28	A	414	SQD	C45-O47-C7	4.58	124.39	117.78
24	d	401	PHO	O1D-CGD-CBD	4.57	131.65	124.72
23	b	605	CLA	C3B-C4B-NB	-4.57	106.45	110.53
23	b	604	CLA	O2D-CGD-O1D	-4.54	115.02	123.85
30	C	516	DGD	O3G-C3G-C2G	-4.53	99.80	110.82
23	C	503	CLA	C7-C6-C5	-4.51	101.23	113.26
23	b	603	CLA	O2D-CGD-CBD	4.49	119.09	111.23
23	b	608	CLA	C4A-NA-C1A	4.48	108.72	106.68
29	e	101	LHG	O4-P-O5	4.47	133.23	112.44
27	m	101	LMG	O7-C10-O9	-4.45	113.30	123.70
29	B	623	LHG	O4-P-O5	4.43	133.06	112.44
23	b	613	CLA	C4A-NA-C1A	4.40	108.69	106.68
23	B	610	CLA	CHB-C4A-NA	4.38	130.72	124.40
24	A	406	PHO	C4D-CHA-CBD	-4.38	106.36	108.45
23	c	501	CLA	O2D-CGD-CBD	4.35	118.84	111.23
29	d	406	LHG	O4-P-O5	4.35	132.67	112.44
28	b	601	SQD	O5-C5-C4	4.35	117.53	109.70
29	D	408	LHG	O4-P-O5	4.33	132.61	112.44
23	c	510	CLA	O2D-CGD-O1D	-4.33	115.41	123.85
23	B	610	CLA	C4A-NA-C1A	4.32	108.65	106.68
29	d	407	LHG	O4-P-O5	4.31	132.48	112.44
33	A	418	BCT	O2-C-O1	4.31	130.69	119.68
24	A	407	PHO	C4D-CHA-CBD	-4.30	106.39	108.45
23	b	611	CLA	O2D-CGD-O1D	-4.28	115.52	123.85
28	B	624	SQD	O7-S-C6	4.27	113.14	106.76
29	l	101	LHG	O4-P-O5	4.22	132.09	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	C3B-C4B-NB	-4.21	106.77	110.53
26	d	405	PL9	C7-C3-C4	4.21	120.38	116.91
30	h	102	DGD	O6E-C5E-C4E	4.20	117.26	109.70
23	B	610	CLA	O2D-CGD-O1D	-4.19	115.70	123.85
23	b	617	CLA	O2D-CGD-O1D	-4.17	115.73	123.85
26	A	410	PL9	C7-C3-C2	-4.17	118.47	123.39
23	c	512	CLA	C1-C2-C3	-4.17	119.37	126.20
25	b	618	BCR	C2-C1-C6	4.16	116.49	110.44
23	C	509	CLA	C4A-NA-C1A	4.15	108.57	106.68
23	c	503	CLA	C3B-C4B-NB	-4.14	106.84	110.53
29	A	413	LHG	O4-P-O5	4.10	131.54	112.44
23	a	411	CLA	C3B-C4B-NB	-4.10	106.87	110.53
29	d	408	LHG	O4-P-O5	4.10	131.50	112.44
23	B	615	CLA	C4A-NA-C1A	4.10	108.55	106.68
23	b	603	CLA	C4A-NA-C1A	4.09	108.55	106.68
35	e	102	HEM	CBD-CAD-C3D	-4.09	101.21	112.53
23	B	611	CLA	O2D-CGD-O1D	-4.07	115.93	123.85
28	A	412	SQD	C1-C2-C3	-4.05	101.48	110.01
23	c	506	CLA	C4A-NA-C1A	4.04	108.52	106.68
29	e	101	LHG	O8-C23-C24	4.03	124.11	111.83
23	C	512	CLA	C3B-C4B-NB	-4.02	106.94	110.53
29	D	407	LHG	O4-P-O5	4.01	131.12	112.44
24	A	406	PHO	CMA-C3A-C4A	-4.01	105.97	114.61
23	B	601	CLA	O1D-CGD-CBD	4.01	132.42	124.52
23	b	603	CLA	CHB-C4A-NA	4.00	130.17	124.40
27	b	622	LMG	C1-O6-C5	-4.00	105.91	113.72
23	b	607	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
26	D	405	PL9	C37-C38-C39	-3.98	118.50	127.62
23	B	603	CLA	O2D-CGD-O1D	-3.98	116.09	123.85
23	a	406	CLA	CHB-C4A-NA	3.97	130.13	124.40
30	H	102	DGD	C1D-O6D-C5D	-3.97	105.97	113.72
25	H	101	BCR	C29-C30-C25	3.97	116.20	110.44
23	C	509	CLA	CHB-C4A-NA	3.96	130.11	124.40
23	B	605	CLA	C3B-C4B-NB	-3.96	107.00	110.53
24	d	401	PHO	C2B-C1B-NB	-3.96	106.57	109.43
28	a	412	SQD	O9-S-O7	-3.95	100.98	113.82
25	B	617	BCR	C29-C30-C25	3.94	116.16	110.44
30	C	517	DGD	O3G-C3G-C2G	-3.94	101.24	110.82
25	K	101	BCR	C39-C30-C25	-3.91	104.11	110.24
23	B	611	CLA	O2D-CGD-CBD	3.90	118.06	111.23
23	a	406	CLA	O2D-CGD-O1D	-3.86	116.34	123.85
29	B	623	LHG	O8-C23-O10	-3.86	113.98	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C3B-C4B-NB	-3.85	107.09	110.53
30	C	515	DGD	C3D-C4D-C5D	-3.83	103.29	110.23
23	b	617	CLA	C4A-NA-C1A	3.81	108.42	106.68
23	B	606	CLA	CHD-C4C-NC	3.80	130.12	124.23
23	B	602	CLA	O2D-CGD-CBD	3.80	117.87	111.23
23	B	614	CLA	CAC-C3C-C4C	3.79	129.72	124.79
28	a	412	SQD	C1-C2-C3	-3.79	102.04	110.01
30	A	415	DGD	C3G-C2G-C1G	-3.78	102.97	111.78
26	d	405	PL9	C45-C44-C46	-3.78	108.67	115.23
23	h	101	CLA	O2D-CGD-CBD	3.76	117.81	111.23
30	h	102	DGD	O2D-C2D-C1D	-3.76	101.12	110.08
28	a	412	SQD	O9-S-C6	3.71	112.30	106.76
28	A	412	SQD	O47-C7-C8	3.70	119.49	111.48
23	b	617	CLA	C3B-C4B-NB	-3.70	107.23	110.53
23	A	405	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
23	a	406	CLA	C3B-C4B-NB	-3.69	107.23	110.53
26	D	405	PL9	C7-C3-C4	3.68	119.94	116.91
23	D	401	CLA	C3B-C4B-NB	-3.67	107.25	110.53
33	a	404	BCT	O2-C-O1	3.67	129.05	119.68
30	c	518	DGD	O3G-C3G-C2G	-3.66	101.91	110.82
23	a	405	CLA	CAC-C3C-C4C	3.65	129.54	124.79
23	b	603	CLA	O2D-CGD-O1D	-3.65	116.75	123.85
23	C	513	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
29	A	413	LHG	O8-C23-C24	3.63	122.91	111.83
23	C	508	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
26	A	410	PL9	C40-C39-C41	3.63	121.52	115.23
30	c	516	DGD	O3G-C3G-C2G	-3.61	102.04	110.82
25	k	101	BCR	C33-C5-C6	-3.60	120.56	124.48
25	H	101	BCR	C27-C26-C25	3.60	127.56	122.70
28	F	101	SQD	O9-S-C6	3.59	112.11	106.76
23	b	604	CLA	C3B-C4B-NB	-3.58	107.33	110.53
23	b	609	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
23	A	404	CLA	C3B-C4B-NB	-3.56	107.35	110.53
23	B	610	CLA	O1D-CGD-CBD	3.56	131.53	124.52
30	A	415	DGD	O5D-C1E-C2E	3.54	113.64	108.27
28	A	412	SQD	O47-C7-O49	-3.53	115.44	123.70
25	A	409	BCR	C2-C1-C6	3.53	115.56	110.44
28	f	101	SQD	O9-S-O7	-3.53	102.35	113.82
23	c	511	CLA	C3B-C4B-NB	-3.52	107.39	110.53
23	C	507	CLA	C3B-C4B-NB	-3.52	107.39	110.53
23	B	606	CLA	C3B-C4B-NB	-3.52	107.39	110.53
28	b	601	SQD	C3-C4-C5	3.51	116.60	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	411	CLA	CHB-C4A-NA	3.50	129.46	124.40
25	D	404	BCR	C2-C1-C6	3.50	115.53	110.44
23	B	610	CLA	O2A-CGA-O1A	-3.50	114.88	123.63
30	C	517	DGD	O3E-C3E-C2E	-3.49	102.15	110.38
26	d	405	PL9	C22-C23-C24	-3.48	119.66	127.62
26	d	405	PL9	C35-C34-C36	3.48	121.27	115.23
24	a	407	PHO	C1-C2-C3	-3.47	120.51	126.20
23	C	504	CLA	C4A-NA-C1A	3.47	108.26	106.68
23	B	605	CLA	C16-C15-C13	-3.47	104.44	115.97
25	c	515	BCR	C36-C18-C17	-3.47	117.20	122.82
23	b	612	CLA	CHD-C1D-ND	-3.46	119.93	124.80
23	a	406	CLA	CED-O2D-CGD	-3.44	108.11	115.92
36	v	201	HEC	CHB-C1B-NB	3.44	128.12	124.42
28	B	624	SQD	O9-S-O7	-3.44	102.65	113.82
25	c	515	BCR	C33-C5-C6	-3.42	120.75	124.48
25	T	101	BCR	C15-C14-C13	-3.42	122.47	127.28
23	B	612	CLA	C3B-C4B-NB	-3.40	107.49	110.53
25	T	101	BCR	C2-C1-C6	3.40	115.38	110.44
23	c	509	CLA	C3B-C4B-NB	-3.39	107.50	110.53
23	C	503	CLA	C4D-CHA-C1A	3.39	125.29	121.24
28	b	601	SQD	C45-O47-C7	3.39	125.90	117.80
24	A	406	PHO	O2D-CGD-CBD	3.39	114.67	110.95
35	E	101	HEM	CBD-CAD-C3D	-3.39	103.17	112.53
27	c	523	LMG	C1-O6-C5	-3.39	107.11	113.72
23	d	403	CLA	C4A-NA-C1A	3.38	108.22	106.68
23	A	404	CLA	CHB-C4A-NA	3.38	129.28	124.40
23	A	408	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
29	D	408	LHG	O8-C23-O10	-3.38	115.18	123.63
23	B	602	CLA	CHB-C4A-NA	3.37	129.27	124.40
23	B	601	CLA	CAA-C2A-C3A	-3.37	103.90	113.00
28	a	413	SQD	O48-C23-O10	-3.37	115.21	123.63
23	b	612	CLA	C4A-NA-C1A	3.36	108.21	106.68
23	c	512	CLA	CHB-C4A-NA	3.35	129.24	124.40
23	c	512	CLA	C3B-C4B-NB	-3.35	107.54	110.53
23	B	605	CLA	C4-C3-C5	3.34	121.03	115.23
23	B	616	CLA	C1-O2A-CGA	3.34	124.73	116.65
25	C	514	BCR	C15-C14-C13	-3.34	122.60	127.28
23	c	509	CLA	O2A-CGA-O1A	-3.34	115.28	123.63
28	b	601	SQD	O7-S-C6	3.33	111.73	106.76
23	C	501	CLA	O2A-CGA-O1A	-3.33	115.30	123.63
30	A	415	DGD	O3G-C3G-C2G	-3.33	102.72	110.82
25	D	404	BCR	C38-C26-C25	-3.33	120.85	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	414	DGD	O1G-C1A-O1A	-3.32	115.32	123.63
23	b	611	CLA	C4A-NA-C1A	3.31	108.19	106.68
25	a	409	BCR	C35-C13-C14	-3.30	117.47	122.82
25	B	619	BCR	C29-C30-C25	3.30	115.23	110.44
23	b	610	CLA	C3B-C4B-NB	-3.30	107.59	110.53
29	B	622	LHG	O4-P-O5	3.29	127.77	112.44
23	B	615	CLA	C6-C7-C8	-3.29	105.04	115.97
25	B	619	BCR	C33-C5-C6	-3.29	120.90	124.48
24	d	401	PHO	CBC-CAC-C3C	3.28	117.57	112.87
30	c	518	DGD	C3G-C2G-C1G	-3.28	104.13	111.78
29	B	623	LHG	O8-C23-C24	3.28	121.82	111.83
25	T	101	BCR	C27-C26-C25	3.27	127.12	122.70
23	A	405	CLA	C3B-C4B-NB	-3.27	107.61	110.53
25	b	618	BCR	C11-C10-C9	-3.27	122.70	127.28
27	A	411	LMG	C38-C37-C36	-3.26	97.87	114.37
23	b	603	CLA	C3B-C4B-NB	-3.26	107.62	110.53
23	A	408	CLA	O2D-CGD-CBD	3.26	116.92	111.23
26	a	410	PL9	C22-C23-C24	-3.26	120.17	127.62
23	B	615	CLA	CHC-C4B-NB	3.25	128.93	124.05
23	c	508	CLA	CHB-C4A-NA	3.25	129.09	124.40
23	C	503	CLA	C3B-C4B-NB	-3.25	107.63	110.53
23	C	510	CLA	C7-C6-C5	-3.23	104.64	113.26
23	B	603	CLA	C3B-C4B-NB	-3.23	107.65	110.53
24	A	407	PHO	C1-C2-C3	-3.23	120.91	126.20
25	Z	101	BCR	C11-C10-C9	-3.23	122.75	127.28
24	d	401	PHO	CMC-C2C-C1C	-3.22	118.94	124.73
23	c	504	CLA	O2D-CGD-CBD	3.22	116.86	111.23
23	b	613	CLA	O1D-CGD-CBD	3.21	130.85	124.52
23	C	501	CLA	C3B-C4B-NB	-3.21	107.67	110.53
23	C	510	CLA	C3B-C4B-NB	-3.21	107.67	110.53
26	d	405	PL9	C50-C49-C48	-3.21	113.03	122.66
25	t	101	BCR	C15-C16-C17	-3.20	116.96	123.52
23	b	612	CLA	CHD-C1D-C2D	3.20	132.15	125.49
23	c	510	CLA	C3B-C4B-NB	-3.20	107.68	110.53
23	C	501	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
30	h	102	DGD	O3G-C3G-C2G	-3.19	103.06	110.82
23	c	502	CLA	C3B-C4B-NB	-3.19	107.68	110.53
23	B	614	CLA	C1-C2-C3	-3.19	120.97	126.20
23	b	609	CLA	O2D-CGD-CBD	3.18	116.78	111.23
30	A	415	DGD	C1D-C2D-C3D	-3.18	103.33	110.01
23	C	501	CLA	O2D-CGD-CBD	3.17	116.77	111.23
30	c	517	DGD	O3G-C1D-C2D	-3.17	103.46	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	521	LMG	C9-C8-C7	-3.17	104.39	111.78
30	C	516	DGD	O6D-C1D-O3G	-3.16	102.57	110.04
26	d	405	PL9	C37-C38-C39	-3.16	120.39	127.62
27	d	409	LMG	O2-C2-C1	-3.16	102.55	110.08
25	c	514	BCR	C27-C26-C25	3.16	126.97	122.70
23	B	602	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
30	c	517	DGD	O3G-C3G-C2G	-3.15	103.14	110.82
25	b	619	BCR	C30-C25-C26	-3.15	118.33	122.64
23	b	604	CLA	C4-C3-C5	3.15	120.70	115.23
35	e	102	HEM	CBA-CAA-C2A	-3.15	103.81	112.53
28	a	412	SQD	O47-C7-C8	3.15	118.30	111.48
30	H	102	DGD	C1D-C2D-C3D	-3.15	103.38	110.01
23	C	503	CLA	C1D-ND-C4D	3.15	108.52	106.31
30	C	517	DGD	CDB-CCB-CBB	-3.15	98.46	114.37
23	A	405	CLA	O2D-CGD-CBD	3.15	116.73	111.23
30	A	415	DGD	C4E-C3E-C2E	-3.14	105.31	110.83
23	b	604	CLA	C4A-NA-C1A	3.14	108.11	106.68
23	b	615	CLA	CHD-C1D-ND	-3.13	120.39	124.80
23	a	405	CLA	C3B-C4B-NB	-3.12	107.74	110.53
23	c	507	CLA	CHB-C4A-NA	3.12	128.91	124.40
23	B	607	CLA	C1C-C2C-C3C	-3.12	103.70	106.98
27	c	521	LMG	O3-C3-C2	-3.12	103.02	110.38
23	B	612	CLA	CHB-C4A-NA	3.12	128.90	124.40
23	b	611	CLA	O1D-CGD-CBD	3.12	130.66	124.52
25	x	101	BCR	C30-C25-C26	-3.12	118.38	122.64
27	c	521	LMG	O6-C1-O1	-3.11	102.70	110.04
26	D	405	PL9	C22-C23-C24	-3.10	120.52	127.62
23	C	511	CLA	CAC-C3C-C4C	3.10	128.83	124.79
35	E	101	HEM	CHC-C4B-NB	3.10	127.76	124.42
23	a	405	CLA	O1D-CGD-CBD	3.09	130.62	124.52
23	D	403	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
26	A	410	PL9	C36-C34-C33	-3.09	114.23	121.17
23	c	512	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
25	k	101	BCR	C27-C26-C25	3.09	126.88	122.70
23	b	609	CLA	O2A-CGA-O1A	-3.09	115.90	123.63
23	b	604	CLA	O2D-CGD-CBD	3.09	116.63	111.23
23	C	507	CLA	CHB-C4A-NA	3.08	128.85	124.40
30	c	518	DGD	O6D-C1D-O3G	-3.08	102.76	110.04
30	h	102	DGD	O5E-C6E-C5E	-3.08	100.84	111.33
23	c	506	CLA	CGD-CBD-CAD	-3.08	100.87	110.85
23	c	508	CLA	C3B-C4B-NB	-3.08	107.78	110.53
23	A	408	CLA	CHB-C4A-NA	3.08	128.84	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	e	102	HEM	CHB-C1B-NB	3.08	128.18	124.37
24	A	406	PHO	CMB-C2B-C3B	3.08	130.83	124.68
25	H	101	BCR	C38-C26-C25	-3.08	121.13	124.48
23	D	402	CLA	CHB-C4A-NA	3.07	128.84	124.40
23	B	604	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
23	C	512	CLA	CHB-C4A-NA	3.07	128.82	124.40
30	c	517	DGD	C8B-C7B-C6B	-3.06	98.90	114.37
28	A	412	SQD	O2-C2-C1	3.06	117.37	110.08
23	C	506	CLA	CHB-C4A-NA	3.06	128.81	124.40
26	d	405	PL9	C40-C39-C41	3.05	120.53	115.23
23	b	615	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
25	b	618	BCR	C33-C5-C6	-3.05	121.15	124.48
23	B	603	CLA	CHD-C4C-NC	3.05	128.96	124.23
23	c	510	CLA	CHB-C4A-NA	3.05	128.80	124.40
29	d	407	LHG	O8-C23-C24	3.05	121.13	111.83
23	d	402	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
25	C	514	BCR	C15-C16-C17	-3.05	117.28	123.52
27	D	406	LMG	O6-C1-O1	-3.05	102.84	110.04
25	A	409	BCR	C11-C10-C9	-3.04	123.02	127.28
29	D	408	LHG	O8-C23-C24	3.04	121.10	111.83
28	b	601	SQD	O2-C2-C1	3.04	117.31	110.08
23	B	615	CLA	CHB-C4A-NA	3.03	128.78	124.40
24	A	406	PHO	O2D-CGD-O1D	-3.03	117.94	123.85
23	B	614	CLA	O1D-CGD-CBD	3.03	130.49	124.52
23	a	411	CLA	C1D-ND-C4D	3.03	108.44	106.31
24	A	407	PHO	O2D-CGD-O1D	-3.03	117.96	123.85
28	B	624	SQD	O8-S-C6	3.02	111.81	105.97
27	M	101	LMG	O1-C1-C2	-3.01	103.70	108.27
30	C	516	DGD	O3E-C3E-C2E	-3.01	103.27	110.38
30	c	517	DGD	O2D-C2D-C1D	-3.01	102.90	110.08
23	C	502	CLA	C3B-C4B-NB	-3.01	107.84	110.53
23	B	614	CLA	O2D-CGD-CBD	3.00	116.48	111.23
25	K	102	BCR	C29-C30-C25	2.99	114.79	110.44
36	V	201	HEC	C3D-C4D-ND	-2.99	107.46	110.35
23	B	606	CLA	CGD-CBD-CAD	-2.99	101.17	110.85
23	b	605	CLA	CHB-C4A-NA	2.99	128.71	124.40
23	B	606	CLA	CHD-C1D-ND	-2.99	120.60	124.80
23	b	609	CLA	CHB-C1B-NB	2.98	128.52	124.05
23	c	504	CLA	C3B-C4B-NB	-2.98	107.87	110.53
23	c	508	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
23	A	405	CLA	O2A-CGA-O1A	-2.98	116.18	123.63
23	B	602	CLA	CHA-C1A-NA	-2.98	119.65	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	CHD-C4C-C3C	-2.97	120.44	124.77
23	h	101	CLA	C3B-C4B-NB	-2.97	107.88	110.53
23	B	608	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
23	B	614	CLA	O2A-CGA-O1A	-2.97	116.20	123.63
25	C	514	BCR	C29-C30-C25	2.97	114.75	110.44
28	b	601	SQD	O8-S-C6	2.97	111.70	105.97
25	b	620	BCR	C29-C30-C25	2.96	114.75	110.44
23	D	402	CLA	C4A-NA-C1A	2.96	108.03	106.68
23	b	606	CLA	C4D-CHA-C1A	2.96	124.78	121.24
35	e	102	HEM	C3B-C2B-C1B	2.96	108.64	106.41
23	b	612	CLA	O2D-CGD-CBD	2.96	116.41	111.23
25	k	102	BCR	C27-C26-C25	2.96	126.70	122.70
26	d	405	PL9	C7-C3-C2	-2.95	119.91	123.39
23	B	603	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
25	Z	101	BCR	C33-C5-C6	-2.95	121.27	124.48
23	A	408	CLA	CHD-C1D-ND	-2.95	120.66	124.80
23	b	613	CLA	C1-C2-C3	-2.94	121.38	126.20
23	C	512	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
23	c	507	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
23	c	503	CLA	CAC-C3C-C4C	2.94	128.61	124.79
25	x	101	BCR	C27-C26-C25	2.94	126.67	122.70
23	b	607	CLA	C6-C5-C3	2.93	120.61	113.47
25	T	101	BCR	C35-C13-C14	-2.93	118.07	122.82
23	C	502	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
25	c	515	BCR	C27-C26-C25	2.93	126.66	122.70
25	b	619	BCR	C15-C14-C13	-2.92	123.18	127.28
23	B	612	CLA	C11-C12-C13	-2.92	106.26	115.97
25	B	619	BCR	C38-C26-C25	-2.92	121.30	124.48
23	c	508	CLA	O2A-CGA-O1A	-2.92	116.33	123.63
28	B	624	SQD	C1-C2-C3	-2.92	103.88	110.01
25	B	618	BCR	C3-C4-C5	-2.91	108.86	114.06
23	b	611	CLA	O2A-CGA-O1A	-2.91	116.35	123.63
23	C	511	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
23	c	513	CLA	CHB-C4A-NA	2.91	128.60	124.40
23	C	507	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
23	d	403	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	B	618	BCR	C15-C14-C13	-2.90	123.20	127.28
23	C	509	CLA	C3B-C4B-NB	-2.90	107.94	110.53
27	D	406	LMG	O3-C3-C2	-2.90	103.54	110.38
28	a	412	SQD	C1-O5-C5	-2.90	108.06	113.72
25	K	101	BCR	C27-C26-C25	2.89	126.61	122.70
25	B	618	BCR	C27-C26-C25	2.89	126.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	410	PL9	C12-C13-C14	-2.88	121.02	127.62
23	c	509	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
30	C	517	DGD	O6D-C1D-O3G	-2.88	103.23	110.04
25	t	101	BCR	C35-C13-C14	-2.88	118.15	122.82
23	a	405	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
23	B	609	CLA	C7-C6-C5	-2.88	105.59	113.26
23	C	508	CLA	CHD-C1D-ND	-2.88	120.76	124.80
28	B	624	SQD	C1-O5-C5	-2.87	108.11	113.72
27	M	101	LMG	O7-C10-O9	-2.87	116.99	123.70
25	Z	101	BCR	C27-C26-C25	2.87	126.58	122.70
25	K	101	BCR	C33-C5-C6	-2.87	121.35	124.48
25	t	101	BCR	C36-C18-C19	2.87	122.47	118.09
28	B	624	SQD	C3-C4-C5	2.86	115.43	110.23
23	b	604	CLA	O2A-CGA-O1A	-2.86	116.46	123.63
23	c	504	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
28	B	624	SQD	O48-C23-C24	2.86	120.55	111.83
28	F	101	SQD	O9-S-O7	-2.86	104.53	113.82
23	C	504	CLA	C3B-C4B-NB	-2.85	107.98	110.53
30	C	515	DGD	O1G-C1A-C2A	-2.85	103.15	111.83
26	A	410	PL9	C22-C23-C24	-2.84	121.11	127.62
28	b	601	SQD	C1-C2-C3	-2.84	104.03	110.01
23	C	510	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
23	a	408	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
25	B	617	BCR	C34-C9-C10	-2.84	118.22	122.82
36	V	201	HEC	CHB-C4A-NA	2.84	127.54	124.45
23	C	512	CLA	CMB-C2B-C3B	2.84	133.22	126.55
23	d	403	CLA	CHD-C1D-ND	-2.84	120.81	124.80
29	d	408	LHG	O8-C23-O10	-2.84	116.53	123.63
23	c	504	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
26	A	410	PL9	O2-C1-C2	-2.83	115.38	121.83
28	A	412	SQD	O5-C1-C2	-2.83	104.55	110.37
23	D	402	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	t	101	BCR	C35-C13-C12	2.83	122.41	118.09
23	C	507	CLA	CHD-C1D-ND	-2.82	120.83	124.80
30	h	102	DGD	C1E-O6E-C5E	2.82	119.23	113.72
29	d	406	LHG	O8-C23-C24	2.81	120.41	111.83
29	e	101	LHG	O8-C23-O10	-2.81	116.61	123.63
25	t	101	BCR	C27-C26-C25	2.81	126.50	122.70
23	h	101	CLA	CBA-CAA-C2A	2.81	122.14	113.79
23	h	101	CLA	C4A-NA-C1A	2.81	107.96	106.68
30	C	515	DGD	O2D-C2D-C1D	-2.80	103.41	110.08
23	B	611	CLA	CHD-C1D-ND	-2.80	120.86	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	d	402	CLA	C1-C2-C3	-2.80	121.62	126.20
23	b	605	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
23	b	605	CLA	CHC-C1C-NC	2.79	128.51	124.31
28	a	413	SQD	O49-C7-C8	-2.79	112.86	123.78
29	d	406	LHG	O8-C6-C5	-2.79	100.35	108.40
23	b	606	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	b	604	CLA	CMB-C2B-C1B	-2.79	121.18	125.42
23	B	616	CLA	C2C-C1C-NC	2.78	112.90	109.98
29	D	407	LHG	O8-C23-C24	2.78	120.31	111.83
25	T	101	BCR	C38-C26-C27	-2.78	107.67	113.60
28	b	601	SQD	O48-C23-C24	2.78	120.31	111.83
28	a	412	SQD	O7-S-C6	2.78	110.90	106.76
28	B	624	SQD	C45-O47-C7	2.78	124.44	117.80
30	C	515	DGD	O3G-C1D-C2D	-2.77	104.06	108.27
25	d	404	BCR	C38-C26-C25	-2.77	121.46	124.48
25	B	618	BCR	C40-C30-C25	2.77	114.59	110.24
23	c	513	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	c	502	CLA	CHB-C1B-NB	2.77	128.20	124.05
23	A	404	CLA	CAA-CBA-CGA	-2.77	105.35	113.21
29	D	407	LHG	O8-C23-O10	-2.76	116.72	123.63
25	K	102	BCR	C2-C1-C6	2.76	114.45	110.44
25	c	515	BCR	C2-C1-C6	2.76	114.45	110.44
26	D	405	PL9	C12-C13-C14	-2.76	121.30	127.62
28	f	101	SQD	C45-O47-C7	2.76	124.40	117.80
23	b	614	CLA	C7-C6-C5	-2.76	105.92	113.26
23	b	609	CLA	CHA-C1A-NA	-2.75	120.15	126.39
27	C	518	LMG	O1-C1-C2	-2.75	104.09	108.27
29	d	406	LHG	C11-C10-C9	-2.75	100.45	114.37
23	B	606	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
25	d	404	BCR	C27-C26-C25	2.75	126.42	122.70
23	B	601	CLA	CAA-CBA-CGA	-2.74	105.42	113.21
23	a	411	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
23	B	603	CLA	CHB-C4A-NA	2.74	128.36	124.40
27	m	101	LMG	C9-C8-C7	-2.74	105.41	111.78
25	a	409	BCR	C27-C26-C25	2.73	126.40	122.70
25	T	101	BCR	C15-C16-C17	-2.73	117.93	123.52
23	b	609	CLA	CMA-C3A-C4A	-2.73	104.43	111.77
28	a	412	SQD	O48-C23-C24	2.73	120.16	111.83
27	d	409	LMG	O6-C1-O1	-2.73	103.60	110.04
25	K	101	BCR	C23-C24-C25	-2.73	119.72	127.00
23	a	408	CLA	O2D-CGD-CBD	2.72	115.98	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	414	DGD	O3G-C3G-C2G	-2.72	104.79	111.77
23	B	616	CLA	CHC-C4B-NB	2.72	128.12	124.05
23	C	503	CLA	C6-C5-C3	2.72	120.09	113.47
23	A	404	CLA	C7-C6-C5	-2.71	106.04	113.26
26	a	410	PL9	C35-C34-C36	2.71	119.93	115.23
23	b	617	CLA	CHB-C4A-NA	2.71	128.31	124.40
23	A	408	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
30	C	517	DGD	C3G-C2G-C1G	-2.70	105.48	111.78
23	b	605	CLA	C1-C2-C3	-2.70	121.77	126.20
24	A	406	PHO	C1-O2A-CGA	2.70	123.19	116.65
23	c	501	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
27	m	101	LMG	O1-C7-C8	-2.69	104.27	110.82
25	K	101	BCR	C15-C16-C17	-2.69	118.01	123.52
23	C	512	CLA	C4A-NA-C1A	2.69	107.91	106.68
23	B	614	CLA	CHB-C4A-NA	2.69	128.28	124.40
27	D	406	LMG	O7-C10-O9	-2.69	117.42	123.70
27	D	406	LMG	O8-C28-O10	-2.68	116.91	123.63
28	A	412	SQD	O48-C23-O10	-2.68	116.91	123.63
27	A	411	LMG	C40-C39-C38	-2.68	100.80	114.37
27	c	519	LMG	C40-C39-C38	-2.68	100.81	114.37
23	B	616	CLA	C5-C3-C2	2.68	127.18	121.17
25	D	404	BCR	C27-C26-C25	2.67	126.32	122.70
30	c	516	DGD	O3G-C1D-C2D	-2.67	104.21	108.27
23	D	401	CLA	CHB-C4A-NA	2.67	128.26	124.40
23	b	613	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
24	A	407	PHO	O1D-CGD-CBD	2.67	128.78	124.72
25	K	101	BCR	C40-C30-C25	2.67	114.42	110.24
26	d	405	PL9	C20-C19-C21	2.66	119.85	115.23
23	b	604	CLA	C6-C5-C3	2.66	119.96	113.47
23	d	402	CLA	C6-C5-C3	2.66	119.95	113.47
23	b	612	CLA	CHD-C4C-NC	2.66	128.36	124.23
29	d	407	LHG	O7-C7-C8	-2.66	105.72	111.48
27	m	101	LMG	O1-C1-C2	-2.66	104.23	108.27
23	c	501	CLA	CED-O2D-CGD	-2.66	109.88	115.92
27	C	518	LMG	O1-C7-C8	-2.66	104.36	110.82
23	c	509	CLA	CHB-C4A-NA	2.65	128.23	124.40
23	c	505	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
25	Z	101	BCR	C34-C9-C10	-2.65	118.52	122.82
23	C	504	CLA	CHD-C1D-ND	-2.65	121.07	124.80
23	b	616	CLA	CHB-C1B-NB	2.65	128.03	124.05
35	e	102	HEM	CHD-C1D-ND	2.65	127.27	124.42
25	b	620	BCR	C37-C22-C21	-2.65	118.52	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	C4-C3-C5	-2.65	110.63	115.23
30	c	516	DGD	CDB-CCB-CBB	-2.65	100.98	114.37
23	c	506	CLA	CBC-CAC-C3C	-2.65	105.24	112.42
23	B	602	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
28	f	101	SQD	O5-C5-C4	2.65	114.47	109.70
23	b	605	CLA	O2A-CGA-O1A	-2.64	117.01	123.63
23	c	506	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
23	C	501	CLA	CHB-C1B-NB	2.64	128.01	124.05
23	c	511	CLA	CHB-C1B-NB	2.64	128.01	124.05
23	B	602	CLA	C2A-C1A-CHA	2.64	128.45	123.87
30	A	415	DGD	O3G-C1D-C2D	-2.64	104.27	108.27
23	C	513	CLA	O2D-CGD-CBD	2.64	115.84	111.23
30	C	516	DGD	C1D-C2D-C3D	-2.64	104.47	110.01
23	A	405	CLA	CHC-C4B-NB	2.64	128.00	124.05
26	A	410	PL9	O2-C1-C6	2.63	124.67	120.48
25	C	514	BCR	C2-C1-C6	2.63	114.26	110.44
28	A	414	SQD	O47-C7-C8	2.63	117.18	111.48
27	m	101	LMG	O8-C28-O10	-2.63	117.05	123.63
23	B	616	CLA	O2D-CGD-CBD	2.63	115.83	111.23
23	c	505	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
23	C	511	CLA	CHB-C4A-NA	2.62	128.19	124.40
29	D	407	LHG	C18-C17-C16	-2.62	101.12	114.37
26	d	405	PL9	C8-C7-C3	2.62	118.80	112.03
23	b	612	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
25	T	101	BCR	C30-C25-C26	-2.62	119.06	122.64
30	c	517	DGD	C1D-C2D-C3D	-2.62	104.50	110.01
23	b	614	CLA	C3B-C4B-NB	-2.62	108.19	110.53
23	B	604	CLA	C6-C5-C3	-2.61	107.10	113.47
27	b	622	LMG	C8-O7-C10	2.61	124.05	117.80
27	D	409	LMG	O1-C7-C8	-2.61	105.06	111.77
29	B	622	LHG	O8-C23-O10	-2.61	117.10	123.63
26	a	410	PL9	C27-C28-C29	-2.61	121.65	127.62
23	b	611	CLA	CHB-C4A-NA	2.61	128.16	124.40
36	v	201	HEC	CBB-CAB-C3B	2.61	119.49	112.42
23	b	608	CLA	O1D-CGD-CBD	2.61	129.66	124.52
25	c	514	BCR	C15-C16-C17	-2.60	118.19	123.52
23	c	512	CLA	O1D-CGD-CBD	2.60	129.65	124.52
28	F	101	SQD	C1-C2-C3	-2.60	104.54	110.01
23	c	503	CLA	C4D-CHA-C1A	2.60	124.34	121.24
27	c	523	LMG	O1-C7-C8	-2.60	104.50	110.82
23	D	402	CLA	C2B-C1B-NB	-2.60	107.63	110.33
23	d	402	CLA	C3B-C4B-NB	-2.60	108.21	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405	CLA	CHB-C1B-NB	2.60	127.95	124.05
23	c	505	CLA	O2D-CGD-CBD	2.60	115.77	111.23
27	B	621	LMG	O7-C10-O9	-2.60	116.66	123.33
30	c	516	DGD	C3D-C4D-C5D	-2.59	105.53	110.23
25	c	514	BCR	C7-C8-C9	-2.59	122.40	126.23
23	C	510	CLA	O2D-CGD-CBD	2.59	115.76	111.23
33	a	404	BCT	O3-C-O1	-2.59	113.05	119.68
23	B	611	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
25	k	101	BCR	C30-C25-C26	-2.59	119.10	122.64
23	b	604	CLA	CHB-C4A-NA	2.59	128.14	124.40
23	C	513	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
36	v	201	HEC	C2A-C1A-NA	-2.59	107.83	110.32
23	b	614	CLA	C1-C2-C3	-2.59	121.96	126.20
23	C	507	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
23	B	601	CLA	CHB-C4A-NA	2.59	128.13	124.40
28	F	101	SQD	C46-C45-C44	-2.59	105.31	113.67
23	B	602	CLA	C1-C2-C3	-2.58	121.96	126.20
29	d	407	LHG	C18-C17-C16	-2.58	101.31	114.37
23	b	613	CLA	CMB-C2B-C3B	2.58	132.62	126.55
25	b	620	BCR	C33-C5-C6	-2.58	121.67	124.48
23	C	508	CLA	O2D-CGD-CBD	2.58	115.73	111.23
27	d	409	LMG	O1-C7-C8	-2.57	104.56	110.82
26	a	410	PL9	C37-C38-C39	-2.57	121.74	127.62
30	H	102	DGD	C8B-C7B-C6B	-2.57	101.38	114.37
27	A	411	LMG	O6-C1-O1	-2.57	103.97	110.04
23	B	608	CLA	CHB-C1B-NB	2.57	127.90	124.05
23	B	604	CLA	C3B-C4B-NB	-2.57	108.24	110.53
25	B	617	BCR	C11-C10-C9	-2.57	123.67	127.28
23	c	505	CLA	CHD-C1D-ND	-2.57	121.19	124.80
23	b	613	CLA	C11-C12-C13	-2.57	107.43	115.97
28	b	601	SQD	O9-S-O7	-2.56	105.48	113.82
23	b	606	CLA	CHD-C1D-ND	-2.56	121.20	124.80
23	B	616	CLA	C1-C2-C3	2.56	130.39	126.20
23	c	510	CLA	CHB-C1B-NB	2.56	127.89	124.05
26	A	410	PL9	C35-C34-C36	2.56	119.67	115.23
27	A	411	LMG	C36-C35-C34	-2.56	101.44	114.37
25	b	618	BCR	C29-C30-C25	2.56	114.15	110.44
29	D	407	LHG	C20-C19-C18	-2.55	101.46	114.37
23	C	504	CLA	C6-C5-C3	2.55	119.68	113.47
25	b	618	BCR	C15-C16-C17	-2.55	118.30	123.52
36	V	201	HEC	C2A-C1A-NA	-2.55	107.86	110.32
23	b	604	CLA	CMB-C2B-C3B	2.55	132.54	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	M	101	LMG	O8-C28-O10	-2.55	117.25	123.63
23	B	609	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
23	C	502	CLA	CHD-C1D-ND	-2.54	121.22	124.80
23	b	608	CLA	CHB-C1B-NB	2.54	127.86	124.05
23	B	612	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
26	D	405	PL9	C8-C7-C3	2.54	118.59	112.03
29	d	407	LHG	C20-C19-C18	-2.54	101.55	114.37
30	c	518	DGD	C3D-C4D-C5D	-2.53	105.64	110.23
25	A	409	BCR	C27-C26-C25	2.53	126.13	122.70
23	c	506	CLA	O1D-CGD-CBD	2.53	129.52	124.52
23	C	508	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	B	617	BCR	C2-C1-C6	2.53	114.11	110.44
25	b	620	BCR	C2-C1-C6	2.53	114.11	110.44
23	b	607	CLA	O2D-CGD-CBD	2.53	115.65	111.23
24	A	407	PHO	C3B-C4B-NB	-2.53	105.82	107.46
23	b	606	CLA	C1-C2-C3	-2.52	122.06	126.20
23	B	611	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
23	a	408	CLA	CAA-CBA-CGA	-2.52	106.04	113.21
23	b	615	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
23	D	401	CLA	O2D-CGD-CBD	2.52	115.63	111.23
23	A	404	CLA	CAA-C2A-C1A	-2.52	103.72	111.97
30	C	515	DGD	O3G-C3G-C2G	-2.52	104.70	110.82
23	B	602	CLA	CHA-C4D-ND	2.51	137.73	132.55
25	Z	101	BCR	C2-C1-C6	2.51	114.09	110.44
23	b	615	CLA	C3B-C4B-NB	-2.51	108.29	110.53
23	C	509	CLA	CED-O2D-CGD	2.51	121.61	115.92
23	a	406	CLA	CMA-C3A-C4A	-2.51	105.03	111.77
23	b	606	CLA	C16-C15-C13	-2.51	107.63	115.97
23	c	509	CLA	O1D-CGD-CBD	2.51	129.47	124.52
23	B	607	CLA	C2C-C1C-NC	2.50	112.61	109.98
23	c	513	CLA	C3B-C4B-NB	-2.50	108.30	110.53
23	c	508	CLA	CHD-C1D-ND	-2.50	121.28	124.80
23	c	508	CLA	C1-C2-C3	-2.50	122.10	126.20
23	h	101	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
23	b	614	CLA	C2B-C1B-NB	-2.50	107.73	110.33
27	m	101	LMG	O3-C3-C2	-2.50	104.49	110.38
23	A	404	CLA	O1D-CGD-CBD	2.50	129.44	124.52
25	T	101	BCR	C7-C8-C9	-2.49	122.54	126.23
23	c	504	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
23	B	605	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
30	A	415	DGD	C3E-C4E-C5E	-2.49	105.72	110.23
23	b	614	CLA	CHA-C1A-NA	-2.49	120.75	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	614	CLA	CHC-C4B-NB	2.49	127.78	124.05
27	C	518	LMG	O6-C1-O1	-2.49	104.17	110.04
26	D	405	PL9	C7-C8-C9	-2.49	122.55	126.83
30	c	517	DGD	C6B-C5B-C4B	-2.48	101.81	114.37
30	C	515	DGD	C4E-C3E-C2E	-2.48	106.47	110.83
25	B	619	BCR	C15-C16-C17	-2.48	118.44	123.52
27	D	406	LMG	O2-C2-C1	-2.48	104.16	110.08
23	b	613	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
23	a	408	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
23	B	608	CLA	C6-C7-C8	-2.48	107.72	115.97
25	B	618	BCR	C11-C10-C9	-2.48	123.80	127.28
28	A	412	SQD	O8-S-C6	2.48	110.76	105.97
23	c	503	CLA	CHD-C1D-ND	-2.48	121.32	124.80
26	a	410	PL9	C40-C39-C38	-2.48	117.27	123.63
27	b	622	LMG	O3-C3-C2	-2.48	104.54	110.38
23	b	613	CLA	C1D-ND-C4D	-2.48	104.58	106.31
36	v	201	HEC	CHD-C1D-ND	2.48	127.43	124.37
23	B	611	CLA	C1-C2-C3	-2.47	122.14	126.20
23	b	617	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
25	B	617	BCR	C30-C25-C26	-2.47	119.25	122.64
23	c	506	CLA	CMC-C2C-C1C	2.47	128.90	125.03
24	A	407	PHO	C2B-C1B-NB	-2.47	107.64	109.43
30	c	518	DGD	C4D-C3D-C2D	-2.47	106.49	110.83
25	K	102	BCR	C37-C22-C21	-2.47	118.81	122.82
27	C	518	LMG	O8-C28-O10	-2.47	117.45	123.63
25	D	404	BCR	C16-C15-C14	-2.47	118.46	123.52
25	a	409	BCR	C30-C25-C26	-2.47	119.26	122.64
27	c	523	LMG	O6-C1-O1	-2.47	104.21	110.04
25	A	409	BCR	C24-C23-C22	-2.47	122.58	126.23
30	a	414	DGD	C1G-O1G-C1A	2.47	126.14	117.12
23	A	408	CLA	C1D-ND-C4D	-2.47	104.58	106.31
23	b	610	CLA	CHC-C4B-NB	2.47	127.75	124.05
23	A	408	CLA	CMB-C2B-C3B	2.46	132.35	126.55
23	B	608	CLA	CHC-C4B-NB	2.46	127.75	124.05
33	A	418	BCT	O3-C-O1	-2.46	113.37	119.68
23	h	101	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	D	403	CLA	C4-C3-C5	2.46	119.50	115.23
30	h	102	DGD	C1D-C2D-C3D	-2.46	104.83	110.01
26	a	410	PL9	O2-C1-C2	-2.46	116.23	121.83
23	A	408	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
23	C	503	CLA	CHC-C4B-NB	2.46	127.73	124.05
36	v	201	HEC	CHA-C1A-C2A	2.46	128.74	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	612	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
23	C	503	CLA	C2A-C1A-CHA	2.45	128.12	123.87
23	C	504	CLA	CHB-C1B-NB	2.45	127.72	124.05
23	B	605	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
30	c	516	DGD	C2G-O2G-C1B	2.45	123.65	117.80
25	T	101	BCR	C3-C4-C5	-2.45	109.69	114.06
25	a	409	BCR	C29-C30-C25	2.45	113.99	110.44
27	d	409	LMG	O1-C1-C2	-2.45	104.56	108.27
23	C	502	CLA	C6-C5-C3	-2.45	107.51	113.47
23	b	609	CLA	CHB-C4A-NA	2.45	127.93	124.40
23	c	507	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
23	d	402	CLA	C4-C3-C5	2.44	119.47	115.23
23	b	604	CLA	CHD-C1D-ND	-2.44	121.36	124.80
23	B	609	CLA	O2D-CGD-CBD	2.44	115.50	111.23
23	b	615	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
25	c	514	BCR	C37-C22-C21	-2.44	118.86	122.82
23	B	611	CLA	CHD-C1D-C2D	2.44	130.56	125.49
23	c	506	CLA	CHC-C4B-NB	2.44	127.71	124.05
23	c	510	CLA	O1D-CGD-CBD	2.44	129.32	124.52
23	a	411	CLA	O2D-CGD-CBD	2.44	115.49	111.23
23	c	502	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
23	b	607	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
23	a	405	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	a	411	CLA	C1-O2A-CGA	2.43	122.53	116.65
30	A	415	DGD	CDB-CCB-CBB	-2.43	102.10	114.37
27	M	101	LMG	C40-C39-C38	-2.43	102.11	114.37
26	D	405	PL9	C42-C43-C44	-2.43	122.07	127.62
23	A	405	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
23	D	401	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
23	C	512	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
24	d	401	PHO	O2D-CGD-CBD	-2.42	108.29	110.95
29	d	408	LHG	C26-C25-C24	2.42	122.02	113.13
30	c	516	DGD	O3E-C3E-C2E	-2.42	104.67	110.38
24	A	407	PHO	CMB-C2B-C3B	2.42	129.52	124.68
25	K	102	BCR	C27-C26-C25	2.42	125.97	122.70
27	A	411	LMG	O7-C10-O9	-2.42	118.05	123.70
25	b	619	BCR	C8-C7-C6	-2.41	120.55	127.00
30	a	414	DGD	O2G-C2G-C1G	2.41	117.00	108.34
23	D	403	CLA	O1D-CGD-CBD	2.41	129.28	124.52
27	M	101	LMG	C1-O6-C5	-2.41	109.01	113.72
23	d	403	CLA	CAC-C3C-C4C	2.41	127.92	124.79
28	B	624	SQD	O5-C5-C4	2.41	114.04	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
23	b	610	CLA	CHA-C1A-NA	-2.41	120.94	126.39
25	C	514	BCR	C33-C5-C6	-2.41	121.86	124.48
23	b	617	CLA	CHC-C4B-NB	2.41	127.66	124.05
23	A	408	CLA	CHC-C1C-C2C	-2.40	120.11	126.95
27	d	409	LMG	C3-C4-C5	-2.40	105.87	110.23
30	C	516	DGD	CCB-CBB-CAB	-2.40	102.22	114.37
23	C	512	CLA	C6-C5-C3	-2.40	107.62	113.47
28	A	412	SQD	O48-C23-C24	2.40	119.16	111.83
23	c	504	CLA	O1A-CGA-CBA	2.40	133.17	123.78
26	D	405	PL9	C50-C49-C48	-2.40	115.46	122.66
23	b	614	CLA	CHB-C1B-NB	2.40	127.65	124.05
23	c	510	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
23	b	606	CLA	CHD-C4C-NC	2.39	127.94	124.23
23	c	511	CLA	CHA-C1A-NA	-2.39	120.97	126.39
25	B	619	BCR	C2-C1-C6	2.39	113.91	110.44
23	b	611	CLA	CAA-CBA-CGA	-2.39	106.42	113.21
26	A	410	PL9	C40-C39-C38	-2.39	117.49	123.63
26	d	405	PL9	C32-C33-C34	-2.39	122.16	127.62
23	B	604	CLA	CMB-C2B-C3B	2.39	132.16	126.55
25	A	409	BCR	C8-C7-C6	-2.39	120.62	127.00
23	D	403	CLA	CMB-C2B-C3B	2.39	132.16	126.55
28	A	412	SQD	O48-C46-C45	2.38	115.27	108.40
23	c	502	CLA	CMD-C2D-C1D	-2.38	120.53	124.73
23	c	512	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
23	B	616	CLA	C4D-CHA-C1A	2.38	124.08	121.24
23	d	402	CLA	CHB-C1B-NB	2.38	127.62	124.05
23	C	512	CLA	CAA-CBA-CGA	-2.38	106.46	113.21
23	B	605	CLA	O1D-CGD-CBD	2.38	129.21	124.52
25	b	618	BCR	C24-C23-C22	-2.37	122.72	126.23
27	m	101	LMG	C1-O6-C5	-2.37	109.08	113.72
30	A	415	DGD	O6E-C1E-O5D	-2.37	104.44	110.04
23	a	408	CLA	CGD-CBD-CAD	-2.37	103.17	110.85
23	b	612	CLA	C1-C2-C3	-2.37	122.31	126.20
27	A	411	LMG	O3-C3-C2	-2.37	104.79	110.38
25	A	409	BCR	C33-C5-C6	-2.37	121.90	124.48
28	a	412	SQD	O5-C5-C4	2.37	113.97	109.70
27	A	411	LMG	C1-O6-C5	-2.37	109.09	113.72
23	C	510	CLA	CHB-C4A-NA	2.37	127.82	124.40
28	F	101	SQD	O48-C23-C24	2.37	119.06	111.83
23	B	613	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
29	B	623	LHG	O3-P-O5	-2.37	99.55	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	410	PL9	C27-C28-C29	-2.37	122.21	127.62
23	c	507	CLA	CHC-C4B-NB	2.37	127.60	124.05
23	d	403	CLA	C1-C2-C3	-2.36	122.32	126.20
23	c	506	CLA	C6-C5-C3	-2.36	107.71	113.47
30	c	516	DGD	C1D-C2D-C3D	-2.36	105.04	110.01
29	B	623	LHG	C18-C17-C16	-2.36	102.43	114.37
23	B	611	CLA	C2C-C1C-NC	2.36	112.46	109.98
23	B	610	CLA	C3B-C4B-NB	-2.35	108.43	110.53
23	C	508	CLA	CHD-C1D-C2D	2.35	130.37	125.49
23	b	605	CLA	CHD-C1D-ND	-2.35	121.50	124.80
23	c	503	CLA	O1D-CGD-CBD	2.35	129.15	124.52
27	d	409	LMG	O7-C10-O9	-2.34	118.22	123.70
27	C	518	LMG	C3-C4-C5	-2.34	105.98	110.23
23	b	617	CLA	O1D-CGD-CBD	2.34	129.14	124.52
25	Z	101	BCR	C38-C26-C25	-2.34	121.93	124.48
23	b	612	CLA	CHB-C1B-NB	2.34	127.56	124.05
23	b	607	CLA	CHB-C1B-NB	2.34	127.55	124.05
23	B	607	CLA	C6-C5-C3	-2.34	107.78	113.47
23	C	512	CLA	CHB-C1B-NB	2.34	127.55	124.05
25	b	618	BCR	C34-C9-C10	-2.34	119.03	122.82
23	b	607	CLA	C4-C3-C5	2.33	119.28	115.23
29	l	101	LHG	C5-O7-C7	-2.33	112.21	117.80
25	c	515	BCR	C35-C13-C14	-2.33	119.04	122.82
23	B	609	CLA	CHB-C1B-NB	2.33	127.54	124.05
23	c	503	CLA	C7-C6-C5	-2.33	107.06	113.26
23	c	501	CLA	C3B-C4B-NB	-2.33	108.45	110.53
23	h	101	CLA	CHD-C1D-ND	-2.33	121.53	124.80
30	H	102	DGD	O2D-C2D-C1D	-2.33	104.53	110.08
25	B	619	BCR	C27-C26-C25	2.33	125.85	122.70
25	b	620	BCR	C38-C26-C25	-2.33	121.94	124.48
25	c	515	BCR	C4-C5-C6	2.33	125.85	122.70
27	M	101	LMG	C8-O7-C10	2.33	123.36	117.80
29	D	408	LHG	C11-C10-C9	-2.32	102.62	114.37
30	H	102	DGD	CDB-CCB-CBB	-2.32	102.63	114.37
23	C	503	CLA	O1D-CGD-CBD	2.32	129.09	124.52
30	h	102	DGD	CAB-C9B-C8B	-2.32	102.64	114.37
23	C	506	CLA	C3B-C4B-NB	-2.32	108.46	110.53
25	c	515	BCR	C1-C6-C5	-2.32	119.47	122.64
23	b	613	CLA	C9-C8-C10	-2.32	103.02	111.27
23	C	503	CLA	CHA-C1A-NA	-2.32	121.14	126.39
23	A	404	CLA	CHD-C4C-C3C	-2.32	121.40	124.77
23	B	603	CLA	CHD-C1D-ND	-2.31	121.55	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	405	PL9	C45-C44-C43	-2.31	117.69	123.63
23	B	605	CLA	CHB-C4A-NA	2.31	127.74	124.40
28	A	412	SQD	O47-C45-C46	2.31	116.64	108.34
27	b	622	LMG	C1-C2-C3	-2.31	105.14	110.01
27	A	411	LMG	O8-C28-O10	-2.31	117.85	123.63
23	A	408	CLA	C2C-C1C-NC	2.31	112.41	109.98
23	a	408	CLA	C2A-C1A-CHA	2.31	127.87	123.87
30	C	515	DGD	C7B-C6B-C5B	-2.31	102.70	114.37
25	b	619	BCR	C27-C26-C25	2.31	125.82	122.70
28	B	624	SQD	O47-C7-O49	-2.30	118.32	123.70
23	B	605	CLA	C4D-C3D-CAD	-2.30	105.60	108.11
30	H	102	DGD	C6D-C5D-C4D	2.30	116.90	112.07
30	C	515	DGD	CBB-CAB-C9B	-2.30	102.73	114.37
23	C	505	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
27	c	523	LMG	O2-C2-C1	-2.30	104.59	110.08
35	E	101	HEM	CHD-C4C-C3C	2.30	129.09	125.21
27	M	101	LMG	C38-C37-C36	-2.30	102.76	114.37
23	c	502	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
30	a	414	DGD	C1G-C2G-C3G	-2.30	106.50	111.80
23	B	609	CLA	C1-O2A-CGA	2.30	122.21	116.65
30	h	102	DGD	C4E-C3E-C2E	-2.30	106.80	110.83
23	B	610	CLA	CHD-C1D-ND	-2.29	121.57	124.80
23	c	502	CLA	CMD-C2D-C3D	2.29	132.95	127.69
25	C	514	BCR	C7-C8-C9	-2.29	122.84	126.23
23	c	501	CLA	CHC-C4B-NB	2.29	127.49	124.05
24	d	401	PHO	C3D-C4D-ND	2.29	110.65	107.71
23	C	509	CLA	C2A-C3A-C4A	2.29	105.57	101.87
25	K	101	BCR	C8-C7-C6	-2.29	120.88	127.00
30	C	516	DGD	CDB-CCB-CBB	-2.29	102.80	114.37
23	B	614	CLA	O1A-CGA-CBA	2.29	132.73	123.78
23	b	606	CLA	C1C-C2C-C3C	-2.29	104.57	106.98
25	b	618	BCR	C27-C26-C25	2.29	125.79	122.70
23	d	403	CLA	CHB-C4A-NA	2.28	127.70	124.40
23	b	606	CLA	C6-C7-C8	-2.28	108.38	115.97
28	b	601	SQD	C44-O6-C1	2.28	118.69	113.80
26	d	405	PL9	C36-C34-C33	-2.28	116.04	121.17
23	d	403	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
23	C	512	CLA	C1-C2-C3	-2.28	122.46	126.20
25	t	101	BCR	C2-C1-C6	2.28	113.75	110.44
26	d	405	PL9	C7-C8-C9	-2.28	122.91	126.83
23	b	609	CLA	CHD-C4C-C3C	-2.28	121.46	124.77
23	c	502	CLA	C1-C2-C3	-2.27	122.47	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	614	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
23	b	608	CLA	C4-C3-C5	2.27	119.17	115.23
23	b	613	CLA	CHB-C4A-NA	2.27	127.68	124.40
25	H	101	BCR	C16-C15-C14	-2.27	118.87	123.52
23	D	401	CLA	C16-C15-C13	-2.27	108.42	115.97
23	B	603	CLA	CHA-C1A-NA	-2.27	121.25	126.39
30	c	516	DGD	O5D-C6D-C5D	-2.27	104.31	109.42
23	C	501	CLA	CHD-C1D-ND	-2.27	121.61	124.80
23	B	610	CLA	C1-C2-C3	-2.27	122.49	126.20
28	f	101	SQD	O48-C23-O10	-2.26	117.96	123.63
25	a	409	BCR	C33-C5-C6	-2.26	122.01	124.48
23	c	510	CLA	O2D-CGD-CBD	2.26	115.19	111.23
30	H	102	DGD	O2G-C1B-O1B	-2.26	118.42	123.70
23	B	604	CLA	CHB-C4A-NA	2.26	127.66	124.40
27	b	622	LMG	O2-C2-C1	-2.26	104.69	110.08
29	D	407	LHG	C11-C10-C9	-2.26	102.94	114.37
25	a	409	BCR	C15-C14-C13	-2.26	124.11	127.28
30	c	518	DGD	O3E-C3E-C2E	-2.26	105.05	110.38
23	C	513	CLA	C6-C7-C8	-2.26	108.45	115.97
23	B	603	CLA	O1D-CGD-CBD	2.26	128.97	124.52
30	c	517	DGD	CDB-CCB-CBB	-2.26	102.96	114.37
27	c	523	LMG	O5-C6-C5	-2.26	103.65	111.33
23	B	604	CLA	CHA-C4D-ND	2.26	137.20	132.55
28	A	412	SQD	C1-O5-C5	-2.25	109.32	113.72
30	h	102	DGD	O6E-C5E-C6E	-2.25	100.85	106.44
23	B	601	CLA	C1-C2-C3	-2.25	122.50	126.20
25	t	101	BCR	C29-C30-C25	2.25	113.71	110.44
30	h	102	DGD	C3E-C4E-C5E	-2.25	106.15	110.23
27	c	519	LMG	O2-C2-C1	-2.25	104.71	110.08
25	c	515	BCR	C30-C25-C26	-2.25	119.56	122.64
23	C	508	CLA	CHC-C1C-NC	2.25	127.70	124.31
30	C	517	DGD	O6E-C1E-O5D	-2.25	104.73	110.04
23	C	502	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
23	c	505	CLA	C6-C7-C8	-2.25	108.49	115.97
27	c	521	LMG	O8-C28-O10	-2.25	118.00	123.63
27	A	411	LMG	O1-C7-C8	-2.25	105.35	110.82
29	d	406	LHG	O8-C23-O10	-2.25	118.01	123.63
26	d	405	PL9	C12-C13-C14	-2.24	122.49	127.62
25	B	618	BCR	C2-C1-C6	2.24	113.70	110.44
30	c	516	DGD	O6E-C5E-C6E	-2.24	100.89	106.44
23	b	612	CLA	CMB-C2B-C3B	2.24	131.82	126.55
27	M	101	LMG	O6-C1-O1	-2.24	104.75	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	m	101	LMG	C21-C20-C19	-2.24	103.04	114.37
27	D	409	LMG	O7-C10-O9	-2.24	118.47	123.70
30	c	518	DGD	O6E-C1E-O5D	-2.24	104.75	110.04
25	b	620	BCR	C27-C26-C25	2.24	125.73	122.70
23	c	511	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
23	c	503	CLA	CHB-C4A-NA	2.24	127.63	124.40
23	C	506	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
23	b	617	CLA	O2D-CGD-CBD	2.23	115.14	111.23
23	C	502	CLA	C4D-CHA-C1A	2.23	123.91	121.24
29	d	407	LHG	O8-C6-C5	-2.23	101.95	108.40
27	C	518	LMG	C9-C8-C7	-2.23	106.58	111.78
23	b	611	CLA	C3B-C4B-NB	-2.23	108.54	110.53
23	B	616	CLA	C1D-ND-C4D	2.23	107.88	106.31
23	b	608	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
23	C	513	CLA	CMB-C2B-C3B	2.23	131.79	126.55
28	b	601	SQD	O9-S-C6	2.23	110.08	106.76
25	H	101	BCR	C1-C6-C5	-2.23	119.59	122.64
23	B	601	CLA	C2A-C1A-CHA	2.23	127.73	123.87
25	B	618	BCR	C8-C7-C6	-2.23	121.05	127.00
23	C	510	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
28	a	413	SQD	O47-C45-C44	2.23	116.22	108.30
25	k	102	BCR	C40-C30-C25	2.23	113.73	110.24
23	C	501	CLA	CAC-C3C-C4C	2.23	127.69	124.79
23	C	508	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
23	b	612	CLA	C2D-C1D-ND	-2.22	107.92	110.13
29	B	622	LHG	C12-C11-C10	-2.22	103.13	114.37
23	B	608	CLA	CHA-C1A-NA	-2.22	121.36	126.39
25	c	514	BCR	C33-C5-C6	-2.22	122.06	124.48
25	B	618	BCR	C30-C25-C26	-2.22	119.60	122.64
23	A	408	CLA	C3D-C4D-ND	2.22	113.60	109.99
24	d	401	PHO	C1-C2-C3	-2.22	122.56	126.20
23	c	506	CLA	CHB-C4A-NA	2.22	127.60	124.40
23	B	613	CLA	C3B-C4B-NB	-2.22	108.55	110.53
23	c	513	CLA	C1-C2-C3	-2.22	122.57	126.20
23	C	507	CLA	CAC-C3C-C4C	-2.22	121.91	124.79
25	K	102	BCR	C8-C7-C6	-2.21	121.08	127.00
23	b	608	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
23	b	617	CLA	CHD-C1D-ND	-2.21	121.69	124.80
23	b	614	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
25	T	101	BCR	C40-C30-C25	2.21	113.71	110.24
27	m	101	LMG	O6-C1-O1	-2.21	104.82	110.04
30	c	518	DGD	C7B-C6B-C5B	-2.21	103.21	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	603	CLA	CGD-CBD-CAD	-2.21	103.70	110.85
23	B	606	CLA	C7-C6-C5	-2.21	107.39	113.26
25	a	409	BCR	C38-C26-C27	-2.20	108.90	113.60
25	B	619	BCR	C15-C14-C13	-2.20	124.19	127.28
25	c	514	BCR	C10-C11-C12	-2.20	116.82	123.20
24	a	407	PHO	O2D-CGD-CBD	2.20	113.37	110.95
25	a	409	BCR	C2-C1-C6	2.20	113.64	110.44
23	D	403	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
30	c	518	DGD	C1D-C2D-C3D	-2.20	105.38	110.01
23	c	508	CLA	O2D-CGD-CBD	2.20	115.08	111.23
30	c	518	DGD	CDB-CCB-CBB	-2.20	103.25	114.37
27	m	101	LMG	C40-C39-C38	-2.20	103.25	114.37
23	B	605	CLA	CAC-C3C-C4C	2.20	127.65	124.79
26	a	410	PL9	C30-C29-C28	-2.20	117.98	123.63
23	c	513	CLA	CAC-C3C-C4C	2.20	127.65	124.79
23	B	605	CLA	CHD-C1D-ND	-2.19	121.71	124.80
30	c	518	DGD	O5E-C6E-C5E	-2.19	103.86	111.33
23	C	506	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
26	d	405	PL9	O1-C4-C3	-2.19	118.42	120.73
23	b	609	CLA	CMB-C2B-C3B	2.19	131.70	126.55
23	C	503	CLA	CHD-C1D-C2D	2.19	130.04	125.49
23	B	609	CLA	CHA-C1A-NA	-2.19	121.44	126.39
29	d	406	LHG	C20-C19-C18	-2.18	103.33	114.37
25	d	404	BCR	C39-C30-C25	-2.18	106.82	110.24
29	B	622	LHG	C20-C19-C18	-2.18	103.33	114.37
23	A	404	CLA	CMB-C2B-C3B	2.18	131.69	126.55
28	A	414	SQD	O48-C23-C24	2.18	118.49	111.83
26	A	410	PL9	C42-C43-C44	-2.18	122.63	127.62
27	M	101	LMG	O1-C7-C8	-2.18	105.51	110.82
23	B	611	CLA	C11-C10-C8	-2.18	108.72	115.97
26	A	410	PL9	C30-C29-C28	-2.18	118.03	123.63
23	C	502	CLA	CAC-C3C-C4C	2.18	127.63	124.79
23	C	506	CLA	CHA-C1A-NA	-2.18	121.45	126.39
23	b	613	CLA	CHD-C1D-ND	-2.18	121.74	124.80
23	B	616	CLA	CED-O2D-CGD	-2.18	110.97	115.92
23	B	610	CLA	C1-O2A-CGA	-2.18	111.38	116.65
23	B	612	CLA	CED-O2D-CGD	-2.18	110.97	115.92
36	V	201	HEC	CHB-C1B-NB	2.18	126.77	124.42
23	C	503	CLA	C2D-C1D-ND	-2.18	107.97	110.13
23	B	605	CLA	OBD-CAD-C3D	2.18	133.50	128.42
23	c	511	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
23	B	607	CLA	C4D-CHA-C1A	2.18	123.84	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	604	CLA	C5-C3-C2	-2.18	116.28	121.17
23	a	411	CLA	CAA-C2A-C3A	-2.17	107.12	113.00
23	b	611	CLA	CHD-C1D-ND	-2.17	121.74	124.80
23	B	604	CLA	CAC-C3C-C4C	2.17	127.62	124.79
23	B	609	CLA	CED-O2D-CGD	2.17	120.84	115.92
23	C	508	CLA	C3B-C4B-NB	-2.17	108.59	110.53
25	B	618	BCR	C15-C16-C17	-2.17	119.08	123.52
29	D	408	LHG	O8-C6-C5	-2.17	102.14	108.40
23	C	503	CLA	CHB-C1B-NB	2.17	127.31	124.05
25	c	514	BCR	C2-C1-C6	2.17	113.59	110.44
23	C	505	CLA	CAC-C3C-C4C	2.17	127.61	124.79
23	B	614	CLA	CHA-C1A-NA	-2.17	121.48	126.39
23	C	512	CLA	C11-C12-C13	-2.17	108.76	115.97
23	c	504	CLA	CMB-C2B-C3B	2.17	131.65	126.55
30	H	102	DGD	O3E-C3E-C2E	-2.17	105.27	110.38
23	B	606	CLA	O2D-CGD-CBD	2.17	115.02	111.23
30	c	518	DGD	C7A-C6A-C5A	-2.17	103.42	114.37
25	x	101	BCR	C11-C10-C9	-2.17	124.24	127.28
23	a	405	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
30	c	517	DGD	O2G-C1B-O1B	-2.16	118.65	123.70
23	B	606	CLA	CHA-C4D-ND	2.16	137.01	132.55
25	c	514	BCR	C15-C14-C13	-2.16	124.24	127.28
23	B	616	CLA	C4-C3-C2	-2.16	118.07	123.63
25	b	619	BCR	C15-C16-C17	-2.16	119.09	123.52
30	h	102	DGD	C3G-C2G-C1G	-2.16	106.74	111.78
27	c	519	LMG	O8-C28-O10	-2.16	118.22	123.63
24	a	407	PHO	OBD-CAD-CBD	-2.16	122.65	125.82
29	l	101	LHG	C27-C26-C25	-2.16	103.44	114.37
23	B	608	CLA	C3B-C4B-NB	-2.16	108.60	110.53
23	B	613	CLA	C16-C15-C13	-2.16	108.79	115.97
23	b	608	CLA	C3B-C4B-NB	-2.16	108.60	110.53
23	A	408	CLA	CHA-C1A-NA	-2.16	121.51	126.39
23	B	611	CLA	CGD-CBD-CAD	-2.16	103.86	110.85
23	b	615	CLA	O2D-CGD-CBD	2.15	115.00	111.23
25	K	102	BCR	C15-C16-C17	-2.15	119.12	123.52
25	Z	101	BCR	C15-C16-C17	-2.15	119.12	123.52
23	D	403	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
23	b	609	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
27	c	521	LMG	C42-C41-C40	-2.15	103.50	114.37
28	a	413	SQD	O48-C23-C24	2.15	118.39	111.83
23	b	615	CLA	C6-C5-C3	-2.15	108.23	113.47
25	x	101	BCR	C34-C9-C8	-2.15	114.81	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f	101	SQD	O47-C7-C8	2.15	118.82	110.93
24	A	407	PHO	CBA-CAA-C2A	-2.15	107.46	113.78
23	c	506	CLA	C3B-C4B-NB	-2.15	108.61	110.53
23	C	509	CLA	CHD-C1D-ND	-2.14	121.79	124.80
23	c	507	CLA	CHD-C1D-ND	-2.14	121.79	124.80
23	C	502	CLA	CHC-C4B-NB	2.14	127.26	124.05
25	k	101	BCR	C38-C26-C25	-2.14	122.15	124.48
27	c	521	LMG	C40-C39-C38	-2.14	103.54	114.37
25	K	101	BCR	C1-C6-C5	-2.14	119.71	122.64
26	a	410	PL9	O2-C1-C6	2.14	123.88	120.48
25	d	404	BCR	C1-C6-C5	-2.14	119.72	122.64
24	a	407	PHO	CMA-C3A-C4A	-2.13	110.01	114.61
29	l	101	LHG	O8-C23-C24	2.13	118.34	111.83
23	C	511	CLA	O2D-CGD-CBD	2.13	114.96	111.23
28	a	412	SQD	O8-S-C6	2.13	110.09	105.97
25	c	514	BCR	C38-C26-C25	-2.13	122.16	124.48
23	C	505	CLA	CHB-C1B-NB	2.13	127.25	124.05
23	D	401	CLA	CHC-C4B-NB	2.13	127.25	124.05
24	a	407	PHO	CBC-CAC-C3C	-2.13	109.82	112.87
30	c	518	DGD	O1G-C1A-C2A	-2.13	105.33	111.83
25	c	514	BCR	C24-C23-C22	-2.13	123.08	126.23
23	b	606	CLA	O1A-CGA-CBA	2.13	132.11	123.78
23	b	613	CLA	C3B-C4B-NB	-2.13	108.63	110.53
23	B	604	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
27	D	406	LMG	C9-C8-C7	-2.13	106.82	111.78
35	E	101	HEM	O2D-CGD-CBD	2.13	120.72	114.00
23	c	506	CLA	CMB-C2B-C3B	2.13	131.55	126.55
23	b	610	CLA	O1D-CGD-CBD	2.13	128.71	124.52
23	A	405	CLA	CED-O2D-CGD	-2.13	111.09	115.92
27	c	523	LMG	O3-C3-C2	-2.13	105.37	110.38
25	Z	101	BCR	C24-C23-C22	-2.13	123.09	126.23
30	C	516	DGD	O3D-C3D-C4D	-2.12	105.37	110.38
23	B	606	CLA	C4D-CHA-C1A	2.12	123.78	121.24
27	c	519	LMG	O6-C1-O1	-2.12	105.02	110.04
23	b	613	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
23	B	606	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
23	B	612	CLA	CMB-C2B-C3B	2.12	131.54	126.55
27	D	406	LMG	O1-C7-C8	-2.12	105.66	110.82
23	c	512	CLA	CHA-C1A-NA	-2.12	121.59	126.39
23	B	605	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	a	409	BCR	C7-C8-C9	-2.12	123.10	126.23
23	b	614	CLA	CHB-C4A-NA	2.12	127.46	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	O1D-CGD-CBD	2.12	128.70	124.52
24	d	401	PHO	O2A-CGA-O1A	-2.12	118.33	123.63
30	c	516	DGD	O6D-C1D-O3G	-2.12	105.04	110.04
23	B	603	CLA	O2D-CGD-CBD	2.12	114.93	111.23
27	C	518	LMG	O2-C2-C1	-2.11	105.04	110.08
25	c	514	BCR	C30-C25-C26	-2.11	119.75	122.64
23	c	501	CLA	CMB-C2B-C3B	2.11	131.52	126.55
23	h	101	CLA	CHD-C1D-C2D	2.11	129.88	125.49
28	a	412	SQD	O5-C1-C2	-2.11	106.03	110.37
25	b	620	BCR	C16-C15-C14	-2.11	119.20	123.52
24	A	407	PHO	O2D-CGD-CBD	2.11	113.27	110.95
26	D	405	PL9	C40-C39-C38	-2.11	118.21	123.63
23	B	606	CLA	CHA-C1A-NA	-2.11	121.61	126.39
23	C	506	CLA	C1-C2-C3	-2.11	122.74	126.20
27	m	101	LMG	O2-C2-C1	-2.11	105.05	110.08
30	c	518	DGD	CBB-CAB-C9B	-2.11	103.71	114.37
28	A	412	SQD	C3-C4-C5	2.11	114.05	110.23
27	b	622	LMG	C24-C23-C22	-2.11	103.72	114.37
23	A	404	CLA	CMD-C2D-C3D	2.11	132.52	127.69
23	A	404	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
23	C	505	CLA	CHD-C1D-ND	-2.11	121.84	124.80
23	B	604	CLA	CHA-C1A-NA	-2.10	121.63	126.39
23	b	608	CLA	CHA-C1A-NA	-2.10	121.63	126.39
23	D	402	CLA	CBA-CAA-C2A	-2.10	107.54	113.79
23	B	615	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
30	c	517	DGD	O5D-C6D-C5D	-2.10	104.68	109.42
23	B	605	CLA	C1-O2A-CGA	-2.10	111.56	116.65
23	D	401	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
23	C	502	CLA	CHA-C1A-NA	-2.10	121.63	126.39
25	B	617	BCR	C39-C30-C25	-2.10	106.95	110.24
23	h	101	CLA	C3A-C2A-C1A	-2.10	98.19	101.34
35	e	102	HEM	CAB-C3B-C2B	-2.10	121.61	128.43
36	v	201	HEC	C3D-C4D-ND	-2.10	108.32	110.35
23	b	606	CLA	CMC-C2C-C1C	2.10	128.31	125.03
25	k	101	BCR	C1-C6-C5	-2.10	119.77	122.64
23	c	506	CLA	CHA-C1A-NA	-2.10	121.64	126.39
23	b	603	CLA	CHC-C1C-NC	2.10	127.47	124.31
23	b	614	CLA	C2C-C1C-NC	2.10	112.18	109.98
25	a	409	BCR	C35-C13-C12	2.10	121.29	118.09
23	B	601	CLA	CHC-C4B-NB	2.10	127.19	124.05
26	d	405	PL9	C46-C47-C48	-2.09	101.66	112.02
23	c	501	CLA	CAC-C3C-C4C	2.09	127.51	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	x	101	BCR	C38-C26-C25	-2.09	122.20	124.48
23	b	609	CLA	C11-C10-C8	-2.09	109.01	115.97
23	b	607	CLA	C3C-C4C-NC	-2.09	107.75	110.43
23	b	616	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
25	x	101	BCR	C2-C1-C6	2.09	113.48	110.44
23	b	612	CLA	CMD-C2D-C1D	2.09	128.41	124.73
30	a	414	DGD	C5B-C4B-C3B	-2.09	103.80	114.37
36	V	201	HEC	CAA-C2A-C3A	-2.09	123.95	127.87
30	h	102	DGD	C3D-C4D-C5D	-2.09	106.44	110.23
23	B	609	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
27	c	523	LMG	C39-C38-C37	-2.09	103.81	114.37
30	C	516	DGD	CAB-C9B-C8B	-2.09	103.81	114.37
23	B	615	CLA	C6-C5-C3	-2.09	108.38	113.47
23	B	601	CLA	CHA-C4D-ND	2.09	136.86	132.55
23	A	405	CLA	CMD-C2D-C3D	2.09	132.48	127.69
23	C	504	CLA	O2D-CGD-CBD	2.09	114.88	111.23
27	c	521	LMG	O1-C1-C2	-2.09	105.11	108.27
23	b	617	CLA	C6-C5-C3	2.09	118.55	113.47
30	C	515	DGD	C5B-C4B-C3B	-2.08	103.83	114.37
23	c	501	CLA	CHA-C1A-NA	-2.08	121.68	126.39
23	b	609	CLA	CAC-C3C-C2C	2.08	131.38	127.56
23	c	507	CLA	CHD-C4C-NC	2.08	127.46	124.23
25	b	618	BCR	C38-C26-C25	-2.08	122.21	124.48
30	C	517	DGD	O3D-C3D-C4D	-2.08	105.47	110.38
25	c	515	BCR	C15-C14-C13	-2.08	124.36	127.28
23	c	505	CLA	C4D-C3D-CAD	-2.08	105.85	108.11
30	C	516	DGD	C7B-C6B-C5B	-2.08	103.86	114.37
23	a	408	CLA	CHA-C1A-NA	-2.08	121.69	126.39
30	h	102	DGD	CDB-CCB-CBB	-2.08	103.87	114.37
25	b	619	BCR	C35-C13-C14	-2.08	119.45	122.82
29	B	623	LHG	C20-C19-C18	-2.08	103.87	114.37
25	k	101	BCR	C4-C5-C6	2.08	125.51	122.70
27	c	519	LMG	O7-C10-O9	-2.08	118.98	122.99
23	B	612	CLA	C16-C15-C13	-2.08	109.07	115.97
26	D	405	PL9	C36-C34-C33	-2.07	116.51	121.17
30	C	516	DGD	O2D-C2D-C1D	-2.07	105.13	110.08
25	A	409	BCR	C40-C30-C39	-2.07	102.70	108.63
23	b	617	CLA	CMB-C2B-C3B	2.07	131.42	126.55
27	D	406	LMG	C3-C4-C5	-2.07	106.48	110.23
27	M	101	LMG	C6-C5-C4	-2.07	107.94	113.02
30	C	517	DGD	C8B-C7B-C6B	-2.07	103.91	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	C4D-C3D-CAD	-2.07	105.86	108.11
23	c	507	CLA	C3B-C4B-NB	-2.07	108.69	110.53
28	F	101	SQD	C1-O5-C5	-2.07	109.68	113.72
23	B	609	CLA	CMC-C2C-C1C	2.07	128.26	125.03
23	B	607	CLA	CHD-C1D-ND	-2.07	121.90	124.80
24	A	406	PHO	C3B-C4B-NB	-2.07	106.12	107.46
23	c	506	CLA	C1C-C2C-C3C	-2.06	104.81	106.98
29	D	407	LHG	C27-C26-C25	-2.06	103.94	114.37
25	d	404	BCR	C10-C11-C12	-2.06	117.22	123.20
23	b	605	CLA	C4-C3-C5	2.06	118.81	115.23
23	B	607	CLA	C1-C2-C3	-2.06	122.82	126.20
23	A	405	CLA	CMB-C2B-C3B	2.06	131.40	126.55
23	b	615	CLA	CHB-C1B-NB	2.06	127.14	124.05
23	a	411	CLA	CHD-C1D-ND	-2.06	121.90	124.80
27	c	521	LMG	O7-C10-O9	-2.06	118.89	123.70
23	d	403	CLA	CHA-C1A-NA	-2.06	121.73	126.39
25	t	101	BCR	C36-C18-C17	-2.06	119.48	122.82
23	b	605	CLA	CHD-C4C-NC	2.06	127.42	124.23
26	d	405	PL9	C27-C28-C29	-2.06	122.92	127.62
27	C	518	LMG	C38-C37-C36	-2.05	103.98	114.37
23	a	405	CLA	C4-C3-C5	2.05	118.79	115.23
36	v	201	HEC	O1D-CGD-CBD	-2.05	116.59	123.09
29	e	101	LHG	C11-C10-C9	-2.05	104.00	114.37
23	B	615	CLA	C1C-C2C-C3C	-2.05	104.83	106.98
23	B	603	CLA	C1-O2A-CGA	-2.05	111.69	116.65
27	d	409	LMG	C1-C2-C3	-2.05	105.70	110.01
25	b	620	BCR	C15-C16-C17	-2.05	119.33	123.52
29	l	101	LHG	O8-C6-C5	-2.05	102.49	108.40
23	b	609	CLA	CHB-C1B-C2B	-2.05	121.49	127.43
30	c	516	DGD	C4D-C3D-C2D	-2.05	107.24	110.83
25	D	404	BCR	C24-C23-C22	-2.05	123.21	126.23
36	V	201	HEC	C1D-ND-C4D	2.05	107.63	105.21
25	k	102	BCR	C33-C5-C6	-2.04	122.25	124.48
23	c	509	CLA	CMB-C2B-C3B	2.04	131.36	126.55
23	B	609	CLA	CHB-C1B-C2B	-2.04	121.49	127.43
24	A	406	PHO	OBD-CAD-CBD	-2.04	122.83	125.82
23	b	606	CLA	C3B-C4B-NB	-2.04	108.71	110.53
23	C	508	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
25	d	404	BCR	C8-C7-C6	-2.04	121.55	127.00
30	C	516	DGD	C1E-O6E-C5E	2.04	117.70	113.72
23	c	504	CLA	C7-C6-C5	-2.04	107.83	113.26
23	B	605	CLA	C6-C7-C8	-2.04	109.19	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	O1A-CGA-CBA	2.04	131.75	123.78
23	b	606	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
25	k	102	BCR	C29-C30-C25	2.04	113.40	110.44
25	b	618	BCR	C15-C14-C13	-2.03	124.42	127.28
28	b	601	SQD	C1-O5-C5	2.03	117.69	113.72
23	C	504	CLA	CHD-C4C-NC	2.03	127.39	124.23
27	c	519	LMG	C9-C8-C7	-2.03	107.05	111.78
30	c	518	DGD	C9B-C8B-C7B	-2.03	104.10	114.37
28	f	101	SQD	O48-C23-C24	2.03	118.02	111.83
23	c	503	CLA	CHD-C1D-C2D	2.03	129.71	125.49
23	D	403	CLA	C2B-C1B-NB	2.03	112.43	110.33
23	c	504	CLA	C1C-C2C-C3C	-2.03	104.85	106.98
23	B	604	CLA	C11-C10-C8	-2.03	109.23	115.97
30	H	102	DGD	C3E-C4E-C5E	-2.03	106.56	110.23
23	c	511	CLA	CHB-C4A-NA	2.02	127.32	124.40
30	h	102	DGD	CCB-CBB-CAB	-2.02	104.14	114.37
23	b	606	CLA	CHD-C1D-C2D	2.02	129.69	125.49
24	d	401	PHO	C3B-C4B-NB	-2.02	106.15	107.46
26	D	405	PL9	O1-C4-C3	-2.02	118.60	120.73
27	b	623	LMG	C37-C36-C35	-2.02	104.15	114.37
23	c	505	CLA	CHB-C4A-NA	2.02	127.32	124.40
23	b	603	CLA	CHD-C1D-ND	-2.02	121.96	124.80
27	B	621	LMG	O8-C28-O10	-2.02	118.14	123.33
25	B	619	BCR	C40-C30-C29	-2.02	101.20	108.95
25	A	409	BCR	C31-C1-C6	-2.02	107.08	110.24
23	c	505	CLA	CHC-C1C-NC	2.02	127.35	124.31
25	B	619	BCR	C11-C10-C9	-2.02	124.45	127.28
25	K	101	BCR	C23-C22-C21	-2.02	115.84	119.01
27	M	101	LMG	O2-C2-C1	-2.02	105.27	110.08
23	B	608	CLA	C2B-C1B-NB	-2.02	108.24	110.33
23	B	613	CLA	CHB-C4A-NA	2.01	127.31	124.40
23	c	513	CLA	O2D-CGD-CBD	2.01	114.75	111.23
29	e	101	LHG	C5-O7-C7	-2.01	112.98	117.80
23	c	504	CLA	C6-C5-C3	-2.01	108.56	113.47
27	D	409	LMG	C38-C37-C36	-2.01	104.20	114.37
23	c	509	CLA	O2A-CGA-CBA	2.01	117.97	111.83
23	C	503	CLA	CHD-C1D-ND	-2.01	121.97	124.80
25	T	101	BCR	C35-C13-C12	2.01	121.16	118.09
27	c	521	LMG	O6-C5-C4	2.01	113.32	109.70
23	c	506	CLA	C1-C2-C3	-2.01	122.90	126.20
25	t	101	BCR	C11-C10-C9	-2.01	124.46	127.28
23	c	506	CLA	CMB-C2B-C1B	-2.01	122.36	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	m	101	LMG	C6-C5-C4	-2.01	108.09	113.02
26	A	410	PL9	C20-C19-C21	2.01	118.71	115.23
23	a	408	CLA	C1-O2A-CGA	-2.01	111.79	116.65
23	d	403	CLA	C3D-C4D-ND	2.01	113.25	109.99
25	H	101	BCR	C35-C13-C12	2.01	121.15	118.09
25	K	101	BCR	C30-C25-C26	-2.01	119.89	122.64
23	B	604	CLA	C11-C12-C13	-2.01	109.30	115.97
23	C	508	CLA	CHB-C1B-NB	2.01	127.06	124.05
23	b	606	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
23	B	605	CLA	CMD-C2D-C3D	2.00	132.28	127.69
29	A	413	LHG	C5-O7-C7	-2.00	113.01	117.80
29	A	413	LHG	O8-C23-O10	-2.00	118.62	123.63
28	F	101	SQD	C3-C4-C5	2.00	113.86	110.23
25	c	514	BCR	C3-C4-C5	-2.00	110.49	114.06

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	V	201	HEC	NA
36	v	201	HEC	NA

