Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2026 – 07:04 AM JST

PDB ID	:	8GN1 / pdb_00008gn1
Title	:	Crystal structure of DBBQ-bound photosystem II complex
Authors	:	Kamada, S.; Nakajima, Y.; Shen, J.-R.
Deposited on	:	2022-08-22
Resolution	:	2.10 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 (i)) were used in the production of this report:

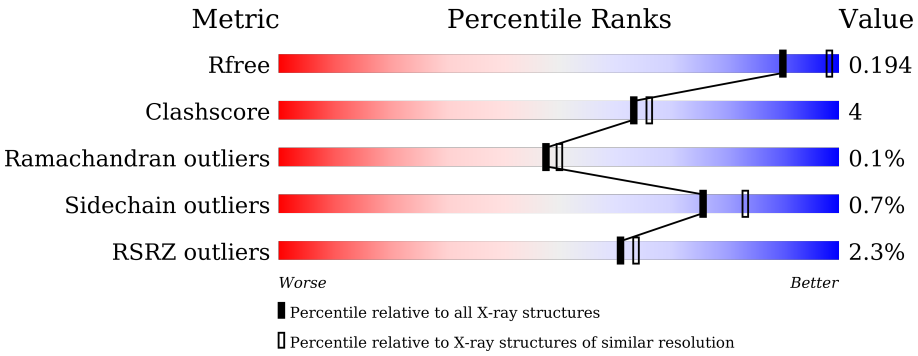
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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.



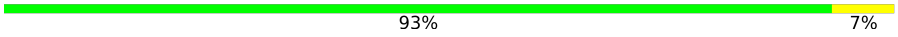
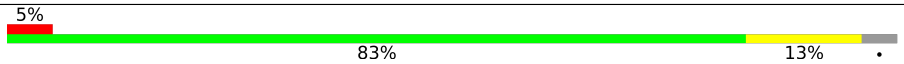
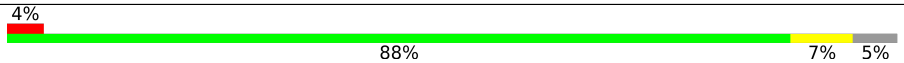
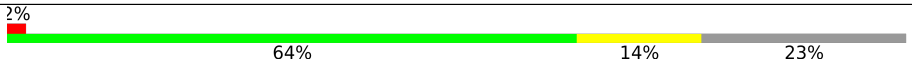
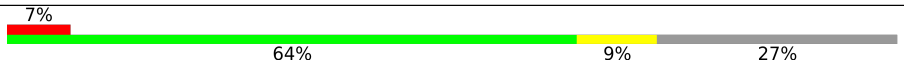
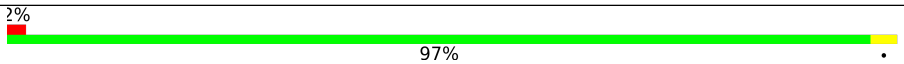
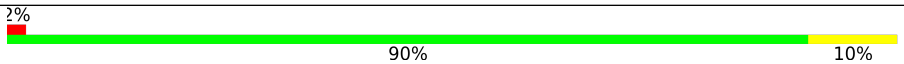
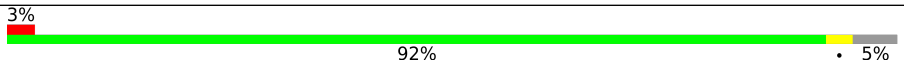
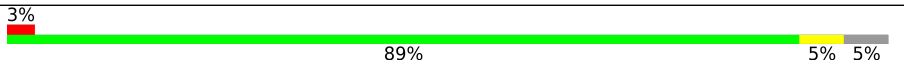
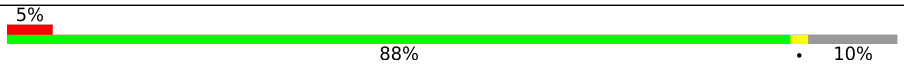
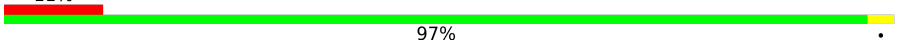
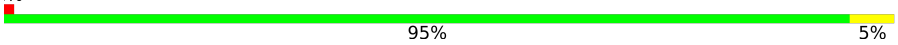
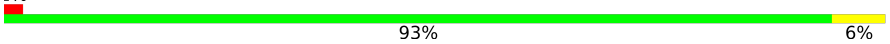
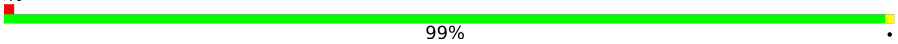
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	344	89% 8%
1	a	344	90% 8%
2	B	505	94% 6%
2	b	505	91% 9%
3	C	455	91% 7%
3	c	455	93% 7%

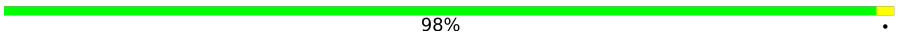
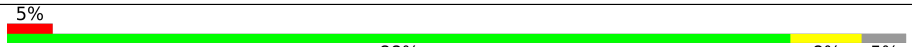
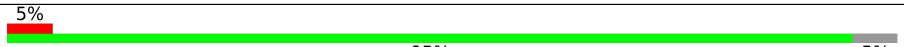
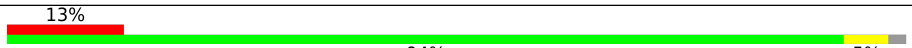
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	41	

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
43	HEC	V	201	X	-	-	-
43	HEC	v	201	X	-	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 54282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2610	1713	428	454	15			
1	a	334	Total	C	N	O	S	0	3	0
			2620	1717	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	5	0
			3997	2623	667	694	13			
2	b	503	Total	C	N	O	S	0	8	0
			3962	2601	660	688	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	2	0
			3494	2286	585	610	13			
3	c	455	Total	C	N	O	S	0	0	0
			3518	2303	589	613	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	342	Total	C	N	O	S	0	4	0
			2743	1819	447	464	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	1	0
			649	425	103	121			
5	e	79	Total	C	N	O	0	0	0
			629	414	99	116			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	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 293	C 198	N 45	O 49	S 1	0	0	0
8	i	36	Total 296	C 200	N 46	O 49	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total 251	C 171	N 37	O 42	S 1	0	0	0
9	j	39	Total 271	C 182	N 40	O 48	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 293	C 205	N 42	O 46	0	1	0
10	k	37	Total 286	C 198	N 42	O 46	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total 298	C 202	N 45	O 51	0	1	0
11	l	36	Total 301	C 204	N 47	O 50	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 261	C 176	N 37	O 47	S 1	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			270	182	39	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	2	0
			1864	1167	313	379	5			
13	o	243	Total	C	N	O	S	0	3	0
			1865	1169	311	379	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	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	N	O	0	1	0
			778	494	132	152			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1059	675	177	203	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			220	146	35	36	3			
17	y	29	Total	C	N	O	S	0	0	0
			212	139	37	33	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			275	185	44	46			
18	x	38	Total	C	N	O	0	1	0
			278	188	44	46			

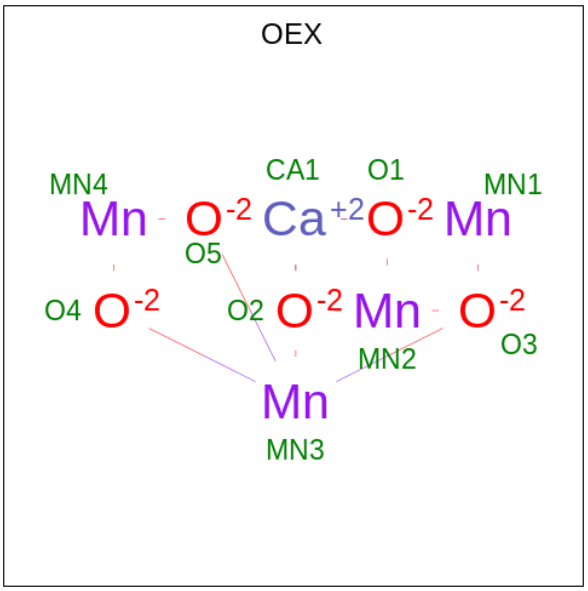
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			458	315	67	74	2			
19	z	61	Total	C	N	O	S	0	0	0
			453	309	70	72	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			207	133	39	35			

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

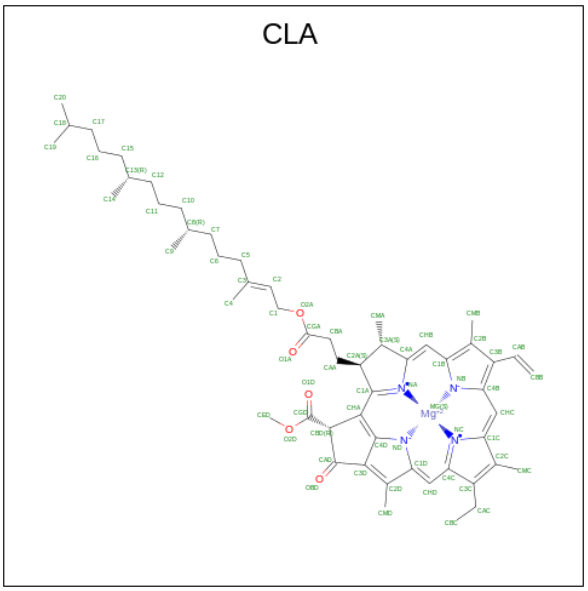
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



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

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

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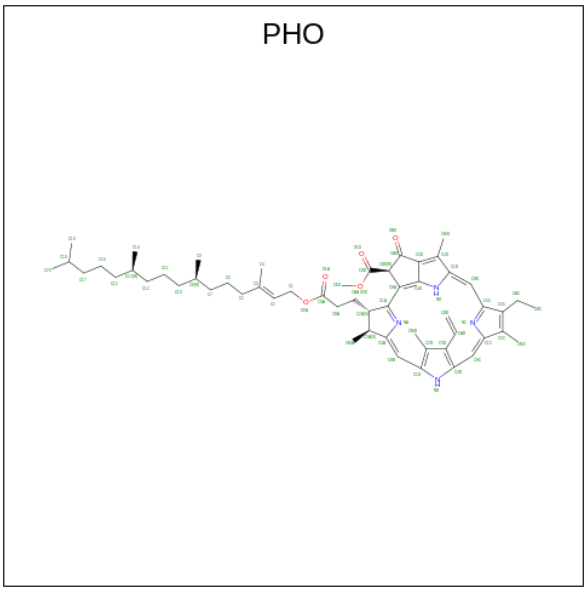
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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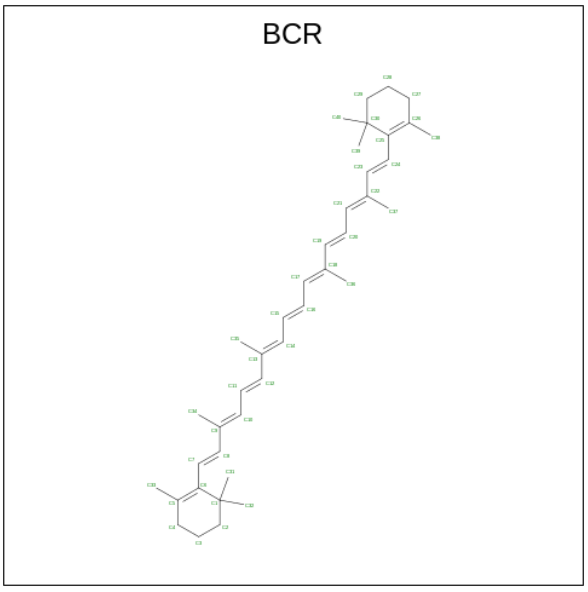
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



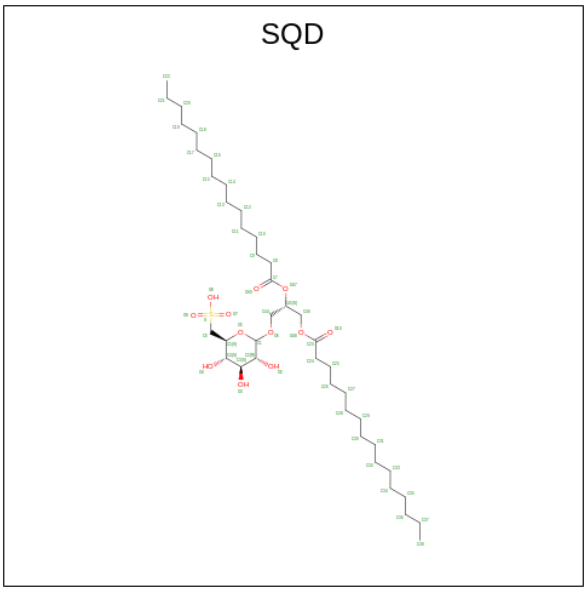
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



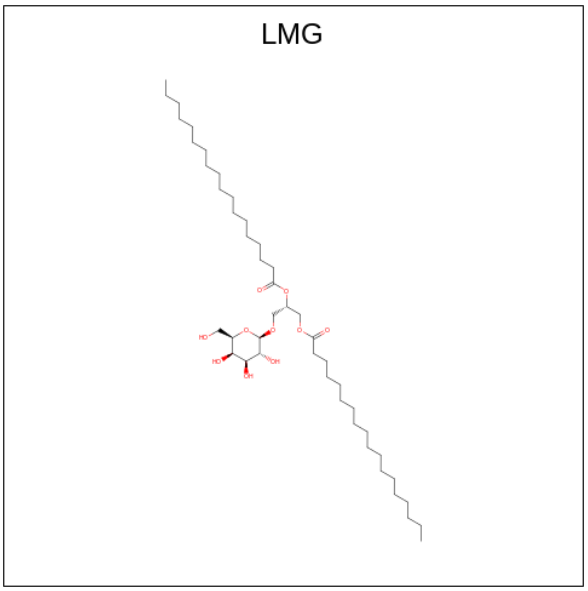
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



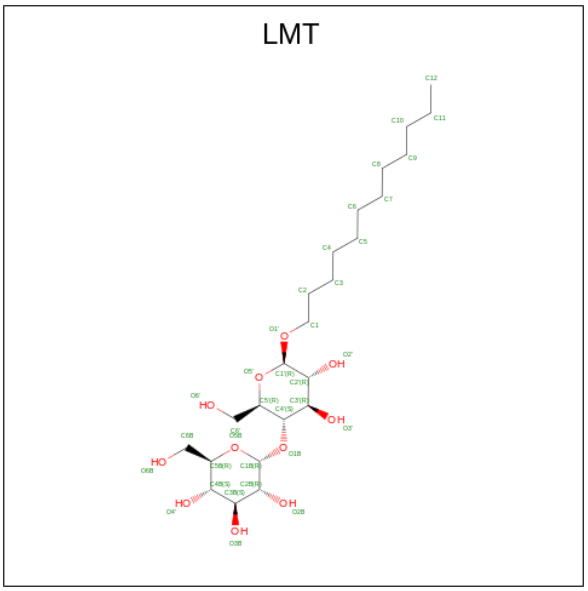
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			49	36	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			45	32	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			53	40	12	1		
27	a	1	Total	C	O	S	0	0
			47	34	12	1		
27	f	1	Total	C	O	S	0	0
			37	27	9	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 51 41 10	0	0
28	B	1	Total C O 51 41 10	0	0
28	C	1	Total C O 51 41 10	0	0
28	C	1	Total C O 48 38 10	0	0
28	D	1	Total C O 44 34 10	0	0
28	b	1	Total C O 51 41 10	0	0
28	c	1	Total C O 49 39 10	0	0
28	c	1	Total C O 48 38 10	0	0
28	d	1	Total C O 48 38 10	0	0
28	i	1	Total C O 51 41 10	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 34 23 11	0	0
29	A	1	Total C O 35 24 11	0	0
29	B	1	Total C O 35 24 11	0	0
29	B	1	Total C O 35 24 11	0	0
29	B	1	Total C O 24 18 6	0	0
29	E	1	Total C O 24 18 6	0	0
29	I	1	Total C O 24 18 6	0	0
29	J	1	Total C O 24 18 6	0	0
29	M	1	Total C O 35 24 11	0	0
29	T	1	Total C O 24 18 6	0	0
29	Z	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	b	1	Total C O 25 19 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	f	1	Total C O 24 18 6	0	0
29	i	1	Total C O 24 18 6	0	0
29	j	1	Total C O 23 17 6	0	0
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	z	1	Total C O 33 22 11	0	0