All (1648) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	C4B-C3B-CAB-CBB
23	B	614	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	C2B-C3B-CAB-CBB
23	a	406	CLA	C4B-C3B-CAB-CBB
23	b	608	CLA	C4-C3-C5-C6
23	b	611	CLA	C2B-C3B-CAB-CBB
23	b	611	CLA	C4B-C3B-CAB-CBB
23	b	615	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	C2B-C3B-CAB-CBB
23	b	616	CLA	C4B-C3B-CAB-CBB
23	c	505	CLA	C2B-C3B-CAB-CBB
23	c	505	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C11-C12-C13-C14
23	c	510	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	CBD-CGD-O2D-CED
25	A	409	BCR	C35-C13-C14-C15
25	A	409	BCR	C16-C17-C18-C36
25	B	617	BCR	C35-C13-C14-C15
25	B	617	BCR	C16-C17-C18-C19
25	B	617	BCR	C20-C21-C22-C37
25	B	618	BCR	C11-C12-C13-C35
25	B	619	BCR	C16-C17-C18-C19
25	D	404	BCR	C22-C23-C24-C25
25	H	101	BCR	C16-C17-C18-C36
25	K	101	BCR	C37-C22-C23-C24
25	K	102	BCR	C37-C22-C23-C24
25	T	101	BCR	C7-C8-C9-C10
25	Z	101	BCR	C10-C11-C12-C13
25	Z	101	BCR	C16-C17-C18-C19
25	Z	101	BCR	C16-C17-C18-C36
25	a	409	BCR	C21-C22-C23-C24
25	c	514	BCR	C7-C8-C9-C10
25	c	514	BCR	C7-C8-C9-C34
25	c	514	BCR	C11-C12-C13-C14
25	c	514	BCR	C20-C21-C22-C37
25	c	515	BCR	C36-C18-C19-C20
25	c	515	BCR	C20-C21-C22-C37
25	d	404	BCR	C21-C22-C23-C24
25	k	101	BCR	C21-C22-C23-C24
25	k	101	BCR	C37-C22-C23-C24
25	k	102	BCR	C7-C8-C9-C10
25	x	101	BCR	C11-C12-C13-C14
26	A	410	PL9	C32-C33-C34-C35
26	A	410	PL9	C35-C34-C36-C37
26	A	410	PL9	C37-C38-C39-C40
26	A	410	PL9	C37-C38-C39-C41
26	D	405	PL9	C22-C23-C24-C25
26	D	405	PL9	C32-C33-C34-C36
26	a	410	PL9	C17-C18-C19-C20
26	a	410	PL9	C22-C23-C24-C25
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C32-C33-C34-C35
26	a	410	PL9	C33-C34-C36-C37
26	d	405	PL9	C32-C33-C34-C36
26	d	405	PL9	C37-C38-C39-C40
27	A	411	LMG	O6-C1-O1-C7
27	A	411	LMG	O9-C10-O7-C8
27	C	518	LMG	C11-C10-O7-C8
27	D	409	LMG	O9-C10-O7-C8
27	D	409	LMG	C11-C10-O7-C8
27	b	622	LMG	O6-C1-O1-C7
27	b	622	LMG	C11-C10-O7-C8
27	c	523	LMG	O6-C1-O1-C7
28	A	412	SQD	O6-C44-C45-O47
28	A	414	SQD	C46-C45-O47-C7
28	B	624	SQD	O5-C1-O6-C44
28	B	624	SQD	O6-C44-C45-O47
28	B	624	SQD	O49-C7-O47-C45
28	B	624	SQD	C8-C7-O47-C45
28	a	412	SQD	C5-C6-S-O7
28	a	413	SQD	O6-C44-C45-O47
28	f	101	SQD	O5-C1-O6-C44
29	A	413	LHG	C4-O6-P-O3
29	A	413	LHG	O10-C23-O8-C6
29	A	413	LHG	C24-C23-O8-C6
29	B	622	LHG	C3-O3-P-O4
29	B	622	LHG	C4-O6-P-O3
29	B	622	LHG	C4-O6-P-O4
29	B	622	LHG	C4-O6-P-O5
29	B	623	LHG	O1-C1-C2-C3
29	B	623	LHG	C3-O3-P-O4
29	B	623	LHG	C3-O3-P-O6
29	D	407	LHG	O1-C1-C2-O2
29	D	407	LHG	O1-C1-C2-C3
29	D	407	LHG	C3-O3-P-O4
29	D	407	LHG	C3-O3-P-O6
29	D	407	LHG	C4-O6-P-O4
29	D	408	LHG	C3-O3-P-O6
29	d	406	LHG	O1-C1-C2-C3
29	d	406	LHG	C3-O3-P-O4
29	d	406	LHG	C3-O3-P-O6
29	d	407	LHG	C3-O3-P-O4
29	d	407	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
29	d	407	LHG	C4-O6-P-O4
29	d	407	LHG	C4-O6-P-O5
29	e	101	LHG	C3-O3-P-O4
29	e	101	LHG	C3-O3-P-O5
29	e	101	LHG	C3-O3-P-O6
29	e	101	LHG	O6-C4-C5-O7
29	e	101	LHG	O10-C23-O8-C6
29	e	101	LHG	C24-C23-O8-C6
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
30	a	414	DGD	O1G-C1G-C2G-O2G
23	b	617	CLA	O1D-CGD-O2D-CED
23	h	101	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
23	h	101	CLA	CBD-CGD-O2D-CED
27	c	523	LMG	O10-C28-O8-C9
30	a	414	DGD	O1A-C1A-O1G-C1G
26	d	405	PL9	C47-C48-C49-C51
23	d	402	CLA	C3-C5-C6-C7
27	M	101	LMG	O10-C28-O8-C9
28	b	601	SQD	O10-C23-O48-C46
23	B	614	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
27	C	518	LMG	O9-C10-O7-C8
27	b	622	LMG	O9-C10-O7-C8
28	a	413	SQD	O49-C7-O47-C45
23	C	512	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
27	c	519	LMG	C29-C28-O8-C9
27	c	523	LMG	C29-C28-O8-C9
28	a	413	SQD	C24-C23-O48-C46
28	b	601	SQD	C24-C23-O48-C46
30	a	414	DGD	C2A-C1A-O1G-C1G
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	CBD-CGD-O2D-CED
23	b	608	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
24	d	401	PHO	CBD-CGD-O2D-CED
27	A	411	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
28	a	413	SQD	C8-C7-O47-C45
23	A	408	CLA	C4-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	D	403	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	606	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
26	A	410	PL9	C20-C19-C21-C22
26	a	410	PL9	C30-C29-C31-C32
23	A	408	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	D	403	CLA	C2-C3-C5-C6
23	b	604	CLA	C2-C3-C5-C6
23	b	606	CLA	C2-C3-C5-C6
23	b	608	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
26	A	410	PL9	C13-C14-C16-C17
26	A	410	PL9	C18-C19-C21-C22
26	A	410	PL9	C38-C39-C41-C42
26	d	405	PL9	C38-C39-C41-C42
36	V	201	HEC	C2C-C3C-CAC-CBC
26	A	410	PL9	C22-C23-C24-C25
26	d	405	PL9	C32-C33-C34-C35
23	b	613	CLA	C13-C15-C16-C17
26	A	410	PL9	C12-C13-C14-C16
26	A	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C32-C33-C34-C36
26	d	405	PL9	C42-C43-C44-C46
30	h	102	DGD	O6E-C5E-C6E-O5E
27	c	521	LMG	O10-C28-O8-C9
28	F	101	SQD	O10-C23-O48-C46
28	a	413	SQD	O10-C23-O48-C46
27	A	411	LMG	O6-C5-C6-O5
23	b	603	CLA	C3-C5-C6-C7
29	d	406	LHG	O2-C2-C3-O3
23	B	601	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C29-C28-O8-C9
28	f	101	SQD	C24-C23-O48-C46
29	A	413	LHG	C8-C7-O7-C5
26	d	405	PL9	C47-C48-C49-C50
23	b	605	CLA	C3-C5-C6-C7
23	B	614	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	A	410	PL9	C40-C39-C41-C42
26	A	410	PL9	C33-C34-C36-C37
26	a	410	PL9	C28-C29-C31-C32
23	c	509	CLA	C13-C15-C16-C17
26	A	410	PL9	C9-C11-C12-C13
26	A	410	PL9	C34-C36-C37-C38
26	a	410	PL9	C19-C21-C22-C23
26	a	410	PL9	C24-C26-C27-C28
26	a	410	PL9	C34-C36-C37-C38
26	d	405	PL9	C9-C11-C12-C13
27	A	411	LMG	C4-C5-C6-O5
23	B	601	CLA	O1A-CGA-O2A-C1
30	C	517	DGD	O1A-C1A-O1G-C1G
29	A	413	LHG	C28-C29-C30-C31
23	C	501	CLA	CBD-CGD-O2D-CED
23	D	403	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	CBD-CGD-O2D-CED
30	h	102	DGD	C4E-C5E-C6E-O5E
27	A	411	LMG	C28-C29-C30-C31
23	b	613	CLA	C3-C5-C6-C7
36	V	201	HEC	C2B-C3B-CAB-CBB
29	d	406	LHG	C1-C2-C3-O3
23	B	614	CLA	CBA-CGA-O2A-C1
23	a	408	CLA	CBA-CGA-O2A-C1
27	C	518	LMG	C29-C28-O8-C9
27	c	521	LMG	C29-C28-O8-C9
28	F	101	SQD	C24-C23-O48-C46
23	c	501	CLA	CBD-CGD-O2D-CED
29	D	407	LHG	C28-C29-C30-C31
23	B	604	CLA	C13-C15-C16-C17
27	A	411	LMG	O10-C28-O8-C9
23	B	614	CLA	C2-C3-C5-C6
26	A	410	PL9	C23-C24-C26-C27
23	B	610	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C12-C13-C14
23	C	502	CLA	C6-C7-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C12-C13-C14
23	a	411	CLA	C14-C13-C15-C16
23	b	607	CLA	C6-C7-C8-C9
23	b	611	CLA	C14-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C12-C13-C14
23	c	511	CLA	C14-C13-C15-C16
23	h	101	CLA	C11-C10-C8-C9
24	A	406	PHO	C14-C13-C15-C16
27	M	101	LMG	O6-C5-C6-O5
23	c	511	CLA	O1D-CGD-O2D-CED
27	b	622	LMG	C2-C1-O1-C7
28	B	624	SQD	C2-C1-O6-C44
29	D	407	LHG	O2-C2-C3-O3
23	B	601	CLA	O1D-CGD-O2D-CED
24	d	401	PHO	O1D-CGD-O2D-CED
23	B	607	CLA	O1D-CGD-O2D-CED
25	A	409	BCR	C36-C18-C19-C20
25	K	101	BCR	C7-C8-C9-C34
25	K	102	BCR	C7-C8-C9-C34
25	T	101	BCR	C7-C8-C9-C34
25	b	620	BCR	C36-C18-C19-C20
25	b	620	BCR	C37-C22-C23-C24
25	c	514	BCR	C11-C12-C13-C35
25	c	514	BCR	C36-C18-C19-C20
25	c	515	BCR	C7-C8-C9-C34
25	d	404	BCR	C11-C12-C13-C35
25	d	404	BCR	C37-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C34
25	x	101	BCR	C11-C12-C13-C35
25	A	409	BCR	C17-C18-C19-C20
23	B	606	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C2A-CAA-CBA-CGA
29	d	406	LHG	C7-C8-C9-C10
30	c	518	DGD	O1A-C1A-O1G-C1G
28	a	412	SQD	O6-C44-C45-O47
30	A	415	DGD	O2G-C2G-C3G-O3G
23	c	510	CLA	C8-C10-C11-C12
23	b	617	CLA	C2-C1-O2A-CGA
23	a	408	CLA	O1A-CGA-O2A-C1
26	D	405	PL9	C32-C33-C34-C35
23	A	404	CLA	C15-C16-C17-C18
23	C	505	CLA	C5-C6-C7-C8
23	c	512	CLA	C13-C15-C16-C17
26	D	405	PL9	C47-C48-C49-C51
29	B	623	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
27	c	523	LMG	C28-C29-C30-C31
27	c	519	LMG	O6-C5-C6-O5
23	b	606	CLA	C11-C10-C8-C7
28	a	412	SQD	C24-C23-O48-C46
29	A	413	LHG	C26-C27-C28-C29
26	A	410	PL9	C15-C14-C16-C17
26	a	410	PL9	C35-C34-C36-C37
23	C	513	CLA	C13-C15-C16-C17
23	c	508	CLA	C13-C15-C16-C17
27	c	519	LMG	O10-C28-O8-C9
23	b	608	CLA	O1D-CGD-O2D-CED
26	A	410	PL9	C44-C46-C47-C48
26	a	410	PL9	C44-C46-C47-C48
26	d	405	PL9	C44-C46-C47-C48
27	c	523	LMG	C4-C5-C6-O5
23	B	614	CLA	C8-C10-C11-C12
23	C	505	CLA	C8-C10-C11-C12
23	b	608	CLA	C10-C11-C12-C13
23	c	506	CLA	C5-C6-C7-C8
27	d	409	LMG	C28-C29-C30-C31
27	m	101	LMG	C10-C11-C12-C13
29	B	623	LHG	C7-C8-C9-C10
29	d	406	LHG	C23-C24-C25-C26
30	a	414	DGD	C1B-C2B-C3B-C4B
23	b	609	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
23	c	513	CLA	C8-C10-C11-C12
23	d	403	CLA	C8-C10-C11-C12
23	B	606	CLA	C15-C16-C17-C18
23	B	607	CLA	C8-C10-C11-C12
23	B	611	CLA	C8-C10-C11-C12
23	B	614	CLA	C13-C15-C16-C17
23	b	612	CLA	C13-C15-C16-C17
23	c	512	CLA	C5-C6-C7-C8
23	d	403	CLA	C5-C6-C7-C8
27	B	621	LMG	C28-C29-C30-C31
27	b	622	LMG	C10-C11-C12-C13
28	A	412	SQD	C7-C8-C9-C10
30	c	517	DGD	C1B-C2B-C3B-C4B
23	C	502	CLA	C3-C5-C6-C7
29	B	622	LHG	C29-C30-C31-C32
23	B	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	B	612	CLA	C13-C15-C16-C17
23	C	509	CLA	C13-C15-C16-C17
23	a	411	CLA	C15-C16-C17-C18
23	b	606	CLA	C15-C16-C17-C18
23	b	612	CLA	C8-C10-C11-C12
23	b	617	CLA	C10-C11-C12-C13
23	c	504	CLA	C5-C6-C7-C8
23	h	101	CLA	C8-C10-C11-C12
29	A	413	LHG	O2-C2-C3-O3
23	B	614	CLA	O1A-CGA-O2A-C1
23	B	605	CLA	C5-C6-C7-C8
23	B	606	CLA	C8-C10-C11-C12
23	a	408	CLA	C13-C15-C16-C17
30	a	414	DGD	O1B-C1B-O2G-C2G
23	B	607	CLA	C13-C15-C16-C17
23	C	506	CLA	C15-C16-C17-C18
23	b	608	CLA	C5-C6-C7-C8
23	b	610	CLA	C15-C16-C17-C18
23	c	510	CLA	C15-C16-C17-C18
27	D	409	LMG	C28-C29-C30-C31
23	c	512	CLA	CBA-CGA-O2A-C1
30	A	415	DGD	C2A-C1A-O1G-C1G
23	b	613	CLA	CBD-CGD-O2D-CED
30	C	517	DGD	C2A-C1A-O1G-C1G
23	B	612	CLA	C10-C11-C12-C13
23	B	613	CLA	C8-C10-C11-C12
23	C	504	CLA	C8-C10-C11-C12
23	D	403	CLA	C5-C6-C7-C8
23	a	408	CLA	C10-C11-C12-C13
23	b	607	CLA	C15-C16-C17-C18
23	b	612	CLA	C15-C16-C17-C18
23	B	603	CLA	C5-C6-C7-C8
23	c	503	CLA	C8-C10-C11-C12
23	h	101	CLA	C15-C16-C17-C18
23	C	508	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
23	b	614	CLA	C13-C15-C16-C17
30	C	515	DGD	O6D-C5D-C6D-O5D
26	A	410	PL9	C25-C24-C26-C27
27	b	622	LMG	O6-C5-C6-O5
28	f	101	SQD	O10-C23-O48-C46
26	d	405	PL9	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
30	c	517	DGD	C2E-C1E-O5D-C6D
23	b	604	CLA	C8-C10-C11-C12
29	e	101	LHG	C23-C24-C25-C26
23	A	405	CLA	C16-C17-C18-C20
23	B	605	CLA	C15-C16-C17-C18
25	B	617	BCR	C11-C10-C9-C34
25	B	617	BCR	C16-C17-C18-C36
25	B	618	BCR	C11-C10-C9-C34
25	B	619	BCR	C35-C13-C14-C15
25	B	619	BCR	C16-C17-C18-C36
25	K	101	BCR	C20-C21-C22-C37
25	K	102	BCR	C20-C21-C22-C37
25	Z	101	BCR	C11-C10-C9-C34
25	Z	101	BCR	C35-C13-C14-C15
25	a	409	BCR	C35-C13-C14-C15
25	a	409	BCR	C16-C17-C18-C36
25	a	409	BCR	C20-C21-C22-C37
25	c	515	BCR	C11-C10-C9-C34
25	c	515	BCR	C35-C13-C14-C15
25	d	404	BCR	C16-C17-C18-C36
25	d	404	BCR	C20-C21-C22-C37
25	k	101	BCR	C16-C17-C18-C36
25	x	101	BCR	C20-C21-C22-C37
23	b	611	CLA	C2C-C3C-CAC-CBC
27	M	101	LMG	C4-C5-C6-O5
23	c	505	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	C5-C6-C7-C8
23	C	509	CLA	C10-C11-C12-C13
25	B	617	BCR	C36-C18-C19-C20
25	Z	101	BCR	C7-C8-C9-C34
25	c	514	BCR	C17-C18-C19-C20
23	b	607	CLA	C2A-CAA-CBA-CGA
23	h	101	CLA	C2A-CAA-CBA-CGA
29	d	408	LHG	O1-C1-C2-C3
29	D	408	LHG	C7-C8-C9-C10
23	B	616	CLA	CBD-CGD-O2D-CED
28	B	624	SQD	C24-C23-O48-C46
23	C	509	CLA	C16-C17-C18-C19
23	c	507	CLA	C16-C17-C18-C20
23	c	512	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	C15-C16-C17-C18
25	A	409	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	B	617	BCR	C12-C13-C14-C15
25	B	617	BCR	C20-C21-C22-C23
25	B	618	BCR	C12-C13-C14-C15
25	B	618	BCR	C16-C17-C18-C19
25	B	619	BCR	C11-C10-C9-C8
25	K	102	BCR	C16-C17-C18-C19
25	b	619	BCR	C12-C13-C14-C15
25	b	620	BCR	C16-C17-C18-C19
25	c	514	BCR	C20-C21-C22-C23
25	x	101	BCR	C11-C10-C9-C8
30	c	517	DGD	O6E-C1E-O5D-C6D
28	a	412	SQD	O47-C45-C46-O48
36	V	201	HEC	C4C-C3C-CAC-CBC
30	C	515	DGD	C1B-C2B-C3B-C4B
23	B	601	CLA	C2-C1-O2A-CGA
23	A	405	CLA	C16-C17-C18-C19
27	c	521	LMG	C36-C37-C38-C39
27	d	409	LMG	C30-C31-C32-C33
28	A	414	SQD	C28-C29-C30-C31
28	a	412	SQD	C10-C11-C12-C13
28	a	412	SQD	C26-C27-C28-C29
29	d	407	LHG	C11-C12-C13-C14
27	D	406	LMG	C14-C15-C16-C17
28	b	601	SQD	C18-C19-C20-C21
29	A	413	LHG	C32-C33-C34-C35
28	A	412	SQD	C23-C24-C25-C26
27	M	101	LMG	C39-C40-C41-C42
27	c	523	LMG	C32-C33-C34-C35
27	c	523	LMG	C34-C35-C36-C37
28	B	624	SQD	C11-C10-C9-C8
29	d	408	LHG	C26-C27-C28-C29
29	e	101	LHG	C26-C27-C28-C29
30	C	516	DGD	C8B-C9B-CAB-CBB
30	c	516	DGD	O6D-C5D-C6D-O5D
27	B	621	LMG	C29-C30-C31-C32
27	B	621	LMG	C36-C37-C38-C39
27	D	406	LMG	C11-C12-C13-C14
27	d	409	LMG	C34-C35-C36-C37
28	A	412	SQD	C24-C25-C26-C27
28	a	412	SQD	C18-C19-C20-C21
28	a	413	SQD	C15-C16-C17-C18
28	b	601	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	A	413	LHG	C33-C34-C35-C36
29	B	622	LHG	C14-C15-C16-C17
29	d	406	LHG	C16-C17-C18-C19
27	c	521	LMG	O9-C10-O7-C8
29	d	406	LHG	O1-C1-C2-O2
27	M	101	LMG	C13-C14-C15-C16
27	M	101	LMG	C16-C17-C18-C19
27	c	523	LMG	C12-C13-C14-C15
28	A	414	SQD	C14-C15-C16-C17
28	a	412	SQD	C15-C16-C17-C18
29	B	623	LHG	C12-C13-C14-C15
30	C	516	DGD	C6A-C7A-C8A-C9A
30	h	102	DGD	C2B-C3B-C4B-C5B
23	d	402	CLA	C4B-C3B-CAB-CBB
29	d	407	LHG	C23-C24-C25-C26
27	D	406	LMG	C18-C19-C20-C21
27	c	523	LMG	O6-C5-C6-O5
23	C	502	CLA	C16-C17-C18-C19
23	B	604	CLA	C10-C11-C12-C13
23	B	606	CLA	C6-C7-C8-C10
23	b	605	CLA	C12-C13-C15-C16
27	b	622	LMG	C15-C16-C17-C18
28	b	601	SQD	C10-C11-C12-C13
29	d	406	LHG	C32-C33-C34-C35
29	B	622	LHG	C27-C28-C29-C30
30	A	415	DGD	C5B-C6B-C7B-C8B
30	C	517	DGD	CCA-CDA-CEA-CFA
23	c	512	CLA	C3A-C2A-CAA-CBA
23	h	101	CLA	C3A-C2A-CAA-CBA
23	b	616	CLA	C8-C10-C11-C12
27	D	406	LMG	C30-C31-C32-C33
30	c	516	DGD	C4B-C5B-C6B-C7B
23	c	510	CLA	C16-C17-C18-C19
29	d	407	LHG	C30-C31-C32-C33
30	A	415	DGD	C9B-CAB-CBB-CCB
29	A	413	LHG	C1-C2-C3-O3
28	a	412	SQD	C44-C45-C46-O48
27	B	621	LMG	C33-C34-C35-C36
27	b	622	LMG	C11-C12-C13-C14
27	b	622	LMG	C34-C35-C36-C37
29	l	101	LHG	C28-C29-C30-C31
30	h	102	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
29	A	413	LHG	C23-C24-C25-C26
27	A	411	LMG	C16-C17-C18-C19
27	b	622	LMG	C16-C17-C18-C19
28	B	624	SQD	C17-C18-C19-C20
28	b	601	SQD	C26-C27-C28-C29
29	d	406	LHG	C25-C26-C27-C28
29	l	101	LHG	C9-C10-C11-C12
30	A	415	DGD	CAA-CBA-CCA-CDA
30	C	515	DGD	C4A-C5A-C6A-C7A
30	H	102	DGD	C3B-C4B-C5B-C6B
30	c	516	DGD	C5B-C6B-C7B-C8B
30	c	517	DGD	C6A-C7A-C8A-C9A
30	c	518	DGD	C3A-C4A-C5A-C6A
27	c	519	LMG	C11-C10-O7-C8
29	d	407	LHG	C29-C30-C31-C32
28	B	624	SQD	C26-C27-C28-C29
29	l	101	LHG	C32-C33-C34-C35
30	h	102	DGD	CAB-CBB-CCB-CDB
23	B	603	CLA	C8-C10-C11-C12
23	b	604	CLA	O1D-CGD-O2D-CED
23	B	606	CLA	C2B-C3B-CAB-CBB
25	D	404	BCR	C23-C24-C25-C26
25	D	404	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	T	101	BCR	C1-C6-C7-C8
25	T	101	BCR	C5-C6-C7-C8
25	c	514	BCR	C1-C6-C7-C8
25	k	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
29	D	408	LHG	C34-C35-C36-C37
29	d	407	LHG	C12-C13-C14-C15
30	A	415	DGD	CDB-CEB-CFB-CGB
30	c	516	DGD	CCB-CDB-CEB-CFB
27	c	521	LMG	C11-C10-O7-C8
23	c	513	CLA	C13-C15-C16-C17
27	c	521	LMG	C32-C33-C34-C35
27	c	521	LMG	C34-C35-C36-C37
29	D	407	LHG	C29-C30-C31-C32
29	e	101	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	d	407	LHG	C26-C27-C28-C29
29	e	101	LHG	C13-C14-C15-C16
30	h	102	DGD	C7A-C8A-C9A-CAA
30	a	414	DGD	C1A-C2A-C3A-C4A
27	m	101	LMG	C29-C30-C31-C32
28	A	412	SQD	C26-C27-C28-C29
28	b	601	SQD	C12-C13-C14-C15
29	A	413	LHG	C12-C13-C14-C15
29	e	101	LHG	C17-C18-C19-C20
30	a	414	DGD	C4A-C5A-C6A-C7A
30	c	517	DGD	C7B-C8B-C9B-CAB
30	c	518	DGD	C7A-C8A-C9A-CAA
27	b	623	LMG	C32-C33-C34-C35
28	A	414	SQD	C12-C13-C14-C15
28	f	101	SQD	C24-C25-C26-C27
30	c	518	DGD	C5B-C6B-C7B-C8B
29	e	101	LHG	O9-C7-O7-C5
23	C	506	CLA	C4-C3-C5-C6
27	b	622	LMG	C31-C32-C33-C34
27	c	521	LMG	C38-C39-C40-C41
29	D	407	LHG	C30-C31-C32-C33
30	C	516	DGD	C9A-CAA-CBA-CCA
30	c	517	DGD	CCA-CDA-CEA-CFA
25	K	102	BCR	C18-C19-C20-C21
25	d	404	BCR	C18-C19-C20-C21
25	k	101	BCR	C18-C19-C20-C21
25	x	101	BCR	C18-C19-C20-C21
26	A	410	PL9	C43-C44-C46-C47
28	a	413	SQD	C10-C11-C12-C13
29	D	408	LHG	C11-C12-C13-C14
30	C	517	DGD	C2A-C3A-C4A-C5A
30	H	102	DGD	C7A-C8A-C9A-CAA
27	A	411	LMG	C29-C28-O8-C9
27	m	101	LMG	C29-C28-O8-C9
30	c	518	DGD	C2A-C1A-O1G-C1G
28	f	101	SQD	C32-C33-C34-C35
29	d	408	LHG	C33-C34-C35-C36
30	C	517	DGD	C8A-C9A-CAA-CBA
28	A	412	SQD	C25-C26-C27-C28
28	a	412	SQD	C30-C31-C32-C33
29	B	623	LHG	C25-C26-C27-C28
29	d	406	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	C8B-C9B-CAB-CBB
30	a	414	DGD	C7B-C8B-C9B-CAB
30	h	102	DGD	C5B-C6B-C7B-C8B
30	h	102	DGD	C7B-C8B-C9B-CAB
25	Z	101	BCR	C22-C23-C24-C25
30	C	516	DGD	O6E-C1E-O5D-C6D
30	C	515	DGD	C4D-C5D-C6D-O5D
30	c	516	DGD	C4D-C5D-C6D-O5D
29	B	623	LHG	C29-C30-C31-C32
29	D	407	LHG	C12-C13-C14-C15
27	c	523	LMG	C2-C1-O1-C7
28	f	101	SQD	C2-C1-O6-C44
30	C	516	DGD	C2E-C1E-O5D-C6D
23	b	615	CLA	C15-C16-C17-C18
27	b	623	LMG	C36-C37-C38-C39
29	A	413	LHG	C16-C17-C18-C19
29	D	407	LHG	C11-C10-C9-C8
30	c	518	DGD	C2A-C3A-C4A-C5A
23	h	101	CLA	C3-C5-C6-C7
25	c	514	BCR	C13-C14-C15-C16
23	C	509	CLA	C16-C17-C18-C20
23	h	101	CLA	C16-C17-C18-C20
30	a	414	DGD	C2B-C1B-O2G-C2G
27	c	521	LMG	C10-C11-C12-C13
23	b	611	CLA	C4C-C3C-CAC-CBC
28	B	624	SQD	C13-C14-C15-C16
23	B	603	CLA	C10-C11-C12-C13
29	d	406	LHG	C10-C11-C12-C13
27	C	518	LMG	C32-C33-C34-C35
27	c	519	LMG	C31-C32-C33-C34
28	F	101	SQD	C33-C34-C35-C36
23	C	507	CLA	C13-C15-C16-C17
23	b	616	CLA	C5-C6-C7-C8
25	Z	101	BCR	C37-C22-C23-C24
28	f	101	SQD	C28-C29-C30-C31
30	H	102	DGD	CBA-CCA-CDA-CEA
27	c	519	LMG	C35-C36-C37-C38
29	d	406	LHG	C31-C32-C33-C34
30	C	516	DGD	C8A-C9A-CAA-CBA
25	b	618	BCR	C21-C22-C23-C24
23	b	615	CLA	CBA-CGA-O2A-C1
28	B	624	SQD	C45-C44-O6-C1

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Mol	Chain	Res	Type	Atoms
28	B	624	SQD	C25-C26-C27-C28
23	B	603	CLA	C16-C17-C18-C19
23	B	603	CLA	C16-C17-C18-C20
23	a	405	CLA	C16-C17-C18-C19
23	a	405	CLA	C16-C17-C18-C20
27	c	521	LMG	C11-C12-C13-C14
29	A	413	LHG	C10-C11-C12-C13
30	A	415	DGD	C2A-C3A-C4A-C5A
30	A	415	DGD	C6B-C7B-C8B-C9B
27	d	409	LMG	C35-C36-C37-C38
27	B	621	LMG	C32-C33-C34-C35
29	B	622	LHG	C32-C33-C34-C35
23	B	602	CLA	C13-C15-C16-C17
23	c	509	CLA	C10-C11-C12-C13
30	c	518	DGD	C1A-C2A-C3A-C4A
28	B	624	SQD	C34-C35-C36-C37
29	A	413	LHG	O9-C7-O7-C5
27	m	101	LMG	C15-C16-C17-C18
26	a	410	PL9	C14-C16-C17-C18
23	b	610	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	C5-C6-C7-C8
23	C	503	CLA	C5-C6-C7-C8
23	c	509	CLA	C15-C16-C17-C18
23	B	611	CLA	C16-C17-C18-C20
23	c	507	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
28	a	413	SQD	C12-C13-C14-C15
27	B	621	LMG	C34-C35-C36-C37
30	H	102	DGD	C4B-C5B-C6B-C7B
30	A	415	DGD	C1A-C2A-C3A-C4A
23	C	501	CLA	O1D-CGD-O2D-CED
28	A	414	SQD	C32-C33-C34-C35
30	C	517	DGD	C5A-C6A-C7A-C8A
30	C	516	DGD	O6E-C5E-C6E-O5E
27	c	519	LMG	O7-C8-C9-O8
27	M	101	LMG	C32-C33-C34-C35
28	F	101	SQD	C34-C35-C36-C37
28	a	413	SQD	C11-C10-C9-C8
28	b	601	SQD	C24-C25-C26-C27
30	H	102	DGD	C9A-CAA-CBA-CCA
28	A	412	SQD	C11-C12-C13-C14
27	D	409	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C18-C19-C20-C21
28	F	101	SQD	C26-C27-C28-C29
29	e	101	LHG	C12-C13-C14-C15
23	c	506	CLA	C2-C1-O2A-CGA
23	C	502	CLA	C16-C17-C18-C20
23	C	512	CLA	C10-C11-C12-C13
27	D	406	LMG	C20-C21-C22-C23
23	C	506	CLA	C2-C3-C5-C6
23	b	610	CLA	C2-C3-C5-C6
30	c	517	DGD	O1B-C1B-O2G-C2G
29	B	623	LHG	C1-C2-C3-O3
29	D	407	LHG	C1-C2-C3-O3
27	D	406	LMG	C33-C34-C35-C36
27	m	101	LMG	C31-C32-C33-C34
28	b	601	SQD	C13-C14-C15-C16
30	a	414	DGD	CBA-CCA-CDA-CEA
27	D	406	LMG	C34-C35-C36-C37
23	b	608	CLA	C8-C10-C11-C12
29	D	408	LHG	C23-C24-C25-C26
28	B	624	SQD	C9-C10-C11-C12
26	a	410	PL9	C47-C48-C49-C50
29	B	622	LHG	C30-C31-C32-C33
30	c	516	DGD	C4A-C5A-C6A-C7A
23	c	505	CLA	C16-C17-C18-C20
23	b	607	CLA	C10-C11-C12-C13
27	d	409	LMG	O6-C5-C6-O5
30	c	516	DGD	O6E-C5E-C6E-O5E
30	c	516	DGD	C8B-C9B-CAB-CBB
23	C	503	CLA	C1A-C2A-CAA-CBA
23	a	408	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	C1A-C2A-CAA-CBA
29	e	101	LHG	C7-C8-C9-C10
23	c	512	CLA	C8-C10-C11-C12
30	c	516	DGD	C7A-C8A-C9A-CAA
30	h	102	DGD	CCA-CDA-CEA-CFA
27	c	523	LMG	C14-C15-C16-C17
29	D	408	LHG	C16-C17-C18-C19
23	B	611	CLA	C15-C16-C17-C18
28	a	413	SQD	C19-C20-C21-C22
27	c	519	LMG	C34-C35-C36-C37
30	A	415	DGD	CDA-CEA-CFA-CGA
23	D	402	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C6-C7-C8-C10
23	C	504	CLA	C11-C10-C8-C7
23	C	508	CLA	C11-C10-C8-C7
23	C	510	CLA	C11-C10-C8-C7
23	D	401	CLA	C11-C12-C13-C15
23	D	403	CLA	C11-C10-C8-C7
23	a	408	CLA	C11-C10-C8-C7
23	b	603	CLA	C6-C7-C8-C10
23	b	605	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	613	CLA	C6-C7-C8-C10
27	c	523	LMG	C11-C12-C13-C14
23	c	506	CLA	C13-C15-C16-C17
23	b	611	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	C13-C15-C16-C17
23	b	605	CLA	C10-C11-C12-C13
27	b	623	LMG	C31-C32-C33-C34
26	d	405	PL9	C28-C29-C31-C32
27	c	523	LMG	C30-C31-C32-C33
29	B	623	LHG	C14-C15-C16-C17
23	C	503	CLA	C8-C10-C11-C12
23	d	403	CLA	C13-C15-C16-C17
23	B	615	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	a	408	CLA	C11-C10-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	b	610	CLA	C14-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C10-C8-C9
27	M	101	LMG	C36-C37-C38-C39
27	b	623	LMG	C34-C35-C36-C37
30	c	516	DGD	C9A-CAA-CBA-CCA
29	A	413	LHG	C7-C8-C9-C10
29	D	408	LHG	C27-C28-C29-C30
23	B	606	CLA	C13-C15-C16-C17
27	c	521	LMG	O6-C5-C6-O5
30	C	515	DGD	O6E-C5E-C6E-O5E
27	M	101	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C15-C16-C17-C18
30	A	415	DGD	C2B-C3B-C4B-C5B
30	C	516	DGD	C5A-C6A-C7A-C8A
30	c	518	DGD	C8B-C9B-CAB-CBB
23	b	613	CLA	O1D-CGD-O2D-CED
27	D	409	LMG	C7-C8-C9-O8
27	b	622	LMG	O1-C7-C8-C9
27	c	519	LMG	C7-C8-C9-O8
27	c	521	LMG	C7-C8-C9-O8
28	A	412	SQD	O6-C44-C45-C46
28	B	624	SQD	O6-C44-C45-C46
28	a	413	SQD	C44-C45-C46-O48
28	b	601	SQD	C44-C45-C46-O48
30	C	515	DGD	O1G-C1G-C2G-C3G
27	D	406	LMG	O6-C5-C6-O5
27	D	406	LMG	C17-C18-C19-C20
28	a	413	SQD	C18-C19-C20-C21
27	A	411	LMG	C14-C15-C16-C17
23	D	403	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	C16-C17-C18-C19
23	b	608	CLA	C16-C17-C18-C20
28	a	413	SQD	C11-C12-C13-C14
29	B	622	LHG	C33-C34-C35-C36
30	A	415	DGD	C8B-C9B-CAB-CBB
30	C	517	DGD	CAA-CBA-CCA-CDA
23	B	616	CLA	O1D-CGD-O2D-CED
26	a	410	PL9	C17-C18-C19-C21
25	Z	101	BCR	C20-C21-C22-C37
25	c	514	BCR	C16-C17-C18-C36
25	k	102	BCR	C35-C13-C14-C15
25	t	101	BCR	C11-C10-C9-C34
27	b	623	LMG	C11-C12-C13-C14
27	m	101	LMG	C11-C12-C13-C14
28	F	101	SQD	C25-C26-C27-C28
29	d	407	LHG	C14-C15-C16-C17
23	b	611	CLA	O1D-CGD-O2D-CED
23	b	610	CLA	C4-C3-C5-C6
26	D	405	PL9	C30-C29-C31-C32
23	c	503	CLA	C5-C6-C7-C8
25	A	409	BCR	C7-C8-C9-C34
28	f	101	SQD	C33-C34-C35-C36
29	A	413	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	D	408	LHG	C25-C26-C27-C28
29	d	407	LHG	C32-C33-C34-C35
30	c	518	DGD	CCB-CDB-CEB-CFB
25	k	101	BCR	C17-C18-C19-C20
23	b	615	CLA	O1A-CGA-O2A-C1
27	C	518	LMG	O10-C28-O8-C9
30	h	102	DGD	C6A-C7A-C8A-C9A
29	D	407	LHG	C32-C33-C34-C35
23	a	408	CLA	C5-C6-C7-C8
28	a	412	SQD	C13-C14-C15-C16
28	a	413	SQD	C24-C25-C26-C27
29	d	407	LHG	C33-C34-C35-C36
30	a	414	DGD	CEA-CFA-CGA-CHA
23	c	503	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	O2A-C1-C2-C3
27	D	409	LMG	C9-C8-O7-C10
27	b	622	LMG	C9-C8-O7-C10
27	b	622	LMG	C39-C40-C41-C42
25	b	619	BCR	C10-C11-C12-C13
27	d	409	LMG	C14-C15-C16-C17
27	m	101	LMG	C40-C41-C42-C43
25	c	514	BCR	C12-C13-C14-C15
28	a	412	SQD	C12-C13-C14-C15
27	c	519	LMG	C36-C37-C38-C39
27	C	518	LMG	C34-C35-C36-C37
29	B	622	LHG	C18-C19-C20-C21
29	D	407	LHG	C25-C26-C27-C28
30	h	102	DGD	CBA-CCA-CDA-CEA
26	d	405	PL9	C40-C39-C41-C42
28	A	412	SQD	C35-C36-C37-C38
28	A	412	SQD	C15-C16-C17-C18
23	c	506	CLA	C16-C17-C18-C19
27	A	411	LMG	C17-C18-C19-C20
30	H	102	DGD	CAA-CBA-CCA-CDA
26	a	410	PL9	C12-C13-C14-C16
27	b	622	LMG	C18-C19-C20-C21
27	c	523	LMG	C13-C14-C15-C16
27	c	523	LMG	C38-C39-C40-C41
27	A	411	LMG	O1-C7-C8-O7
27	M	101	LMG	C35-C36-C37-C38
29	e	101	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
30	a	414	DGD	C2A-C3A-C4A-C5A
26	A	410	PL9	C19-C21-C22-C23
29	A	413	LHG	C19-C20-C21-C22
29	e	101	LHG	C28-C29-C30-C31
27	M	101	LMG	C10-C11-C12-C13
27	d	409	LMG	C33-C34-C35-C36
29	D	408	LHG	C9-C10-C11-C12
27	D	409	LMG	C37-C38-C39-C40
23	c	508	CLA	C16-C17-C18-C19
27	b	623	LMG	C37-C38-C39-C40
23	C	510	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
26	d	405	PL9	C30-C29-C31-C32
29	d	406	LHG	C24-C25-C26-C27
30	C	516	DGD	O1B-C1B-O2G-C2G
28	F	101	SQD	C45-C44-O6-C1
23	B	603	CLA	C6-C7-C8-C9
23	B	615	CLA	C6-C7-C8-C9
23	C	504	CLA	C11-C10-C8-C9
23	C	508	CLA	C11-C10-C8-C9
23	C	509	CLA	C14-C13-C15-C16
23	C	510	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C10-C8-C9
23	D	401	CLA	C11-C12-C13-C14
23	D	403	CLA	C11-C10-C8-C9
23	a	406	CLA	C14-C13-C15-C16
23	b	605	CLA	C6-C7-C8-C9
23	b	605	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C14
23	b	607	CLA	C11-C10-C8-C9
23	c	508	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C12-C13-C14
23	d	402	CLA	C6-C7-C8-C9
23	c	501	CLA	O1D-CGD-O2D-CED
23	D	401	CLA	C13-C15-C16-C17
23	B	603	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
23	h	101	CLA	C4B-C3B-CAB-CBB
29	B	623	LHG	C32-C33-C34-C35
29	D	408	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	H	102	DGD	CCB-CDB-CEB-CFB
27	D	406	LMG	C15-C16-C17-C18
27	b	623	LMG	C30-C31-C32-C33
29	l	101	LHG	O6-C4-C5-C6
30	C	517	DGD	C3A-C4A-C5A-C6A
23	B	615	CLA	C6-C7-C8-C10
23	B	615	CLA	C11-C12-C13-C15
23	C	505	CLA	C12-C13-C15-C16
23	C	509	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	D	403	CLA	C12-C13-C15-C16
23	a	406	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C10-C8-C7
23	b	610	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C7
23	c	505	CLA	C6-C7-C8-C10
23	c	508	CLA	C12-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C10
23	d	402	CLA	C6-C7-C8-C10
23	h	101	CLA	C10-C11-C12-C13
29	B	623	LHG	C19-C20-C21-C22
29	D	408	LHG	O2-C2-C3-O3
26	A	410	PL9	C47-C48-C49-C50
27	d	409	LMG	C40-C41-C42-C43
23	a	408	CLA	C16-C17-C18-C19
23	b	612	CLA	C16-C17-C18-C19
30	A	415	DGD	CCB-CDB-CEB-CFB
30	C	517	DGD	C9B-CAB-CBB-CCB
23	B	602	CLA	C3A-C2A-CAA-CBA
23	C	505	CLA	C4-C3-C5-C6
23	c	512	CLA	C4-C3-C5-C6
26	a	410	PL9	C15-C14-C16-C17
23	b	604	CLA	C13-C15-C16-C17
23	c	510	CLA	C5-C6-C7-C8
23	C	505	CLA	C2-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
26	D	405	PL9	C28-C29-C31-C32
30	c	518	DGD	CCA-CDA-CEA-CFA
23	c	503	CLA	O1A-CGA-O2A-C1
28	A	414	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
29	l	101	LHG	C29-C30-C31-C32
23	c	506	CLA	CBA-CGA-O2A-C1
23	A	404	CLA	C2C-C3C-CAC-CBC
29	D	408	LHG	C33-C34-C35-C36
25	B	619	BCR	C7-C8-C9-C34
30	H	102	DGD	O2G-C1B-C2B-C3B
23	c	511	CLA	C13-C15-C16-C17
28	f	101	SQD	C31-C32-C33-C34
30	C	515	DGD	CBA-CCA-CDA-CEA
30	c	516	DGD	CAB-CBB-CCB-CDB
27	M	101	LMG	C7-C8-C9-O8
28	a	412	SQD	O6-C44-C45-C46
30	A	415	DGD	C1G-C2G-C3G-O3G
30	a	414	DGD	O1G-C1G-C2G-C3G
30	c	518	DGD	C5A-C6A-C7A-C8A
27	D	406	LMG	C35-C36-C37-C38
23	C	511	CLA	C8-C10-C11-C12
28	B	624	SQD	C11-C12-C13-C14
30	a	414	DGD	C6A-C7A-C8A-C9A
30	c	518	DGD	CBB-CCB-CDB-CEB
23	c	507	CLA	C8-C10-C11-C12
29	B	622	LHG	C19-C20-C21-C22
23	c	512	CLA	C2-C3-C5-C6
26	d	405	PL9	C13-C14-C16-C17
29	d	406	LHG	C19-C20-C21-C22
28	A	414	SQD	O47-C45-C46-O48
23	B	616	CLA	C11-C12-C13-C14
23	c	506	CLA	C16-C17-C18-C20
23	h	101	CLA	C16-C17-C18-C19
29	l	101	LHG	O6-C4-C5-O7
25	K	102	BCR	C23-C24-C25-C30
25	b	618	BCR	C1-C6-C7-C8
25	k	101	BCR	C23-C24-C25-C30
28	F	101	SQD	O6-C44-C45-C46
27	M	101	LMG	C40-C41-C42-C43
23	B	615	CLA	C16-C17-C18-C20
23	b	606	CLA	C5-C6-C7-C8
27	D	409	LMG	O7-C8-C9-O8
27	c	523	LMG	O7-C8-C9-O8
26	D	405	PL9	C4-C3-C7-C8
26	a	410	PL9	C4-C3-C7-C8
27	c	521	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
26	d	405	PL9	C15-C14-C16-C17
27	c	521	LMG	C40-C41-C42-C43
29	d	406	LHG	C33-C34-C35-C36
29	d	408	LHG	C29-C30-C31-C32
25	B	617	BCR	C18-C19-C20-C21
23	C	510	CLA	C2-C3-C5-C6
29	d	406	LHG	C17-C18-C19-C20
30	c	516	DGD	C9B-CAB-CBB-CCB
30	c	518	DGD	C6B-C7B-C8B-C9B
23	B	615	CLA	C16-C17-C18-C19
23	B	616	CLA	C11-C12-C13-C15
23	b	612	CLA	C16-C17-C18-C20
29	d	407	LHG	C25-C26-C27-C28
30	C	515	DGD	C9B-CAB-CBB-CCB
23	B	616	CLA	C6-C7-C8-C9
23	b	603	CLA	C11-C10-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	b	609	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
29	D	407	LHG	C15-C16-C17-C18
30	C	516	DGD	CCB-CDB-CEB-CFB
27	D	406	LMG	C39-C40-C41-C42
25	T	101	BCR	C6-C7-C8-C9
25	d	404	BCR	C22-C23-C24-C25
23	c	508	CLA	O1A-CGA-O2A-C1
27	c	519	LMG	C4-C5-C6-O5
25	D	404	BCR	C14-C15-C16-C17
25	a	409	BCR	C14-C15-C16-C17
28	A	414	SQD	C44-C45-O47-C7
29	B	623	LHG	C27-C28-C29-C30
23	A	408	CLA	C6-C7-C8-C9
27	c	523	LMG	C33-C34-C35-C36
27	m	101	LMG	C17-C18-C19-C20
26	A	410	PL9	C29-C31-C32-C33
30	c	518	DGD	C9A-CAA-CBA-CCA
27	D	406	LMG	C40-C41-C42-C43
27	b	622	LMG	C42-C43-C44-C45
29	d	408	LHG	C24-C23-O8-C6
30	C	515	DGD	O1G-C1A-C2A-C3A
26	a	410	PL9	C13-C14-C16-C17
27	c	523	LMG	C40-C41-C42-C43
27	c	521	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	e	101	LHG	C1-C2-C3-O3
27	A	411	LMG	C12-C13-C14-C15
28	F	101	SQD	C27-C28-C29-C30
29	d	407	LHG	C28-C29-C30-C31
30	a	414	DGD	C5B-C6B-C7B-C8B
25	A	409	BCR	C20-C21-C22-C37
25	B	619	BCR	C11-C10-C9-C34
25	K	102	BCR	C16-C17-C18-C36
25	b	618	BCR	C16-C17-C18-C36
25	b	618	BCR	C20-C21-C22-C37
25	b	620	BCR	C20-C21-C22-C37
25	c	514	BCR	C11-C10-C9-C34
25	k	102	BCR	C20-C21-C22-C37
25	t	101	BCR	C16-C17-C18-C36
25	t	101	BCR	C20-C21-C22-C37
23	c	509	CLA	CAA-CBA-CGA-O2A
29	B	622	LHG	C23-C24-C25-C26
30	H	102	DGD	C8B-C9B-CAB-CBB
23	B	610	CLA	C8-C10-C11-C12
29	e	101	LHG	O6-C4-C5-C6
23	b	610	CLA	O1D-CGD-O2D-CED
27	C	518	LMG	C37-C38-C39-C40
28	A	414	SQD	C16-C17-C18-C19
23	a	405	CLA	C15-C16-C17-C18
29	D	408	LHG	C30-C31-C32-C33
23	B	616	CLA	C6-C7-C8-C10
23	C	505	CLA	C11-C12-C13-C15
23	C	510	CLA	C12-C13-C15-C16
23	C	513	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C12-C13-C15
23	a	406	CLA	C11-C10-C8-C7
23	a	411	CLA	C12-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C12-C13-C15
23	b	611	CLA	C12-C13-C15-C16
23	c	505	CLA	C11-C10-C8-C7
23	c	509	CLA	C12-C13-C15-C16
23	c	510	CLA	C11-C12-C13-C15
30	C	517	DGD	CBA-CCA-CDA-CEA
30	C	516	DGD	CDA-CEA-CFA-CGA
23	b	617	CLA	CBA-CGA-O2A-C1
28	a	412	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
28	a	412	SQD	C5-C6-S-O8
30	C	516	DGD	C2G-C3G-O3G-C1D
30	C	516	DGD	C5D-C6D-O5D-C1E
30	c	517	DGD	C2G-C3G-O3G-C1D
30	c	517	DGD	C5D-C6D-O5D-C1E
30	c	517	DGD	CDB-CEB-CFB-CGB
29	B	623	LHG	C9-C10-C11-C12
23	C	511	CLA	O1A-CGA-O2A-C1
28	F	101	SQD	C45-C46-O48-C23
28	A	412	SQD	C10-C11-C12-C13
27	m	101	LMG	C22-C23-C24-C25
23	C	511	CLA	CBA-CGA-O2A-C1
29	D	407	LHG	C11-C12-C13-C14
29	e	101	LHG	C14-C15-C16-C17
27	A	411	LMG	C9-C8-O7-C10
28	b	601	SQD	C44-C45-O47-C7
30	a	414	DGD	C1G-C2G-O2G-C1B
23	c	506	CLA	O1A-CGA-O2A-C1
23	B	611	CLA	C16-C17-C18-C19
28	A	412	SQD	C11-C10-C9-C8
29	B	622	LHG	O10-C23-O8-C6
30	c	516	DGD	O1A-C1A-O1G-C1G
30	c	517	DGD	O1A-C1A-O1G-C1G
25	A	409	BCR	C11-C10-C9-C8
25	A	409	BCR	C20-C21-C22-C23
25	c	514	BCR	C11-C10-C9-C8
30	a	414	DGD	CFA-CGA-CHA-CIA
30	C	516	DGD	C3B-C4B-C5B-C6B
29	l	101	LHG	O9-C7-O7-C5
28	F	101	SQD	O48-C23-C24-C25
28	a	413	SQD	C9-C10-C11-C12
29	d	407	LHG	C34-C35-C36-C37
26	A	410	PL9	C39-C41-C42-C43
35	E	101	HEM	C4C-C3C-CAC-CBC
35	e	102	HEM	C4B-C3B-CAB-CBB
23	B	607	CLA	C16-C17-C18-C19
23	c	505	CLA	C16-C17-C18-C19
29	e	101	LHG	C19-C20-C21-C22
27	b	622	LMG	C41-C42-C43-C44
29	B	623	LHG	C24-C25-C26-C27
27	B	621	LMG	C14-C15-C16-C17
27	b	622	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
28	A	412	SQD	O47-C45-C46-O48
23	C	505	CLA	C11-C12-C13-C14
23	C	505	CLA	C14-C13-C15-C16
23	a	406	CLA	C11-C10-C8-C9
28	A	412	SQD	C14-C15-C16-C17
30	A	415	DGD	O6D-C5D-C6D-O5D
29	e	101	LHG	C10-C11-C12-C13
36	V	201	HEC	C4B-C3B-CAB-CBB
29	d	407	LHG	C31-C32-C33-C34
28	b	601	SQD	C15-C16-C17-C18
29	l	101	LHG	C11-C12-C13-C14
23	C	505	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
29	A	413	LHG	C2-C3-O3-P
28	A	414	SQD	C17-C18-C19-C20
23	B	601	CLA	C4-C3-C5-C6
23	C	504	CLA	C4-C3-C5-C6
23	C	513	CLA	C10-C11-C12-C13
30	H	102	DGD	C5A-C6A-C7A-C8A
27	D	409	LMG	C12-C13-C14-C15
29	D	407	LHG	C23-C24-C25-C26
23	C	506	CLA	C13-C15-C16-C17
23	B	611	CLA	CBA-CGA-O2A-C1
27	C	518	LMG	O6-C5-C6-O5
27	b	622	LMG	C13-C14-C15-C16
28	A	414	SQD	C10-C11-C12-C13
29	d	407	LHG	C17-C18-C19-C20
23	B	605	CLA	C4B-C3B-CAB-CBB
23	C	512	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	O1D-CGD-O2D-CED
30	H	102	DGD	C9B-CAB-CBB-CCB
25	B	619	BCR	C22-C23-C24-C25
25	H	101	BCR	C21-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C10
29	d	408	LHG	C32-C33-C34-C35
27	C	518	LMG	C29-C30-C31-C32
28	a	412	SQD	C32-C33-C34-C35
23	c	507	CLA	CBD-CGD-O2D-CED
27	d	409	LMG	O9-C10-O7-C8
28	a	412	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C12-C13-C15-C16
23	B	604	CLA	C12-C13-C15-C16
23	B	605	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C7
23	C	512	CLA	C12-C13-C15-C16
23	D	402	CLA	C6-C7-C8-C10
23	c	501	CLA	C11-C12-C13-C15
23	c	511	CLA	C12-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C15
23	h	101	CLA	C11-C10-C8-C7
24	A	406	PHO	C12-C13-C15-C16
24	a	407	PHO	C6-C7-C8-C10
30	A	415	DGD	CEB-CFB-CGB-CHB
23	B	610	CLA	C16-C17-C18-C19
29	d	407	LHG	C19-C20-C21-C22
30	a	414	DGD	C7A-C8A-C9A-CAA
27	d	409	LMG	C37-C38-C39-C40
28	a	412	SQD	C34-C35-C36-C37
30	c	517	DGD	CBB-CCB-CDB-CEB
28	a	412	SQD	C17-C18-C19-C20
30	a	414	DGD	C4B-C5B-C6B-C7B
27	D	406	LMG	C37-C38-C39-C40
30	C	515	DGD	C6A-C7A-C8A-C9A
30	C	515	DGD	CBB-CCB-CDB-CEB
23	b	617	CLA	O1A-CGA-O2A-C1
27	m	101	LMG	C38-C39-C40-C41
30	C	517	DGD	C2B-C3B-C4B-C5B
28	A	414	SQD	C7-C8-C9-C10
30	h	102	DGD	CBB-CCB-CDB-CEB
23	B	601	CLA	C3-C5-C6-C7
29	e	101	LHG	C8-C7-O7-C5
23	b	611	CLA	C2A-CAA-CBA-CGA
23	b	609	CLA	C11-C12-C13-C14
23	c	506	CLA	C6-C7-C8-C9
23	c	509	CLA	C14-C13-C15-C16
30	c	516	DGD	C6A-C7A-C8A-C9A
23	C	502	CLA	C15-C16-C17-C18
29	D	407	LHG	C27-C28-C29-C30
23	b	603	CLA	C13-C15-C16-C17
30	C	516	DGD	C3A-C4A-C5A-C6A
30	c	518	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
28	A	414	SQD	C15-C16-C17-C18
29	D	407	LHG	C33-C34-C35-C36
27	M	101	LMG	O7-C8-C9-O8
27	c	521	LMG	O7-C8-C9-O8
28	a	413	SQD	O47-C45-C46-O48
28	b	601	SQD	O6-C44-C45-O47
28	b	601	SQD	O47-C45-C46-O48
28	f	101	SQD	O6-C44-C45-O47
29	e	101	LHG	O7-C5-C6-O8
30	C	515	DGD	O1G-C1G-C2G-O2G
23	B	613	CLA	C5-C6-C7-C8
27	c	523	LMG	C7-C8-C9-O8
28	A	412	SQD	C44-C45-C46-O48
23	B	615	CLA	C4-C3-C5-C6
23	a	408	CLA	C4-C3-C5-C6
27	b	622	LMG	C35-C36-C37-C38
23	B	601	CLA	C2-C3-C5-C6
28	A	414	SQD	C9-C10-C11-C12
23	B	610	CLA	C2C-C3C-CAC-CBC
30	c	516	DGD	C1A-C2A-C3A-C4A
23	B	603	CLA	CBD-CGD-O2D-CED
30	A	415	DGD	CFA-CGA-CHA-CIA
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	O1D-CGD-O2D-CED
29	B	622	LHG	C15-C16-C17-C18
23	b	617	CLA	C5-C6-C7-C8
23	B	606	CLA	C16-C17-C18-C19
23	D	403	CLA	C16-C17-C18-C20
23	a	408	CLA	C16-C17-C18-C20
23	C	506	CLA	C3-C5-C6-C7
27	D	409	LMG	C15-C16-C17-C18
23	c	510	CLA	C10-C11-C12-C13
23	B	611	CLA	O1A-CGA-O2A-C1
28	F	101	SQD	C23-C24-C25-C26
27	m	101	LMG	C14-C15-C16-C17
23	A	405	CLA	C2C-C3C-CAC-CBC
29	e	101	LHG	C15-C16-C17-C18
23	B	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
24	d	401	PHO	CHA-CBD-CGD-O1D
24	d	401	PHO	CHA-CBD-CGD-O2D
25	A	409	BCR	C13-C14-C15-C16
25	k	102	BCR	C15-C16-C17-C18
29	A	413	LHG	C3-O3-P-O4
29	A	413	LHG	C3-O3-P-O5
29	A	413	LHG	C4-O6-P-O5
29	B	623	LHG	C3-O3-P-O5
29	D	408	LHG	C3-O3-P-O5
29	l	101	LHG	C4-O6-P-O5
30	C	516	DGD	C7A-C8A-C9A-CAA
23	B	603	CLA	C2B-C3B-CAB-CBB
23	D	402	CLA	C2B-C3B-CAB-CBB
23	d	402	CLA	C2B-C3B-CAB-CBB
23	h	101	CLA	C2B-C3B-CAB-CBB
30	h	102	DGD	O2G-C1B-C2B-C3B
29	d	408	LHG	C2-C3-O3-P
29	A	413	LHG	C13-C14-C15-C16
29	D	408	LHG	C11-C10-C9-C8
26	A	410	PL9	C4-C3-C7-C8
30	c	516	DGD	C1B-C2B-C3B-C4B
28	f	101	SQD	C46-C45-O47-C7
30	A	415	DGD	C8A-C9A-CAA-CBA
23	B	607	CLA	O1A-CGA-O2A-C1
23	B	603	CLA	C11-C12-C13-C14
23	B	604	CLA	C11-C12-C13-C14
23	B	605	CLA	C11-C12-C13-C14
23	C	513	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
23	b	614	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	c	505	CLA	C14-C13-C15-C16
23	c	508	CLA	C11-C12-C13-C14
30	A	415	DGD	C4B-C5B-C6B-C7B
23	C	502	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	c	505	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C7
29	D	408	LHG	C29-C30-C31-C32
25	c	515	BCR	C12-C13-C14-C15
30	A	415	DGD	O1A-C1A-O1G-C1G
23	C	504	CLA	C2-C3-C5-C6
29	D	407	LHG	C35-C36-C37-C38
23	c	513	CLA	C3-C5-C6-C7
23	c	506	CLA	C10-C11-C12-C13
30	c	516	DGD	O1G-C1G-C2G-O2G
23	B	607	CLA	CBA-CGA-O2A-C1
30	A	415	DGD	C4D-C5D-C6D-O5D
28	A	414	SQD	C18-C19-C20-C21
23	C	507	CLA	C5-C6-C7-C8
30	a	414	DGD	CEB-CFB-CGB-CHB
30	c	517	DGD	C9B-CAB-CBB-CCB
29	e	101	LHG	C4-C5-C6-O8
30	c	517	DGD	CDA-CEA-CFA-CGA
23	D	402	CLA	C2C-C3C-CAC-CBC
25	t	101	BCR	C7-C8-C9-C34
28	f	101	SQD	C25-C26-C27-C28
29	l	101	LHG	C33-C34-C35-C36
30	c	518	DGD	C8A-C9A-CAA-CBA
25	K	102	BCR	C7-C8-C9-C10
23	c	510	CLA	CBA-CGA-O2A-C1
30	H	102	DGD	C7B-C8B-C9B-CAB
30	c	516	DGD	C5D-C6D-O5D-C1E
28	B	624	SQD	C35-C36-C37-C38
23	b	603	CLA	C2A-CAA-CBA-CGA
25	c	515	BCR	C15-C16-C17-C18
27	c	523	LMG	C35-C36-C37-C38
29	l	101	LHG	C24-C25-C26-C27
30	C	516	DGD	C6B-C7B-C8B-C9B
26	d	405	PL9	C45-C44-C46-C47
23	a	406	CLA	C8-C10-C11-C12
29	d	407	LHG	C35-C36-C37-C38
29	d	408	LHG	O1-C1-C2-O2
23	d	402	CLA	C2C-C3C-CAC-CBC
23	B	614	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	D	403	CLA	C14-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	D	408	LHG	C2-C3-O3-P
27	B	621	LMG	C35-C36-C37-C38
23	B	601	CLA	C4B-C3B-CAB-CBB
23	D	402	CLA	C4B-C3B-CAB-CBB
30	c	516	DGD	C2A-C3A-C4A-C5A
23	d	402	CLA	C16-C17-C18-C19
27	C	518	LMG	C28-C29-C30-C31
23	c	508	CLA	C4-C3-C5-C6
26	A	410	PL9	C30-C29-C31-C32
30	C	515	DGD	C5B-C6B-C7B-C8B
28	F	101	SQD	C30-C31-C32-C33
25	c	514	BCR	C15-C16-C17-C18
23	b	609	CLA	C5-C6-C7-C8
29	l	101	LHG	C35-C36-C37-C38
30	h	102	DGD	CDA-CEA-CFA-CGA
29	B	623	LHG	C31-C32-C33-C34
23	c	509	CLA	C11-C12-C13-C15
23	c	510	CLA	O1A-CGA-O2A-C1
23	b	607	CLA	C3-C5-C6-C7
27	c	521	LMG	C30-C31-C32-C33
29	D	407	LHG	C34-C35-C36-C37
30	C	516	DGD	C9B-CAB-CBB-CCB
23	a	406	CLA	C13-C15-C16-C17
29	l	101	LHG	C13-C14-C15-C16
30	h	102	DGD	C5A-C6A-C7A-C8A
23	d	402	CLA	C16-C17-C18-C20
29	d	406	LHG	C27-C28-C29-C30
30	A	415	DGD	C4A-C5A-C6A-C7A
23	d	403	CLA	C3A-C2A-CAA-CBA
29	B	622	LHG	C25-C26-C27-C28
23	B	615	CLA	C2-C3-C5-C6
23	B	604	CLA	C2C-C3C-CAC-CBC
23	c	503	CLA	C15-C16-C17-C18
30	C	515	DGD	O6E-C1E-O5D-C6D
28	a	412	SQD	O49-C7-O47-C45
29	B	622	LHG	C12-C13-C14-C15
29	d	408	LHG	C23-C24-C25-C26
25	K	102	BCR	C13-C14-C15-C16
23	d	403	CLA	C16-C17-C18-C20
29	A	413	LHG	C35-C36-C37-C38
27	m	101	LMG	C16-C17-C18-C19
30	h	102	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
30	c	517	DGD	C8A-C9A-CAA-CBA
23	a	408	CLA	C2-C3-C5-C6
27	b	622	LMG	C4-C5-C6-O5
23	C	507	CLA	C15-C16-C17-C18
26	d	405	PL9	C34-C36-C37-C38
29	l	101	LHG	C4-C5-C6-O8
27	C	518	LMG	C18-C19-C20-C21
23	b	605	CLA	C13-C15-C16-C17
29	d	406	LHG	O10-C23-O8-C6
23	B	601	CLA	C6-C7-C8-C9
23	B	606	CLA	C11-C10-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	b	605	CLA	C11-C12-C13-C14
23	b	607	CLA	C14-C13-C15-C16
23	b	603	CLA	C16-C17-C18-C19
28	F	101	SQD	C32-C33-C34-C35
28	A	412	SQD	C17-C18-C19-C20
27	D	409	LMG	O1-C7-C8-C9
27	m	101	LMG	C36-C37-C38-C39
28	B	624	SQD	C18-C19-C20-C21
29	d	407	LHG	C7-C8-C9-C10
23	c	512	CLA	C16-C17-C18-C19
27	c	521	LMG	C41-C42-C43-C44
23	c	508	CLA	C2-C3-C5-C6
27	D	409	LMG	C11-C12-C13-C14
27	B	621	LMG	C37-C38-C39-C40
23	b	615	CLA	C2A-CAA-CBA-CGA
27	b	622	LMG	C19-C20-C21-C22
28	A	414	SQD	C11-C12-C13-C14
28	a	413	SQD	C27-C28-C29-C30
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	606	CLA	C16-C17-C18-C20
27	b	622	LMG	C17-C18-C19-C20
23	B	601	CLA	C2B-C3B-CAB-CBB
23	B	605	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	512	CLA	C2B-C3B-CAB-CBB
23	c	512	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C1-C6-C7-C8
25	K	102	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	b	618	BCR	C5-C6-C7-C8
25	c	514	BCR	C5-C6-C7-C8
30	c	518	DGD	C4B-C5B-C6B-C7B
29	B	623	LHG	O2-C2-C3-O3
29	D	407	LHG	C10-C11-C12-C13
29	l	101	LHG	C30-C31-C32-C33
30	a	414	DGD	CDB-CEB-CFB-CGB
23	B	607	CLA	C16-C17-C18-C20
23	B	613	CLA	C4-C3-C5-C6
26	D	405	PL9	C43-C44-C46-C47
27	c	523	LMG	C31-C32-C33-C34
35	e	102	HEM	CAD-CBD-CGD-O1D
23	A	404	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	C12-C13-C15-C16
23	B	604	CLA	C11-C12-C13-C15
23	B	605	CLA	C11-C12-C13-C15
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	b	605	CLA	C11-C12-C13-C15
23	b	607	CLA	C11-C12-C13-C15
23	d	402	CLA	C11-C12-C13-C15
23	h	101	CLA	C12-C13-C15-C16
23	C	505	CLA	C16-C17-C18-C20
28	A	414	SQD	C26-C27-C28-C29
30	a	414	DGD	C5A-C6A-C7A-C8A
35	E	101	HEM	CAD-CBD-CGD-O1D
27	b	623	LMG	C33-C34-C35-C36
26	A	410	PL9	C12-C13-C14-C15
26	a	410	PL9	C37-C38-C39-C40
23	B	610	CLA	C15-C16-C17-C18
23	c	511	CLA	C16-C17-C18-C20
29	d	407	LHG	O9-C7-O7-C5
30	c	517	DGD	C3B-C4B-C5B-C6B
25	b	618	BCR	C11-C12-C13-C35
36	v	201	HEC	CAD-CBD-CGD-O2D
29	A	413	LHG	C9-C10-C11-C12
29	B	622	LHG	C28-C29-C30-C31
28	a	413	SQD	C31-C32-C33-C34
23	b	615	CLA	C16-C17-C18-C19
23	b	613	CLA	C6-C7-C8-C9
23	C	510	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	a	412	SQD	C24-C25-C26-C27
30	C	515	DGD	C2B-C3B-C4B-C5B
27	c	523	LMG	C18-C19-C20-C21
30	c	516	DGD	C3B-C4B-C5B-C6B
30	c	518	DGD	C4A-C5A-C6A-C7A
26	D	405	PL9	C45-C44-C46-C47
26	a	410	PL9	C20-C19-C21-C22
26	a	410	PL9	C25-C24-C26-C27
25	A	409	BCR	C14-C15-C16-C17
23	C	501	CLA	CBA-CGA-O2A-C1
35	e	102	HEM	CAD-CBD-CGD-O2D
30	C	515	DGD	C2E-C1E-O5D-C6D
23	C	510	CLA	C15-C16-C17-C18
30	C	515	DGD	C9A-CAA-CBA-CCA
27	b	622	LMG	C7-C8-C9-O8
35	E	101	HEM	CAD-CBD-CGD-O2D
27	D	409	LMG	O1-C7-C8-O7
27	A	411	LMG	C39-C40-C41-C42
23	B	616	CLA	O1A-CGA-O2A-C1
23	c	501	CLA	C2A-CAA-CBA-CGA
23	B	603	CLA	C13-C15-C16-C17
30	c	516	DGD	O1G-C1A-C2A-C3A
23	c	506	CLA	C4-C3-C5-C6
23	c	511	CLA	C16-C17-C18-C19
29	D	407	LHG	C13-C14-C15-C16
23	A	405	CLA	C4C-C3C-CAC-CBC
23	B	615	CLA	C13-C15-C16-C17
23	b	610	CLA	C13-C15-C16-C17
23	c	502	CLA	O1A-CGA-O2A-C1
36	V	201	HEC	CAD-CBD-CGD-O2D
36	v	201	HEC	CAD-CBD-CGD-O1D
23	C	513	CLA	C16-C17-C18-C20
23	B	603	CLA	O1D-CGD-O2D-CED
27	d	409	LMG	C32-C33-C34-C35
25	C	514	BCR	C35-C13-C14-C15
25	C	514	BCR	C16-C17-C18-C36
25	D	404	BCR	C20-C21-C22-C37
25	T	101	BCR	C35-C13-C14-C15
25	c	515	BCR	C16-C17-C18-C36
28	B	624	SQD	O10-C23-O48-C46
23	a	406	CLA	C10-C11-C12-C13
23	B	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	l	101	LHG	O7-C5-C6-O8
30	C	517	DGD	CBB-CCB-CDB-CEB
27	m	101	LMG	O6-C1-O1-C7
23	B	607	CLA	C10-C11-C12-C13
23	C	505	CLA	C6-C7-C8-C10
23	b	617	CLA	C11-C10-C8-C7
36	V	201	HEC	CAD-CBD-CGD-O1D
27	m	101	LMG	C35-C36-C37-C38
23	B	602	CLA	C11-C12-C13-C14
23	B	604	CLA	C11-C10-C8-C9
23	D	402	CLA	C6-C7-C8-C9
23	a	406	CLA	C6-C7-C8-C9
24	A	407	PHO	C6-C7-C8-C9
24	a	407	PHO	C6-C7-C8-C9
30	A	415	DGD	CBB-CCB-CDB-CEB
27	A	411	LMG	C8-C7-O1-C1
27	M	101	LMG	C8-C7-O1-C1
23	C	506	CLA	C2-C1-O2A-CGA
23	D	402	CLA	C2-C1-O2A-CGA
30	C	517	DGD	O6D-C5D-C6D-O5D
23	b	603	CLA	C16-C17-C18-C20
28	F	101	SQD	C35-C36-C37-C38
29	d	408	LHG	C9-C10-C11-C12
27	c	523	LMG	C15-C16-C17-C18
28	b	601	SQD	C29-C30-C31-C32
23	h	101	CLA	C4-C3-C5-C6
30	c	516	DGD	C3A-C4A-C5A-C6A
29	B	623	LHG	C23-C24-C25-C26
23	b	615	CLA	C8-C10-C11-C12
24	A	406	PHO	C15-C16-C17-C18
30	a	414	DGD	O2G-C1B-C2B-C3B
28	f	101	SQD	C26-C27-C28-C29
23	B	601	CLA	C16-C17-C18-C20
29	d	407	LHG	C15-C16-C17-C18
30	c	517	DGD	CAA-CBA-CCA-CDA
25	c	515	BCR	C20-C21-C22-C23
26	D	405	PL9	C24-C26-C27-C28
27	A	411	LMG	O1-C7-C8-C9
27	C	518	LMG	O1-C7-C8-C9
27	c	523	LMG	O1-C7-C8-C9
27	m	101	LMG	O1-C7-C8-C9
30	c	516	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
30	c	516	DGD	C1G-C2G-C3G-O3G
23	C	501	CLA	O1A-CGA-O2A-C1
23	C	509	CLA	C8-C10-C11-C12
29	D	408	LHG	C35-C36-C37-C38
29	d	407	LHG	O1-C1-C2-O2
28	b	601	SQD	C17-C18-C19-C20
29	D	408	LHG	C15-C16-C17-C18
23	b	615	CLA	C16-C17-C18-C20
28	A	414	SQD	C27-C28-C29-C30
29	A	413	LHG	C34-C35-C36-C37
27	C	518	LMG	C15-C16-C17-C18
28	B	624	SQD	O47-C7-C8-C9
23	b	611	CLA	C8-C10-C11-C12
29	d	408	LHG	C30-C31-C32-C33
30	a	414	DGD	C8B-C9B-CAB-CBB
23	c	509	CLA	CAA-CBA-CGA-O1A
23	c	504	CLA	C11-C12-C13-C15
23	B	604	CLA	C11-C10-C8-C7
23	B	615	CLA	C12-C13-C15-C16
23	C	510	CLA	C11-C12-C13-C15
23	a	406	CLA	C6-C7-C8-C10
23	b	604	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
23	c	506	CLA	C3-C5-C6-C7
23	A	404	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C30
25	k	101	BCR	C23-C24-C25-C26
23	B	613	CLA	C2-C1-O2A-CGA
23	d	402	CLA	C2-C1-O2A-CGA
29	l	101	LHG	C16-C17-C18-C19
28	A	412	SQD	O47-C7-C8-C9
28	B	624	SQD	C32-C33-C34-C35
23	c	504	CLA	C11-C12-C13-C14
23	B	609	CLA	C4-C3-C5-C6
23	B	609	CLA	C2-C3-C5-C6
29	e	101	LHG	O2-C2-C3-O3
23	C	501	CLA	C2A-CAA-CBA-CGA
23	B	607	CLA	C15-C16-C17-C18
23	C	513	CLA	C15-C16-C17-C18
23	b	605	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	C16-C17-C18-C20
29	D	407	LHG	C14-C15-C16-C17
23	B	612	CLA	CAA-CBA-CGA-O2A
27	b	622	LMG	O7-C10-C11-C12
30	c	518	DGD	O1G-C1A-C2A-C3A
28	A	412	SQD	C27-C28-C29-C30
23	C	510	CLA	C8-C10-C11-C12
35	e	102	HEM	CAA-CBA-CGA-O2A
27	d	409	LMG	C15-C16-C17-C18
27	m	101	LMG	O7-C10-C11-C12
28	a	412	SQD	O47-C7-C8-C9
25	a	409	BCR	C11-C10-C9-C34
28	b	601	SQD	C11-C12-C13-C14
30	c	516	DGD	O2G-C1B-C2B-C3B
28	B	624	SQD	C12-C13-C14-C15
28	A	412	SQD	C12-C13-C14-C15
27	B	621	LMG	O8-C28-C29-C30
23	B	601	CLA	C14-C13-C15-C16
23	B	605	CLA	C14-C13-C15-C16
23	C	505	CLA	C6-C7-C8-C9
23	b	613	CLA	C11-C10-C8-C9
27	c	523	LMG	C17-C18-C19-C20
27	c	521	LMG	C37-C38-C39-C40
30	C	516	DGD	CAA-CBA-CCA-CDA
23	c	512	CLA	C2C-C3C-CAC-CBC
23	C	504	CLA	C4B-C3B-CAB-CBB
23	b	612	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C8-C10-C11-C12
30	C	516	DGD	O6D-C1D-O3G-C3G
29	B	622	LHG	O7-C7-C8-C9
27	B	621	LMG	O7-C10-C11-C12
25	t	101	BCR	C13-C14-C15-C16
23	B	604	CLA	CBD-CGD-O2D-CED
28	a	413	SQD	C29-C30-C31-C32
30	C	517	DGD	C4E-C5E-C6E-O5E
30	C	515	DGD	O2G-C1B-C2B-C3B
23	B	603	CLA	C2A-CAA-CBA-CGA
29	B	622	LHG	C24-C25-C26-C27
23	B	606	CLA	C5-C6-C7-C8
29	l	101	LHG	C7-C8-C9-C10
29	D	407	LHG	C26-C27-C28-C29
27	c	519	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
30	H	102	DGD	CCA-CDA-CEA-CFA
23	b	607	CLA	C6-C7-C8-C10
23	A	405	CLA	C13-C15-C16-C17
29	d	408	LHG	C28-C29-C30-C31
28	B	624	SQD	C30-C31-C32-C33
24	a	407	PHO	O2A-C1-C2-C3
27	c	523	LMG	C7-C8-O7-C10
30	h	102	DGD	CDB-CEB-CFB-CGB
29	A	413	LHG	C11-C12-C13-C14
29	B	623	LHG	C18-C19-C20-C21
23	c	507	CLA	C5-C6-C7-C8
27	C	518	LMG	C19-C20-C21-C22
23	c	509	CLA	C2A-CAA-CBA-CGA
23	C	501	CLA	C16-C17-C18-C20
26	D	405	PL9	C36-C37-C38-C39
23	c	506	CLA	C8-C10-C11-C12
24	a	407	PHO	C3A-C2A-CAA-CBA
27	A	411	LMG	C33-C34-C35-C36
27	A	411	LMG	C8-C9-O8-C28
24	A	406	PHO	C8-C10-C11-C12
28	B	624	SQD	O49-C7-C8-C9
28	A	412	SQD	C32-C33-C34-C35
23	B	603	CLA	C14-C13-C15-C16
23	B	604	CLA	C14-C13-C15-C16
23	C	512	CLA	C14-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C14
23	b	612	CLA	C6-C7-C8-C9
23	c	503	CLA	C11-C10-C8-C9
23	h	101	CLA	C14-C13-C15-C16
27	M	101	LMG	C38-C39-C40-C41
25	b	620	BCR	C13-C14-C15-C16
29	d	406	LHG	C11-C10-C9-C8
23	c	502	CLA	C15-C16-C17-C18
28	a	412	SQD	O10-C23-C24-C25
35	e	102	HEM	CAA-CBA-CGA-O1A
28	a	412	SQD	O49-C7-C8-C9
23	b	615	CLA	C13-C15-C16-C17
29	B	623	LHG	C16-C17-C18-C19
30	C	515	DGD	C4B-C5B-C6B-C7B
30	c	517	DGD	C2A-C3A-C4A-C5A
30	C	515	DGD	CDB-CEB-CFB-CGB
23	b	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	d	409	LMG	O7-C10-C11-C12
29	d	406	LHG	O10-C23-C24-C25
30	c	516	DGD	O1B-C1B-C2B-C3B
27	A	411	LMG	C38-C39-C40-C41
30	C	516	DGD	C2A-C3A-C4A-C5A
23	B	612	CLA	CAA-CBA-CGA-O1A
23	C	503	CLA	C15-C16-C17-C18
23	B	613	CLA	CAA-CBA-CGA-O2A
27	m	101	LMG	O8-C28-C29-C30
24	a	407	PHO	O1D-CGD-O2D-CED
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D
23	B	609	CLA	C3-C5-C6-C7
28	F	101	SQD	C44-C45-C46-O48
23	A	404	CLA	C2-C1-O2A-CGA
23	C	513	CLA	C2-C1-O2A-CGA
29	e	101	LHG	O10-C23-C24-C25
23	B	605	CLA	C16-C17-C18-C20
29	D	408	LHG	C31-C32-C33-C34
30	C	515	DGD	C8A-C9A-CAA-CBA
23	b	612	CLA	C10-C11-C12-C13
23	C	512	CLA	C4-C3-C5-C6
27	M	101	LMG	C28-C29-C30-C31
23	B	613	CLA	C11-C12-C13-C15
27	b	623	LMG	C39-C40-C41-C42
27	C	518	LMG	O7-C10-C11-C12
23	b	613	CLA	CAA-CBA-CGA-O1A
27	c	521	LMG	C39-C40-C41-C42
27	c	523	LMG	O8-C28-C29-C30
23	h	101	CLA	C13-C15-C16-C17
28	b	601	SQD	O49-C7-C8-C9
24	d	401	PHO	C2C-C3C-CAC-CBC

There are no ring outliers.

106 monomers are involved in 194 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	d	404	BCR	3	0
35	E	101	HEM	5	0
23	c	506	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	409	BCR	2	0
29	D	407	LHG	1	0
23	B	612	CLA	2	0
23	h	101	CLA	3	0
23	c	507	CLA	1	0
24	A	407	PHO	1	0
24	d	401	PHO	2	0
28	a	413	SQD	3	0
25	K	101	BCR	2	0
29	B	623	LHG	2	0
25	k	102	BCR	2	0
25	x	101	BCR	2	0
23	b	614	CLA	4	0
23	C	505	CLA	2	0
23	b	615	CLA	3	0
28	B	624	SQD	1	0
25	c	514	BCR	1	0
28	f	101	SQD	2	0
23	c	501	CLA	1	0
23	B	601	CLA	2	0
29	l	101	LHG	1	0
23	b	608	CLA	2	0
28	A	414	SQD	1	0
29	d	406	LHG	5	0
23	c	502	CLA	1	0
29	A	413	LHG	4	0
23	B	606	CLA	3	0
23	C	501	CLA	1	0
29	e	101	LHG	2	0
25	B	619	BCR	3	0
23	B	603	CLA	1	0
32	A	417[B]	OEY	2	0
23	b	604	CLA	3	0
25	H	101	BCR	2	0
29	D	408	LHG	2	0
23	C	508	CLA	2	0
25	b	618	BCR	4	0
30	H	102	DGD	1	0
35	e	102	HEM	3	0
29	d	407	LHG	3	0
23	b	606	CLA	6	0
23	b	607	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	d	409	LMG	1	0
23	c	508	CLA	1	0
23	b	603	CLA	2	0
23	D	401	CLA	2	0
25	b	619	BCR	3	0
23	b	613	CLA	2	0
25	T	101	BCR	3	0
23	B	614	CLA	1	0
23	b	616	CLA	3	0
23	C	513	CLA	3	0
25	K	102	BCR	1	0
23	C	506	CLA	1	0
32	a	417[B]	OEY	1	0
25	k	101	BCR	2	0
23	c	509	CLA	1	0
25	t	101	BCR	6	0
23	a	411	CLA	4	0
27	D	406	LMG	1	0
23	B	608	CLA	1	0
23	d	403	CLA	1	0
23	B	605	CLA	2	0
25	c	515	BCR	1	0
23	B	604	CLA	3	0
25	C	514	BCR	1	0
27	A	411	LMG	1	0
23	A	405	CLA	1	0
23	C	504	CLA	2	0
23	B	615	CLA	2	0
29	d	408	LHG	1	0
26	A	410	PL9	6	0
30	h	102	DGD	1	0
25	B	618	BCR	5	0
23	C	511	CLA	1	0
28	a	412	SQD	1	0
36	V	201	HEC	1	0
25	D	404	BCR	5	0
23	c	511	CLA	1	0
23	B	613	CLA	2	0
23	A	404	CLA	3	0
23	c	504	CLA	1	0
27	c	521	LMG	2	0
28	b	601	SQD	1	0

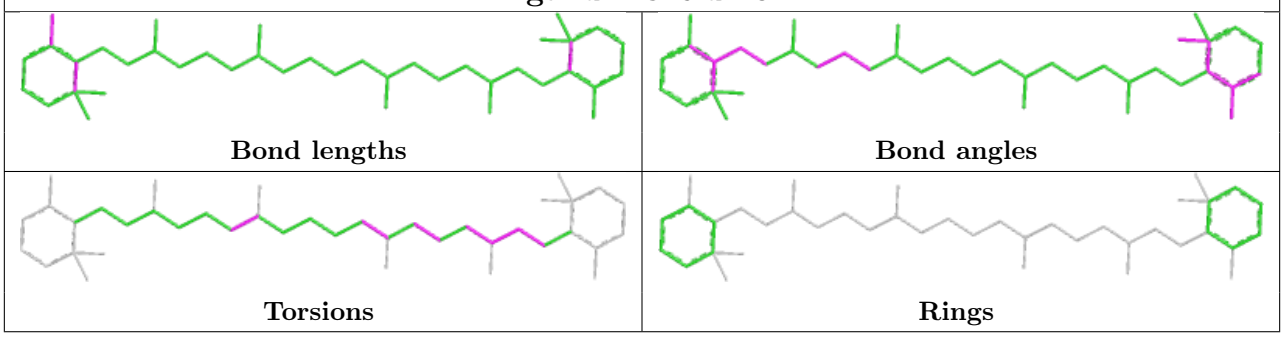
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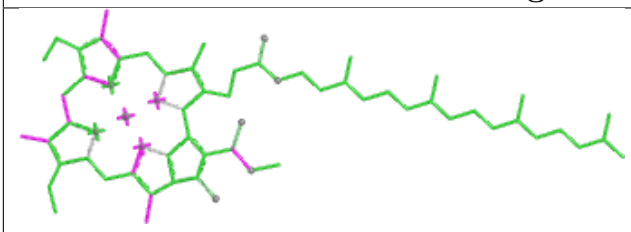
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	412	SQD	1	0
23	C	509	CLA	1	0
27	m	101	LMG	1	0
23	a	405	CLA	1	0
23	D	403	CLA	1	0
23	B	609	CLA	2	0
25	b	620	BCR	1	0
27	c	523	LMG	2	0
25	Z	101	BCR	4	0
26	a	410	PL9	6	0
26	d	405	PL9	2	0
30	A	415	DGD	3	0
25	a	409	BCR	2	0
23	b	611	CLA	4	0
23	b	605	CLA	2	0
23	B	602	CLA	3	0
27	b	622	LMG	2	0
23	c	510	CLA	2	0
30	a	414	DGD	3	0

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

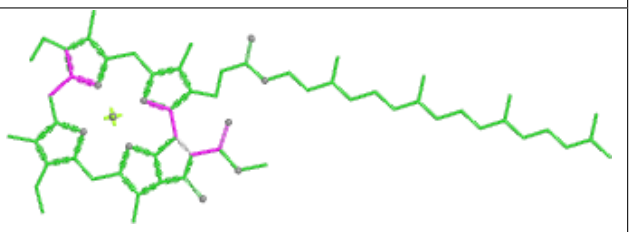
Ligand BCR d 404



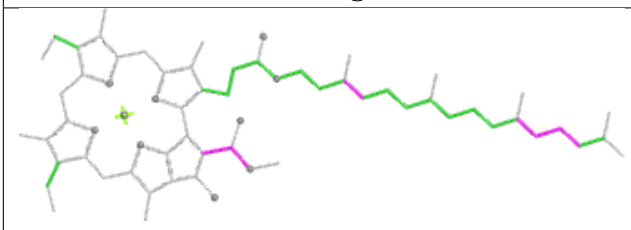
Ligand CLA b 610



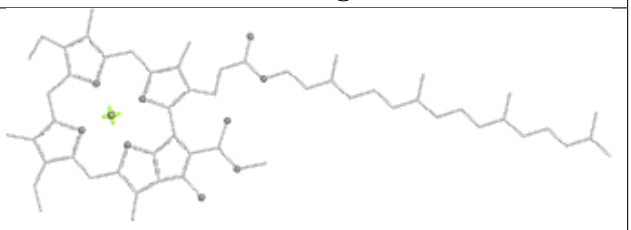
Bond lengths



Bond angles

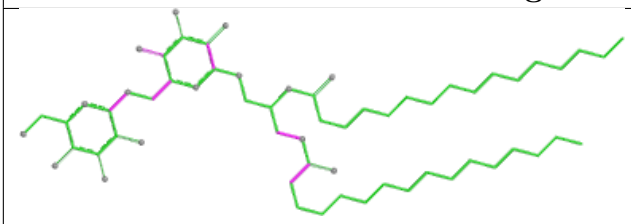


Torsions

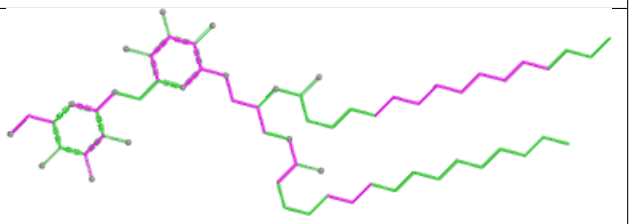


Rings

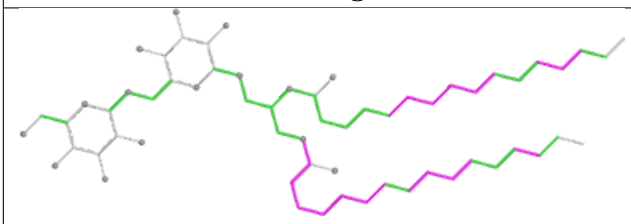
Ligand DGD c 518



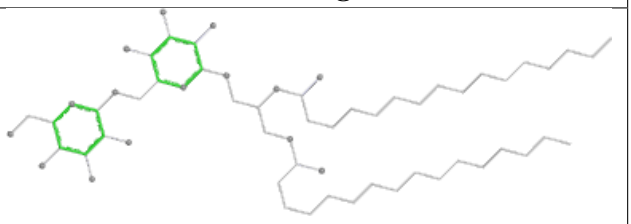
Bond lengths



Bond angles

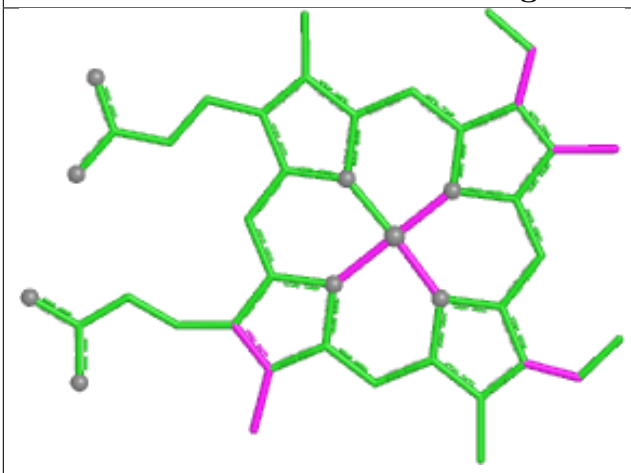


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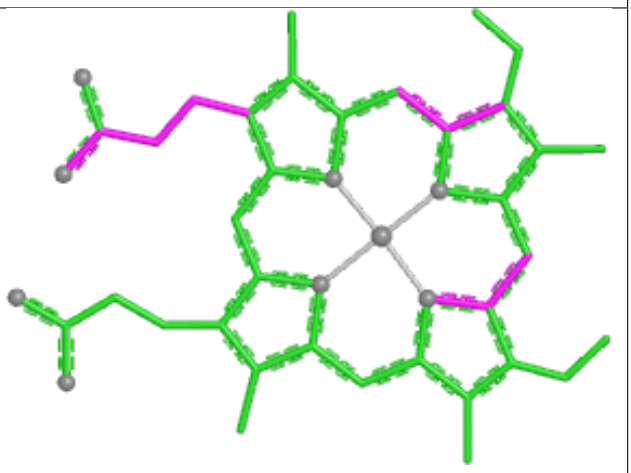


Rings

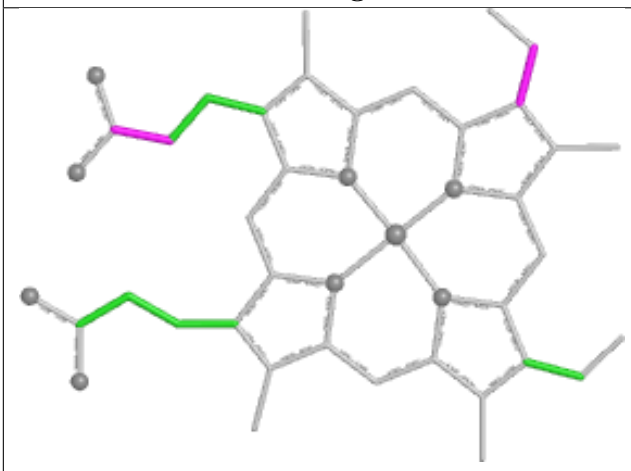
Ligand HEM E 101



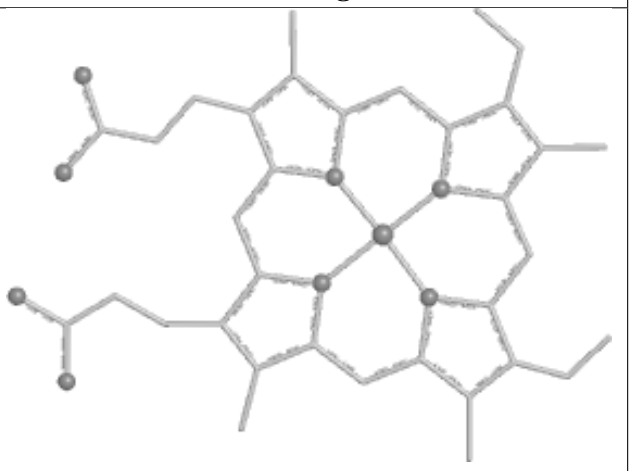
Bond lengths



Bond angles

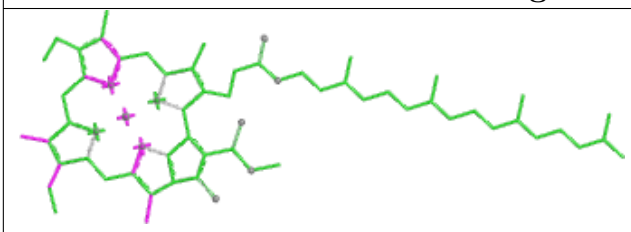


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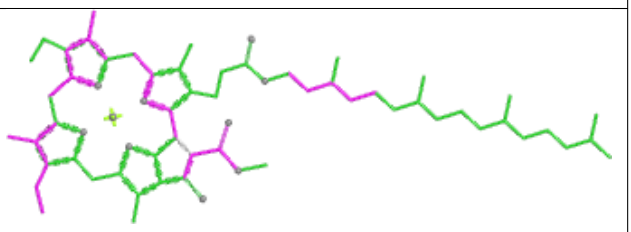


Rings

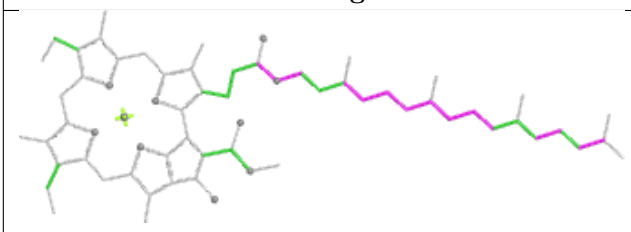
Ligand CLA c 506



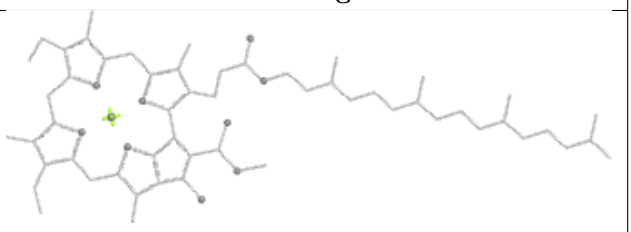
Bond lengths



Bond angles

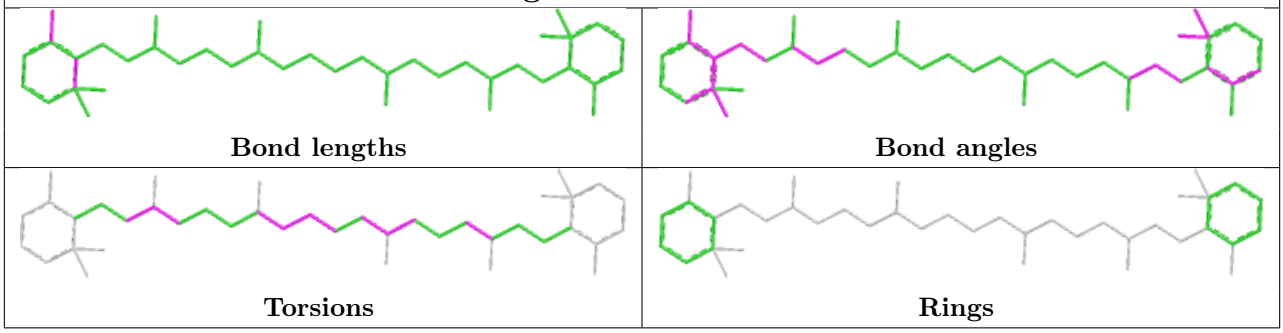


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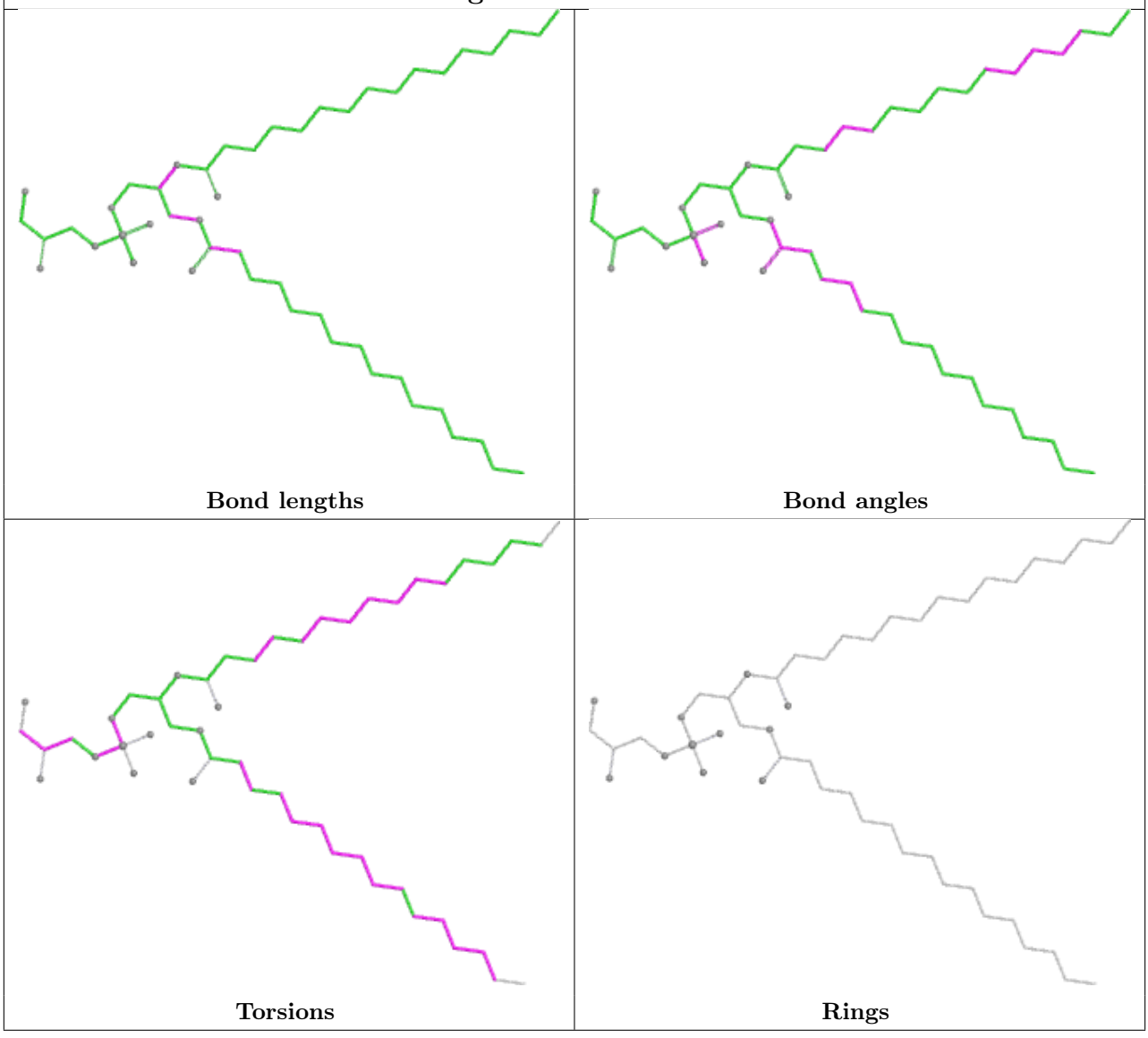


Rings

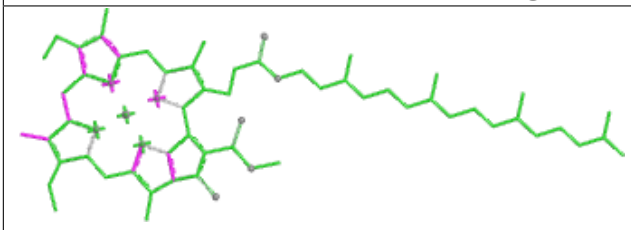
Ligand BCR A 409



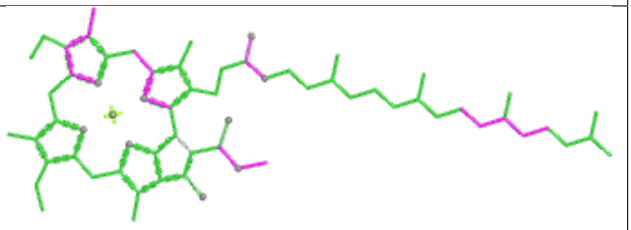
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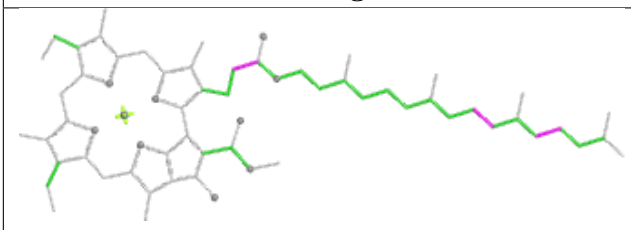
Ligand CLA B 612



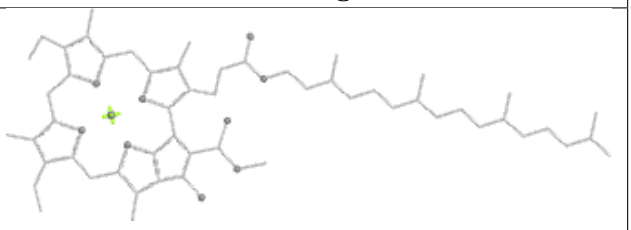
Bond lengths



Bond angles



Torsions

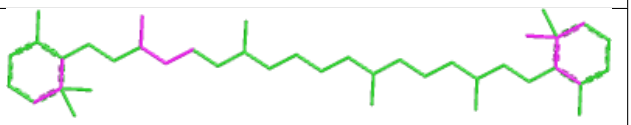


Rings

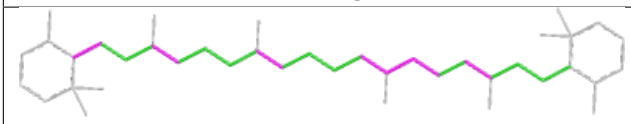
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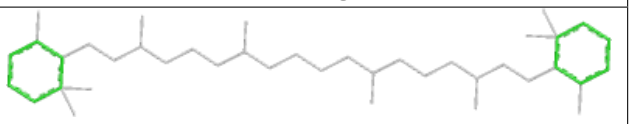
Bond lengths



Bond angles

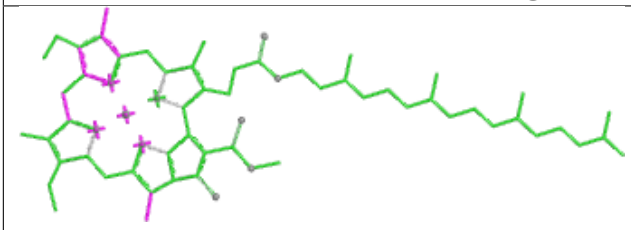


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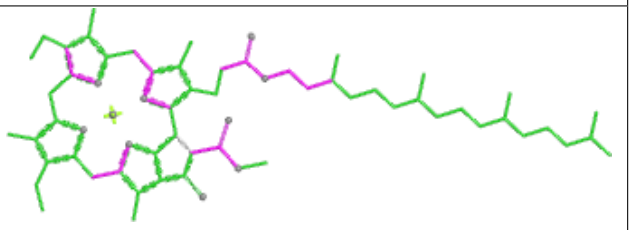


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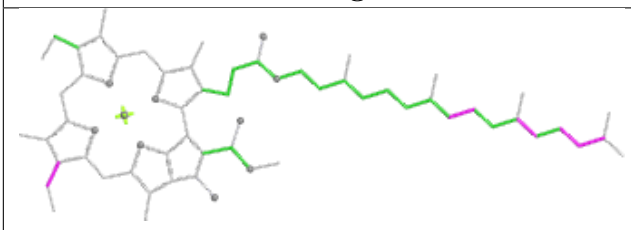
Ligand CLA B 610



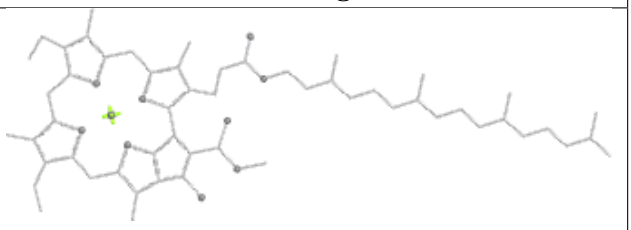
Bond lengths



Bond angles

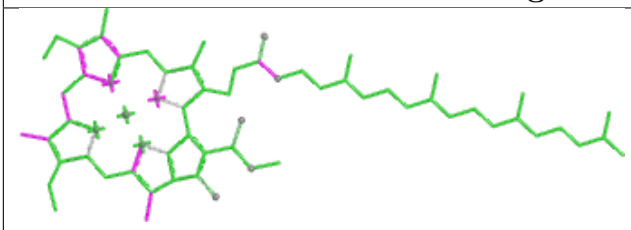


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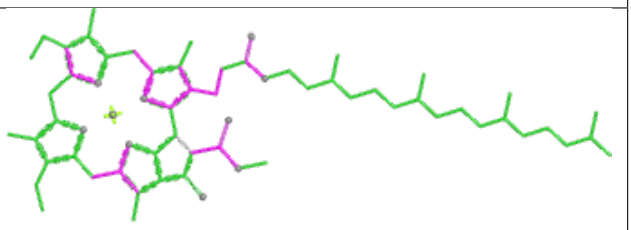


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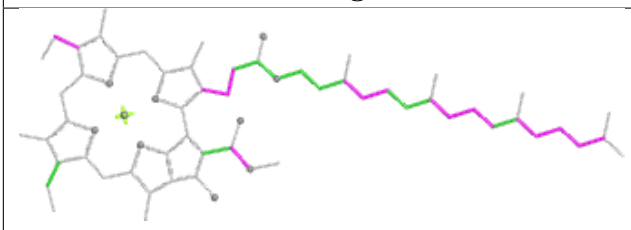
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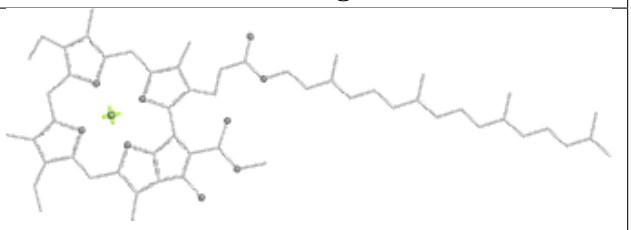
Bond lengths



Bond angles

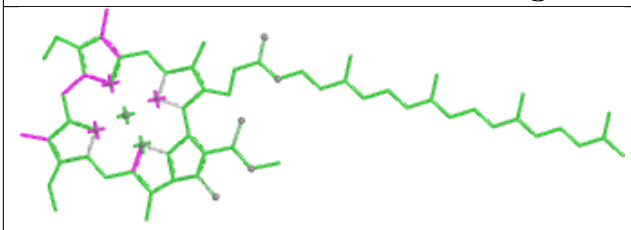


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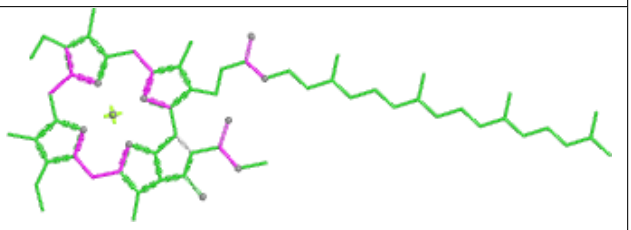


Rings

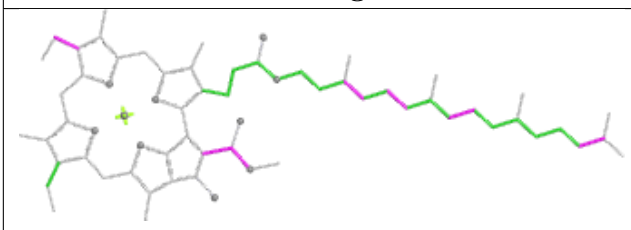
Ligand CLA c 507



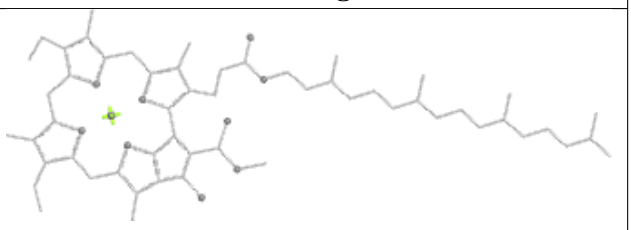
Bond lengths



Bond angles

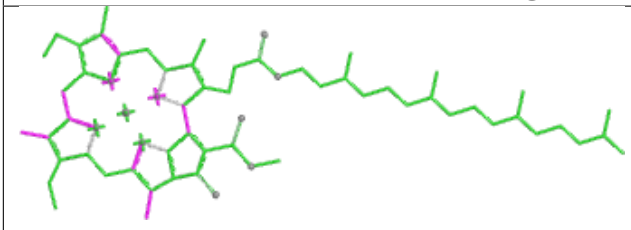


Torsions

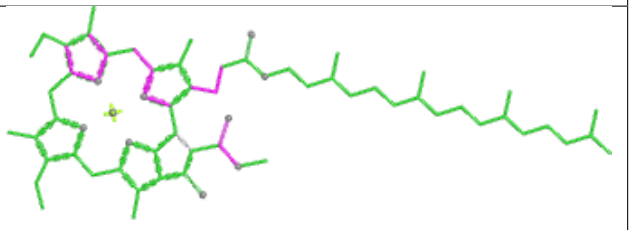


Rings

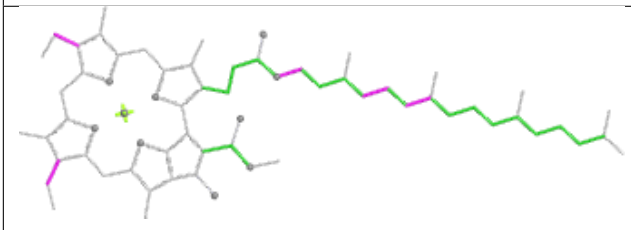
Ligand CLA D 402



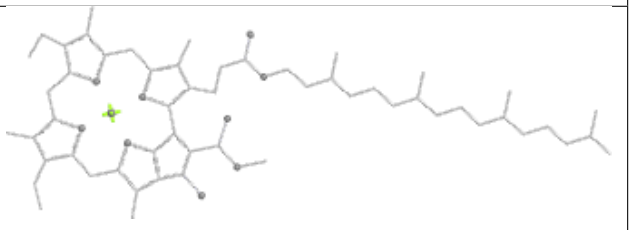
Bond lengths



Bond angles

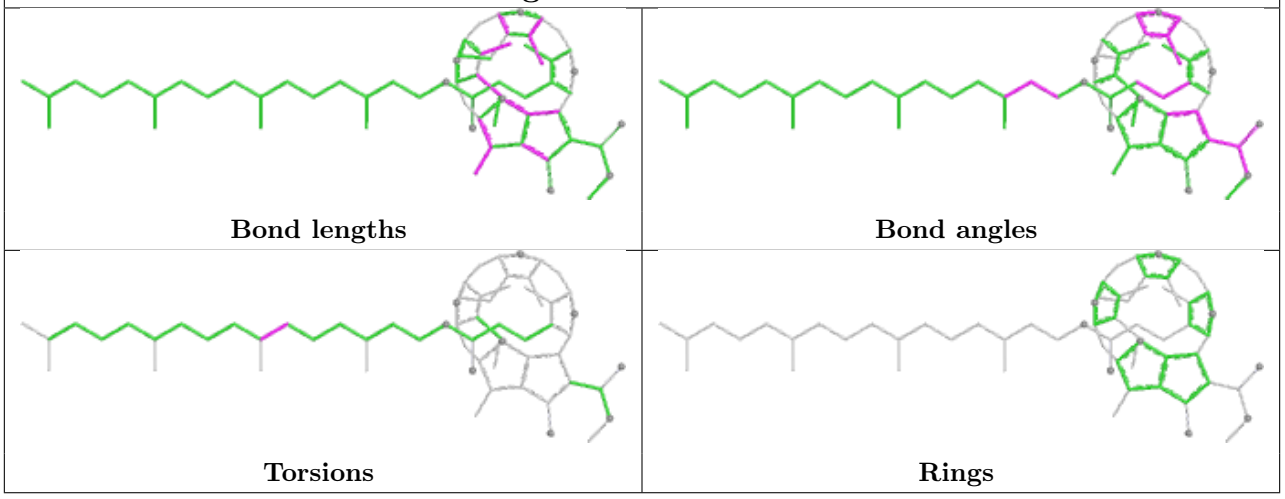


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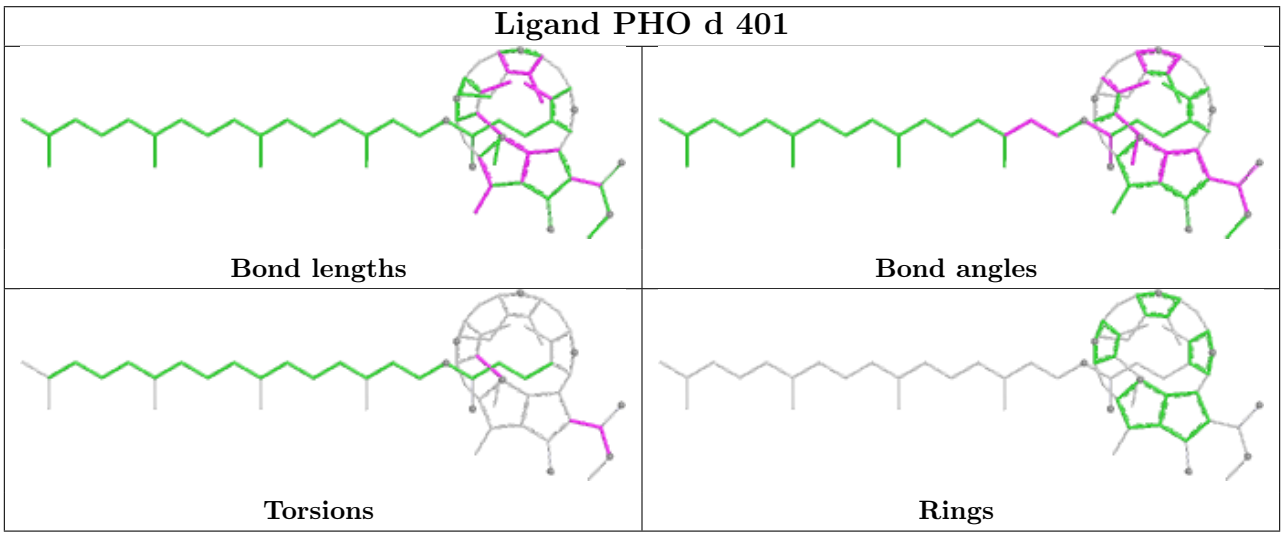


Rings

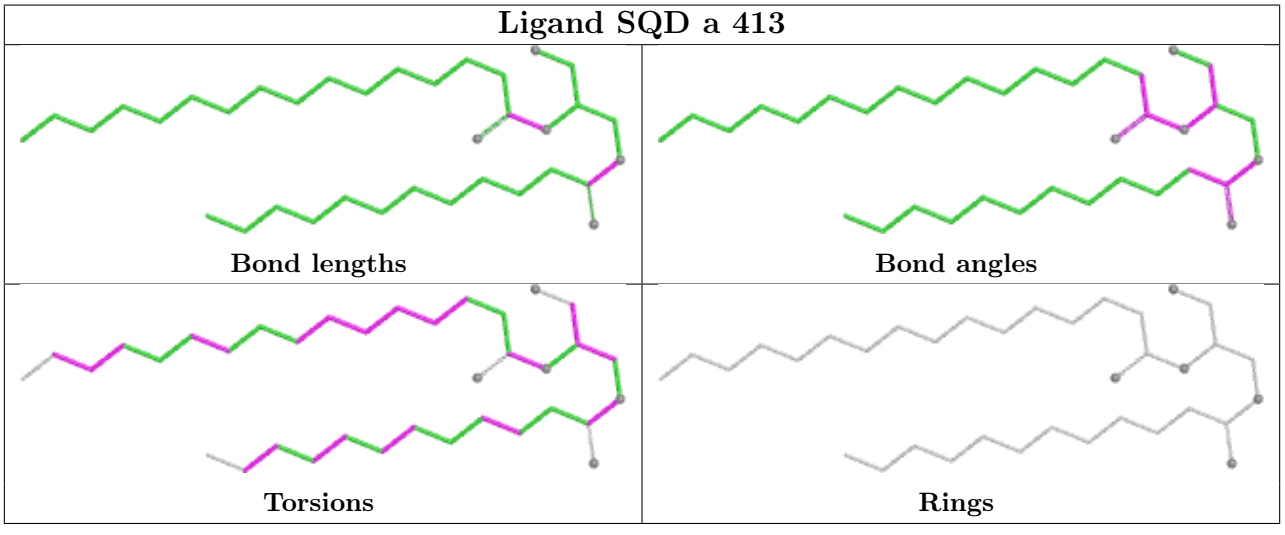
Ligand PHO A 407



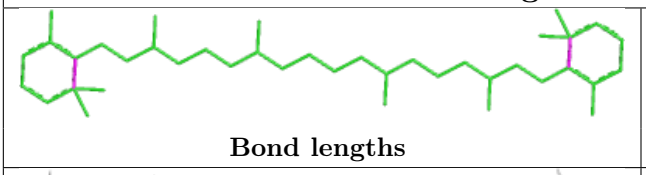
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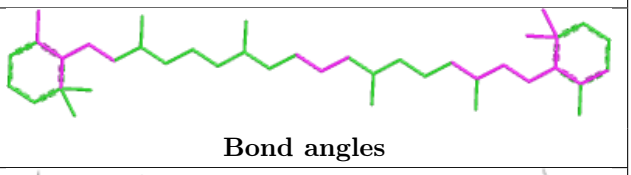
Ligand SQD a 413



Ligand BCR K 101



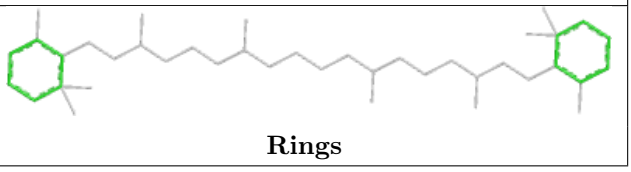
Bond lengths



Bond angles

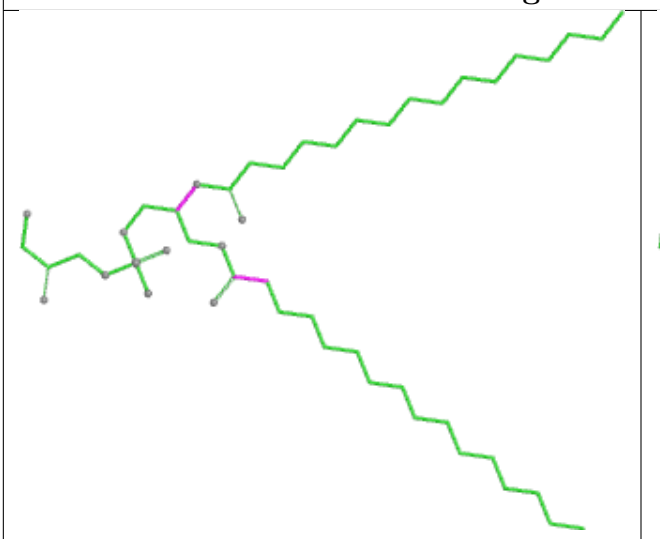


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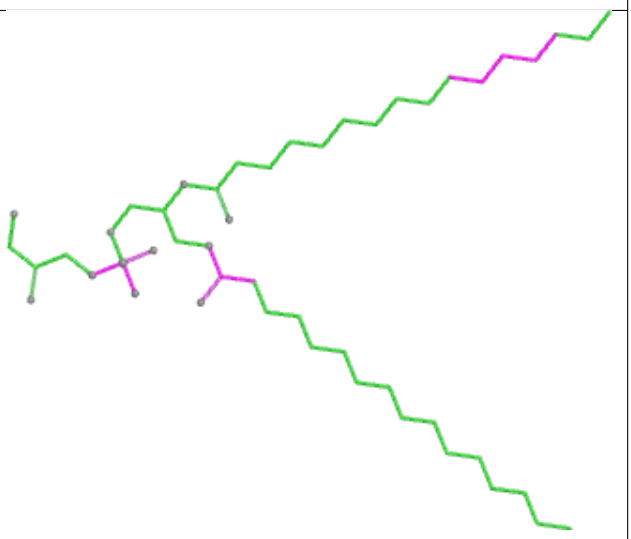


Rings

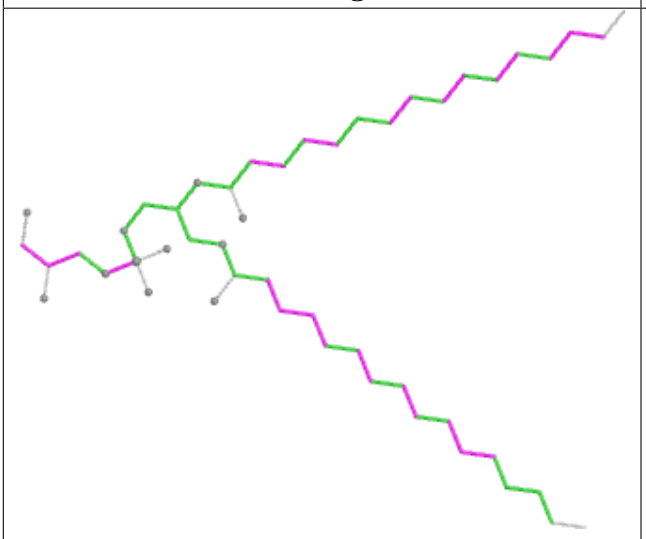
Ligand LHG B 623



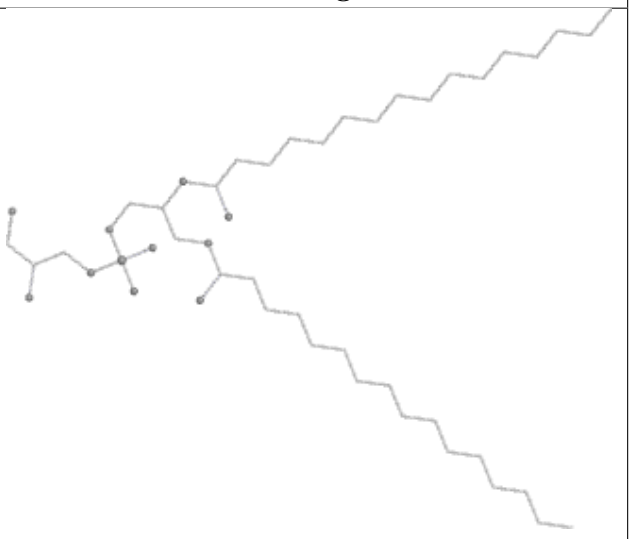
Bond lengths



Bond angles

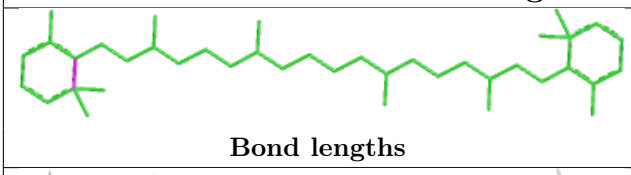


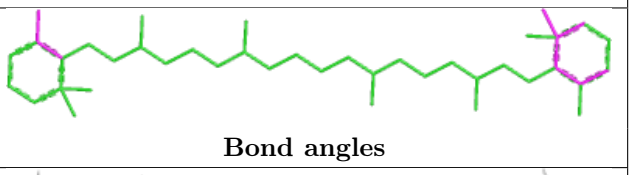
Torsions

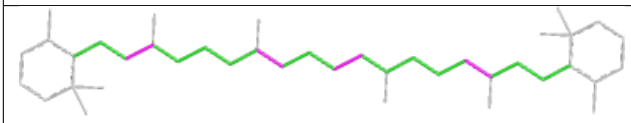


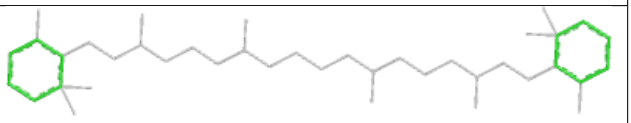
Rings

Ligand BCR k 102


Bond lengths

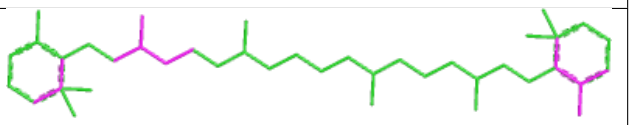

Bond angles

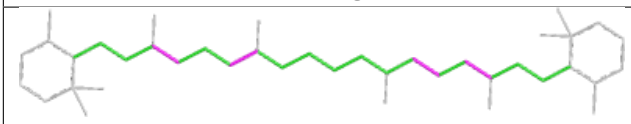

Torsions

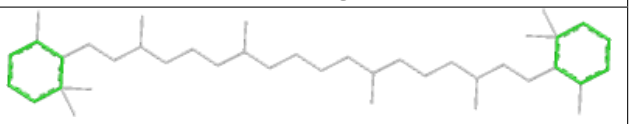

Rings

Ligand BCR x 101

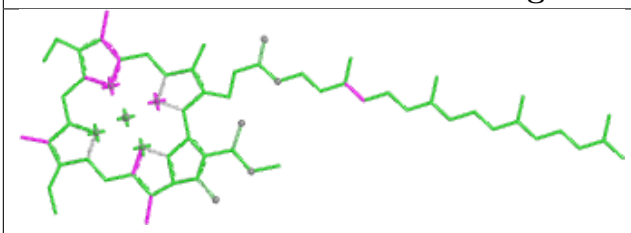

Bond lengths

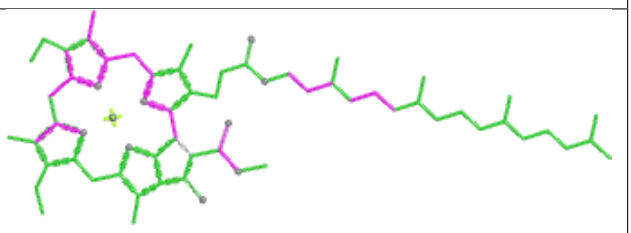

Bond angles

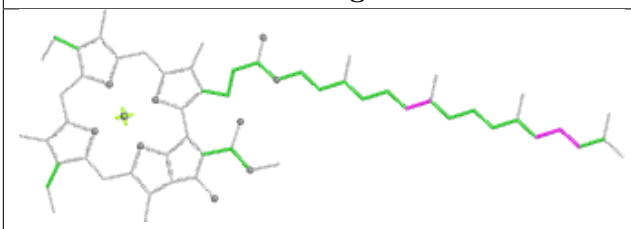

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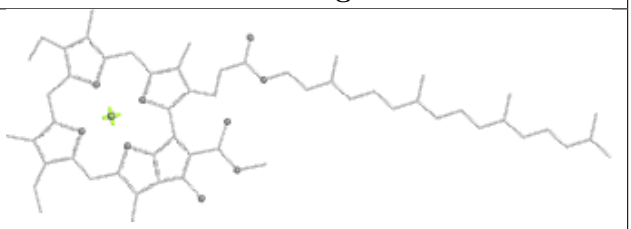

Rings

Ligand CLA b 614

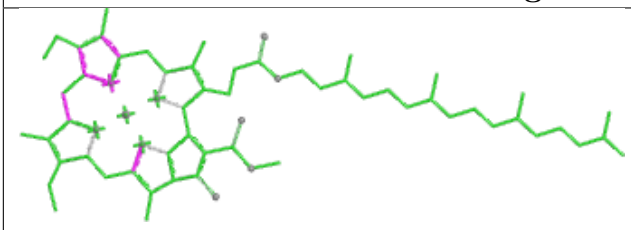

Bond lengths


Bond angles

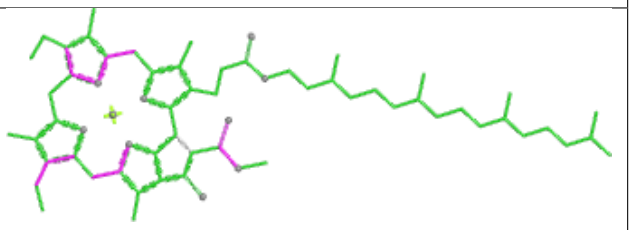

Torsions


Rings

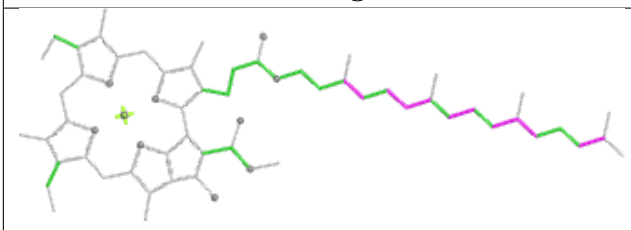
Ligand CLA C 505



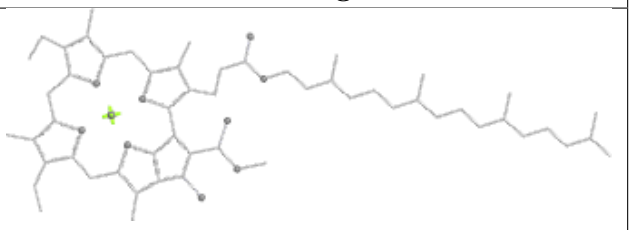
Bond lengths



Bond angles

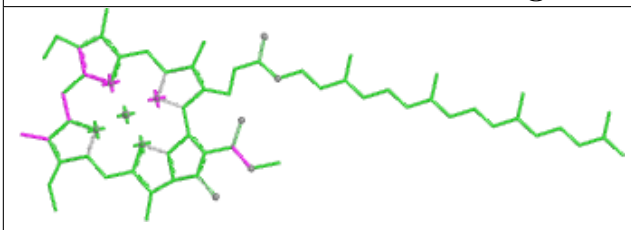


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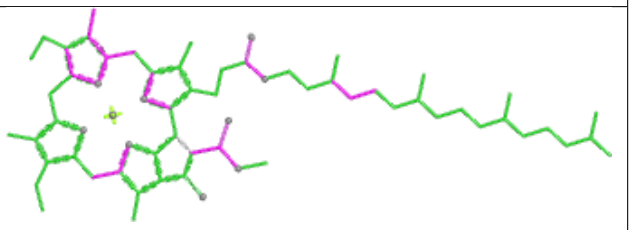


Rings

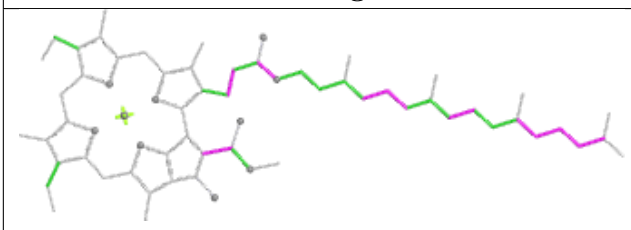
Ligand CLA b 615



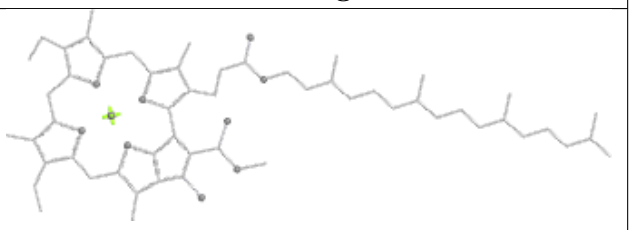
Bond lengths



Bond angles

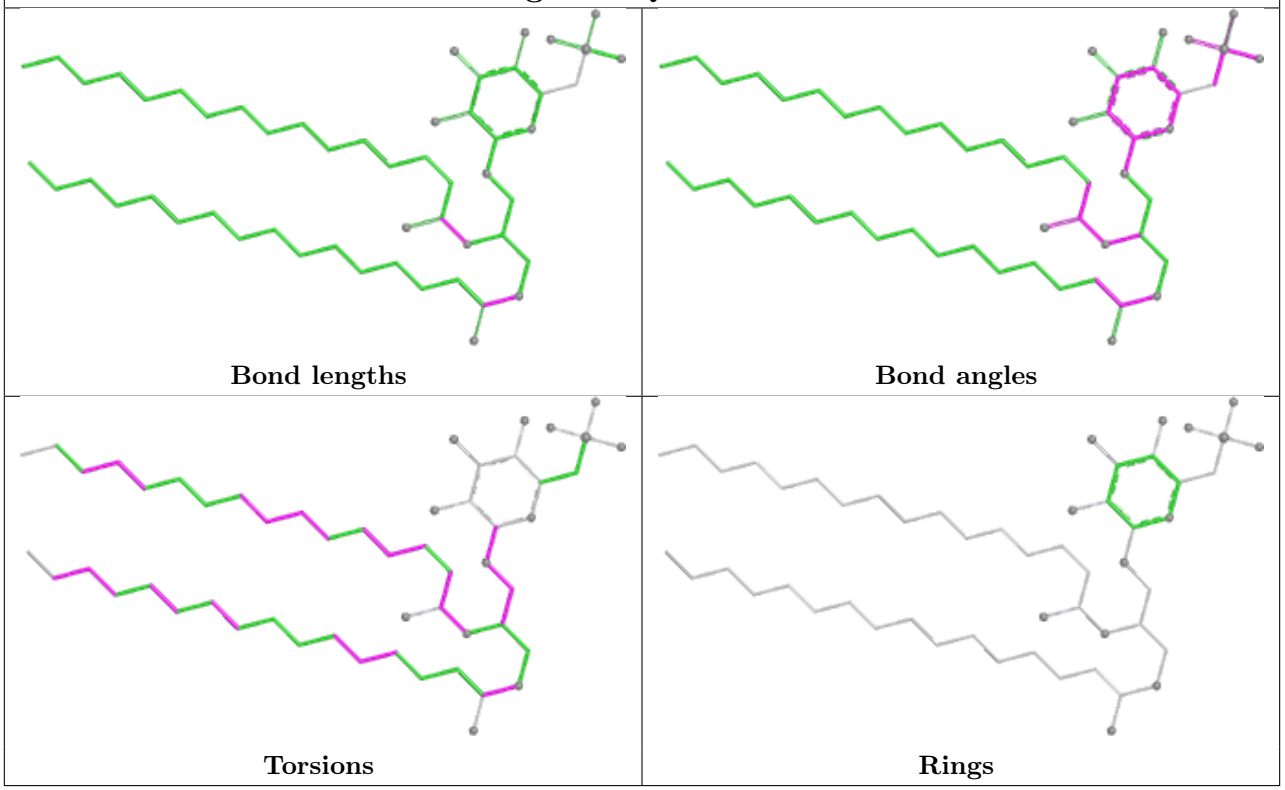


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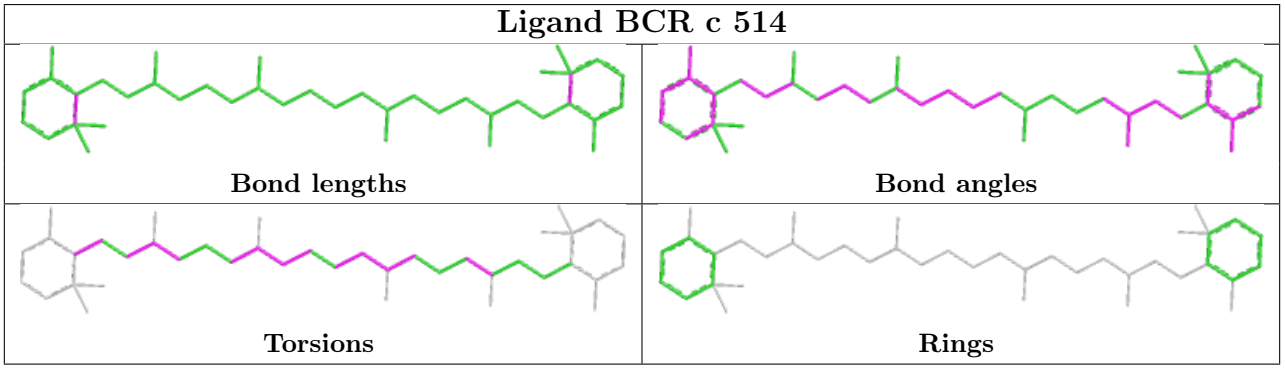


Rings

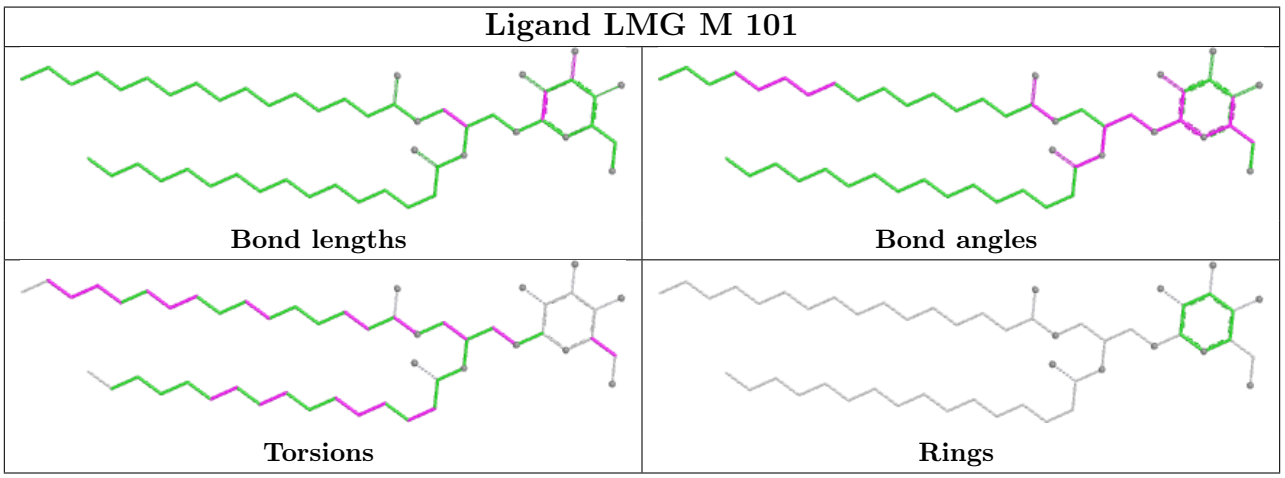
Ligand SQD B 624



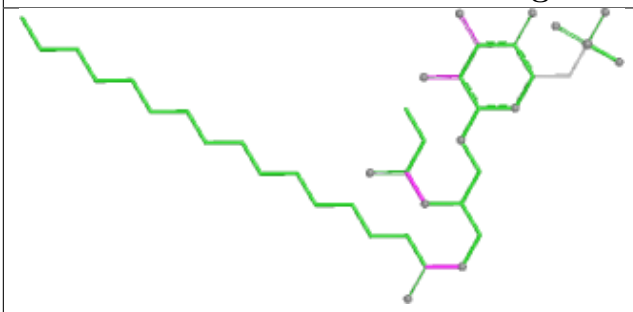
Ligand BCR c 514



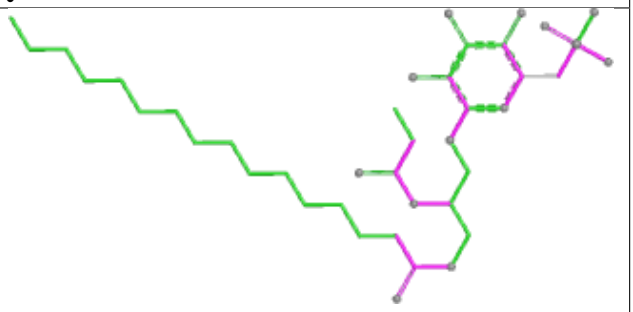
Ligand LMG M 101



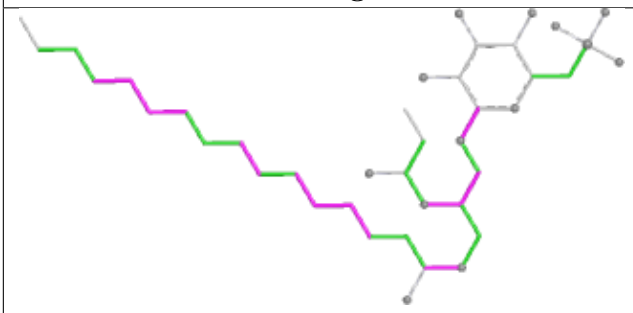
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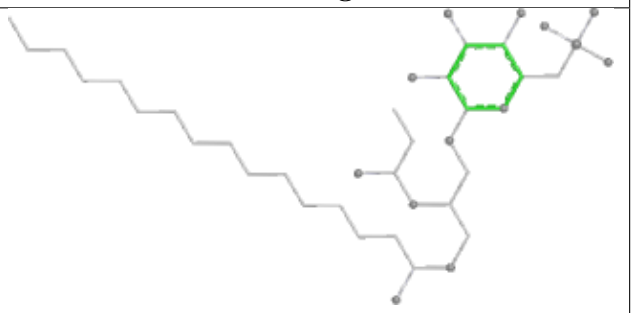
Bond lengths



Bond angles

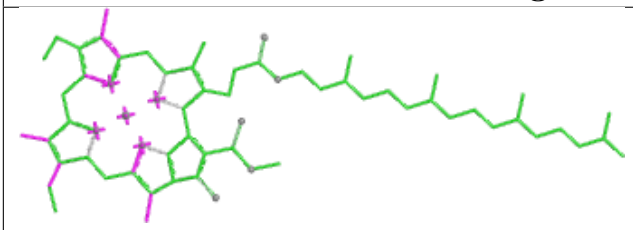


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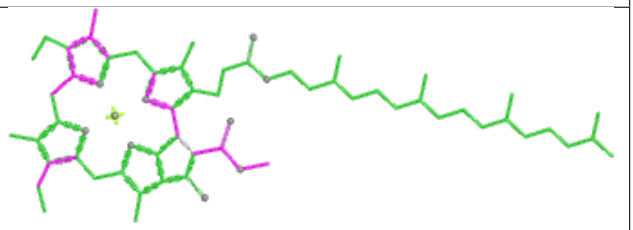


Rings

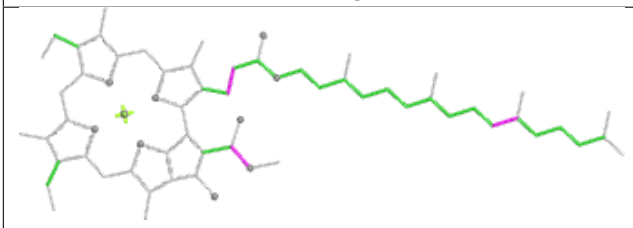
Ligand CLA c 501



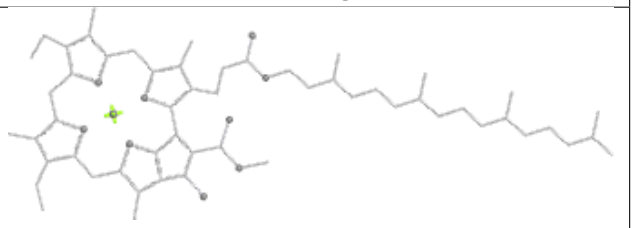
Bond lengths



Bond angles

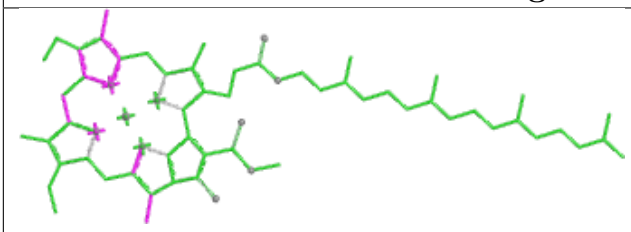


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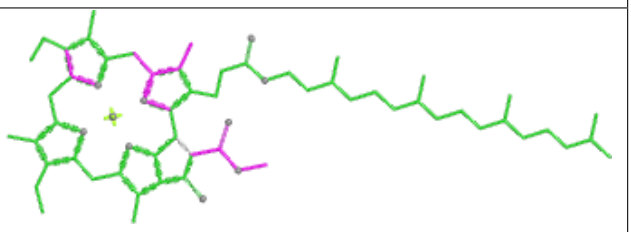


Rings

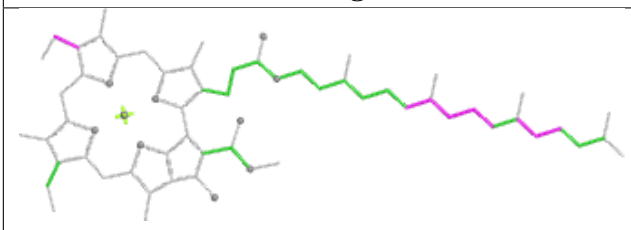
Ligand CLA a 406



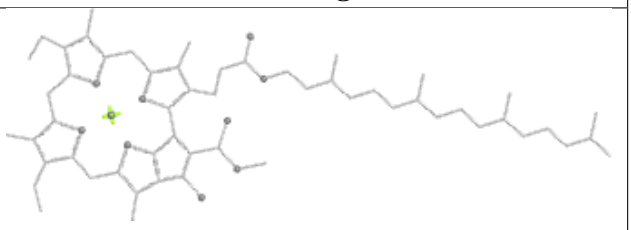
Bond lengths



Bond angles

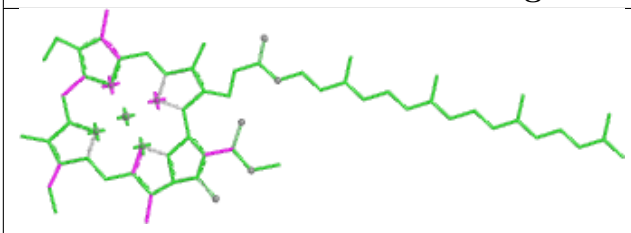


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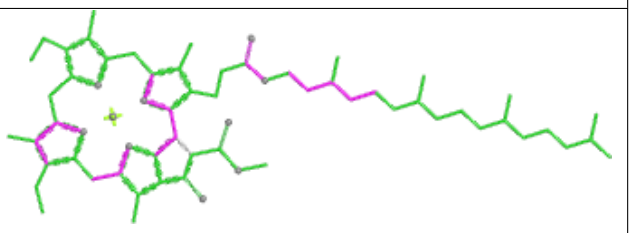


Rings

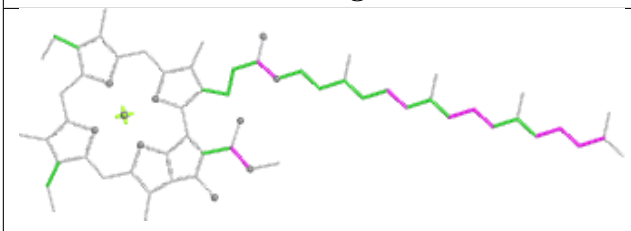
Ligand CLA B 607



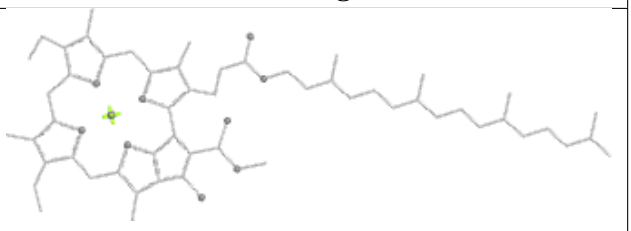
Bond lengths



Bond angles

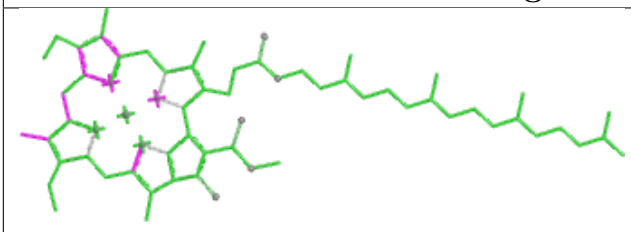


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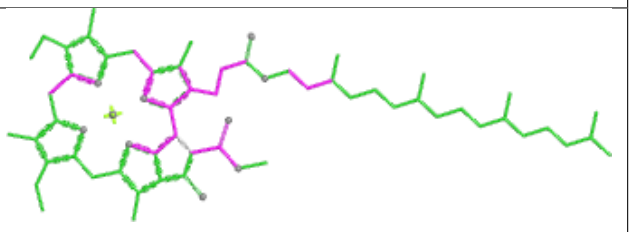


Rings

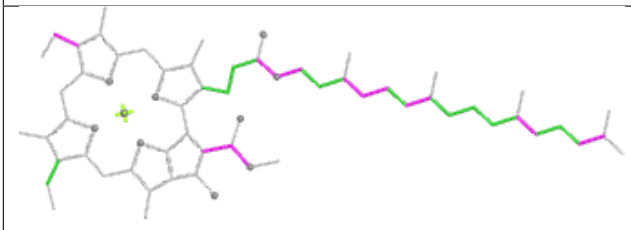
Ligand CLA B 601



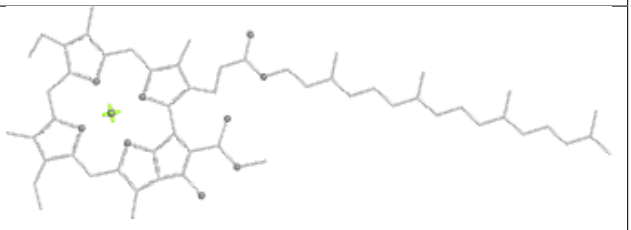
Bond lengths



Bond angles

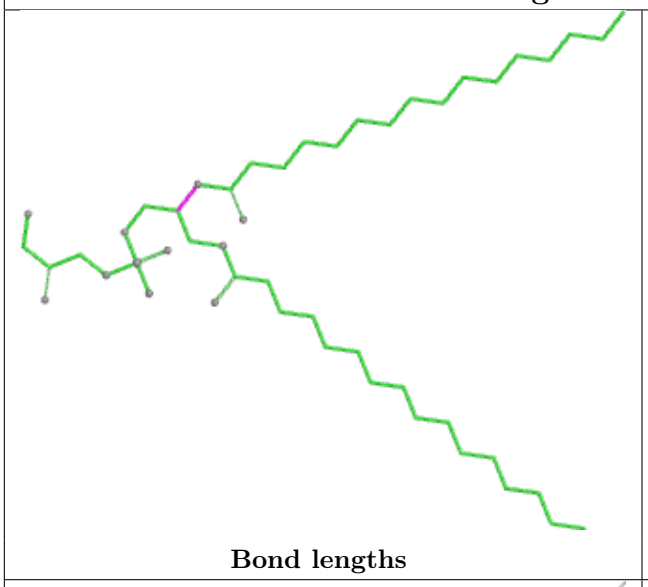


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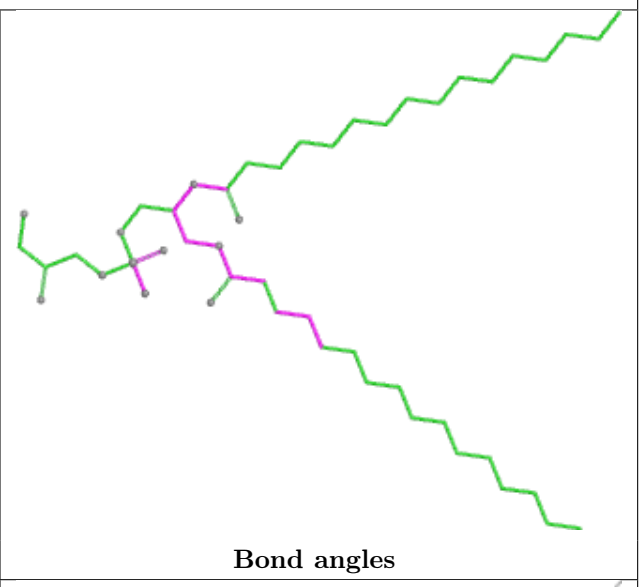


Rings

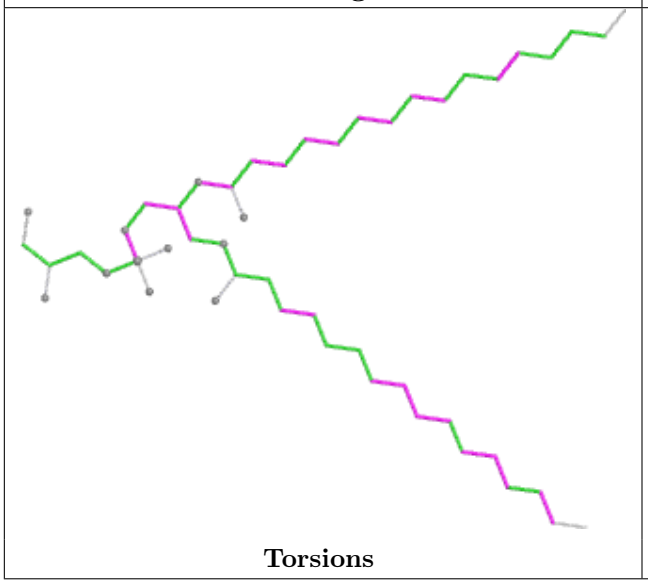
Ligand LHG l 101



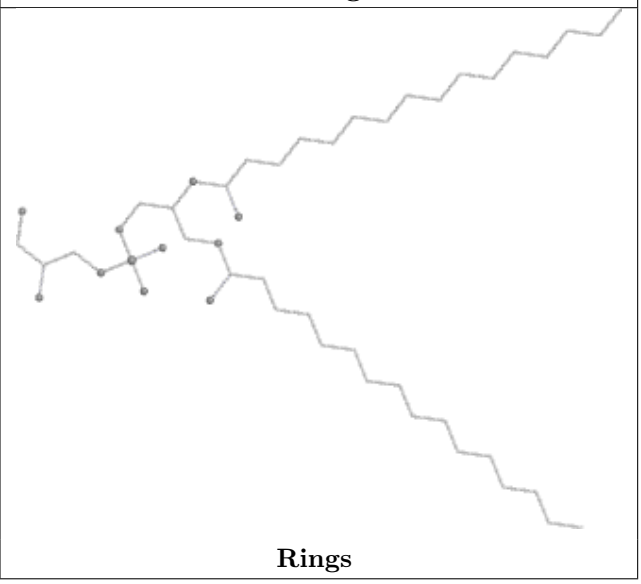
Bond lengths



Bond angles

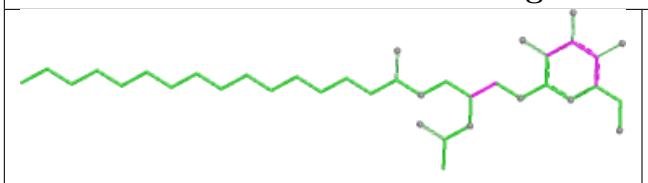


Torsions

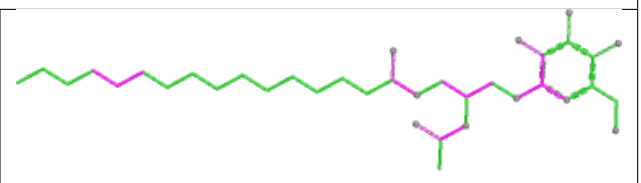


Rings

Ligand LMG c 519



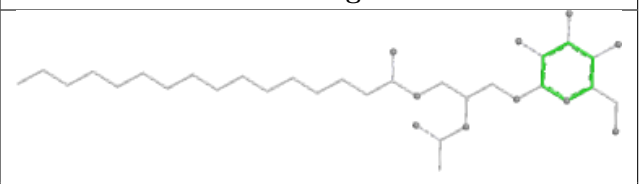
Bond lengths



Bond angles

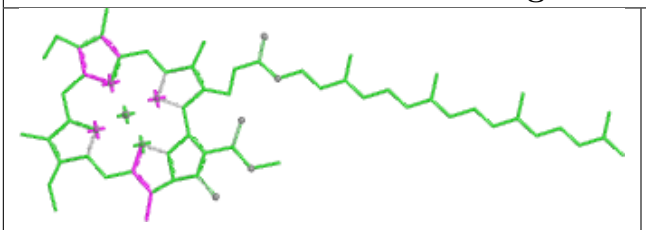


Torsions

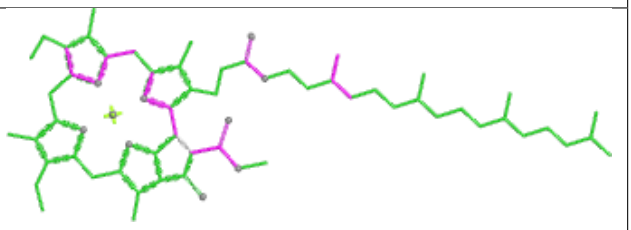


Rings

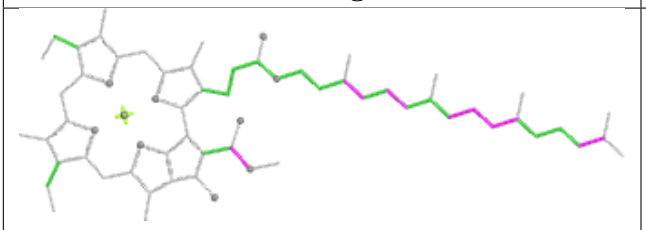
Ligand CLA b 608



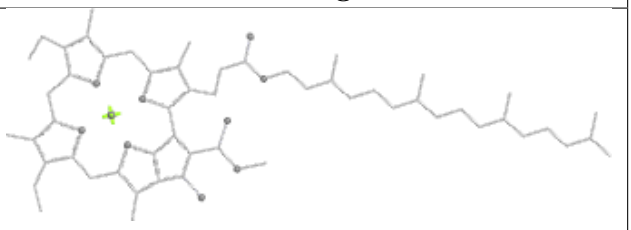
Bond lengths



Bond angles

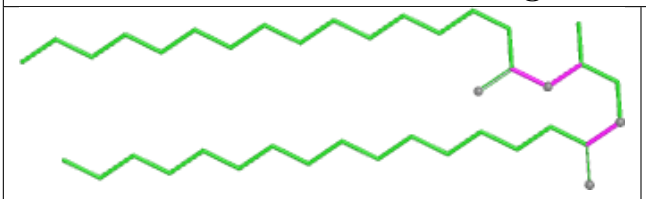


Torsions

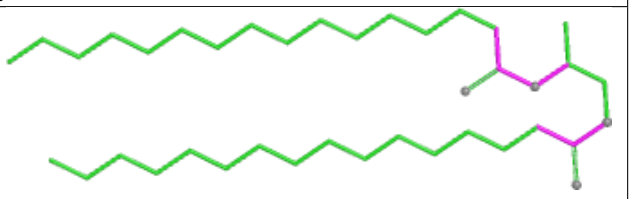


Rings

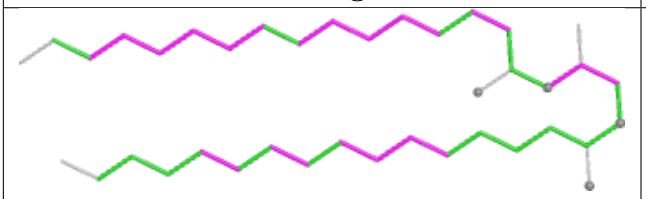
Ligand SQD A 414



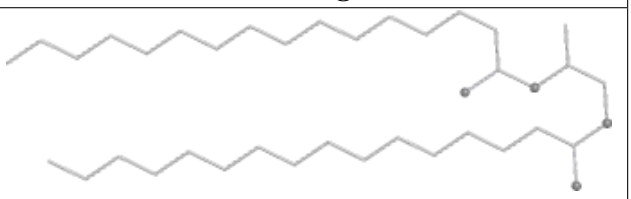
Bond lengths



Bond angles

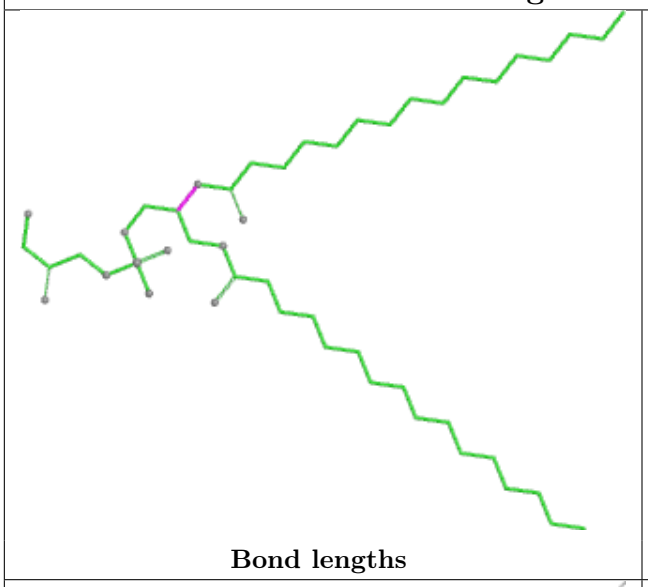


Torsions

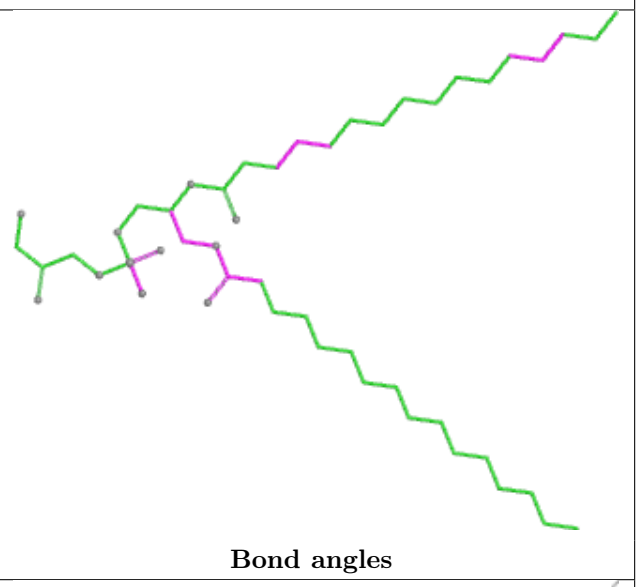


Rings

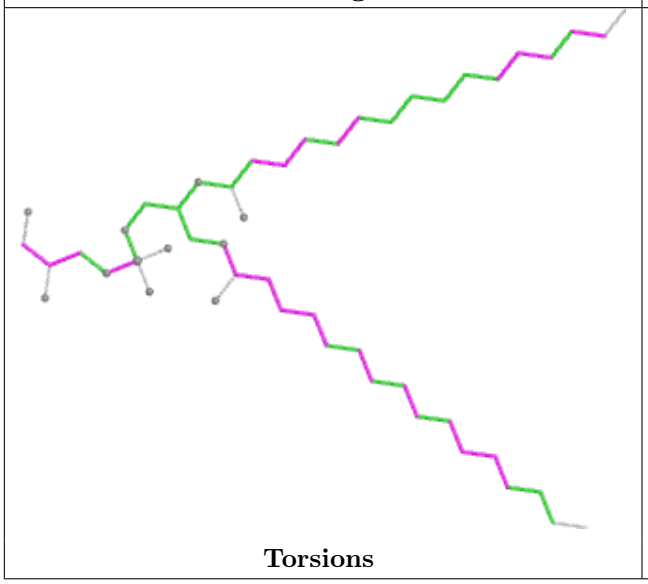
Ligand LHG d 406



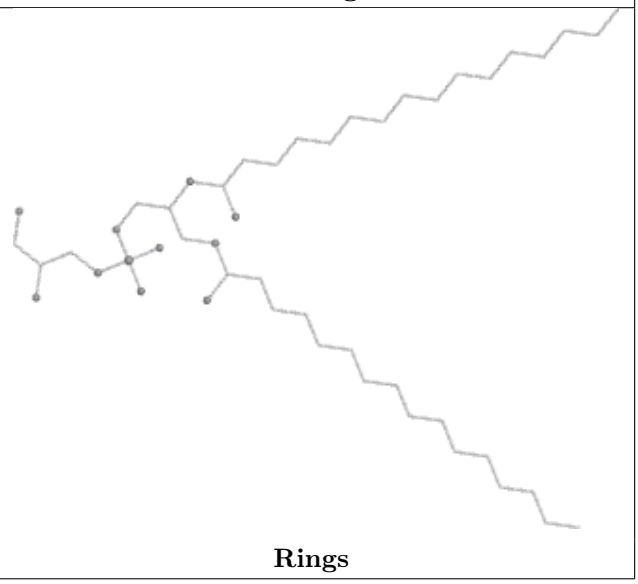
Bond lengths



Bond angles

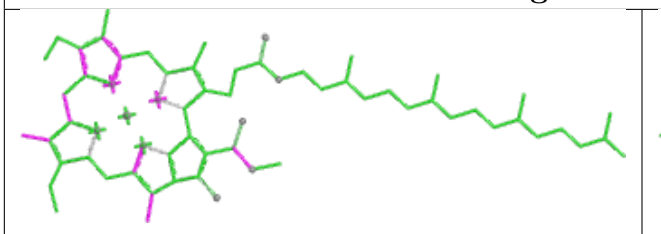


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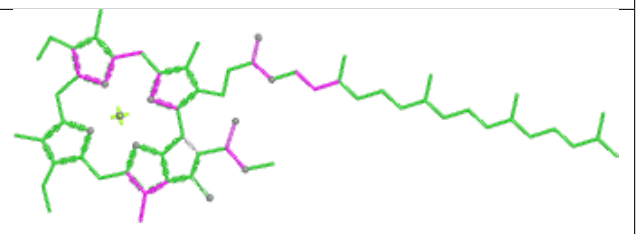


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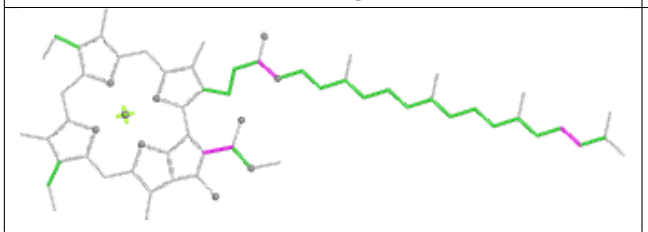
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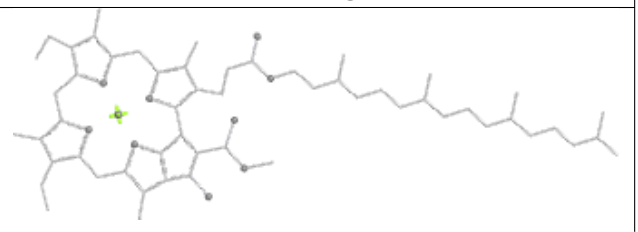
Bond lengths



Bond angles

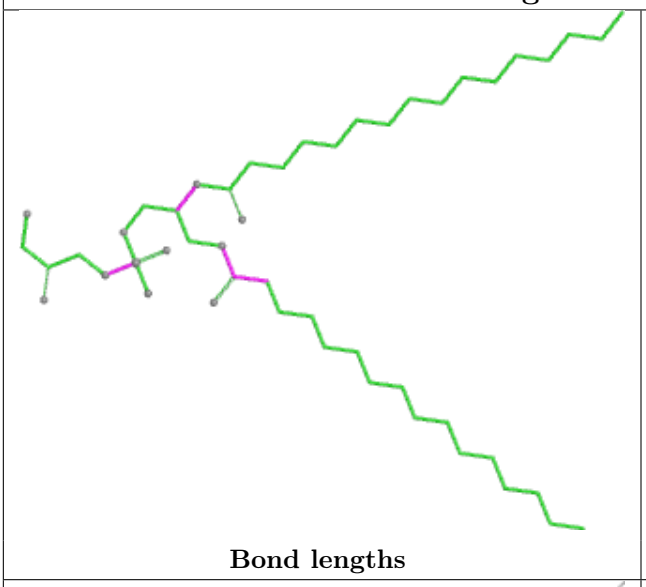


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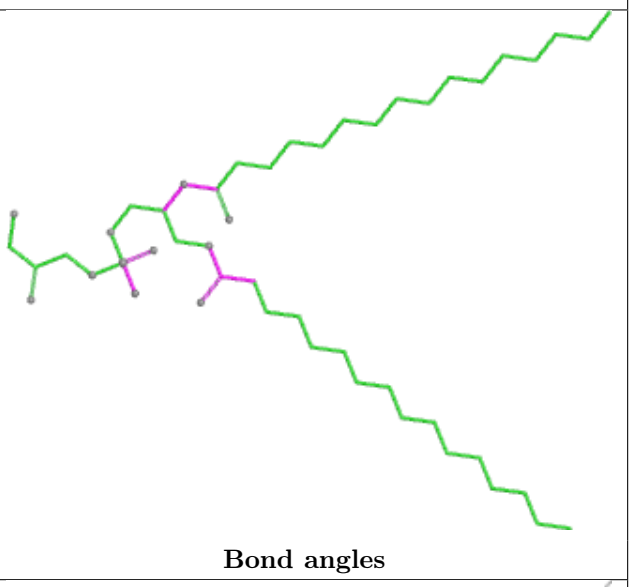


Rings

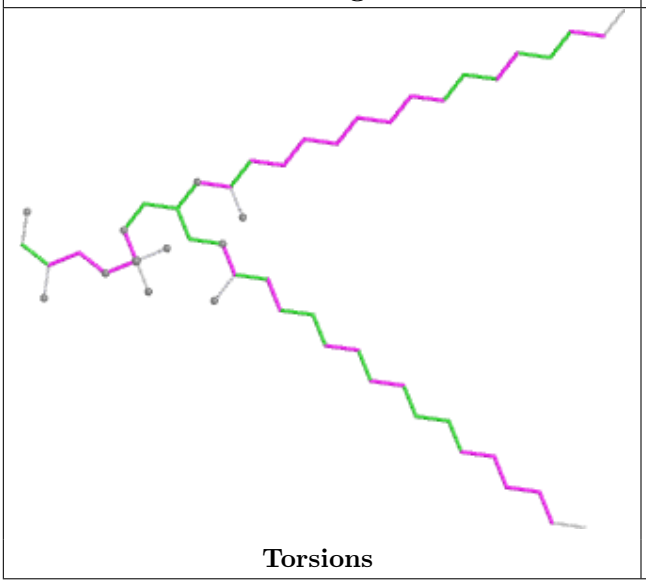
Ligand LHG A 413



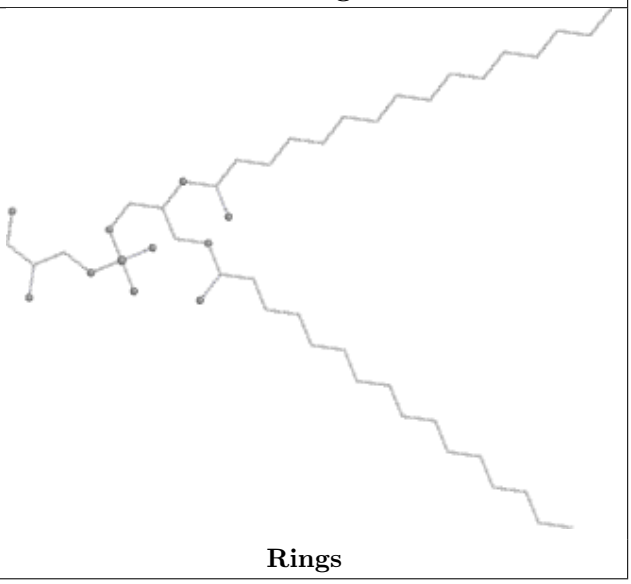
Bond lengths



Bond angles

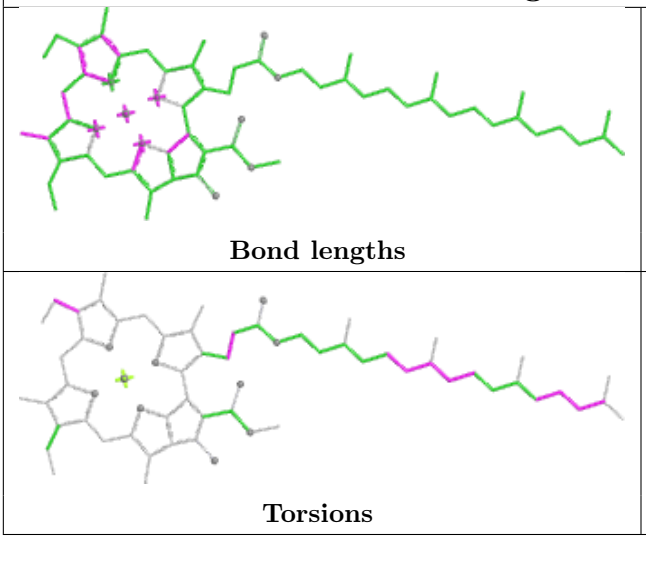


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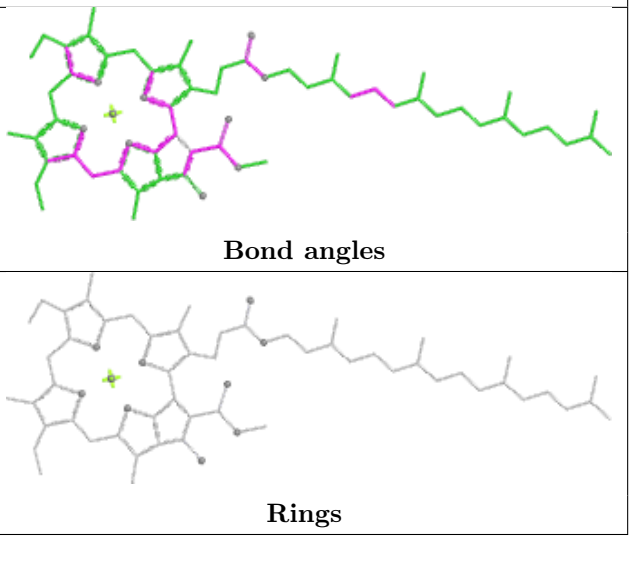


Rings

Ligand CLA B 606



Bond lengths

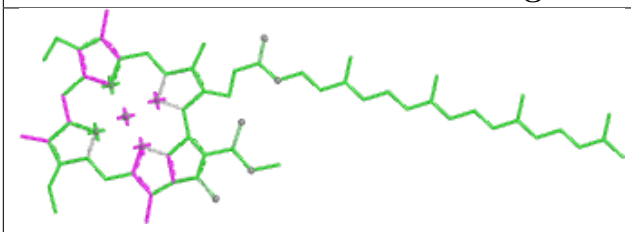


Bond angles

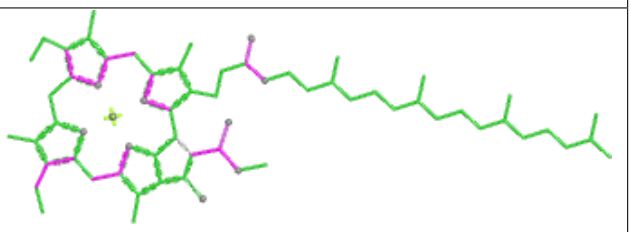
Torsions

Rings

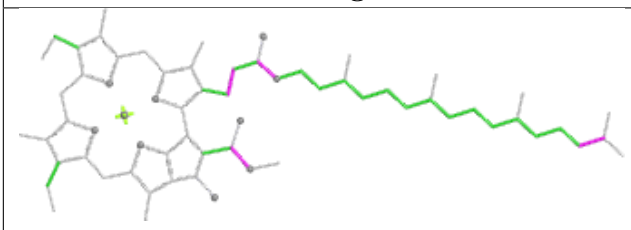
Ligand CLA C 501



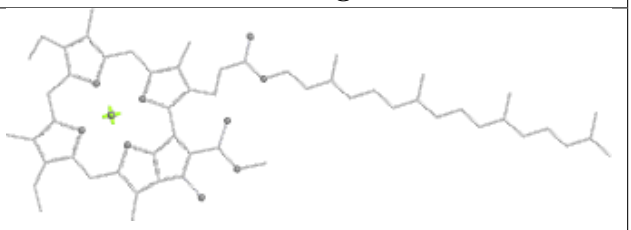
Bond lengths



Bond angles

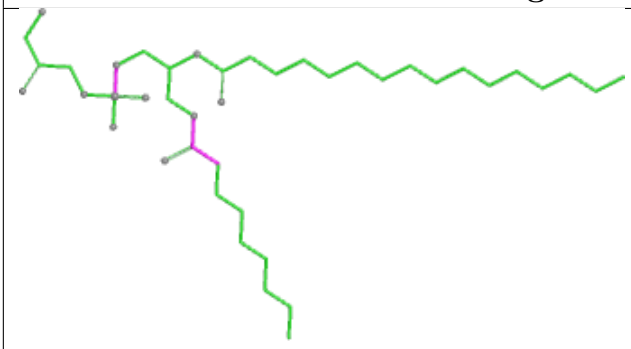


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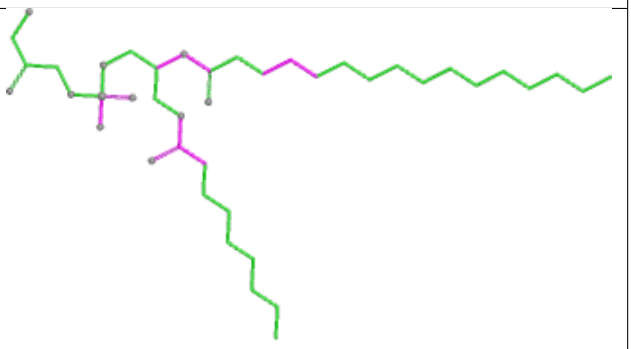


Rings

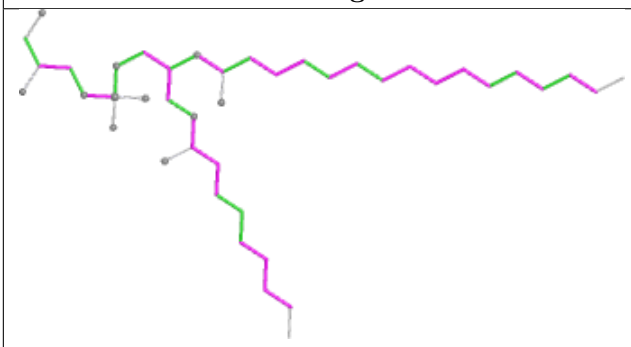
Ligand LHG e 101



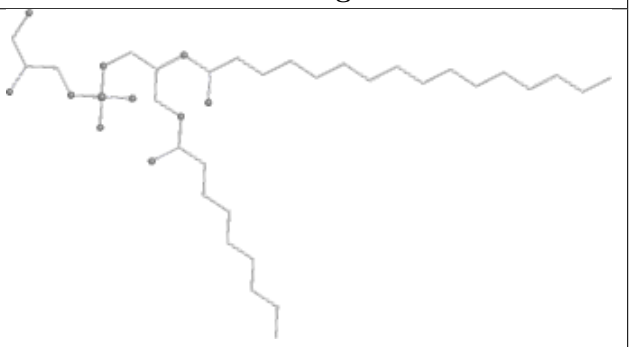
Bond lengths



Bond angles

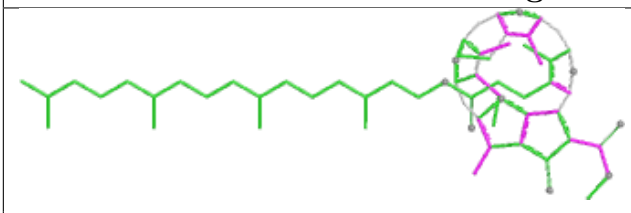


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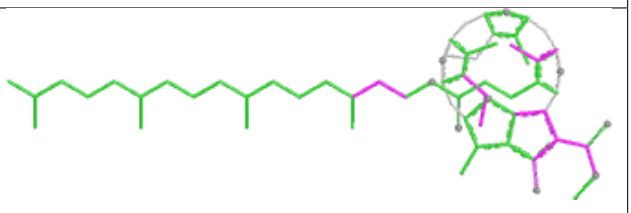


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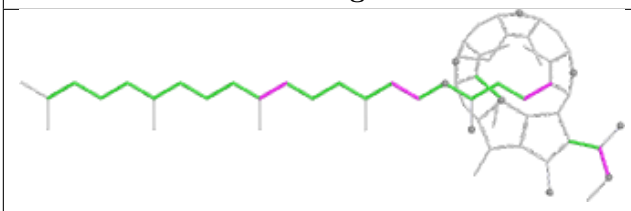
Ligand PHO a 407



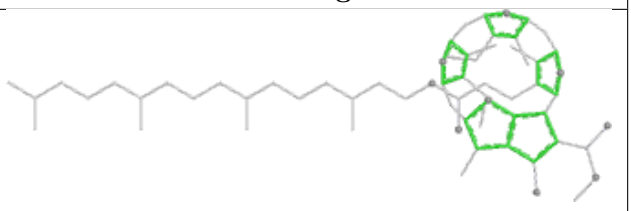
Bond lengths



Bond angles



Torsions

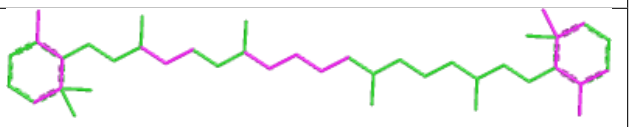


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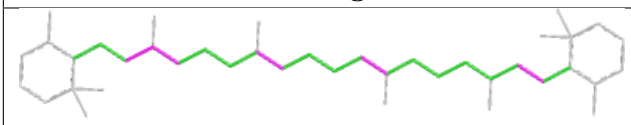
Ligand BCR B 619



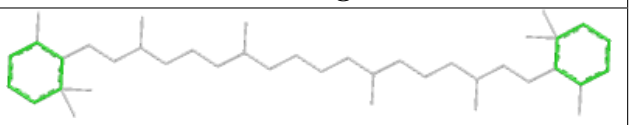
Bond lengths



Bond angles

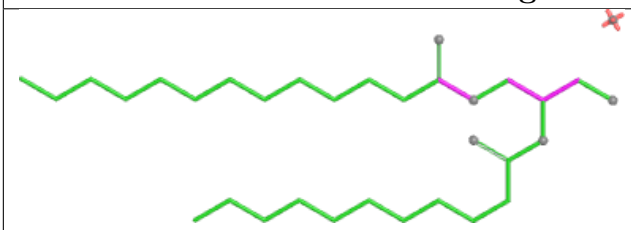


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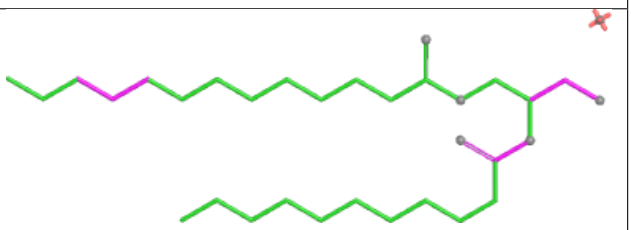


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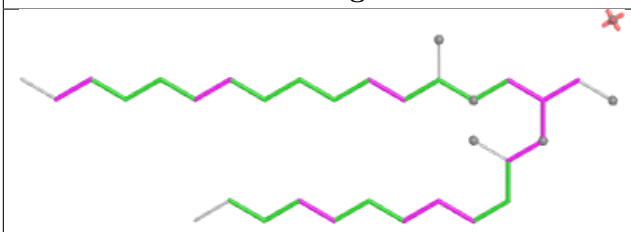
Ligand LMG D 409



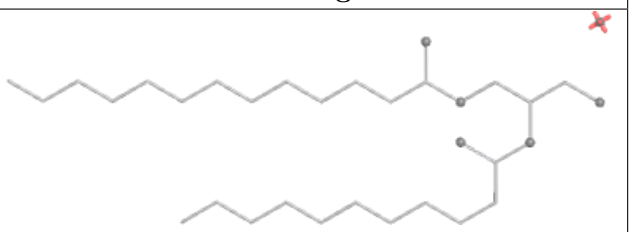
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Bond angles

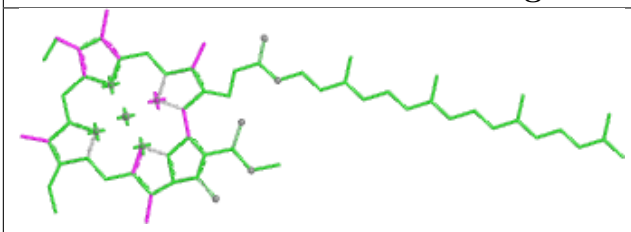


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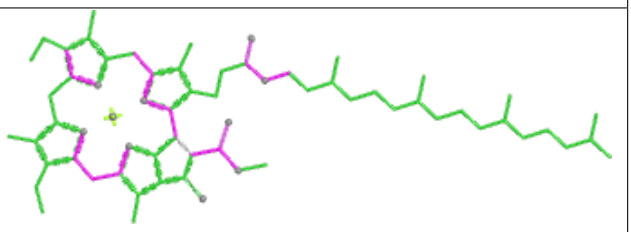


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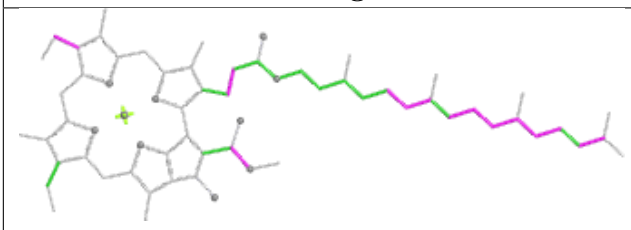
Ligand CLA B 603



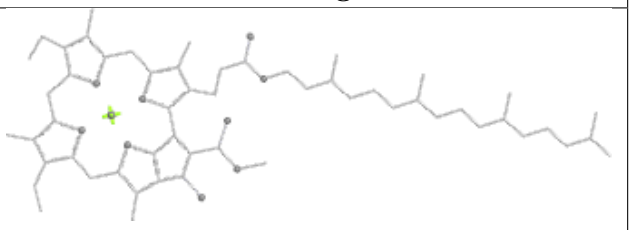
Bond lengths



Bond angles

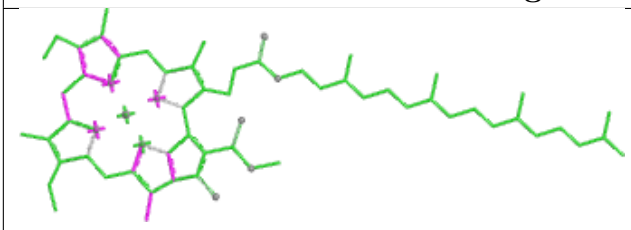


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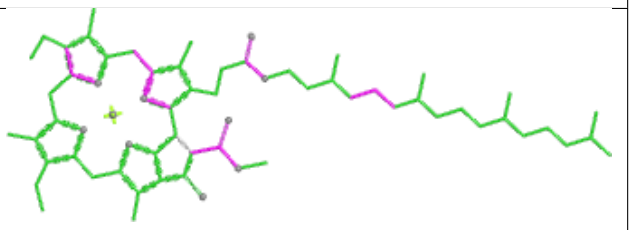


Rings

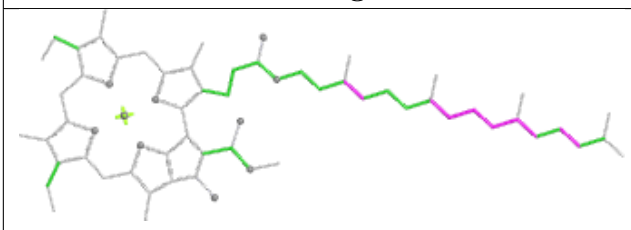
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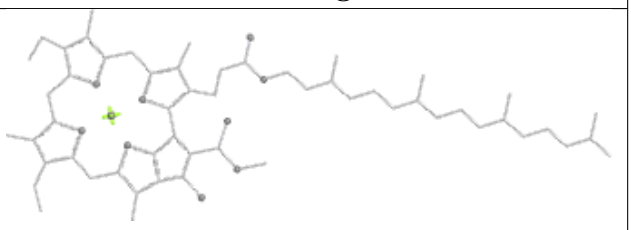
Bond lengths



Bond angles

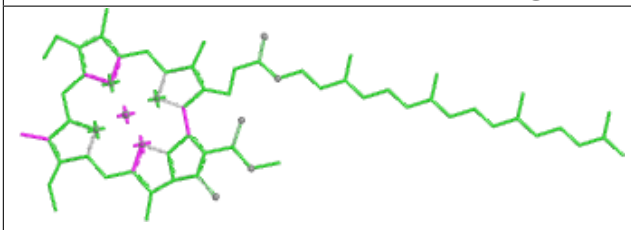


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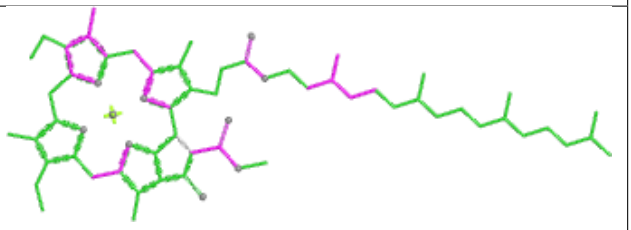


Rings

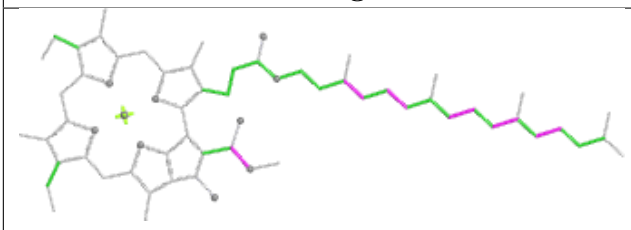
Ligand CLA b 604



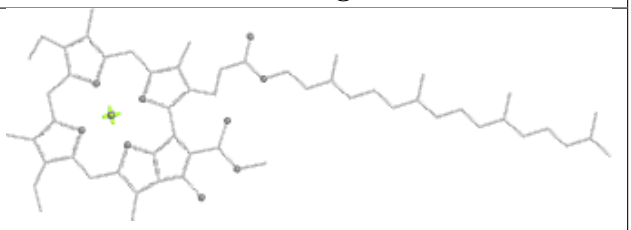
Bond lengths



Bond angles

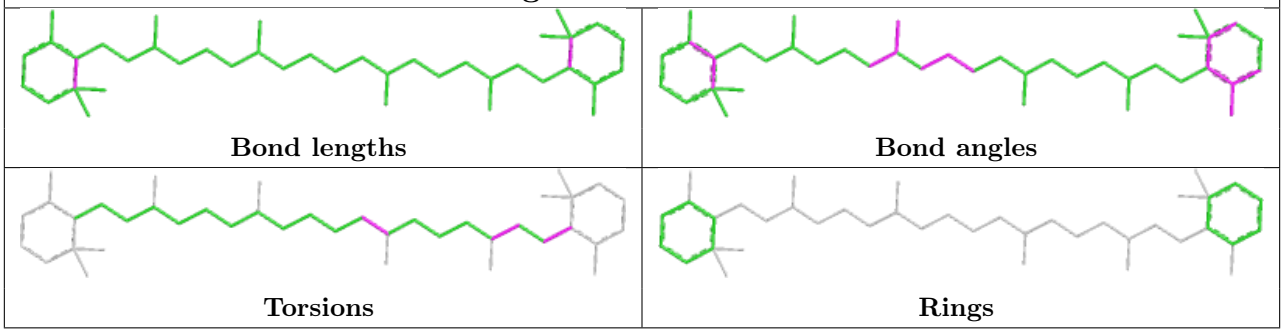


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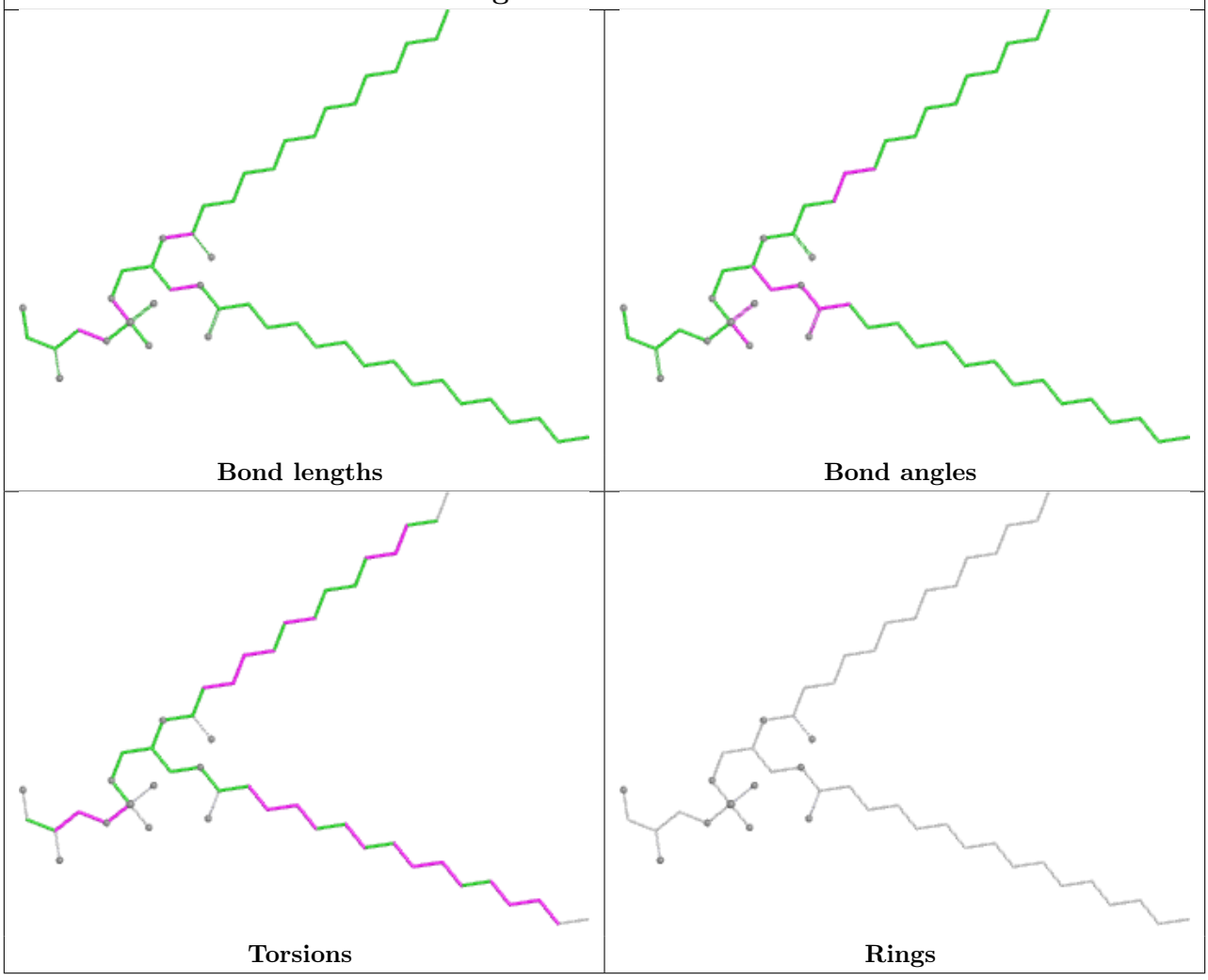


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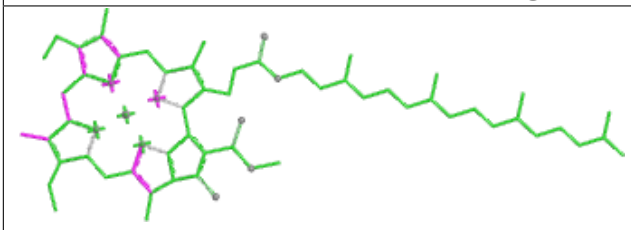
Ligand BCR H 101



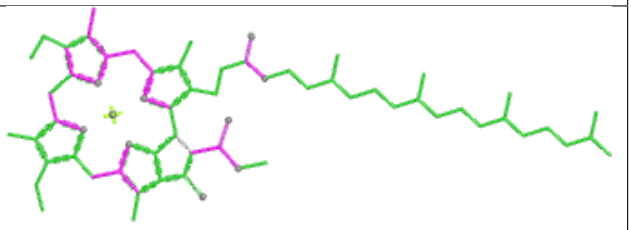
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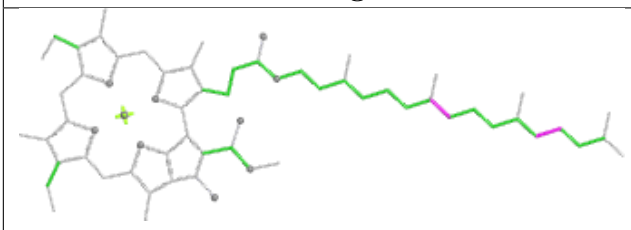
Ligand CLA C 508



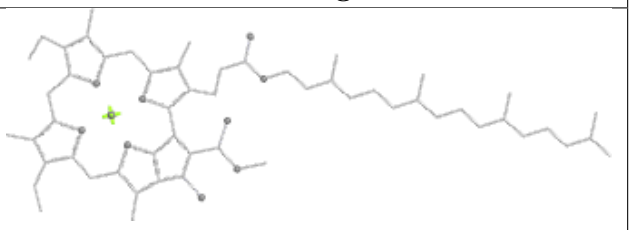
Bond lengths



Bond angles



Torsions

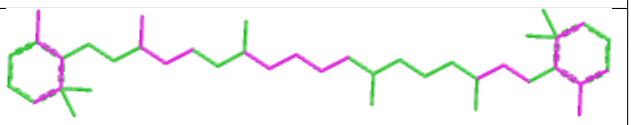


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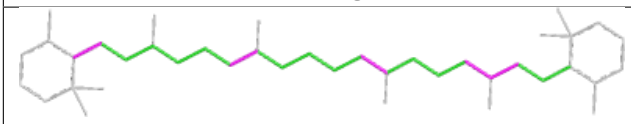
Ligand BCR b 618



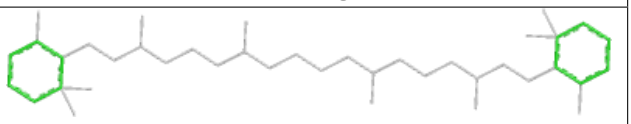
Bond lengths



Bond angles

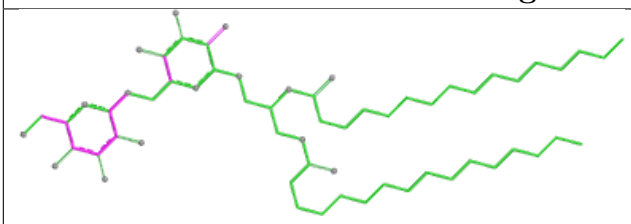


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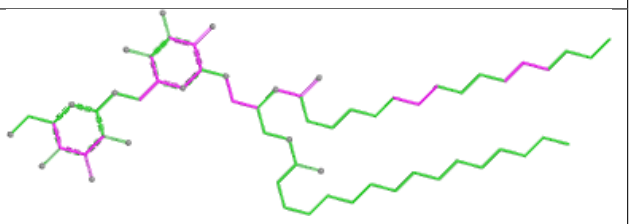


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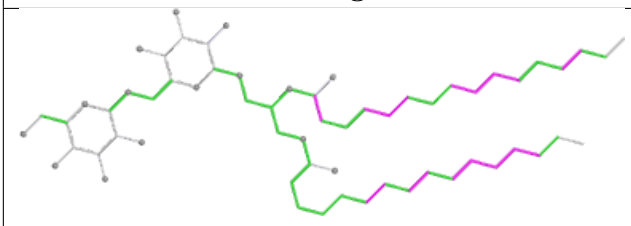
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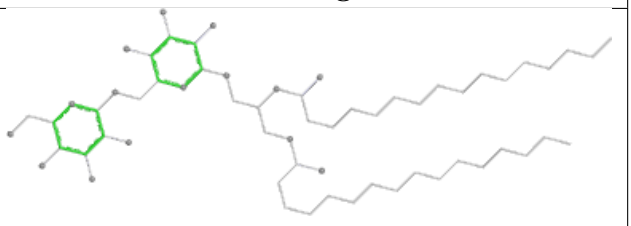
Bond lengths



Bond angles

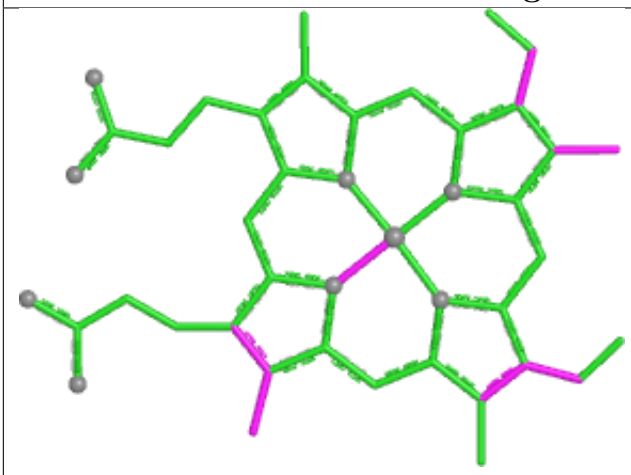


Torsions

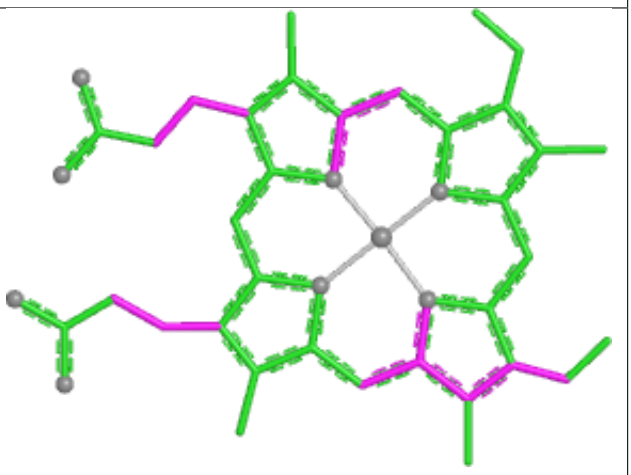


Rings

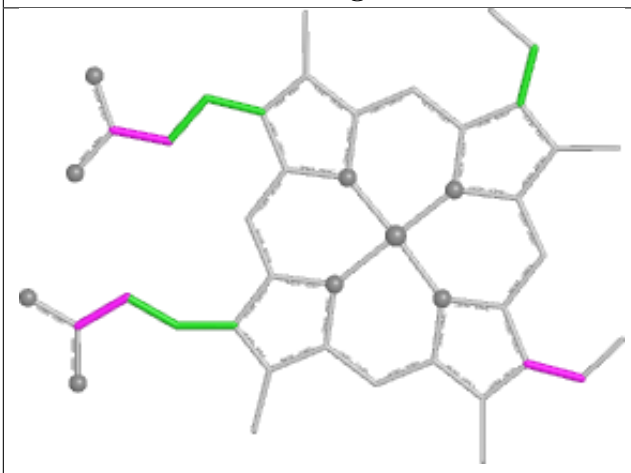
Ligand HEM e 102



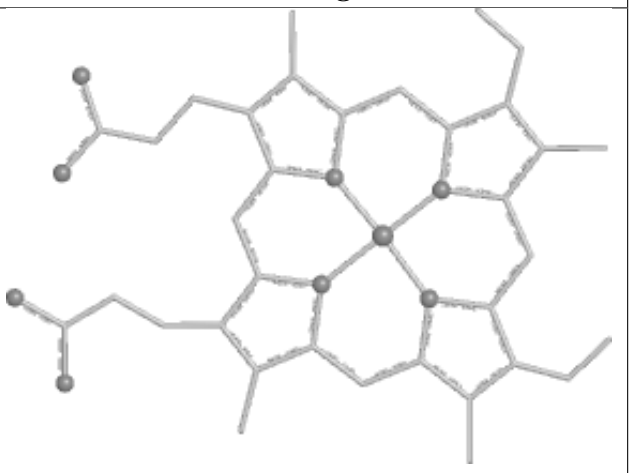
Bond lengths



Bond angles

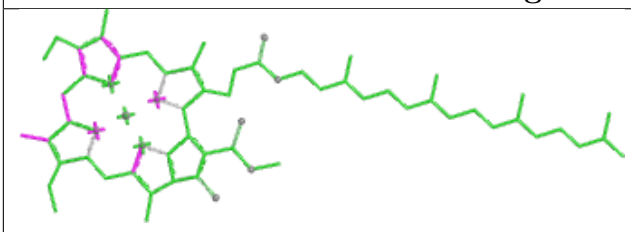


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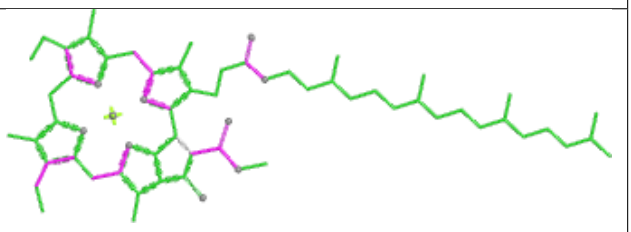