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

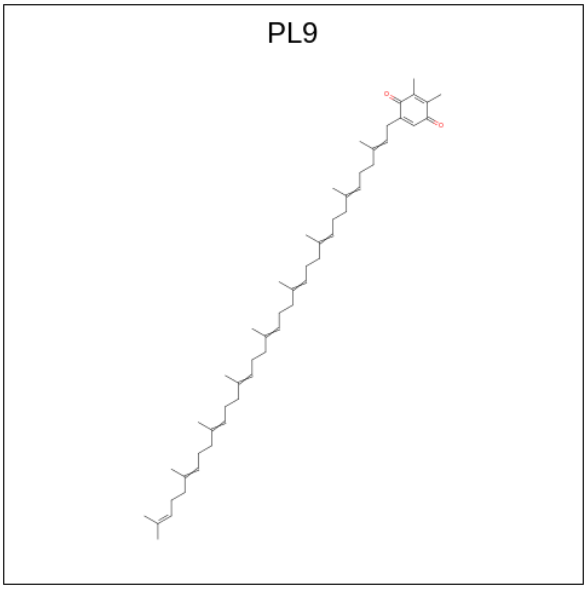
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	2	Total C O 55 50 5	0	0
30	B	5	Total C O 74 68 6	0	0
30	C	2	Total C O 50 45 5	0	0
30	D	3	Total C O 65 60 5	0	0
30	E	4	Total C 43 43	0	0
30	I	2	Total C 29 29	0	0
30	J	1	Total C 15 15	0	0
30	M	1	Total C O 15 13 2	0	0
30	T	1	Total C 9 9	0	0
30	Y	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0
30	a	2	Total C O 26 22 4	0	0
30	b	4	Total C O 56 52 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	c	2	Total C O 48 43 5	0	0
30	d	4	Total C O 82 75 7	0	0
30	e	1	Total C 15 15	0	0
30	h	2	Total C 23 23	0	0
30	i	2	Total C O 29 25 4	0	0
30	j	1	Total C 16 16	0	0
30	k	1	Total C 12 12	0	0
30	m	1	Total C 13 13	0	0
30	t	1	Total C 8 8	0	0

- Molecule 31 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



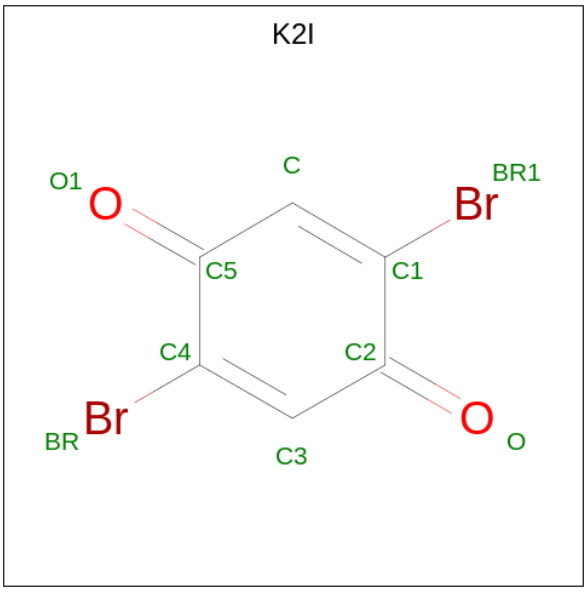
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C 39 39	0	0

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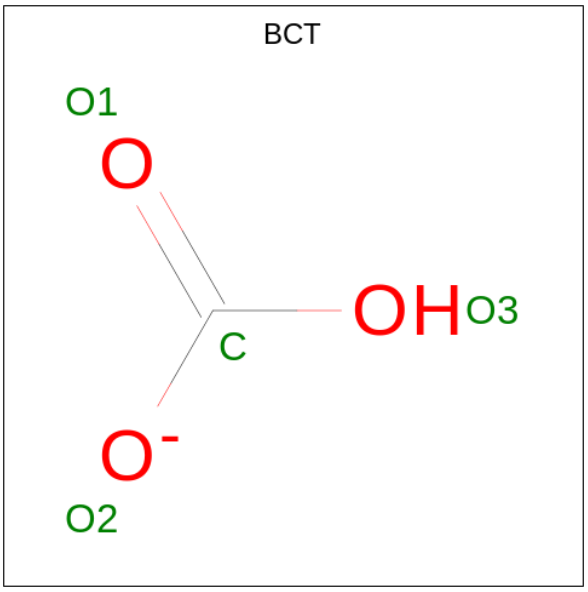
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	D	1	Total C O 55 53 2	0	0
31	d	1	Total C O 55 53 2	0	0
31	x	1	Total C 39 39	0	0

- Molecule 32 is 2,5-bis(bromanyl)cyclohexa-2,5-diene-1,4-dione (CCD ID: K2I) (formula: $C_6H_2Br_2O_2$) (labeled as "Ligand of Interest" by depositor).



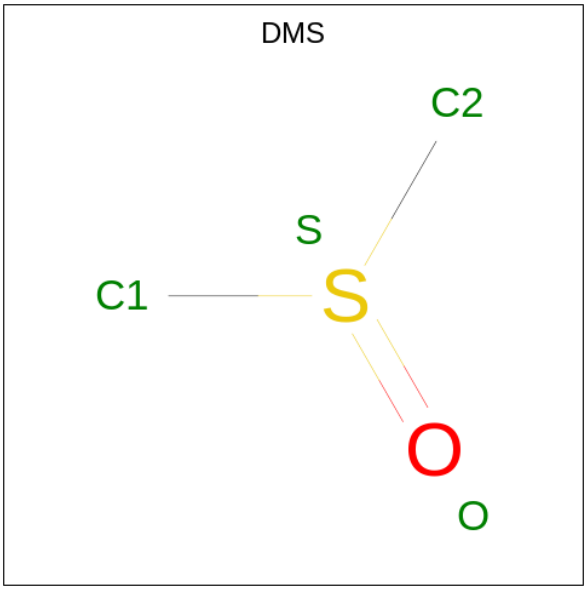
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Br C O 20 4 12 4	0	1
32	A	1	Total Br C O 10 2 6 2	0	0
32	a	1	Total Br C O 20 4 12 4	0	1
32	a	1	Total Br C O 10 2 6 2	0	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	E	1	Total	C	O	S	0	0
			4	2	1	1		
34	E	1	Total	C	O	S	0	0
			4	2	1	1		
34	F	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	U	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	a	1	Total	C	O	S	0	0
			4	2	1	1		
34	a	1	Total	C	O	S	0	0
			4	2	1	1		
34	a	1	Total	C	O	S	0	0
			4	2	1	1		
34	a	1	Total	C	O	S	0	0
			4	2	1	1		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	e	1	Total	C	O	S	0	0
			4	2	1	1		
34	i	1	Total	C	O	S	0	0
			4	2	1	1		
34	j	1	Total	C	O	S	0	0
			4	2	1	1		
34	k	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		

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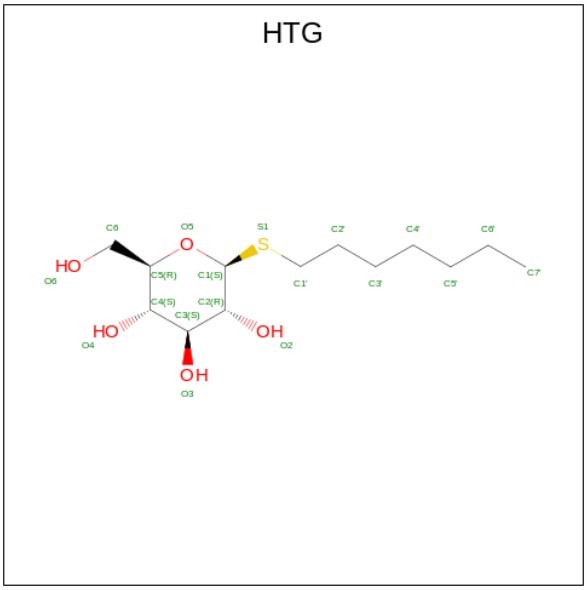
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	t	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	x	1	Total	C	O	S	0	0
			4	2	1	1		
34	z	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



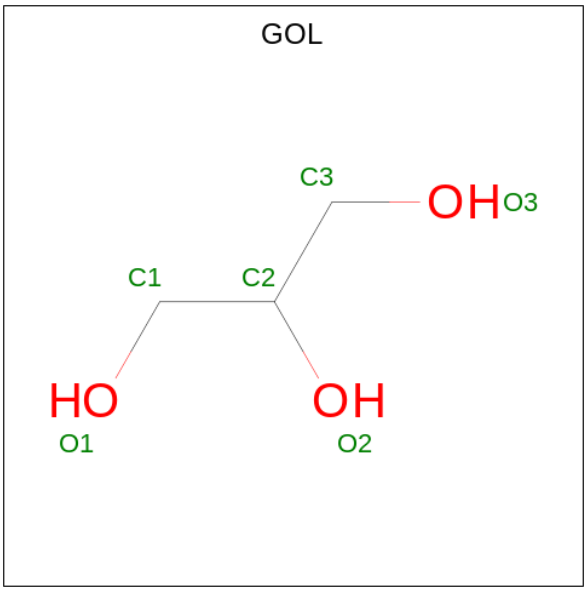
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 38 26 10 2	0	1
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			19	13	5	1		
36	I	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	i	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 37 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



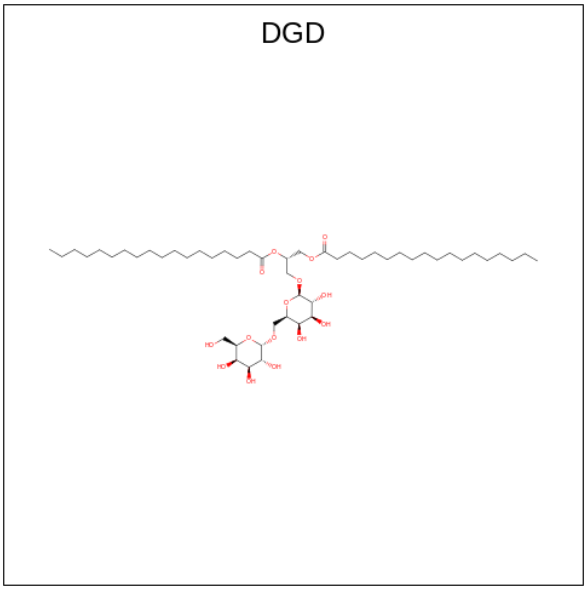
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	B	1	Total C O 6 3 3	0	0
37	B	1	Total C O 6 3 3	0	0
37	C	1	Total C O 6 3 3	0	0
37	C	1	Total C O 6 3 3	0	0
37	D	1	Total C O 6 3 3	0	0
37	H	1	Total C O 6 3 3	0	0
37	O	1	Total C O 6 3 3	0	0
37	U	1	Total C O 6 3 3	0	0
37	U	1	Total C O 6 3 3	0	0
37	V	1	Total C O 6 3 3	0	0
37	Z	1	Total C O 6 3 3	0	0
37	a	1	Total C O 6 3 3	0	0
37	b	1	Total C O 6 3 3	0	0
37	c	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	d	1	Total C O 6 3 3	0	0
37	k	1	Total C O 6 3 3	0	0
37	o	1	Total C O 6 3 3	0	0
37	o	1	Total C O 6 3 3	0	0
37	v	1	Total C O 6 3 3	0	0
37	v	1	Total C O 6 3 3	0	0
37	v	1	Total C O 6 3 3	0	0

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



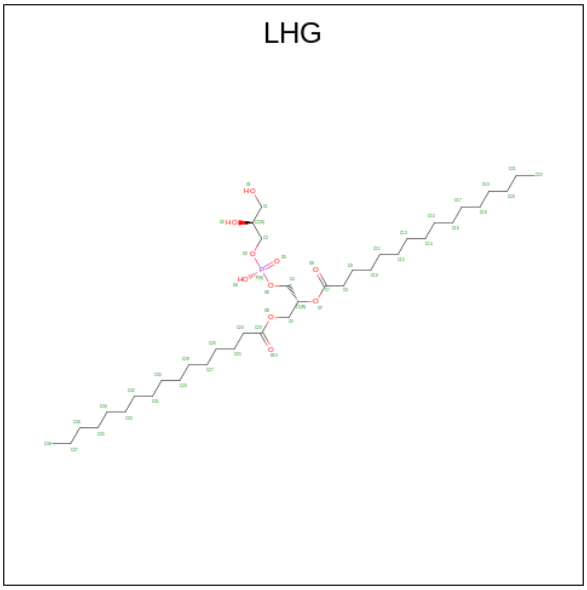
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	C	1	Total C O 62 47 15	0	0
38	C	1	Total C O 62 47 15	0	0
38	C	1	Total C O 62 47 15	0	0
38	D	1	Total C O 46 35 11	0	0

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

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



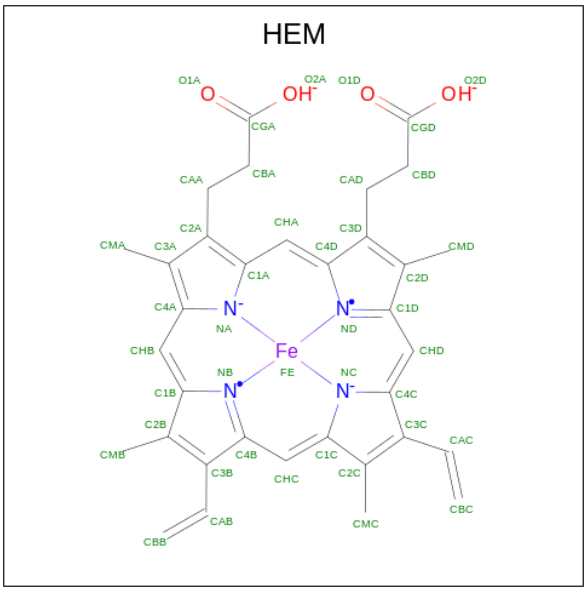
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	D	1	Total C O P 49 38 10 1	0	0
39	D	1	Total C O P 49 38 10 1	0	0
39	D	1	Total C O P 44 33 10 1	0	0
39	E	1	Total C O P 49 38 10 1	0	0
39	L	1	Total C O P 49 38 10 1	0	0
39	d	1	Total C O P 49 38 10 1	0	0

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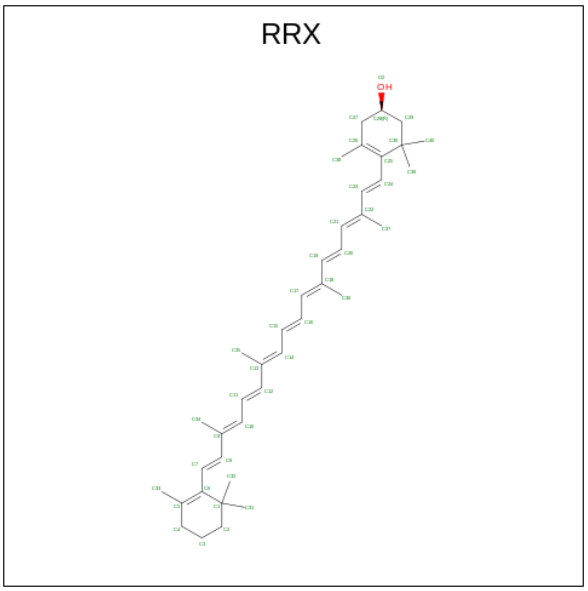
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	d	1	Total C O P 49 38 10 1	0	0
39	d	1	Total C O P 36 25 10 1	0	0
39	e	1	Total C O P 32 22 9 1	0	0
39	l	1	Total C O P 49 38 10 1	0	0

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 41 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).