Rings

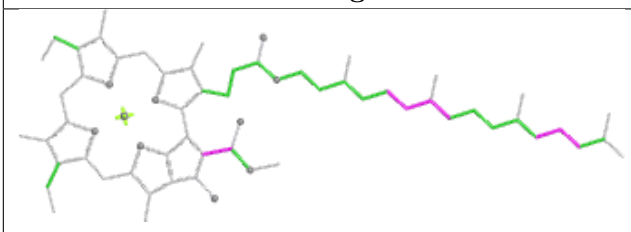
Ligand CLA C 507



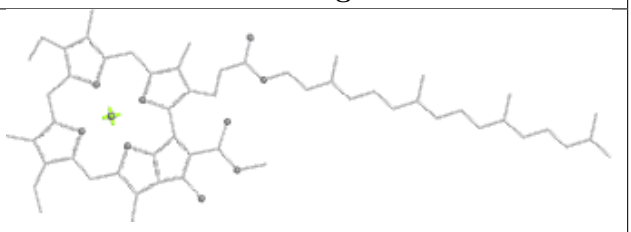
Bond lengths



Bond angles

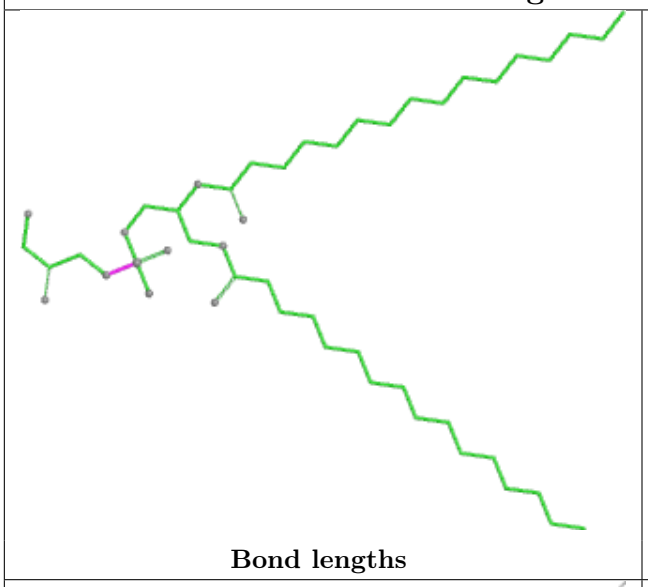


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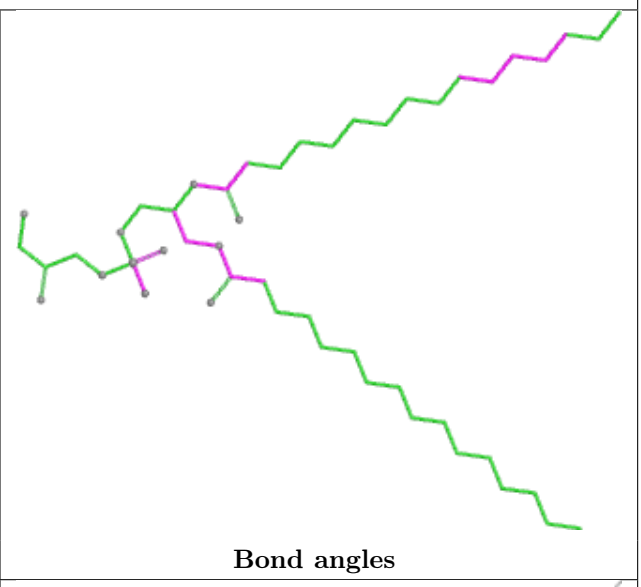


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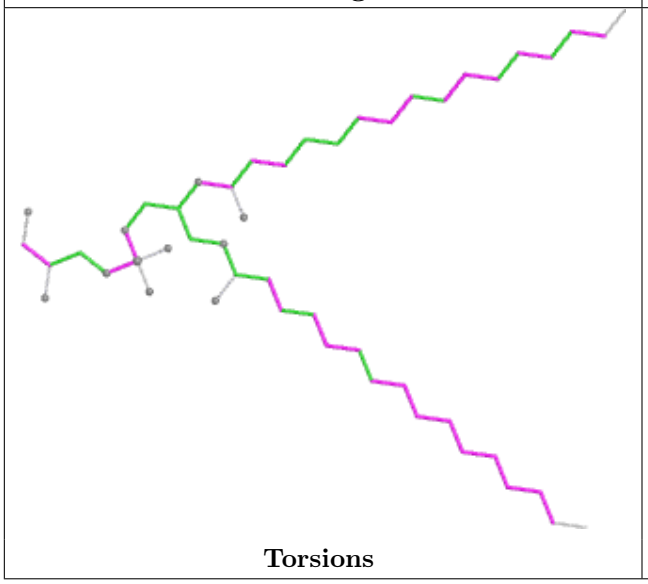
Ligand LHG d 407



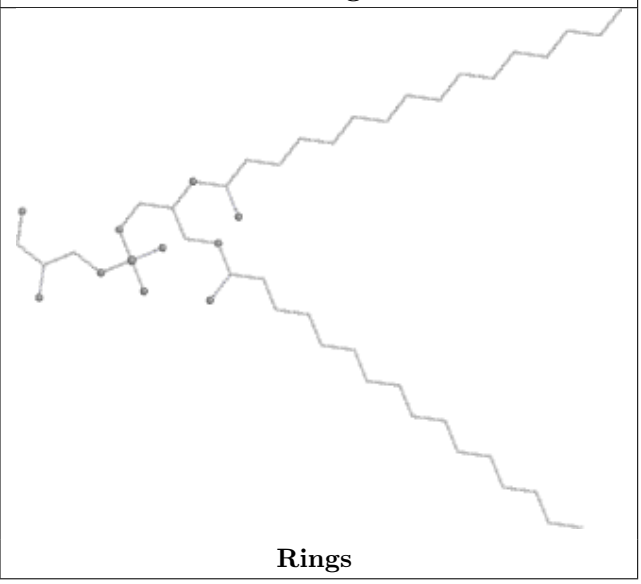
Bond lengths



Bond angles

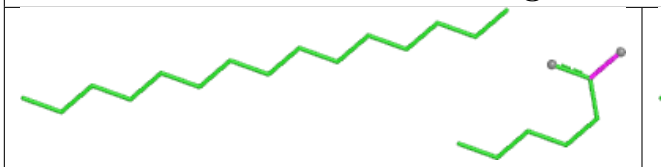


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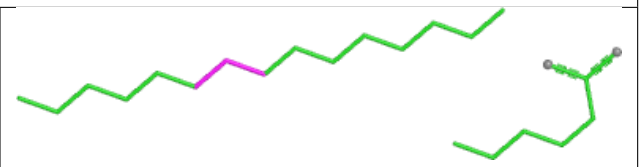


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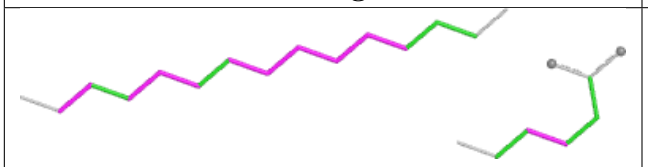
Ligand LMG b 623



Bond lengths



Bond angles

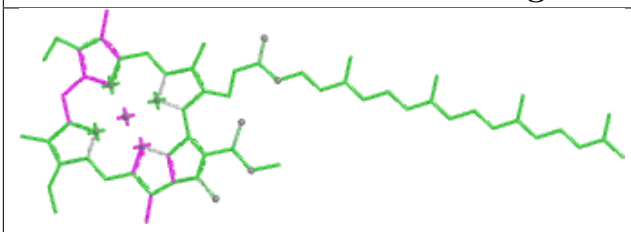


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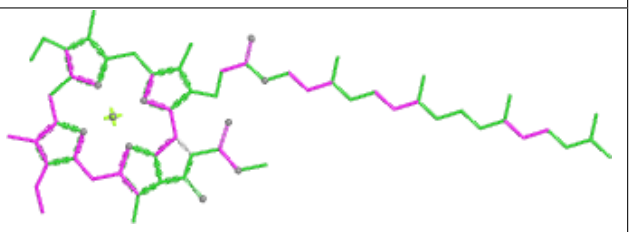


Rings

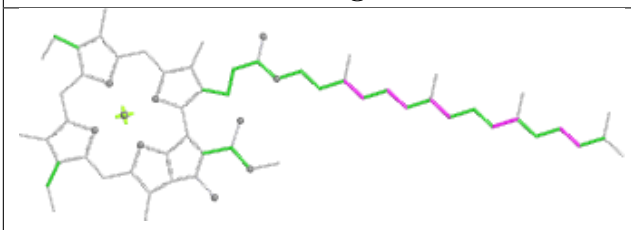
Ligand CLA b 606



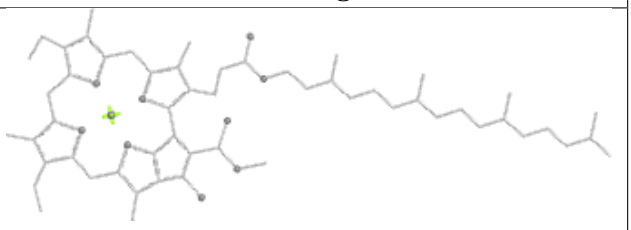
Bond lengths



Bond angles

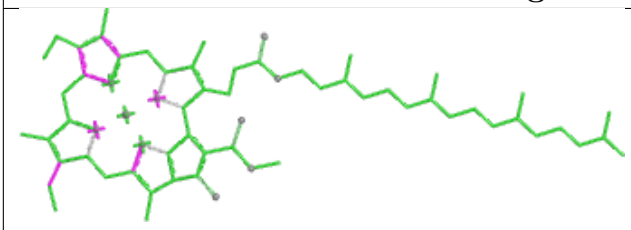


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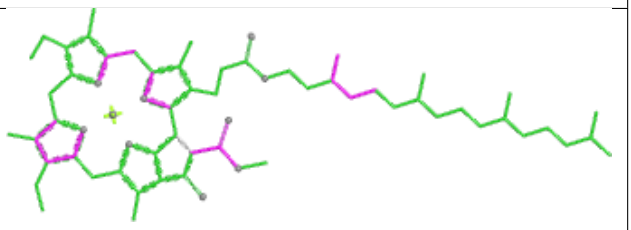


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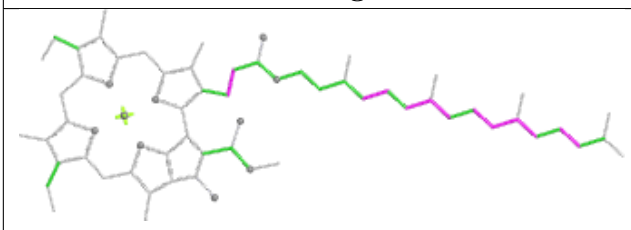
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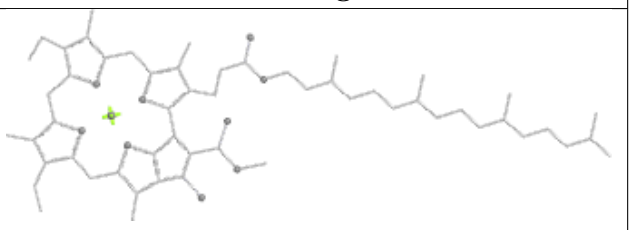
Bond lengths



Bond angles

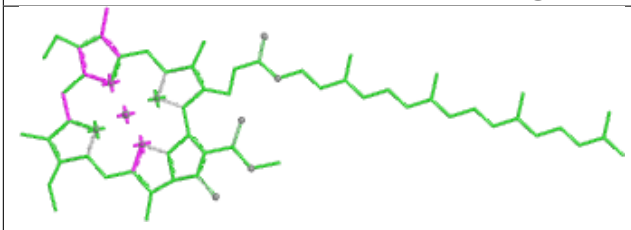


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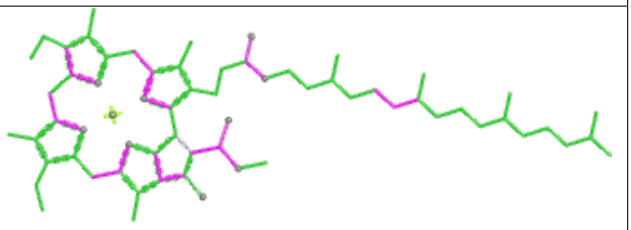


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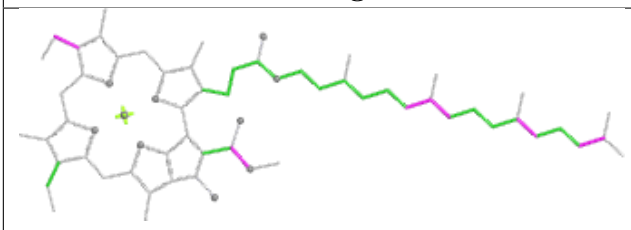
Ligand CLA c 505



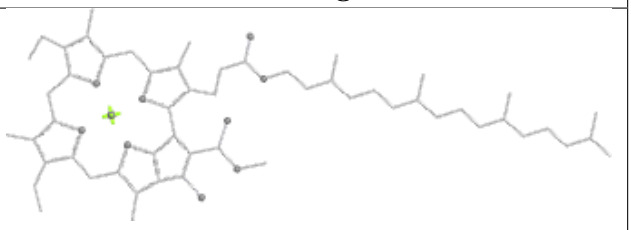
Bond lengths



Bond angles

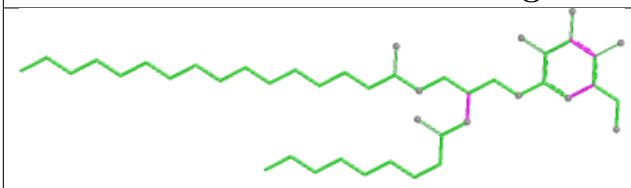


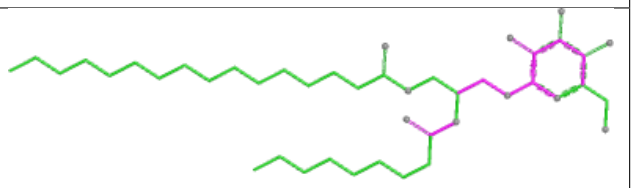
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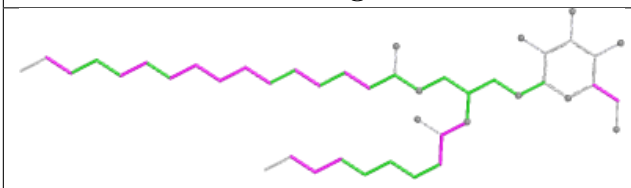


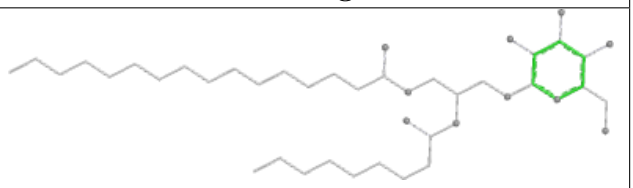
Rings

Ligand LMG d 409

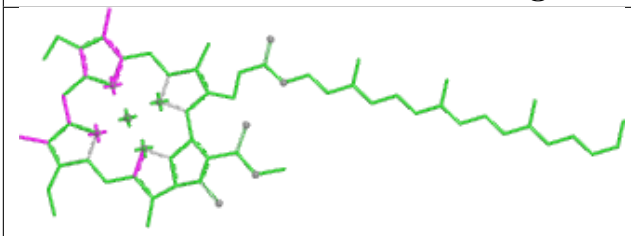

Bond lengths

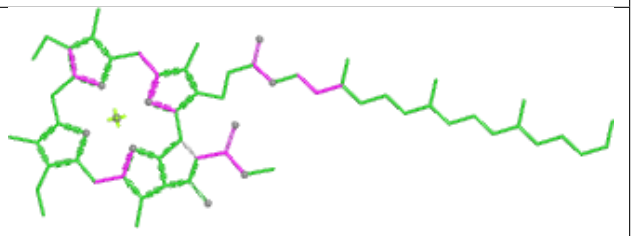

Bond angles

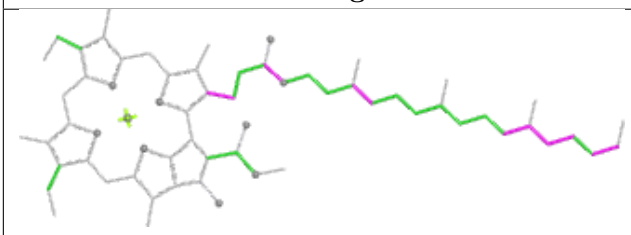

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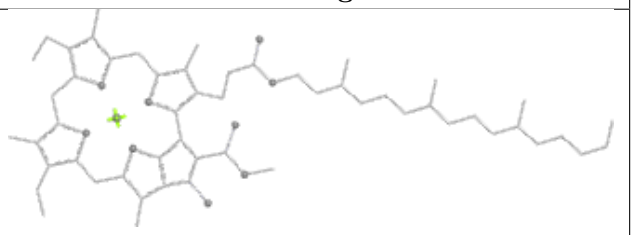

Rings

Ligand CLA c 508

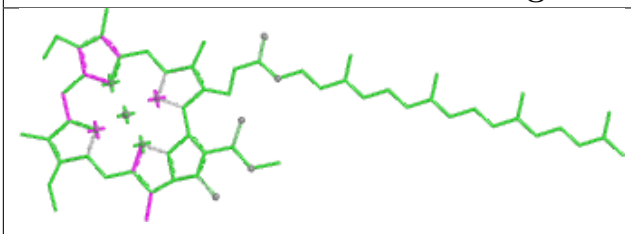

Bond lengths

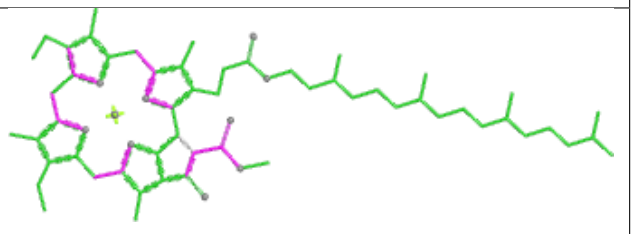

Bond angles

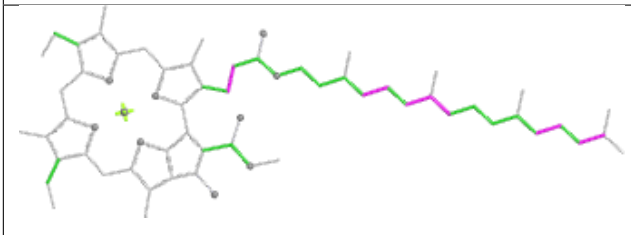

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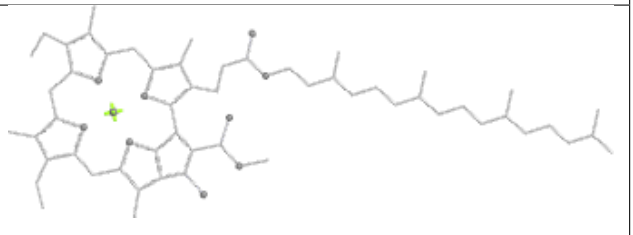

Rings

Ligand CLA b 603

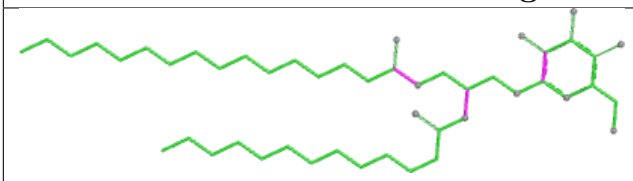

Bond lengths


Bond angles

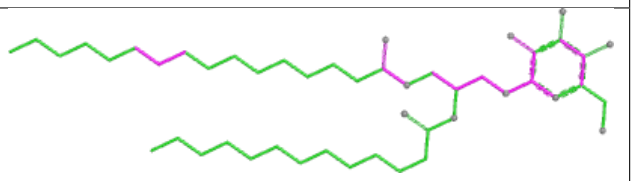

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Rings

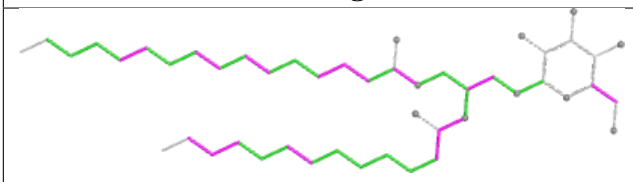
Ligand LMG C 518



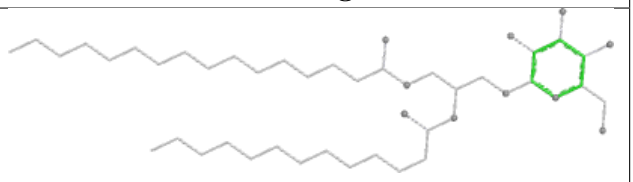
Bond lengths



Bond angles

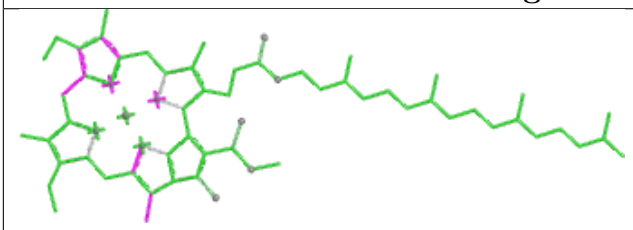


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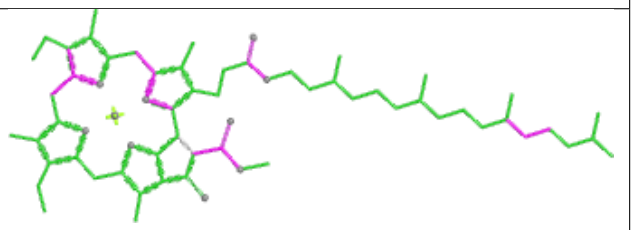


Rings

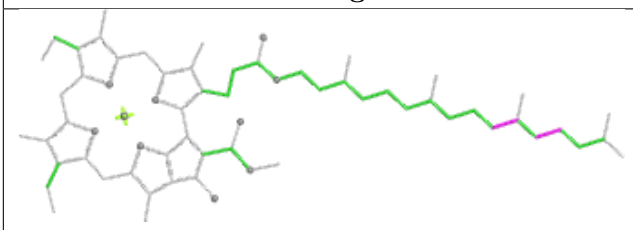
Ligand CLA D 401



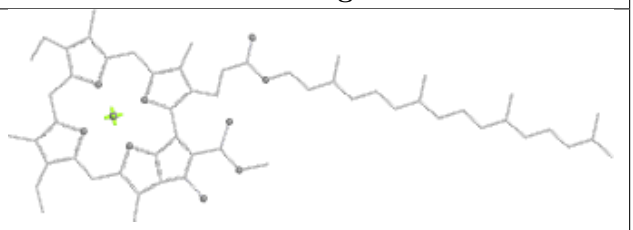
Bond lengths



Bond angles



Torsions

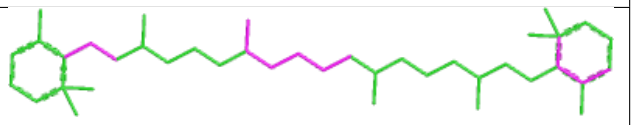


Rings

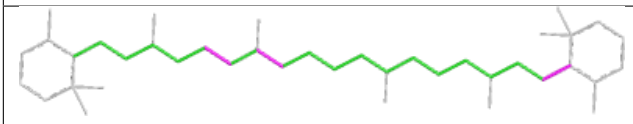
Ligand BCR b 619



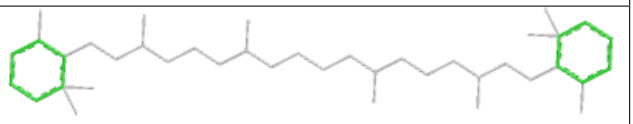
Bond lengths



Bond angles

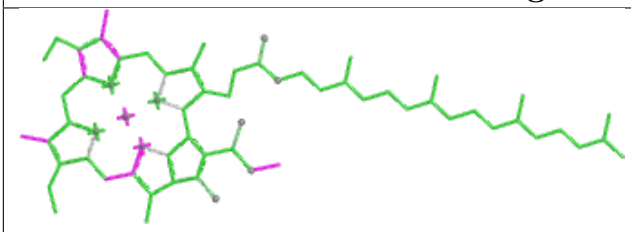


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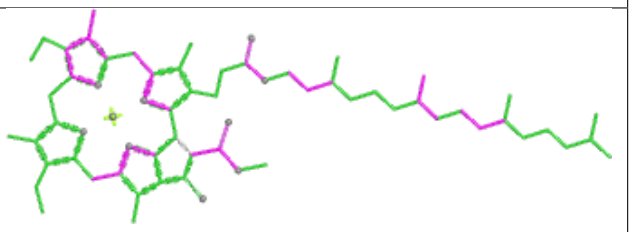


Rings

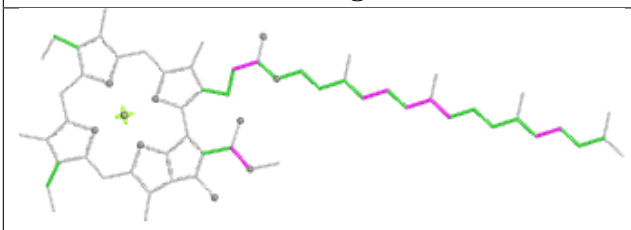
Ligand CLA b 613



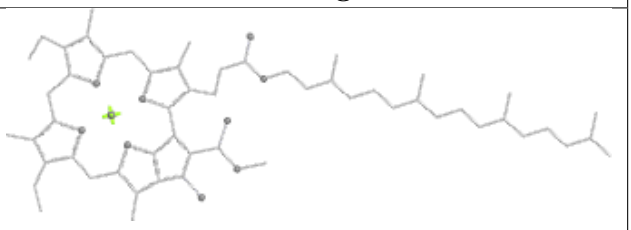
Bond lengths



Bond angles

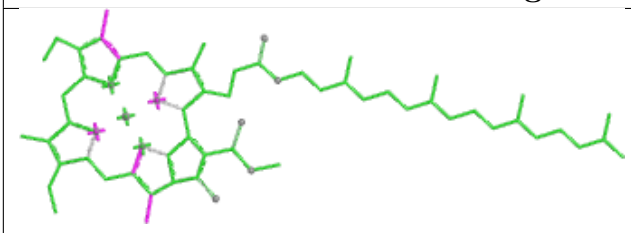


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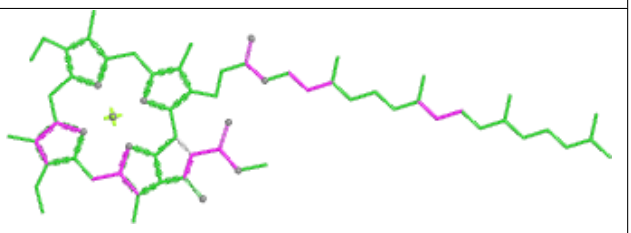


Rings

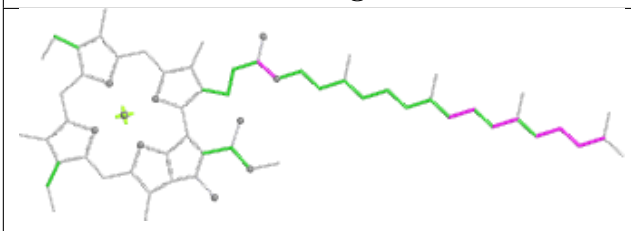
Ligand CLA B 611



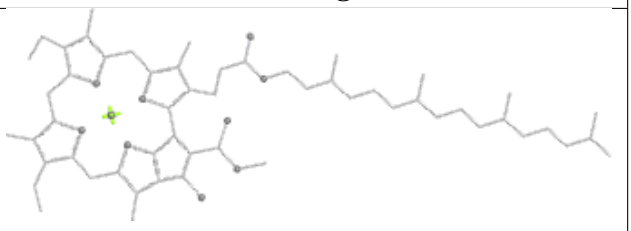
Bond lengths



Bond angles

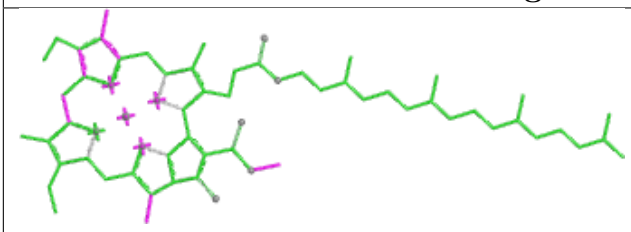


Torsions

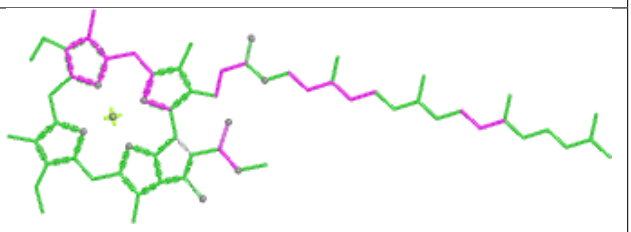


Rings

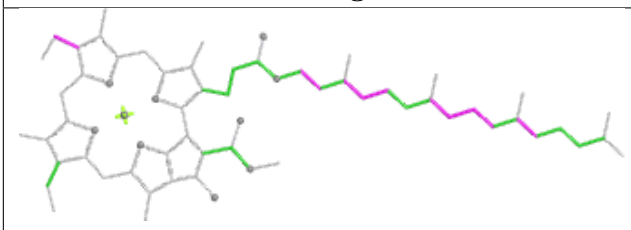
Ligand CLA C 512



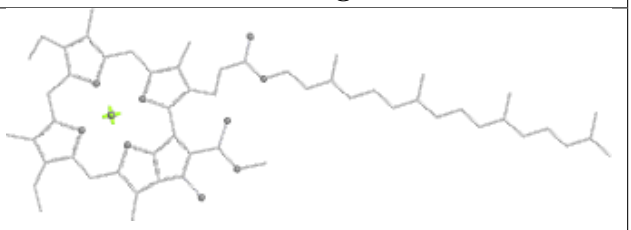
Bond lengths



Bond angles

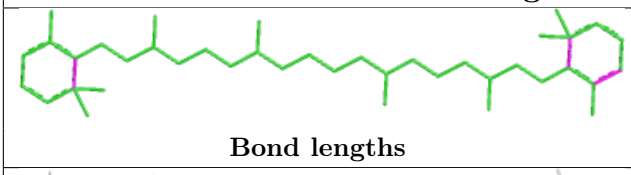


Torsions

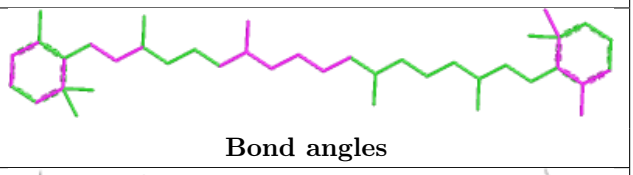


Rings

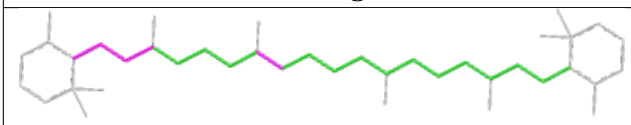
Ligand BCR T 101



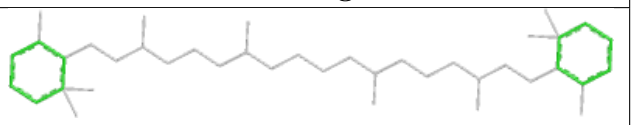
Bond lengths



Bond angles

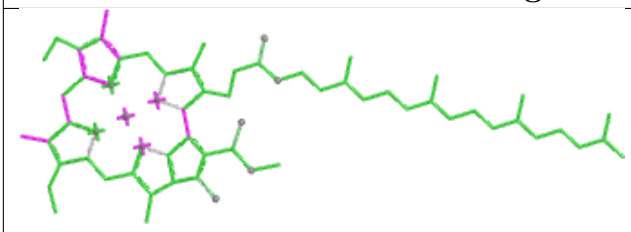


Torsions

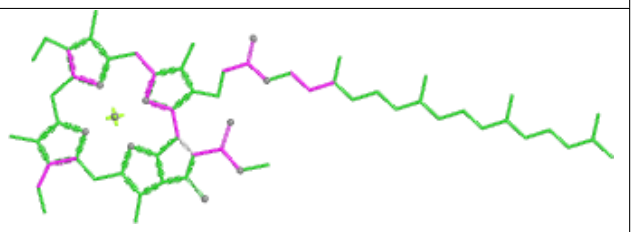


Rings

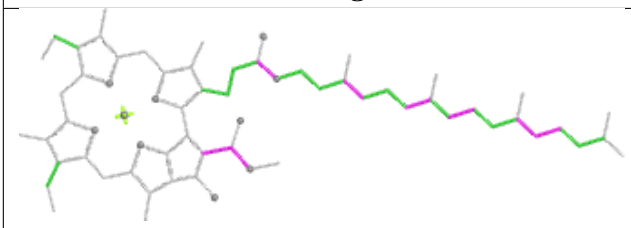
Ligand CLA B 614



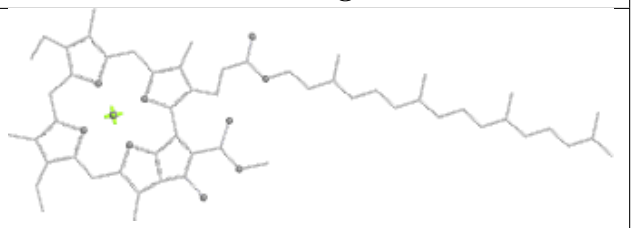
Bond lengths



Bond angles

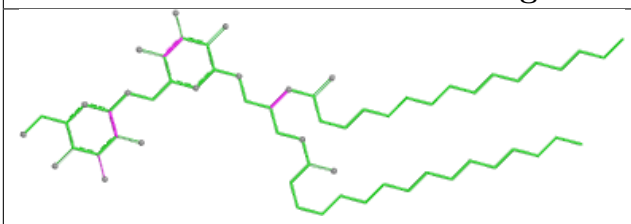


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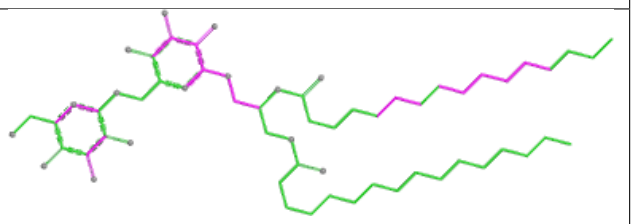


Rings

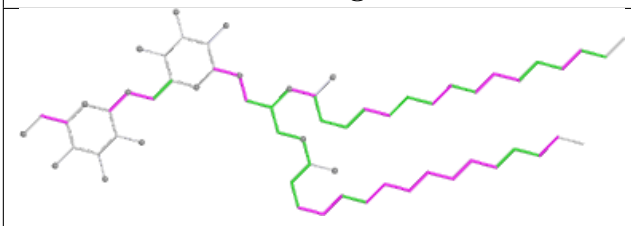
Ligand DGD C 516



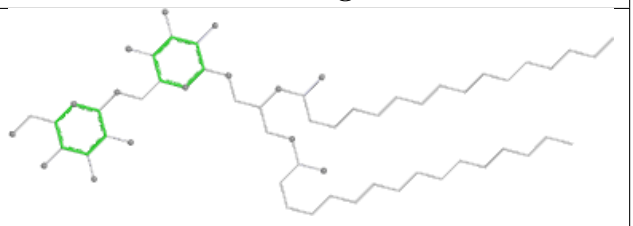
Bond lengths



Bond angles

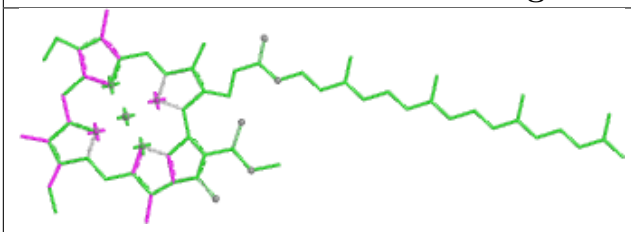


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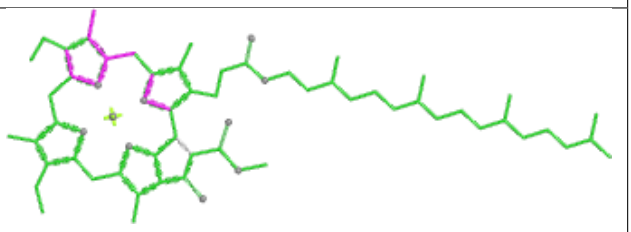


Rings

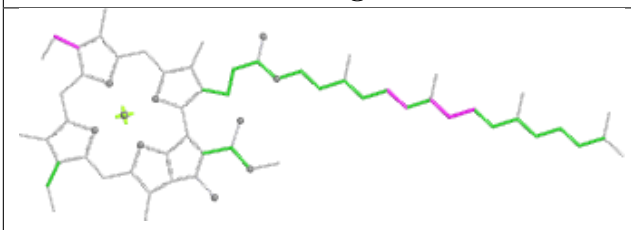
Ligand CLA b 616



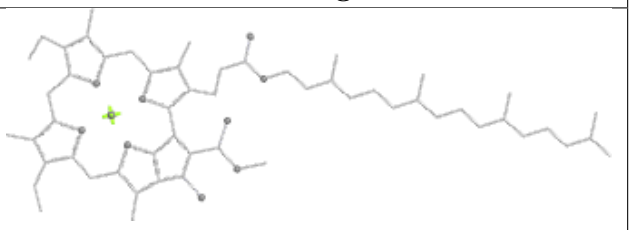
Bond lengths



Bond angles



Torsions



Rings

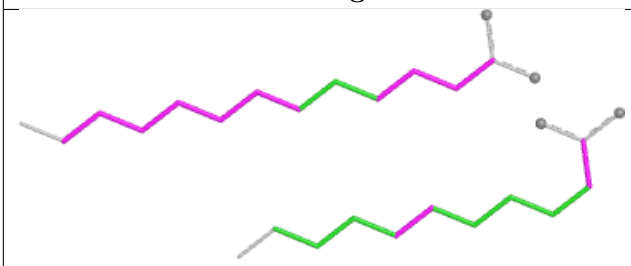
Ligand LMG B 621



Bond lengths



Bond angles

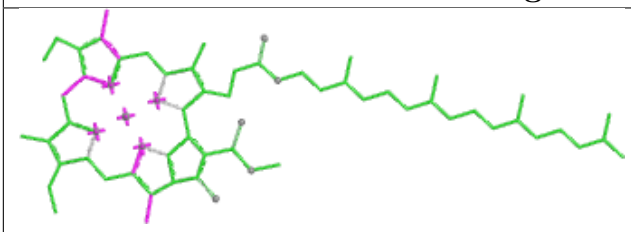


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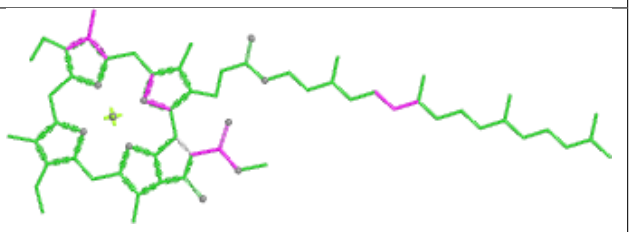


Rings

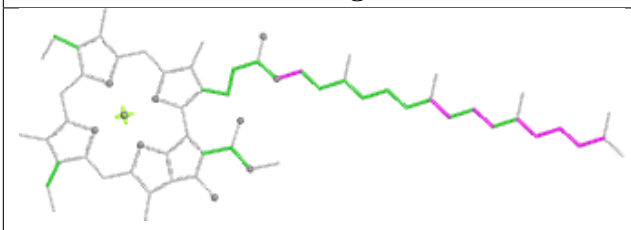
Ligand CLA C 513



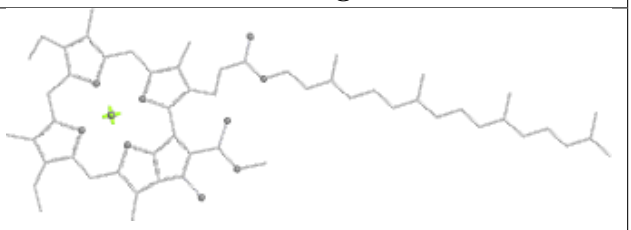
Bond lengths



Bond angles



Torsions

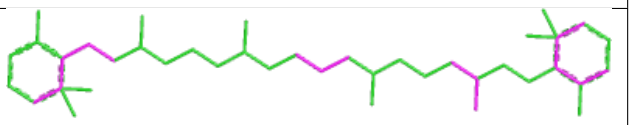


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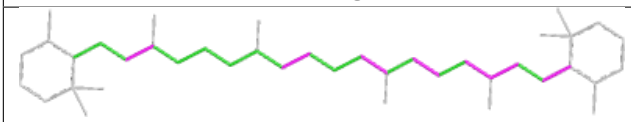
Ligand BCR K 102



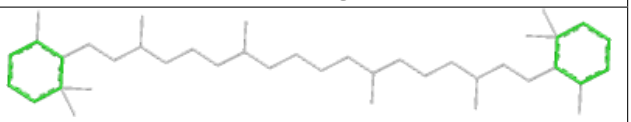
Bond lengths



Bond angles

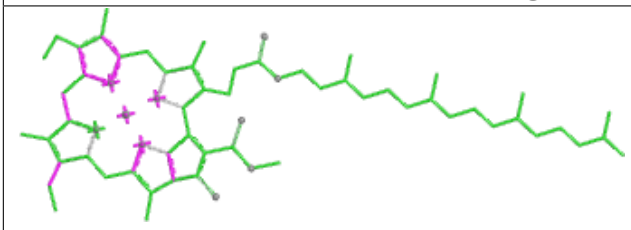


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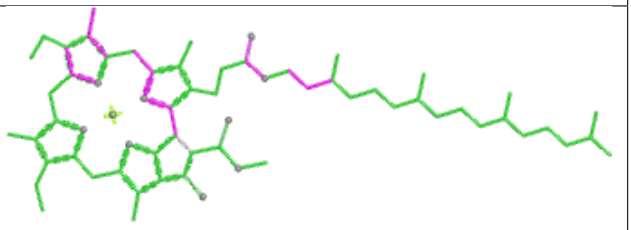


Rings

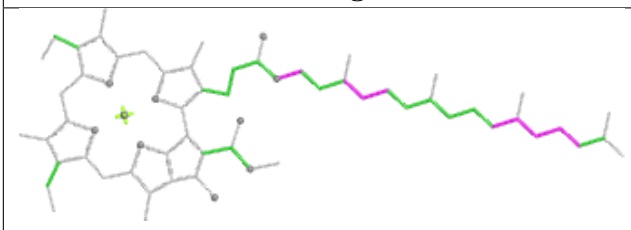
Ligand CLA C 506



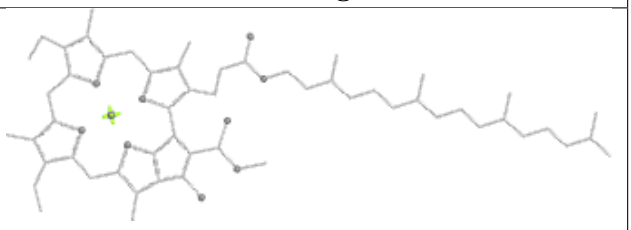
Bond lengths



Bond angles

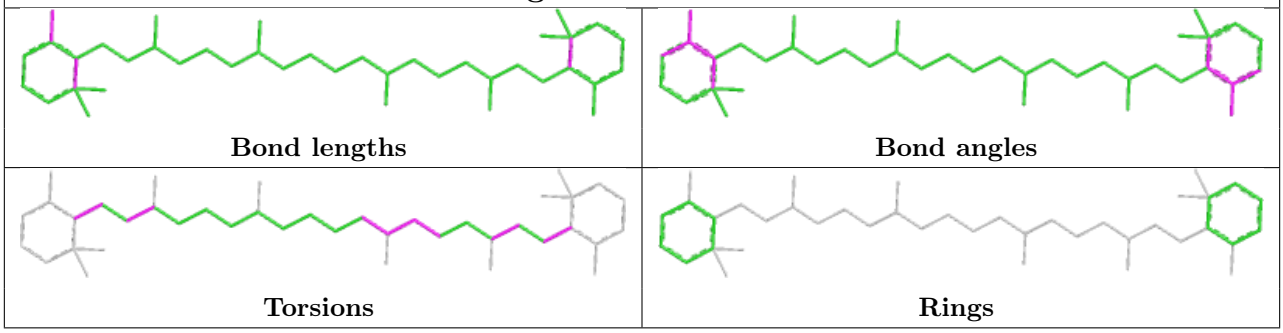


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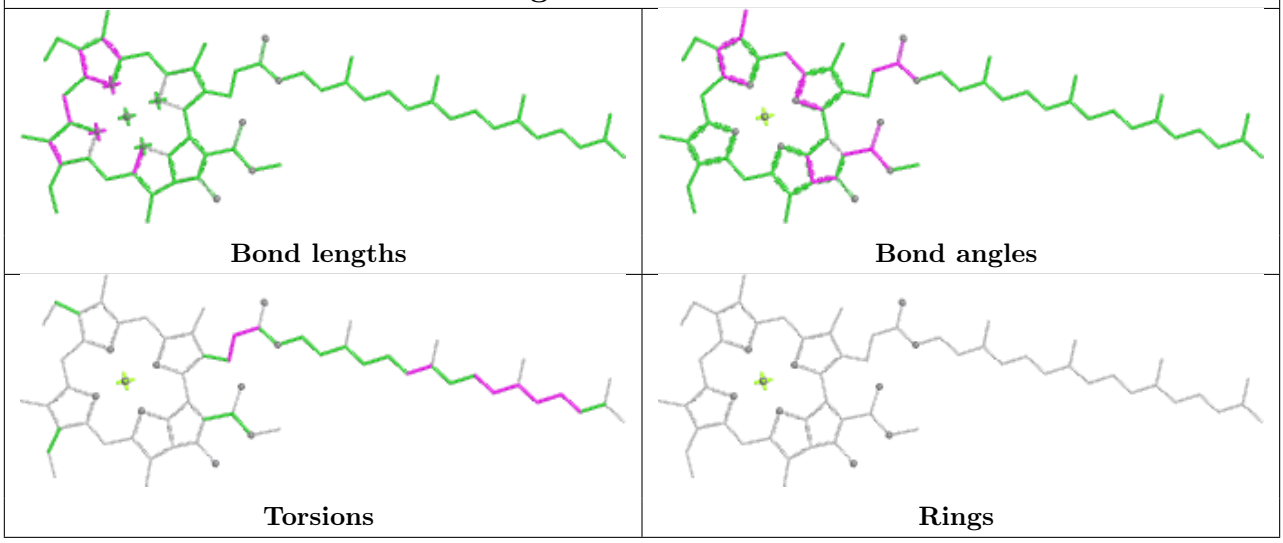


Rings

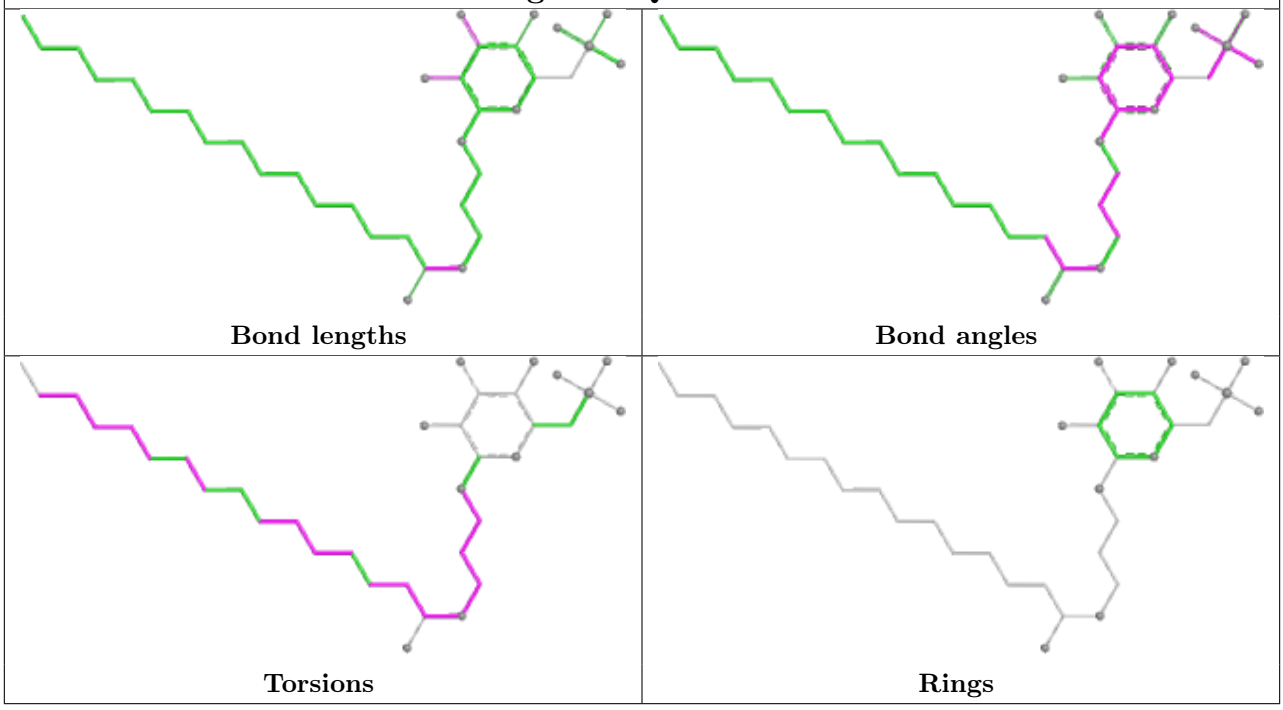
Ligand BCR k 101



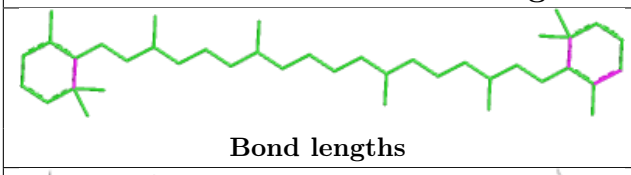
Ligand CLA c 509



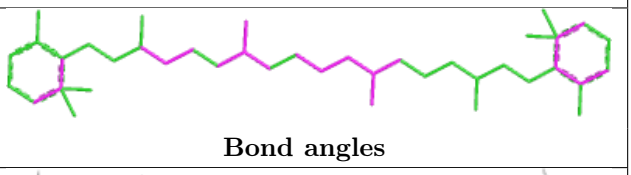
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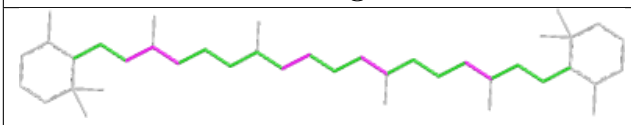
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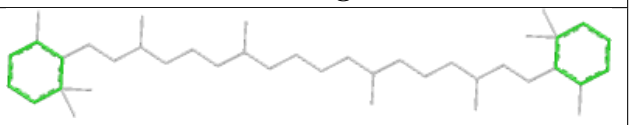
Bond lengths



Bond angles

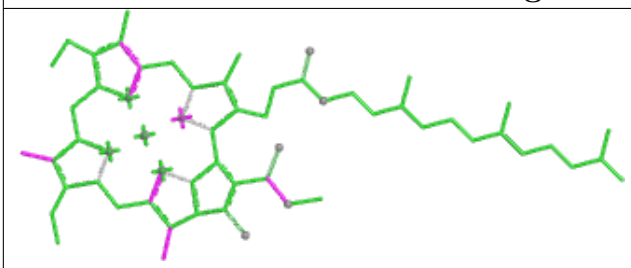


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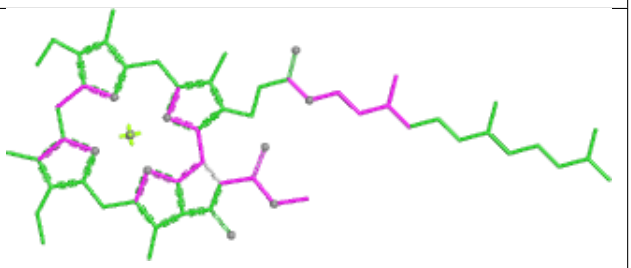


Rings

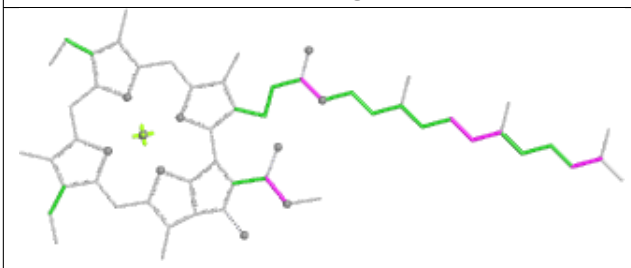
Ligand CLA B 616



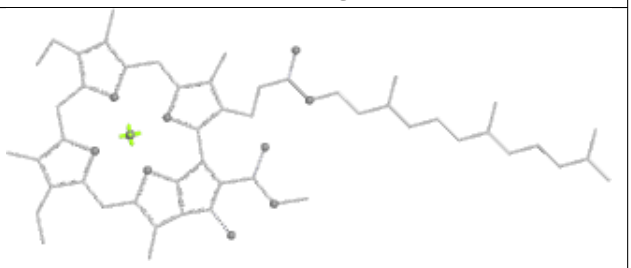
Bond lengths



Bond angles

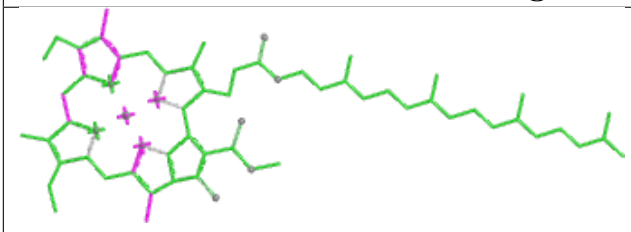


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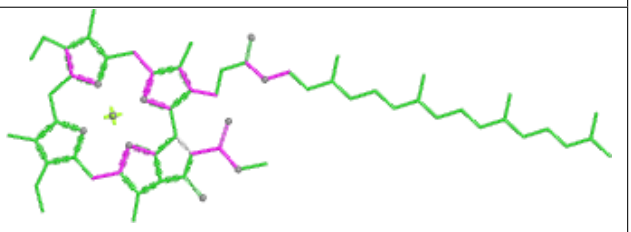


Rings

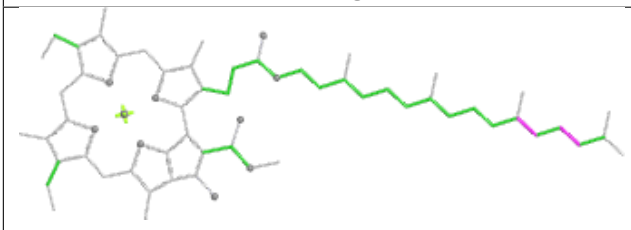
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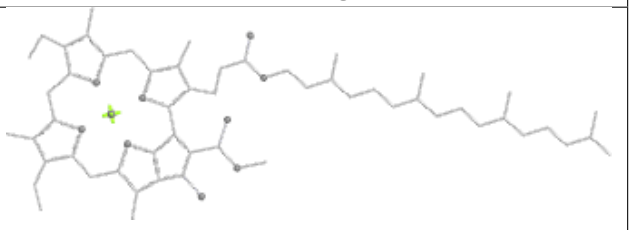
Bond lengths



Bond angles

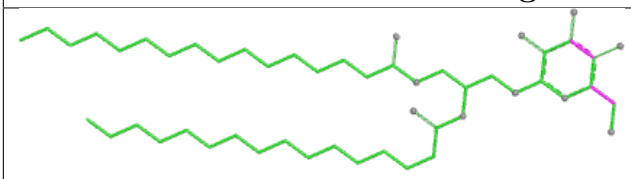


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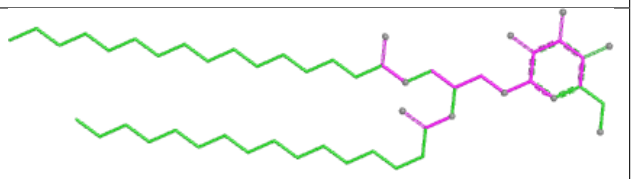


Rings

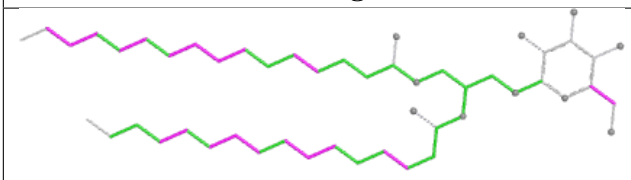
Ligand LMG D 406



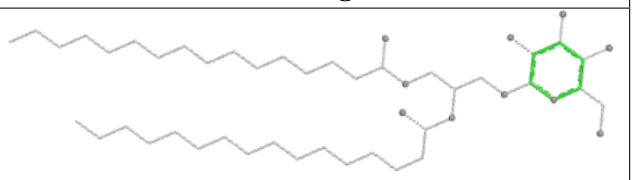
Bond lengths



Bond angles

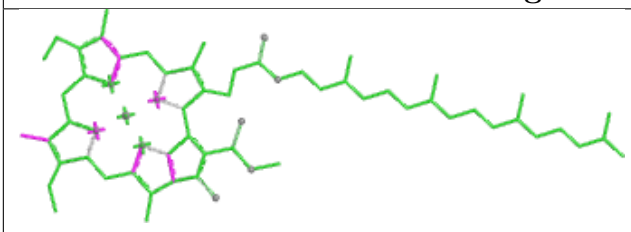


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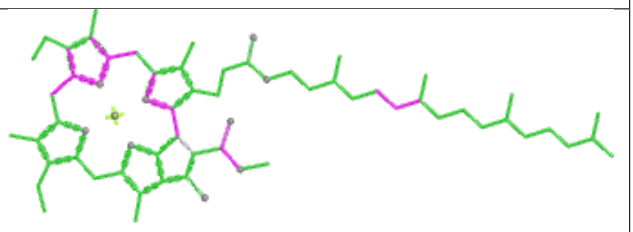


Rings

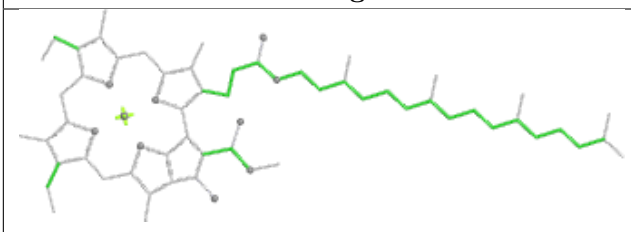
Ligand CLA B 608



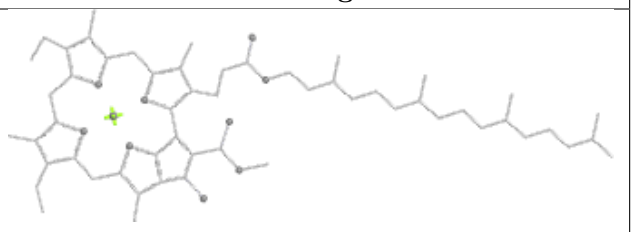
Bond lengths



Bond angles

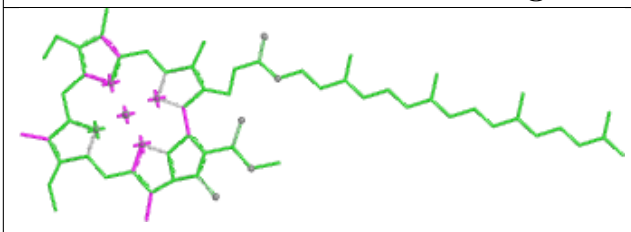


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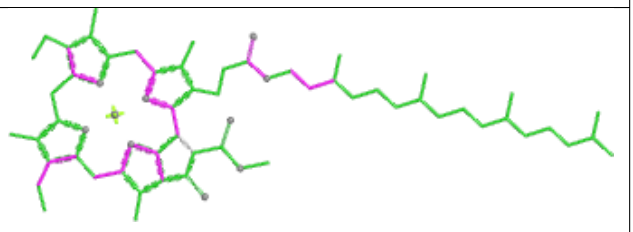


Rings

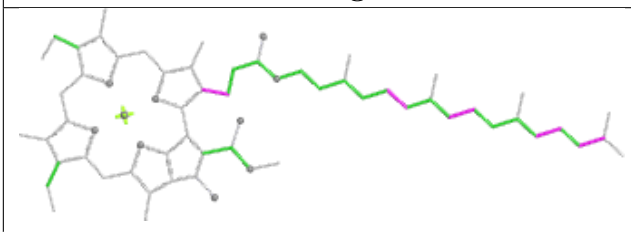
Ligand CLA d 403



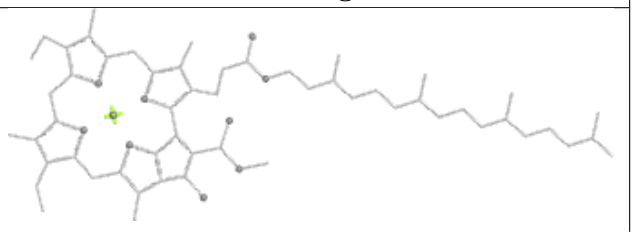
Bond lengths



Bond angles

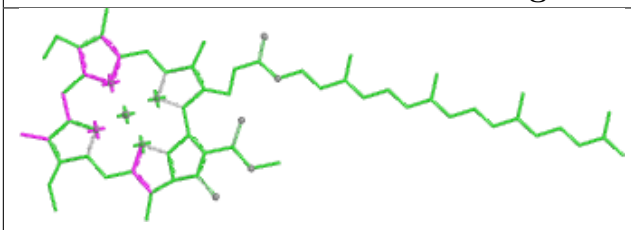


Torsions

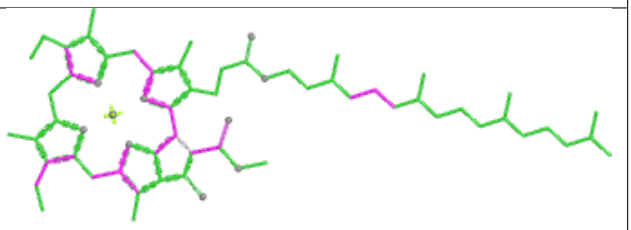


Rings

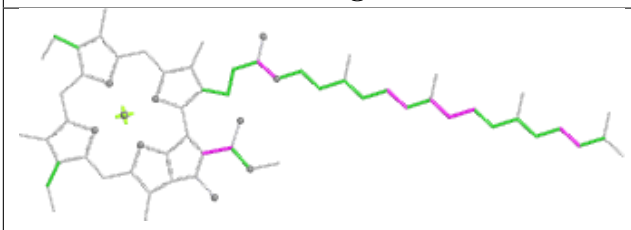
Ligand CLA c 503



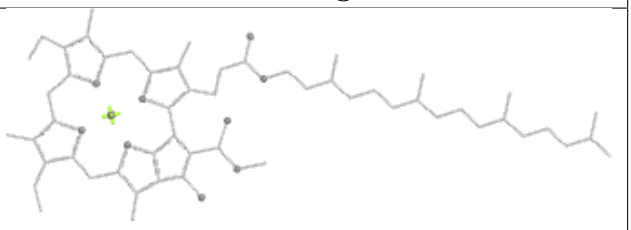
Bond lengths



Bond angles

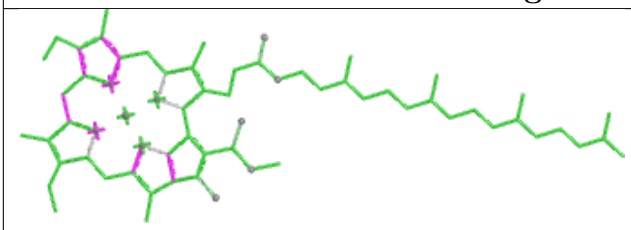


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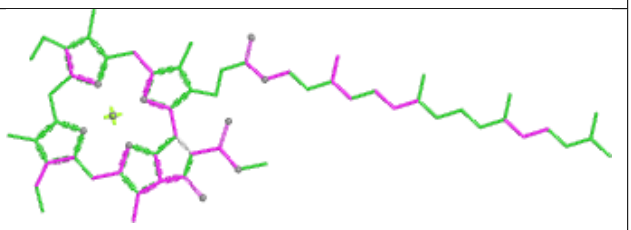


Rings

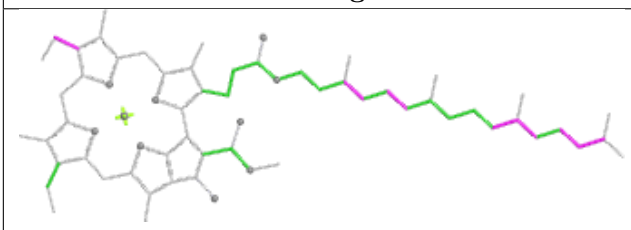
Ligand CLA B 605



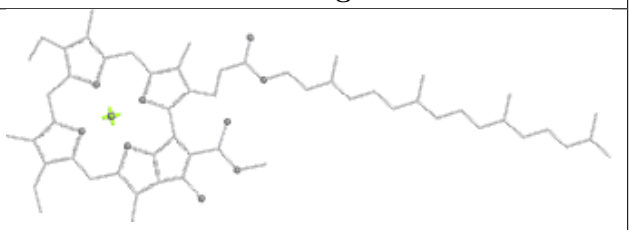
Bond lengths



Bond angles



Torsions

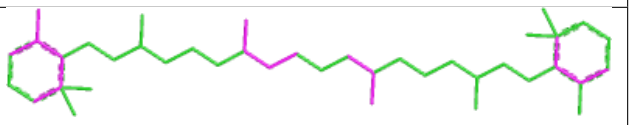


Rings

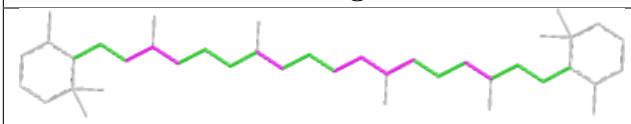
Ligand BCR c 515



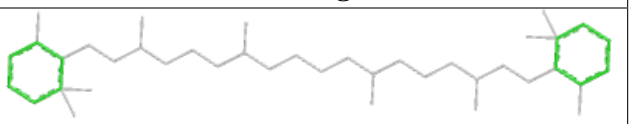
Bond lengths



Bond angles

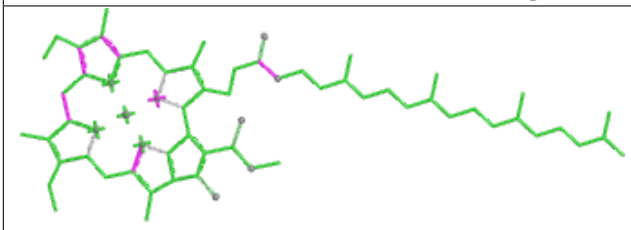


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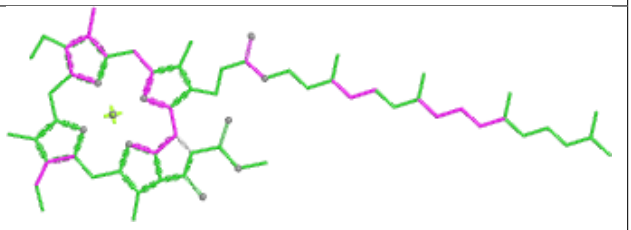


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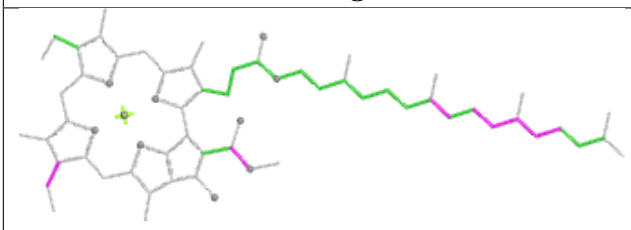
Ligand CLA B 604



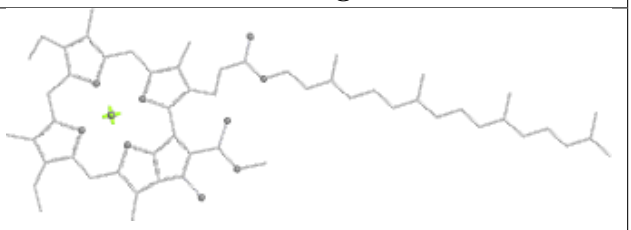
Bond lengths



Bond angles



Torsions

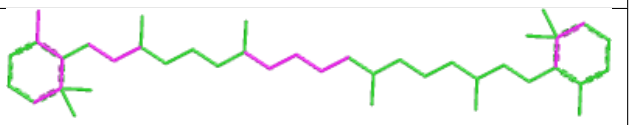


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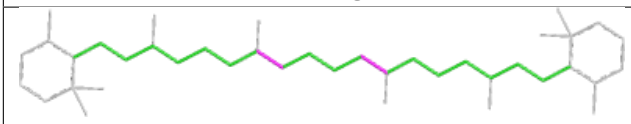
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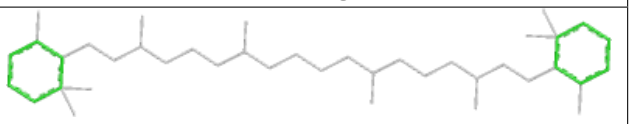
Bond lengths



Bond angles

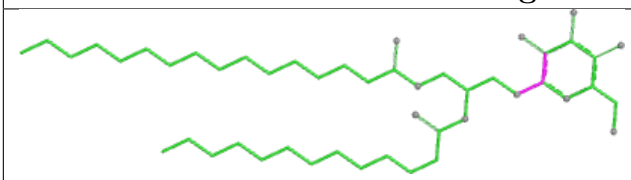


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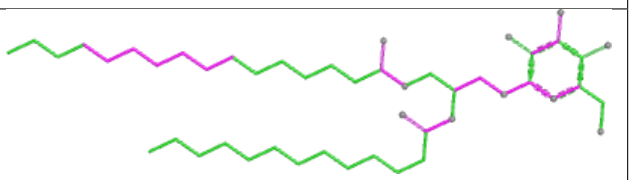


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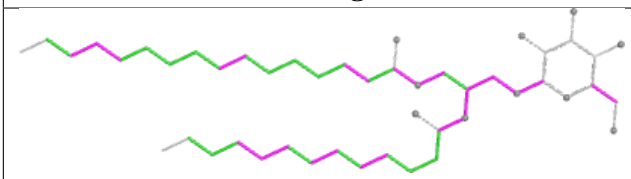
Ligand LMG A 411



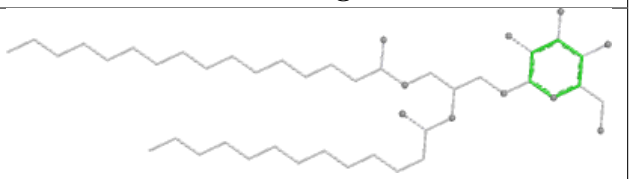
Bond lengths



Bond angles

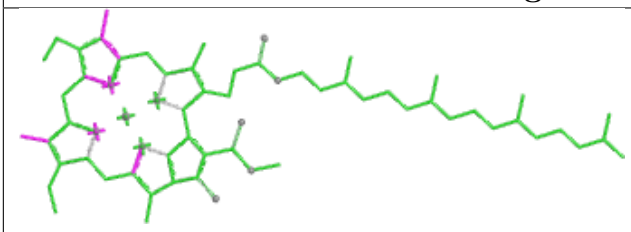


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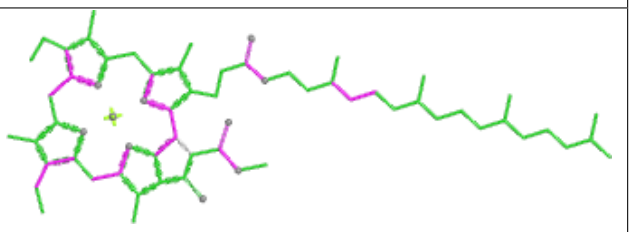


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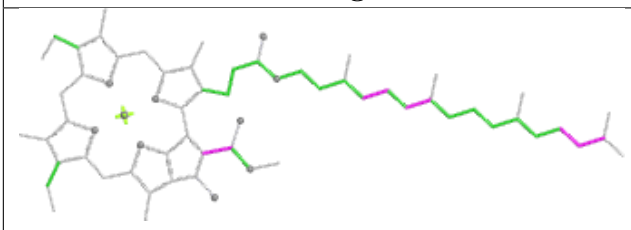
Ligand CLA C 502



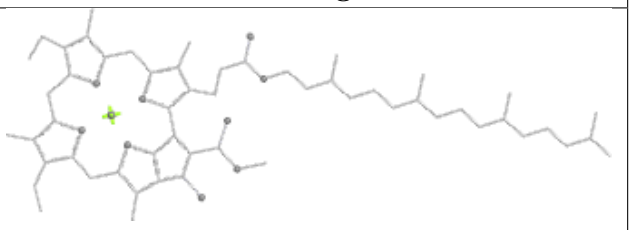
Bond lengths



Bond angles



Torsions

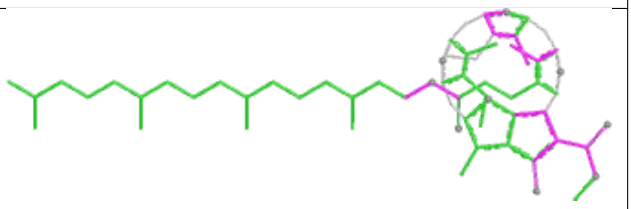


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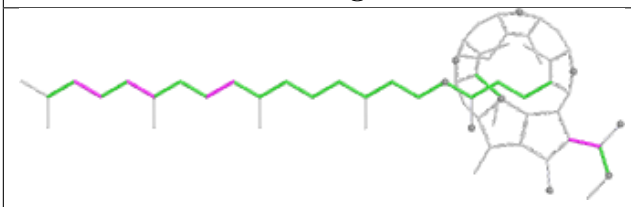
Ligand PHO A 406



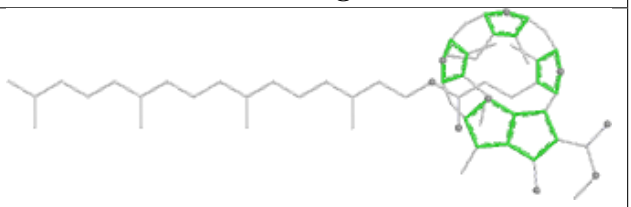
Bond lengths



Bond angles

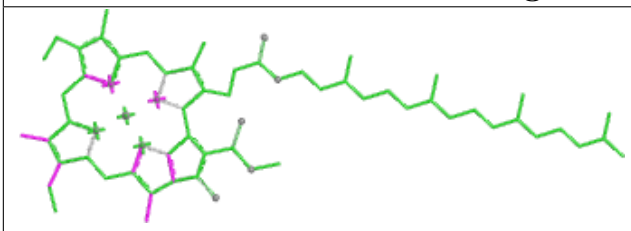


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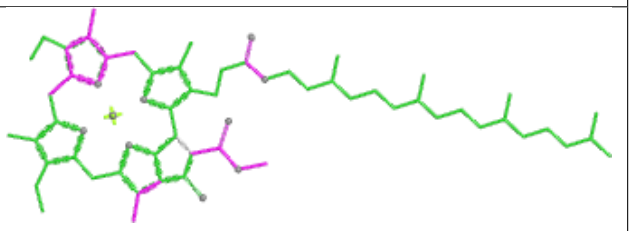


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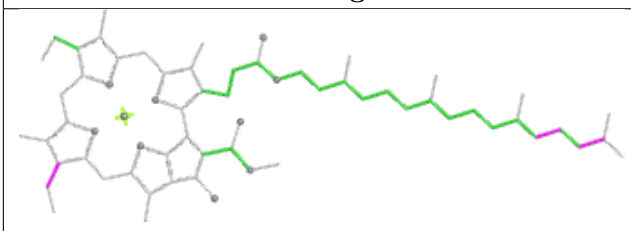
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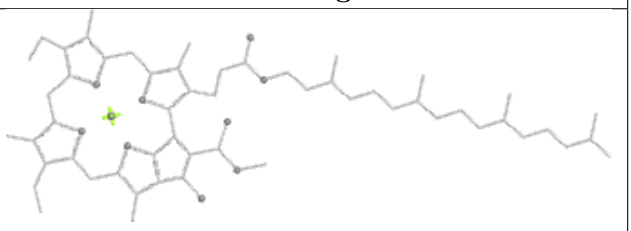
Bond lengths



Bond angles

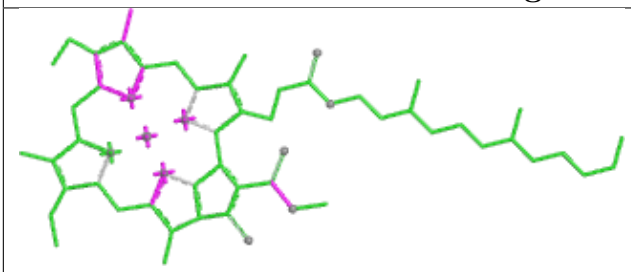


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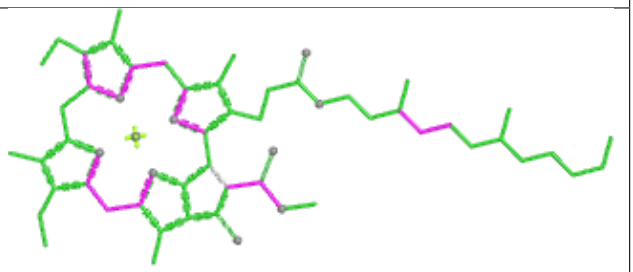


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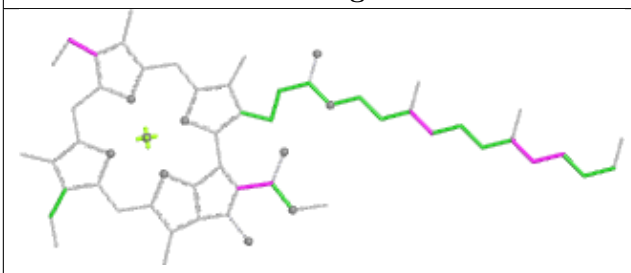
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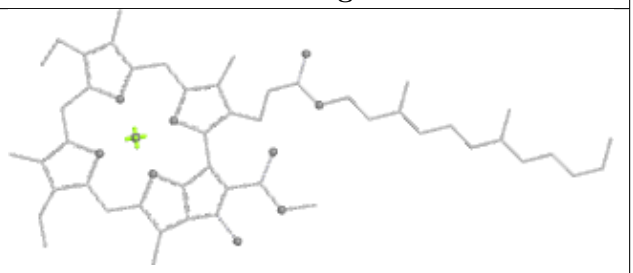
Bond lengths



Bond angles

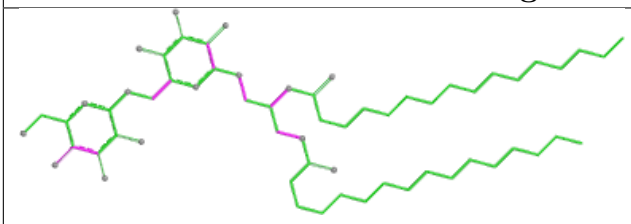


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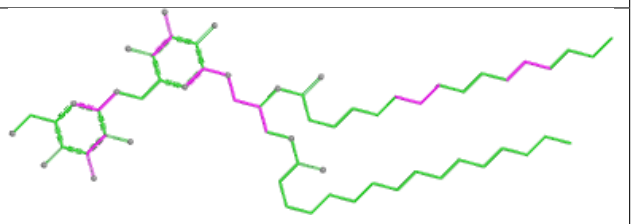


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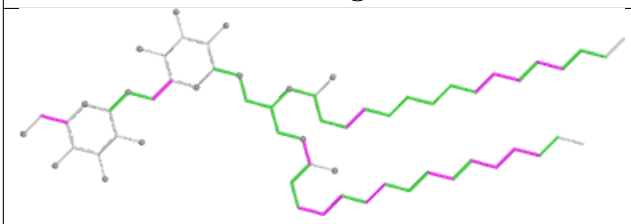
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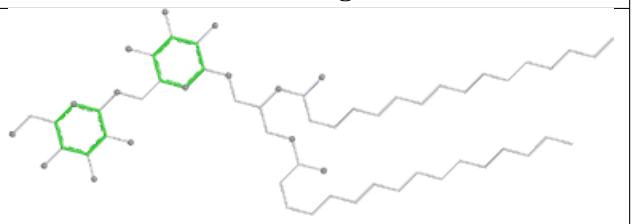
Bond lengths



Bond angles

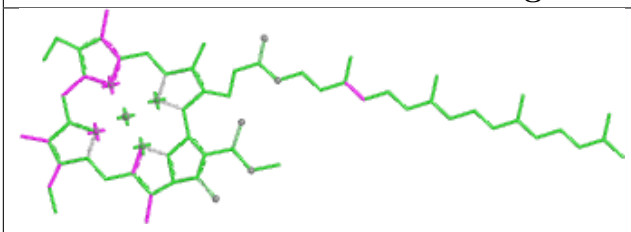


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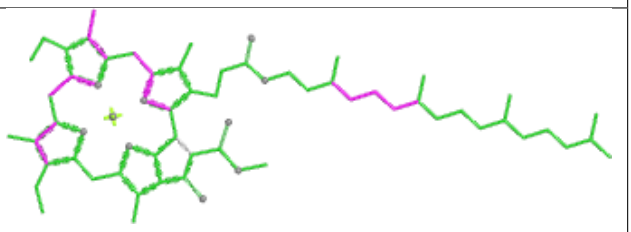


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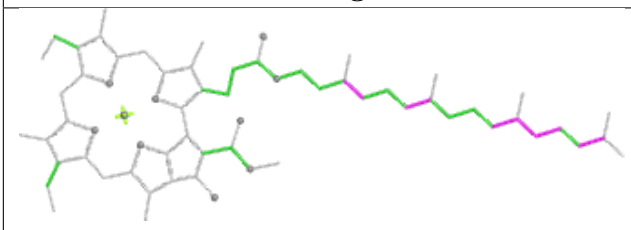
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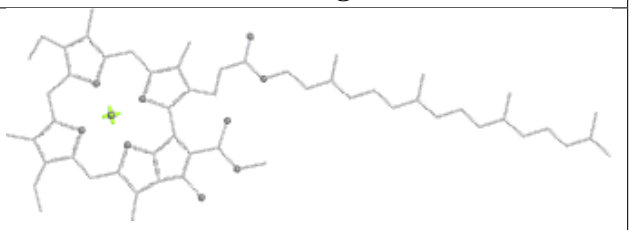
Bond lengths



Bond angles

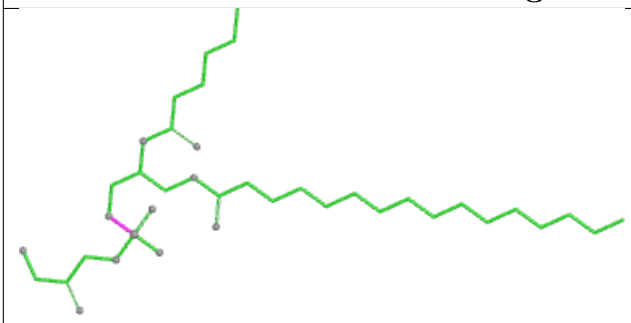


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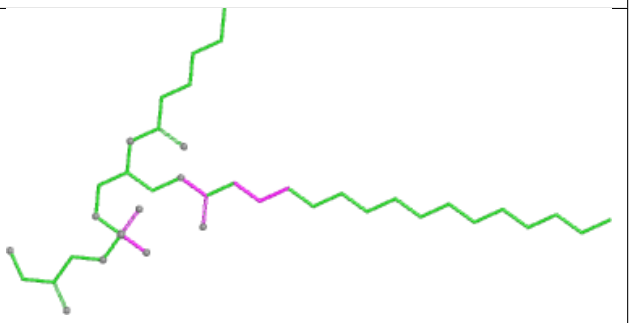


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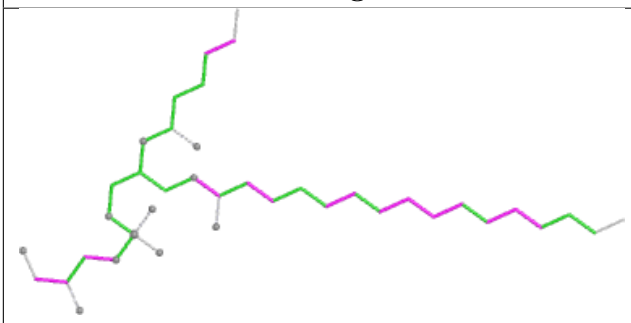
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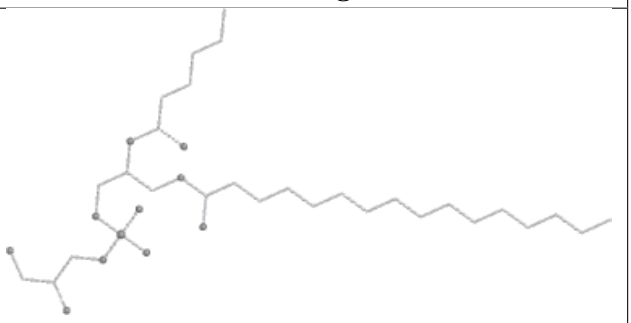
Bond lengths



Bond angles

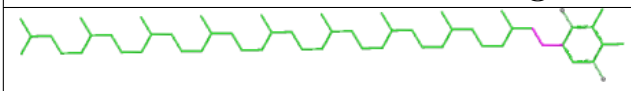


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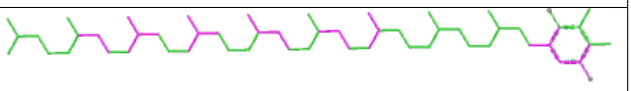


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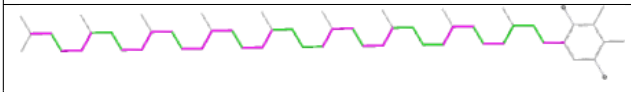
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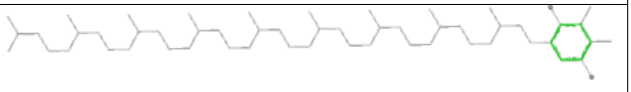
Bond lengths



Bond angles

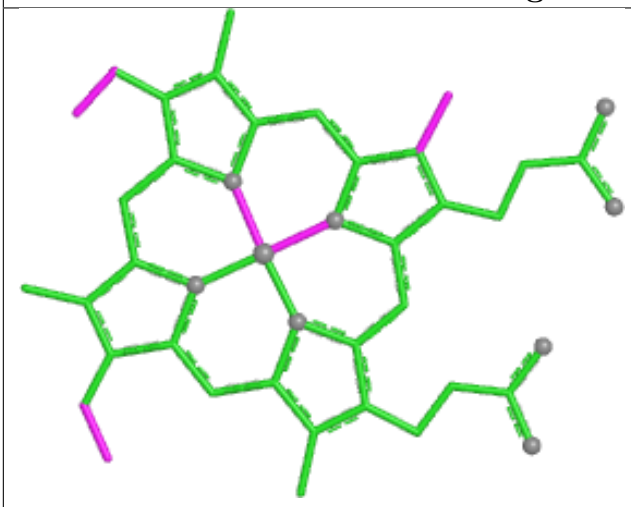


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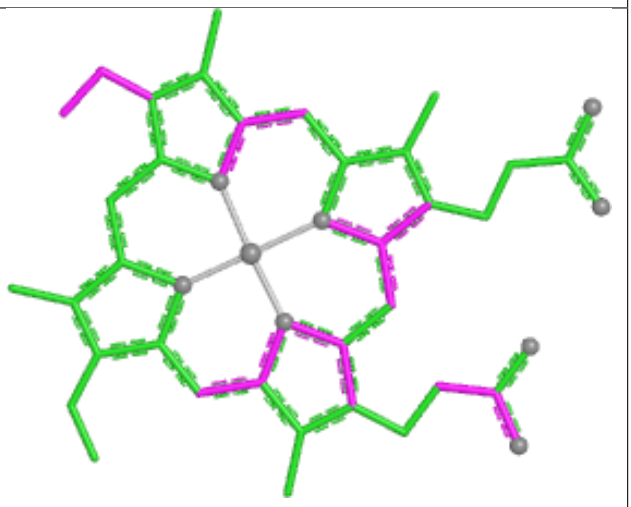


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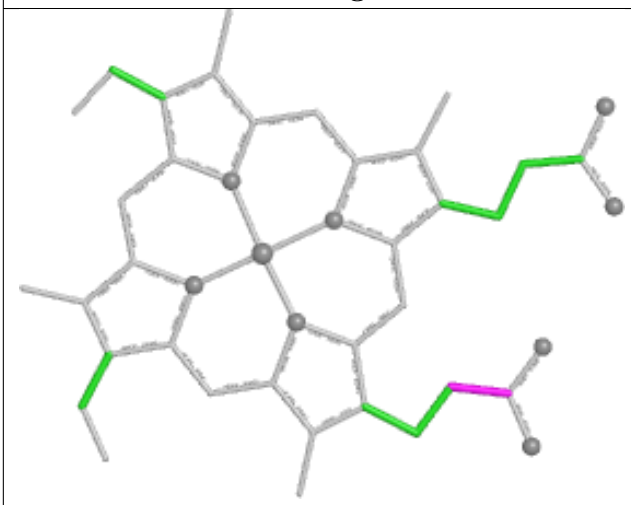
Ligand HEC v 201



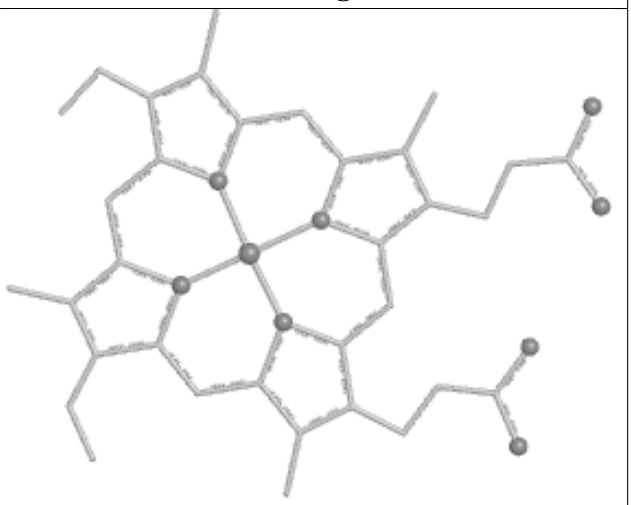
Bond lengths



Bond angles

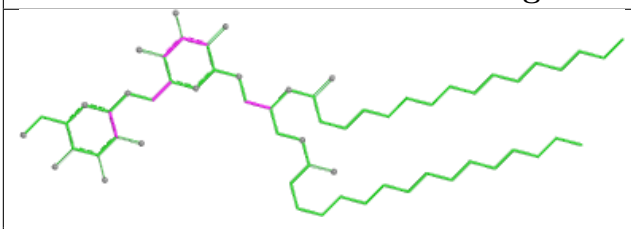


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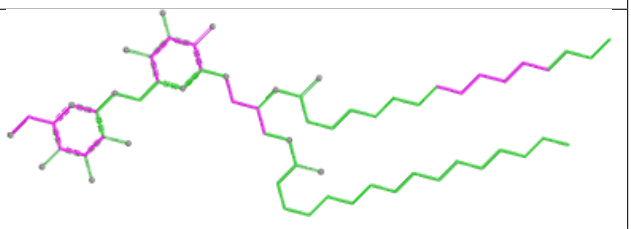