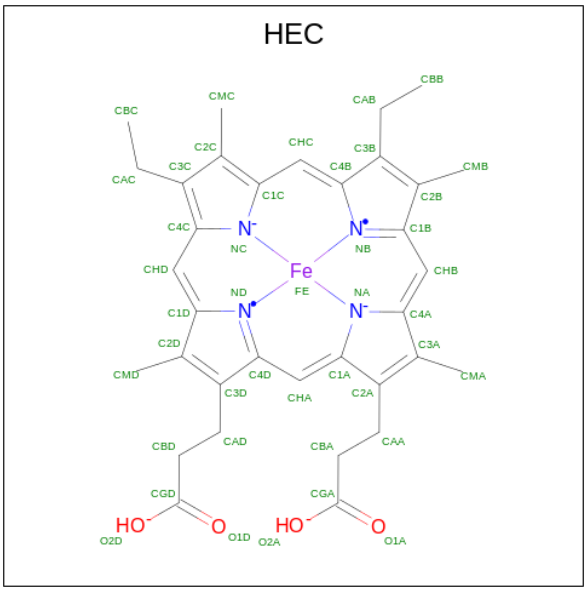


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	H	1	Total C O 41 40 1	0	0
41	h	1	Total C O 41 40 1	0	0

- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 43 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
44	A	142	Total	O	0	0
			142	142		
44	B	291	Total	O	0	0
			291	291		
44	C	231	Total	O	0	0
			231	231		
44	D	140	Total	O	0	2
			142	142		
44	E	34	Total	O	0	0
			34	34		
44	F	6	Total	O	0	0
			6	6		
44	H	47	Total	O	0	0
			47	47		
44	I	11	Total	O	0	0
			11	11		
44	J	13	Total	O	0	0
			13	13		
44	K	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	L	19	Total O 19 19	0	0
44	M	6	Total O 6 6	0	0
44	O	148	Total O 148 148	0	0
44	T	13	Total O 13 13	0	0
44	U	80	Total O 80 80	0	0
44	V	121	Total O 121 121	0	0
44	Y	5	Total O 5 5	0	0
44	X	14	Total O 14 14	0	0
44	Z	1	Total O 1 1	0	0
44	a	135	Total O 135 135	0	0
44	b	265	Total O 268 268	0	3
44	c	229	Total O 229 229	0	0
44	d	135	Total O 135 135	0	0
44	e	23	Total O 23 23	0	0
44	f	9	Total O 9 9	0	0
44	h	32	Total O 32 32	0	0
44	i	12	Total O 12 12	0	0
44	j	15	Total O 15 15	0	0
44	k	8	Total O 8 8	0	0
44	l	13	Total O 14 14	0	1
44	m	9	Total O 9 9	0	0

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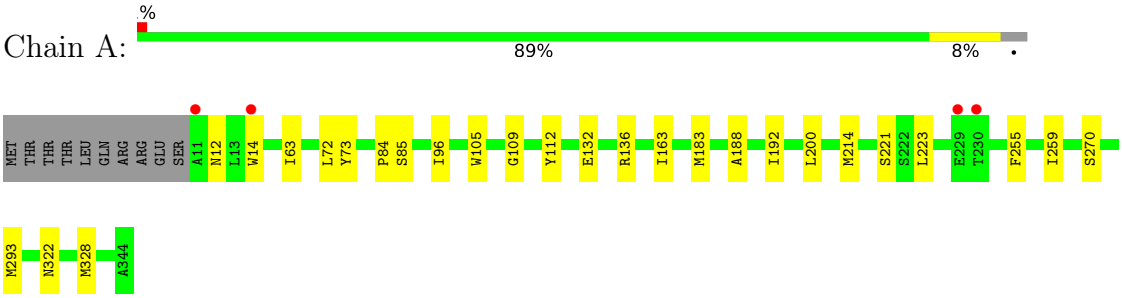
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	o	130	Total O 131 131	0	1
44	t	11	Total O 11 11	0	0
44	u	90	Total O 91 91	0	1
44	v	98	Total O 100 100	0	2
44	y	8	Total O 8 8	0	0
44	x	12	Total O 12 12	0	0
44	z	4	Total O 4 4	0	0
44	R	1	Total O 1 1	0	0

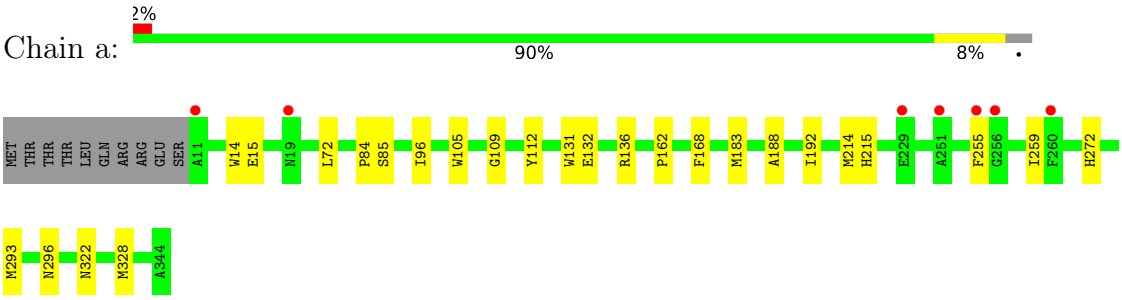
3 Residue-property plots

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

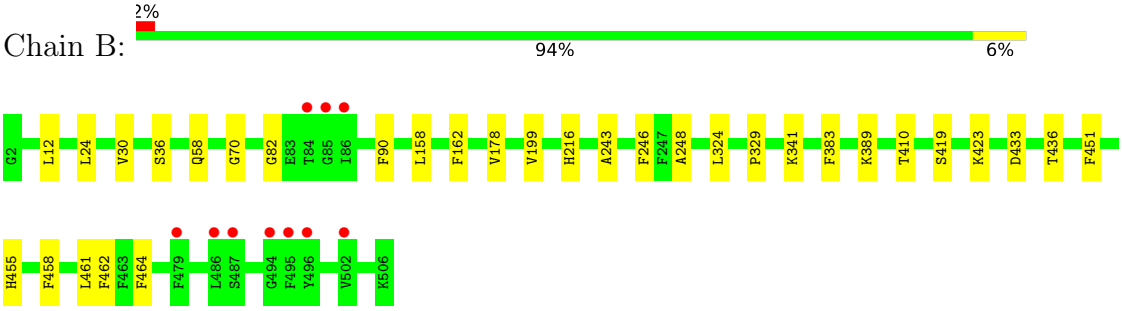
• Molecule 1: Photosystem II protein D1



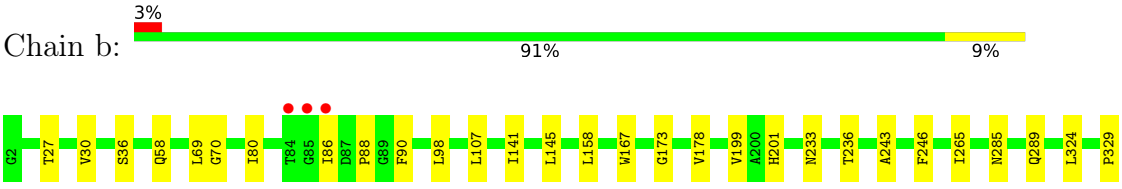
• Molecule 1: Photosystem II protein D1

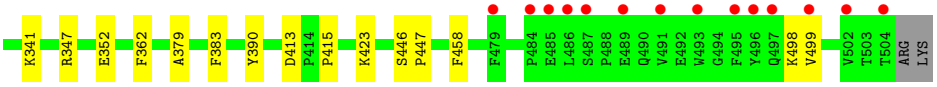


• Molecule 2: Photosystem II CP47 reaction center protein

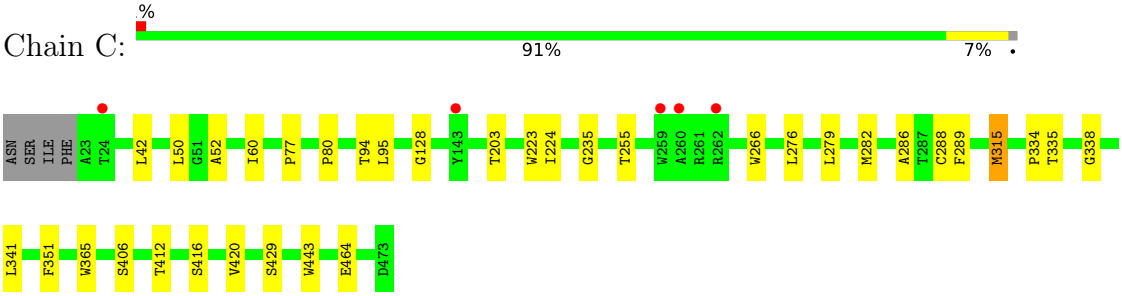


• Molecule 2: Photosystem II CP47 reaction center protein

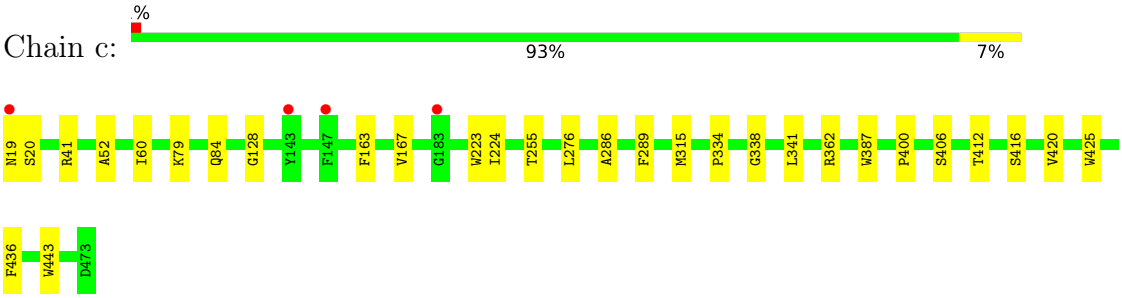




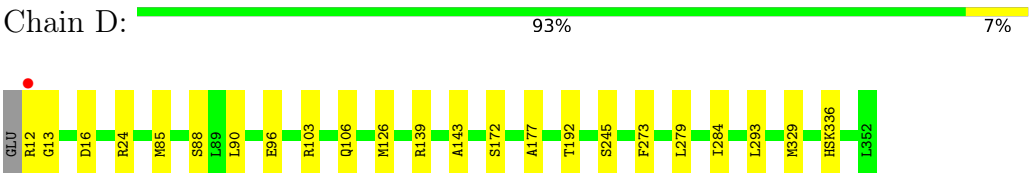
• Molecule 3: Photosystem II CP43 reaction center protein



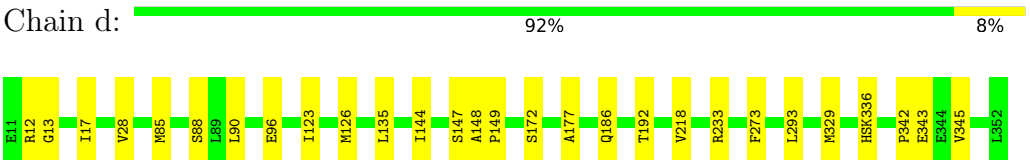
• Molecule 3: Photosystem II CP43 reaction center protein



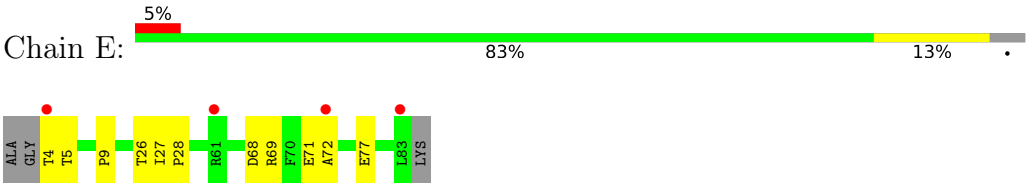
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein



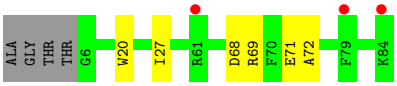
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

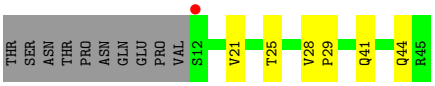




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

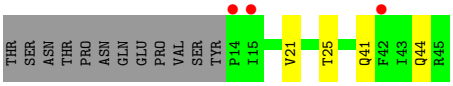




• Molecule 6: Cytochrome b559 subunit beta

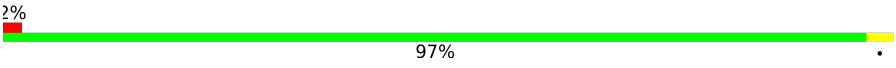
Chain f:





• Molecule 7: Photosystem II reaction center protein H

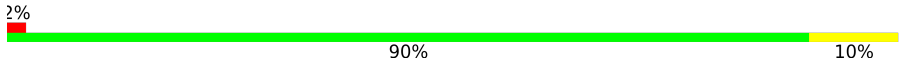
Chain H:

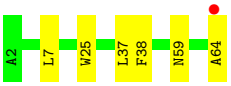




• Molecule 7: Photosystem II reaction center protein H

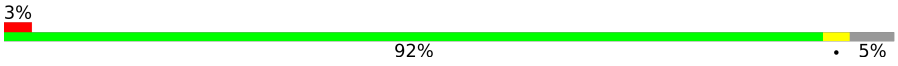
Chain h:





• Molecule 8: Photosystem II reaction center protein I

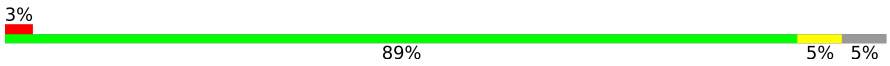
Chain I:

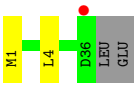




• Molecule 8: Photosystem II reaction center protein I

Chain i:

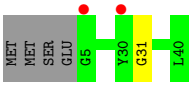




• Molecule 9: Photosystem II reaction center protein J

Chain J:

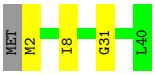




• Molecule 9: Photosystem II reaction center protein J

Chain j:

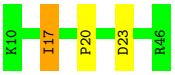




• Molecule 10: Photosystem II reaction center protein K

Chain K:





• Molecule 10: Photosystem II reaction center protein K

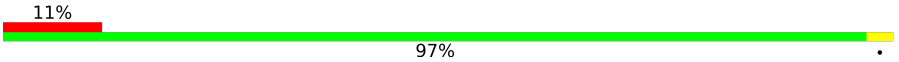
Chain k:

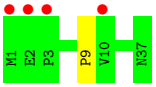




• Molecule 11: Photosystem II reaction center protein L

Chain L:

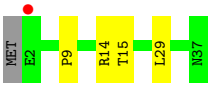




• Molecule 11: Photosystem II reaction center protein L

Chain l:

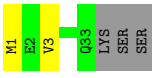




• Molecule 12: Photosystem II reaction center protein M

Chain M:

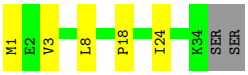




• Molecule 12: Photosystem II reaction center protein M

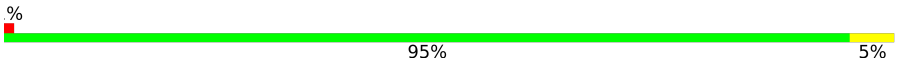
Chain m:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

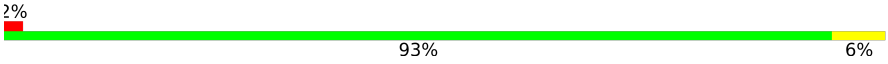
Chain O:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

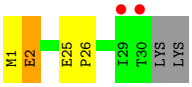




• Molecule 14: Photosystem II reaction center protein T

Chain T:

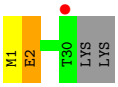




• Molecule 14: Photosystem II reaction center protein T

Chain t:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

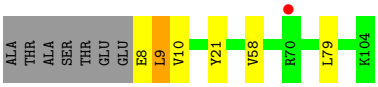




• Molecule 15: Photosystem II 12 kDa extrinsic protein

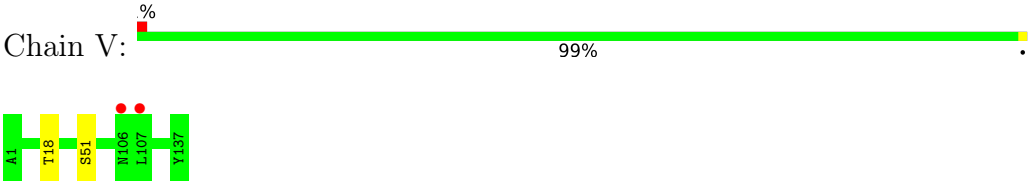
Chain u:





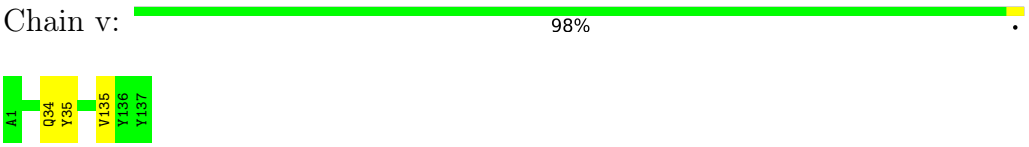
• Molecule 16: Cytochrome c-550

Chain V:



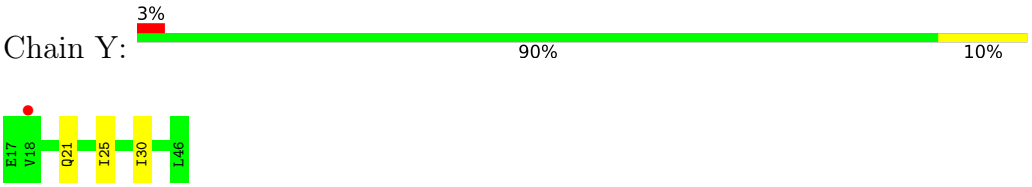
• Molecule 16: Cytochrome c-550

Chain v:



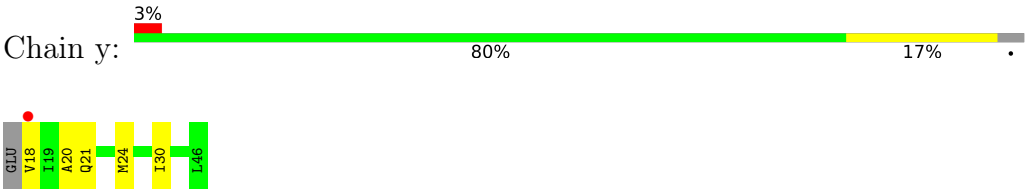
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



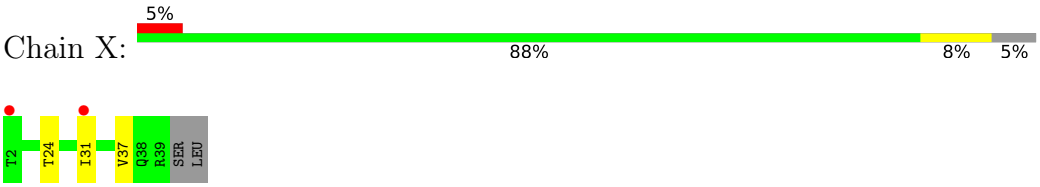
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



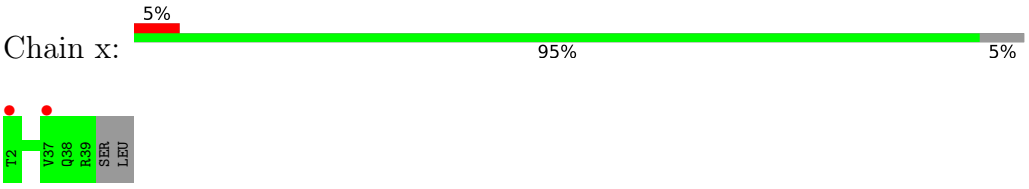
• Molecule 18: Photosystem II reaction center protein X

Chain X:



• Molecule 18: Photosystem II reaction center protein X

Chain x:



• Molecule 19: Photosystem II reaction center protein Z

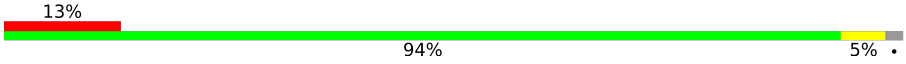
Chain Z:

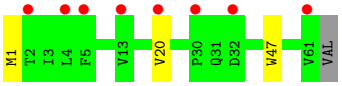




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

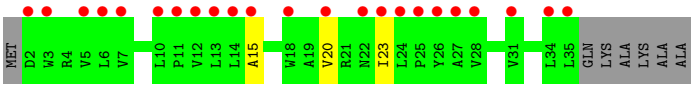




• Molecule 20: Photosystem II protein Y

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.19Å 228.46Å 286.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.10 49.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.02-2.10) 88.1 (49.02-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.46 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.157 , 0.191 0.163 , 0.194	Depositor DCC
R_{free} test set	22959 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	54282	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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, HTG, LMT, BCR, SQD, LMG, LHG, PL9, RRX, CL, DMS, FE2, UNL, HEM, BCT, CLA, HSK, HEC, CA, K2I, FME, PHO, GOL, MG, OEX

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	0.35	0/2704	0.53	0/3690
1	a	0.34	0/2713	0.52	0/3700
2	B	0.33	0/4149	0.49	0/5652
2	b	0.32	0/4123	0.47	0/5619
3	C	0.30	0/3613	0.46	0/4919
3	c	0.28	0/3632	0.46	0/4945
4	D	0.36	0/2804	0.50	0/3820
4	d	0.34	0/2827	0.48	0/3850
5	E	0.27	0/671	0.45	0/918
5	e	0.24	0/648	0.44	0/887
6	F	0.24	0/284	0.43	0/387
6	f	0.25	0/265	0.45	0/360
7	H	0.28	0/511	0.42	0/697
7	h	0.26	0/511	0.43	0/697
8	I	0.21	0/290	0.40	0/393
8	i	0.25	0/293	0.43	0/396
9	J	0.23	0/257	0.40	0/349
9	j	0.22	0/277	0.36	0/376
10	K	0.25	0/306	0.45	0/422
10	k	0.24	0/296	0.42	0/408
11	L	0.39	0/308	0.43	0/420
11	l	0.35	0/314	0.44	0/428
12	M	0.30	0/257	0.52	0/352
12	m	0.32	0/266	0.46	0/363
13	O	0.31	0/1901	0.50	0/2579
13	o	0.28	0/1905	0.49	0/2583
14	T	0.34	0/255	0.42	0/346
14	t	0.33	0/255	0.40	0/346
15	U	0.32	0/792	0.49	0/1073
15	u	0.31	0/785	0.47	0/1064
16	V	0.32	0/1083	0.46	0/1470

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.26	0/1073	0.44	0/1461
17	Y	0.22	0/221	0.37	0/296
17	y	0.24	0/213	0.40	0/285
18	X	0.21	0/278	0.34	0/376
18	x	0.20	0/284	0.35	0/384
19	Z	0.20	0/459	0.38	0/630
19	z	0.17	0/454	0.35	0/622
20	R	0.16	0/209	0.33	0/290
All	All	0.31	0/42486	0.47	0/57853

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2610	0	2506	20	0
1	a	2620	0	2527	18	0
2	B	3997	0	3860	31	0
2	b	3962	0	3813	30	0
3	C	3494	0	3418	27	0
3	c	3518	0	3434	23	0
4	D	2726	0	2629	19	0
4	d	2743	0	2652	21	0
5	E	649	0	627	8	0
5	e	629	0	600	6	0
6	F	275	0	282	3	0
6	f	257	0	269	2	0
7	H	498	0	518	3	0
7	h	498	0	518	5	0
8	I	293	0	302	0	0
8	i	296	0	311	1	0
9	J	251	0	257	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	271	0	270	4	0
10	K	293	0	303	3	0
10	k	286	0	285	4	0
11	L	298	0	309	1	0
11	l	301	0	320	4	0
12	M	261	0	280	1	0
12	m	270	0	293	4	0
13	O	1864	0	1835	9	0
13	o	1865	0	1842	10	0
14	T	256	0	256	2	0
14	t	256	0	256	1	0
15	U	778	0	782	6	0
15	u	774	0	773	3	0
16	V	1059	0	1074	2	0
16	v	1052	0	1040	3	0
17	Y	220	0	245	3	0
17	y	212	0	237	4	0
18	X	275	0	301	3	0
18	x	278	0	305	0	0
19	Z	458	0	472	0	0
19	z	453	0	459	3	0
20	R	207	0	157	2	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	195	0	216	4	0
24	B	1040	0	1152	25	0
24	C	845	0	936	29	0
24	D	195	0	216	5	0
24	a	195	0	216	6	0
24	b	1040	0	1152	27	0
24	c	845	0	936	28	0
24	d	195	0	216	7	0
25	A	128	0	148	2	0
25	a	128	0	148	1	0
26	A	40	0	56	1	0
26	B	120	0	168	6	0
26	C	80	0	112	7	0
26	D	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	K	40	0	56	1	0
26	T	40	0	56	5	0
26	Y	40	0	56	3	0
26	a	40	0	56	1	0
26	b	120	0	168	6	0
26	c	120	0	168	6	0
26	d	40	0	56	1	0
26	k	40	0	56	1	0
26	t	40	0	56	6	0
27	A	103	0	143	2	0
27	B	54	0	78	3	0
27	F	45	0	57	2	0
27	L	54	0	78	1	0
27	a	100	0	131	2	0
27	f	37	0	45	1	0
28	A	51	0	72	1	0
28	B	51	0	72	2	0
28	C	99	0	138	2	0
28	D	44	0	58	0	0
28	b	51	0	72	1	0
28	c	97	0	134	1	0
28	d	48	0	66	0	0
28	i	51	0	72	2	0
29	A	69	0	87	3	0
29	B	94	0	127	2	0
29	E	24	0	35	0	0
29	I	24	0	35	0	0
29	J	24	0	35	1	0
29	M	35	0	46	2	0
29	T	24	0	35	0	0
29	Z	35	0	46	0	0
29	a	70	0	92	4	0
29	b	25	0	35	0	0
29	f	24	0	35	0	0
29	i	24	0	35	1	0
29	j	23	0	22	0	0
29	m	70	0	92	2	0
29	z	33	0	35	2	0
30	A	55	0	0	0	0
30	B	74	0	0	0	0
30	C	50	0	0	0	0
30	D	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	E	43	0	0	0	0
30	I	29	0	0	0	0
30	J	15	0	0	0	0
30	M	15	0	0	0	0
30	T	9	0	0	0	0
30	X	18	0	0	0	0
30	Y	10	0	0	0	0
30	a	26	0	0	0	0
30	b	56	0	0	0	0
30	c	48	0	0	0	0
30	d	82	0	0	0	0
30	e	15	0	0	0	0
30	h	23	0	0	0	0
30	i	29	0	0	0	0
30	j	16	0	0	0	0
30	k	12	0	0	0	0
30	m	13	0	0	0	0
30	t	8	0	0	0	0
31	A	39	0	59	2	0
31	D	55	0	80	0	0
31	d	55	0	80	1	0
31	x	39	0	59	1	0
32	A	30	0	0	3	0
32	a	30	0	0	3	0
33	A	4	0	0	0	0
33	a	4	0	0	0	0
34	A	20	0	30	0	0
34	B	52	0	78	2	0
34	C	52	0	78	3	0
34	D	20	0	30	0	0
34	E	8	0	12	0	0
34	F	4	0	6	0	0
34	O	44	0	66	2	0
34	T	12	0	18	0	0
34	U	4	0	6	2	0
34	V	28	0	42	1	0
34	a	16	0	24	0	0
34	b	48	0	72	2	0
34	c	56	0	84	2	0
34	d	28	0	42	3	0
34	e	4	0	6	0	0
34	i	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	j	4	0	6	0	0
34	k	4	0	6	0	0
34	o	36	0	54	1	0
34	t	4	0	6	0	0
34	u	16	0	24	0	0
34	v	40	0	60	1	0
34	x	4	0	6	0	0
34	z	4	0	6	0	0
35	B	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	1	0	0	0	0
35	o	1	0	0	0	0
36	B	114	0	156	8	0
36	C	38	0	52	0	0
36	D	19	0	26	3	0
36	I	19	0	26	1	0
36	O	19	0	26	1	0
36	V	19	0	26	0	0
36	b	76	0	104	7	0
36	c	57	0	78	0	0
36	d	38	0	52	2	0
36	i	19	0	26	0	0
37	B	12	0	16	2	0
37	C	12	0	16	0	0
37	D	6	0	8	1	0
37	H	6	0	8	0	0
37	O	6	0	8	0	0
37	U	12	0	16	0	0
37	V	6	0	8	0	0
37	Z	6	0	8	0	0
37	a	6	0	8	0	0
37	b	6	0	8	0	0
37	c	6	0	8	2	0
37	d	6	0	8	0	0
37	k	6	0	8	0	0
37	o	12	0	16	2	0
37	v	18	0	24	0	0
38	C	186	0	246	9	0
38	D	46	0	57	0	0
38	H	62	0	82	0	0
38	c	186	0	246	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	62	0	82	1	0
39	D	142	0	209	5	0
39	E	49	0	74	5	0
39	L	49	0	74	2	0
39	d	134	0	190	3	0
39	e	32	0	43	1	0
39	l	49	0	74	1	0
40	F	43	0	30	1	0
40	e	43	0	30	2	0
41	H	41	0	56	3	0
41	h	41	0	56	3	0
42	J	1	0	0	0	0
42	j	1	0	0	0	0
43	V	43	0	30	0	0
43	v	43	0	30	0	0
44	A	142	0	0	0	0
44	B	291	0	0	2	0
44	C	231	0	0	1	0
44	D	142	0	0	0	0
44	E	34	0	0	0	0
44	F	6	0	0	0	0
44	H	47	0	0	0	0
44	I	11	0	0	0	0
44	J	13	0	0	0	0
44	K	12	0	0	0	0
44	L	19	0	0	0	0
44	M	6	0	0	0	0
44	O	148	0	0	1	0
44	R	1	0	0	0	0
44	T	13	0	0	0	0
44	U	80	0	0	4	0
44	V	121	0	0	0	0
44	X	14	0	0	0	0
44	Y	5	0	0	0	0
44	Z	1	0	0	0	0
44	a	135	0	0	0	0
44	b	268	0	0	4	0
44	c	229	0	0	0	0
44	d	135	0	0	0	0
44	e	23	0	0	0	0
44	f	9	0	0	0	0
44	h	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	i	12	0	0	0	0
44	j	15	0	0	1	0
44	k	8	0	0	0	0
44	l	14	0	0	0	0
44	m	9	0	0	0	0
44	o	131	0	0	3	0
44	t	11	0	0	0	0
44	u	91	0	0	0	0
44	v	100	0	0	1	0
44	x	12	0	0	0	0
44	y	8	0	0	0	0
44	z	4	0	0	0	0
All	All	54282	0	52476	414	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 4.

All (414) 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)
1:a:14:TRP:HD1	29:a:2120:LMT:H6B	0.98	0.91
1:a:14:TRP:CD1	29:a:2120:LMT:H6B	1.91	0.86
4:D:13:GLY:HA3	36:D:413:HTG:H62	1.62	0.82
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.68	0.76
24:b:618:CLA:H2	24:b:619:CLA:HBB2	1.71	0.73
3:C:315:MET:HG3	3:C:365:TRP:HZ3	1.55	0.72
2:B:410:THR:H	37:B:635:GOL:H2	1.53	0.72
2:B:248:ALA:HA	24:B:604:CLA:H42	1.73	0.70
4:d:13:GLY:HA3	36:d:403:HTG:H62	1.75	0.69
36:B:624:HTG:H1	29:a:2103:LMT:H21	1.74	0.69
36:b:601:HTG:O2	36:b:602:HTG:S1	2.48	0.68
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.75	0.68
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.74	0.68
24:c:513:CLA:H171	19:z:20:VAL:HA	1.76	0.67
2:B:90:PHE:H	36:B:628:HTG:H62	1.59	0.66
24:B:612:CLA:H142	39:L:101:LHG:H372	1.78	0.65
13:o:23:ASP:OD1	13:o:23:ASP:N	2.28	0.64
26:B:618:BCR:H383	27:B:621:SQD:H91	1.79	0.64
24:c:503:CLA:C4D	24:c:505:CLA:H2	2.27	0.64
4:d:233:ARG:NH2	34:d:423:DMS:S	2.71	0.64
3:C:315:MET:HG2	3:C:351:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:ILE:HG12	40:F:102:HEM:HMC3	1.79	0.63
25:A:408:PHO:HBC3	4:D:279:LEU:HD22	1.81	0.62
36:I:1202:HTG:H1	36:b:602:HTG:H1	1.80	0.61
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.82	0.61
38:c:518:DGD:HB52	28:i:101:LMG:H382	1.81	0.61
5:e:68:ASP:OD2	5:e:71:GLU:HB2	2.01	0.61
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.82	0.61
24:b:608:CLA:HHC	24:b:608:CLA:HBB1	1.82	0.61
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.83	0.61
4:D:192:THR:HG23	24:D:404:CLA:HBC2	1.83	0.60
11:L:9:PRO:HA	29:m:102:LMT:H6D	1.84	0.60
26:B:619:BCR:H363	26:t:102:BCR:H19C	1.84	0.59
1:a:183:MET:HA	24:a:2109:CLA:HMD1	1.83	0.59
20:R:20:VAL:HA	20:R:23:ILE:HG22	1.85	0.59
15:U:70[B]:ARG:NH1	44:U:603:HOH:O	2.34	0.59
3:c:286:ALA:HB2	24:c:504:CLA:HMD1	1.84	0.58
24:C:505:CLA:H42	38:C:518:DGD:HB52	1.86	0.58
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.86	0.57
5:E:68:ASP:OD2	5:E:71:GLU:HB2	2.04	0.57
24:C:503:CLA:H61	24:C:513:CLA:H42	1.85	0.57
2:B:82:GLY:O	37:o:2601:GOL:O1	2.22	0.57
15:u:8:GLU:HG3	15:u:9:LEU:HD13	1.86	0.57
28:C:520:LMG:H172	17:Y:25:ILE:HG12	1.86	0.57
24:C:514:CLA:HAB	26:C:515:BCR:H24C	1.86	0.56
26:c:528:BCR:H321	26:c:528:BCR:HC8	1.87	0.56
36:d:403:HTG:H1	7:h:25:TRP:CD1	2.40	0.56
24:b:618:CLA:H2	24:b:619:CLA:CBB	2.35	0.56
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.89	0.56
24:b:604:CLA:H72	24:b:604:CLA:H2	1.88	0.55
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.42	0.55
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.87	0.55
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.42	0.55
24:B:605:CLA:H43	24:B:606:CLA:H2	1.89	0.55
24:c:504:CLA:H61	24:c:514:CLA:H42	1.89	0.55
24:c:508:CLA:HMC2	24:c:509:CLA:H102	1.89	0.54
13:O:111:ALA:HB3	34:O:309:DMS:H12	1.89	0.54
1:a:215:HIS:ND1	32:a:2118[B]:K2I:O	2.30	0.54
24:C:514:CLA:H171	26:C:515:BCR:H373	1.90	0.54
24:B:603:CLA:H101	24:B:610:CLA:H193	1.90	0.54
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	1.90	0.54
15:U:81:HIS:HE1	44:U:670:HOH:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.38	0.53
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.44	0.53
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.42	0.53
2:b:499:VAL:HG12	4:d:135:LEU:HB3	1.90	0.53
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.07	0.53
27:B:621:SQD:H242	11:l:14:ARG:HD3	1.90	0.53
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.73	0.53
3:c:60:ILE:HG22	24:c:505:CLA:HHD	1.91	0.53
3:c:52:ALA:HB2	24:c:513:CLA:HMA2	1.91	0.53
38:c:519:DGD:HAT2	38:c:520:DGD:HBN2	1.90	0.52
10:k:20:PRO:HB3	17:y:21:GLN:HG3	1.91	0.52
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.91	0.52
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.92	0.52
34:c:531:DMS:H11	34:v:205:DMS:H22	1.92	0.52
24:B:615:CLA:H18	28:B:622:LMG:H422	1.90	0.52
1:a:84:PRO:HA	1:a:112:TYR:CG	2.45	0.52
24:c:507:CLA:HAA1	24:c:507:CLA:HBD	1.92	0.52
13:O:194:LYS:HE2	44:O:534:HOH:O	2.10	0.51
2:B:162:PHE:O	24:B:607:CLA:HHD	2.11	0.51
9:j:2:MET:N	44:j:1701:HOH:O	2.43	0.51
13:o:180:GLU:CD	13:o:180:GLU:H	2.18	0.51
1:A:200:LEU:HG	38:C:519:DGD:HAT2	1.93	0.51
24:C:510:CLA:H141	24:C:513:CLA:HMD3	1.93	0.51
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.93	0.51
24:b:613:CLA:HHC	24:b:613:CLA:HBB1	1.93	0.51
3:C:279:LEU:HD22	24:C:510:CLA:HED2	1.93	0.51
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.10	0.50
24:b:607:CLA:H43	24:b:608:CLA:H2	1.93	0.50
2:B:341:LYS:NZ	36:B:625[B]:HTG:S1	2.83	0.50
26:T:101:BCR:H19C	26:b:621:BCR:H363	1.93	0.50
24:b:604:CLA:H122	24:b:604:CLA:C4B	2.42	0.50
28:B:622:LMG:H242	4:D:284:ILE:HD13	1.93	0.50
24:C:506:CLA:HBC2	26:C:516:BCR:H341	1.92	0.50
7:h:59:ASN:O	7:h:64:ALA:HB3	2.12	0.50
1:a:215:HIS:HA	32:a:2118[B]:K2I:O	2.12	0.50
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.94	0.50
17:y:20:ALA:O	17:y:24:MET:HG2	2.12	0.50
24:C:502:CLA:C3D	24:C:504:CLA:H2	2.42	0.49
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.48	0.49
34:U:503:DMS:H23	16:V:51:SER:HA	1.94	0.49
4:d:126[B]:MET:HE1	4:d:147:SER:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.49
24:A:409:CLA:H172	24:C:507:CLA:H91	1.95	0.49
2:b:69:LEU:HD12	24:b:608:CLA:HBA1	1.93	0.49
2:b:233:ASN:O	2:b:236:THR:HG22	2.12	0.49
24:B:617:CLA:H101	24:B:617:CLA:H142	1.93	0.49
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.93	0.49
3:C:338:GLY:HA3	3:C:341:LEU:O	2.12	0.49
3:c:41:ARG:NH1	24:c:513:CLA:HMD1	2.28	0.49
26:Y:302:BCR:H321	26:Y:302:BCR:HC8	1.93	0.49
10:K:17:ILE:H	10:K:17:ILE:HD13	1.78	0.49
26:T:101:BCR:HC7	26:T:101:BCR:H331	1.52	0.49
2:b:58:GLN:C	2:b:329:PRO:HB3	2.38	0.49
24:c:503:CLA:H202	24:c:509:CLA:HBB1	1.94	0.49
2:b:145:LEU:HB3	24:b:607:CLA:H162	1.95	0.48
36:b:625:HTG:H6'1	44:b:898:HOH:O	2.13	0.48
13:o:69:LYS:NZ	44:o:2705:HOH:O	2.45	0.48
1:A:255:PHE:CD2	32:A:418[B]:K2I:BR	3.22	0.48
3:C:266:TRP:CZ3	24:C:508:CLA:HAC2	2.48	0.48
24:c:503:CLA:C3D	24:c:505:CLA:H2	2.43	0.48
8:i:4:LEU:HD22	29:i:104:LMT:H61	1.96	0.48
17:y:18:VAL:HG22	17:y:20:ALA:H	1.79	0.48
16:V:18:THR:H	34:V:206:DMS:H13	1.78	0.48
3:c:79:LYS:HB3	3:c:84:GLN:NE2	2.27	0.48
2:b:36:SER:OG	26:b:621:BCR:H362	2.13	0.48
29:B:623:LMT:O6'	4:D:16:ASP:OD1	2.30	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.48
27:F:101:SQD:H321	18:X:24:THR:HA	1.96	0.48
34:B:643:DMS:H23	44:B:888:HOH:O	2.14	0.47
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.49	0.47
26:t:102:BCR:HC7	26:t:102:BCR:H331	1.54	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.96	0.47
3:C:286:ALA:HB2	24:C:503:CLA:HMD2	1.96	0.47
15:U:33:ALA:HB1	34:U:503:DMS:H22	1.95	0.47
24:b:618:CLA:H161	7:h:7:LEU:HD21	1.95	0.47
19:z:47:TRP:CE2	29:z:1801:LMT:H102	2.50	0.47
4:d:273:PHE:CZ	39:l:101:LHG:H101	2.49	0.47
24:c:510:CLA:HBC3	24:c:512:CLA:H71	1.95	0.47
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.96	0.47
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.96	0.47
34:o:2606:DMS:H23	44:o:2751:HOH:O	2.15	0.47
2:B:341:LYS:NZ	36:B:625[A]:HTG:S1	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:347[A]:ARG:NH2	44:b:710:HOH:O	2.47	0.47
24:b:612:CLA:NC	41:h:702:RRX:H56	2.29	0.47
5:e:27:ILE:HG12	40:e:103:HEM:HMC3	1.97	0.47
26:Y:302:BCR:HC7	26:Y:302:BCR:H331	1.78	0.47
2:b:324:LEU:HA	4:d:293[A]:LEU:HG	1.96	0.47
3:c:387:TRP:CG	37:c:527:GOL:H2	2.49	0.47
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.79	0.47
13:o:42:ARG:O	13:o:241:ALA:HA	2.15	0.47
1:a:131:TRP:CH2	24:c:507:CLA:HAA2	2.49	0.47
24:b:610:CLA:H42	28:b:623:LMG:H311	1.97	0.47
2:B:389:LYS:NZ	37:D:403:GOL:O3	2.48	0.47
3:c:436:PHE:CE2	24:c:506:CLA:H152	2.50	0.47
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.50	0.47
2:b:498:LYS:NZ	44:b:713:HOH:O	2.48	0.46
2:B:24:LEU:HD21	24:B:617:CLA:CAB	2.45	0.46
3:c:387:TRP:CD2	37:c:527:GOL:H2	2.50	0.46
6:f:21:VAL:O	6:f:25:THR:HG23	2.15	0.46
4:D:273:PHE:CZ	39:L:101:LHG:H101	2.50	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
36:b:626:HTG:H1	34:b:643:DMS:S	2.56	0.46
24:c:513:CLA:HAA1	24:c:513:CLA:HBD	1.96	0.46
13:o:180:GLU:OE2	44:o:2701:HOH:O	2.21	0.46
24:B:602:CLA:H91	41:H:101:RRX:H25	1.98	0.46
24:C:504:CLA:HMC3	24:C:514:CLA:H191	1.96	0.46
13:O:39:ARG:HG2	13:O:246:ALA:HB2	1.96	0.46
24:c:511:CLA:HBB1	24:c:511:CLA:HMB1	1.98	0.46
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.98	0.46
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.98	0.46
31:A:417:PL9:H351	31:A:417:PL9:H372	1.44	0.46
5:E:68:ASP:O	5:E:72:ALA:HB2	2.15	0.46
26:T:101:BCR:H311	26:T:101:BCR:HC8	1.97	0.46
5:E:9:PRO:HA	39:E:101:LHG:HC31	1.97	0.46
3:c:362:ARG:HD3	34:c:532:DMS:O	2.16	0.46
4:d:12:ARG:HG3	4:d:17:ILE:HD11	1.97	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	1.98	0.45
24:c:508:CLA:H72	26:c:517:BCR:H10C	1.98	0.45
1:A:85:SER:HA	1:A:109:GLY:HA3	1.98	0.45
3:C:42:LEU:HD21	24:C:512:CLA:H2A	1.98	0.45
26:C:515:BCR:H11C	26:C:515:BCR:H341	1.84	0.45
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.16	0.45
4:D:85:MET:CE	4:D:96:GLU:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.99	0.45
2:B:423:LYS:HG3	36:B:625[B]:HTG:H1'1	1.99	0.45
24:D:401:CLA:H203	24:D:401:CLA:H162	1.70	0.45
3:c:334:PRO:HA	13:o:153:THR:OG1	2.16	0.45
4:d:343:GLU:HG2	16:v:135:VAL:HG11	1.98	0.45
34:B:647:DMS:O	44:B:701:HOH:O	2.21	0.45
4:d:342:PRO:O	4:d:345:VAL:HG22	2.17	0.45
40:e:103:HEM:HBB2	40:e:103:HEM:HMB2	1.98	0.45
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.45
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.97	0.45
24:b:604:CLA:H203	24:b:604:CLA:H162	1.82	0.45
24:B:615:CLA:H72	29:m:102:LMT:H92	1.99	0.45
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.46	0.45
2:b:201:HIS:HB2	24:b:605:CLA:CHB	2.47	0.45
27:f:102:SQD:H241	27:f:102:SQD:H272	1.66	0.45
26:C:516:BCR:H15C	26:C:516:BCR:H351	1.88	0.45
2:b:341:LYS:NZ	36:b:625:HTG:S1	2.89	0.45
26:c:516:BCR:H15C	26:c:516:BCR:H351	1.73	0.45
27:F:101:SQD:H242	18:X:31:ILE:HD13	1.99	0.44
24:a:2109:CLA:CBD	24:d:401:CLA:HAC2	2.46	0.44
26:c:516:BCR:H11C	26:c:516:BCR:H341	1.87	0.44
31:d:407:PL9:H411	11:l:29:LEU:HD23	1.98	0.44
1:A:255:PHE:CE2	32:A:418[B]:K2I:BR	3.26	0.44
24:B:617:CLA:H202	24:B:617:CLA:H162	1.79	0.44
24:c:506:CLA:H101	38:c:520:DGD:HBF2	1.99	0.44
7:h:38:PHE:HB2	41:h:702:RRX:C10	2.46	0.44
28:i:101:LMG:H161	28:i:101:LMG:H192	1.83	0.44
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.52	0.44
26:t:102:BCR:HC8	26:t:102:BCR:H311	1.99	0.44
26:t:102:BCR:HC8	26:t:102:BCR:H321	1.99	0.44
6:F:21:VAL:O	6:F:25:THR:HG23	2.16	0.44
1:A:14:TRP:NE1	29:A:420:LMT:H2B	2.32	0.44
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.18	0.44
26:Y:302:BCR:H15C	26:Y:302:BCR:H351	1.89	0.44
1:a:132:GLU:O	1:a:136:ARG:HG2	2.17	0.44
24:b:616:CLA:H72	24:b:616:CLA:H111	1.76	0.44
3:c:406:SER:HA	3:c:420:VAL:HG23	1.99	0.44
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.99	0.44
2:B:58:GLN:C	2:B:329:PRO:HB3	2.42	0.44
2:b:458:PHE:HB3	24:b:607:CLA:HBC2	1.99	0.44
24:d:401:CLA:H203	24:d:401:CLA:H162	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:SER:HB2	36:B:625[B]:HTG:H6'2	2.00	0.44
2:B:423:LYS:HG3	36:B:625[A]:HTG:H1'1	2.00	0.44
24:b:608:CLA:H41	24:b:608:CLA:H62	1.75	0.44
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.99	0.44
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.53	0.44
24:D:404:CLA:HAA2	24:D:404:CLA:HBD	2.00	0.44
24:b:619:CLA:H143	24:b:619:CLA:H162	1.83	0.43
24:c:506:CLA:H143	24:c:510:CLA:H143	1.98	0.43
2:B:462:PHE:CE2	24:B:614:CLA:HMB2	2.53	0.43
39:D:411:LHG:H223	39:D:411:LHG:H191	1.85	0.43
29:M:101:LMT:H6D	11:l:9:PRO:HA	1.99	0.43