Rings

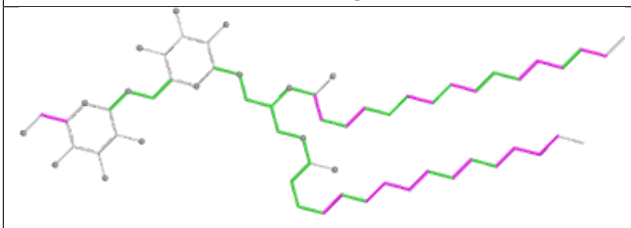
Ligand DGD h 102



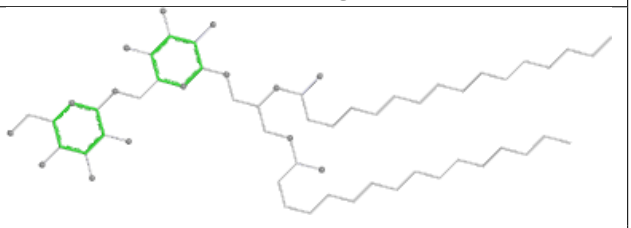
Bond lengths



Bond angles

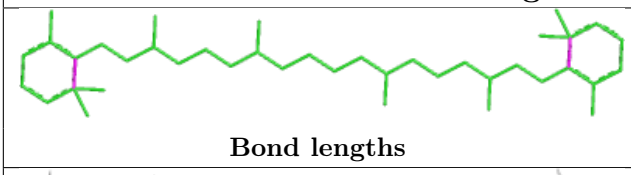


Torsions

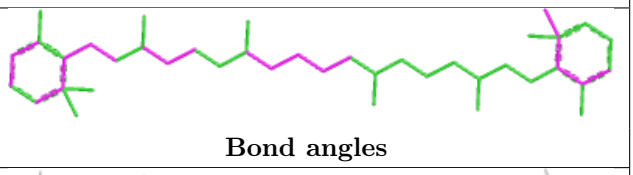


Rings

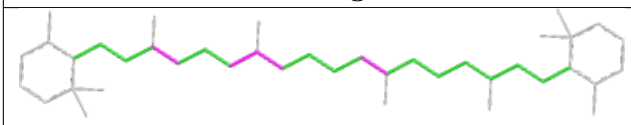
Ligand BCR B 618



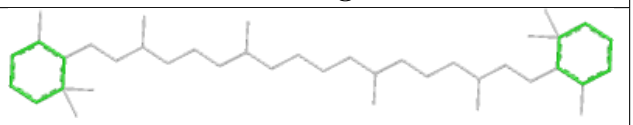
Bond lengths



Bond angles

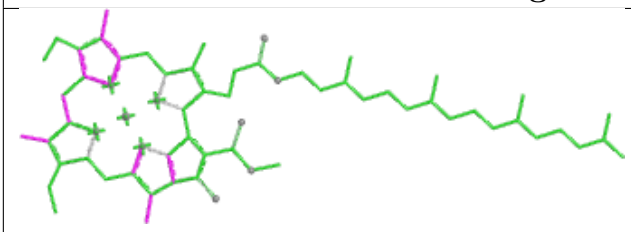


Torsions

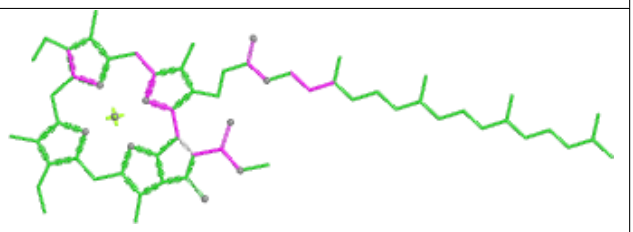


Rings

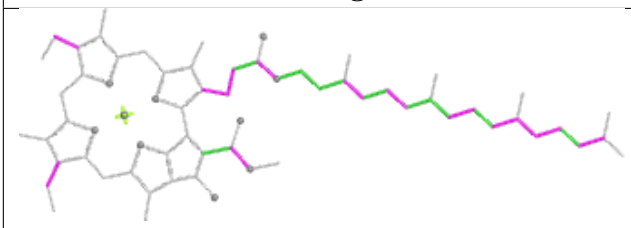
Ligand CLA c 512



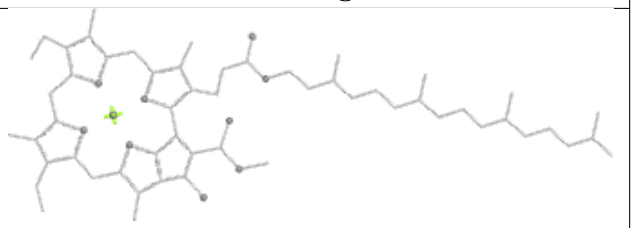
Bond lengths



Bond angles

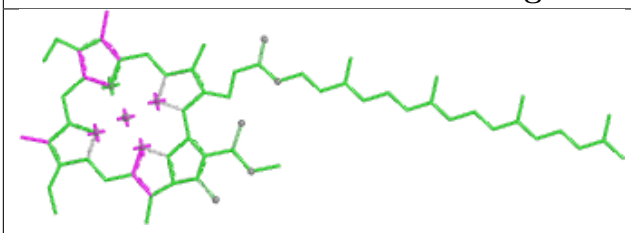


Torsions

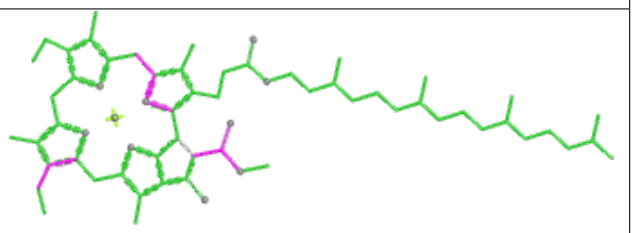


Rings

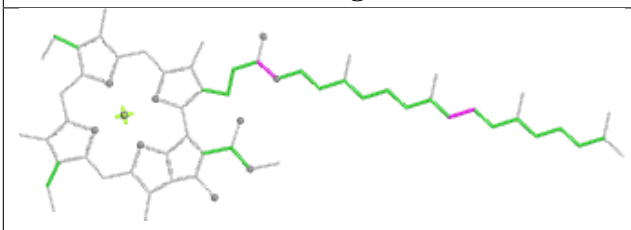
Ligand CLA C 511



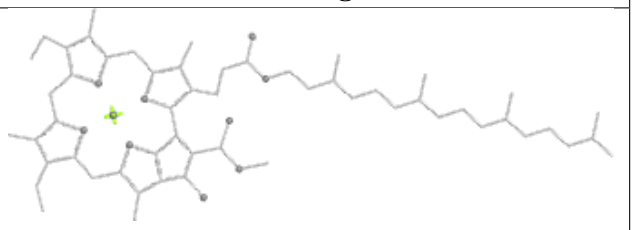
Bond lengths



Bond angles

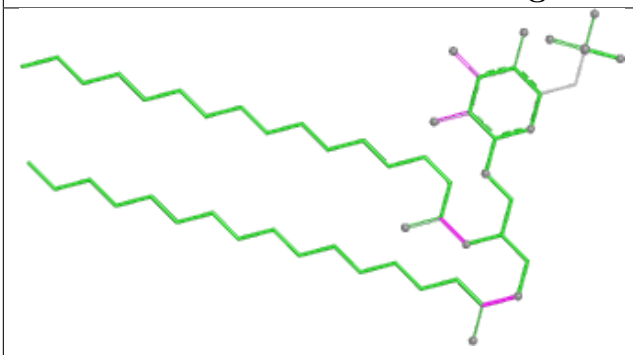


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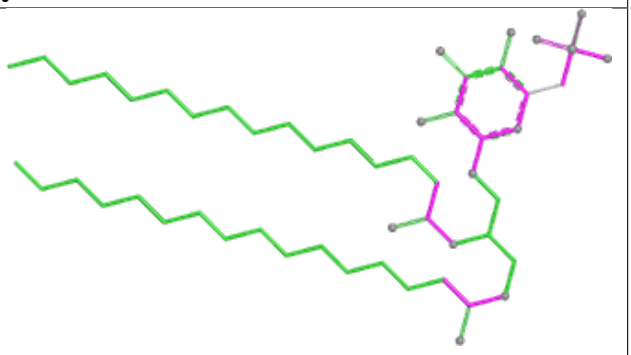


Rings

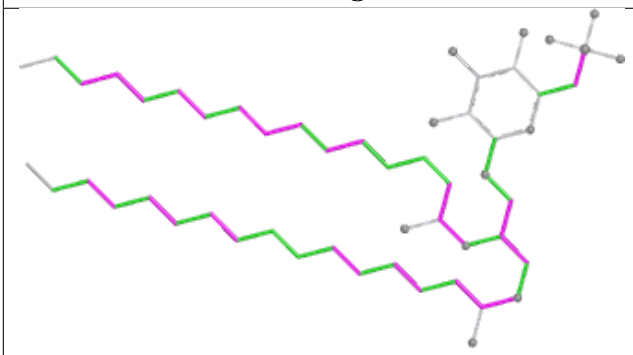
Ligand SQD a 412



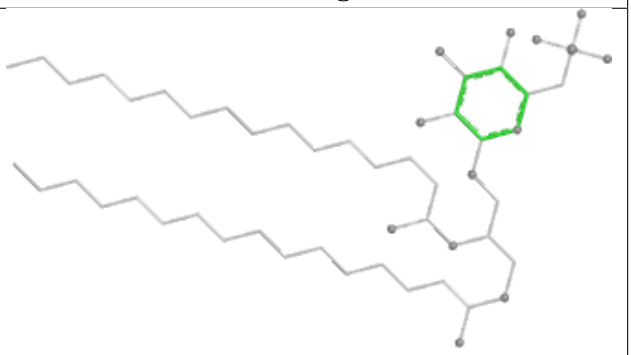
Bond lengths



Bond angles

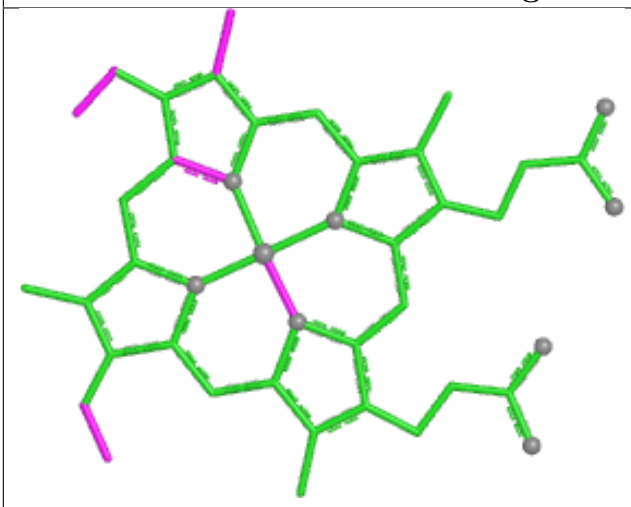


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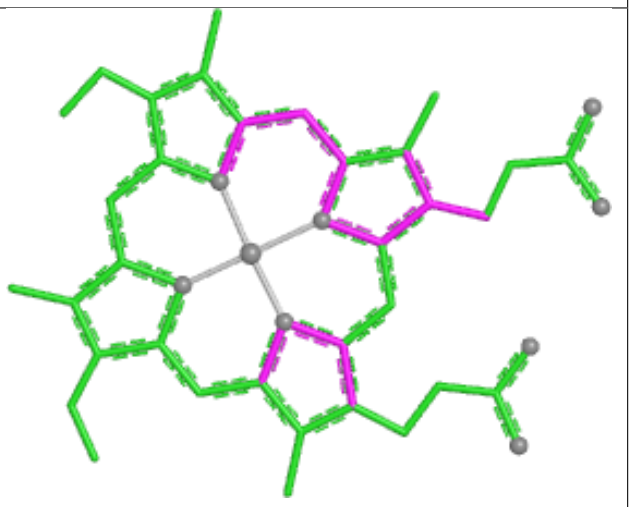


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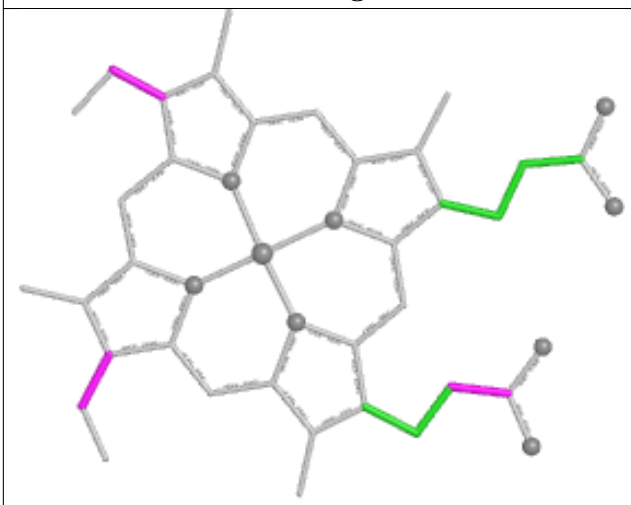
Ligand HEC V 201



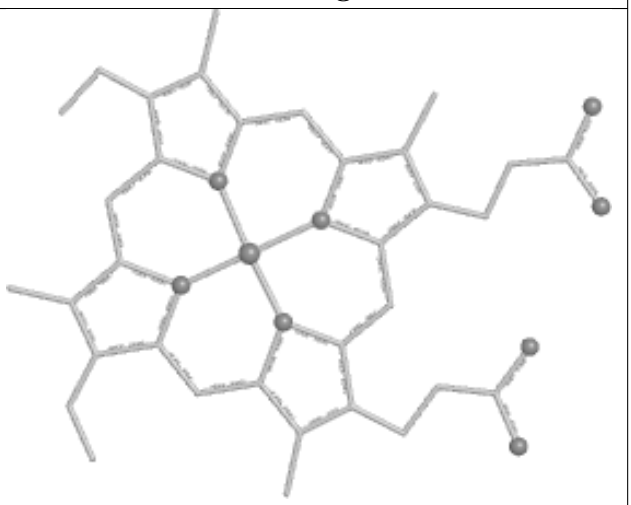
Bond lengths



Bond angles



Torsions

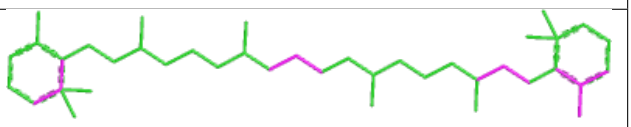


Rings

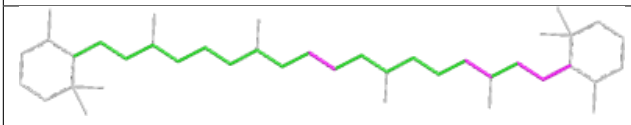
Ligand BCR D 404



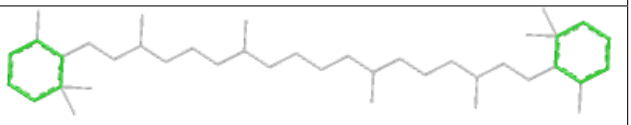
Bond lengths



Bond angles

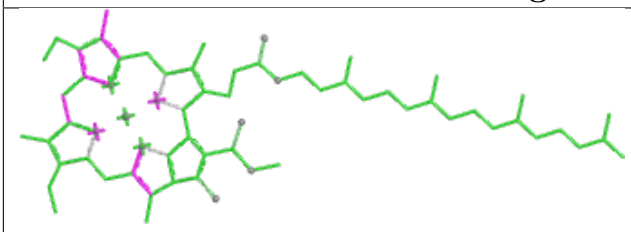


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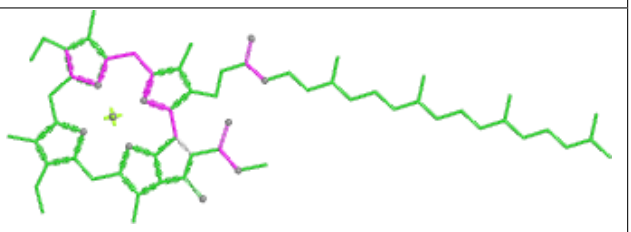


Rings

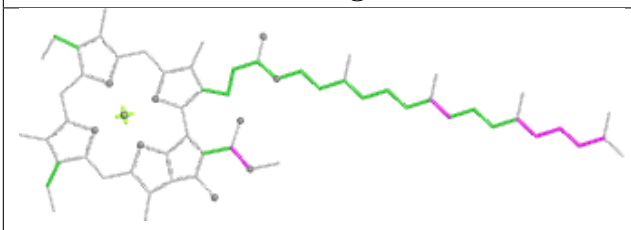
Ligand CLA c 511



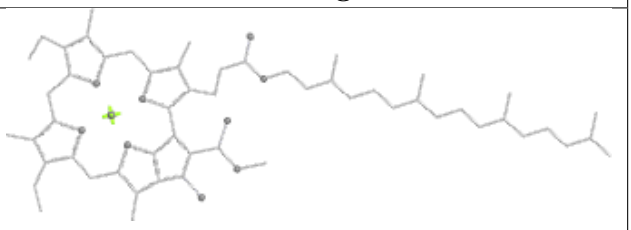
Bond lengths



Bond angles

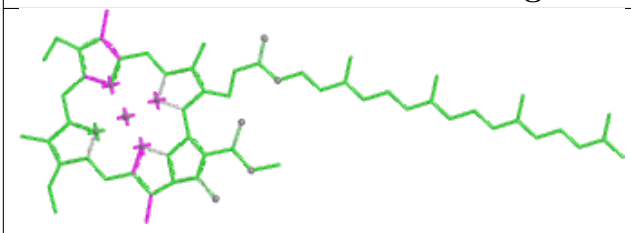


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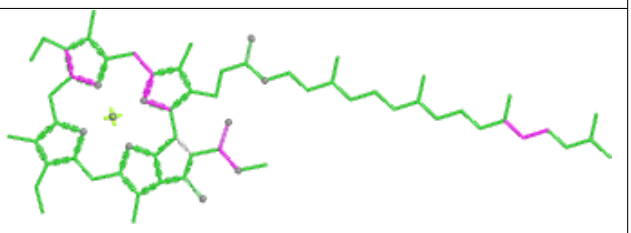


Rings

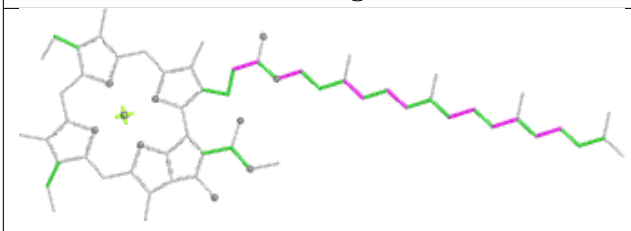
Ligand CLA B 613



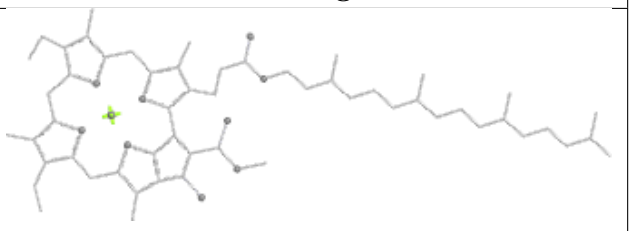
Bond lengths



Bond angles

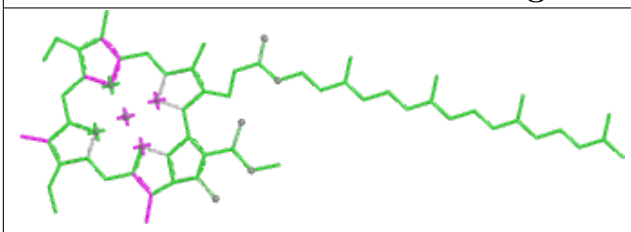


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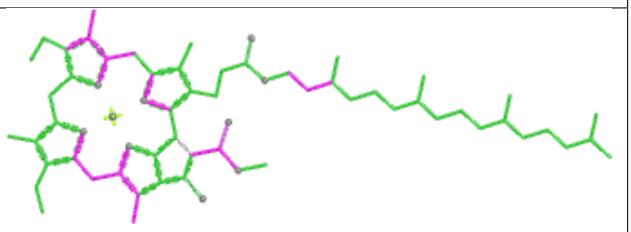


Rings

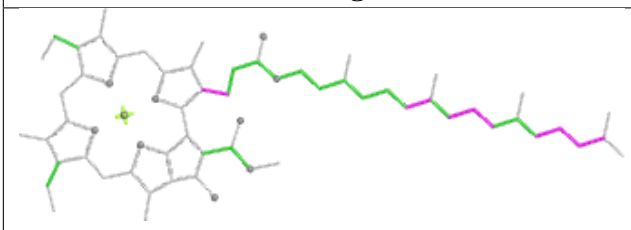
Ligand CLA b 612



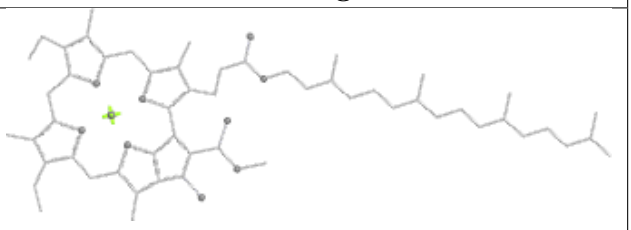
Bond lengths



Bond angles

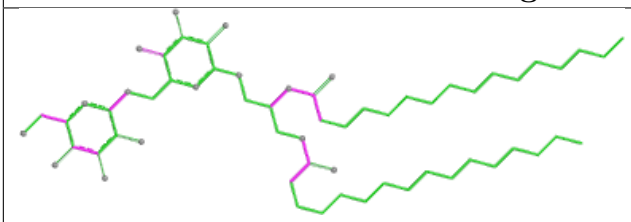


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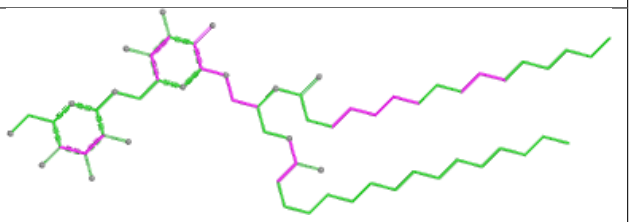


Rings

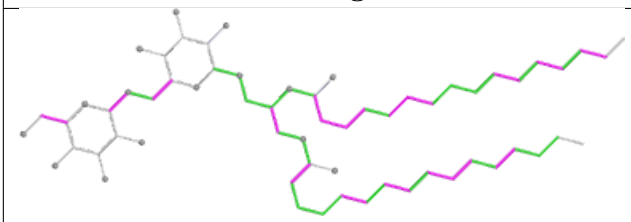
Ligand DGD C 515



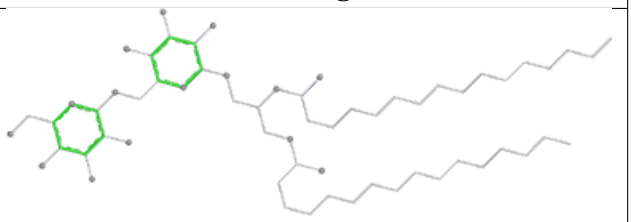
Bond lengths



Bond angles

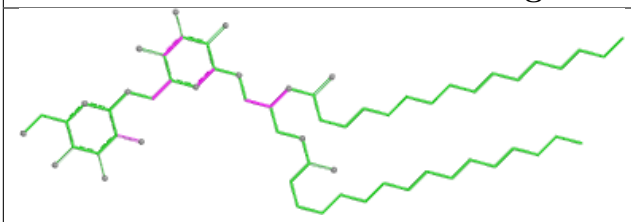


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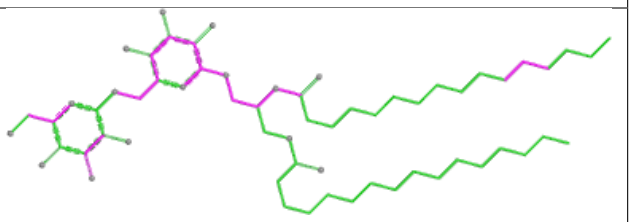


Rings

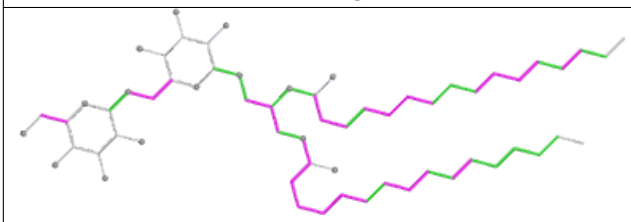
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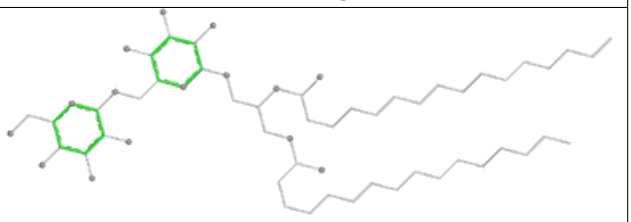
Bond lengths



Bond angles

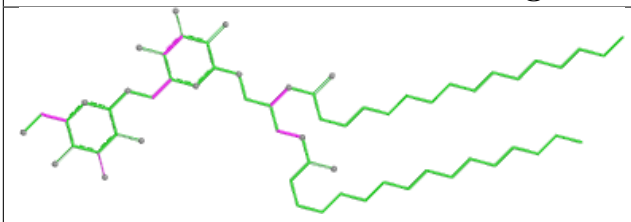


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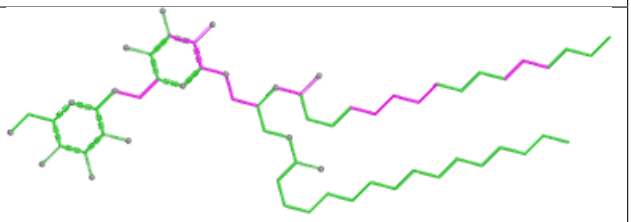


Rings

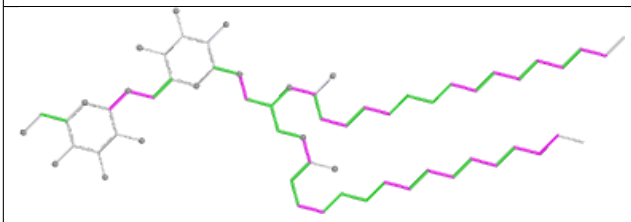
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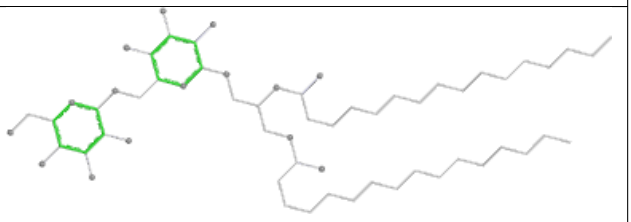
Bond lengths



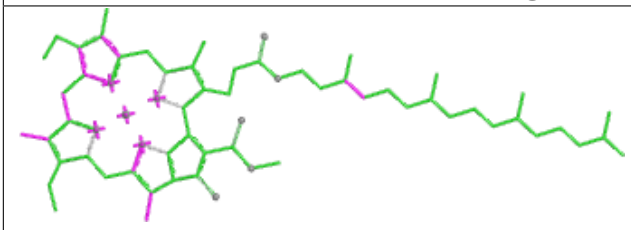
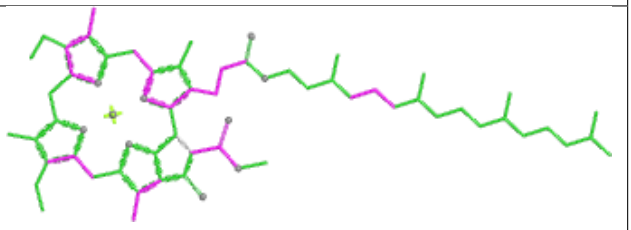
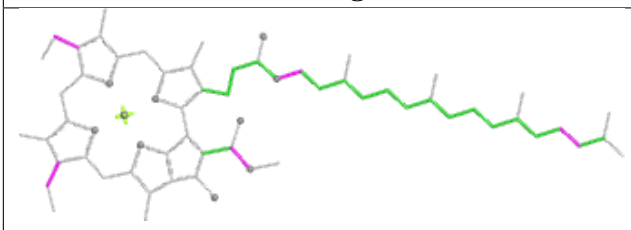
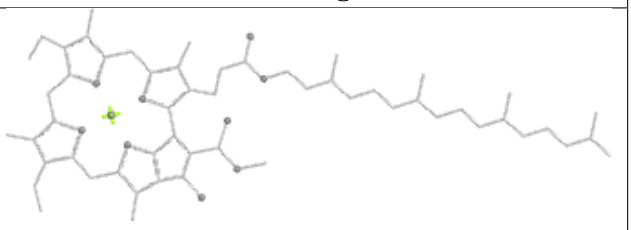
Bond angles

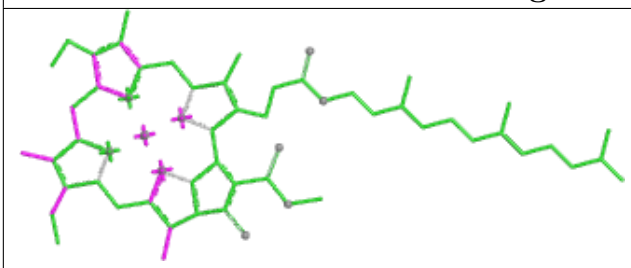
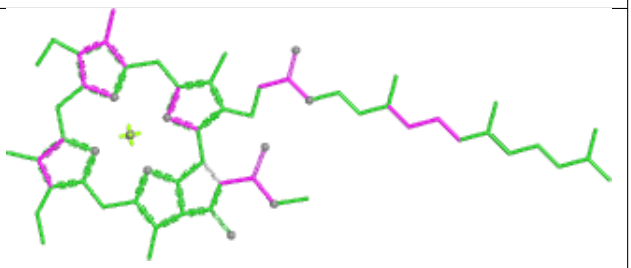
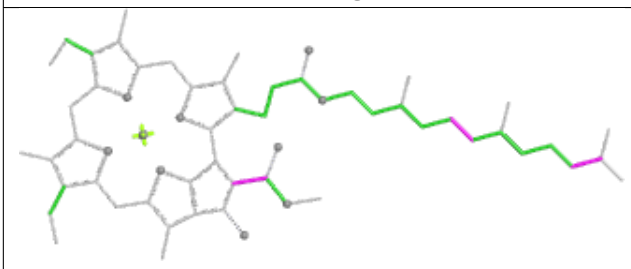
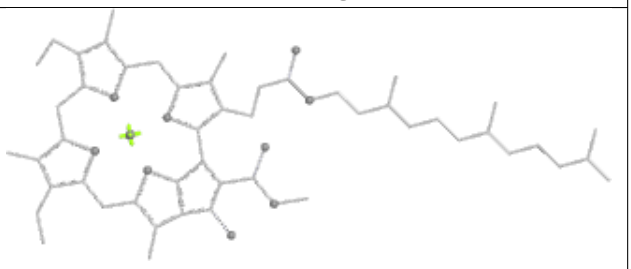


Torsions

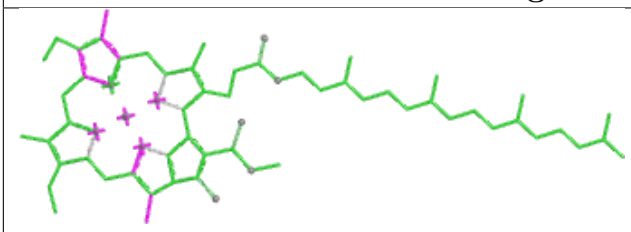


Rings

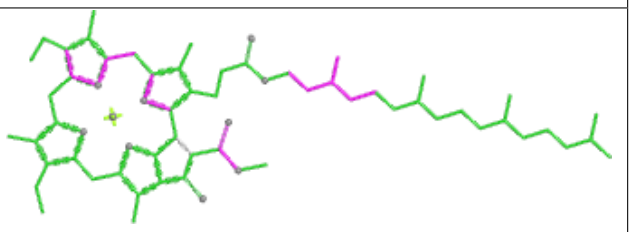
Ligand CLA A 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

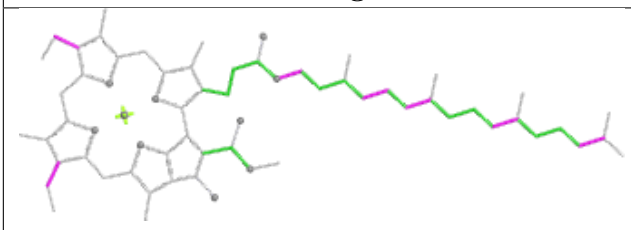
Ligand CLA d 402



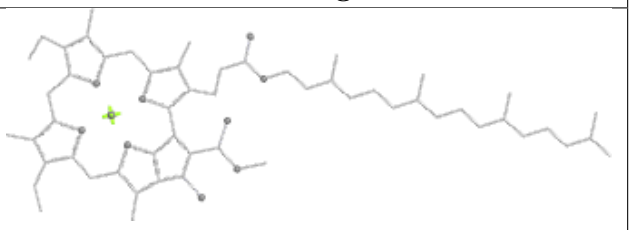
Bond lengths



Bond angles

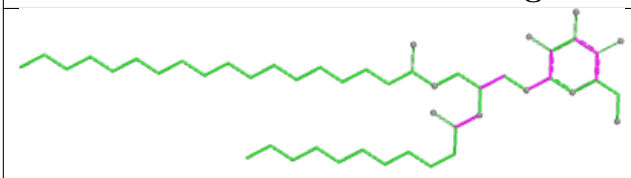


Torsions

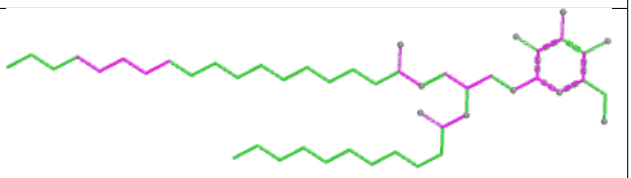


Rings

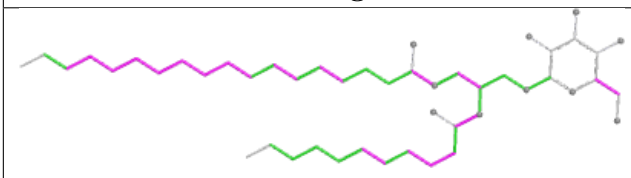
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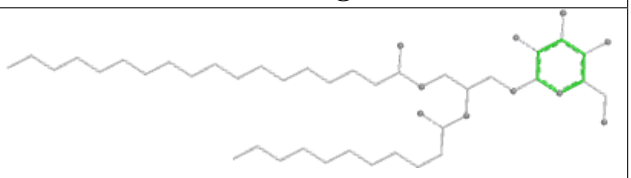
Bond lengths



Bond angles

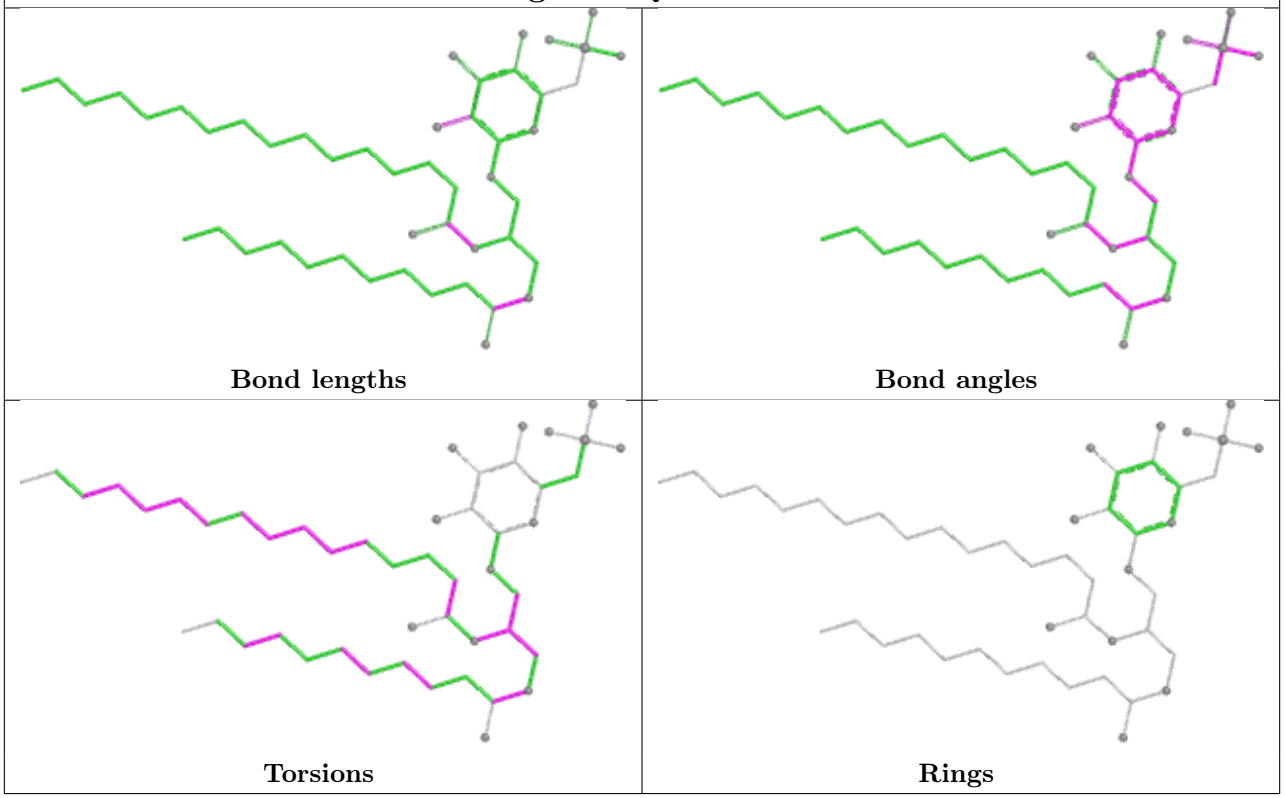


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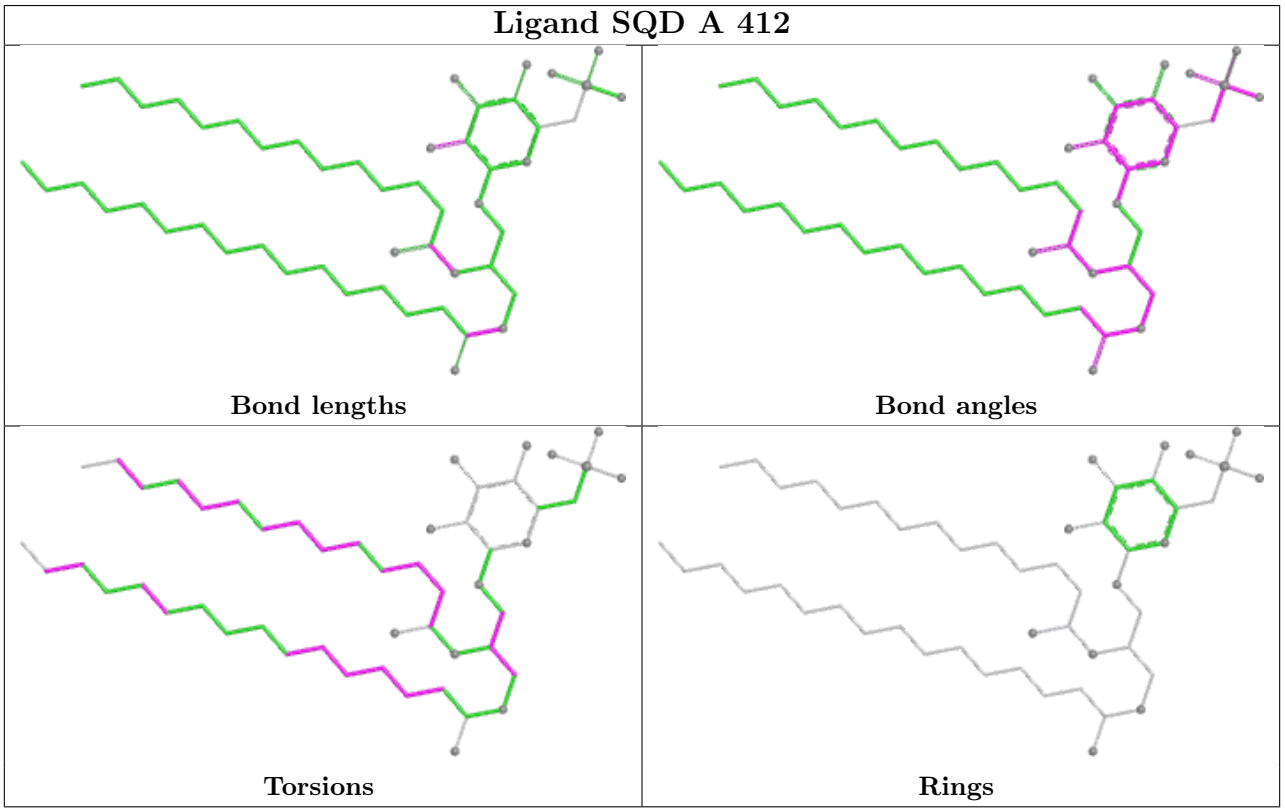


Rings

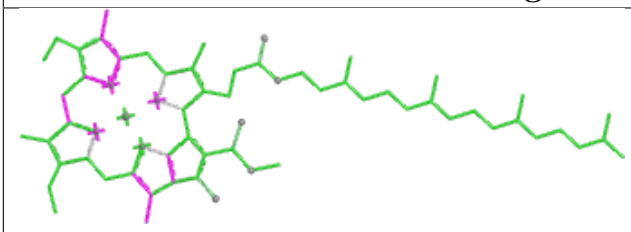
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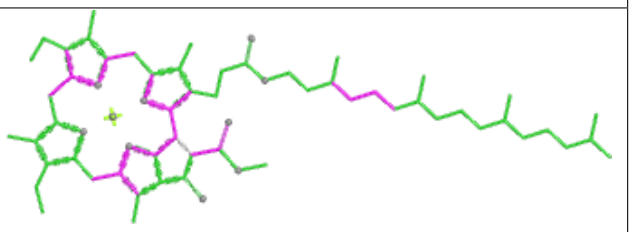
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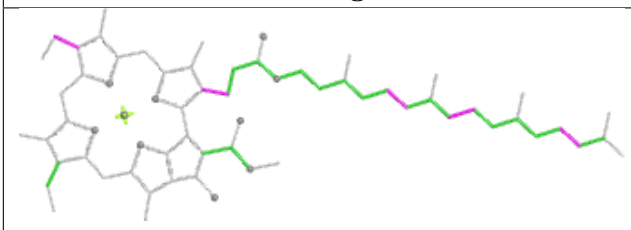
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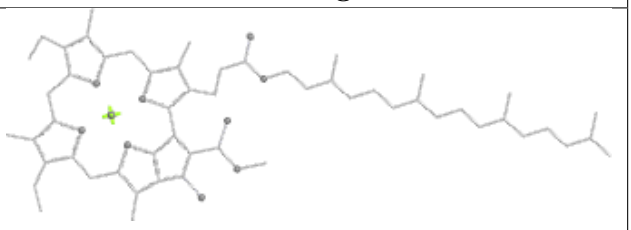
Bond lengths



Bond angles

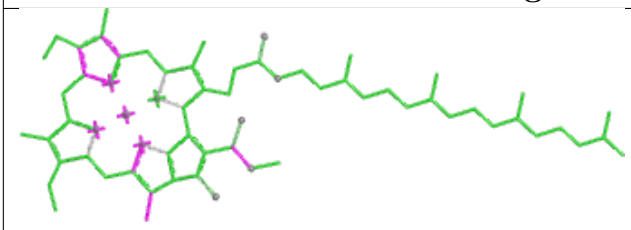


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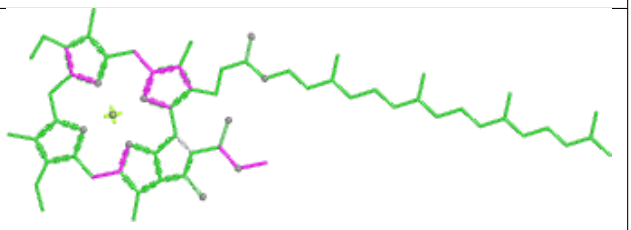


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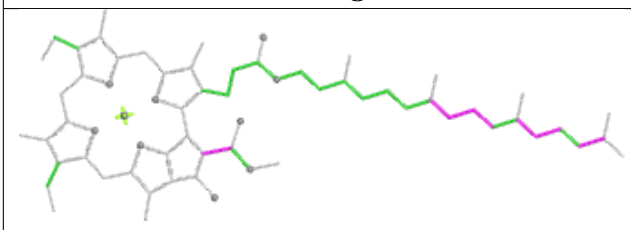
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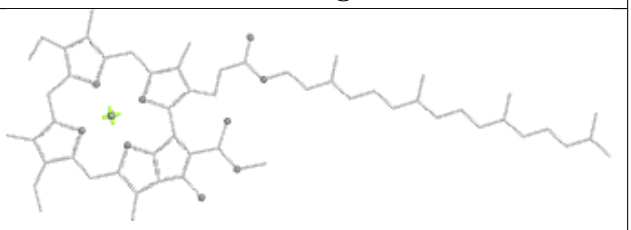
Bond lengths



Bond angles

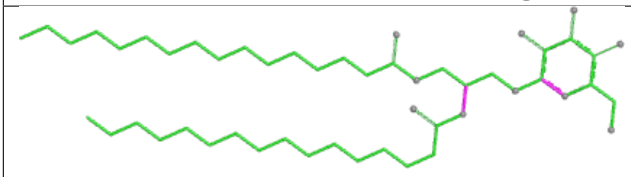


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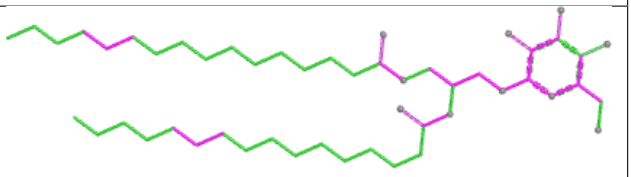


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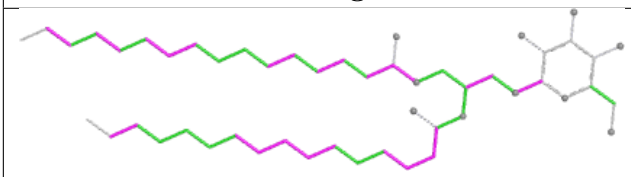
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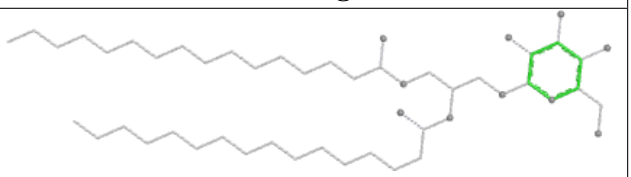
Bond lengths



Bond angles

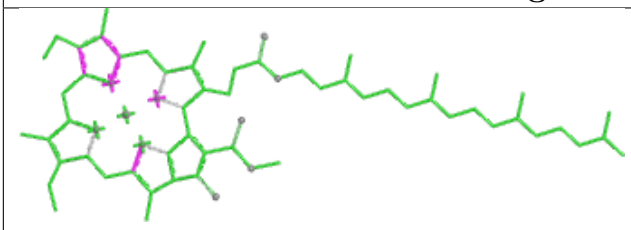


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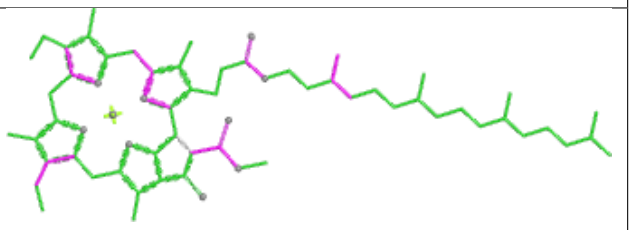


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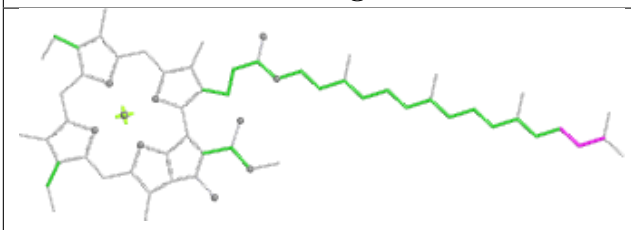
Ligand CLA a 405



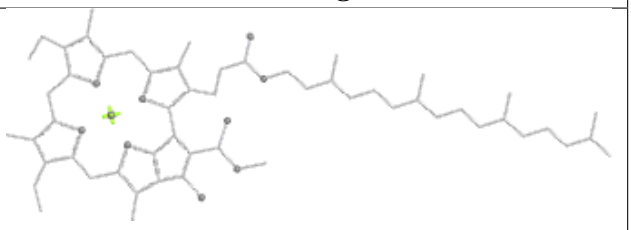
Bond lengths



Bond angles

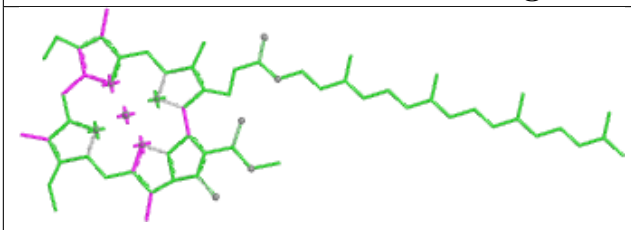


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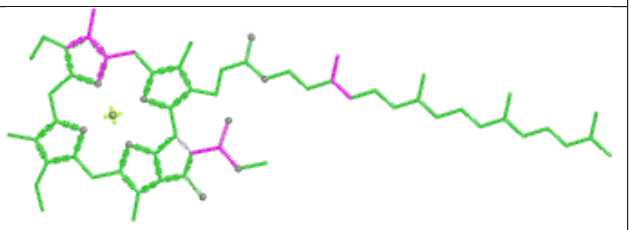


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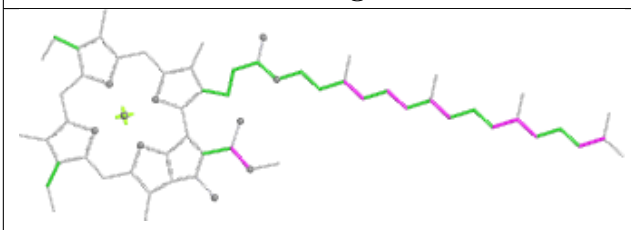
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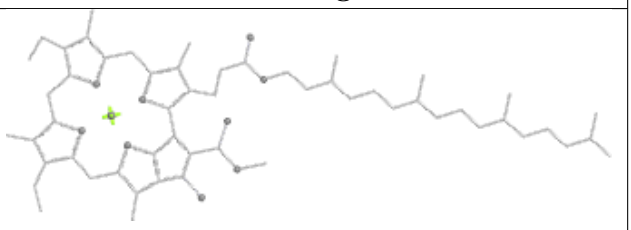
Bond lengths



Bond angles

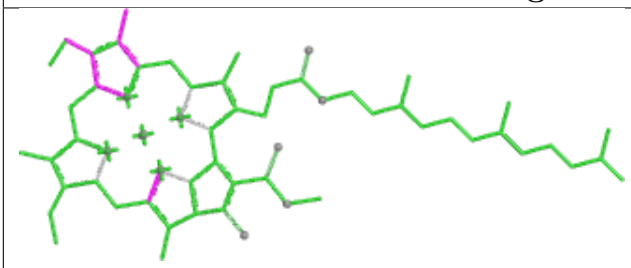


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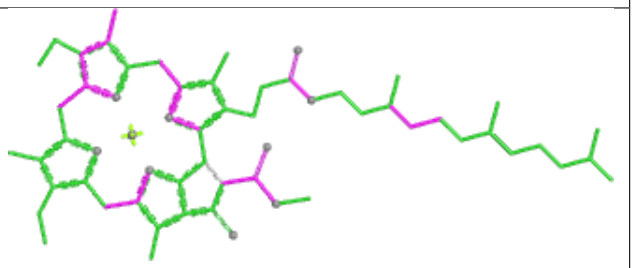


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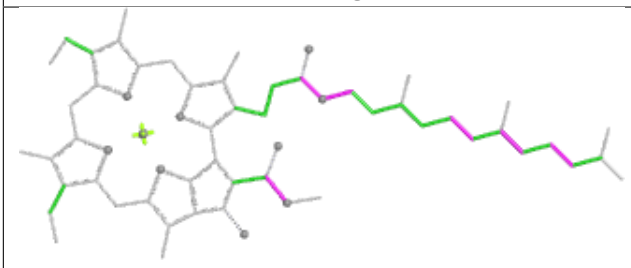
Ligand CLA b 617



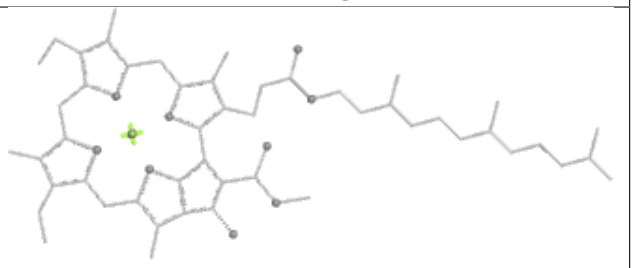
Bond lengths



Bond angles

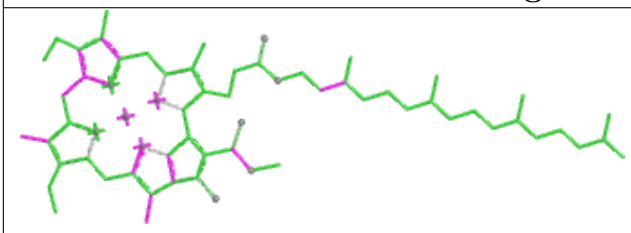


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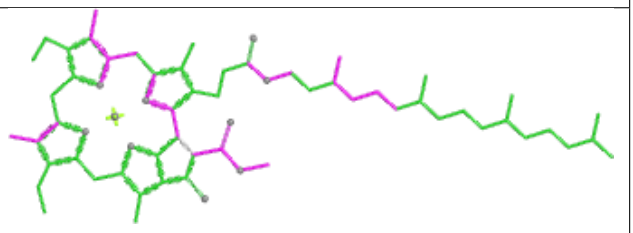


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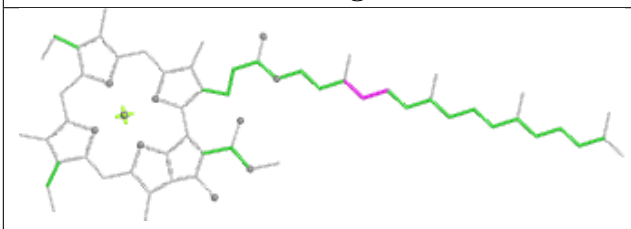
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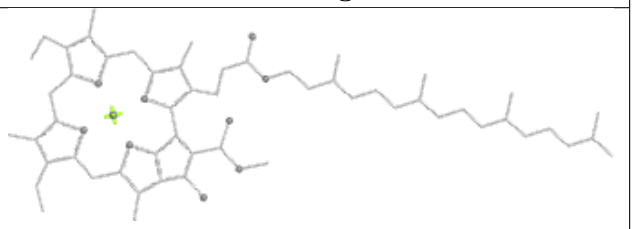
Bond lengths



Bond angles



Torsions

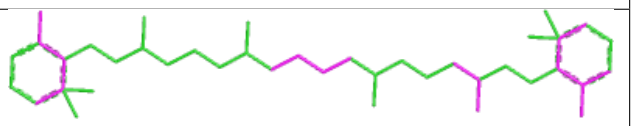


Rings

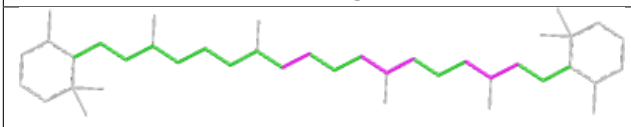
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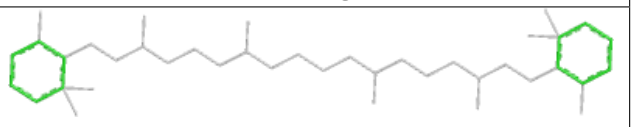
Bond lengths



Bond angles

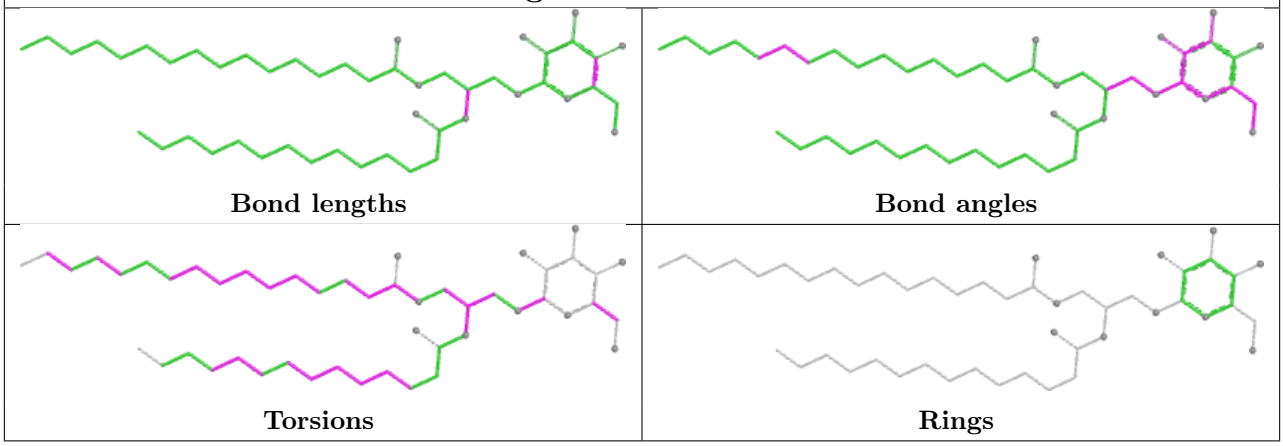


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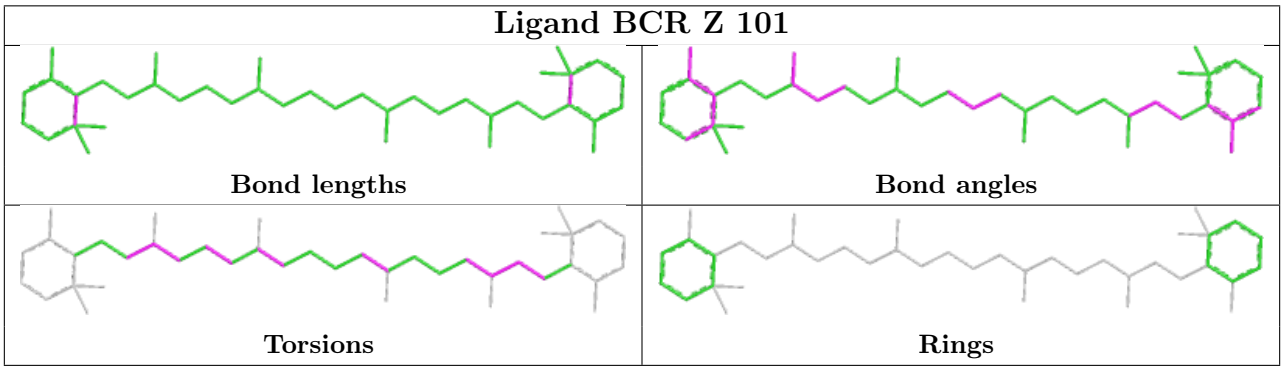


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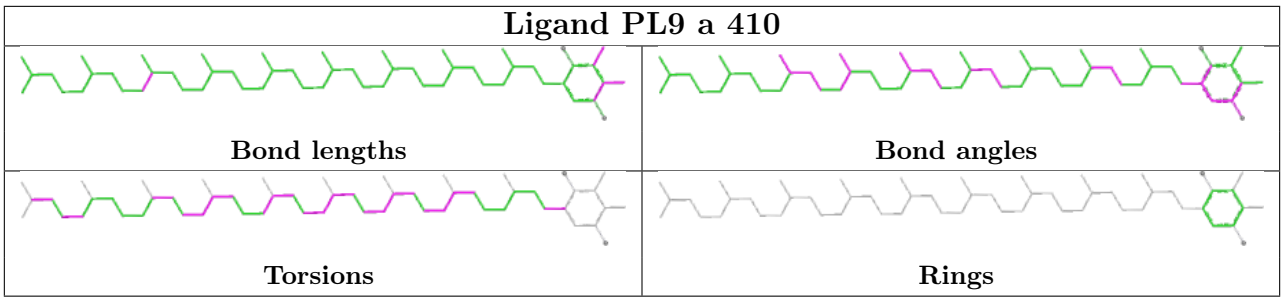
Ligand LMG c 523



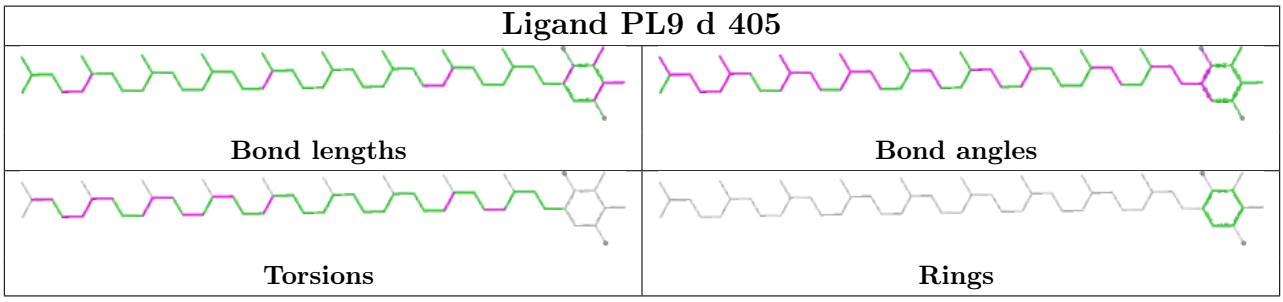
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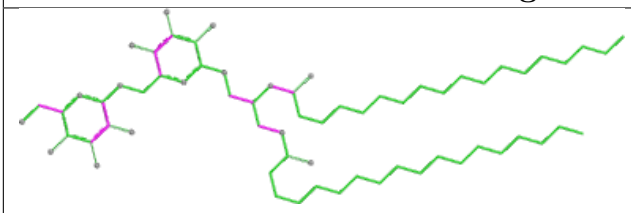
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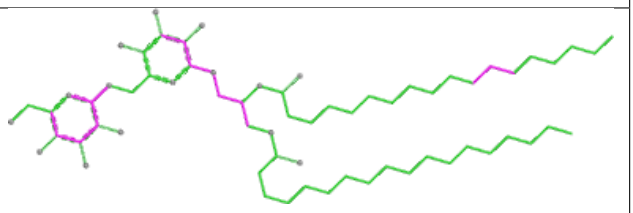
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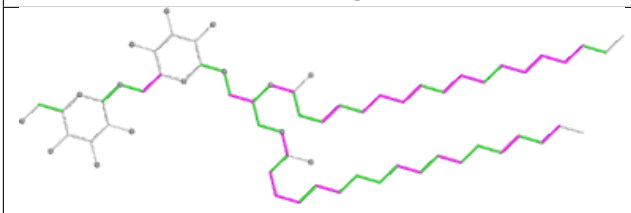
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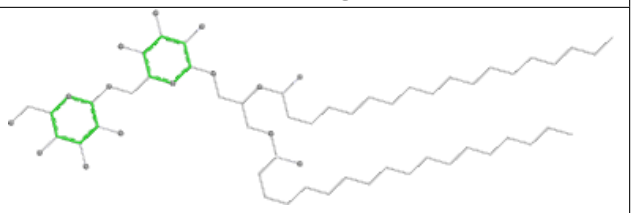
Bond lengths



Bond angles

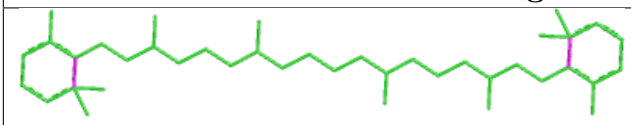


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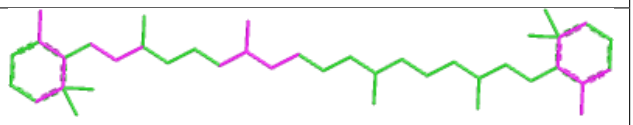


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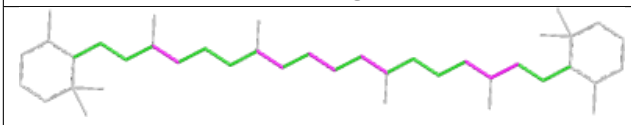
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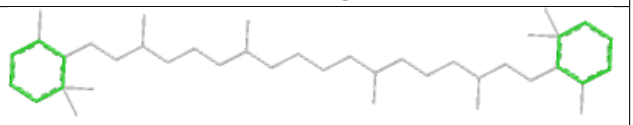
Bond lengths



Bond angles

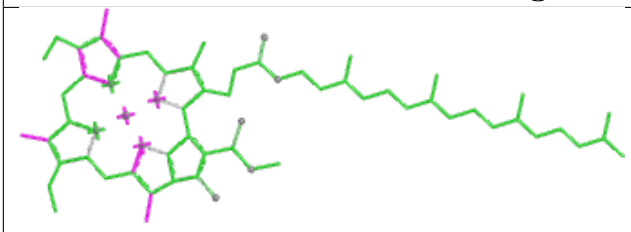


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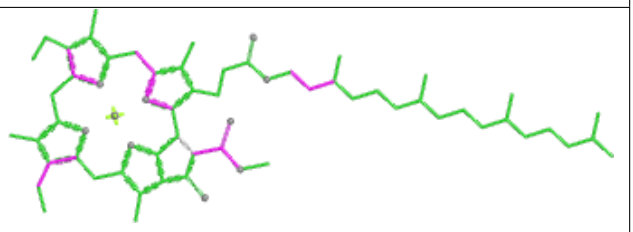


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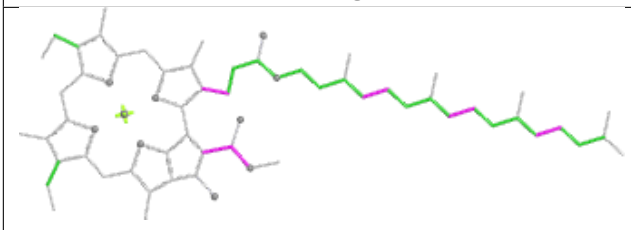
Ligand CLA c 513



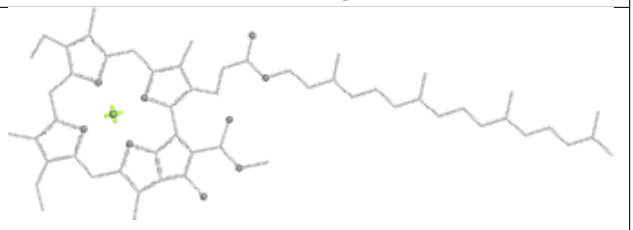
Bond lengths



Bond angles

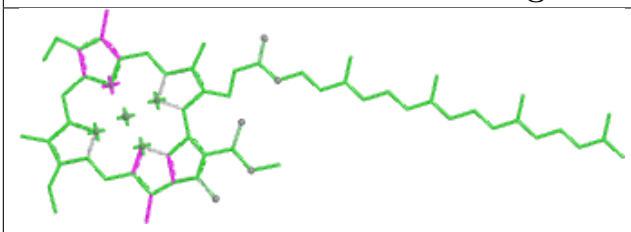


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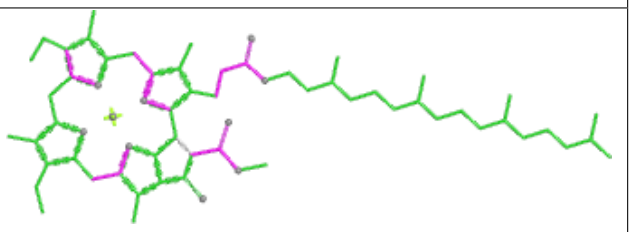


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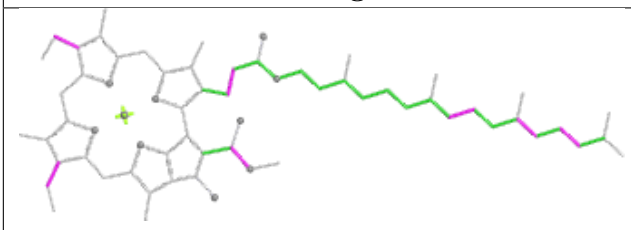
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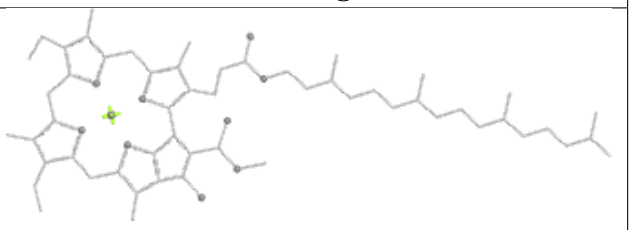
Bond lengths



Bond angles

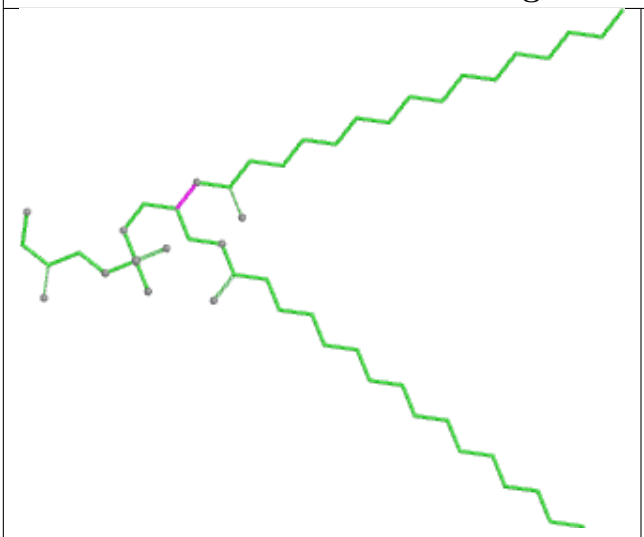


Torsions

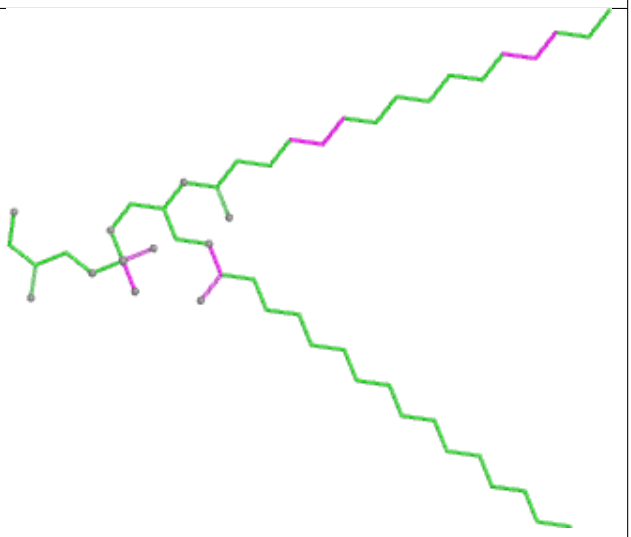


Rings

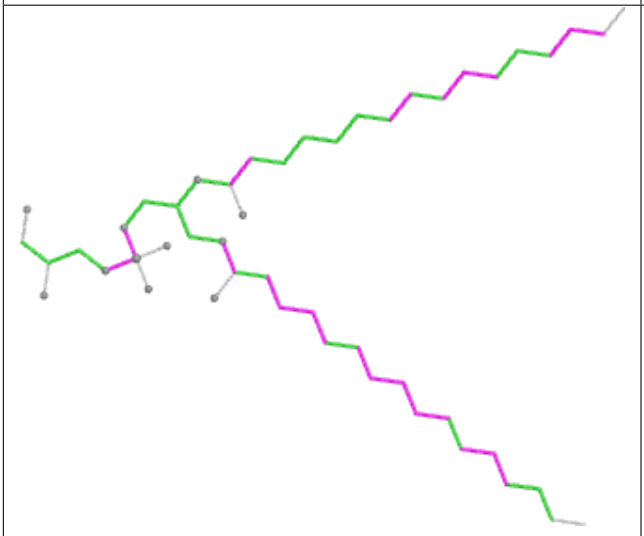
Ligand LHG B 622



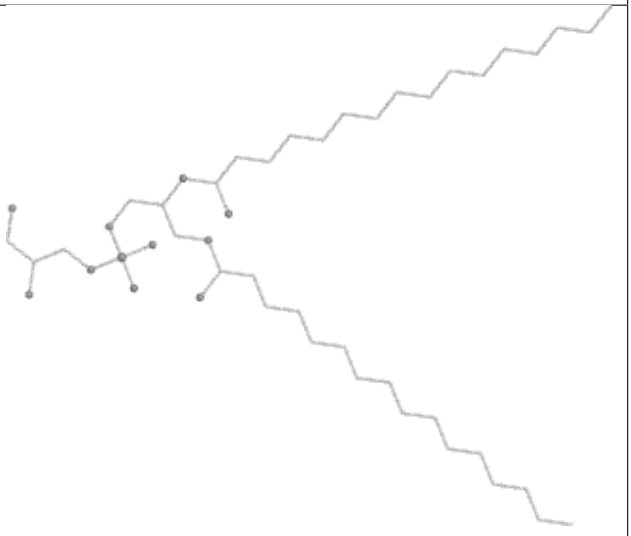
Bond lengths



Bond angles

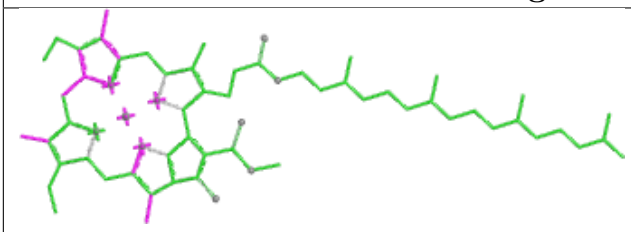


Torsions

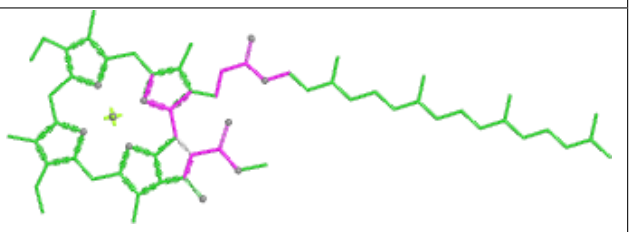


Rings

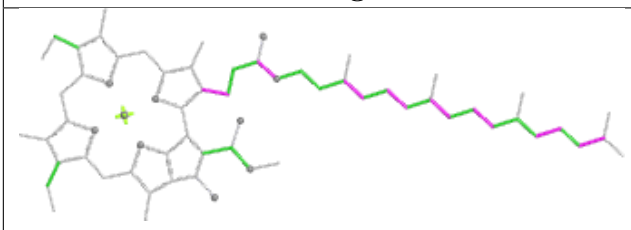
Ligand CLA a 408



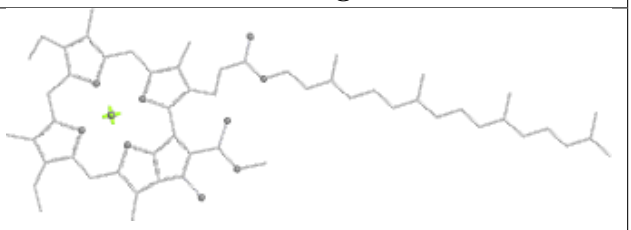
Bond lengths



Bond angles

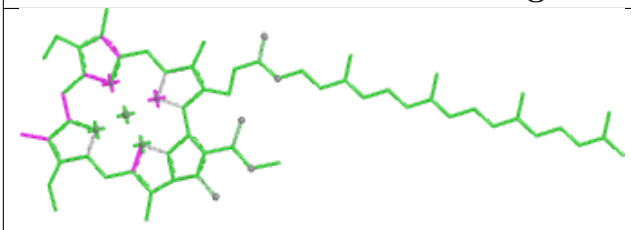


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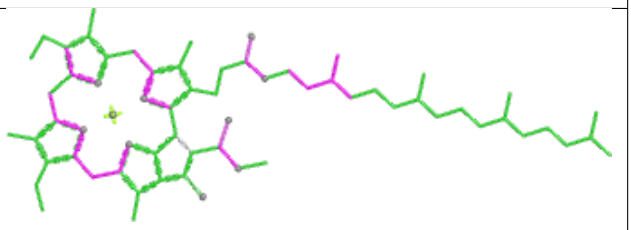


Rings

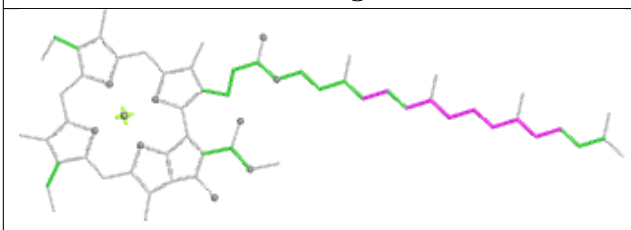
Ligand CLA b 605



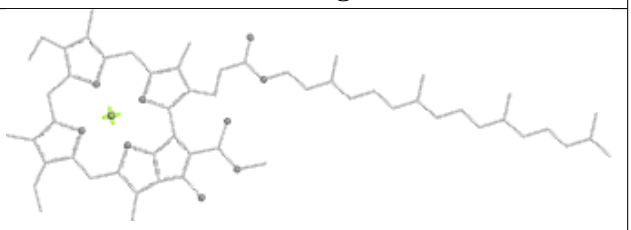
Bond lengths



Bond angles

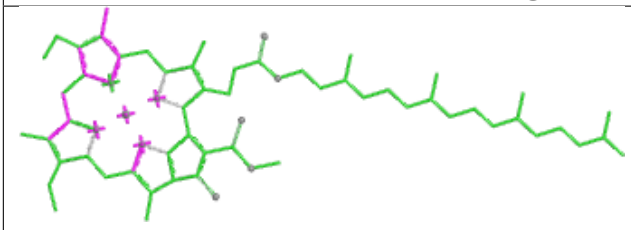


Torsions

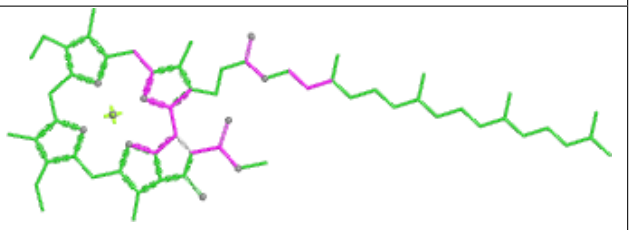


Rings

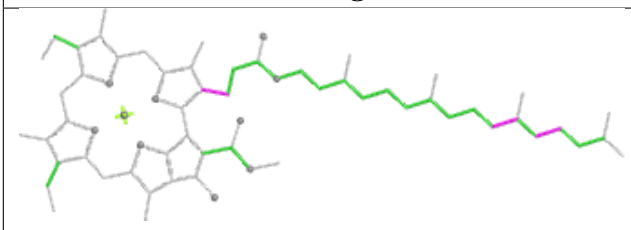
Ligand CLA B 602



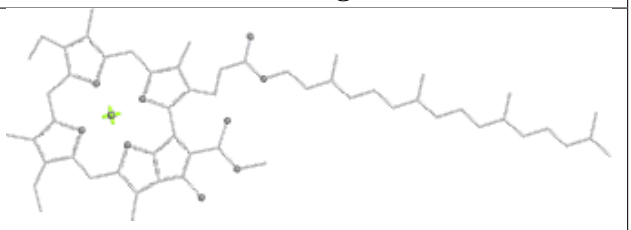
Bond lengths



Bond angles

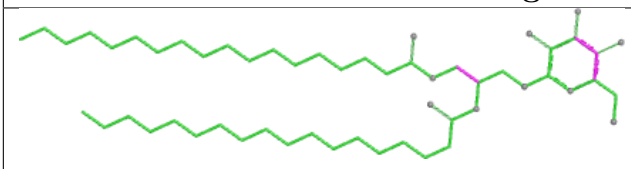


Torsions

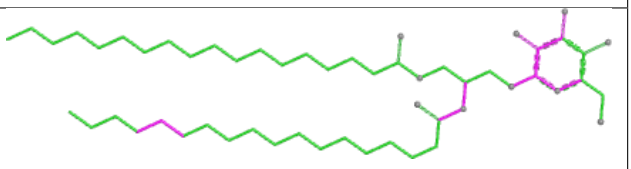


Rings

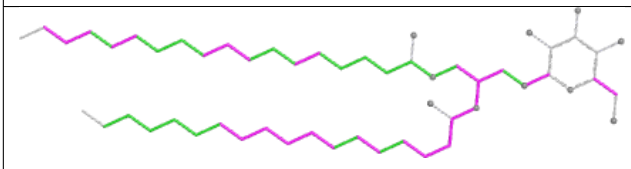
Ligand LMG b 622



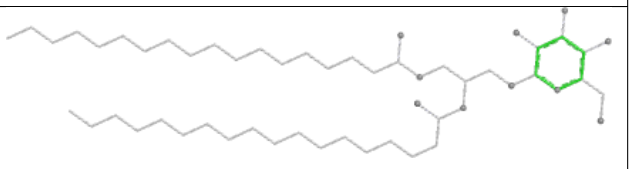
Bond lengths



Bond angles

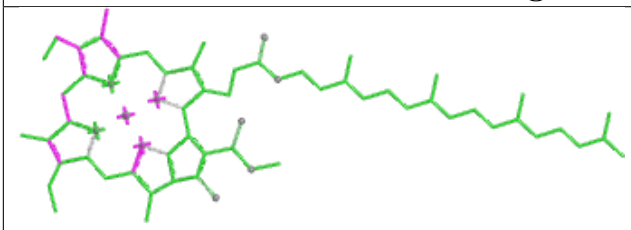


Torsions

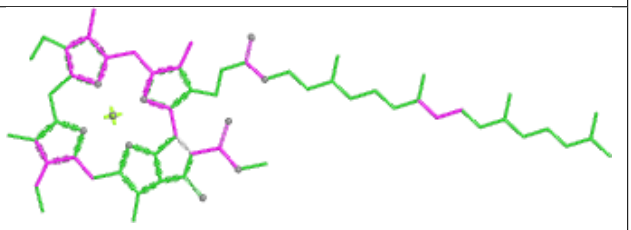


Rings

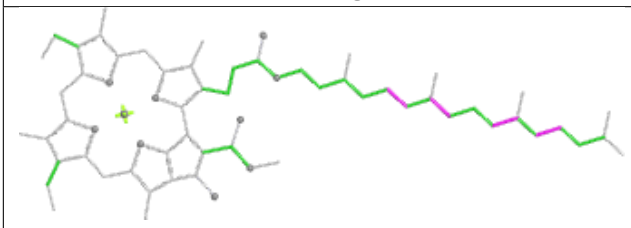
Ligand CLA b 609



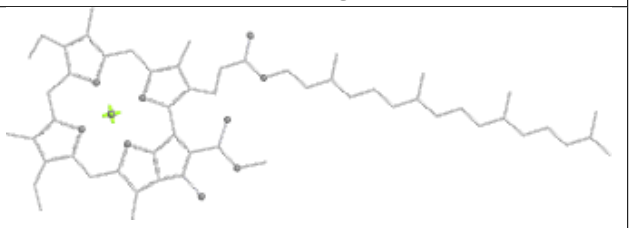
Bond lengths



Bond angles

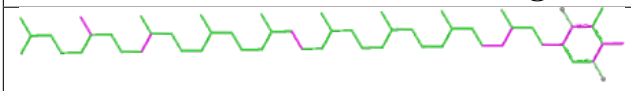


Torsions



Rings

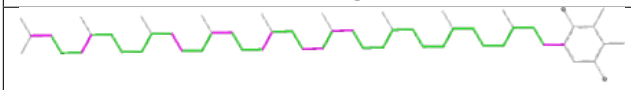
Ligand PL9 D 405



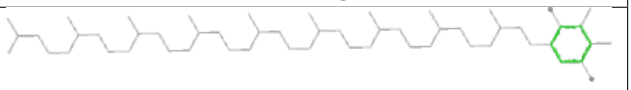
Bond lengths



Bond angles

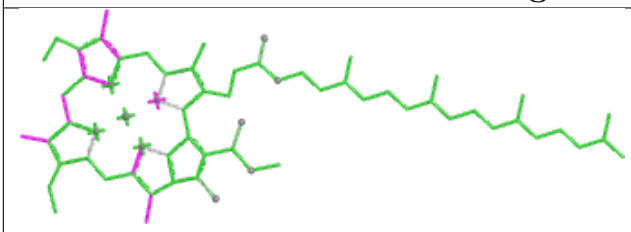


Torsions

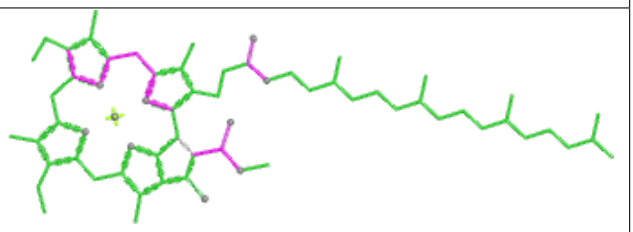


Rings

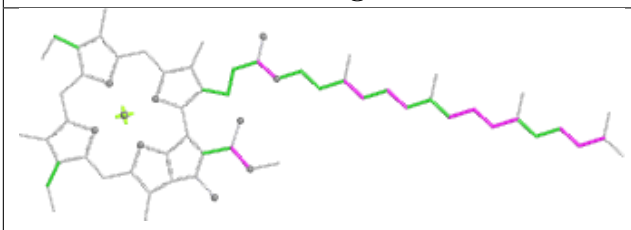
Ligand CLA c 510



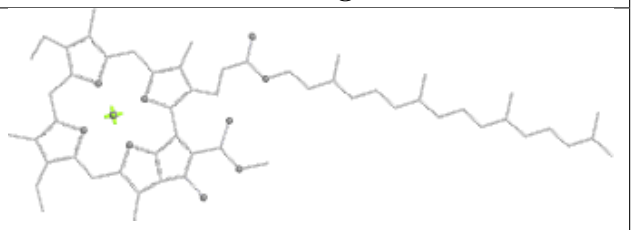
Bond lengths



Bond angles

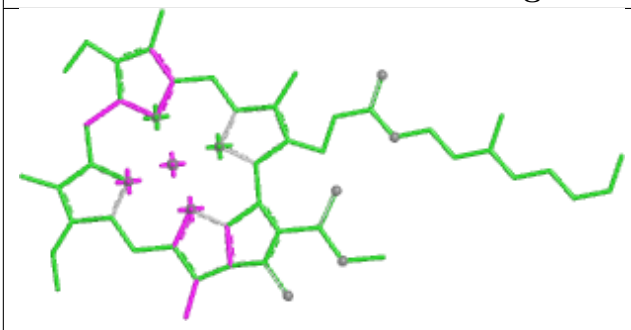


Torsions

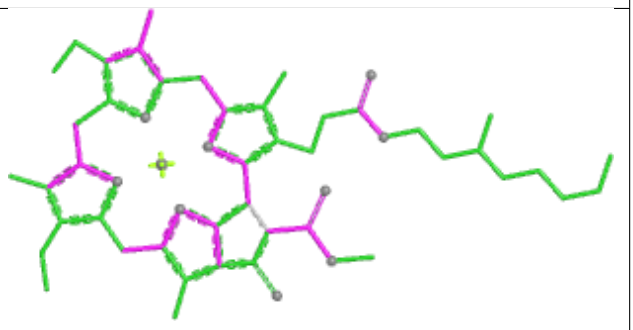


Rings

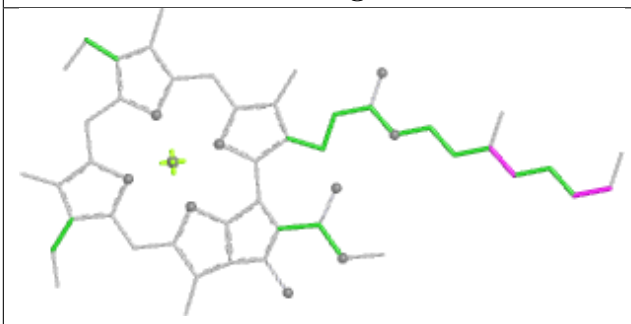
Ligand CLA A 408



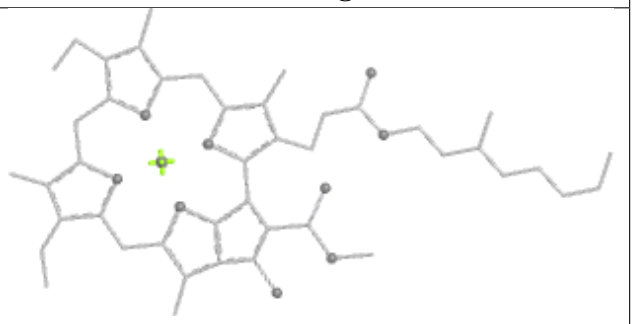
Bond lengths



Bond angles

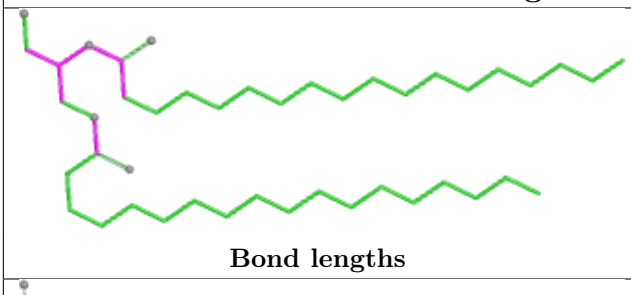


Torsions

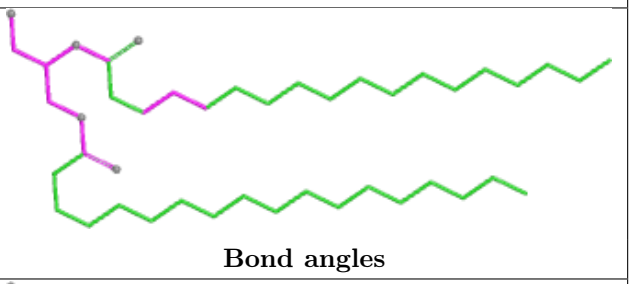


Rings

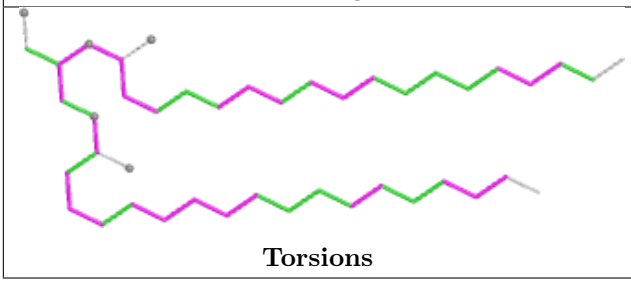
Ligand DGD a 414



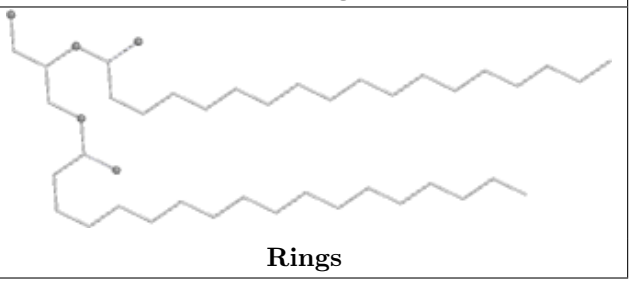
Bond lengths



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%)	-0.64	1 (0%) 90 92	12, 30, 52, 79	59 (17%)
1	a	334/334 (100%)	-0.53	1 (0%) 90 92	12, 32, 65, 89	59 (17%)
2	B	505/505 (100%)	-0.55	0 100 100	17, 35, 68, 108	4 (0%)
2	b	505/505 (100%)	-0.43	3 (0%) 85 88	21, 39, 79, 114	0
3	C	442/451 (98%)	-0.52	0 100 100	14, 39, 58, 83	7 (1%)
3	c	451/451 (100%)	-0.39	0 100 100	14, 43, 68, 105	8 (1%)
4	D	341/341 (100%)	-0.69	0 100 100	15, 32, 52, 99	1 (0%)
4	d	341/341 (100%)	-0.52	0 100 100	17, 36, 62, 92	2 (0%)
5	E	81/82 (98%)	0.07	1 (1%) 76 78	30, 55, 75, 92	1 (1%)
5	e	82/82 (100%)	0.19	0 100 100	40, 65, 90, 102	0
6	F	34/34 (100%)	-0.23	0 100 100	38, 46, 68, 86	0
6	f	34/34 (100%)	0.16	0 100 100	45, 55, 82, 95	0
7	H	65/65 (100%)	-0.33	1 (1%) 72 74	35, 44, 65, 86	0
7	h	63/65 (96%)	-0.02	0 100 100	42, 52, 70, 81	0
8	I	35/36 (97%)	-0.45	0 100 100	33, 41, 72, 88	0
8	i	35/36 (97%)	-0.22	1 (2%) 53 55	34, 43, 78, 88	0
9	J	36/36 (100%)	-0.23	0 100 100	39, 54, 81, 104	0
9	j	36/36 (100%)	0.13	0 100 100	43, 57, 94, 98	0
10	K	37/37 (100%)	-0.06	0 100 100	31, 57, 76, 78	1 (2%)
10	k	37/37 (100%)	0.20	0 100 100	48, 62, 79, 89	0
11	L	37/37 (100%)	-0.68	0 100 100	26, 32, 71, 77	0
11	l	36/37 (97%)	-0.59	0 100 100	27, 33, 82, 92	0
12	M	32/33 (96%)	-0.53	0 100 100	30, 35, 62, 80	0
12	m	31/33 (93%)	-0.54	0 100 100	28, 37, 53, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.34	0 100 100	22, 44, 91, 155	1 (0%)
13	o	244/244 (100%)	-0.34	1 (0%) 88 90	26, 43, 86, 142	0
14	T	29/30 (96%)	-0.65	0 100 100	26, 35, 64, 78	0
14	t	29/30 (96%)	-0.52	1 (3%) 48 48	26, 34, 87, 99	0
15	U	97/97 (100%)	-0.34	0 100 100	33, 47, 73, 105	0
15	u	97/97 (100%)	-0.38	1 (1%) 79 82	30, 43, 62, 97	0
16	V	137/137 (100%)	-0.49	0 100 100	29, 43, 60, 87	0
16	v	137/137 (100%)	-0.23	0 100 100	34, 51, 74, 89	0
17	Y	27/30 (90%)	0.97	3 (11%) 10 10	58, 84, 125, 131	0
17	y	30/30 (100%)	0.57	0 100 100	65, 81, 97, 118	0
18	X	38/38 (100%)	-0.03	0 100 100	42, 54, 83, 86	0
18	x	38/38 (100%)	0.09	1 (2%) 57 59	50, 63, 95, 108	0
19	Z	62/62 (100%)	0.57	2 (3%) 50 50	53, 71, 122, 140	0
19	z	62/62 (100%)	0.71	2 (3%) 50 50	59, 76, 119, 136	0
20	R	34/34 (100%)	0.75	1 (2%) 53 55	65, 77, 100, 106	0
20	r	31/34 (91%)	1.08	1 (3%) 50 50	75, 93, 109, 117	0
All	All	5300/5326 (99%)	-0.38	21 (0%) 88 90	12, 40, 81, 155	143 (2%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	35	LEU	3.6
19	z	33	TRP	3.4
1	A	13	LEU	3.0
15	u	53	ALA	2.9
13	o	58	ASN	2.9
19	Z	62	VAL	2.8
17	Y	22	LEU	2.8
14	t	30	THR	2.7
17	Y	20	ALA	2.6
5	E	79	PHE	2.6
2	b	499	VAL	2.4
19	z	62	VAL	2.4
2	b	486	LEU	2.3
20	r	14	LEU	2.3
17	Y	26	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
7	H	66	GLY	2.2
1	a	249	VAL	2.2
2	b	495	PHE	2.1
19	Z	33	TRP	2.1
8	i	36	ASP	2.0
18	x	2	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
12	FME	M	1	10/11	0.95	0.08	34,48,63,68	0
14	FME	t	1	10/11	0.95	0.08	29,37,64,69	0
8	FME	i	1	10/11	0.96	0.07	35,48,60,64	0
12	FME	m	1	10/11	0.96	0.08	31,46,65,72	0
8	FME	I	1	10/11	0.96	0.07	35,54,65,68	0
14	FME	T	1	10/11	0.97	0.07	27,44,65,71	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
34	UNL	H	103	53/-	0.78	0.15	43,73,86,90	0
34	UNL	b	627	26/-	0.80	0.16	42,58,69,74	0
27	LMG	b	623	23/55	0.81	0.17	43,70,95,98	0
29	LHG	e	101	42/49	0.82	0.12	57,87,116,139	0
27	LMG	c	521	48/55	0.82	0.14	44,77,121,128	0
29	LHG	A	413	49/49	0.82	0.14	51,85,125,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	LMG	b	622	55/55	0.83	0.15	35,73,101,104	0
34	UNL	c	522	28/-	0.83	0.12	46,66,88,93	0
34	UNL	a	415	28/-	0.84	0.11	39,66,77,79	0
34	UNL	b	626	55/-	0.84	0.12	44,61,77,81	0
34	UNL	E	102	28/-	0.84	0.13	52,79,91,94	0
30	DGD	A	415	66/66	0.84	0.12	45,68,93,108	0
34	UNL	t	103	26/-	0.84	0.13	42,64,76,81	0
26	PL9	a	410	55/55	0.85	0.14	36,67,91,98	0
34	UNL	b	625	44/-	0.85	0.14	34,58,80,84	0
30	DGD	a	414	44/66	0.86	0.13	36,58,84,92	0
34	UNL	B	626	46/-	0.86	0.12	44,64,84,93	0
34	UNL	B	627	28/-	0.86	0.14	42,64,86,91	0
34	UNL	B	628	47/-	0.86	0.13	47,65,78,89	0
28	SQD	a	413	36/54	0.86	0.12	31,67,87,96	0
34	UNL	d	411	55/-	0.86	0.11	42,58,72,73	0
34	UNL	m	102	28/-	0.86	0.12	42,59,73,78	0
23	CLA	h	101	65/65	0.86	0.11	45,69,93,104	0
27	LMG	D	409	33/55	0.87	0.12	32,54,107,111	0
27	LMG	c	519	37/55	0.87	0.11	44,70,88,97	0
26	PL9	A	410	55/55	0.87	0.14	39,62,83,94	135
34	UNL	b	602	47/-	0.87	0.12	35,50,64,73	0
34	UNL	b	624	40/-	0.87	0.12	46,63,83,85	0
28	SQD	A	414	39/54	0.87	0.12	36,69,93,99	0
27	LMG	C	518	48/55	0.88	0.11	43,72,96,103	0
34	UNL	b	621	55/-	0.88	0.10	39,57,86,91	0
27	LMG	c	523	49/55	0.88	0.10	32,56,87,111	0
34	UNL	c	520	55/-	0.88	0.11	39,61,79,86	0
34	UNL	B	620	43/-	0.89	0.10	34,51,68,74	0
28	SQD	b	601	49/54	0.89	0.10	38,60,102,112	0
28	SQD	f	101	41/54	0.89	0.12	54,87,117,125	0
25	BCR	x	101	40/40	0.89	0.10	35,57,76,82	0
34	UNL	C	521	47/-	0.89	0.10	37,56,73,74	0
27	LMG	A	411	48/55	0.89	0.10	37,62,78,103	0
28	SQD	B	624	54/54	0.89	0.10	39,58,90,100	0
34	UNL	I	101	41/-	0.89	0.12	37,53,75,79	0
34	UNL	d	410	43/-	0.89	0.13	39,58,70,78	0
34	UNL	J	101	28/-	0.89	0.11	52,64,78,86	0
34	UNL	X	101	55/-	0.89	0.10	34,49,75,79	0
27	LMG	B	621	28/55	0.89	0.11	31,47,60,70	0
27	LMG	m	101	51/55	0.90	0.09	30,51,81,97	0
34	UNL	j	101	28/-	0.90	0.10	42,56,67,67	0
25	BCR	K	101	40/40	0.91	0.09	36,53,73,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	UNL	B	625	28/-	0.91	0.10	31,46,69,70	0
25	BCR	c	514	40/40	0.91	0.09	40,59,77,79	0
28	SQD	a	412	54/54	0.91	0.10	34,69,91,95	0
25	BCR	k	101	40/40	0.91	0.09	39,65,81,83	0
34	UNL	C	519	28/-	0.91	0.10	34,46,55,56	0
34	UNL	C	520	28/-	0.91	0.09	42,51,64,65	0
34	UNL	l	102	53/-	0.91	0.11	33,50,87,91	0
23	CLA	B	601	65/65	0.91	0.10	32,61,99,105	0
34	UNL	t	102	34/-	0.91	0.09	35,50,58,65	0
30	DGD	h	102	62/66	0.91	0.09	33,52,65,70	0
25	BCR	d	404	40/40	0.92	0.08	36,54,90,102	0
25	BCR	D	404	40/40	0.92	0.10	25,46,103,108	0
25	BCR	k	102	40/40	0.92	0.10	37,57,66,73	0
30	DGD	C	516	62/66	0.92	0.09	30,54,108,129	0
23	CLA	c	512	65/65	0.92	0.10	40,58,97,107	0
23	CLA	C	513	65/65	0.92	0.10	45,68,95,101	0
27	LMG	M	101	51/55	0.92	0.08	25,47,72,84	0
28	SQD	A	412	52/54	0.93	0.09	32,61,93,101	0
25	BCR	b	619	40/40	0.93	0.07	27,39,55,58	0
23	CLA	c	513	65/65	0.93	0.09	47,72,109,114	0
34	UNL	M	102	37/-	0.93	0.09	26,45,54,69	0
34	UNL	M	103	26/-	0.93	0.10	24,49,57,63	0
28	SQD	F	101	36/54	0.93	0.10	41,71,87,95	0
25	BCR	c	515	40/40	0.93	0.09	31,48,64,72	0
30	DGD	H	102	62/66	0.93	0.08	30,49,61,74	0
27	LMG	d	409	44/55	0.93	0.09	31,58,89,105	0
30	DGD	c	517	62/66	0.93	0.08	31,52,86,96	0
25	BCR	Z	101	40/40	0.93	0.09	34,57,72,75	0
23	CLA	C	503	65/65	0.94	0.07	29,42,52,55	0
25	BCR	b	618	40/40	0.94	0.07	22,43,54,58	0
23	CLA	c	503	65/65	0.94	0.07	32,45,56,62	0
27	LMG	D	406	51/55	0.94	0.09	26,56,89,97	0
25	BCR	b	620	40/40	0.94	0.07	28,47,61,67	0
25	BCR	B	618	40/40	0.94	0.06	23,39,54,56	0
25	BCR	B	619	40/40	0.94	0.07	27,42,65,78	0
25	BCR	C	514	40/40	0.94	0.08	27,39,54,59	0
29	LHG	d	406	49/49	0.94	0.10	36,52,82,94	0
29	LHG	d	408	39/49	0.94	0.08	26,47,73,78	0
23	CLA	c	511	65/65	0.94	0.09	34,57,74,76	0
25	BCR	H	101	40/40	0.94	0.07	31,47,57,62	0
25	BCR	t	101	40/40	0.94	0.06	25,36,53,61	0
23	CLA	C	512	65/65	0.94	0.09	33,56,102,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	K	102	40/40	0.94	0.10	34,58,73,76	0
25	BCR	T	101	40/40	0.94	0.06	27,40,60,62	0
23	CLA	c	504	60/65	0.95	0.08	30,44,86,93	0
23	CLA	c	505	65/65	0.95	0.07	23,43,68,72	0
23	CLA	c	506	65/65	0.95	0.09	28,51,111,120	0
29	LHG	B	623	49/49	0.95	0.08	25,44,76,87	0
29	LHG	D	408	47/49	0.95	0.09	26,46,84,100	0
23	CLA	c	508	64/65	0.95	0.08	30,45,93,113	0
23	CLA	c	509	65/65	0.95	0.08	30,48,67,68	0
25	BCR	a	409	40/40	0.95	0.06	22,33,42,46	0
29	LHG	l	101	49/49	0.95	0.08	29,48,59,64	0
23	CLA	c	510	65/65	0.95	0.07	33,50,69,76	0
30	DGD	C	515	62/66	0.95	0.08	21,40,86,103	0
23	CLA	C	508	65/65	0.95	0.08	23,41,119,127	0
23	CLA	C	509	65/65	0.95	0.08	26,45,65,79	0
23	CLA	C	510	65/65	0.95	0.07	29,46,75,87	0
23	CLA	C	511	65/65	0.95	0.08	35,51,67,69	0
30	DGD	c	518	62/66	0.95	0.07	29,52,82,94	0
24	PHO	d	401	64/64	0.95	0.06	27,38,50,59	0
25	BCR	A	409	40/40	0.95	0.06	24,34,43,47	0
25	BCR	B	617	40/40	0.95	0.07	26,40,54,56	0
23	CLA	B	609	65/65	0.95	0.07	24,35,57,66	0
23	CLA	C	502	65/65	0.95	0.07	24,44,56,64	0
23	CLA	b	617	60/65	0.95	0.08	28,44,105,113	0
23	CLA	B	606	65/65	0.95	0.07	21,35,73,83	0
26	PL9	d	405	55/55	0.95	0.06	21,35,44,47	0
23	CLA	B	612	65/65	0.96	0.06	21,32,46,51	0
23	CLA	C	504	59/65	0.96	0.07	24,44,83,93	0
23	CLA	a	405	65/65	0.96	0.06	17,29,50,61	0
23	CLA	a	406	65/65	0.96	0.07	24,40,100,112	0
23	CLA	a	408	65/65	0.96	0.08	16,36,95,107	0
23	CLA	d	403	65/65	0.96	0.07	29,49,97,109	0
23	CLA	b	607	65/65	0.96	0.07	24,40,74,83	0
24	PHO	A	407	64/64	0.96	0.05	22,32,44,50	0
24	PHO	a	407	64/64	0.96	0.06	22,31,40,48	0
29	LHG	B	622	49/49	0.96	0.07	26,42,57,74	0
26	PL9	D	405	55/55	0.96	0.06	17,32,48,52	0
23	CLA	b	609	65/65	0.96	0.07	24,41,70,74	0
23	CLA	b	610	65/65	0.96	0.07	30,46,71,89	0
29	LHG	d	407	49/49	0.96	0.07	24,44,61,72	0
23	CLA	b	611	65/65	0.96	0.07	24,38,51,57	0
23	CLA	b	613	65/65	0.96	0.07	20,34,49,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	615	65/65	0.96	0.08	20,37,81,97	0
23	CLA	b	616	65/65	0.96	0.07	26,39,62,68	0
23	CLA	C	505	65/65	0.96	0.08	25,43,73,83	0
23	CLA	c	501	65/65	0.96	0.06	25,39,52,59	0
30	DGD	C	517	62/66	0.96	0.07	23,45,82,93	0
23	CLA	c	502	65/65	0.96	0.07	27,43,65,69	0
23	CLA	C	506	65/65	0.96	0.07	27,42,95,110	0
30	DGD	c	516	62/66	0.96	0.07	21,43,78,84	0
23	CLA	B	614	65/65	0.96	0.07	21,38,83,95	0
23	CLA	B	615	65/65	0.96	0.06	24,36,70,87	0
23	CLA	B	616	60/65	0.96	0.09	23,41,93,102	0
23	CLA	c	507	65/65	0.96	0.07	21,43,62,66	0
23	CLA	B	603	65/65	0.96	0.06	16,32,70,72	0
23	CLA	B	611	65/65	0.97	0.05	17,30,46,53	0
24	PHO	A	406	64/64	0.97	0.05	15,28,37,41	0
23	CLA	C	507	65/65	0.97	0.06	23,40,57,62	0
23	CLA	A	405	65/65	0.97	0.08	18,34,99,118	0
23	CLA	b	612	65/65	0.97	0.06	20,33,51,57	0
29	LHG	D	407	49/49	0.97	0.06	21,41,54,68	0
23	CLA	B	613	65/65	0.97	0.05	13,30,63,74	0
23	CLA	b	614	65/65	0.97	0.06	18,32,77,84	0
23	CLA	B	604	65/65	0.97	0.07	18,31,79,87	0
23	CLA	B	605	65/65	0.97	0.06	18,30,44,46	0
23	CLA	A	404	65/65	0.97	0.05	17,27,47,57	0
23	CLA	C	501	65/65	0.97	0.06	18,34,52,58	0
23	CLA	D	401	65/65	0.97	0.05	18,29,53,61	0
23	CLA	D	402	65/65	0.97	0.06	15,32,58,67	0
23	CLA	D	403	65/65	0.97	0.07	23,40,121,137	0
23	CLA	B	607	65/65	0.97	0.06	14,33,65,72	0
23	CLA	B	608	65/65	0.97	0.05	19,35,56,61	0
23	CLA	B	602	65/65	0.97	0.06	22,36,61,63	0
23	CLA	a	411	65/65	0.97	0.06	17,31,44,50	0
23	CLA	b	603	65/65	0.97	0.07	26,42,73,83	0
23	CLA	b	604	65/65	0.97	0.06	18,37,70,77	0
23	CLA	b	605	65/65	0.97	0.07	21,34,88,99	0
33	BCT	a	404	4/4	0.97	0.06	23,23,41,49	0
23	CLA	b	606	65/65	0.97	0.06	21,35,52,57	0
23	CLA	B	610	65/65	0.97	0.06	16,31,44,48	0
23	CLA	d	402	65/65	0.97	0.06	19,33,64,73	0
23	CLA	b	608	65/65	0.97	0.07	18,35,66,74	0
35	HEM	e	102	43/43	0.97	0.09	43,57,78,80	0
33	BCT	A	418	4/4	0.98	0.06	26,33,39,47	0

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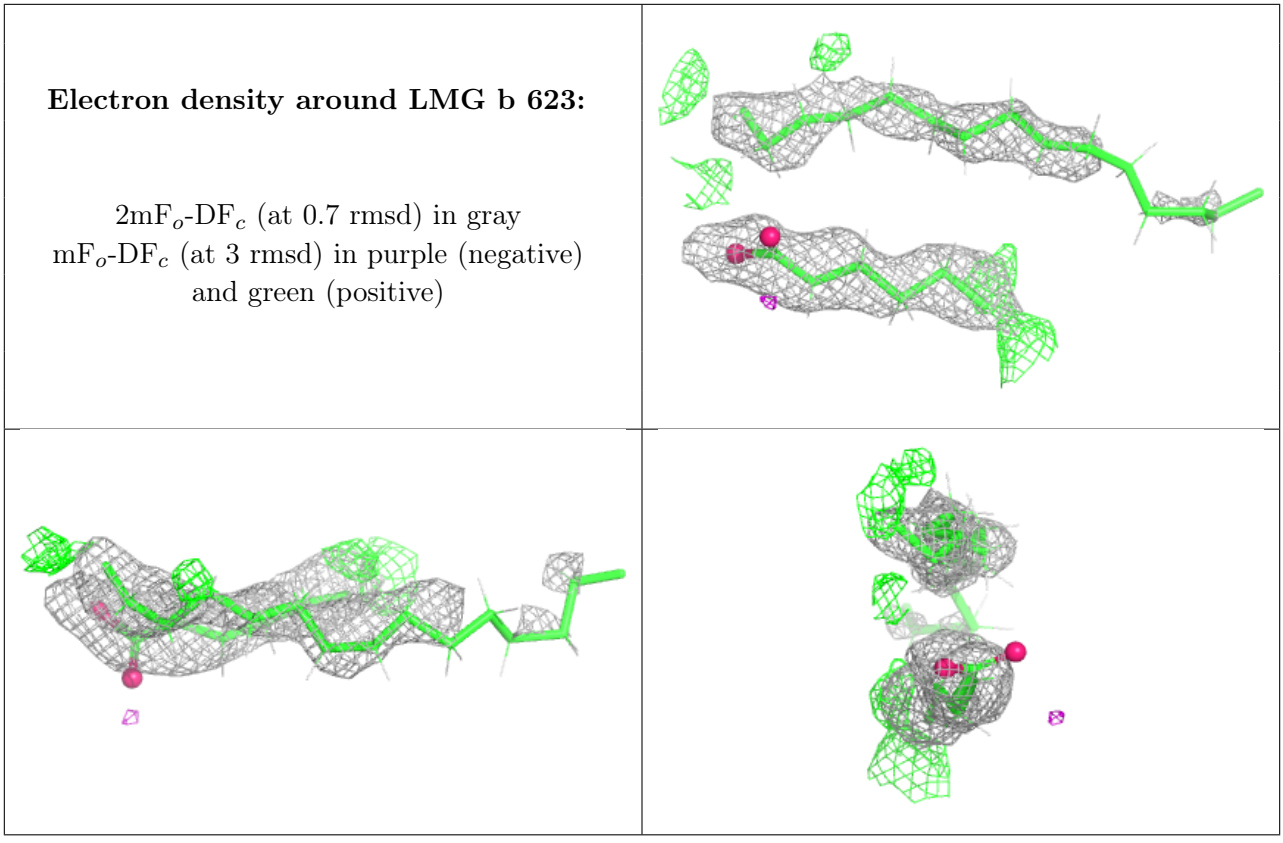
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	HEM	E	101	43/43	0.98	0.08	35,50,67,72	0
23	CLA	A	408	54/65	0.98	0.06	16,30,74,77	0
32	OEY	a	417[B]	11/11	0.99	0.03	22,28,30,30	11
22	CL	A	403	1/1	0.99	0.04	24,24,24,24	0
22	CL	a	402	1/1	0.99	0.03	28,28,28,28	0
22	CL	a	403	1/1	0.99	0.09	27,27,27,27	0
21	FE2	A	401	1/1	0.99	0.01	30,30,30,30	0
21	FE2	a	401	1/1	0.99	0.02	35,35,35,35	0
22	CL	A	402	1/1	0.99	0.05	29,29,29,29	0
31	OEX	A	416[A]	10/10	0.99	0.03	21,30,34,35	10
32	OEY	A	417[B]	11/11	0.99	0.03	22,26,29,30	11
36	HEC	V	201	43/43	0.99	0.04	24,31,41,41	0
36	HEC	v	201	43/43	0.99	0.05	27,35,51,54	0
31	OEX	a	416[A]	10/10	1.00	0.02	25,31,34,35	10

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.