13:O:180:GLU:H	13:O:180:GLU:CD	2.26	0.43
25:a:2112:PHO:ND	25:a:2112:PHO:NC	2.66	0.43
5:e:68:ASP:O	5:e:72:ALA:HB2	2.17	0.43
1:a:72:LEU:HD22	29:a:2103:LMT:O2'	2.17	0.43
24:a:2113:CLA:H161	24:a:2113:CLA:H122	1.73	0.43
24:b:616:CLA:H18	39:d:408:LHG:H202	1.99	0.43
26:b:620:BCR:H24C	26:b:620:BCR:H371	1.79	0.43
3:c:223:TRP:CG	3:c:224:ILE:H	2.36	0.43
38:c:519:DGD:HBF2	38:c:519:DGD:HBE2	1.72	0.43
25:A:408:PHO:NC	25:A:408:PHO:ND	2.67	0.43
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.52	0.43
24:B:610:CLA:NC	41:H:101:RRX:H56	2.33	0.43
3:C:50:LEU:HD11	24:C:514:CLA:HBB1	2.01	0.43
24:b:619:CLA:H61	24:b:619:CLA:H2	1.54	0.43
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.52	0.43
27:a:2115:SQD:H131	32:a:2119:K2I:BR1	2.73	0.43
24:b:609:CLA:H111	24:b:609:CLA:H142	1.79	0.43
24:c:504:CLA:H102	24:c:505:CLA:CHB	2.48	0.43
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.00	0.43
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.83	0.43
24:b:609:CLA:H61	24:b:609:CLA:H102	1.60	0.43
26:c:517:BCR:H15C	26:c:517:BCR:H351	1.85	0.43
5:e:20:TRP:CD1	9:j:8:ILE:HD12	2.54	0.43
1:A:163:ILE:HD11	38:C:517:DGD:HA22	2.01	0.43
31:A:417:PL9:H201	39:E:101:LHG:H181	2.00	0.43
36:b:625:HTG:H6'2	36:b:625:HTG:H3'2	1.83	0.43
3:c:19:ASN:HB3	3:c:20:SER:H	1.64	0.43
39:d:409:LHG:HC62	11:l:15:THR:HG23	1.99	0.43
31:x:801:PL9:H272	31:x:801:PL9:H251	1.80	0.43
39:E:101:LHG:H172	39:E:101:LHG:H202	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:128:GLY:HA3	24:c:515:CLA:C3C	2.48	0.43
3:c:276:LEU:HD23	24:c:511:CLA:HED1	2.01	0.43
24:d:401:CLA:HBA1	24:d:401:CLA:C4A	2.47	0.43
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.00	0.43
2:B:458:PHE:HB3	24:B:605:CLA:HBC2	2.01	0.43
27:B:621:SQD:H312	27:B:621:SQD:H341	1.64	0.43
3:C:80:PRO:HG3	34:C:528:DMS:H11	2.00	0.43
38:C:518:DGD:HA41	29:J:102:LMT:H82	2.01	0.43
44:b:894:HOH:O	37:o:2603:GOL:H32	2.18	0.43
4:d:144:ILE:HD11	34:d:417:DMS:H21	2.01	0.43
27:A:411:SQD:H111	27:A:411:SQD:H141	1.75	0.43
36:D:413:HTG:H3'2	7:H:25:TRP:CZ3	2.54	0.43
27:L:102:SQD:H311	27:L:102:SQD:H341	1.72	0.43
1:a:85:SER:HA	1:a:109:GLY:HA3	2.01	0.43
26:a:2114:BCR:H15C	26:a:2114:BCR:H351	1.94	0.43
24:b:614:CLA:H112	24:b:614:CLA:H72	1.75	0.43
4:d:85:MET:CE	4:d:96:GLU:HG2	2.44	0.43
26:k:2003:BCR:H15C	26:k:2003:BCR:H351	1.89	0.43
24:B:605:CLA:H192	24:B:605:CLA:H162	1.92	0.42
3:C:52:ALA:HB2	24:C:512:CLA:HMA2	1.99	0.42
3:C:429:SER:HB3	38:C:518:DGD:HBT2	2.00	0.42
34:C:528:DMS:H23	34:C:529:DMS:H22	2.01	0.42
41:H:101:RRX:H43	41:H:101:RRX:H47	1.83	0.42
26:T:101:BCR:H11C	26:T:101:BCR:H341	1.90	0.42
2:b:141:ILE:HG21	24:b:618:CLA:HBB1	2.01	0.42
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.31	0.42
24:a:2110:CLA:HED1	38:c:520:DGD:HAE2	2.01	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.49	0.42
26:T:101:BCR:HC8	26:T:101:BCR:H321	2.02	0.42
24:c:506:CLA:HAA1	24:c:506:CLA:HBD	2.02	0.42
24:c:514:CLA:C1B	26:c:516:BCR:H401	2.49	0.42
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.84	0.42
2:b:86:ILE:HD12	2:b:88:PRO:HD3	2.01	0.42
38:c:519:DGD:HB62	28:c:521:LMG:H401	2.01	0.42
39:e:101:LHG:H112	39:e:101:LHG:HC82	1.82	0.42
2:B:324:LEU:HA	4:D:293[A]:LEU:HG	2.01	0.42
24:C:504:CLA:C3B	28:C:526:LMG:H221	2.50	0.42
4:D:12:ARG:HB2	4:D:16:ASP:HB2	2.02	0.42
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.01	0.42
4:d:123:ILE:HD11	38:h:703:DGD:HAH1	2.02	0.42
3:C:77:PRO:HB2	34:C:534:DMS:H23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:C:518:DGD:HAT2	38:C:518:DGD:HA71	1.76	0.42
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.00	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.19	0.42
2:b:30:VAL:HG12	24:b:608:CLA:HHD	2.01	0.42
24:b:608:CLA:HAA1	24:b:608:CLA:HBD	2.01	0.42
2:B:410:THR:O	37:B:635:GOL:H32	2.20	0.42
26:B:620:BCR:H15C	26:B:620:BCR:H351	1.95	0.42
26:C:516:BCR:H341	26:C:516:BCR:H11C	1.92	0.42
36:D:413:HTG:H1	7:H:25:TRP:CD1	2.55	0.42
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.01	0.42
3:c:79:LYS:HD2	16:v:35:TYR:CE1	2.55	0.42
41:h:702:RRX:H32	41:h:702:RRX:H28	1.86	0.42
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.08	0.42
3:C:276:LEU:HD23	24:C:510:CLA:HED1	2.02	0.42
38:C:518:DGD:HAT2	38:C:518:DGD:HAH2	1.39	0.42
24:a:2113:CLA:H102	24:a:2113:CLA:H61	1.64	0.42
2:b:27:THR:HG22	2:b:107:LEU:HD13	2.02	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.38	0.42
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.50	0.42
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.41
2:b:80:ILE:HD11	2:b:167:TRP:CZ3	2.55	0.41
2:b:285:ASN:O	2:b:289:GLN:HG2	2.20	0.41
3:c:167:VAL:HG13	24:c:514:CLA:H72	2.01	0.41
3:c:443:TRP:CZ2	24:c:510:CLA:HMD1	2.54	0.41
1:A:223:LEU:HD12	4:D:139:ARG:HH12	1.84	0.41
3:C:95:LEU:HD21	24:C:502:CLA:OBD	2.21	0.41
24:C:513:CLA:H203	24:C:513:CLA:H161	1.87	0.41
13:O:218:GLU:HG3	34:O:310:DMS:H13	2.01	0.41
24:a:2110:CLA:H142	24:a:2110:CLA:H112	1.85	0.41
16:v:34:GLN:NE2	44:v:305:HOH:O	2.50	0.41
24:B:606:CLA:H62	24:B:606:CLA:H41	1.80	0.41
24:C:513:CLA:H92	24:C:513:CLA:H62	1.81	0.41
38:C:518:DGD:HBF1	38:C:518:DGD:HBE2	1.78	0.41
4:D:126:MET:HE3	4:D:143:ALA:O	2.21	0.41
24:b:604:CLA:H141	24:b:604:CLA:H161	1.80	0.41
26:b:622:BCR:H15C	26:b:622:BCR:H351	1.92	0.41
24:A:405:CLA:CBD	24:D:401:CLA:HAC2	2.50	0.41
26:A:410:BCR:H15C	26:A:410:BCR:H351	1.92	0.41
24:D:405:CLA:H161	24:D:405:CLA:H141	1.87	0.41
13:O:42:ARG:O	13:O:241:ALA:HA	2.20	0.41
13:O:54:GLU:O	13:O:56:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:338:GLY:HA3	3:c:341:LEU:O	2.20	0.41
26:t:102:BCR:H11C	26:t:102:BCR:H341	1.94	0.41
2:B:419:SER:HB2	36:B:625[A]:HTG:H6'2	2.01	0.41
3:C:60:ILE:HG22	24:C:504:CLA:HHD	2.02	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.41
36:O:302:HTG:H7'3	2:b:98:LEU:HB2	2.02	0.41
15:U:76:ARG:NH1	44:U:609:HOH:O	2.53	0.41
24:B:616:CLA:H51	26:B:620:BCR:H341	2.02	0.41
3:C:94:THR:HG22	24:C:502:CLA:HED1	2.01	0.41
3:C:443:TRP:CZ2	24:C:509:CLA:HMD1	2.56	0.41
4:d:144:ILE:CD1	34:d:417:DMS:H21	2.51	0.41
2:B:461:LEU:HD22	39:D:409:LHG:H301	2.02	0.41
24:B:616:CLA:H161	7:H:7:LEU:HD21	2.03	0.41
39:d:408:LHG:H212	12:m:18:PRO:HG3	2.02	0.41
1:A:73:TYR:OH	29:A:414:LMT:H6E	2.21	0.41
2:b:90:PHE:H	36:b:602:HTG:H62	1.86	0.41
3:c:163:PHE:CD2	24:c:514:CLA:HAB	2.56	0.41
28:A:412:LMG:H182	28:A:412:LMG:H151	1.73	0.41
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.41
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.36	0.41
24:C:514:CLA:CAB	26:C:515:BCR:H24C	2.51	0.41
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	2.02	0.41
15:U:16:LYS:NZ	44:U:608:HOH:O	2.53	0.41
34:b:633:DMS:H21	15:u:21:TYR:CZ	2.55	0.41
3:c:425:TRP:CD1	24:c:506:CLA:HMA3	2.55	0.41
4:d:186:GLN:HB2	24:d:404:CLA:HBC1	2.03	0.41
4:d:293[A]:LEU:HD12	4:d:293[A]:LEU:HA	1.91	0.41
10:k:24:VAL:O	10:k:27:VAL:HG22	2.21	0.41
13:o:193:THR:HG21	13:o:220:LEU:HD12	2.01	0.41
19:z:47:TRP:CD2	29:z:1801:LMT:H102	2.55	0.41
1:A:322:ASN:OD1	3:C:412:THR:HA	2.21	0.41
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.03	0.41
26:d:406:BCR:H15C	26:d:406:BCR:H351	1.90	0.41
24:C:508:CLA:H61	24:C:508:CLA:H92	1.83	0.40
44:C:604:HOH:O	39:E:101:LHG:H361	2.21	0.40
1:a:296:ASN:HB2	3:c:400:PRO:O	2.21	0.40
1:a:322:ASN:OD1	3:c:412:THR:HA	2.20	0.40
24:d:401:CLA:HMB1	24:d:401:CLA:HBB1	2.02	0.40
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	2.03	0.40
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.51	0.40
29:B:636:LMT:H81	12:m:8:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:464:GLU:OE2	4:D:245:SER:OG	2.27	0.40
5:E:26:THR:HA	20:R:15:ALA:HB1	2.04	0.40
26:b:621:BCR:H15C	26:b:621:BCR:H351	1.96	0.40
1:A:72:LEU:HD11	29:A:414:LMT:H52	2.02	0.40
24:A:406:CLA:H142	24:A:406:CLA:H112	1.90	0.40
24:B:610:CLA:HBA1	24:B:610:CLA:H3A	1.91	0.40
3:C:288:CYS:SG	38:C:517:DGD:HB32	2.61	0.40
39:D:409:LHG:H282	39:D:409:LHG:H312	1.83	0.40
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.82	0.40
24:d:405:CLA:H162	7:h:37:LEU:HD23	2.04	0.40
3:C:128:GLY:HA3	24:C:514:CLA:C3C	2.52	0.40
39:E:101:LHG:H321	39:E:101:LHG:H351	1.96	0.40
14:T:25:GLU:HA	14:T:26:PRO:HD3	1.97	0.40
27:a:2102:SQD:H141	26:t:102:BCR:HC41	2.04	0.40
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.03	0.40
26:b:622:BCR:H24C	26:b:622:BCR:H371	1.88	0.40
1:A:270[B]:SER:OG	27:A:411:SQD:H3	2.22	0.40
32:A:419:K2I:BR1	39:D:411:LHG:H222	2.77	0.40
2:B:464:PHE:CZ	39:D:409:LHG:H252	2.57	0.40
24:B:603:CLA:H203	24:B:603:CLA:H162	1.92	0.40
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.54	0.40
29:M:101:LMT:H71	12:m:24:ILE:HD13	2.04	0.40
15:U:10:VAL:HG11	15:U:15:GLU:OE2	2.22	0.40
2:b:413:ASP:CG	2:b:415:PRO:HD2	2.46	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	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	36 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	36	36
2	B	508/505 (101%)	502 (99%)	6 (1%)	0	100	100
2	b	509/505 (101%)	503 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	442 (98%)	8 (2%)	1 (0%)	43	44
3	c	453/455 (100%)	443 (98%)	9 (2%)	1 (0%)	43	44
4	D	339/342 (99%)	331 (98%)	8 (2%)	0	100	100
4	d	342/342 (100%)	335 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	77/83 (93%)	77 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
7	h	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	244/244 (100%)	239 (98%)	5 (2%)	0	100	100
13	o	244/244 (100%)	239 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5244/5387 (97%)	5155 (98%)	85 (2%)	4 (0%)	48	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	416	SER
3	C	416	SER
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/279 (96%)	266 (100%)	1 (0%)	84	89
1	a	270/279 (97%)	269 (100%)	1 (0%)	84	89
2	B	405/403 (100%)	405 (100%)	0	100	100
2	b	398/403 (99%)	395 (99%)	3 (1%)	73	81
3	C	354/356 (99%)	351 (99%)	3 (1%)	73	81
3	c	355/356 (100%)	352 (99%)	3 (1%)	73	81
4	D	275/276 (100%)	273 (99%)	2 (1%)	76	83
4	d	278/276 (101%)	275 (99%)	3 (1%)	65	74
5	E	70/72 (97%)	68 (97%)	2 (3%)	37	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	66/72 (92%)	66 (100%)	0	100	100
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	34
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	32
7	H	53/53 (100%)	53 (100%)	0	100	100
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	37
10	k	28/30 (93%)	28 (100%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	205/207 (99%)	205 (100%)	0	100	100
13	o	206/207 (100%)	203 (98%)	3 (2%)	57	65
14	T	25/28 (89%)	24 (96%)	1 (4%)	28	29
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	29
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	49
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	49
16	V	115/117 (98%)	115 (100%)	0	100	100
16	v	114/117 (97%)	114 (100%)	0	100	100
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24	25
17	y	21/23 (91%)	20 (95%)	1 (5%)	23	23
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	45/51 (88%)	45 (100%)	0	100	100
19	z	43/51 (84%)	43 (100%)	0	100	100
20	R	11/33 (33%)	11 (100%)	0	100	100
All	All	4252/4401 (97%)	4220 (99%)	32 (1%)	76	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
3	C	255	THR
3	C	289	PHE
3	C	315	MET
4	D	90	LEU
4	D	329	MET
5	E	4	THR
5	E	5	THR
6	F	44	GLN
10	K	17	ILE
14	T	2	GLU
15	U	70[A]	ARG
15	U	70[B]	ARG
17	Y	30	ILE
1	a	15	GLU
2	b	352[A]	GLU
2	b	352[B]	GLU
2	b	362	PHE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	28	VAL
4	d	90	LEU
4	d	329	MET
6	f	44	GLN
13	o	23	ASP
13	o	64	GLU
13	o	179	GLU
14	t	2	GLU
15	u	9	LEU
15	u	10	VAL
17	y	30	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	296	ASN
2	B	179	GLN
2	B	289	GLN
2	B	374	ASN