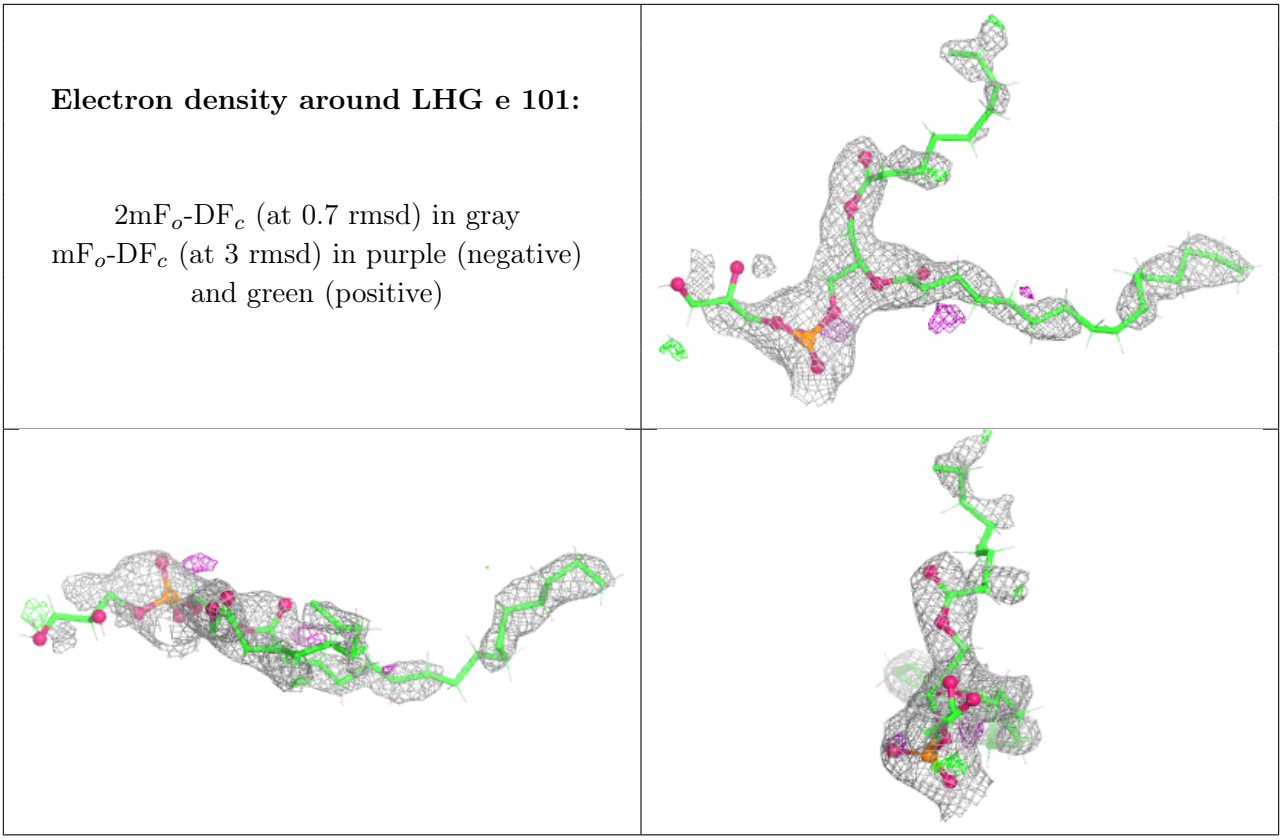
Electron density around LMG b 623:

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



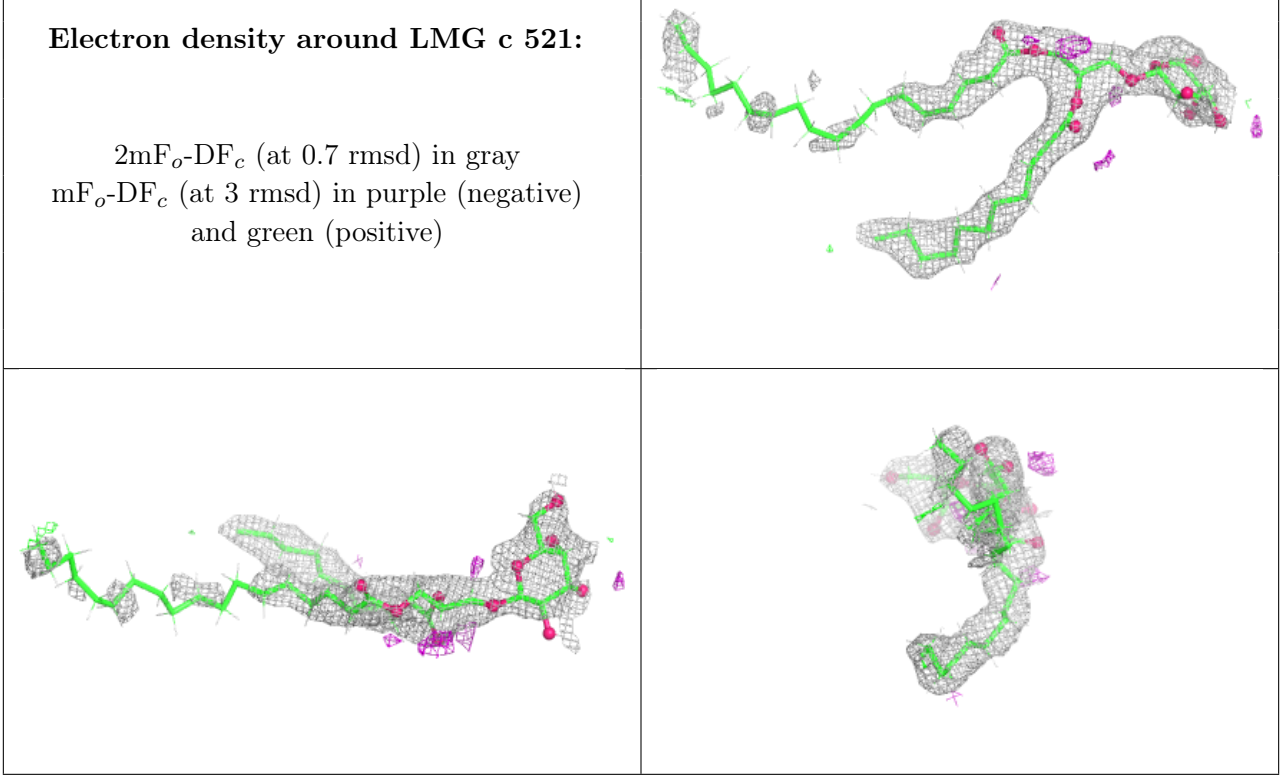
Electron density around LHG e 101:

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



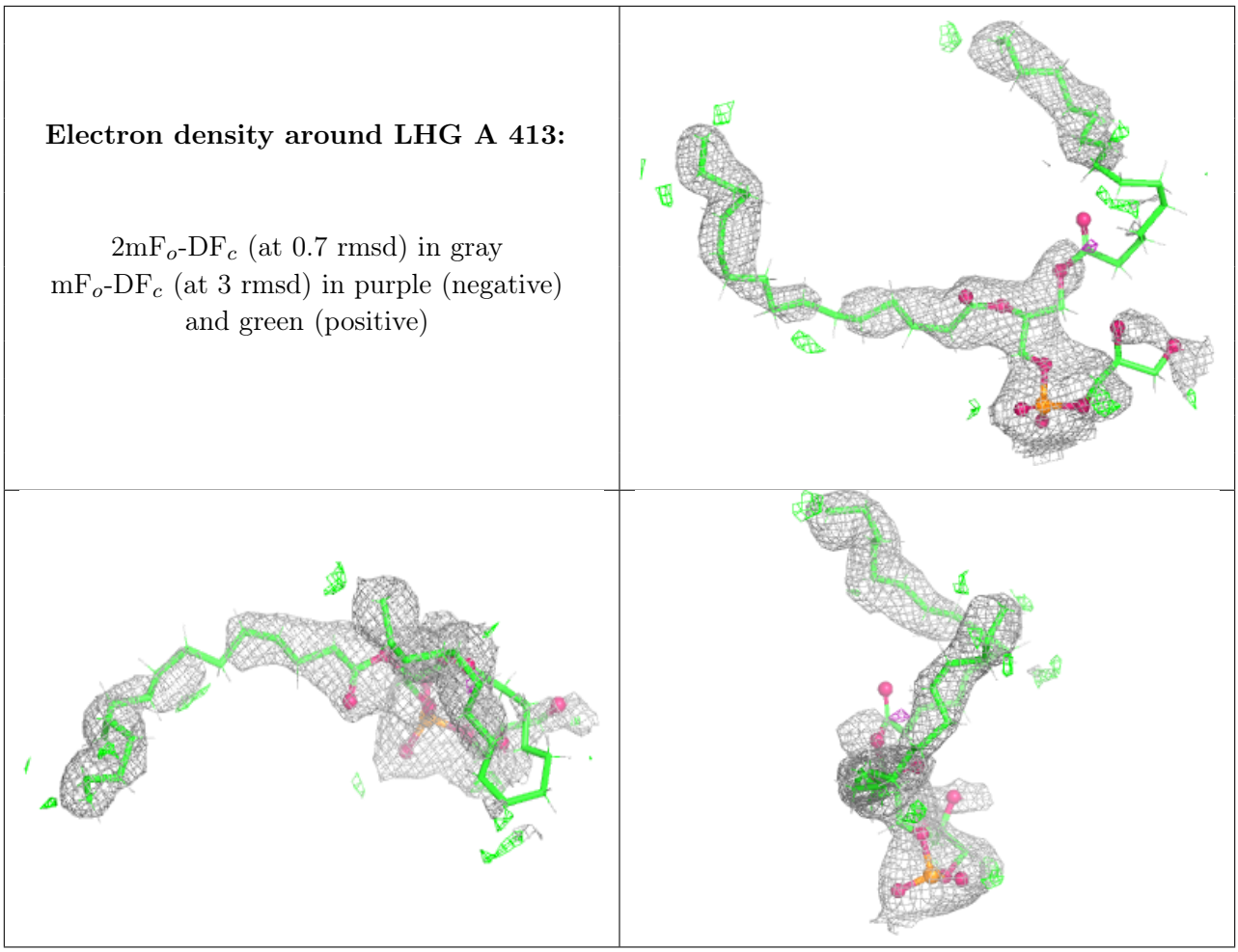
Electron density around LMG c 521:

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



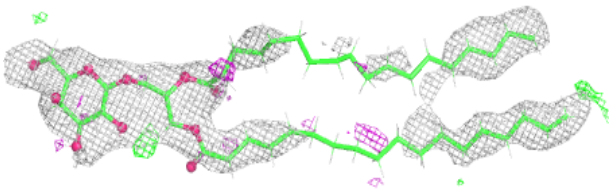
Electron density around LHG A 413:

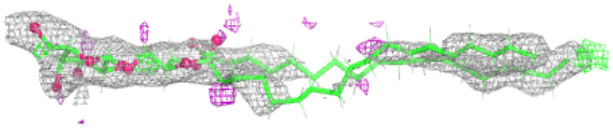
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 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)

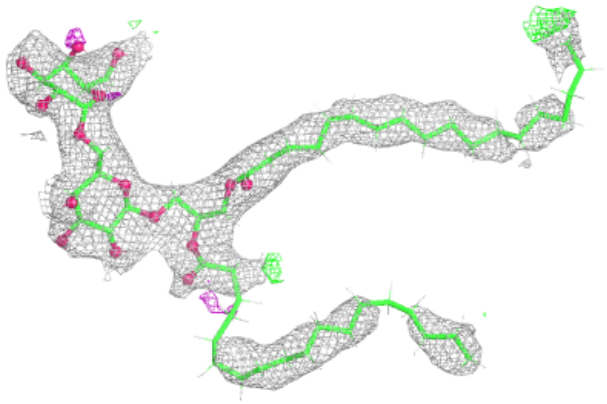


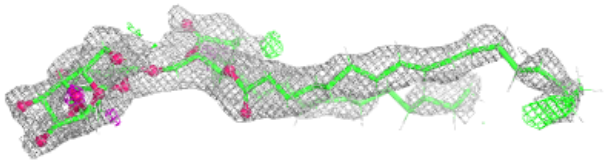


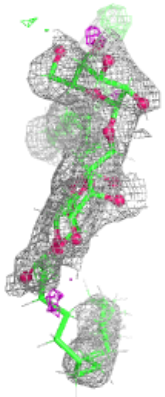


Electron density around DGD A 415:

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

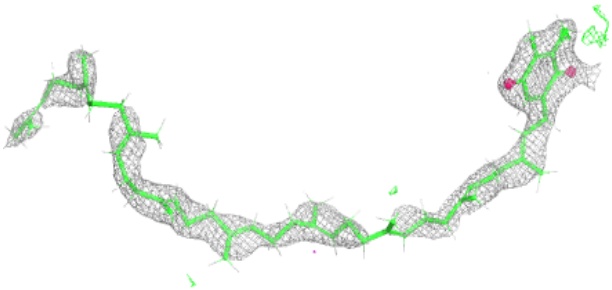


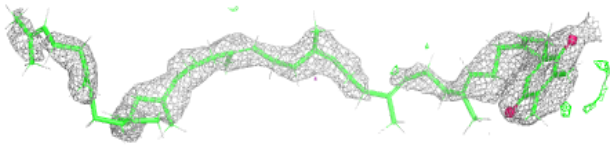


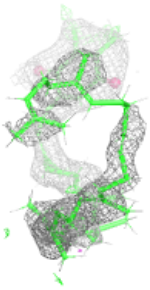


Electron density around PL9 a 410:

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

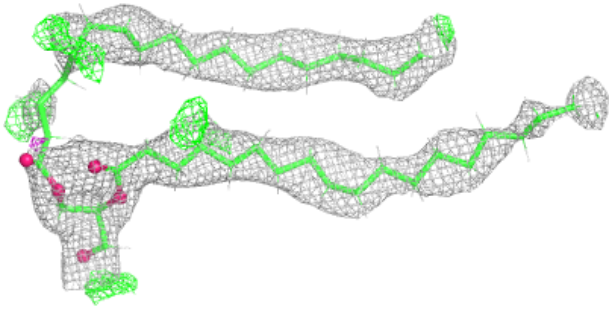


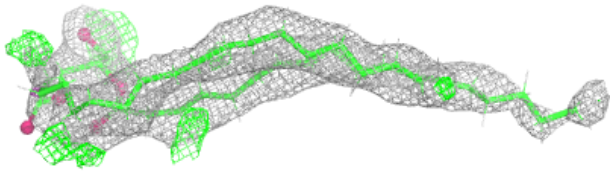


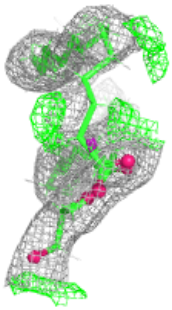


Electron density around DGD a 414:

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

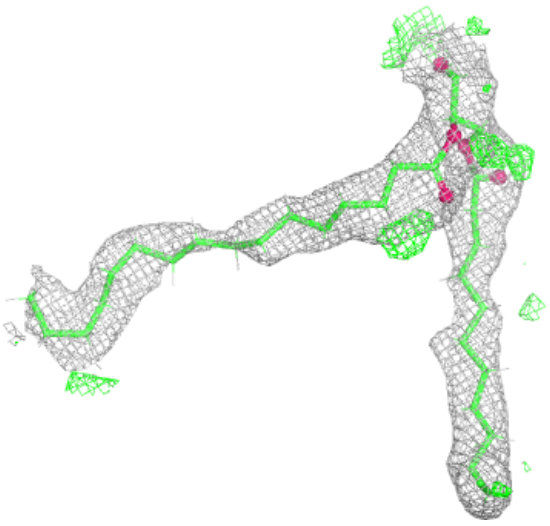


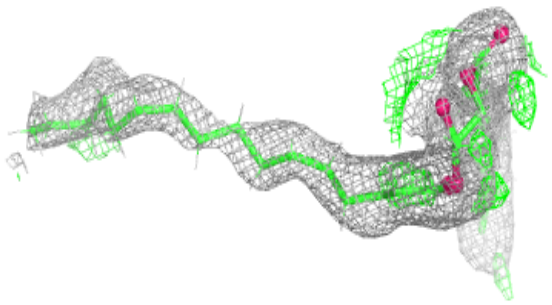


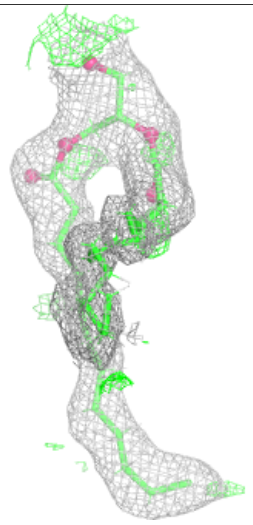


Electron density around SQD a 413:

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

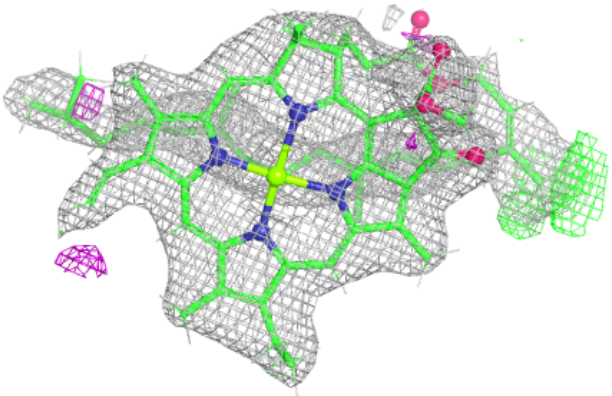


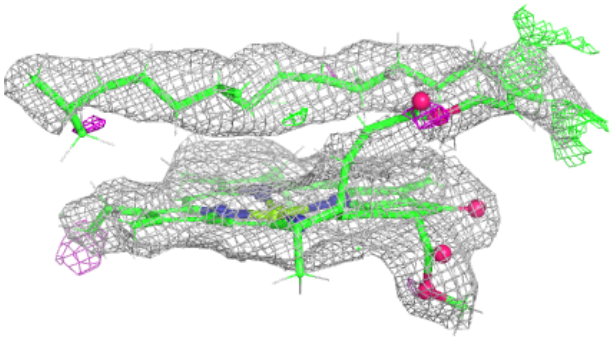


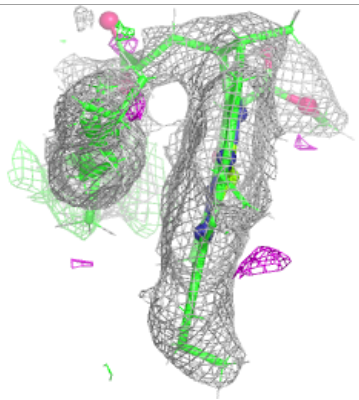


Electron density around CLA h 101:

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

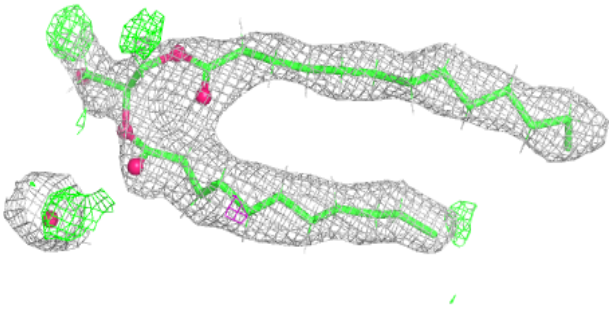


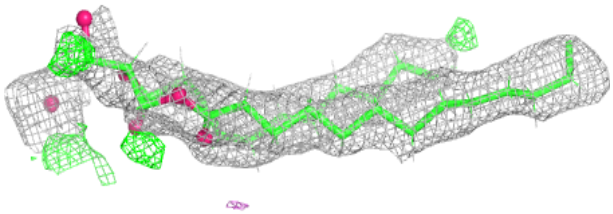


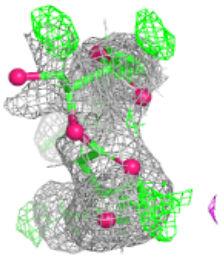


Electron density around LMG D 409:

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

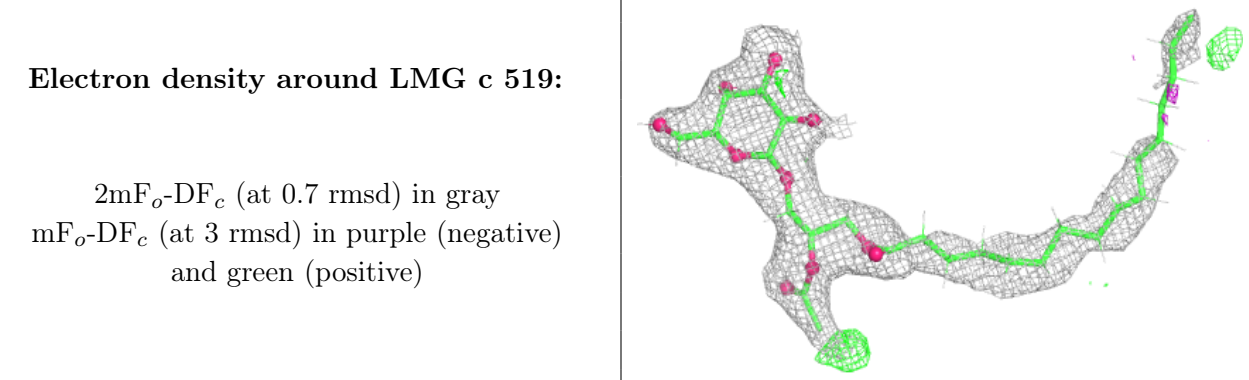


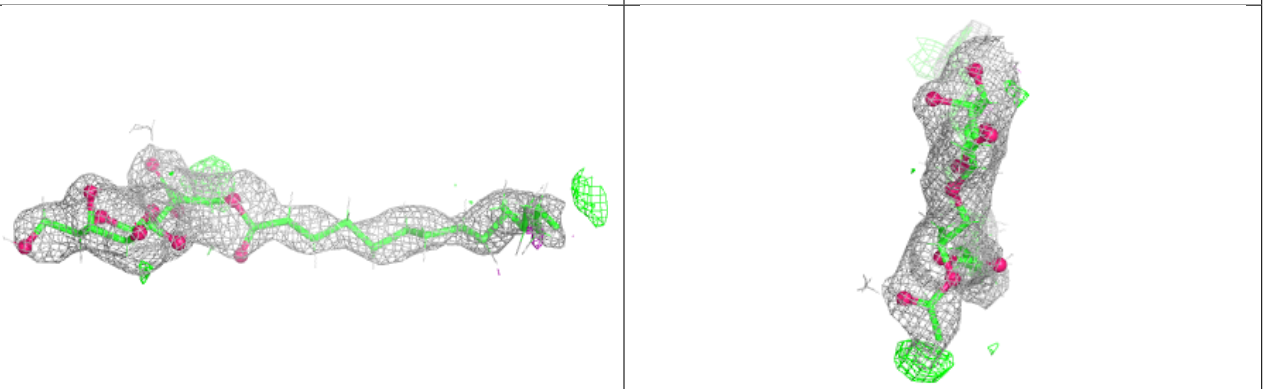




Electron density around LMG c 519:

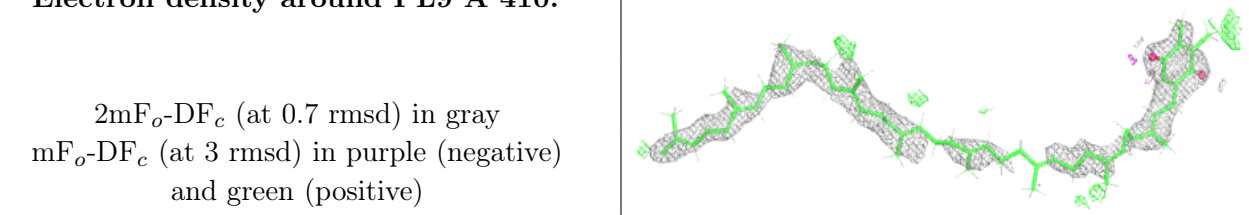
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

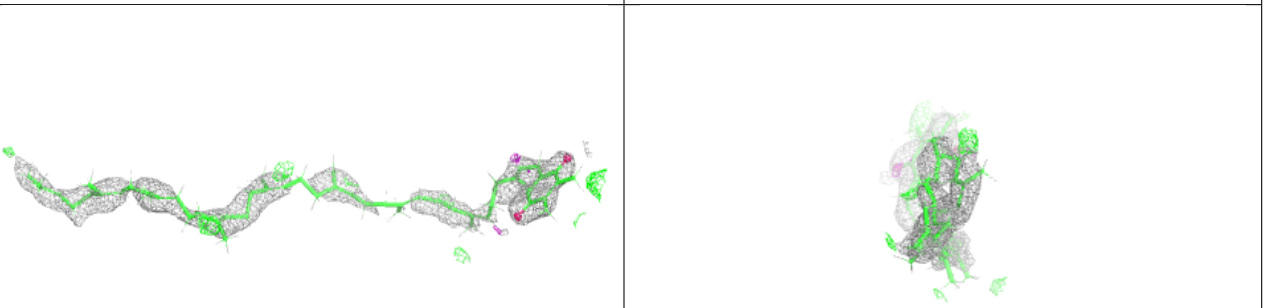




Electron density around PL9 A 410:

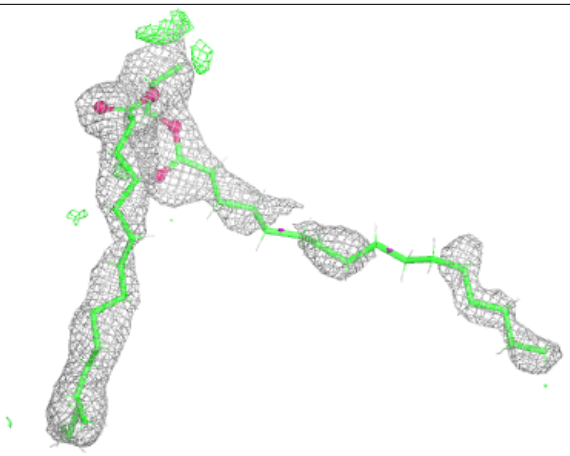
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

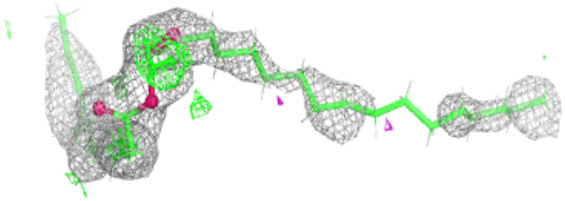


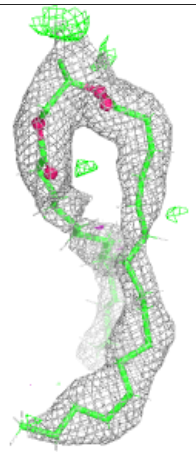


Electron density around SQD A 414:

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

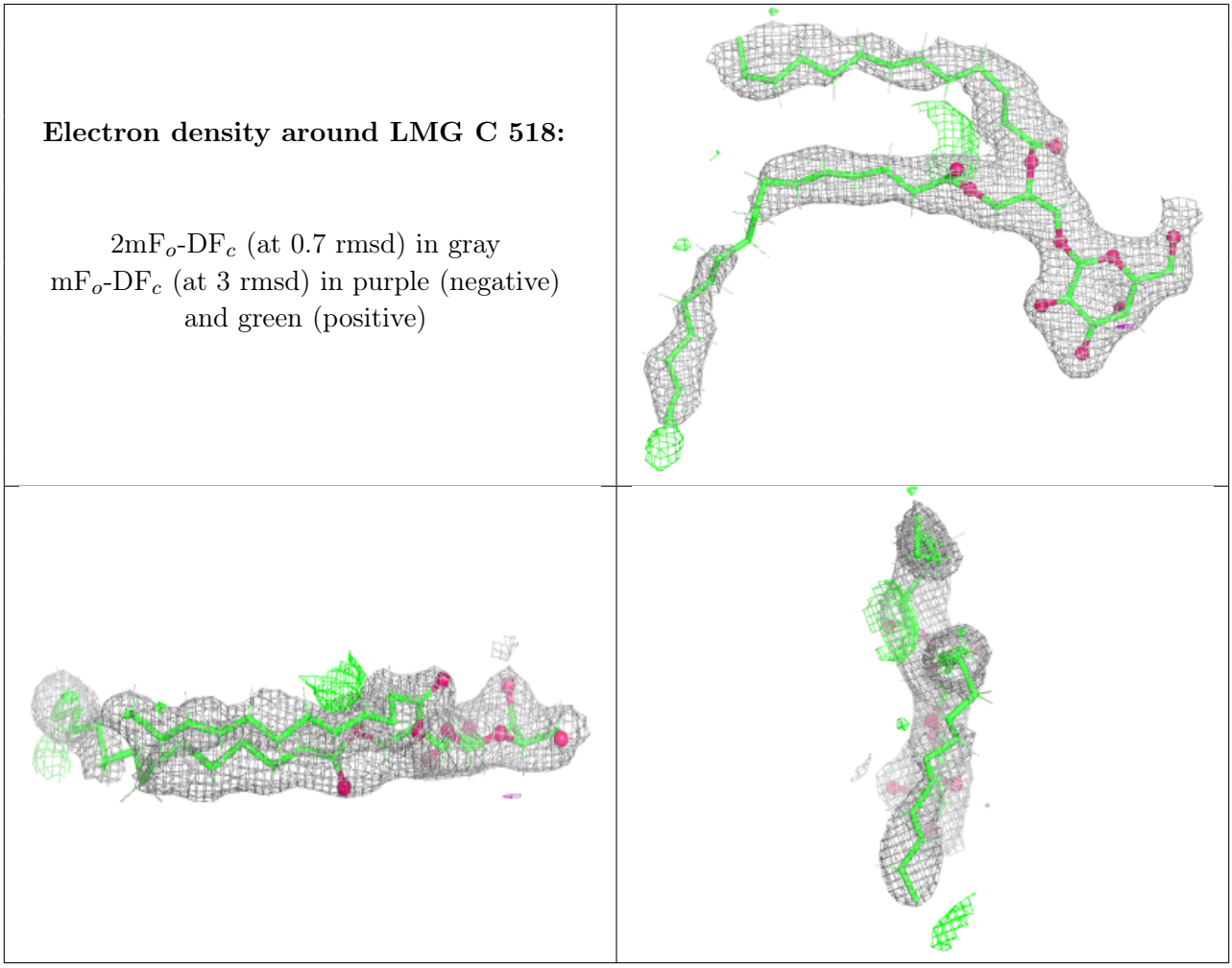






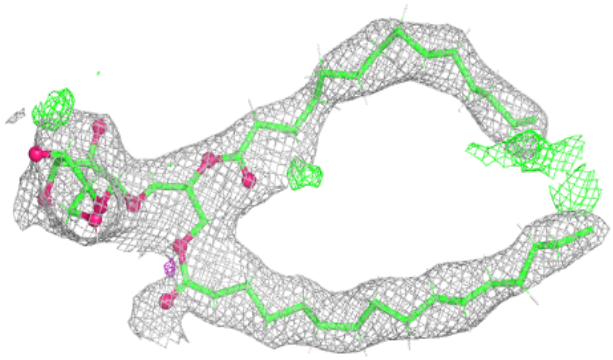
Electron density around LMG C 518:

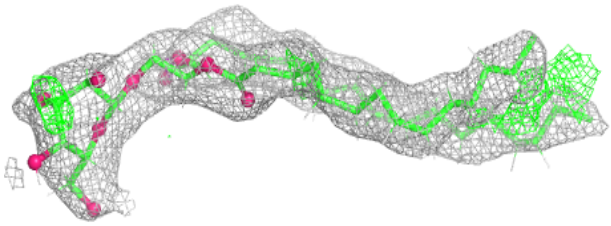
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

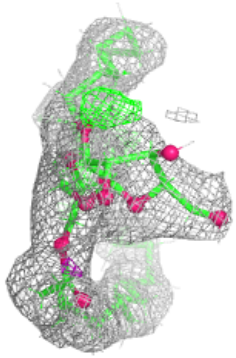


Electron density around LMG c 523:

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

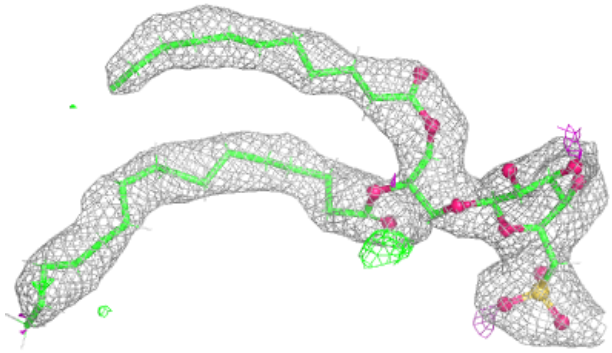


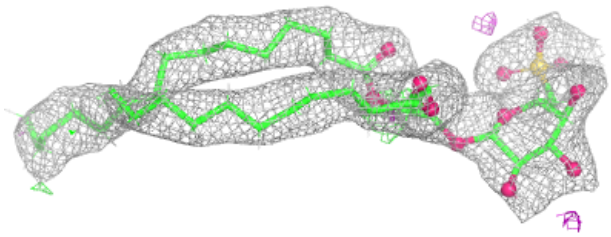


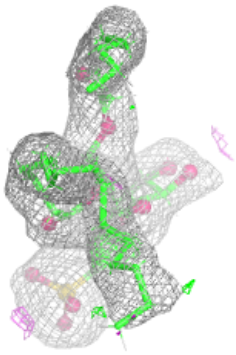


Electron density around SQD b 601:

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

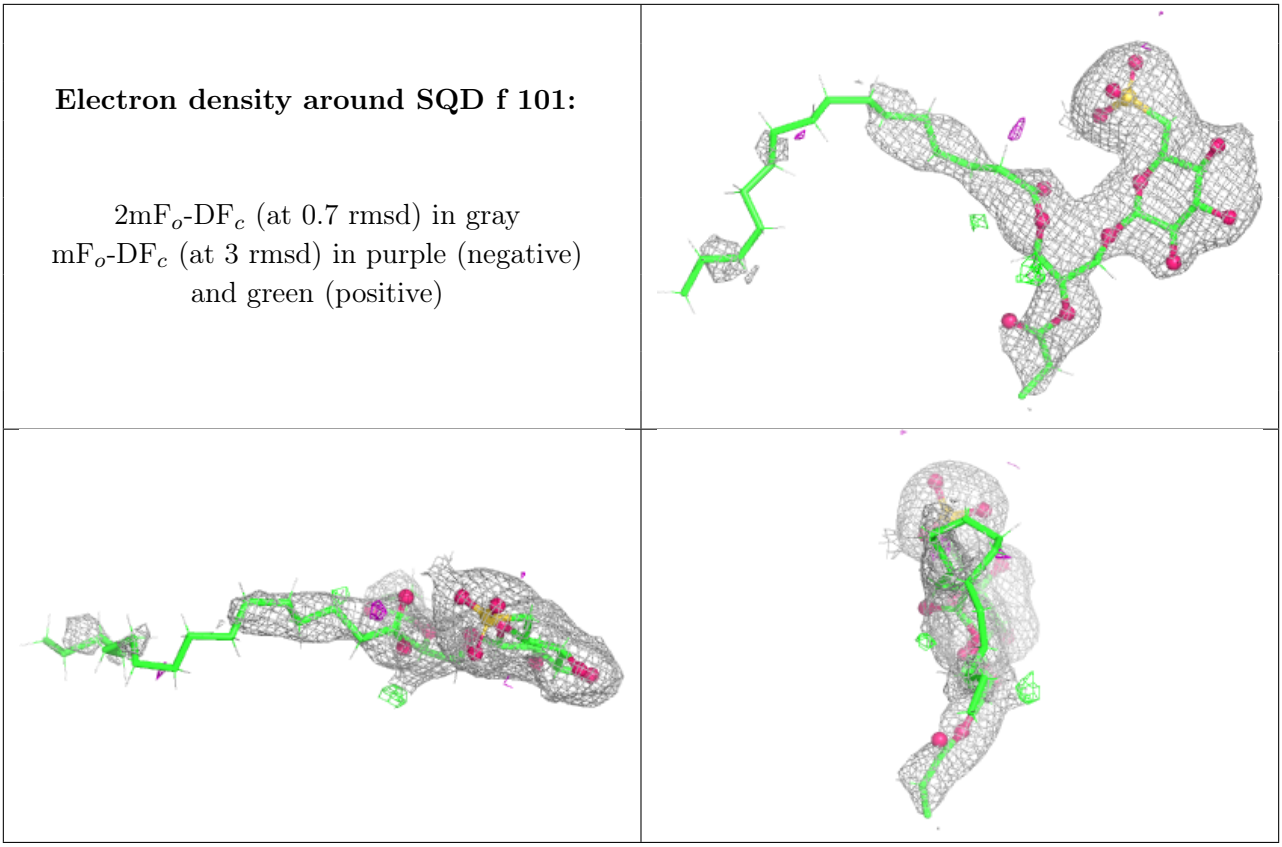






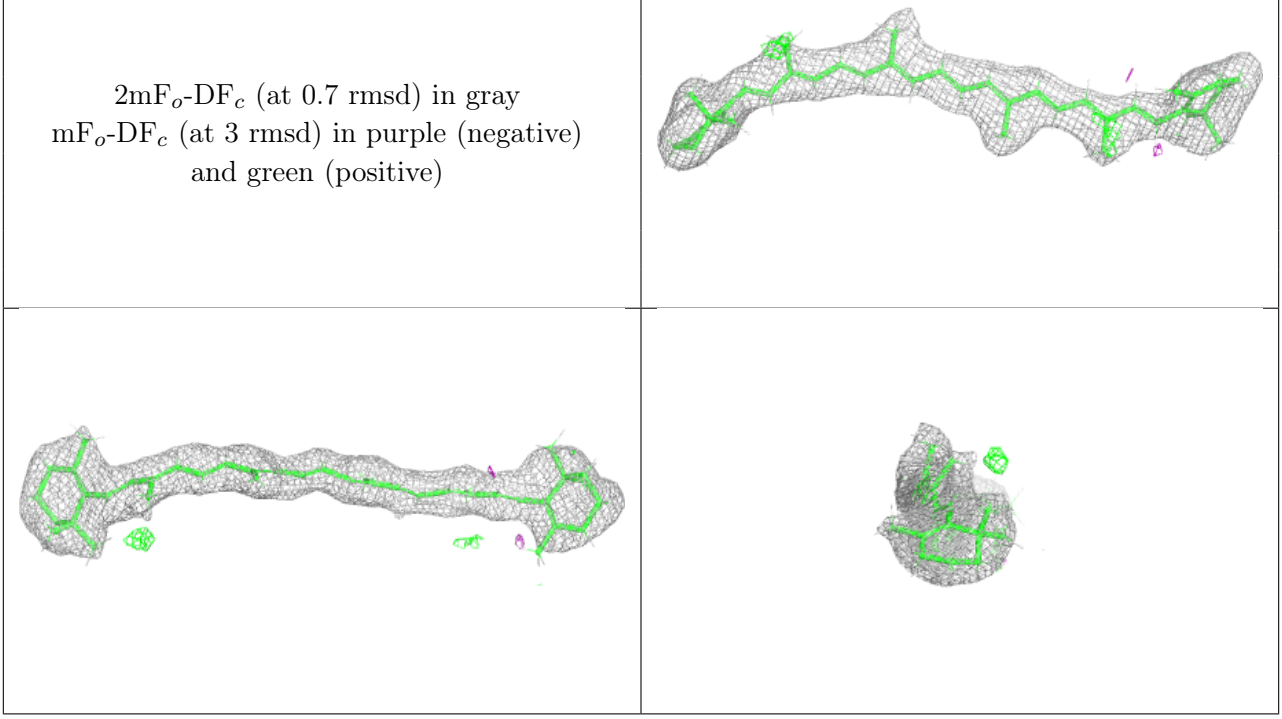
Electron density around SQD f 101:

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



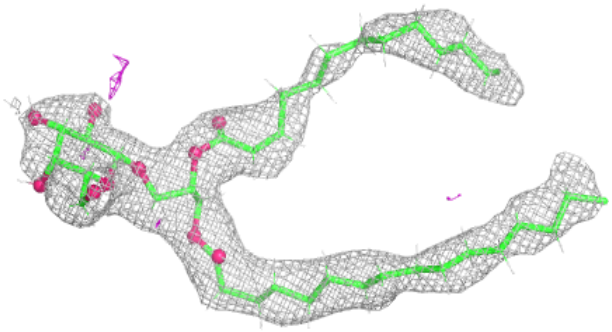
Electron density around BCR x 101:

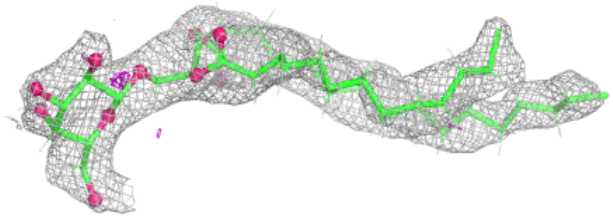
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

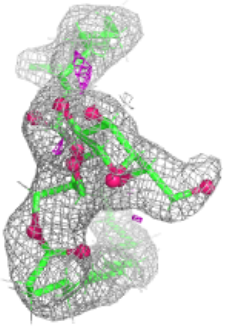


Electron density around LMG A 411:

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

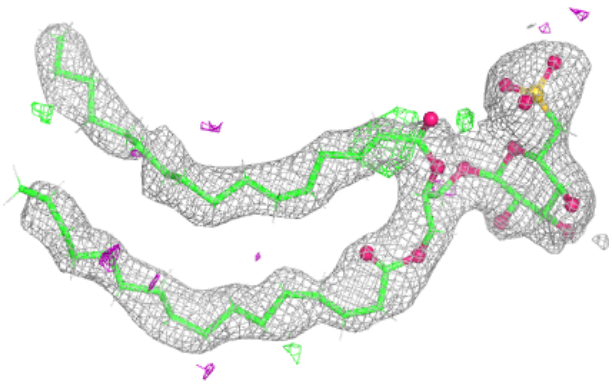


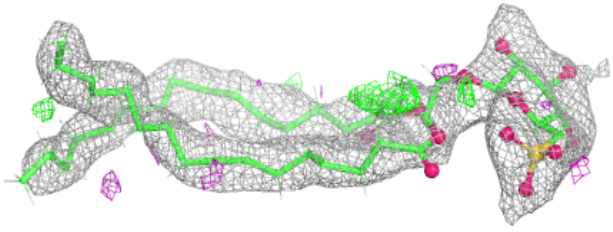


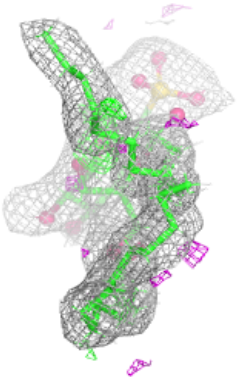


Electron density around SQD B 624:

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

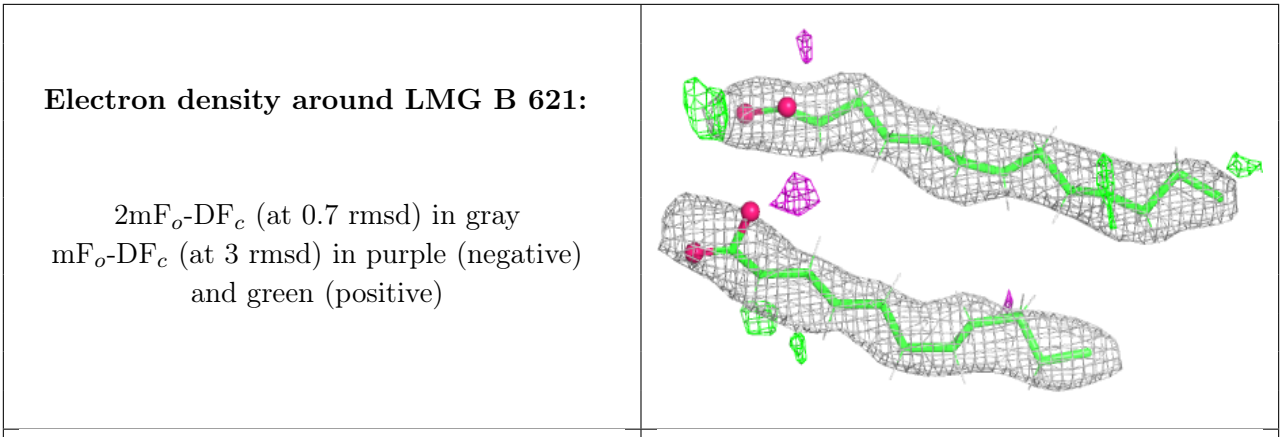






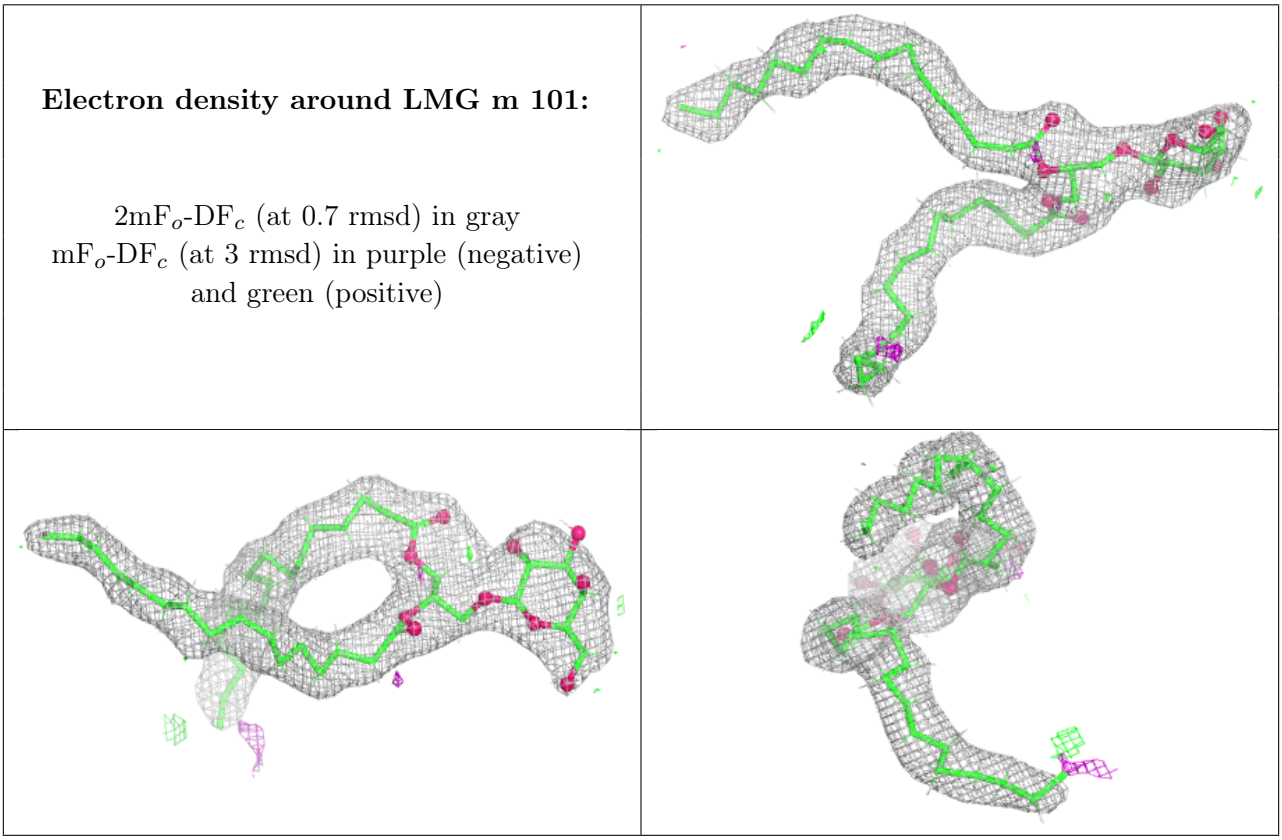
Electron density around LMG B 621:

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



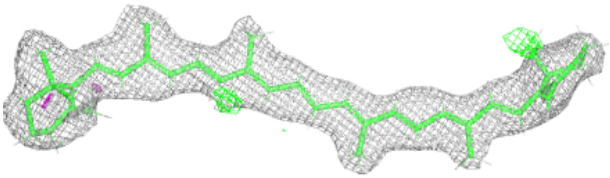
Electron density around LMG m 101:

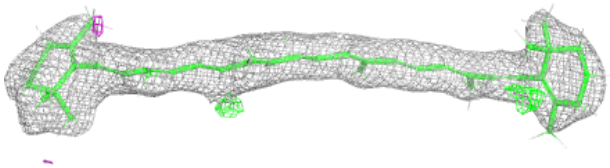
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

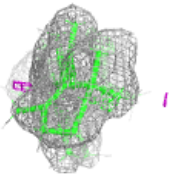


Electron density around BCR K 101:

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

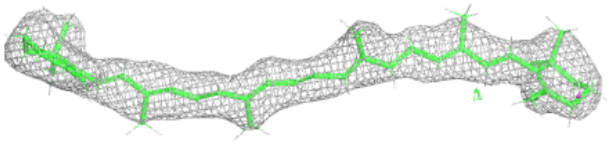


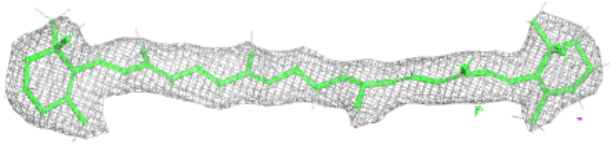


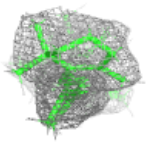


Electron density around BCR c 514:

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

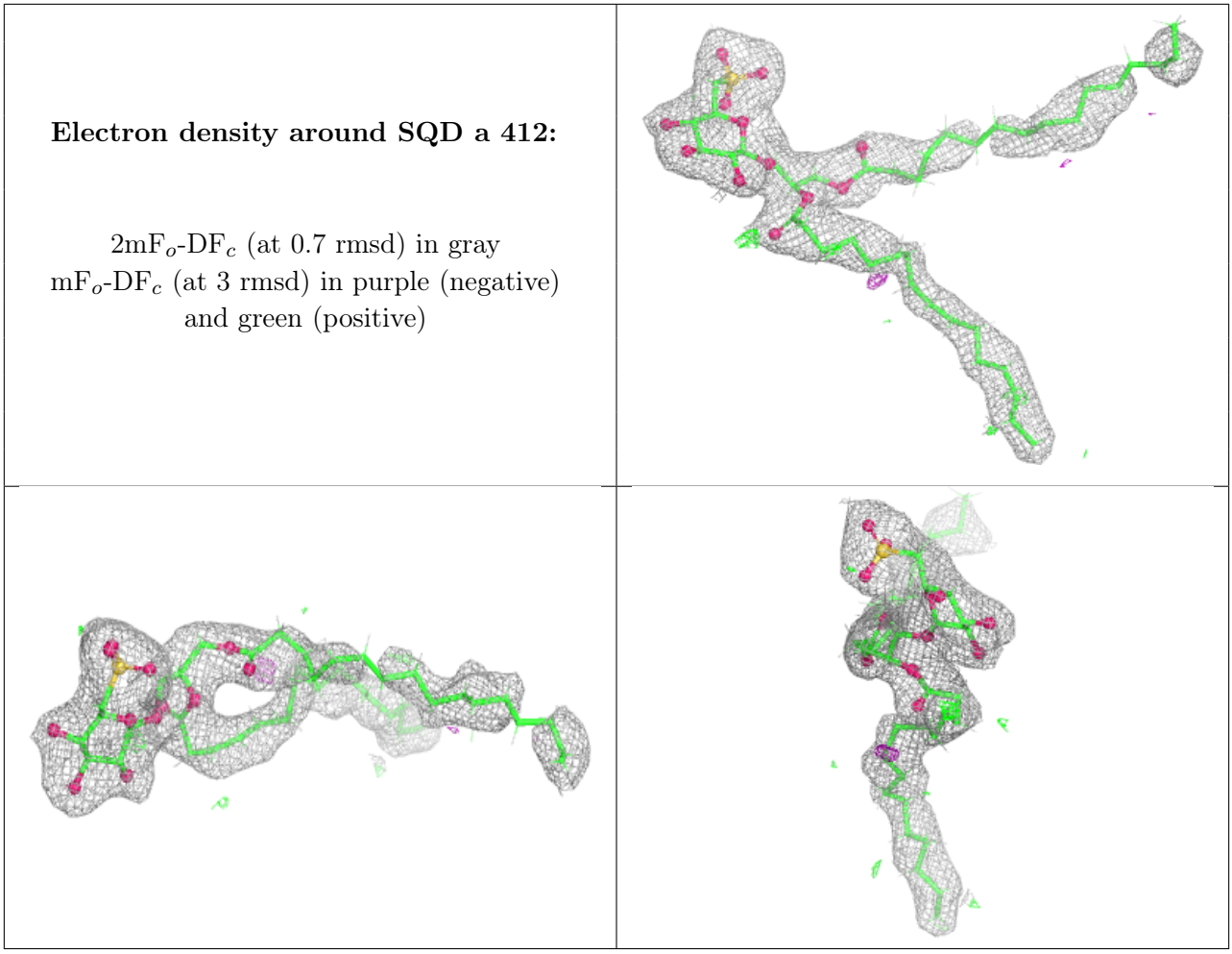






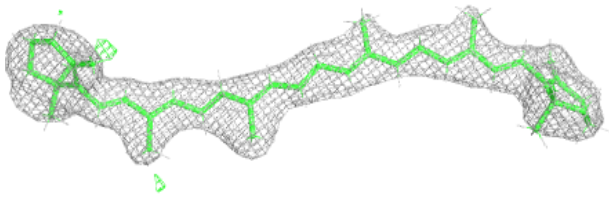
Electron density around SQD a 412:

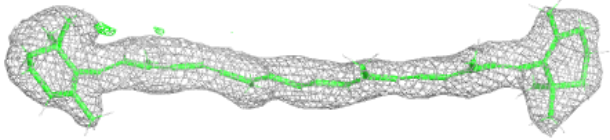
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

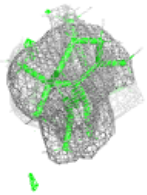


Electron density around BCR k 101:

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

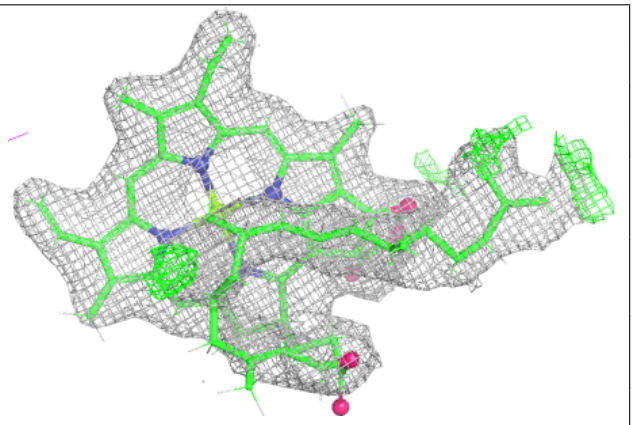


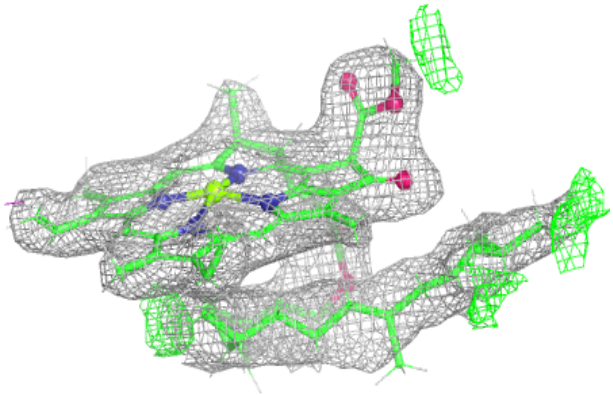


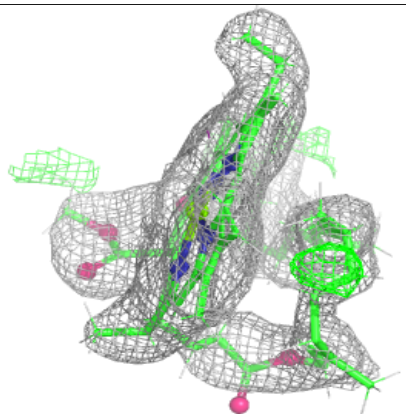


Electron density around CLA B 601:

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

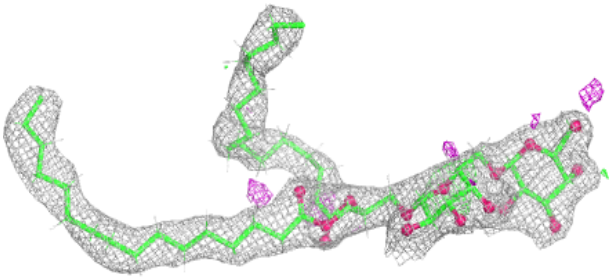


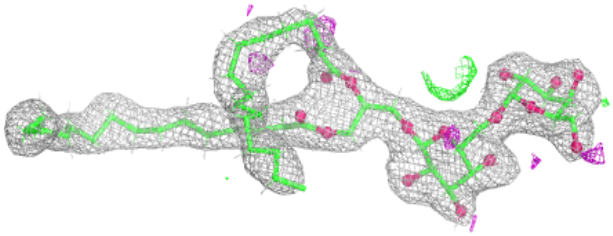


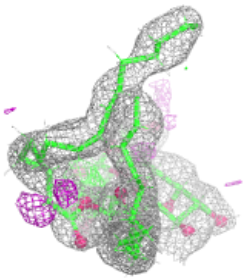


Electron density around DGD h 102:

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

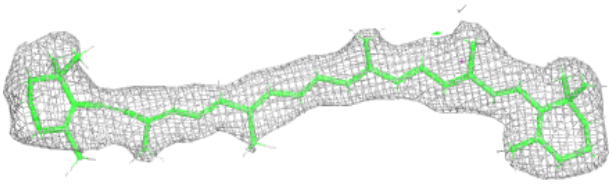


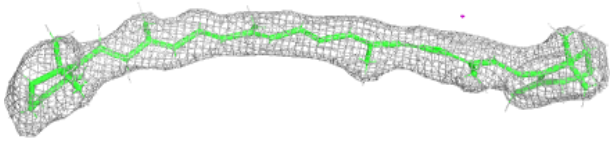


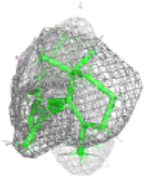


Electron density around BCR d 404:

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

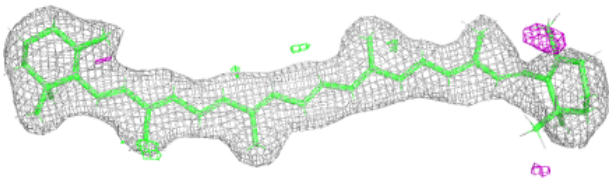


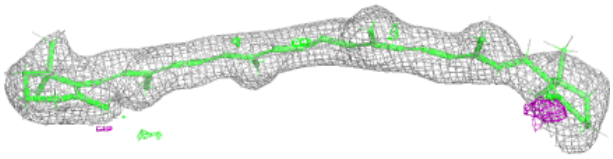


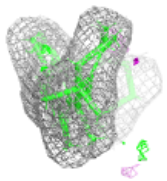


Electron density around BCR D 404:

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

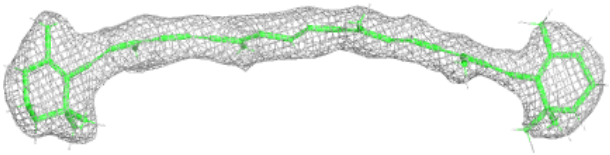


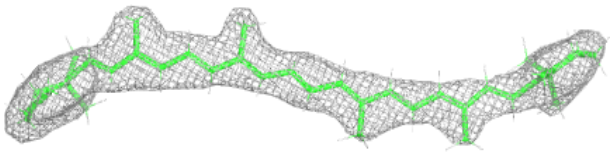


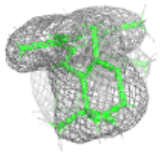


Electron density around BCR k 102:

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

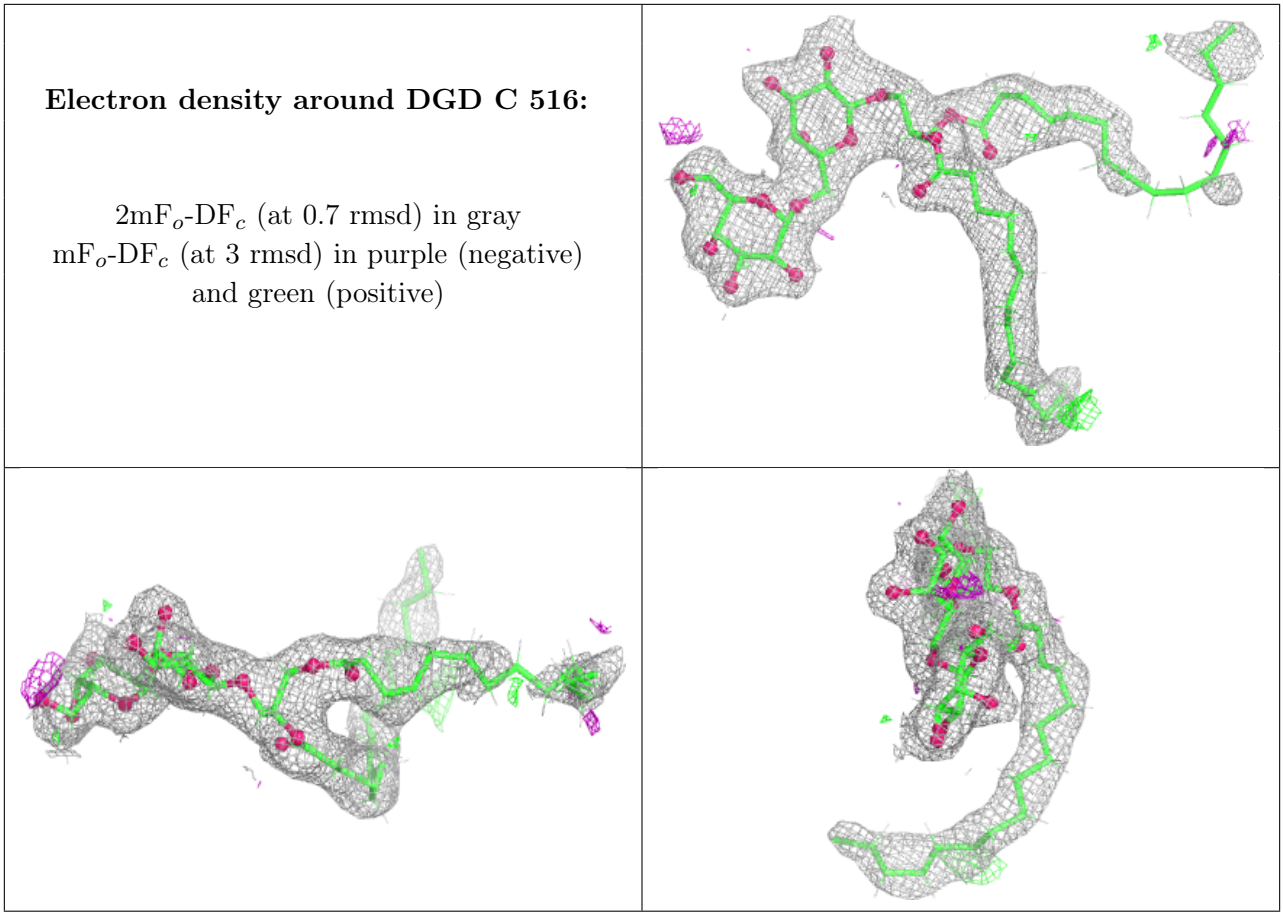






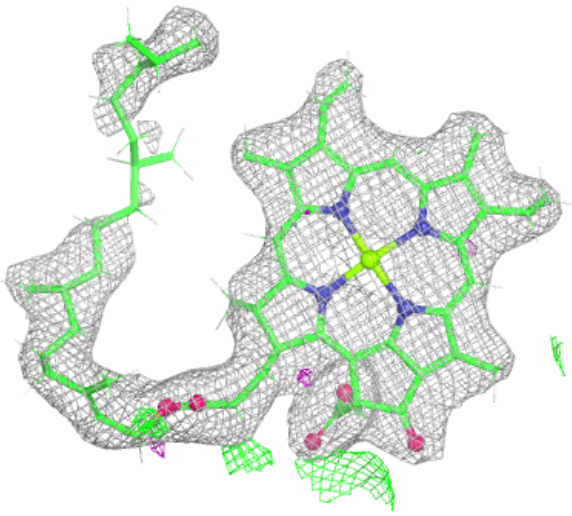
Electron density around DGD C 516:

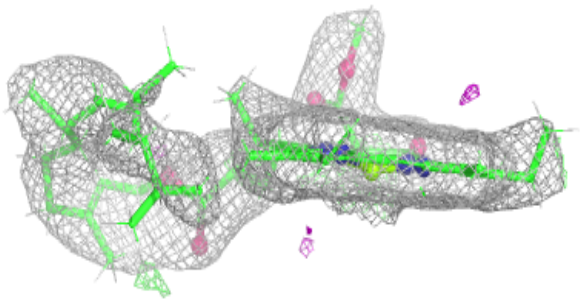
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

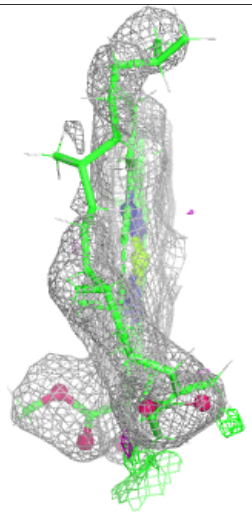


Electron density around CLA c 512:

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

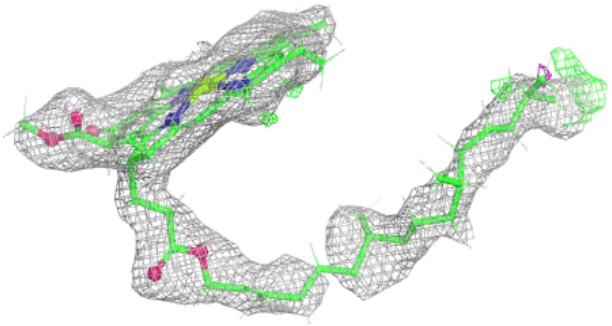


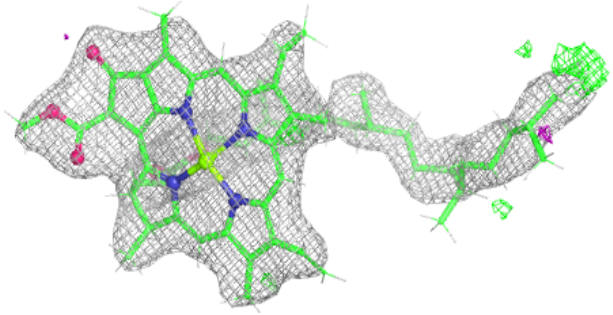


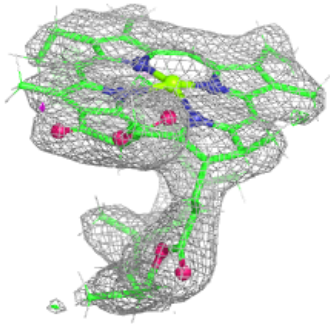


Electron density around CLA C 513:

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

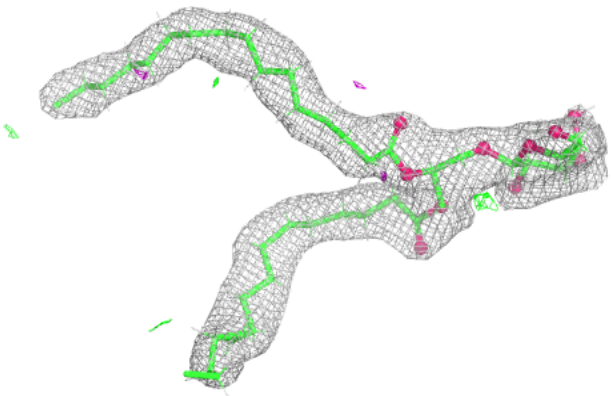


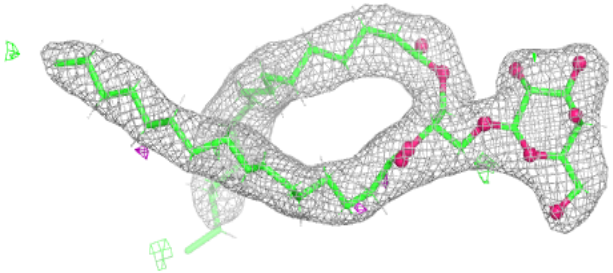


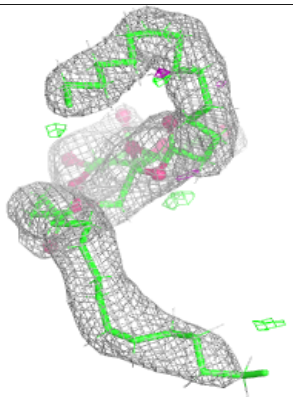


Electron density around LMG M 101:

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

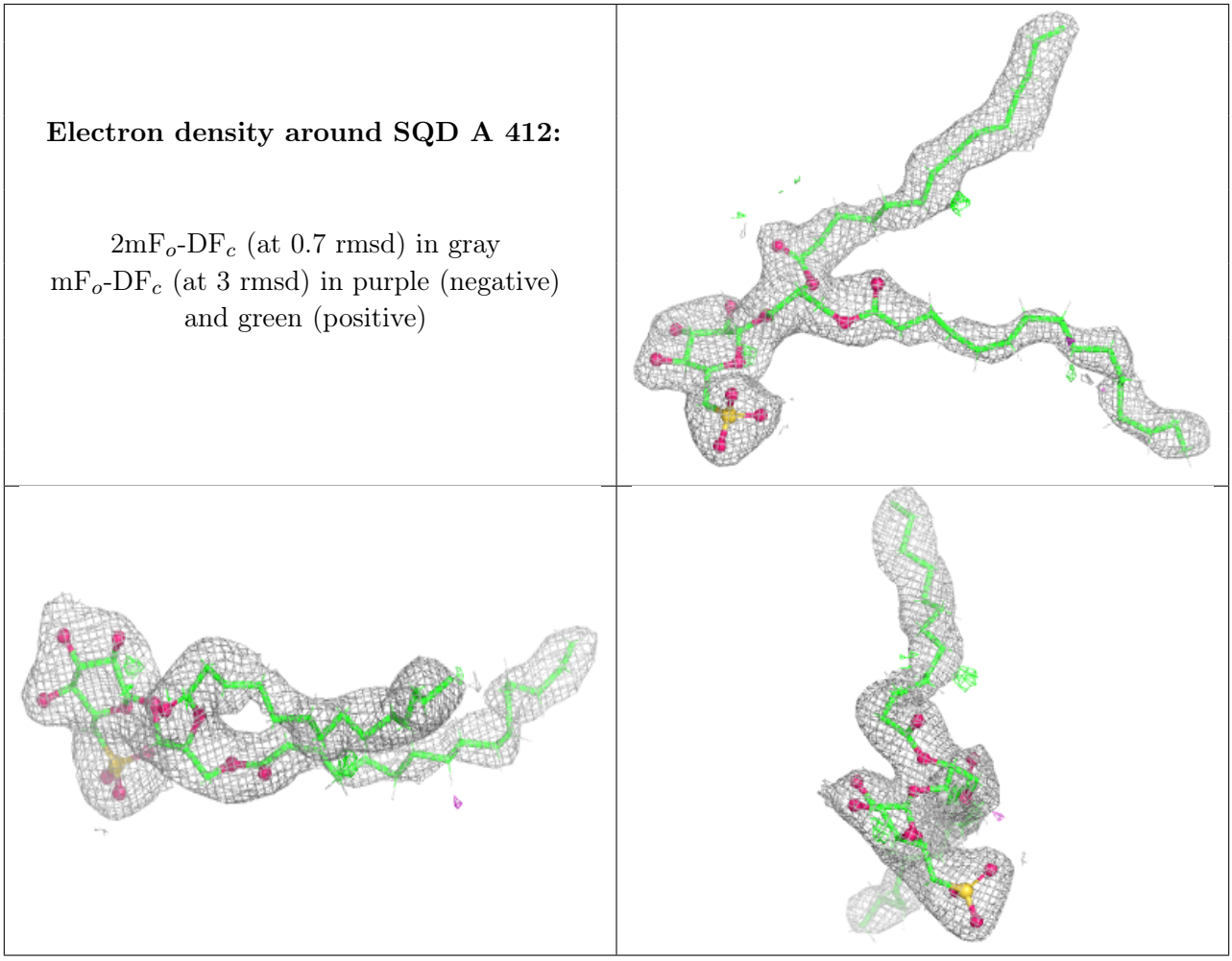






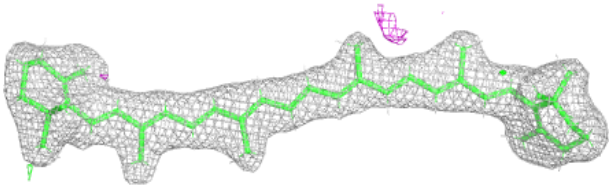
Electron density around SQD A 412:

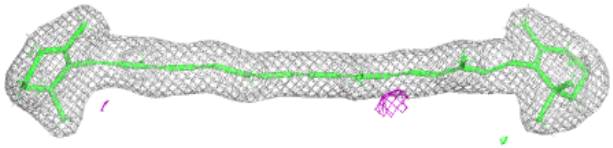
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

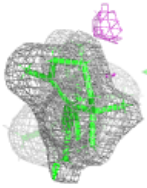


Electron density around BCR b 619:

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

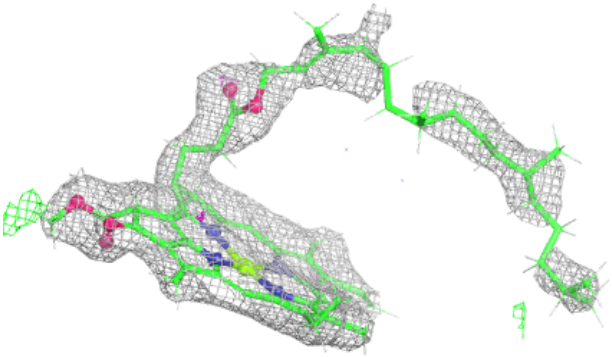


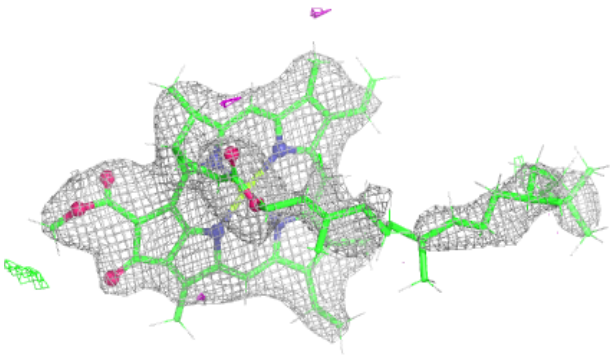


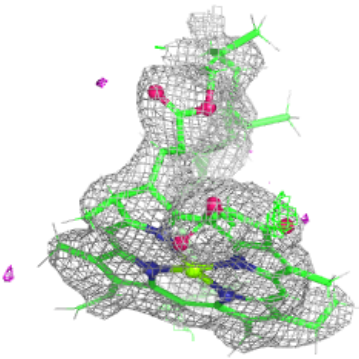


Electron density around CLA c 513:

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

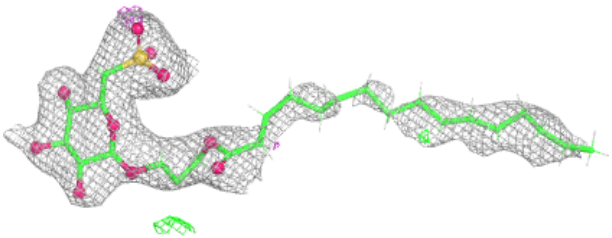


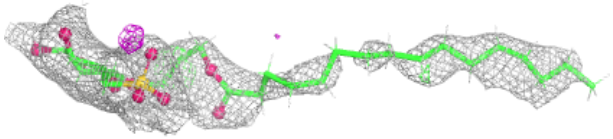


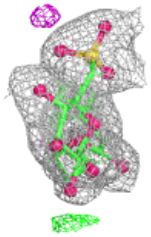


Electron density around SQD F 101:

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

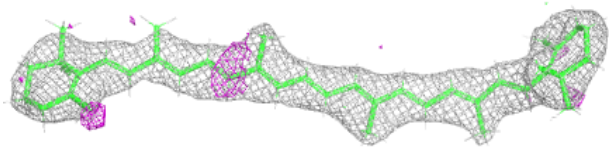


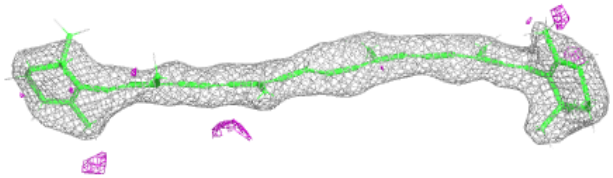


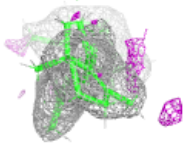


Electron density around BCR c 515:

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

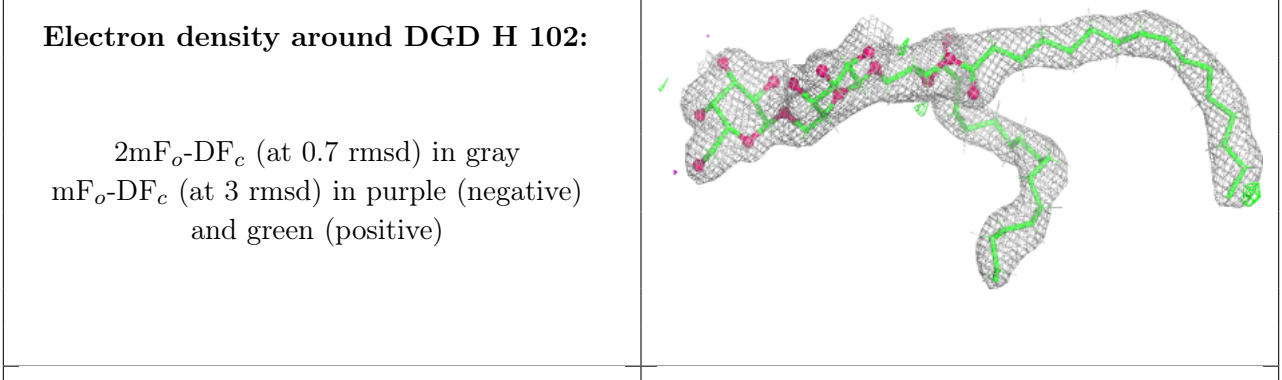






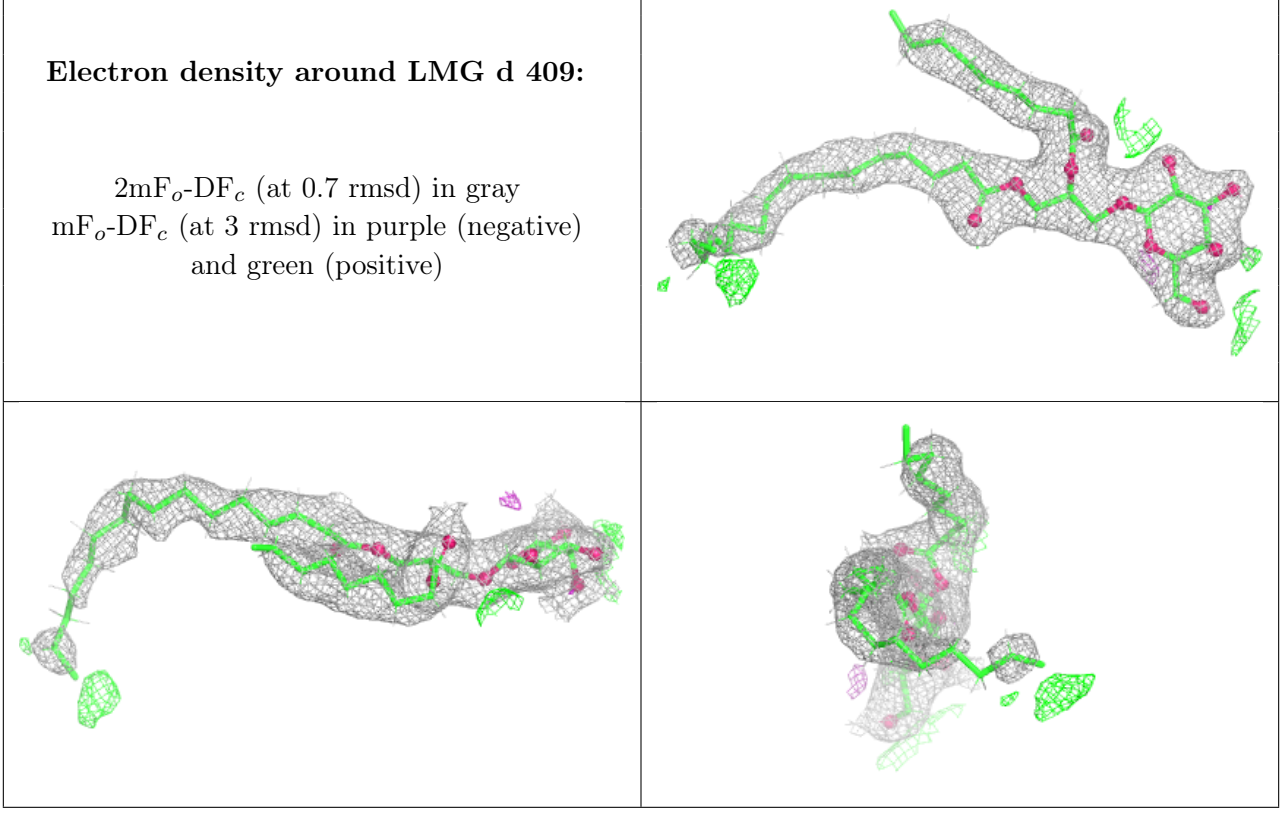
Electron density around DGD H 102:

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



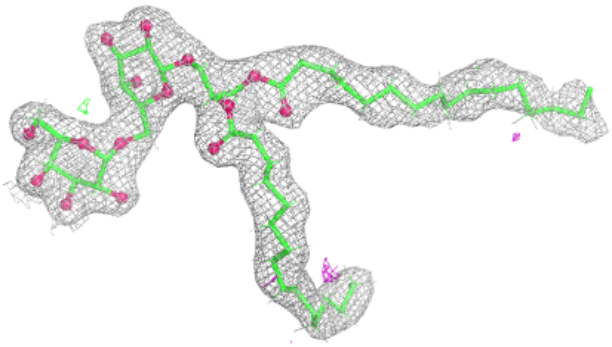
Electron density around LMG d 409:

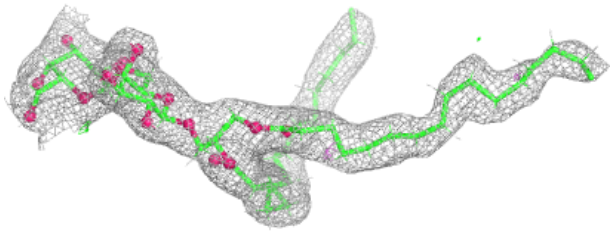
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

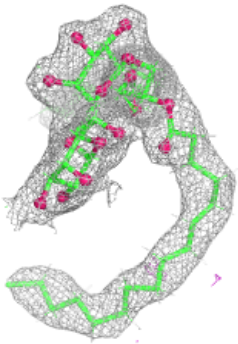


Electron density around DGD c 517:

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

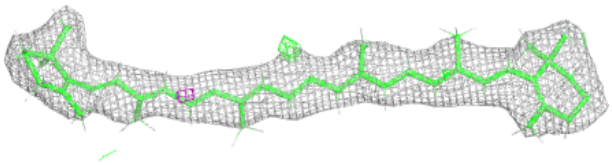


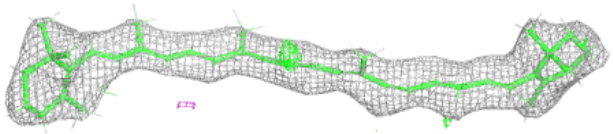


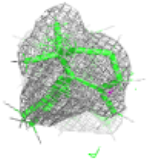


Electron density around BCR Z 101:

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

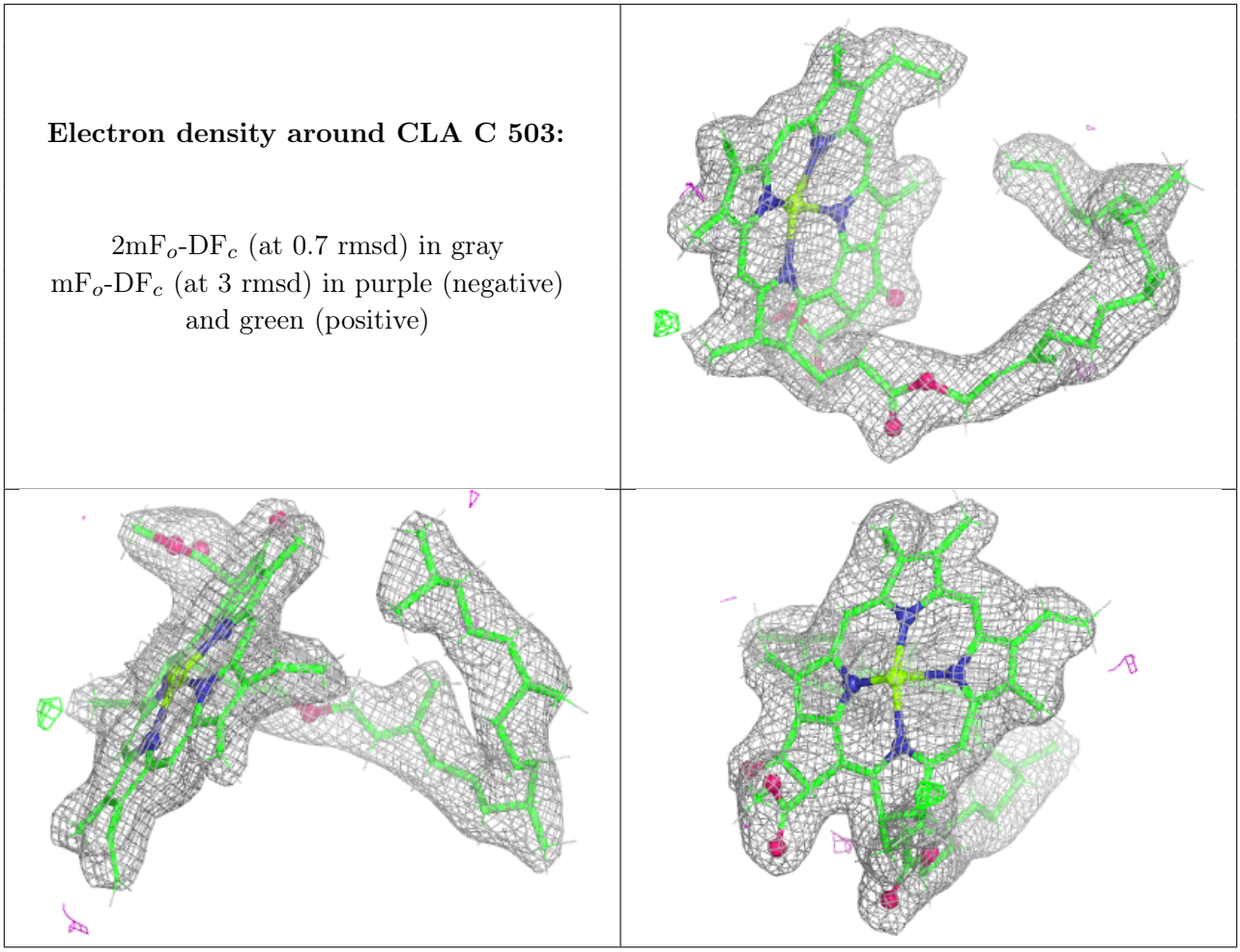






Electron density around CLA C 503:

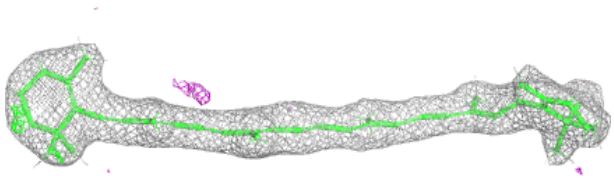
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

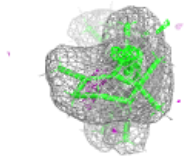


Electron density around BCR b 618:

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

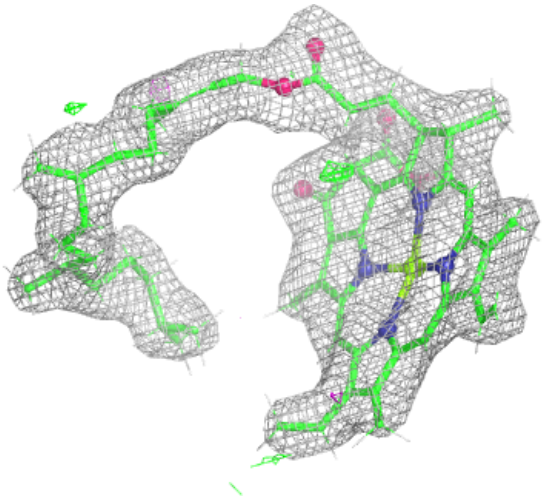


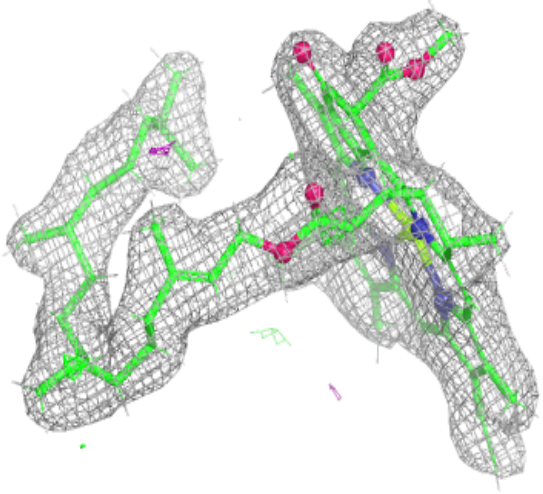


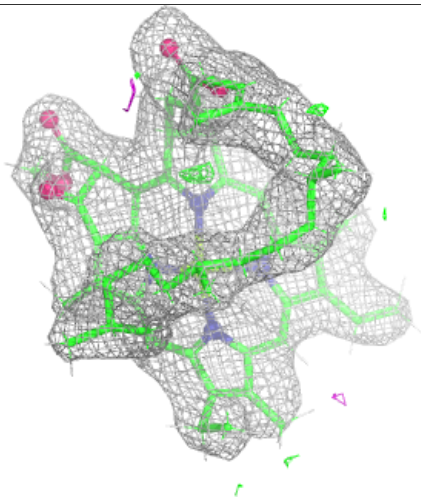


Electron density around CLA c 503:

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

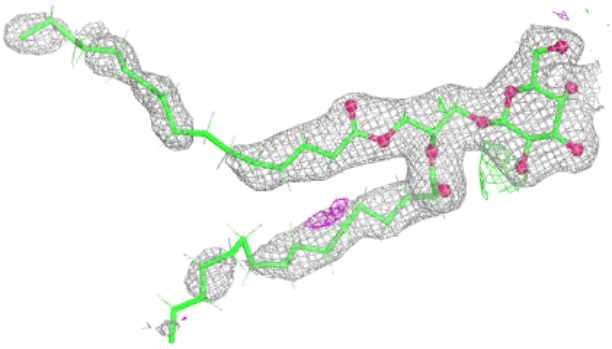


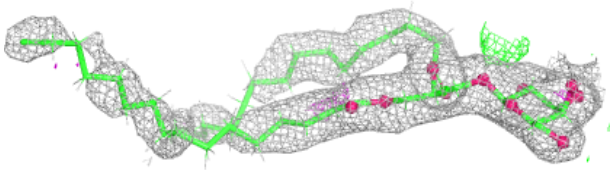


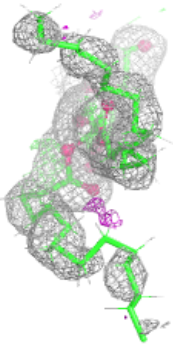


Electron density around LMG D 406:

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

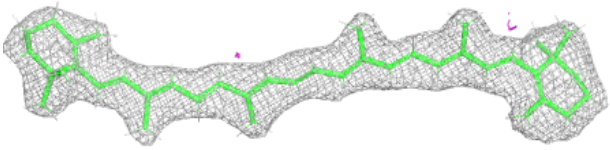


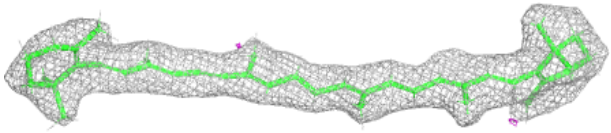


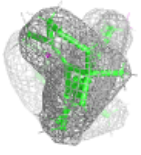


Electron density around BCR b 620:

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

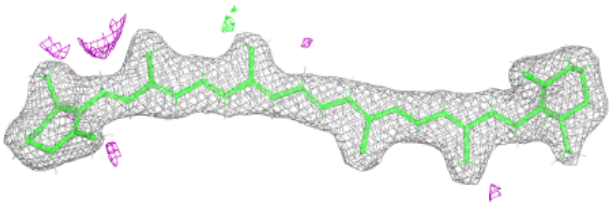


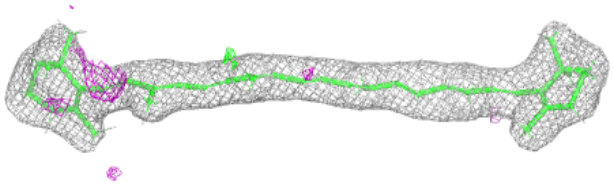


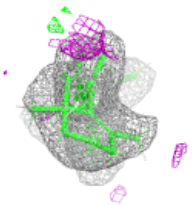


Electron density around BCR B 618:

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

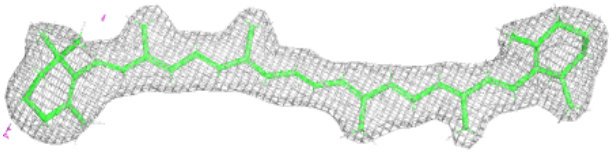


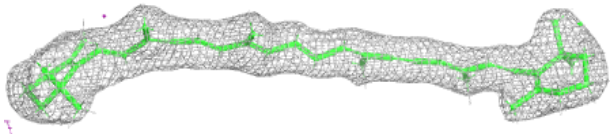


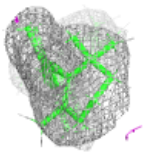


Electron density around BCR B 619:

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

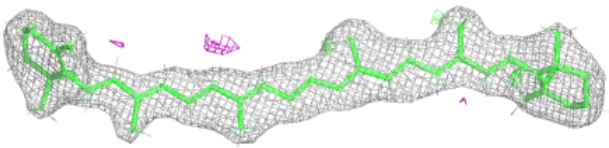


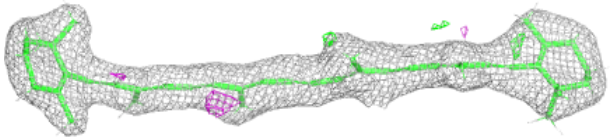


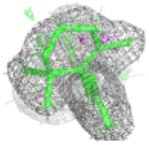


Electron density around BCR C 514:

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

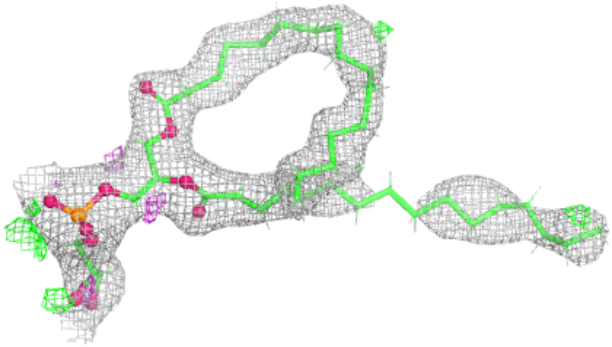


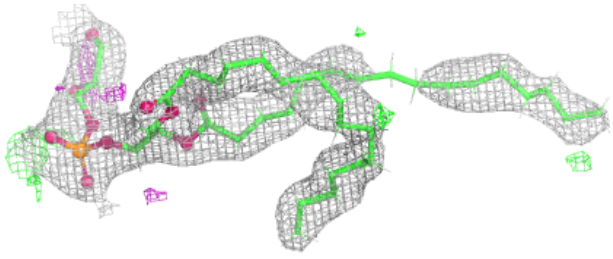


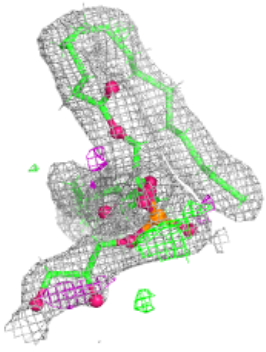


Electron density around LHG d 406:

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

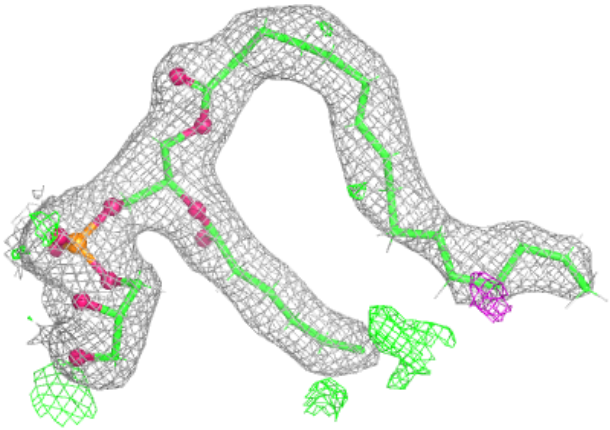


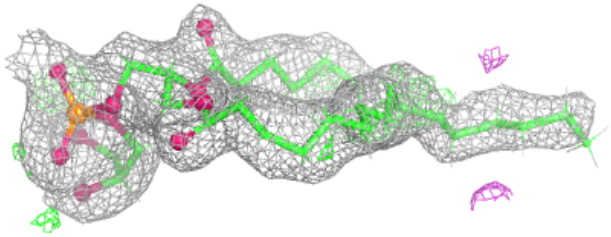


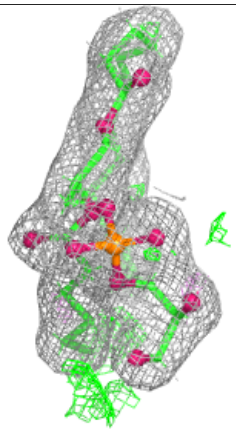


Electron density around LHG d 408:

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

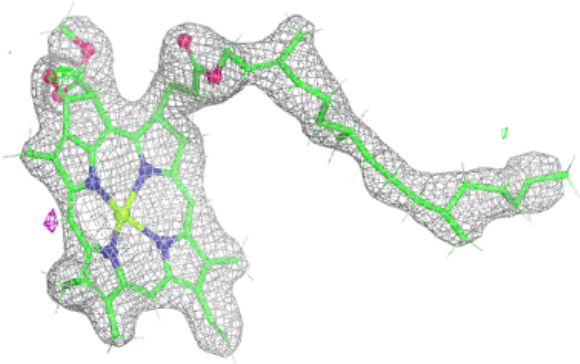


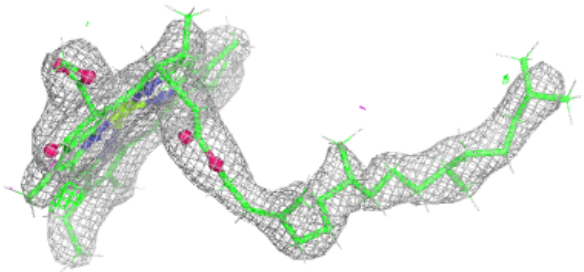


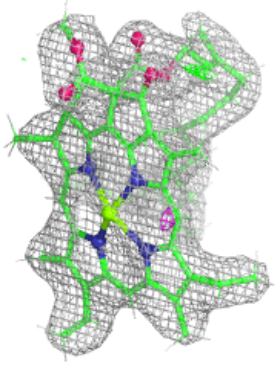


Electron density around CLA c 511:

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

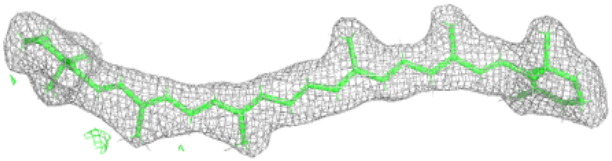


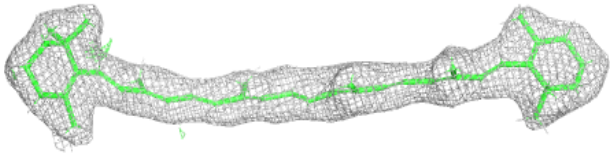


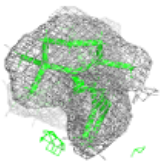


Electron density around BCR H 101:

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

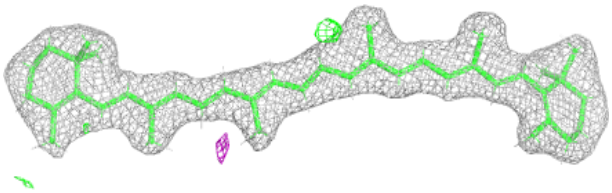


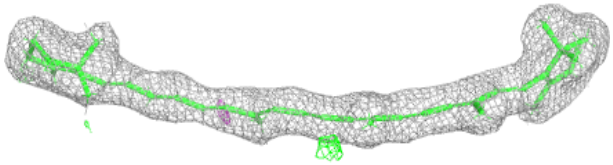


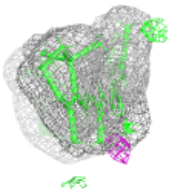


Electron density around BCR t 101:

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

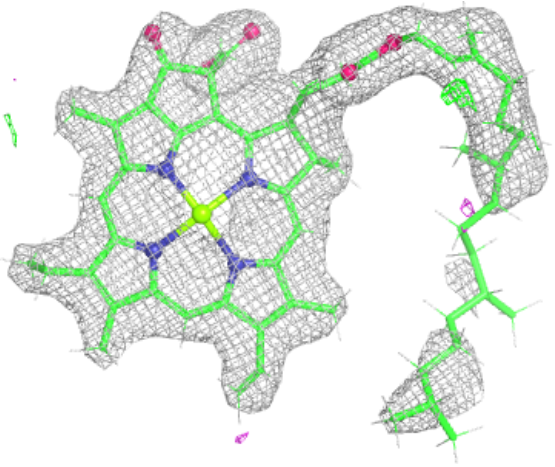


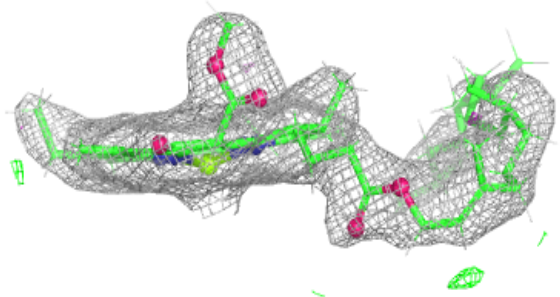


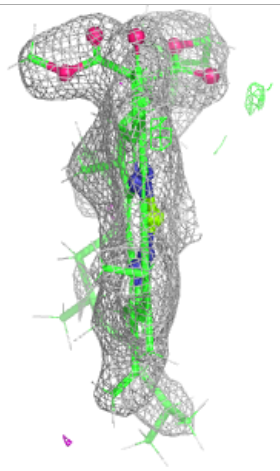


Electron density around CLA C 512:

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

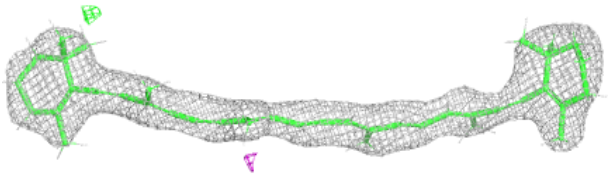


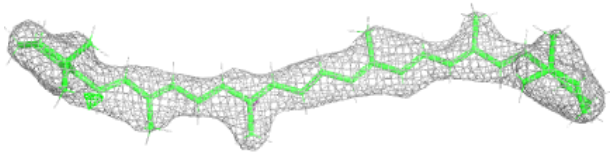


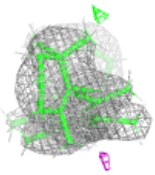


Electron density around BCR K 102:

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

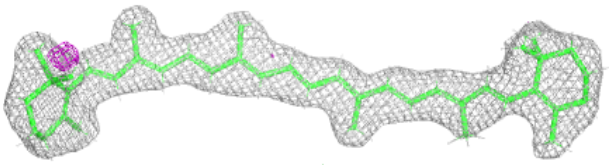


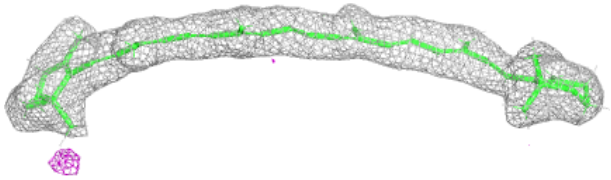


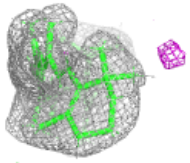


Electron density around BCR T 101:

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

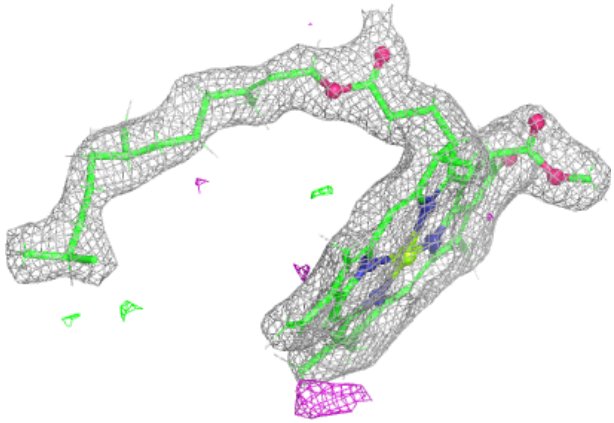


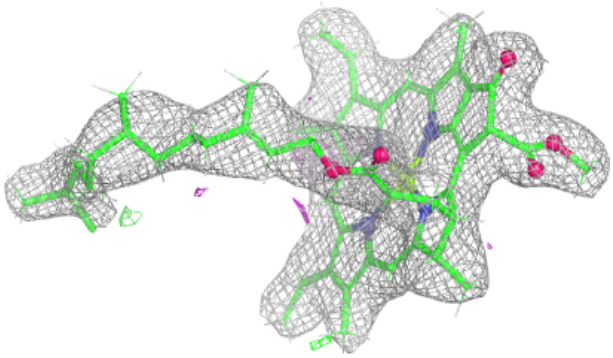


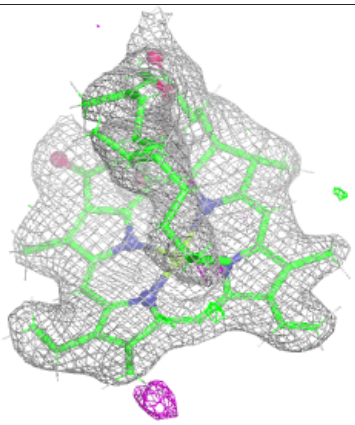


Electron density around CLA c 504:

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

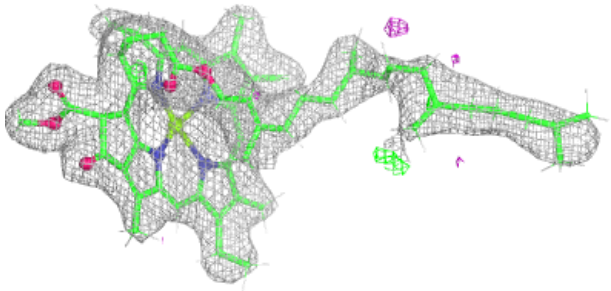


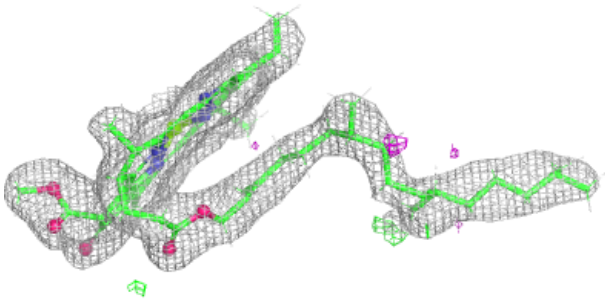


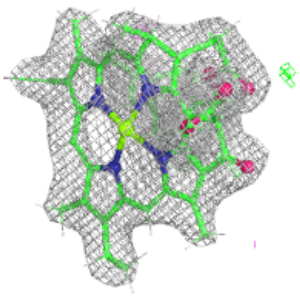


Electron density around CLA c 505:

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

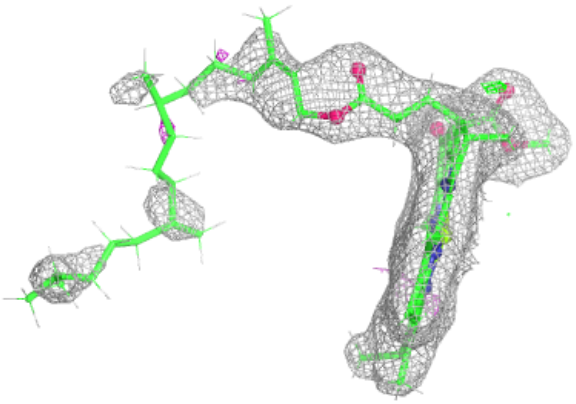


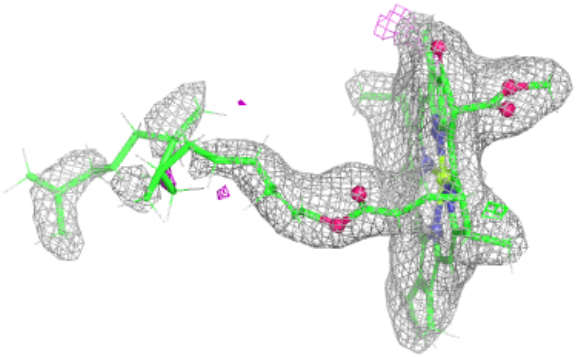


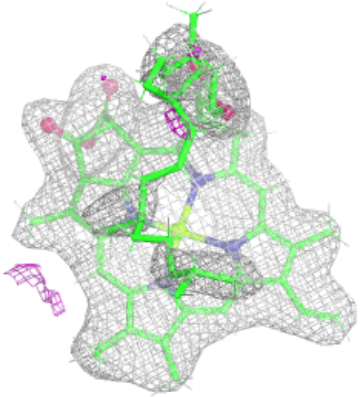


Electron density around CLA c 506:

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

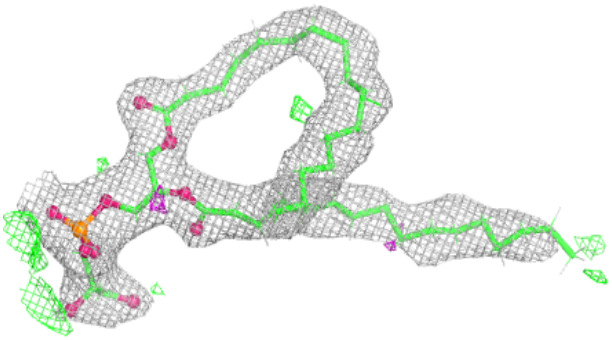


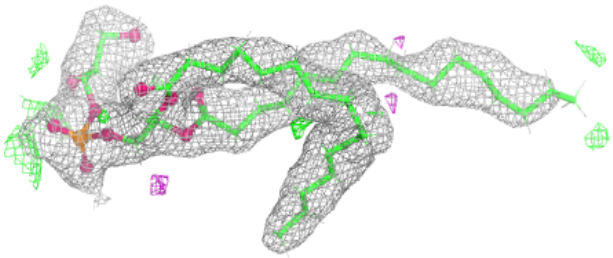


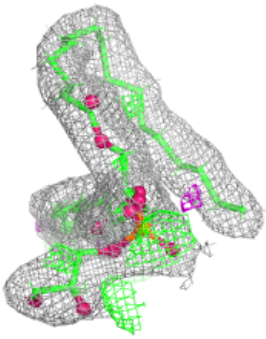


Electron density around LHG B 623:

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

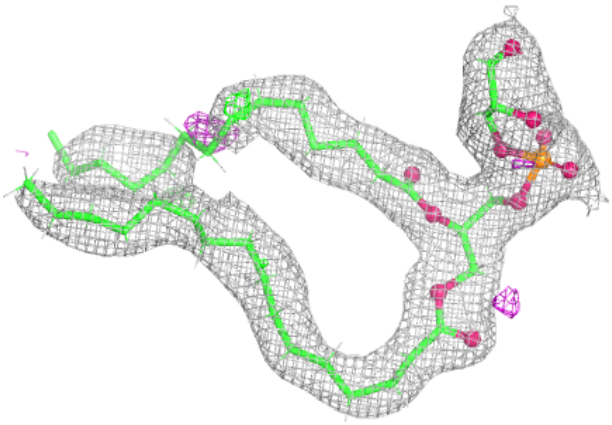


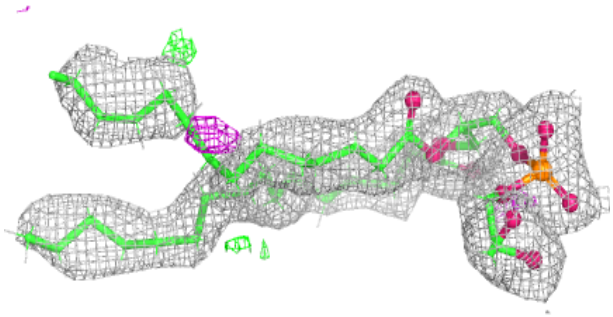


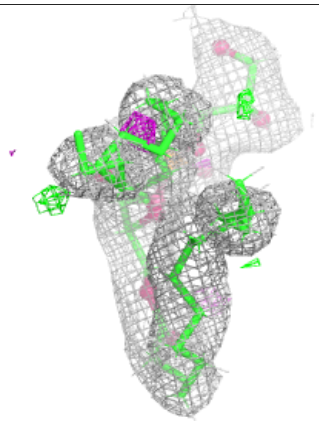


Electron density around LHG D 408:

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

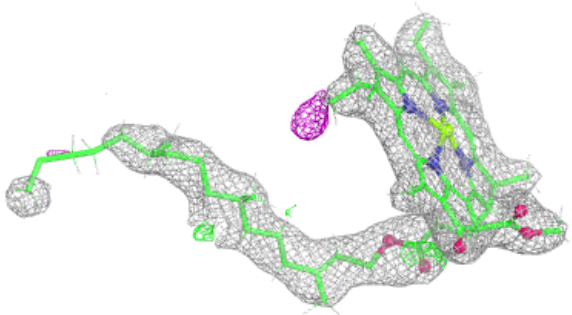


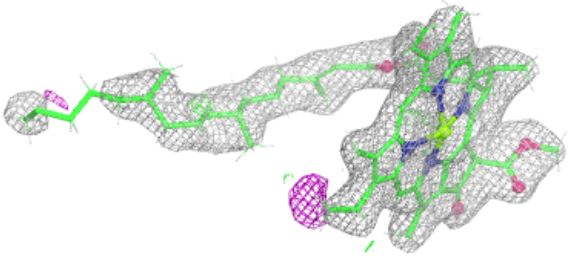


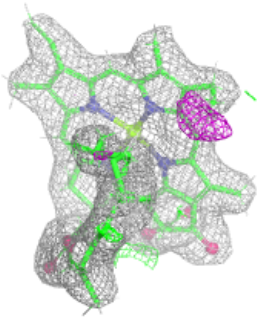


Electron density around CLA c 508:

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

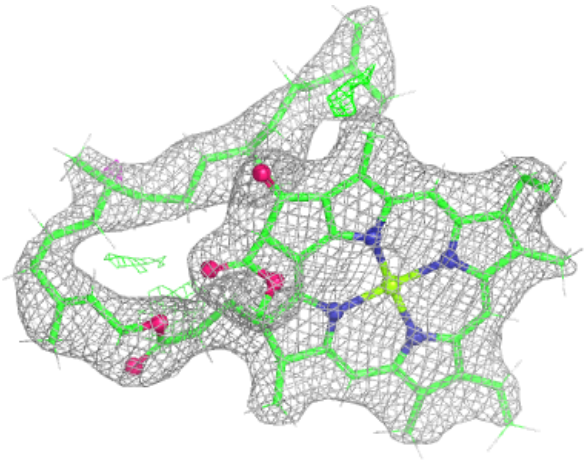


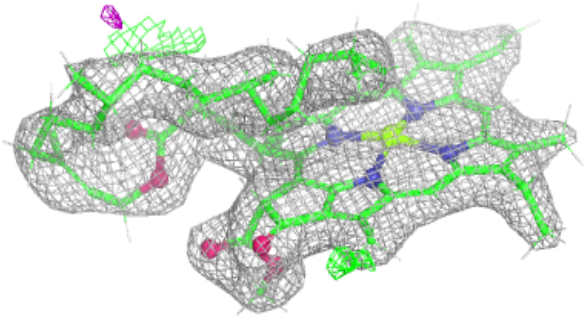


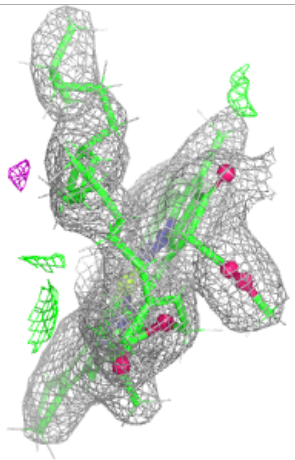


Electron density around CLA c 509:

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

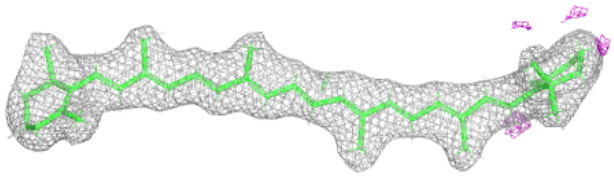


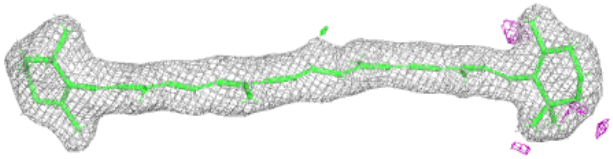


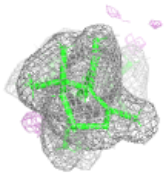


Electron density around BCR a 409:

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

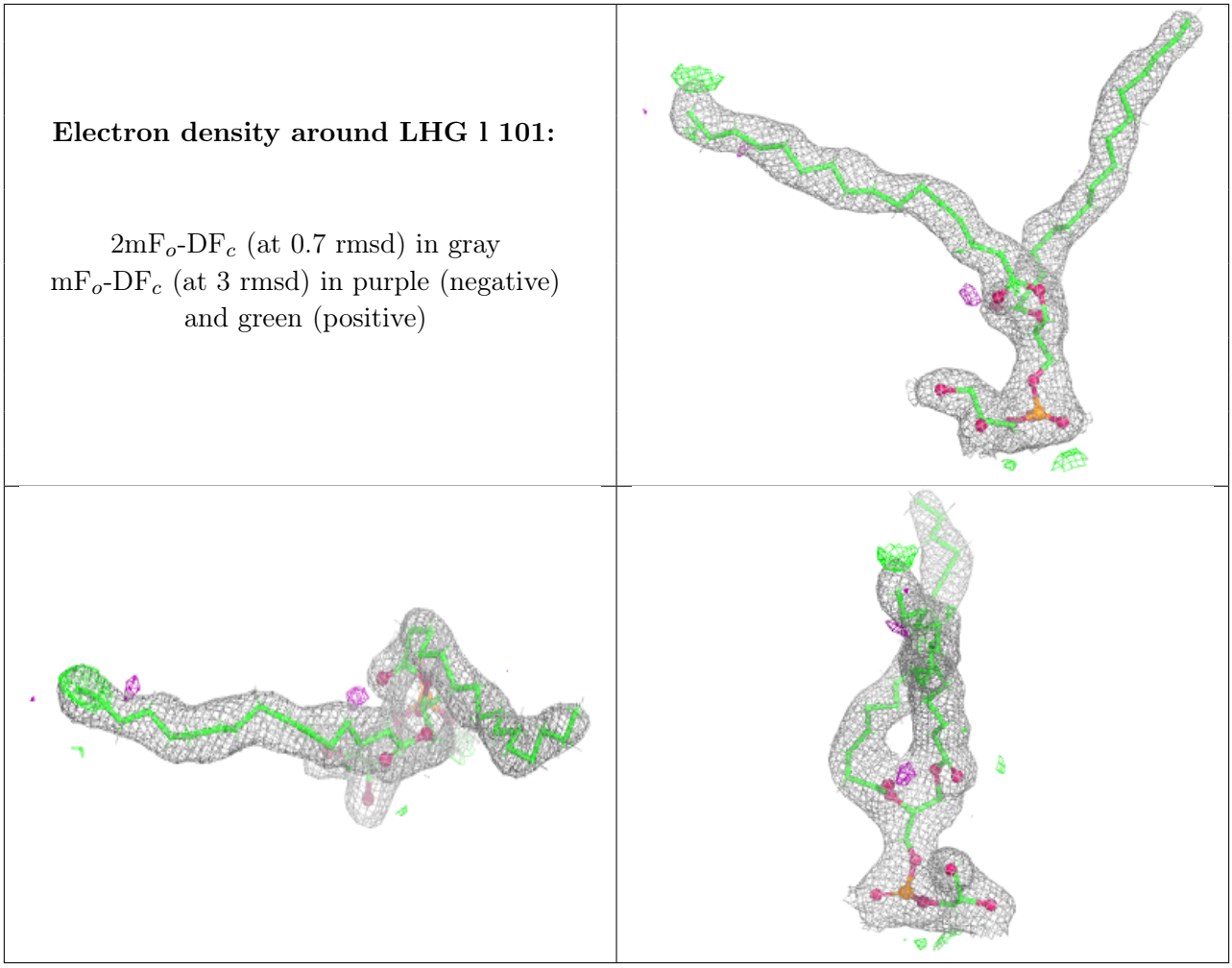






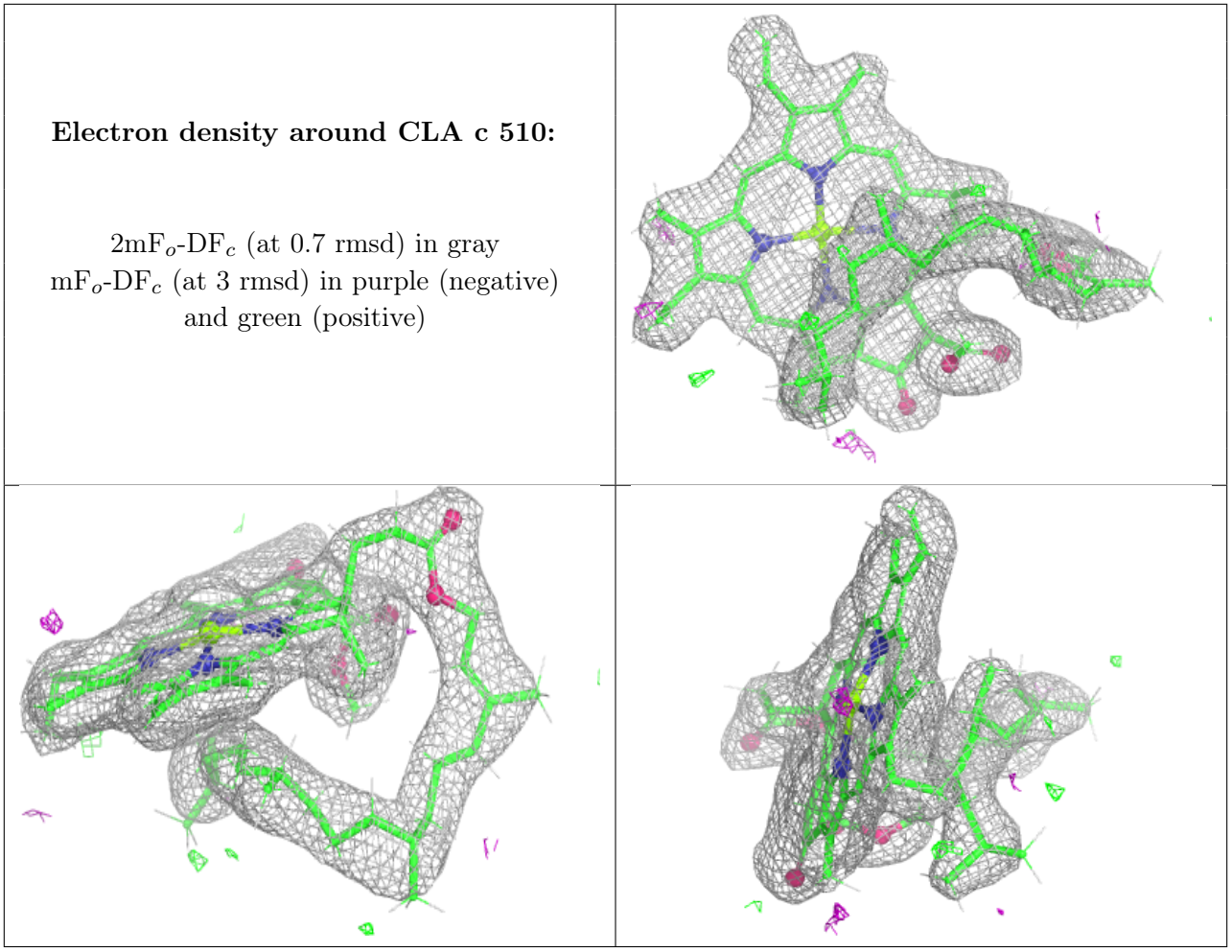
Electron density around LHG l 101:

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



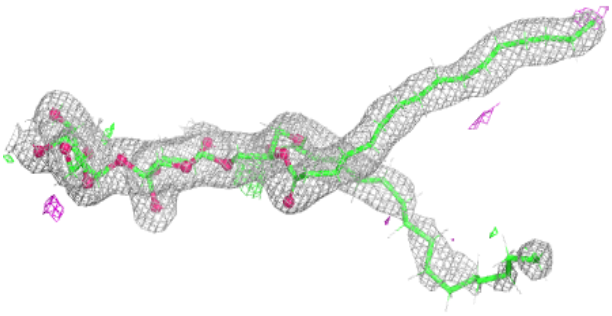
Electron density around CLA c 510:

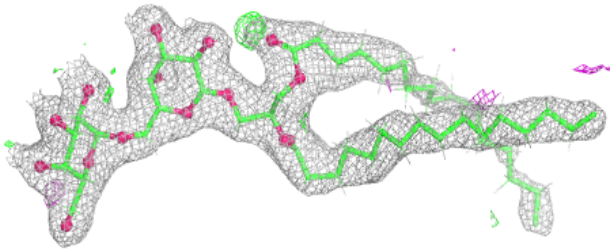
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

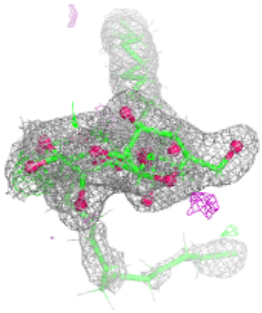


Electron density around DGD C 515:

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

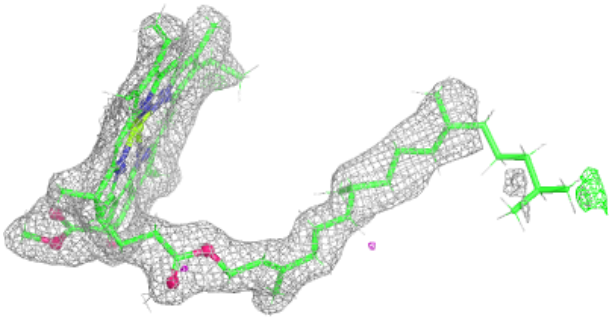


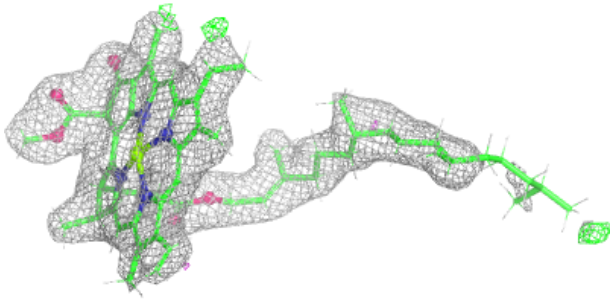


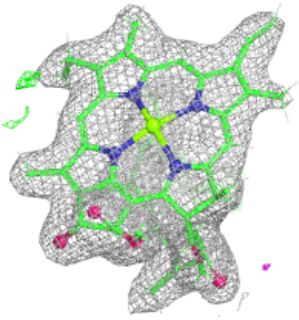


Electron density around CLA C 508:

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

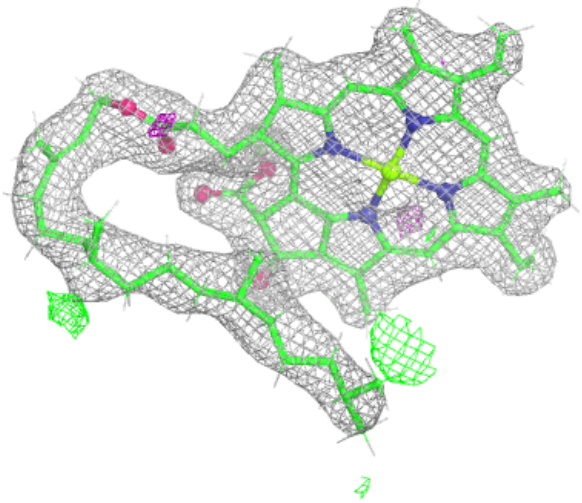


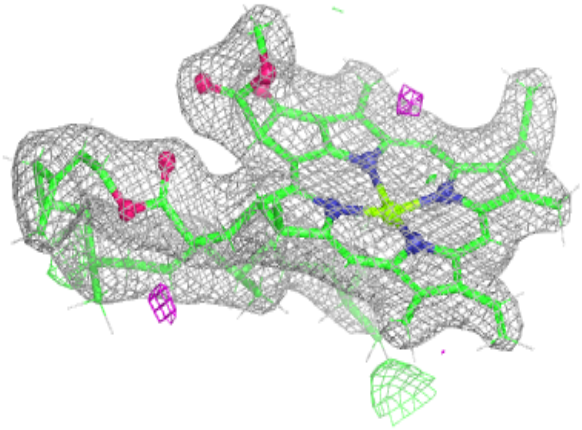


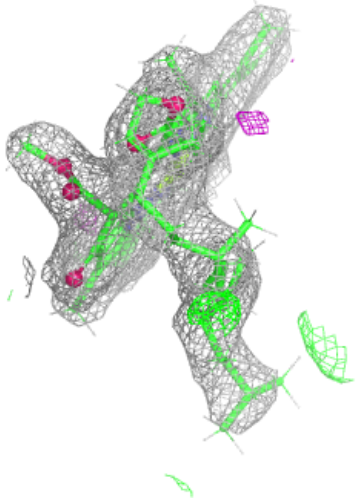


Electron density around CLA C 509:

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

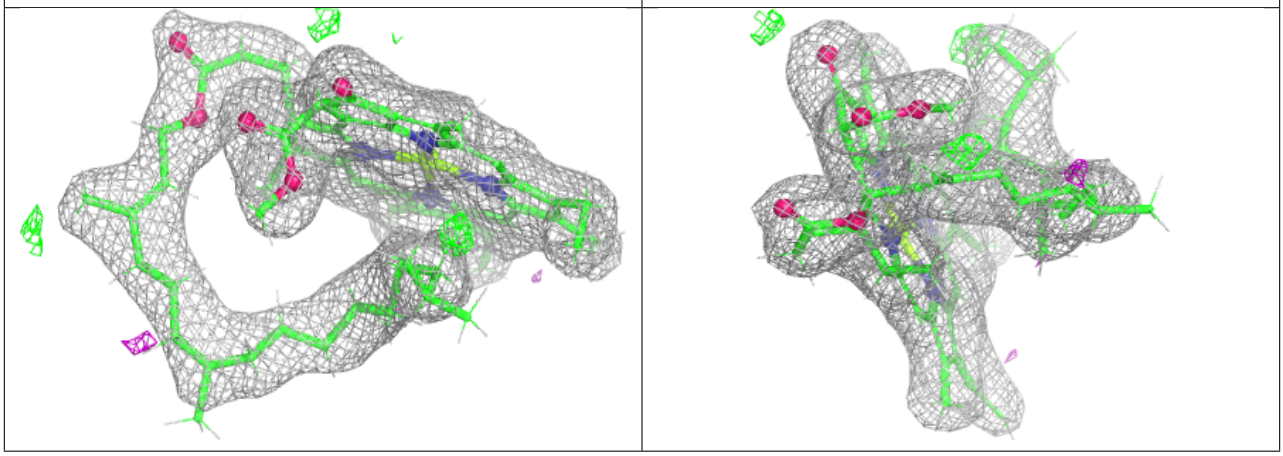






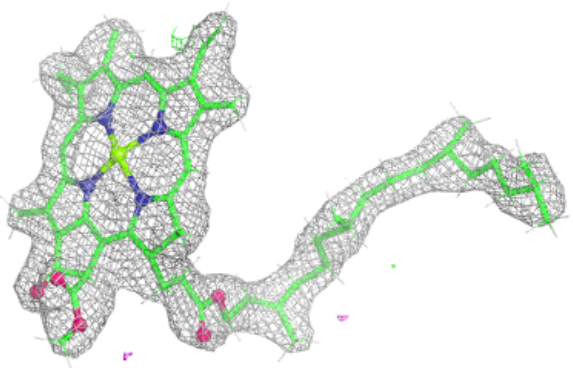
Electron density around CLA C 510:

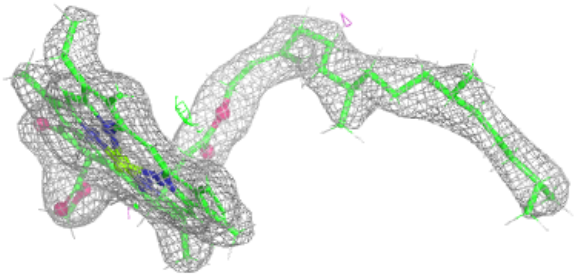
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

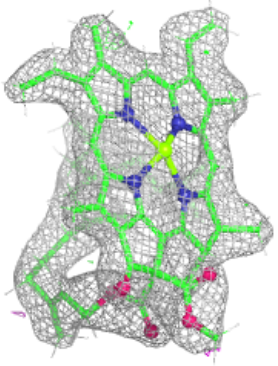


Electron density around CLA C 511:

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

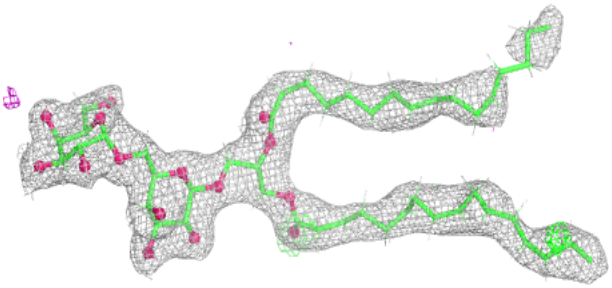


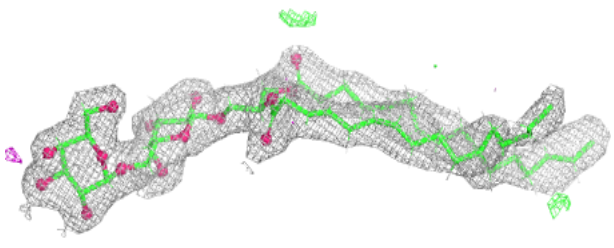


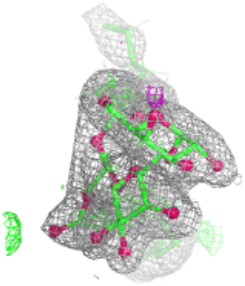


Electron density around DGD c 518:

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

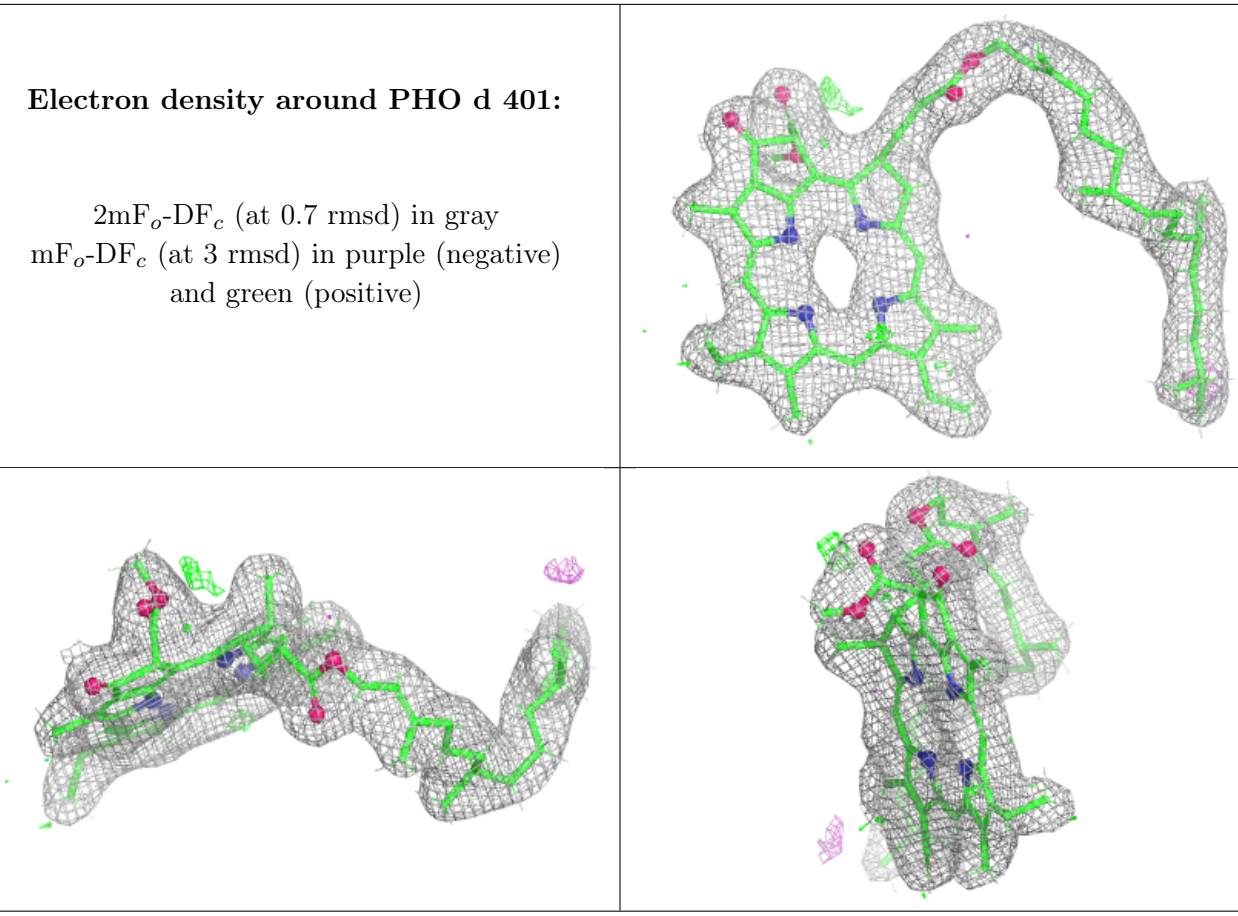






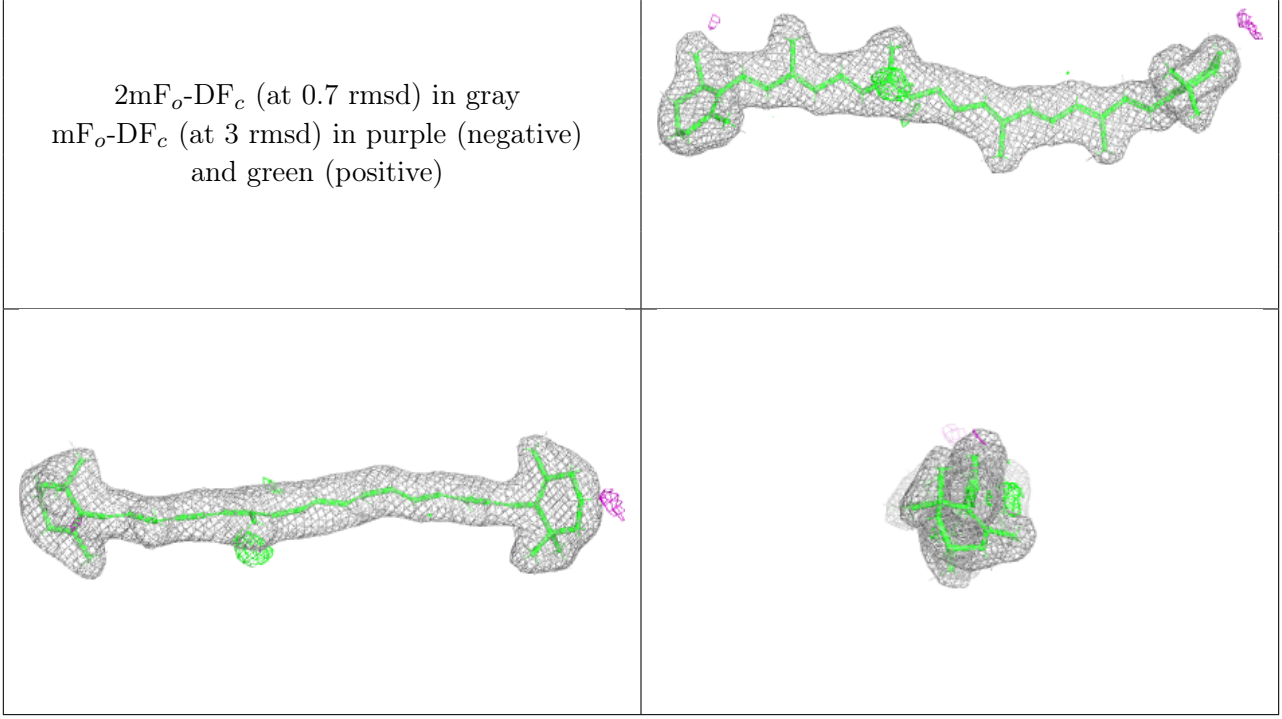
Electron density around PHO d 401:

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



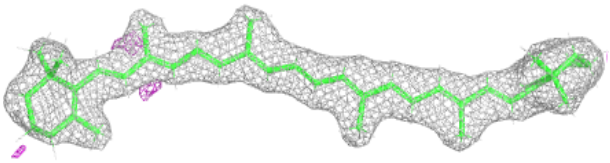
Electron density around BCR A 409:

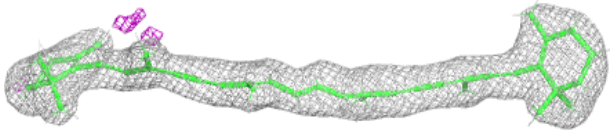
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

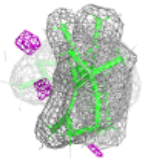


Electron density around BCR B 617:

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

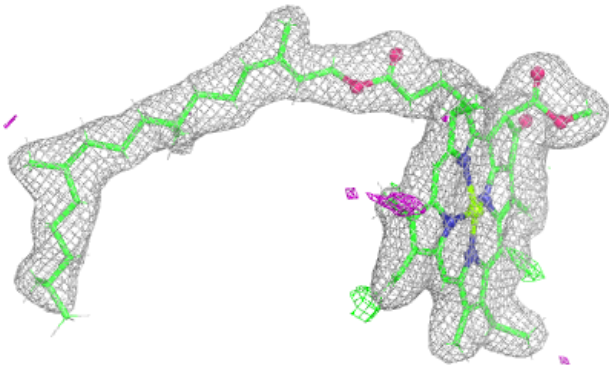


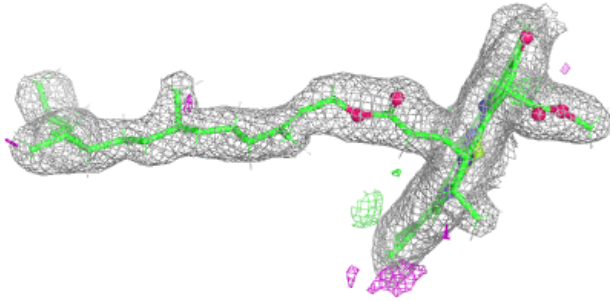


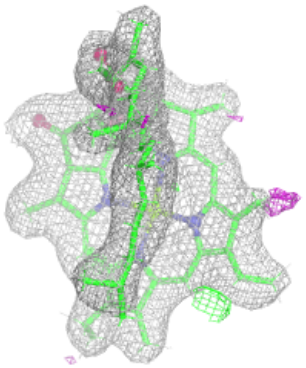


Electron density around CLA B 609:

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

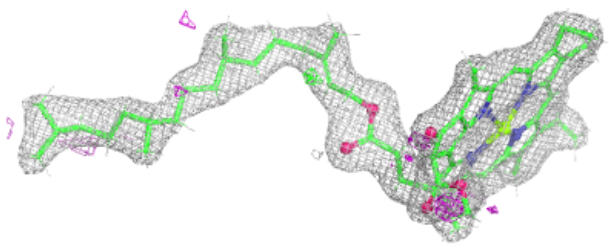


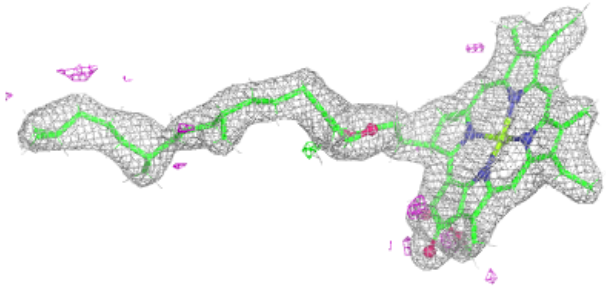


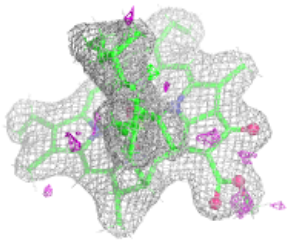


Electron density around CLA C 502:

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

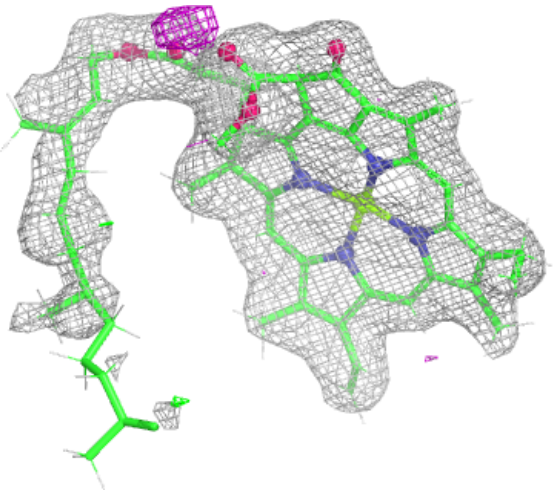


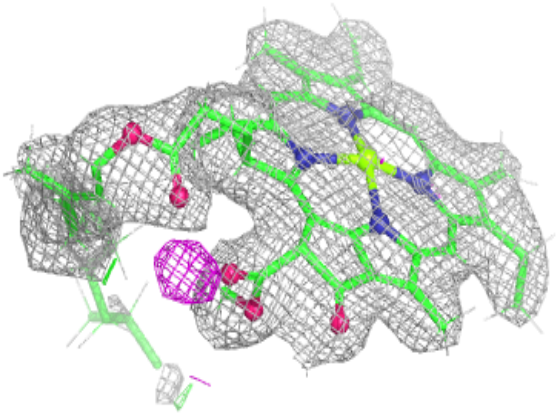


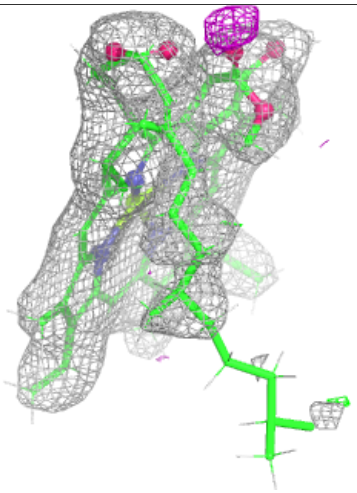


Electron density around CLA b 617:

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

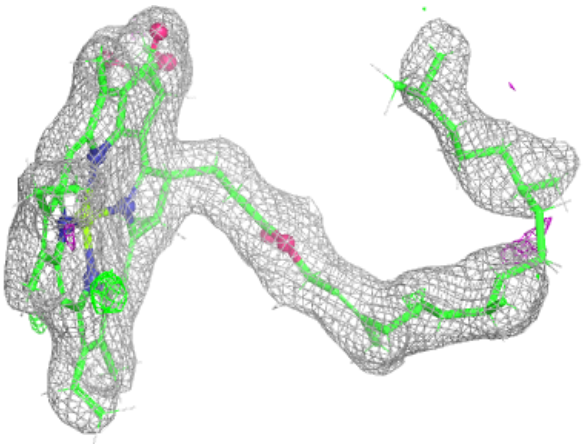


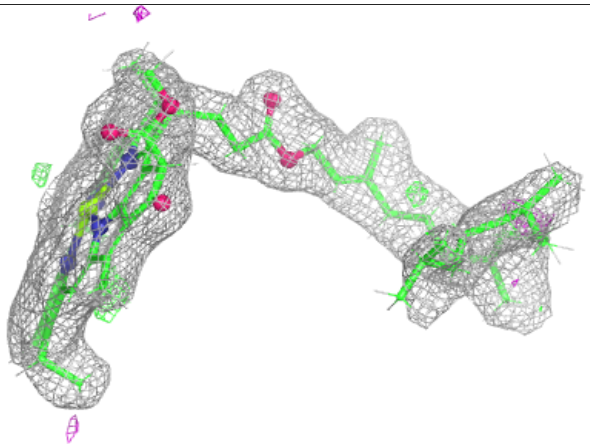


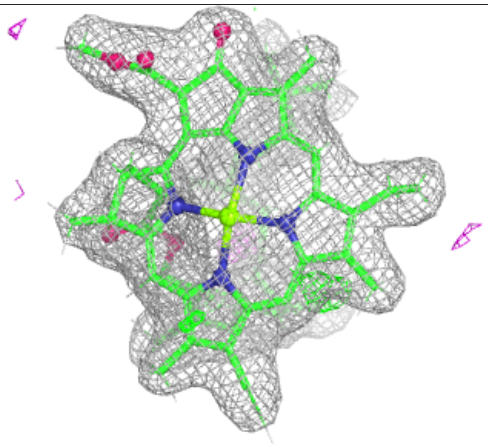


Electron density around CLA B 606:

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

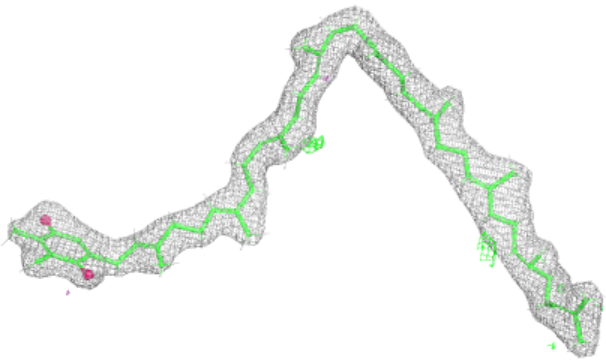


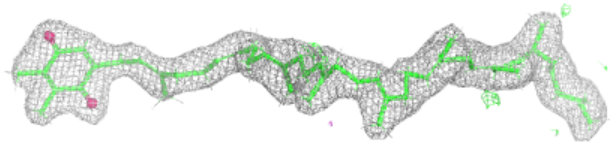




Electron density around PL9 d 405:

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

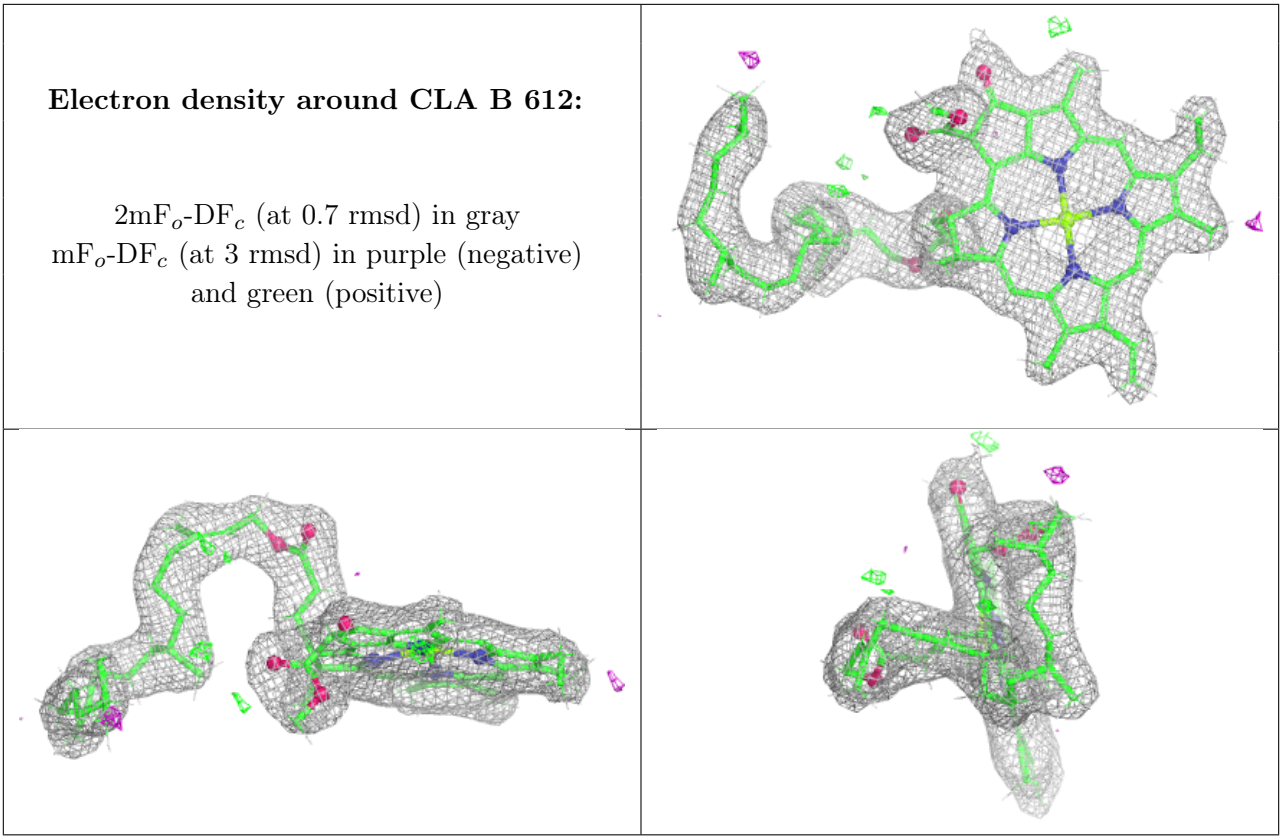






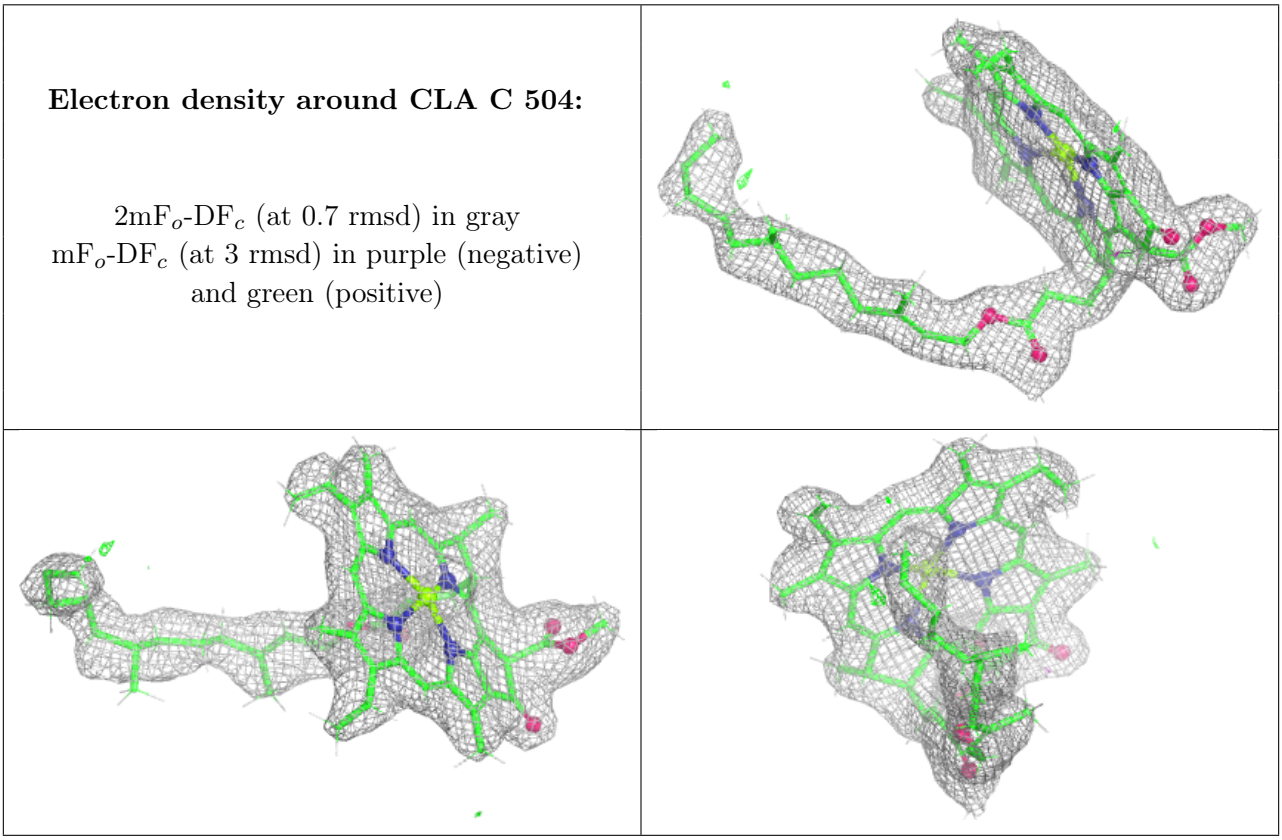
Electron density around CLA B 612:

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



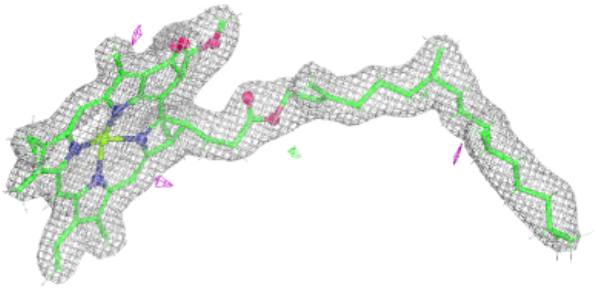
Electron density around CLA C 504:

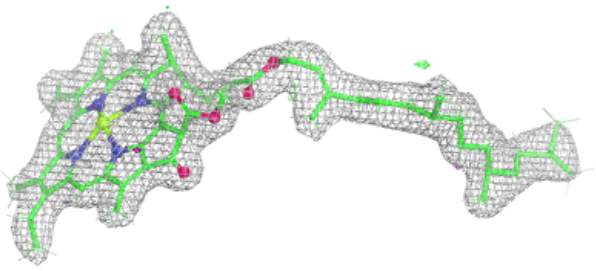
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

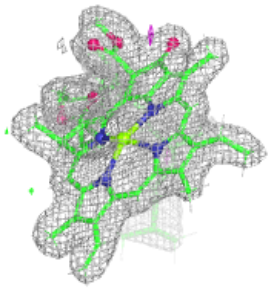


Electron density around CLA a 405:

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

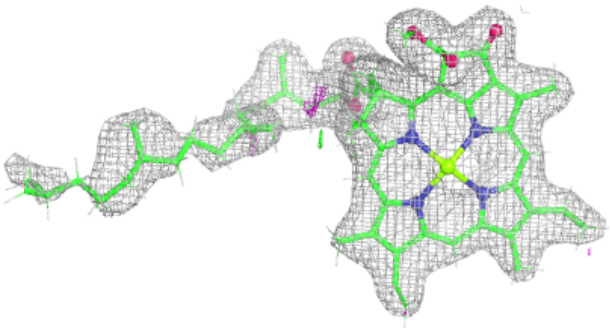


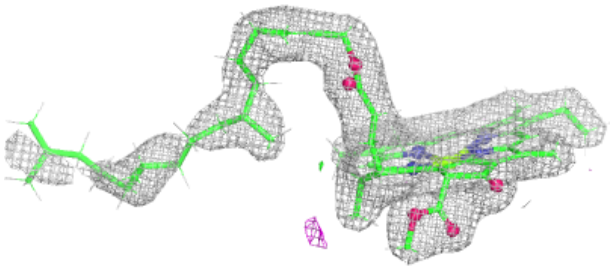


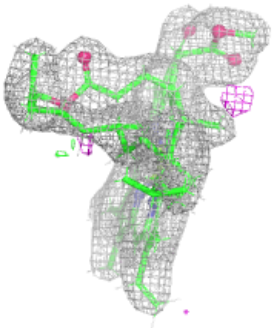


Electron density around CLA a 406:

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

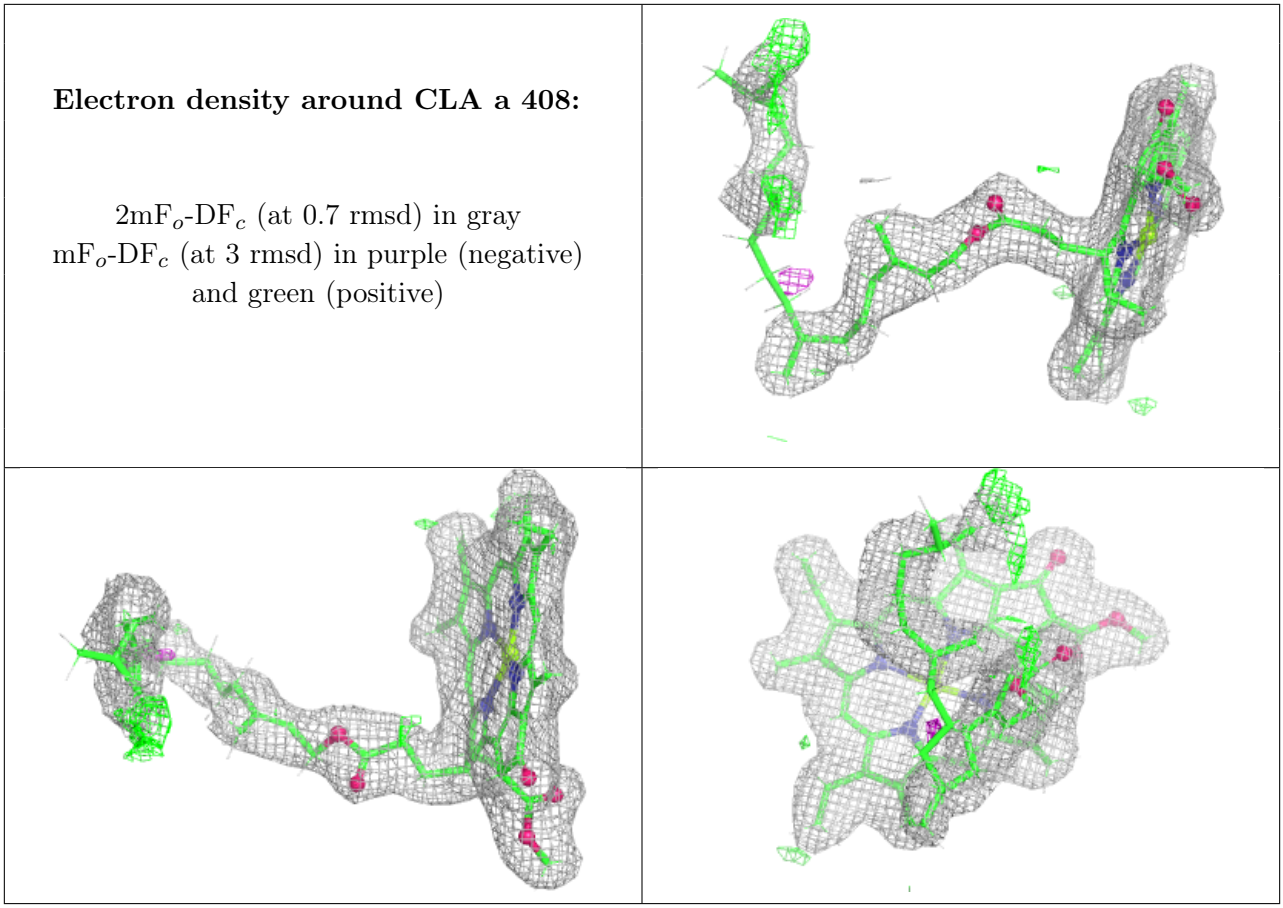






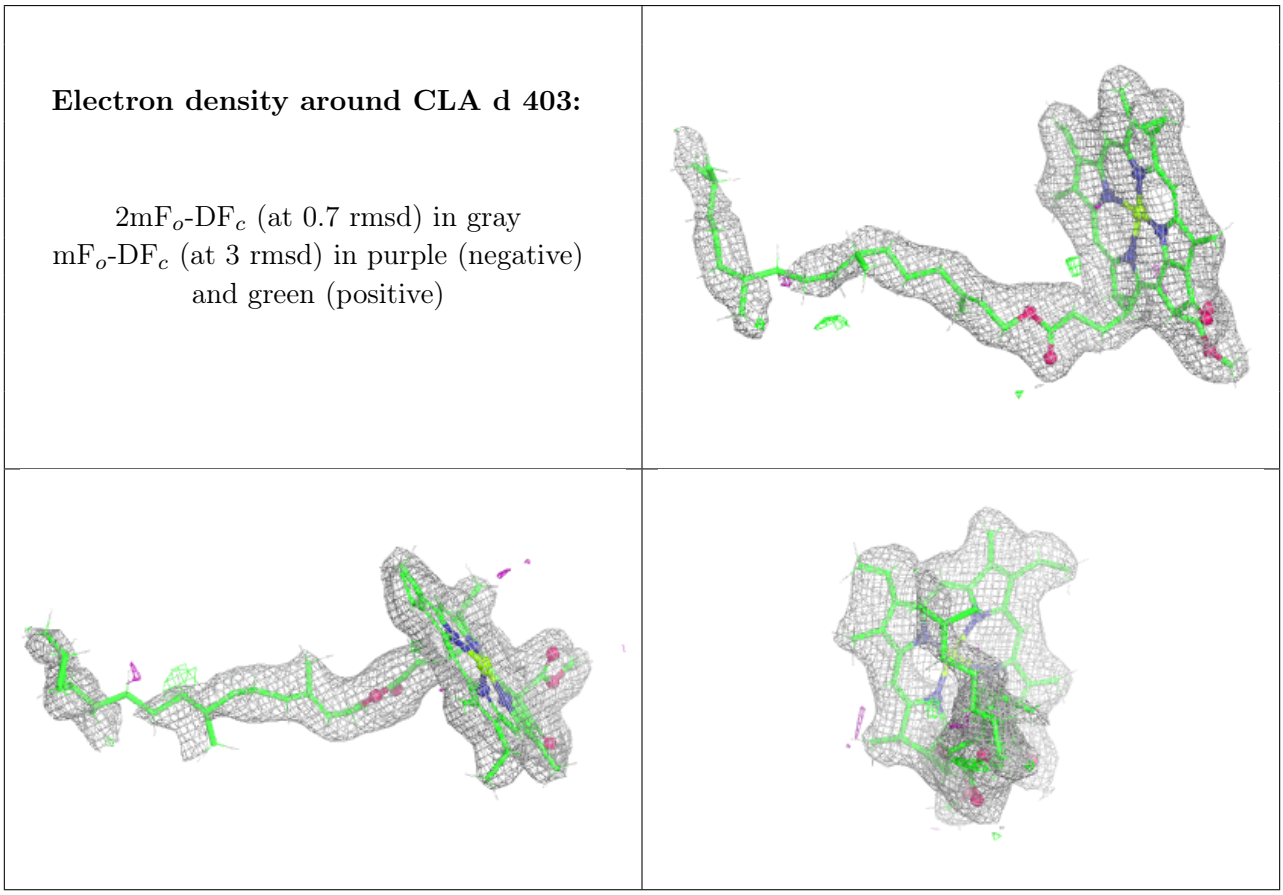
Electron density around CLA a 408:

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



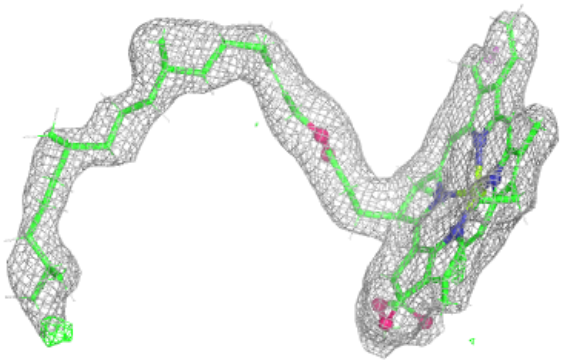
Electron density around CLA d 403:

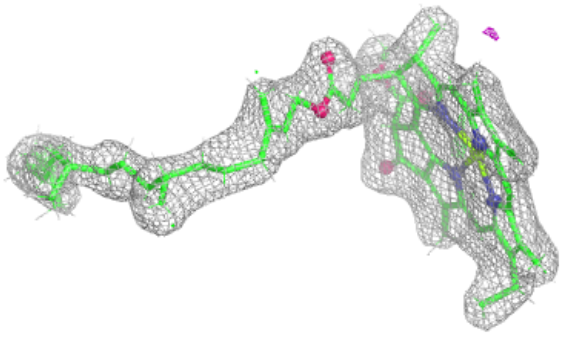
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

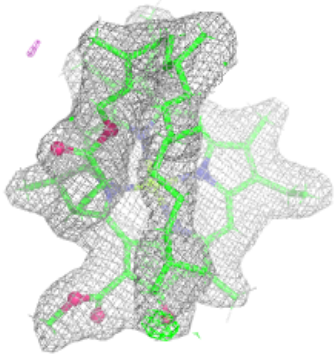


Electron density around CLA b 607:

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

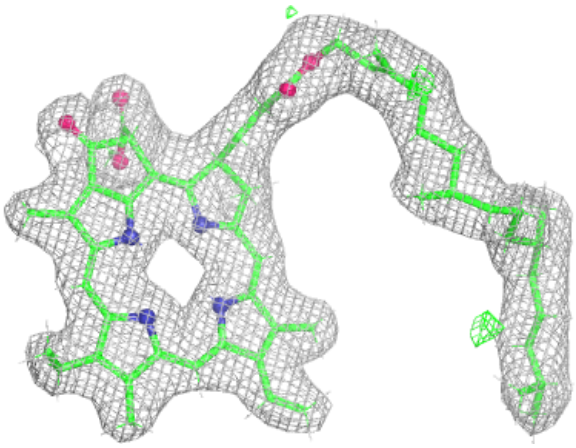


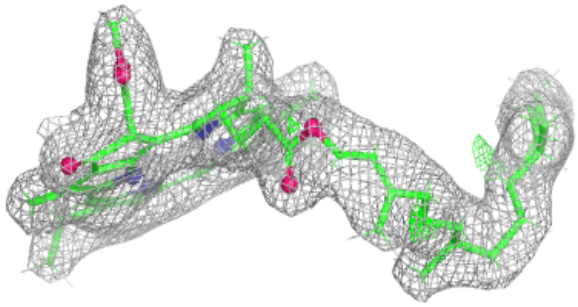


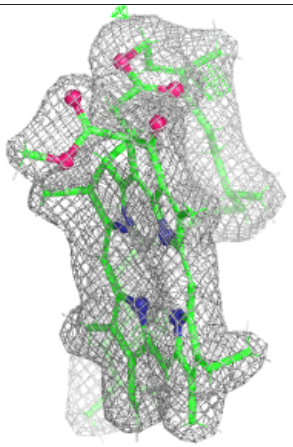


Electron density around PHO A 407:

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

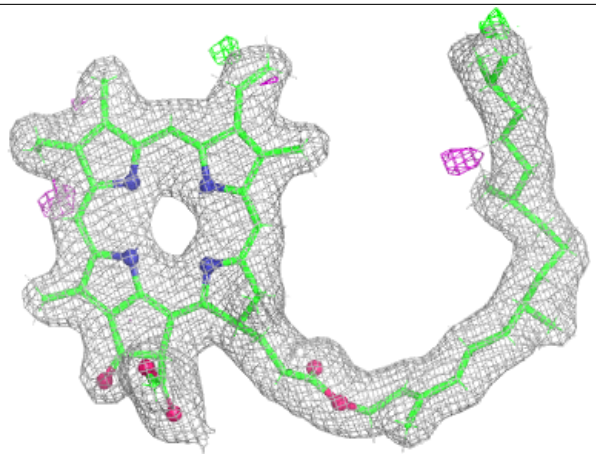


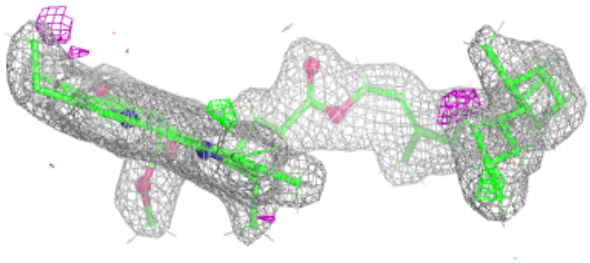


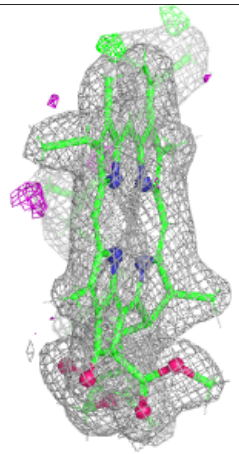


Electron density around PHO a 407:

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

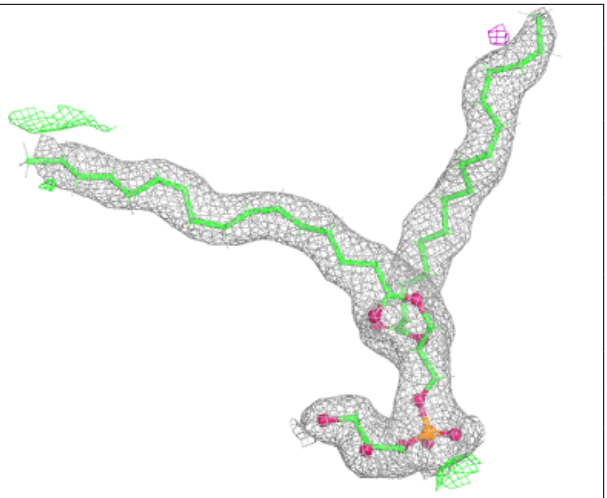


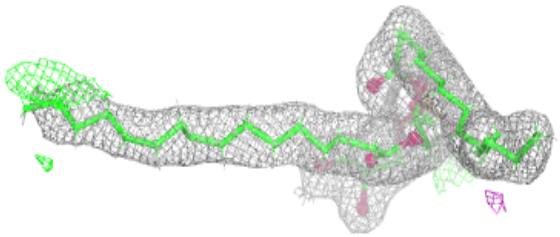


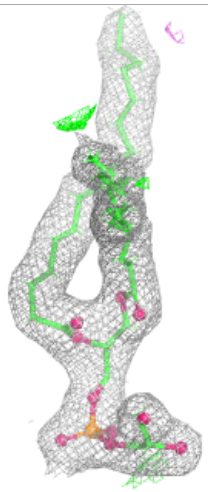


Electron density around LHG B 622:

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

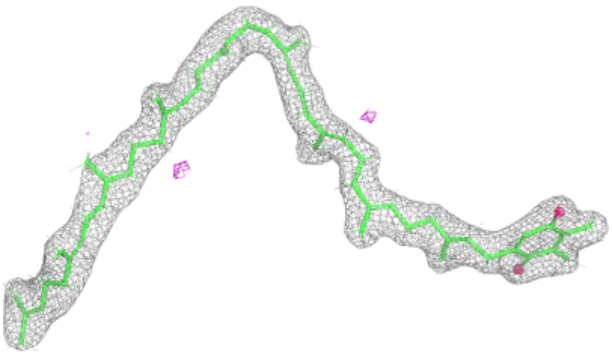


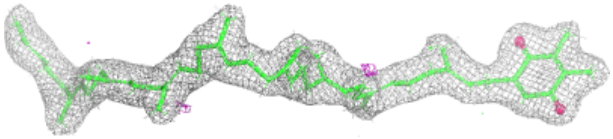


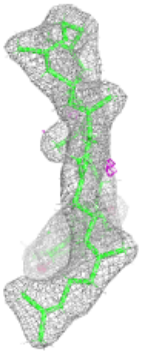


Electron density around PL9 D 405:

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

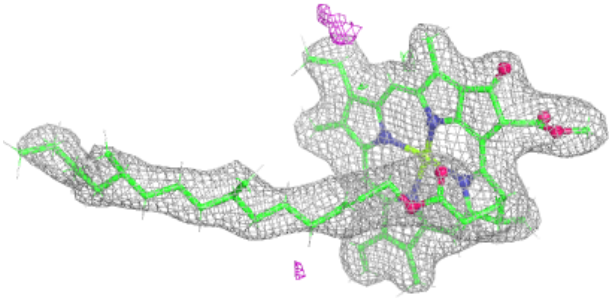


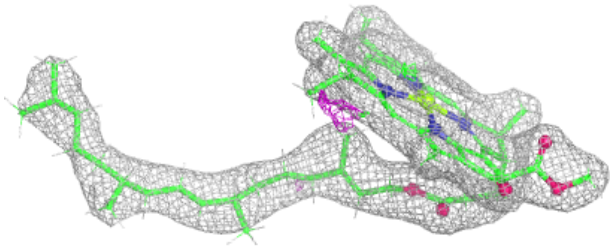


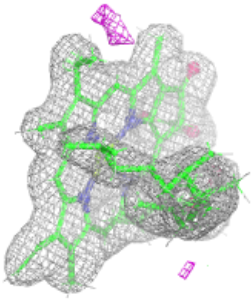


Electron density around CLA b 609:

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

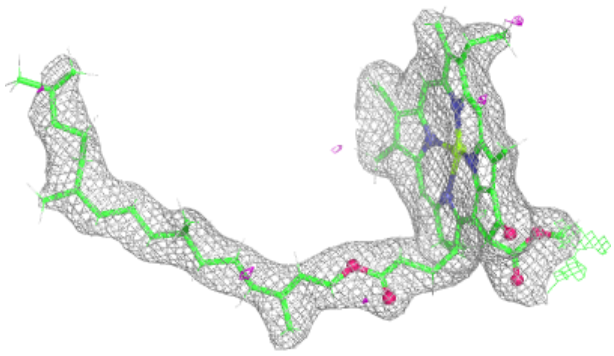


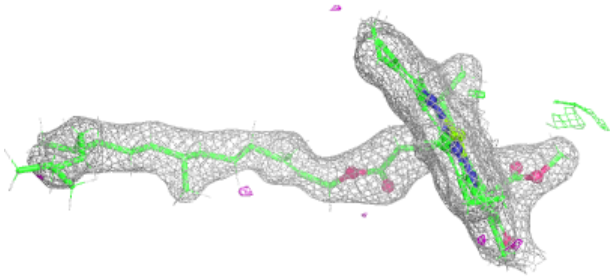


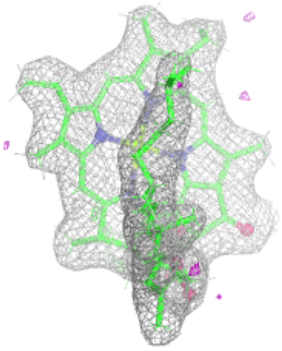


Electron density around CLA b 610:

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

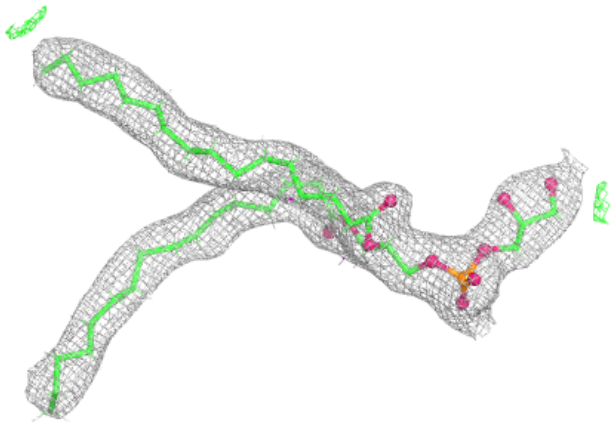


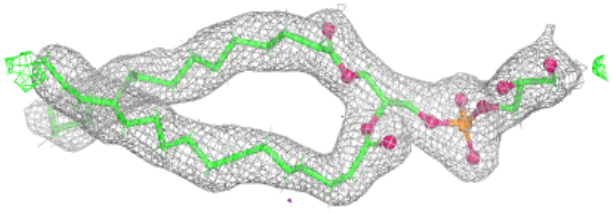


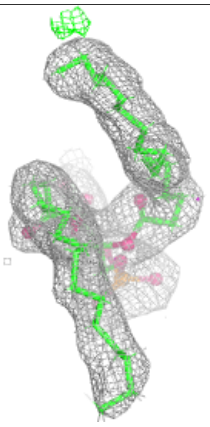


Electron density around LHG d 407:

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

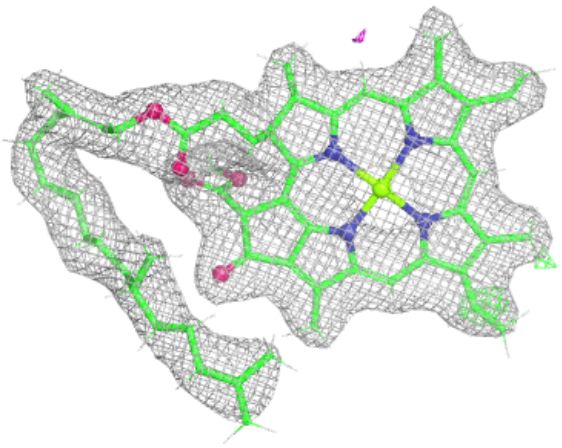


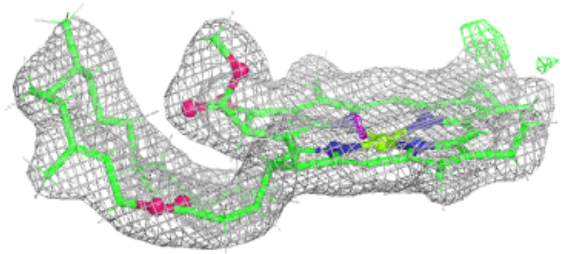




Electron density around CLA b 611:

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

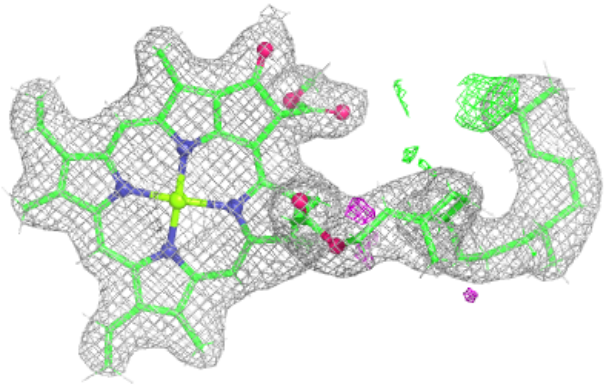


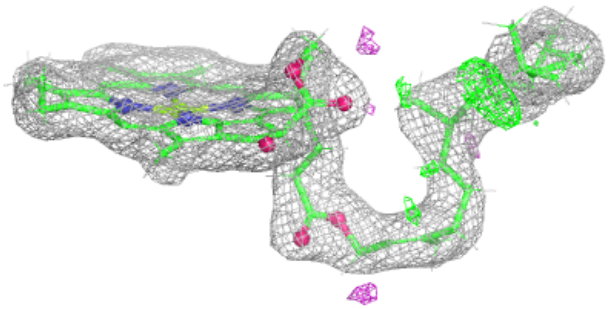


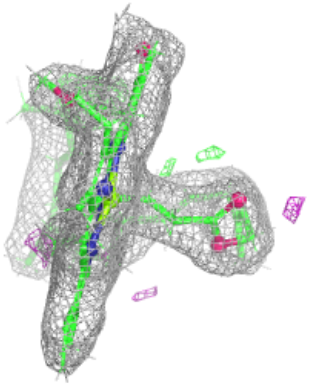


Electron density around CLA b 613:

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

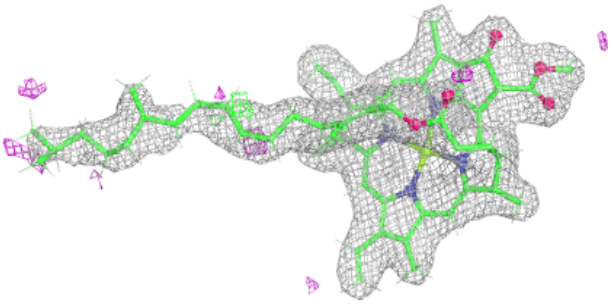


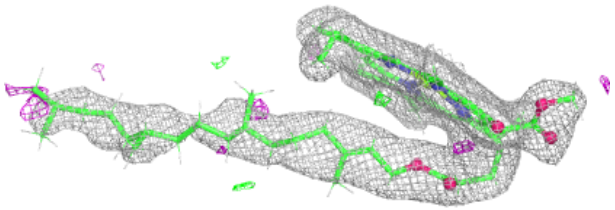




Electron density around CLA b 615:

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

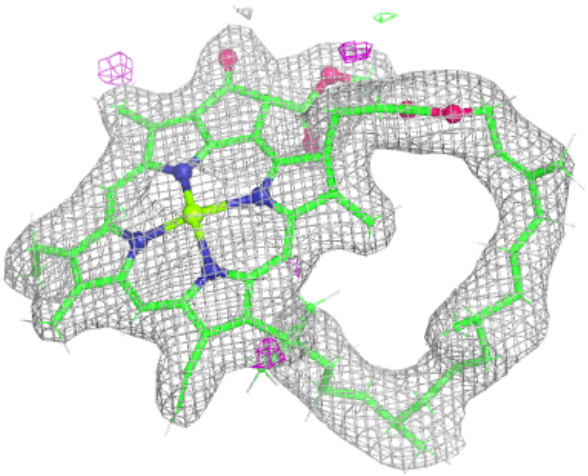


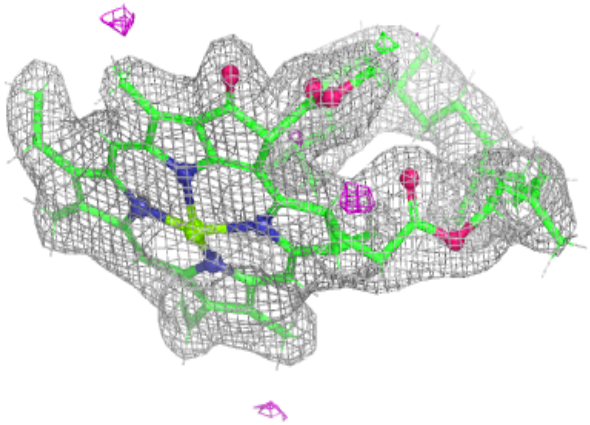


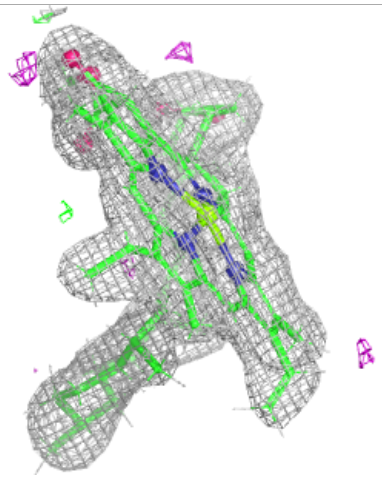


Electron density around CLA b 616:

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

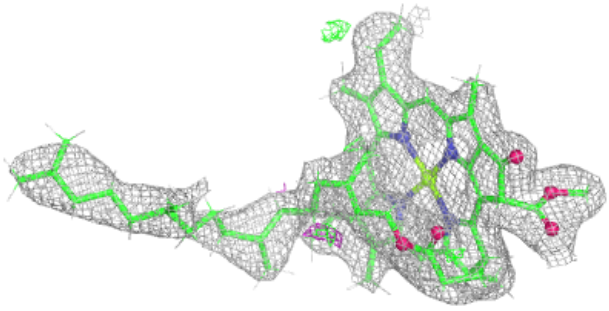


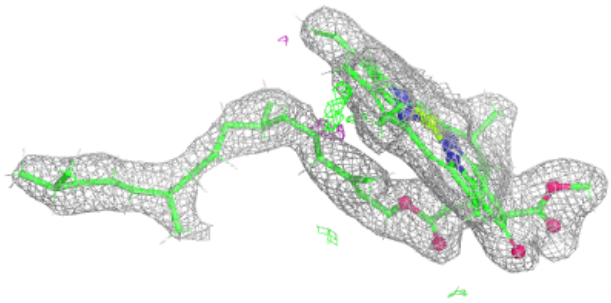


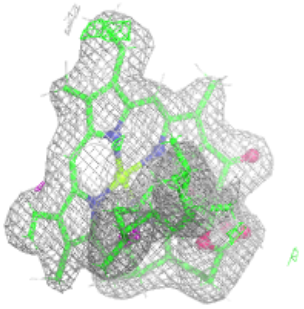


Electron density around CLA C 505:

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

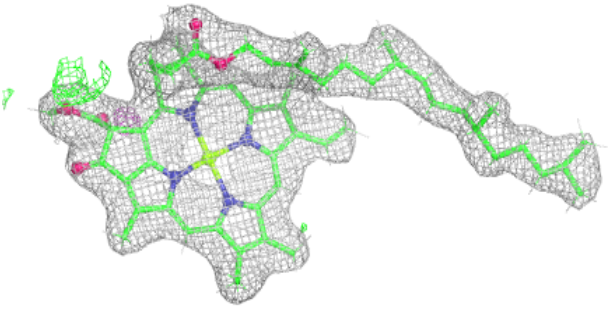


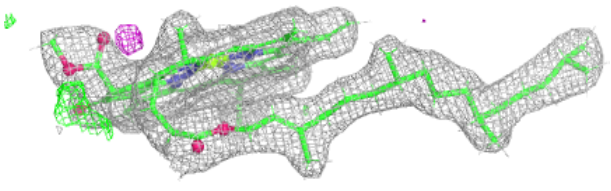


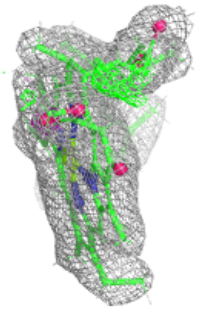


Electron density around CLA c 501:

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

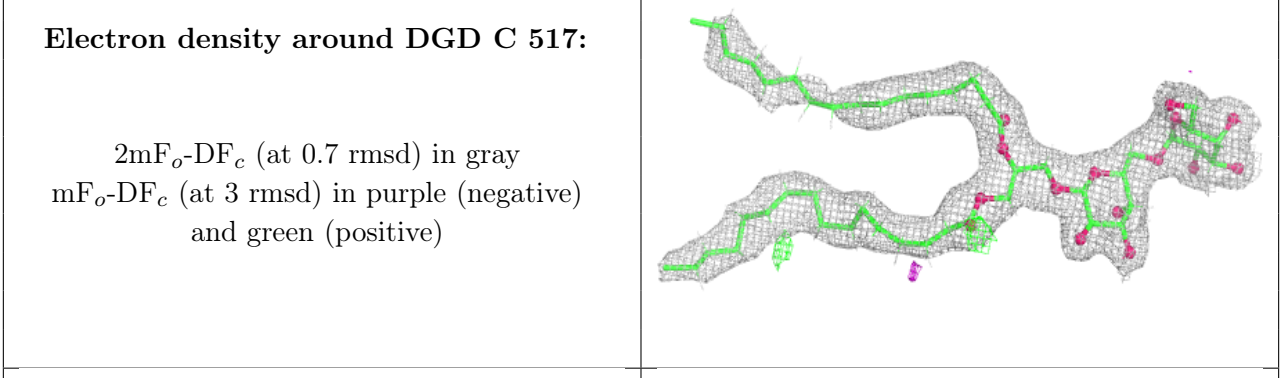






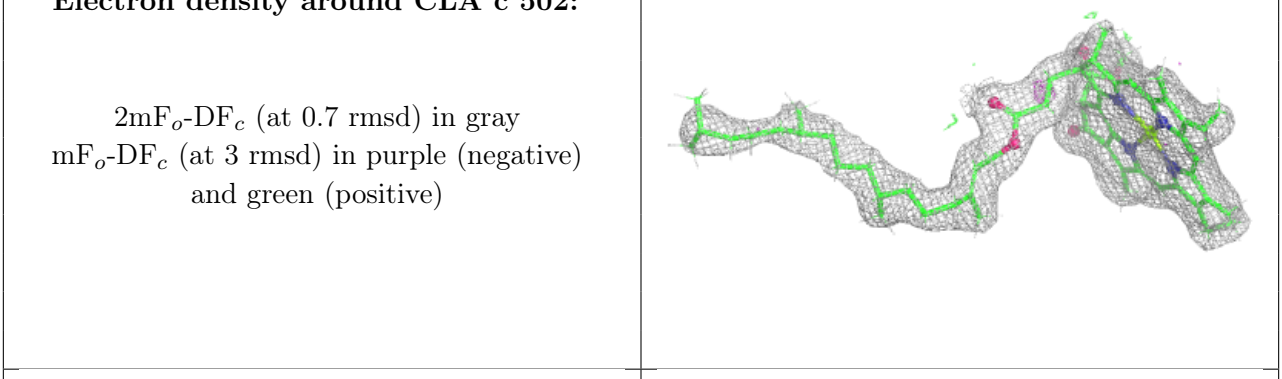
Electron density around DGD C 517:

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



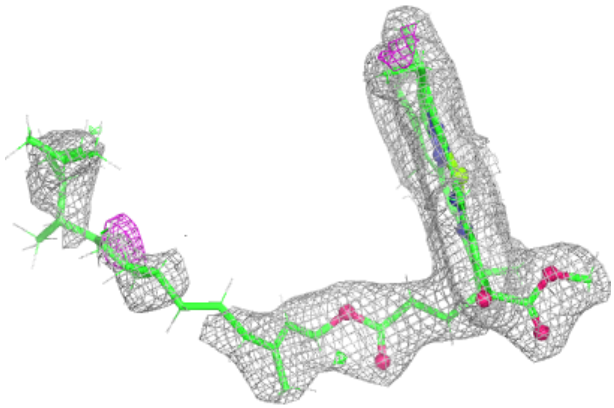
Electron density around CLA c 502:

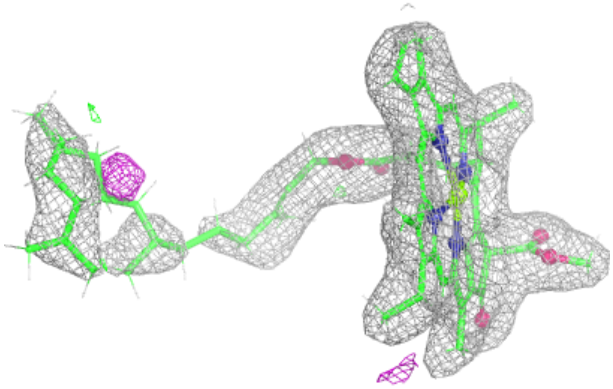
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

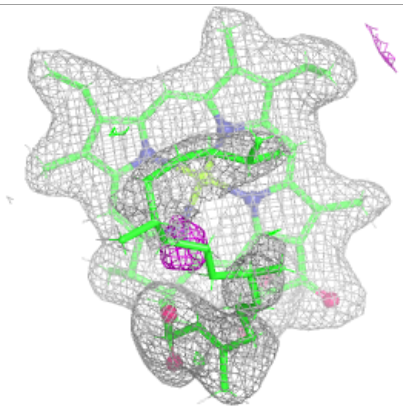


Electron density around CLA C 506:

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

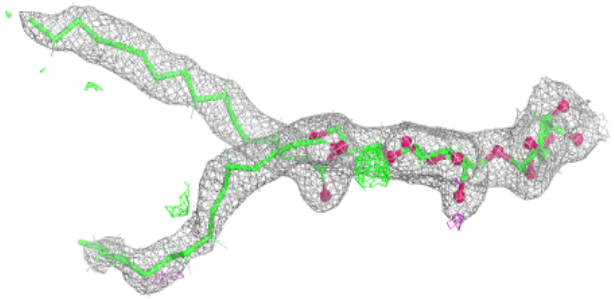


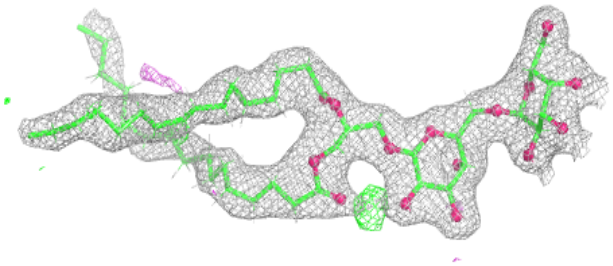


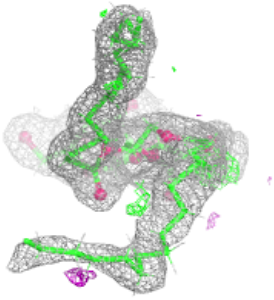


Electron density around DGD c 516:

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

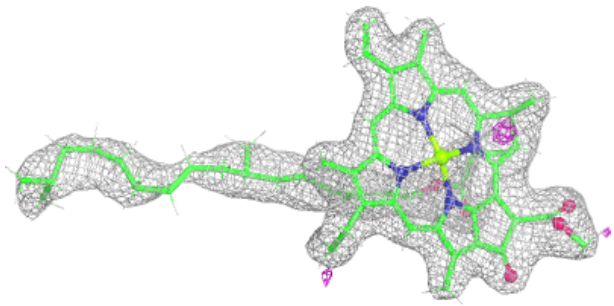


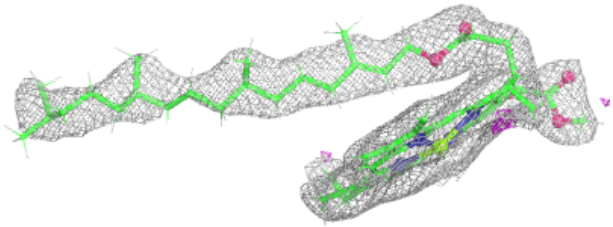


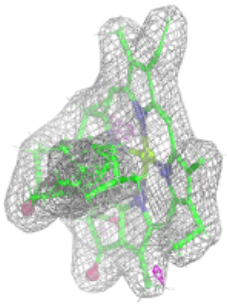


Electron density around CLA B 614:

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

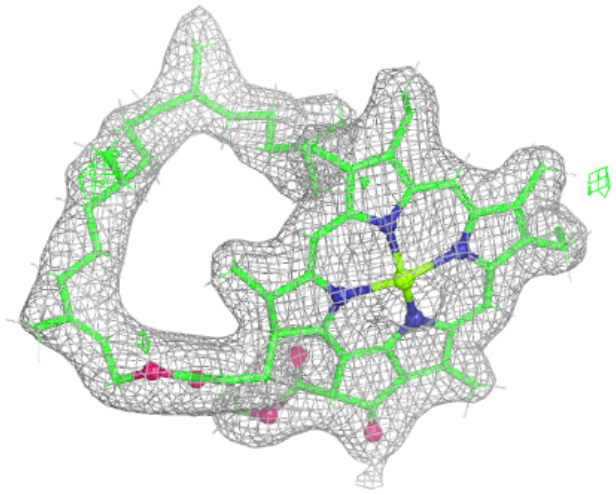


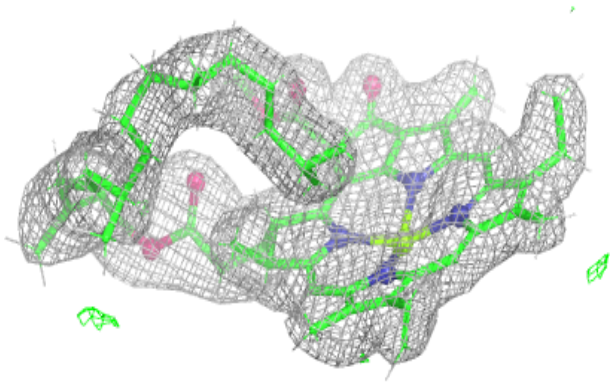


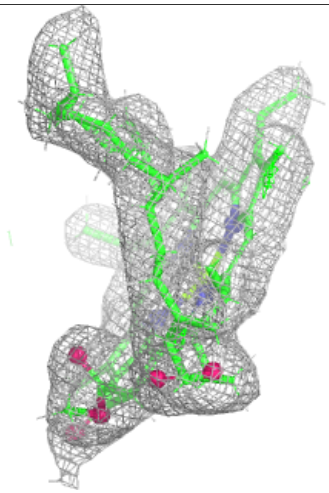


Electron density around CLA B 615:

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

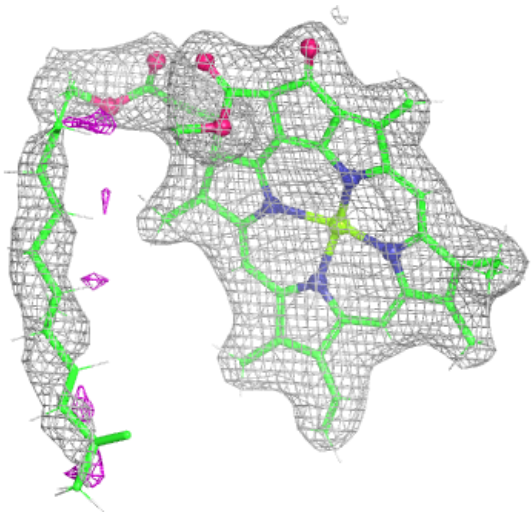


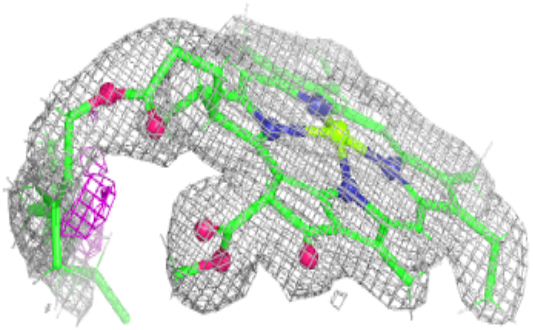


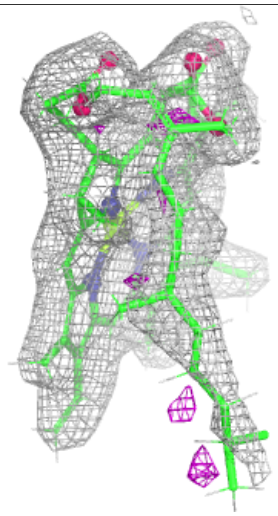


Electron density around CLA B 616:

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

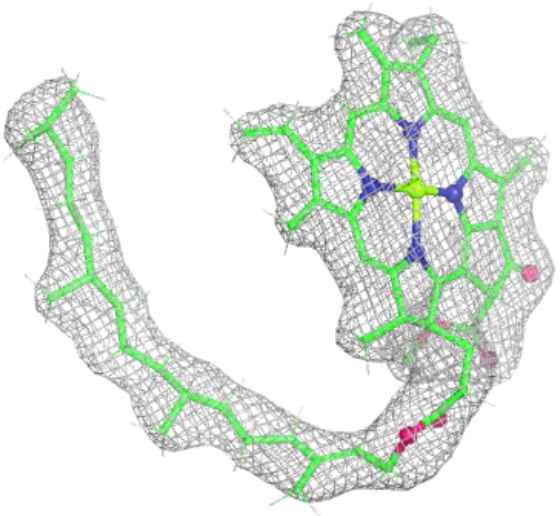


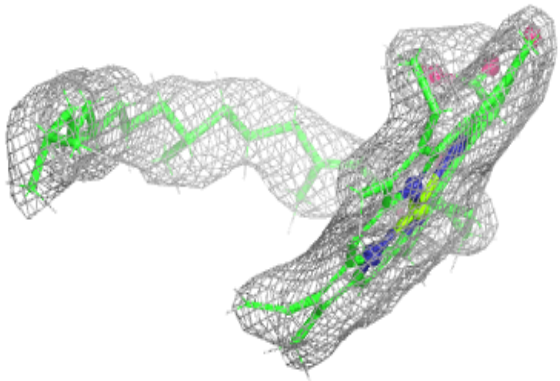


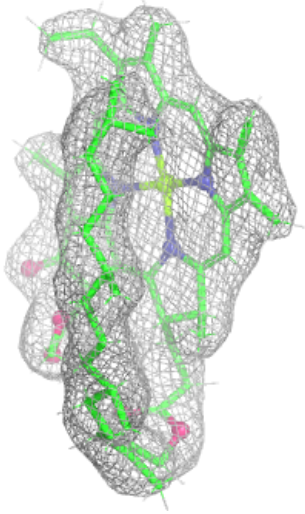


Electron density around CLA c 507:

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

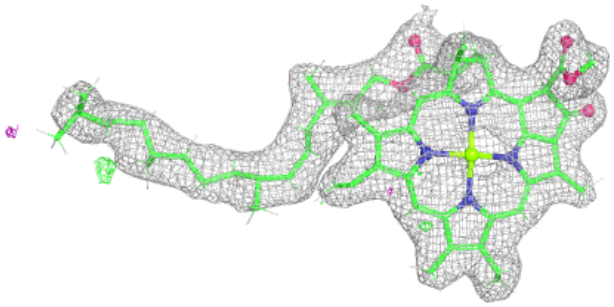


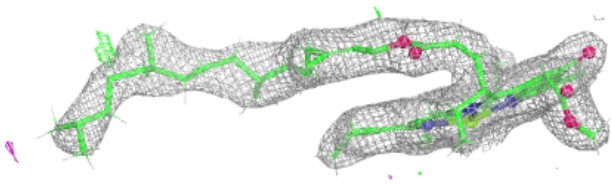


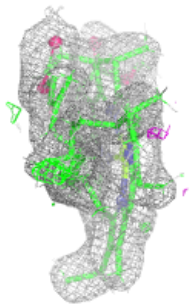


Electron density around CLA B 603:

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

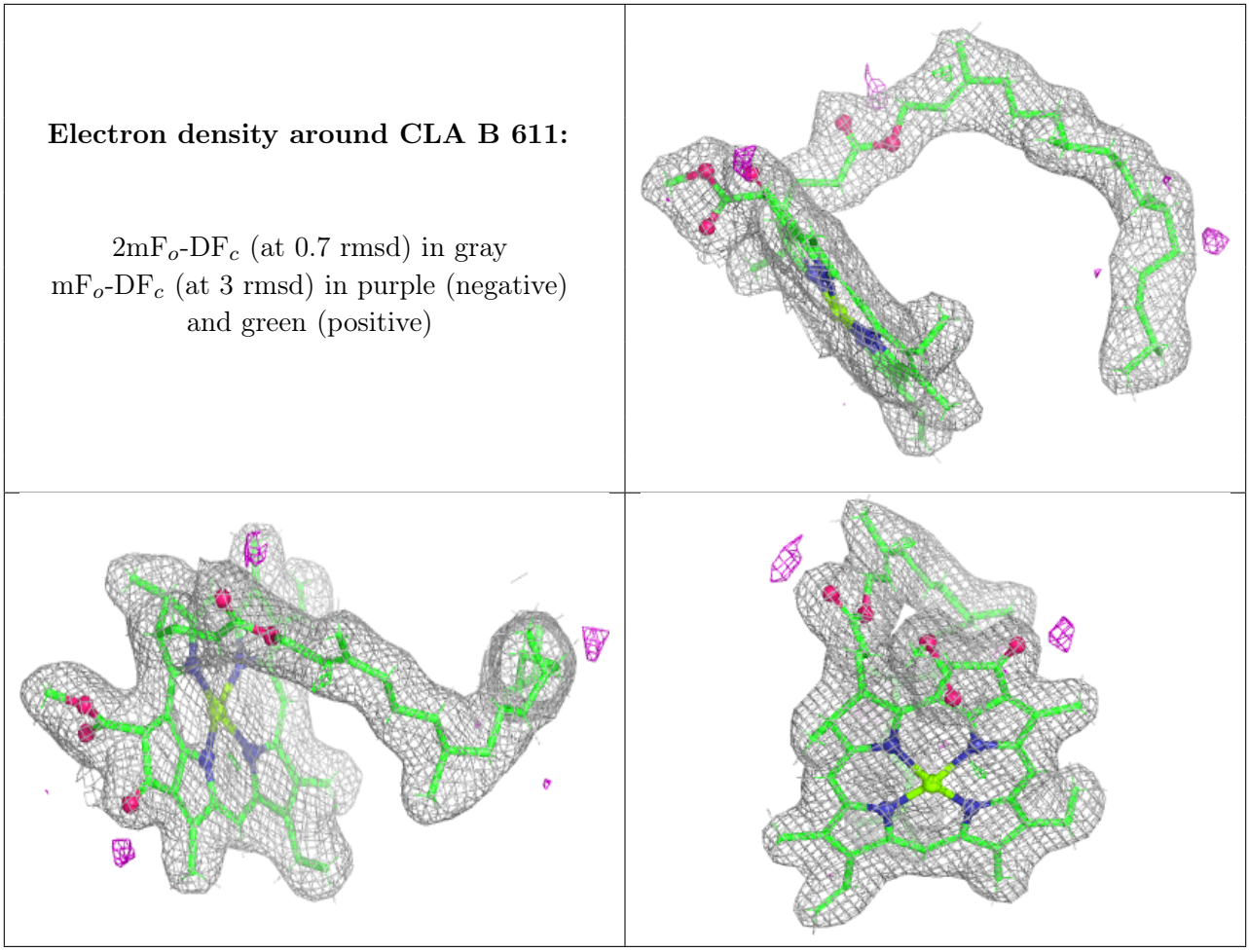






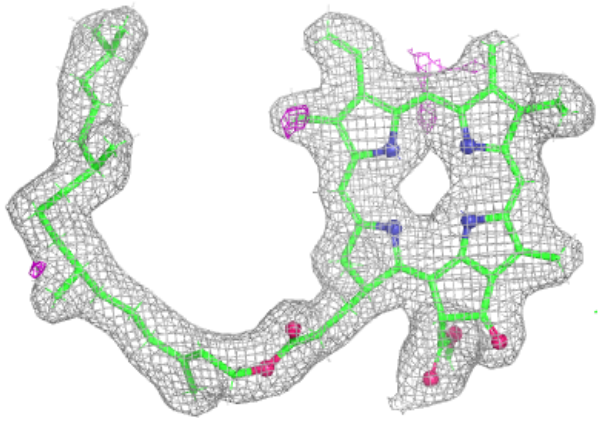
Electron density around CLA B 611:

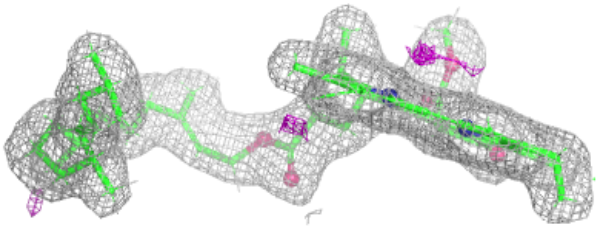
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

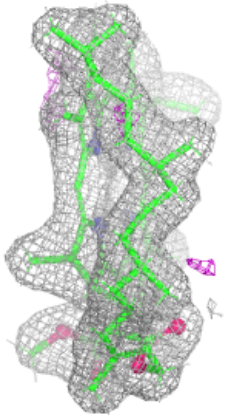


Electron density around PHO A 406:

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

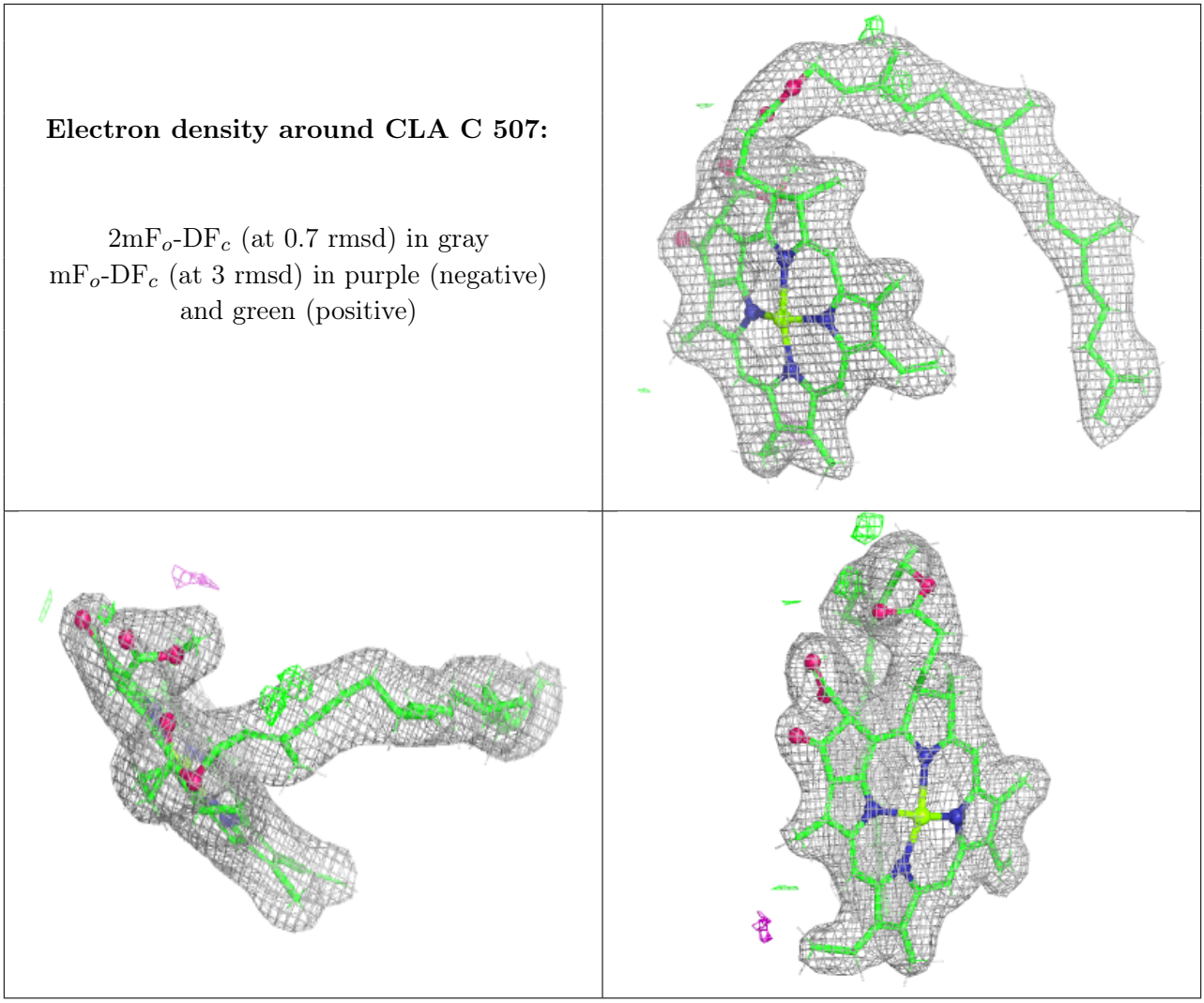






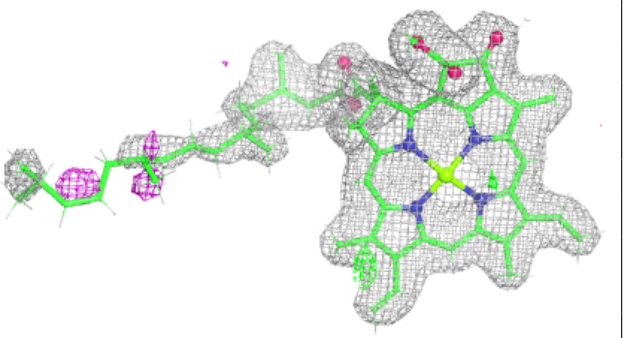
Electron density around CLA C 507:

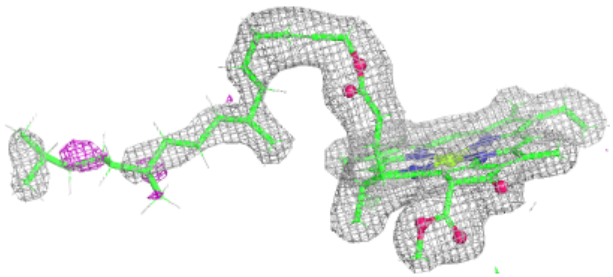
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

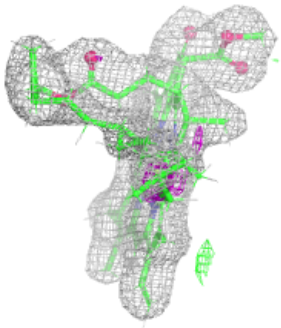


Electron density around CLA A 405:

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

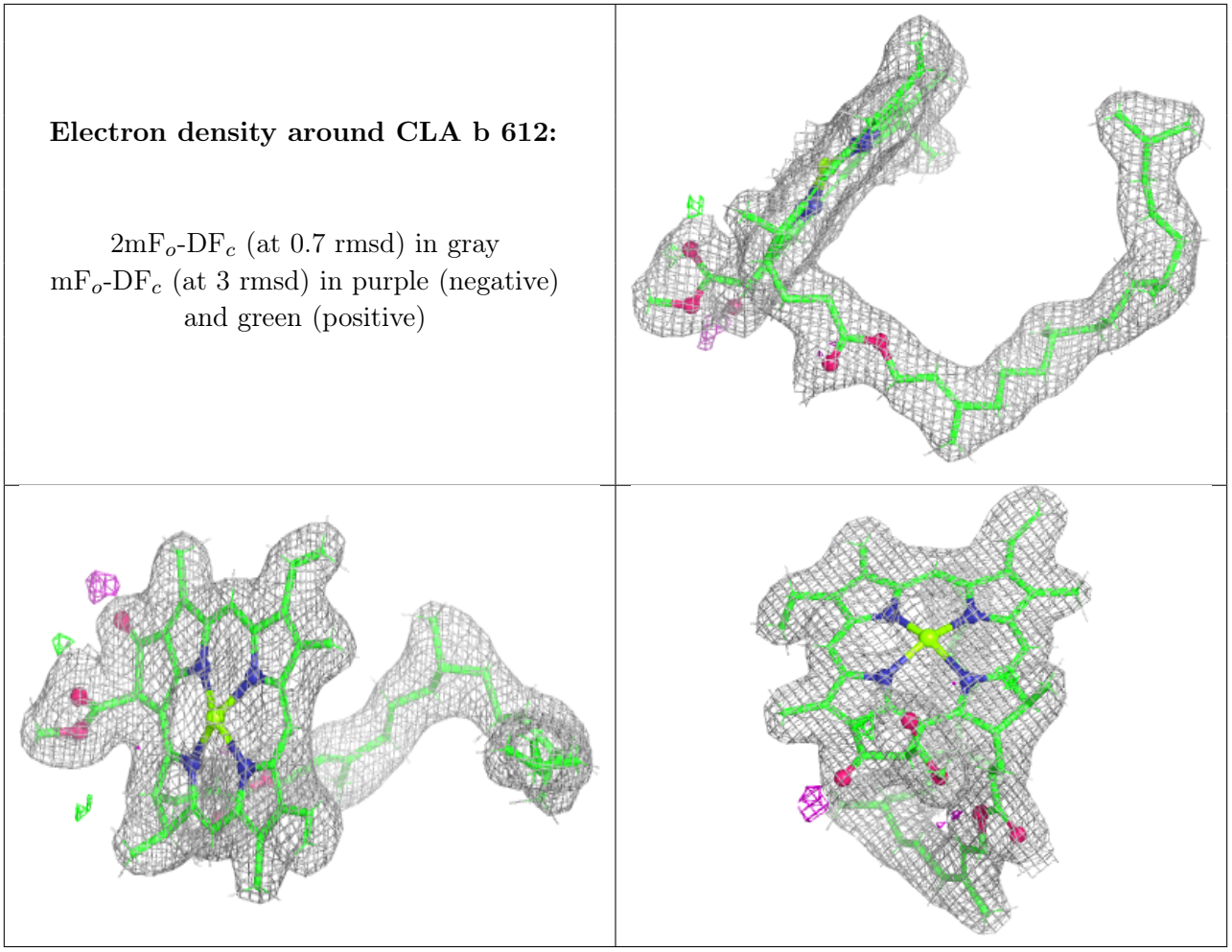






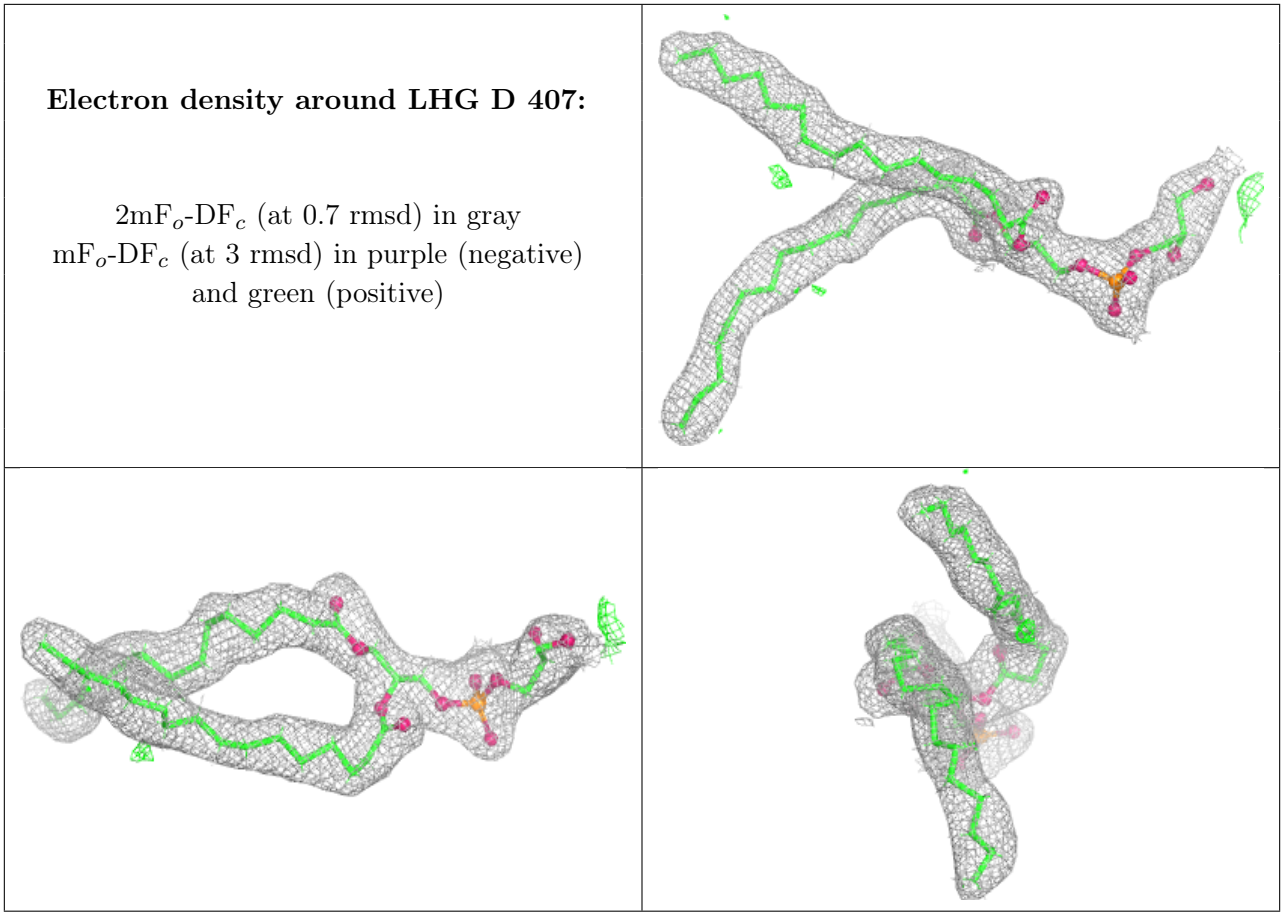
Electron density around CLA b 612:

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



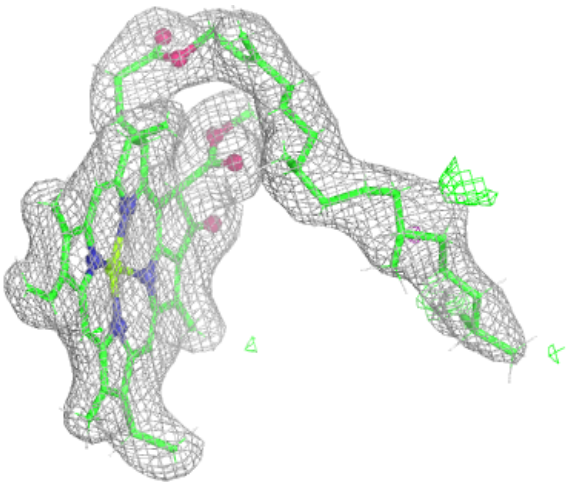
Electron density around LHG D 407:

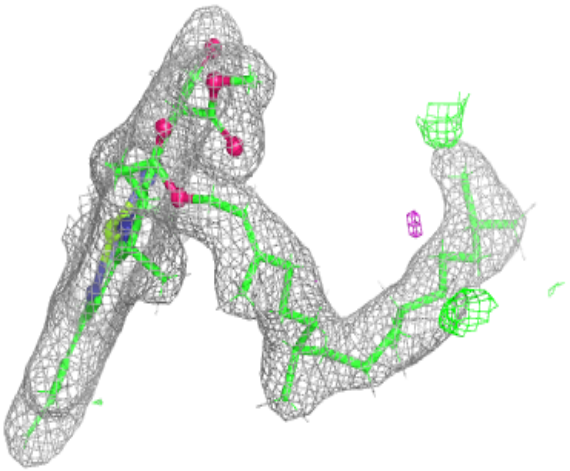
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

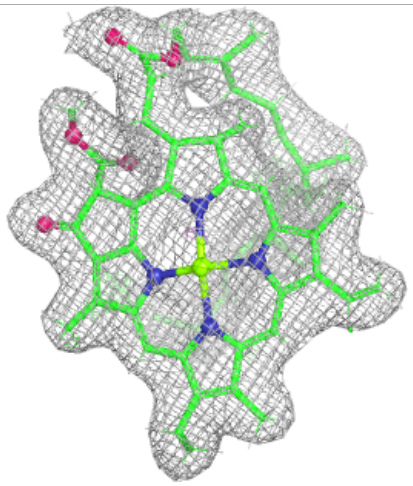


Electron density around CLA B 613:

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

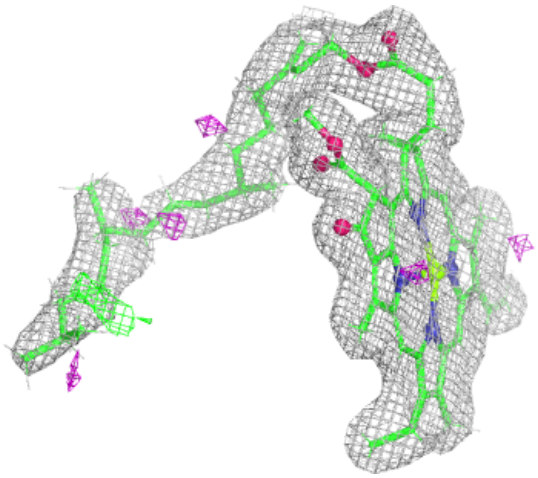


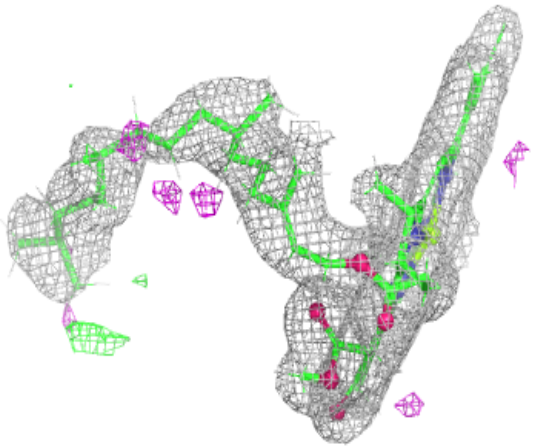


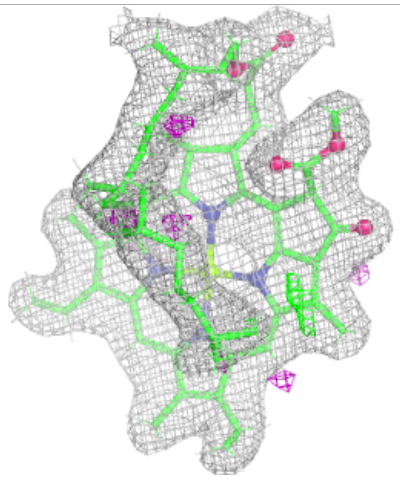


Electron density around CLA b 614:

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

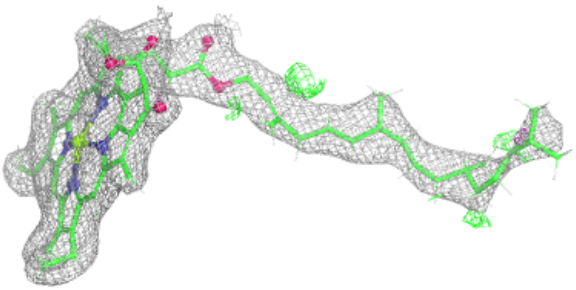


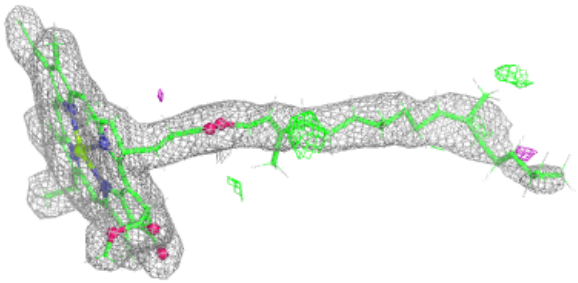


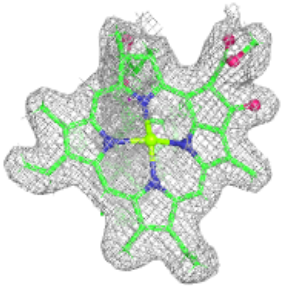


Electron density around CLA B 604:

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

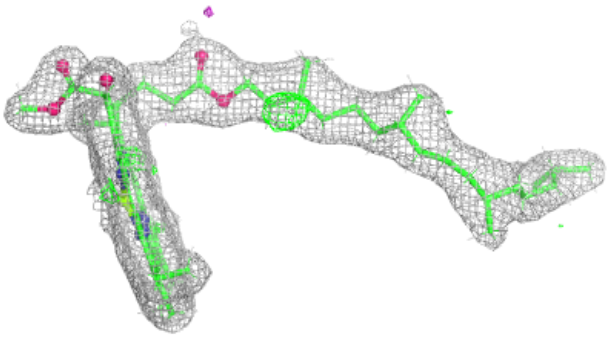


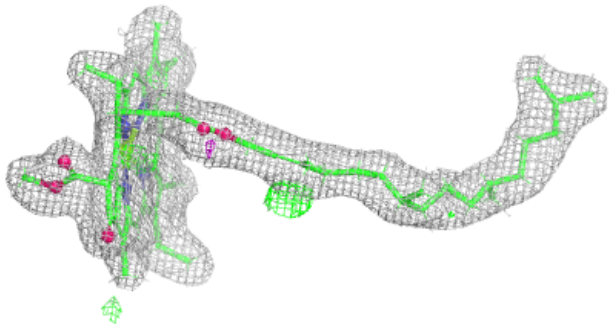


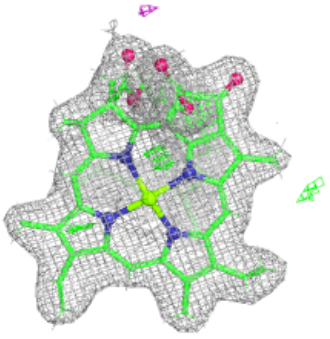


Electron density around CLA B 605:

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

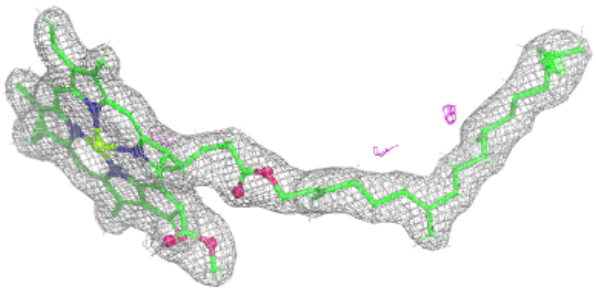


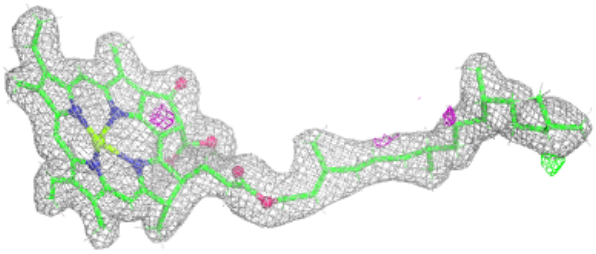


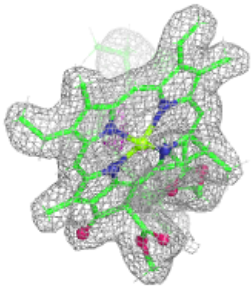


Electron density around CLA A 404:

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

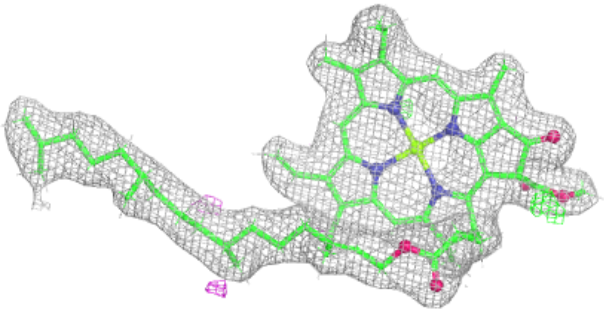


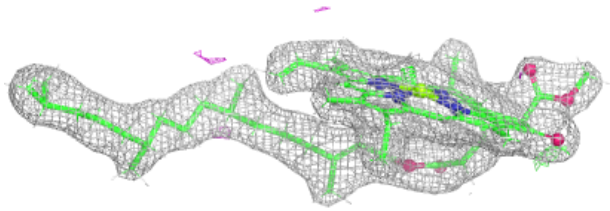


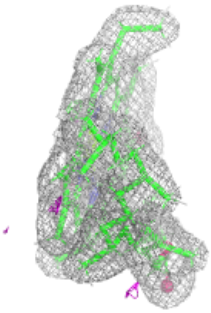


Electron density around CLA C 501:

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

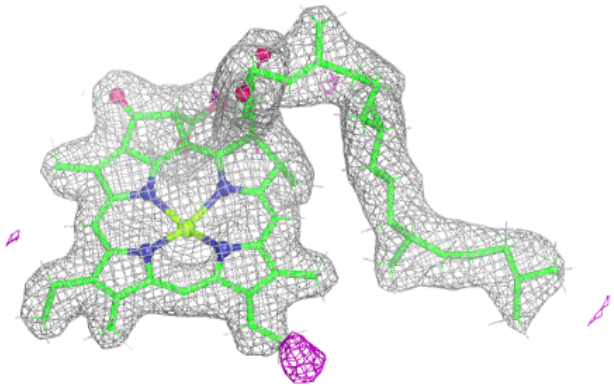


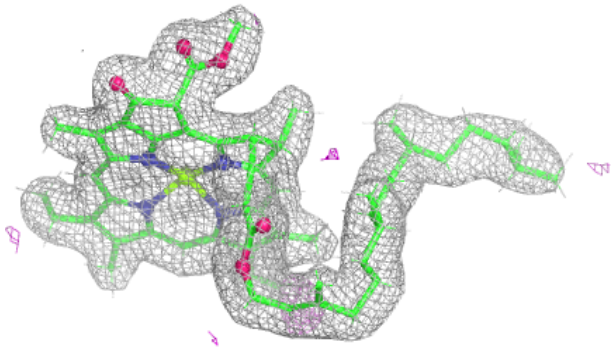


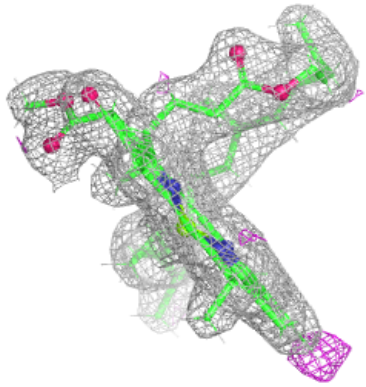


Electron density around CLA D 401:

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

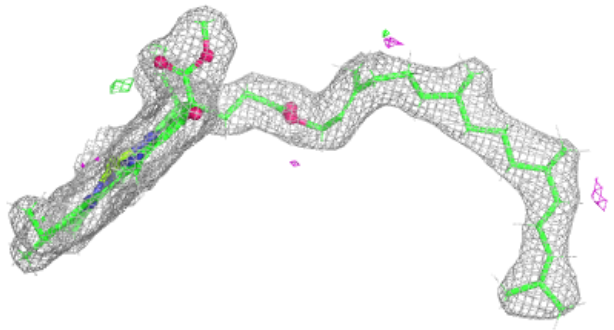


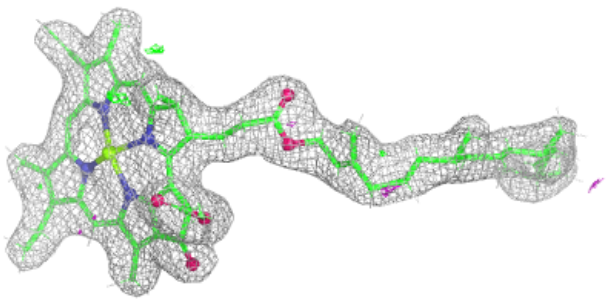


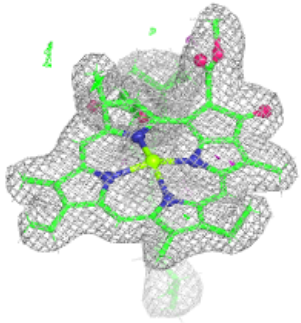


Electron density around CLA D 402:

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

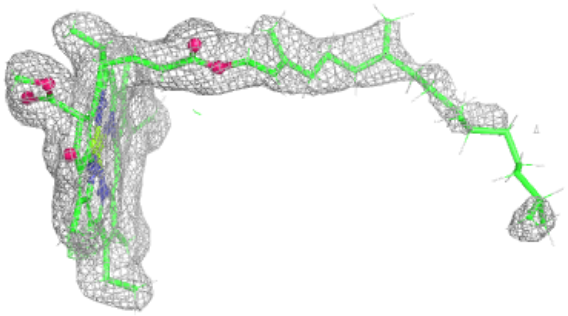


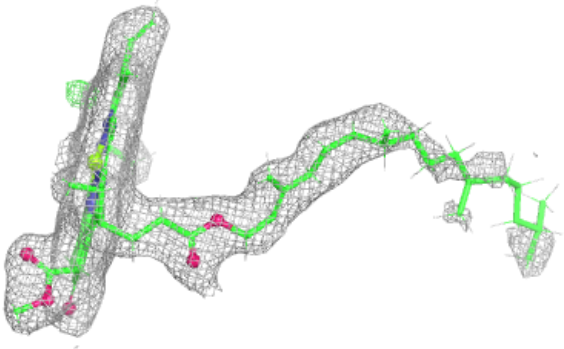


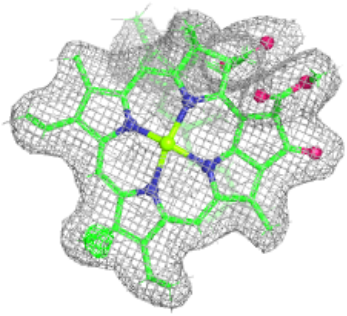


Electron density around CLA D 403:

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

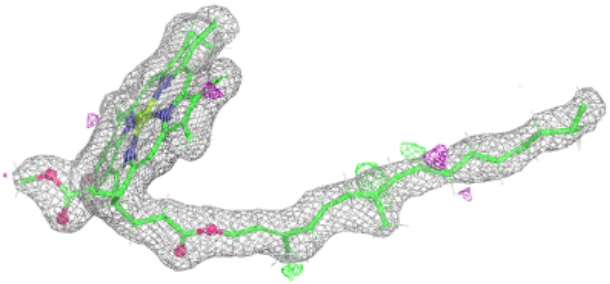


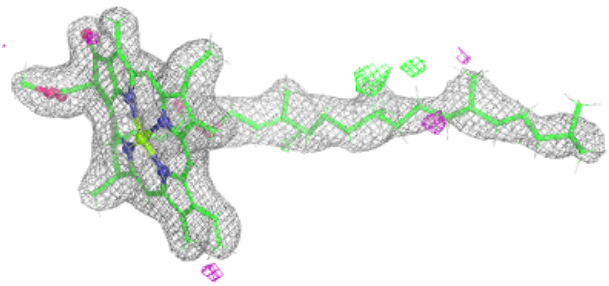


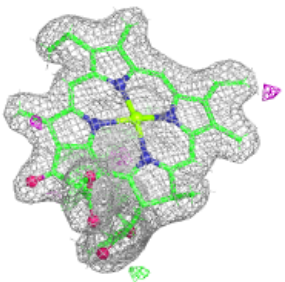


Electron density around CLA B 607:

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

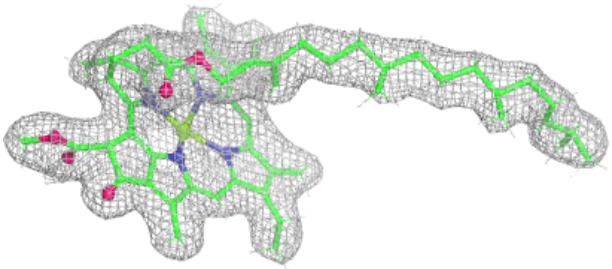


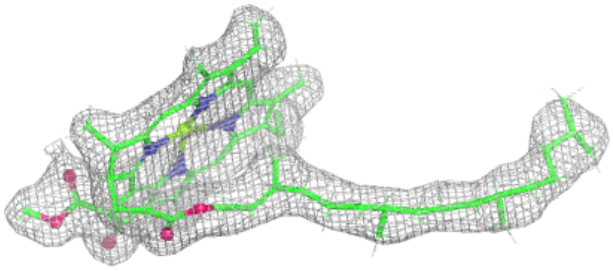


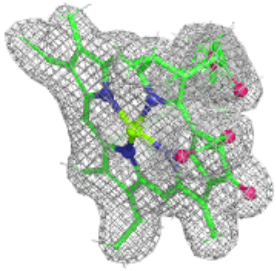


Electron density around CLA B 608:

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

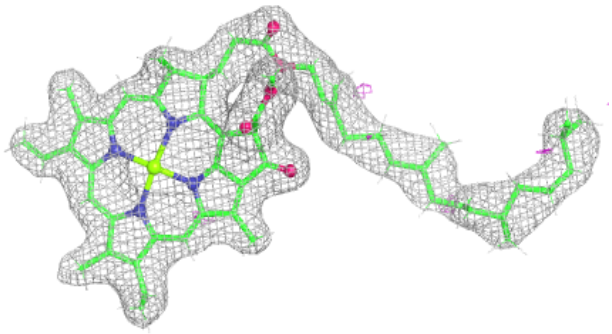


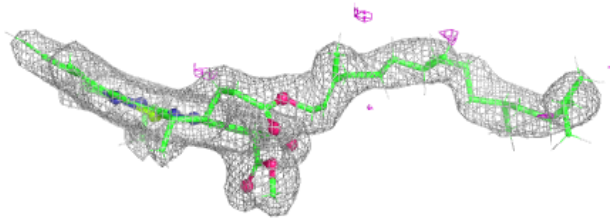


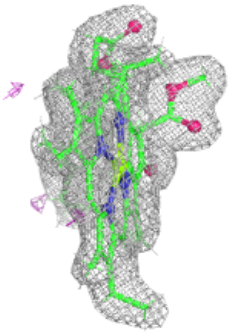


Electron density around CLA B 602:

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

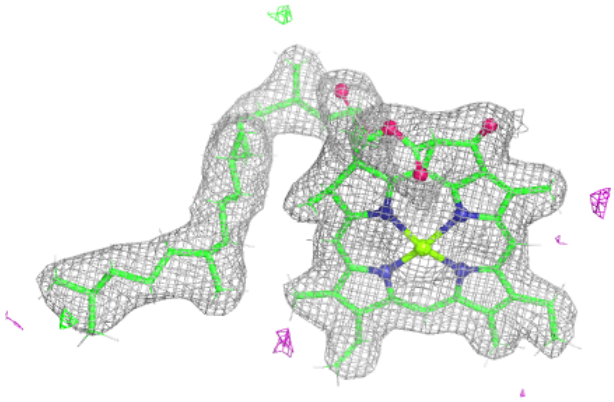


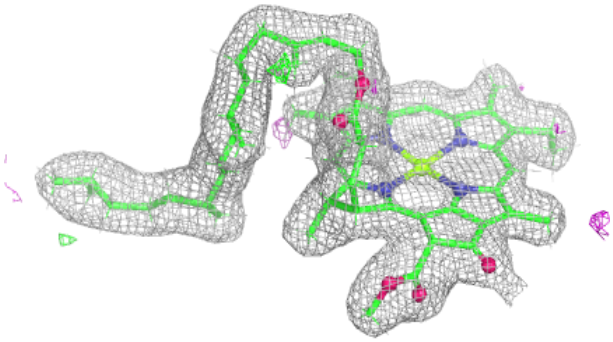


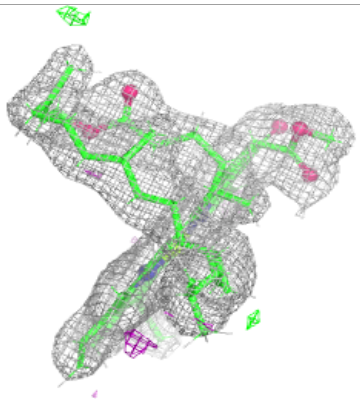


Electron density around CLA a 411:

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

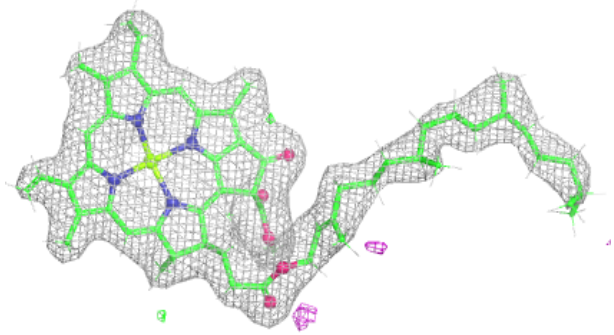


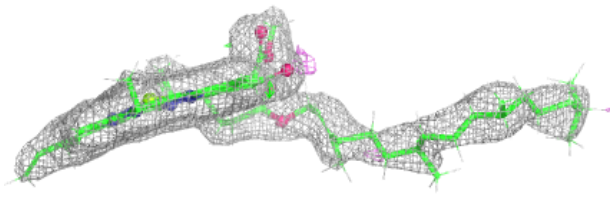


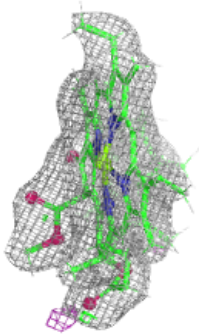


Electron density around CLA b 603:

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

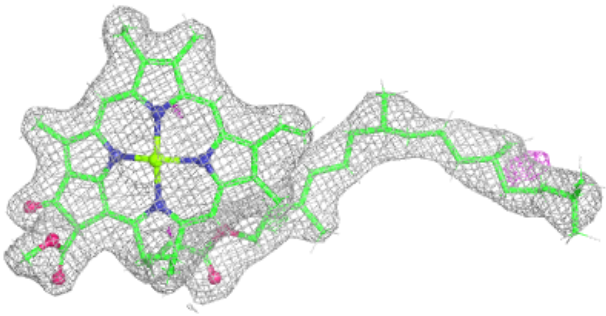


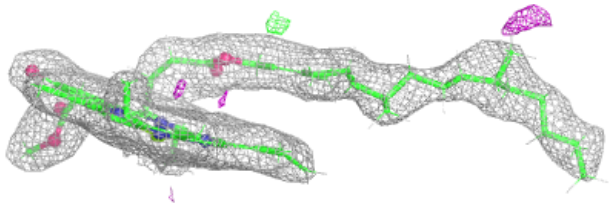


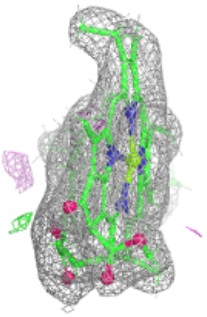


Electron density around CLA b 604:

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

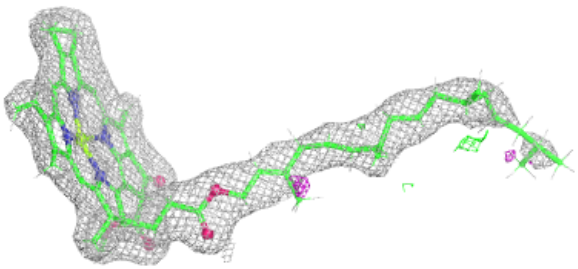


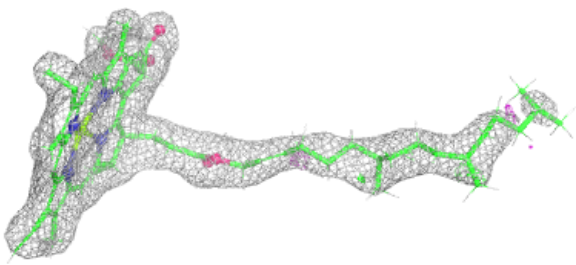


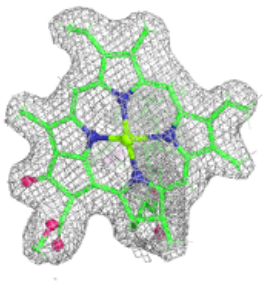


Electron density around CLA b 605:

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

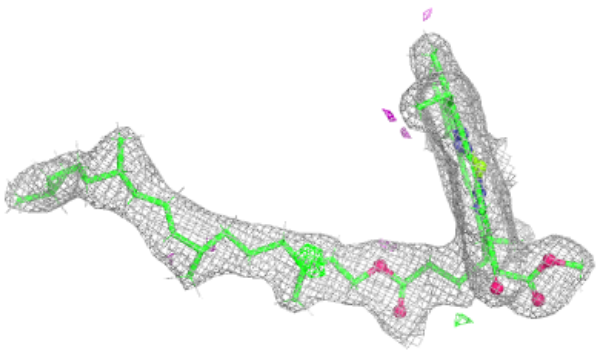


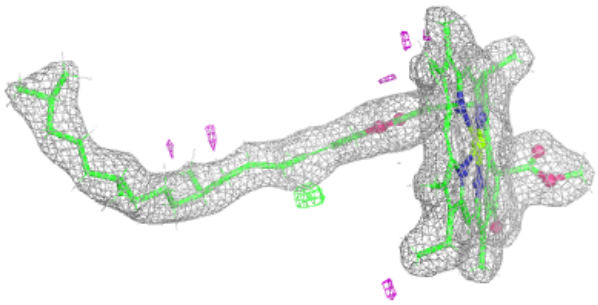


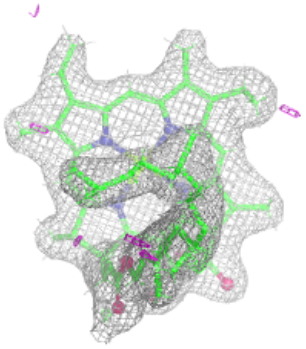


Electron density around CLA b 606:

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

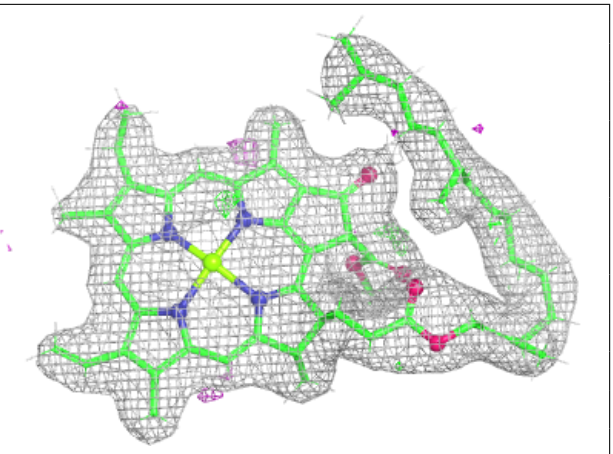


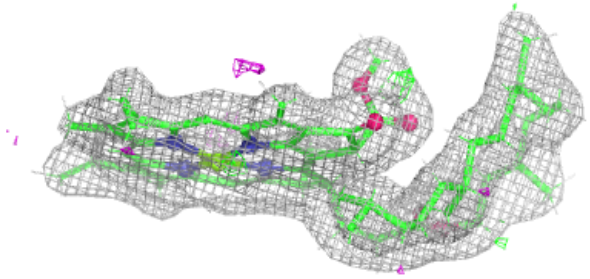


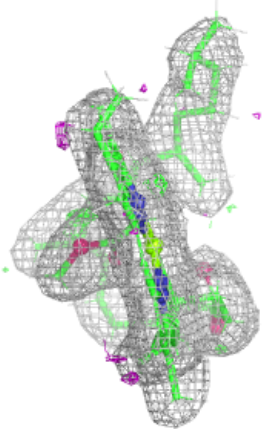


Electron density around CLA B 610:

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

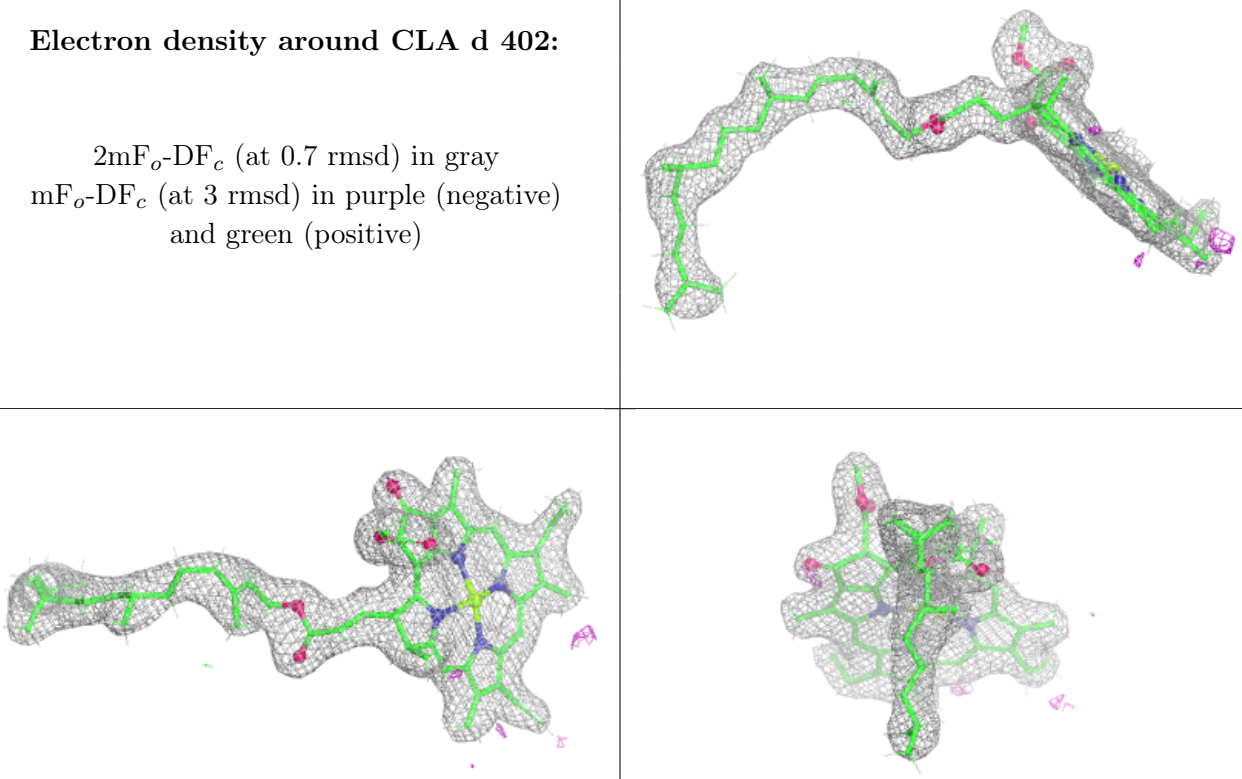






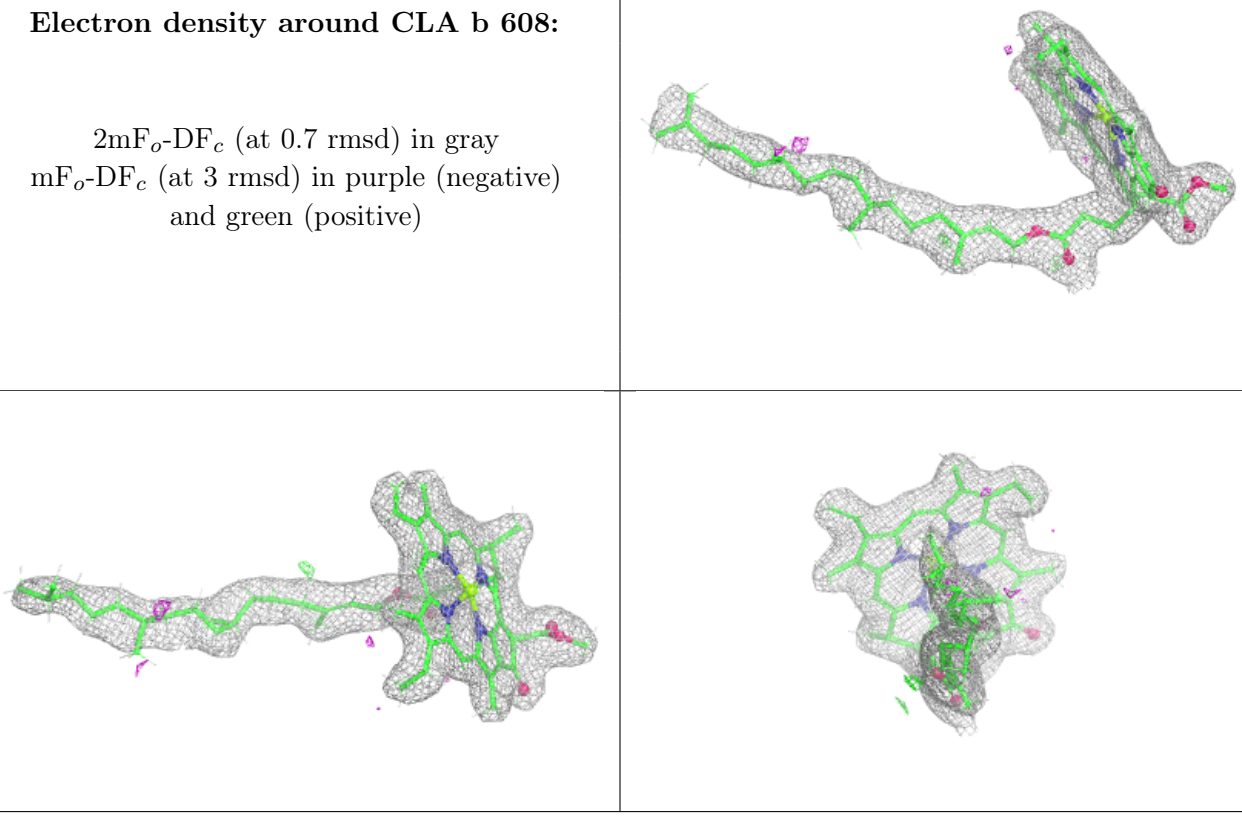
Electron density around CLA d 402:

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



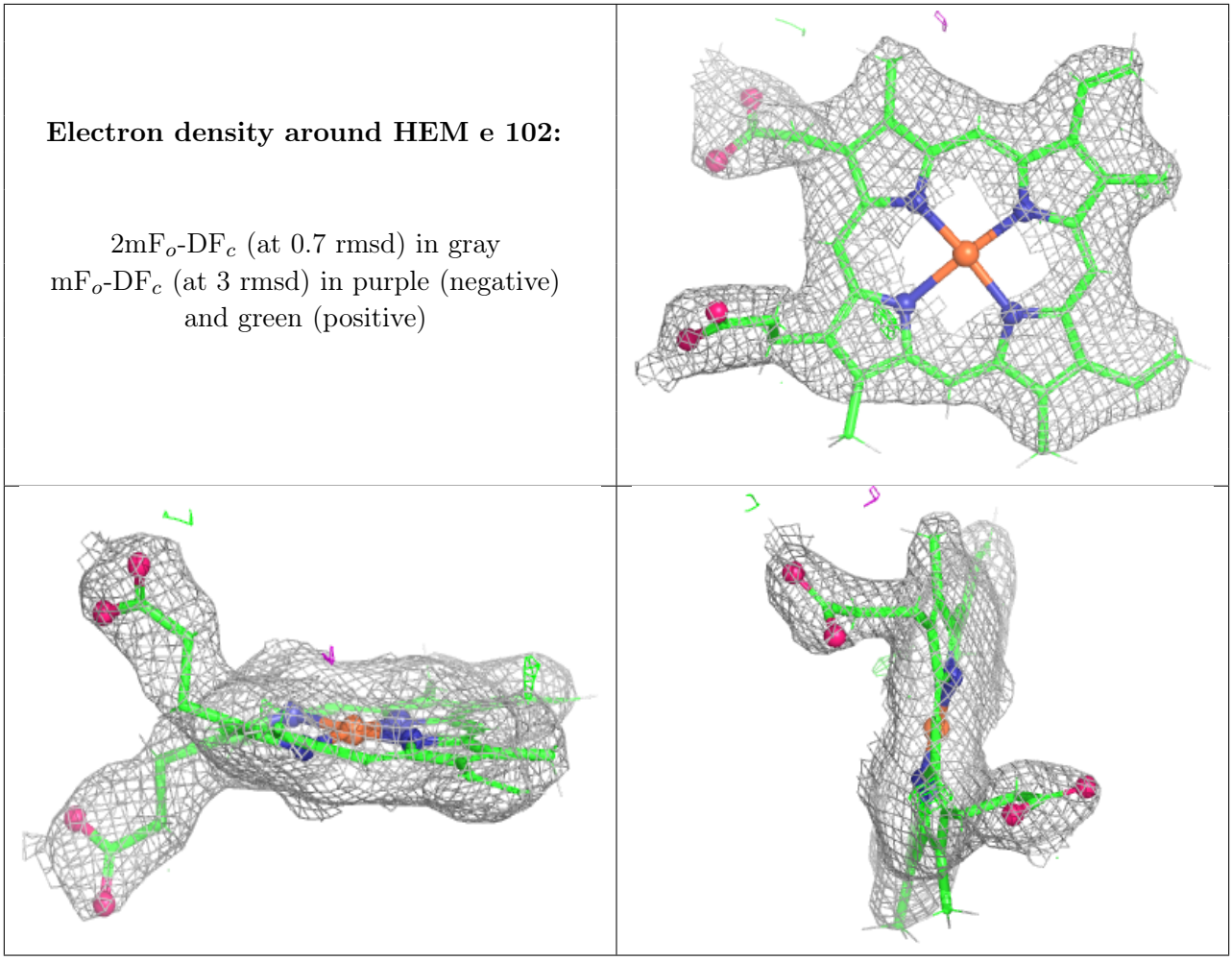
Electron density around CLA b 608:

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



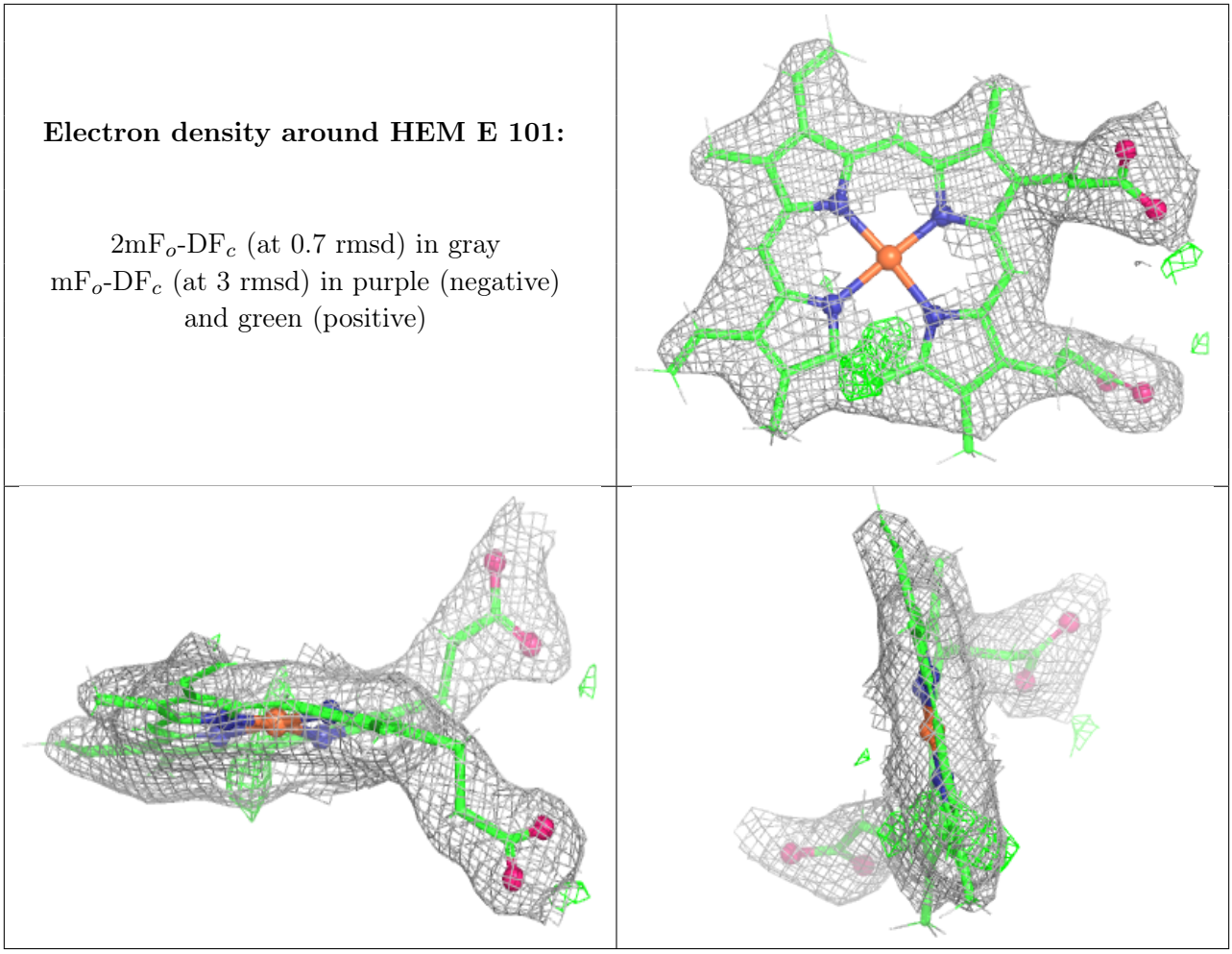
Electron density around HEM e 102:

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



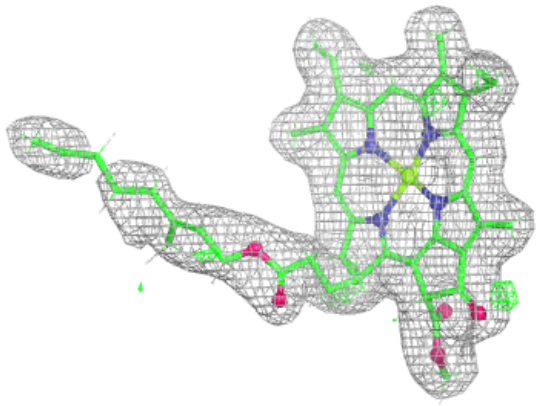
Electron density around HEM E 101:

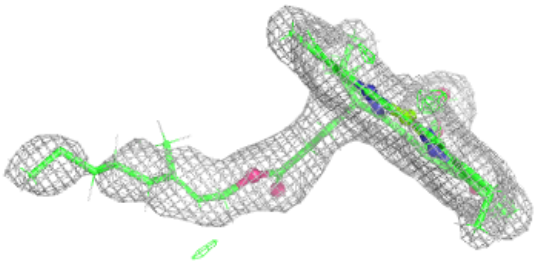
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

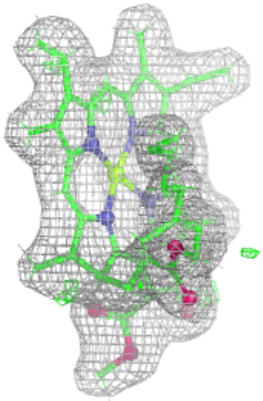


Electron density around CLA A 408:

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

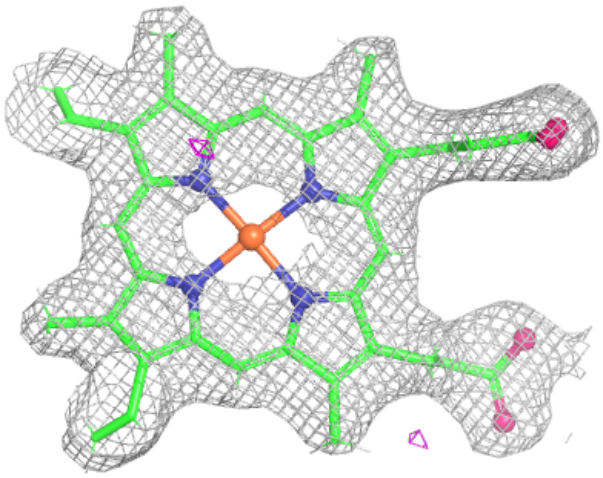


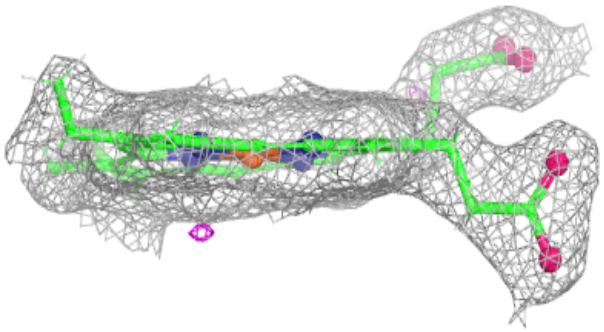


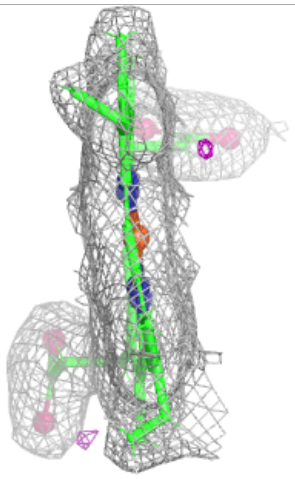


Electron density around HEC V 201:

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

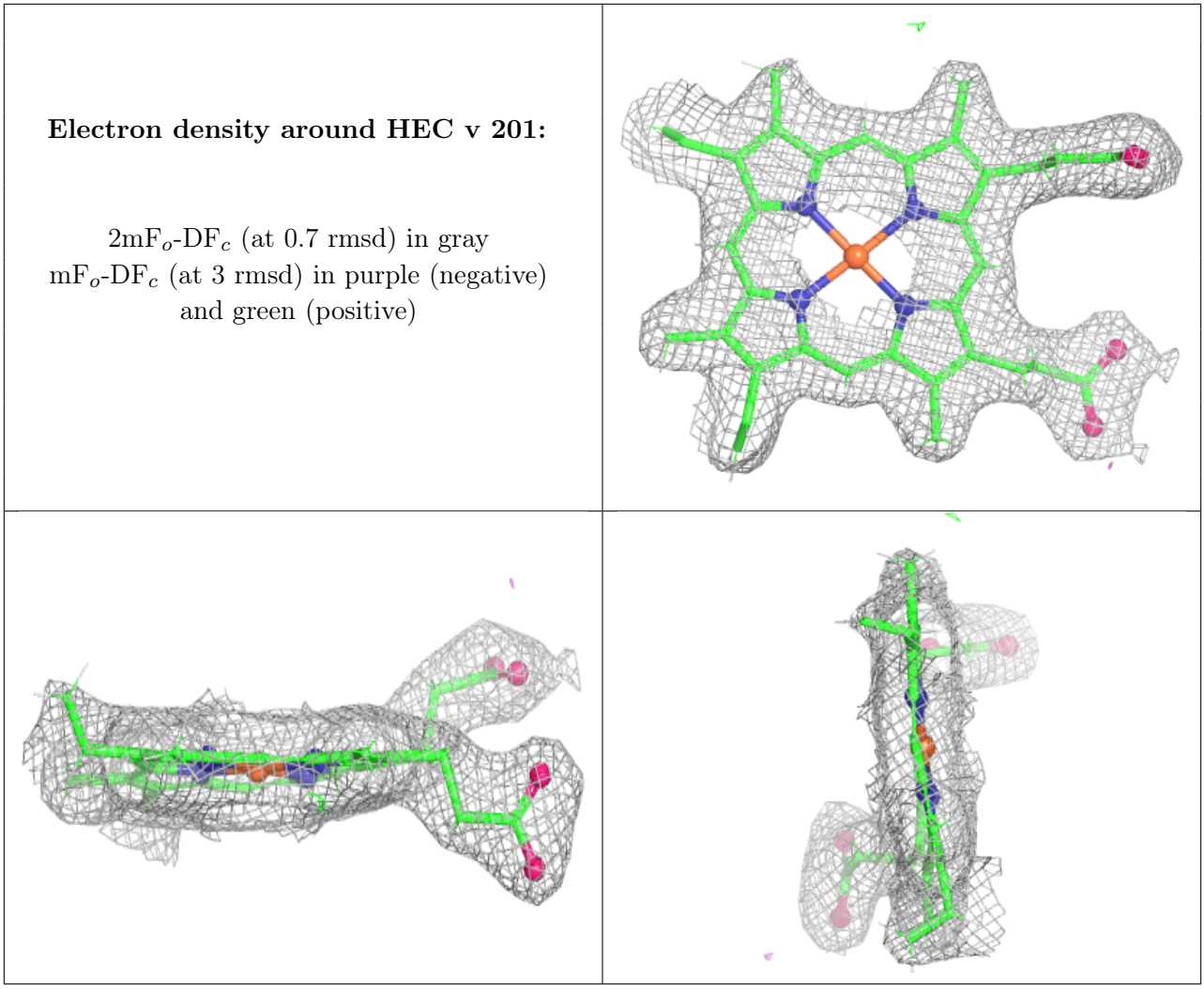






Electron density around HEC v 201:

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



6.5 Other polymers

There are no such residues in this entry.