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Mol	Chain	Res	Type
3	C	44	ASN
4	D	186	GLN
4	D	255	GLN
5	E	60	GLN
13	O	61	GLN
13	O	155	ASN
15	U	37	GLN
15	U	78	ASN
1	a	165	GLN
1	a	296	ASN
2	b	282	GLN
2	b	289	GLN
2	b	331	ASN
3	c	385	GLN
4	d	186	GLN
4	d	255	GLN
4	d	301	GLN
16	v	118	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	$\#\|Z\| > 2$
4	HSK	D	336[A]	-	9,10,12	10.51	2 (22%)	6,12,16	2.12	2 (33%)
8	FME	I	1	8	8,9,10	0.60	0	7,9,11	1.56	2 (28%)
14	FME	T	1	14	8,9,10	0.66	0	7,9,11	1.66	2 (28%)
4	HSK	D	336[B]	-	9,11,12	1.84	2 (22%)	6,14,16	3.92	4 (66%)

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	0.56	0	7,9,11	1.32	1 (14%)
19	FME	Z	1	19	8,9,10	0.63	0	7,9,11	1.81	2 (28%)
4	HSK	d	336[A]	-	9,10,12	5.62	1 (11%)	6,12,16	1.85	3 (50%)
8	FME	i	1	8	8,9,10	0.58	0	7,9,11	1.59	2 (28%)
19	FME	z	1	19	8,9,10	0.62	0	7,9,11	1.63	4 (57%)
4	HSK	d	336[B]	-	9,11,12	1.78	2 (22%)	6,14,16	3.96	4 (66%)
12	FME	M	1	12	8,9,10	0.73	0	7,9,11	1.33	1 (14%)
14	FME	t	1	14	8,9,10	0.66	0	7,9,11	1.79	2 (28%)

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
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
12	FME	m	1	12	-	1/7/9/11	-
19	FME	Z	1	19	-	3/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
19	FME	z	1	19	-	4/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-31.36	0.97	1.38
4	d	336[A]	HSK	OM-ND1	-16.46	1.17	1.38
4	D	336[B]	HSK	OM-ND1	4.06	1.44	1.38
4	d	336[B]	HSK	OM-ND1	3.70	1.43	1.38
4	D	336[B]	HSK	CE1-ND1	-2.44	1.33	1.37
4	d	336[B]	HSK	CE1-ND1	-2.39	1.33	1.37
4	D	336[A]	HSK	CE1-ND1	-2.03	1.33	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	336[B]	HSK	ND1-CE1-NE2	-6.13	104.08	111.75
4	D	336[B]	HSK	ND1-CE1-NE2	-6.04	104.20	111.75
4	d	336[B]	HSK	CE1-ND1-CG	5.87	114.88	107.37
4	D	336[B]	HSK	CE1-ND1-CG	5.66	114.61	107.37
4	d	336[B]	HSK	CD2-NE2-CE1	3.62	109.63	105.22
4	D	336[B]	HSK	CD2-NE2-CE1	3.53	109.52	105.22
4	D	336[A]	HSK	ND1-CE1-NE2	-3.14	107.82	111.75
4	D	336[B]	HSK	CB-CG-ND1	3.05	128.04	122.89
19	Z	1	FME	CE-SD-CG	2.98	110.64	100.40
4	D	336[A]	HSK	CD2-NE2-CE1	2.91	108.76	105.22
4	d	336[B]	HSK	CB-CG-ND1	2.73	127.50	122.89
4	d	336[A]	HSK	ND1-CE1-NE2	-2.54	108.57	111.75
14	t	1	FME	O-C-CA	-2.54	118.12	124.78
14	T	1	FME	CE-SD-CG	2.53	109.10	100.40
4	d	336[A]	HSK	CD2-NE2-CE1	2.48	108.25	105.22
14	t	1	FME	CE-SD-CG	2.38	108.57	100.40
14	T	1	FME	O-C-CA	-2.34	118.65	124.78
19	Z	1	FME	CA-N-CN	-2.25	119.36	122.82
19	z	1	FME	CE-SD-CG	2.16	107.81	100.40
12	m	1	FME	CE-SD-CG	2.15	107.80	100.40
19	z	1	FME	CA-N-CN	-2.12	119.57	122.82
8	I	1	FME	CA-N-CN	-2.09	119.61	122.82
4	d	336[A]	HSK	CB-CG-ND1	2.06	126.37	122.89
19	z	1	FME	O-C-CA	-2.05	119.41	124.78
12	M	1	FME	CA-N-CN	-2.05	119.67	122.82
8	i	1	FME	C-CA-N	2.05	113.43	109.73
8	I	1	FME	O-C-CA	-2.03	119.46	124.78
8	i	1	FME	O-C-CA	-2.01	119.51	124.78
19	z	1	FME	O1-CN-N	-2.00	120.00	125.27

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	Z	1	FME	CA-CB-CG-SD
12	m	1	FME	O1-CN-N-CA
14	t	1	FME	N-CA-CB-CG
19	z	1	FME	N-CA-CB-CG
19	z	1	FME	C-CA-CB-CG
19	z	1	FME	CA-CB-CG-SD
14	t	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	O1-CN-N-CA
19	Z	1	FME	O1-CN-N-CA
8	I	1	FME	CB-CA-N-CN
19	Z	1	FME	CB-CA-N-CN
19	z	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 399 ligands modelled in this entry, 13 are monoatomic and 44 are unknown - leaving 342 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	$\#\|Z\| > 2$
34	DMS	a	2123	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
36	HTG	C	521	-	19,19,19	1.02	2 (10%)	23,24,24	1.07	2 (8%)
24	CLA	B	604	2	69,73,73	2.48	24 (34%)	83,113,113	2.49	27 (32%)
21	OEX	A	401	1,44,3	0,14,14	-	-	-		
33	BCT	a	2108	22	2,3,3	0.57	0	2,3,3	1.08	0
34	DMS	B	648	-	3,3,3	2.66	1 (33%)	3,3,3	0.36	0
27	SQD	F	101	-	44,45,54	1.10	3 (6%)	53,56,65	1.57	10 (18%)
34	DMS	T	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LHG	D	410	-	48,48,48	0.89	2 (4%)	51,54,54	0.92	3 (5%)
25	PHO	A	407	-	58,69,69	2.67	13 (22%)	56,99,99	2.91	16 (28%)
34	DMS	b	642	-	3,3,3	2.71	1 (33%)	3,3,3	0.59	0
29	LMT	Z	101	-	36,36,36	0.40	0	47,47,47	0.83	0
26	BCR	d	406	-	41,41,41	0.86	1 (2%)	56,56,56	1.70	8 (14%)
24	CLA	B	606	2	69,73,73	2.35	22 (31%)	83,113,113	2.51	24 (28%)
34	DMS	V	207	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
34	DMS	B	639	-	3,3,3	2.60	1 (33%)	3,3,3	0.60	0
34	DMS	D	420	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
24	CLA	B	608	44	69,73,73	2.50	22 (31%)	83,113,113	2.40	30 (36%)
34	DMS	b	632	-	3,3,3	2.45	1 (33%)	3,3,3	0.57	0
29	LMT	A	414	-	35,35,36	0.44	0	46,46,47	1.13	4 (8%)
28	LMG	b	623	-	51,51,55	0.93	2 (3%)	59,59,63	1.01	2 (3%)
36	HTG	B	625[A]	-	19,19,19	1.01	1 (5%)	23,24,24	1.23	1 (4%)
34	DMS	B	643	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
34	DMS	c	538	-	3,3,3	2.71	1 (33%)	3,3,3	0.62	0
29	LMT	E	105	-	24,24,36	0.51	1 (4%)	29,29,47	0.88	1 (3%)
34	DMS	T	106	-	3,3,3	2.70	1 (33%)	3,3,3	0.56	0
34	DMS	C	539	-	3,3,3	2.76	1 (33%)	3,3,3	0.70	0
24	CLA	C	511	3	69,73,73	2.58	25 (36%)	83,113,113	2.42	29 (34%)
34	DMS	O	311	-	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
34	DMS	v	208	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
37	GOL	a	2101	-	5,5,5	1.02	0	5,5,5	1.12	0
34	DMS	d	419	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
24	CLA	a	2110	44	69,73,73	2.34	22 (31%)	83,113,113	2.73	30 (36%)
34	DMS	c	529	-	3,3,3	2.61	1 (33%)	3,3,3	0.34	0
34	DMS	V	210	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
38	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.18	8 (10%)
24	CLA	c	510	3	69,73,73	2.52	23 (33%)	83,113,113	2.51	24 (28%)
24	CLA	C	504	3	69,73,73	2.56	22 (31%)	83,113,113	2.38	26 (31%)
24	CLA	b	607	2	69,73,73	2.87	24 (34%)	83,113,113	2.50	30 (36%)
24	CLA	B	613	2	69,73,73	2.31	25 (36%)	83,113,113	2.56	24 (28%)
24	CLA	B	605	2	69,73,73	2.54	23 (33%)	83,113,113	2.36	25 (30%)
24	CLA	b	604	44	69,73,73	2.49	25 (36%)	83,113,113	2.42	24 (28%)
34	DMS	E	107	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	D	401	44	69,73,73	2.27	23 (33%)	83,113,113	2.75	29 (34%)
26	BCR	T	101	-	41,41,41	0.72	0	56,56,56	1.67	14 (25%)
24	CLA	b	610	44	69,73,73	2.69	24 (34%)	83,113,113	2.44	30 (36%)
36	HTG	b	625	-	19,19,19	0.91	1 (5%)	23,24,24	1.80	6 (26%)
37	GOL	v	204	-	5,5,5	0.80	0	5,5,5	0.94	0
34	DMS	U	503	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
29	LMT	i	104	-	24,24,36	0.54	1 (4%)	29,29,47	1.38	3 (10%)
34	DMS	O	308	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	T	105	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
34	DMS	B	642	-	3,3,3	2.66	1 (33%)	3,3,3	0.40	0
24	CLA	c	507	3	69,73,73	2.58	24 (34%)	83,113,113	2.42	25 (30%)
29	LMT	B	636	-	36,36,36	0.49	0	47,47,47	1.06	4 (8%)
36	HTG	b	601	-	19,19,19	1.04	2 (10%)	23,24,24	1.57	4 (17%)
34	DMS	O	312	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
34	DMS	C	533	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
24	CLA	D	404	4	69,73,73	2.23	22 (31%)	83,113,113	2.74	30 (36%)
43	HEC	V	201	16	50,50,50	1.95	7 (14%)	68,82,82	1.56	9 (13%)
43	HEC	v	201	16	50,50,50	1.95	10 (20%)	68,82,82	1.58	12 (17%)
34	DMS	d	420	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
36	HTG	D	413	-	19,19,19	1.06	2 (10%)	23,24,24	1.24	3 (13%)
34	DMS	b	633	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
34	DMS	a	2124	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
34	DMS	v	207	-	3,3,3	2.63	1 (33%)	3,3,3	0.48	0
24	CLA	C	506	3	69,73,73	2.68	24 (34%)	83,113,113	2.27	26 (31%)
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	1.09	4 (8%)
34	DMS	B	640	-	3,3,3	2.70	1 (33%)	3,3,3	0.56	0
24	CLA	C	510	3	69,73,73	2.61	25 (36%)	83,113,113	2.51	27 (32%)
36	HTG	d	414	-	19,19,19	1.01	2 (10%)	23,24,24	1.26	1 (4%)
38	DGD	C	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.06	5 (6%)
32	K2I	A	418[A]	-	8,10,10	1.34	0	10,14,14	2.63	4 (40%)
34	DMS	c	532	-	3,3,3	2.58	1 (33%)	3,3,3	0.34	0
27	SQD	A	411	-	48,49,54	1.03	3 (6%)	57,60,65	1.71	10 (17%)
27	SQD	a	2115	-	46,47,54	1.03	3 (6%)	55,58,65	1.78	11 (20%)
37	GOL	o	2603	-	5,5,5	0.83	0	5,5,5	1.08	0
34	DMS	B	641	-	3,3,3	2.55	1 (33%)	3,3,3	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	615	2	69,73,73	2.32	22 (31%)	83,113,113	2.68	27 (32%)
24	CLA	b	608	2	69,73,73	2.24	24 (34%)	83,113,113	2.66	25 (30%)
26	BCR	c	517	-	41,41,41	0.77	0	56,56,56	1.53	10 (17%)
34	DMS	a	2122	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
34	DMS	b	637	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
34	DMS	A	422	-	3,3,3	2.53	1 (33%)	3,3,3	0.65	0
34	DMS	u	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.59	0
32	K2I	a	2118[B]	-	8,10,10	1.37	1 (12%)	10,14,14	2.26	3 (30%)
37	GOL	U	502	-	5,5,5	0.85	0	5,5,5	0.97	0
26	BCR	c	528	-	41,41,41	0.72	0	56,56,56	1.45	9 (16%)
28	LMG	D	412	42	44,44,55	0.93	2 (4%)	52,52,63	0.90	4 (7%)
34	DMS	C	531	-	3,3,3	2.61	1 (33%)	3,3,3	0.52	0
34	DMS	O	314	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
28	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.16	5 (8%)
29	LMT	a	2120	-	36,36,36	0.48	0	47,47,47	1.20	6 (12%)
25	PHO	A	408	-	58,69,69	2.80	14 (24%)	56,99,99	2.89	14 (25%)
24	CLA	d	404	4	69,73,73	2.41	24 (34%)	83,113,113	2.42	28 (33%)
34	DMS	B	638	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
34	DMS	i	106	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
34	DMS	c	536	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
24	CLA	c	511	3	69,73,73	2.75	24 (34%)	83,113,113	2.37	26 (31%)
34	DMS	v	214	-	3,3,3	2.76	1 (33%)	3,3,3	0.77	0
24	CLA	d	401	44	69,73,73	2.42	21 (30%)	83,113,113	2.69	32 (38%)
37	GOL	C	525	-	5,5,5	0.93	0	5,5,5	0.95	0
24	CLA	c	509	44	69,73,73	2.52	24 (34%)	83,113,113	2.59	30 (36%)
32	K2I	A	418[B]	-	8,10,10	1.35	1 (12%)	10,14,14	2.12	4 (40%)
34	DMS	B	649	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
34	DMS	F	103	-	3,3,3	2.67	1 (33%)	3,3,3	0.71	0
34	DMS	e	104	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
24	CLA	C	509	3	69,73,73	2.62	24 (34%)	83,113,113	2.41	21 (25%)
37	GOL	U	501	-	5,5,5	1.12	0	5,5,5	0.89	0
24	CLA	B	609	2	69,73,73	2.50	25 (36%)	83,113,113	2.42	27 (32%)
24	CLA	C	512	3	69,73,73	2.78	25 (36%)	83,113,113	2.43	29 (34%)
29	LMT	b	624	-	25,25,36	0.44	0	30,30,47	1.15	3 (10%)
34	DMS	u	202	-	3,3,3	2.68	1 (33%)	3,3,3	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	514	3	69,73,73	2.58	24 (34%)	83,113,113	2.45	27 (32%)
37	GOL	v	202	-	5,5,5	0.97	0	5,5,5	0.93	0
34	DMS	o	2612	-	3,3,3	2.72	1 (33%)	3,3,3	0.65	0
34	DMS	C	535	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
34	DMS	o	2611	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
34	DMS	B	647	-	3,3,3	2.69	1 (33%)	3,3,3	0.46	0
34	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.47	0
34	DMS	o	2606	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
37	GOL	H	103	-	5,5,5	0.95	0	5,5,5	0.86	0
40	HEM	e	103	6,5	50,50,50	1.94	10 (20%)	66,82,82	1.41	8 (12%)
26	BCR	C	516	-	41,41,41	0.73	0	56,56,56	1.54	10 (17%)
31	PL9	D	407	-	55,55,55	0.72	2 (3%)	68,69,69	1.58	15 (22%)
32	K2I	a	2119	-	8,10,10	1.37	2 (25%)	10,14,14	1.56	3 (30%)
34	DMS	o	2608	-	3,3,3	2.65	1 (33%)	3,3,3	0.42	0
26	BCR	K	101	-	41,41,41	0.73	0	56,56,56	1.35	8 (14%)
36	HTG	c	526	-	19,19,19	1.08	2 (10%)	23,24,24	1.17	1 (4%)
38	DGD	h	703	-	63,63,67	0.92	3 (4%)	77,77,81	1.06	6 (7%)
34	DMS	c	535	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
37	GOL	D	403	-	5,5,5	1.15	0	5,5,5	0.87	0
34	DMS	B	650	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	O	305	-	3,3,3	2.64	1 (33%)	3,3,3	0.52	0
34	DMS	o	2604	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
37	GOL	Z	102	-	5,5,5	0.97	0	5,5,5	0.83	0
24	CLA	b	614	2	69,73,73	2.62	25 (36%)	83,113,113	2.49	30 (36%)
36	HTG	c	524	-	19,19,19	1.08	2 (10%)	23,24,24	1.58	2 (8%)
24	CLA	C	505	44	69,73,73	2.54	24 (34%)	83,113,113	2.41	25 (30%)
34	DMS	u	201	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
37	GOL	d	415	-	5,5,5	0.90	0	5,5,5	0.99	0
34	DMS	V	208	-	3,3,3	2.67	1 (33%)	3,3,3	0.60	0
26	BCR	A	410	-	41,41,41	0.82	0	56,56,56	1.43	8 (14%)
34	DMS	E	108	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
31	PL9	d	407	-	55,55,55	0.74	1 (1%)	68,69,69	1.58	15 (22%)
34	DMS	d	422	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
29	LMT	j	1601	-	22,22,36	0.64	1 (4%)	26,26,47	1.18	2 (7%)
26	BCR	t	102	-	41,41,41	0.72	0	56,56,56	1.55	17 (30%)
34	DMS	d	418	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	DGD	C	517	-	63,63,67	0.84	3 (4%)	77,77,81	1.07	6 (7%)
34	DMS	C	534	-	3,3,3	2.66	1 (33%)	3,3,3	0.61	0
24	CLA	B	617	2	69,73,73	2.35	23 (33%)	83,113,113	2.61	26 (31%)
34	DMS	o	2607	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
34	DMS	C	537	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
32	K2I	a	2118[A]	-	8,10,10	1.38	1 (12%)	10,14,14	2.37	4 (40%)
34	DMS	V	202	-	3,3,3	2.67	1 (33%)	3,3,3	0.63	0
36	HTG	O	302	-	19,19,19	0.99	1 (5%)	23,24,24	0.96	2 (8%)
41	RRX	H	101	-	42,42,42	0.74	0	57,58,58	1.33	8 (14%)
39	LHG	D	411	-	43,43,48	0.93	2 (4%)	46,49,54	1.00	3 (6%)
26	BCR	B	618	-	41,41,41	0.75	0	56,56,56	1.39	6 (10%)
36	HTG	b	602	-	19,19,19	1.13	2 (10%)	23,24,24	1.81	4 (17%)
34	DMS	v	211	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
39	LHG	D	409	-	48,48,48	0.88	2 (4%)	51,54,54	1.16	6 (11%)
24	CLA	b	605	2	69,73,73	2.51	24 (34%)	83,113,113	2.44	29 (34%)
37	GOL	B	635	-	5,5,5	1.08	0	5,5,5	0.90	0
24	CLA	B	612	2	69,73,73	2.66	24 (34%)	83,113,113	2.55	28 (33%)
38	DGD	D	408	-	46,46,67	1.03	2 (4%)	53,54,81	1.16	4 (7%)
29	LMT	a	2103	-	36,36,36	0.39	0	47,47,47	1.22	5 (10%)
24	CLA	b	612	2	69,73,73	2.56	24 (34%)	83,113,113	2.47	30 (36%)
36	HTG	C	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.77	4 (17%)
24	CLA	b	618	2	69,73,73	2.38	21 (30%)	83,113,113	2.37	28 (33%)
28	LMG	B	622	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	4 (6%)
26	BCR	k	2003	-	41,41,41	0.66	0	56,56,56	1.48	11 (19%)
24	CLA	B	614	2	69,73,73	2.30	23 (33%)	83,113,113	2.48	28 (33%)
37	GOL	k	2001	-	5,5,5	0.93	0	5,5,5	0.92	0
24	CLA	B	607	2	69,73,73	2.49	24 (34%)	83,113,113	2.52	27 (32%)
27	SQD	B	621	-	53,54,54	1.07	4 (7%)	62,65,65	1.52	8 (12%)
24	CLA	b	619	2	69,73,73	2.47	23 (33%)	83,113,113	2.51	26 (31%)
34	DMS	k	2004	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
24	CLA	C	513	3	69,73,73	2.53	22 (31%)	83,113,113	2.56	30 (36%)
29	LMT	m	103	-	36,36,36	0.47	0	47,47,47	1.03	4 (8%)
34	DMS	c	531	-	3,3,3	2.65	1 (33%)	3,3,3	0.41	0
24	CLA	B	611	44	69,73,73	2.39	24 (34%)	83,113,113	2.52	29 (34%)
24	CLA	b	616	2	69,73,73	2.57	24 (34%)	83,113,113	2.48	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	B	644	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
34	DMS	O	306	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
37	GOL	O	303	-	5,5,5	0.94	0	5,5,5	0.92	0
29	LMT	B	623	-	36,36,36	0.39	0	47,47,47	1.33	7 (14%)
24	CLA	C	508	44	69,73,73	2.62	24 (34%)	83,113,113	2.48	29 (34%)
28	LMG	d	411	42	48,48,55	0.95	2 (4%)	56,56,63	1.04	2 (3%)
26	BCR	D	406	-	41,41,41	0.82	1 (2%)	56,56,56	1.60	8 (14%)
34	DMS	u	204	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
37	GOL	o	2601	-	5,5,5	1.01	0	5,5,5	0.85	0
33	BCT	A	421	22	2,3,3	0.60	0	2,3,3	0.98	0
34	DMS	x	802	-	3,3,3	2.71	1 (33%)	3,3,3	0.65	0
37	GOL	C	524	-	5,5,5	0.90	0	5,5,5	0.97	0
39	LHG	e	101	-	31,31,48	0.89	1 (3%)	33,36,54	1.07	1 (3%)
29	LMT	A	420	-	36,36,36	0.56	1 (2%)	47,47,47	1.35	5 (10%)
37	GOL	v	203	-	5,5,5	1.05	0	5,5,5	1.19	1 (20%)
34	DMS	C	536	-	3,3,3	2.69	1 (33%)	3,3,3	0.60	0
34	DMS	o	2605	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
36	HTG	V	204	-	19,19,19	0.97	2 (10%)	23,24,24	1.88	5 (21%)
34	DMS	O	304	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	A	425	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
34	DMS	v	209	-	3,3,3	2.67	1 (33%)	3,3,3	0.62	0
34	DMS	b	643	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
24	CLA	C	502	3	69,73,73	2.48	24 (34%)	83,113,113	2.32	22 (26%)
37	GOL	V	203	-	5,5,5	0.96	0	5,5,5	0.89	0
37	GOL	b	631	-	5,5,5	0.87	0	5,5,5	0.99	0
34	DMS	V	209	-	3,3,3	2.64	1 (33%)	3,3,3	0.57	0
39	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
21	OEX	a	2104	1,44,3	0,14,14	-	-	-		
27	SQD	a	2102	-	52,53,54	1.02	3 (5%)	61,64,65	1.22	5 (8%)
36	HTG	B	627	-	19,19,19	1.04	2 (10%)	23,24,24	1.59	3 (13%)
28	LMG	C	526	-	48,48,55	0.98	2 (4%)	56,56,63	1.26	5 (8%)
37	GOL	B	632	-	5,5,5	0.98	0	5,5,5	0.81	0
24	CLA	c	505	3	69,73,73	2.83	23 (33%)	83,113,113	2.33	29 (34%)
24	CLA	D	405	4	69,73,73	2.47	25 (36%)	83,113,113	2.47	28 (33%)
36	HTG	d	403	-	19,19,19	1.10	2 (10%)	23,24,24	1.06	2 (8%)
24	CLA	C	503	3	69,73,73	2.66	24 (34%)	83,113,113	2.51	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	PL9	x	801	-	38,38,55	0.40	0	45,45,69	1.77	15 (33%)
34	DMS	D	418	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
34	DMS	C	527	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
24	CLA	b	613	44	69,73,73	2.43	24 (34%)	83,113,113	2.49	28 (33%)
34	DMS	C	532	-	3,3,3	2.64	1 (33%)	3,3,3	0.38	0
34	DMS	b	639	-	3,3,3	2.63	1 (33%)	3,3,3	0.42	0
29	LMT	I	1201	-	24,24,36	0.44	0	29,29,47	1.14	3 (10%)
34	DMS	v	213	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
37	GOL	c	527	-	5,5,5	0.76	0	5,5,5	1.03	0
24	CLA	c	515	3	69,73,73	2.58	25 (36%)	83,113,113	2.37	25 (30%)
29	LMT	T	102	-	24,24,36	0.40	0	29,29,47	0.97	1 (3%)
36	HTG	I	1202	-	19,19,19	1.15	2 (10%)	23,24,24	1.95	4 (17%)
34	DMS	C	530	-	3,3,3	2.69	1 (33%)	3,3,3	0.63	0
41	RRX	h	702	-	42,42,42	0.71	0	57,58,58	1.37	9 (15%)
34	DMS	A	424	-	3,3,3	2.58	1 (33%)	3,3,3	0.47	0
34	DMS	t	103	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
26	BCR	b	622	-	41,41,41	0.79	1 (2%)	56,56,56	1.40	6 (10%)
26	BCR	a	2114	-	41,41,41	0.75	0	56,56,56	1.32	6 (10%)
34	DMS	b	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
34	DMS	c	542	-	3,3,3	2.64	1 (33%)	3,3,3	0.56	0
36	HTG	B	624	-	19,19,19	1.10	1 (5%)	23,24,24	1.27	2 (8%)
29	LMT	z	1801	-	33,33,36	0.43	0	43,43,47	0.97	2 (4%)
34	DMS	b	636	-	3,3,3	2.74	1 (33%)	3,3,3	0.69	0
24	CLA	b	615	2	69,73,73	2.32	22 (31%)	83,113,113	2.62	25 (30%)
34	DMS	o	2609	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
38	DGD	c	518	-	63,63,67	0.81	2 (3%)	77,77,81	1.20	6 (7%)
39	LHG	d	410	-	35,35,48	1.10	2 (5%)	38,41,54	1.01	3 (7%)
29	LMT	m	102	-	36,36,36	0.50	0	47,47,47	1.16	5 (10%)
34	DMS	v	205	-	3,3,3	2.63	1 (33%)	3,3,3	0.54	0
36	HTG	B	628	-	19,19,19	1.02	2 (10%)	23,24,24	1.58	4 (17%)
32	K2I	A	419	-	8,10,10	1.30	1 (12%)	10,14,14	1.44	3 (30%)
34	DMS	b	635	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
24	CLA	B	616	2	69,73,73	2.47	22 (31%)	83,113,113	2.57	30 (36%)
26	BCR	b	621	-	41,41,41	0.84	0	56,56,56	1.20	6 (10%)
28	LMG	i	101	-	51,51,55	0.93	2 (3%)	59,59,63	1.12	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	V	205	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
34	DMS	C	538	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
24	CLA	c	513	3	69,73,73	2.48	22 (31%)	83,113,113	2.42	31 (37%)
24	CLA	C	507	3	69,73,73	2.73	22 (31%)	83,113,113	2.57	28 (33%)
25	PHO	a	2112	-	58,69,69	2.74	13 (22%)	56,99,99	2.86	14 (25%)
38	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.07	4 (5%)
40	HEM	F	102	6,5	50,50,50	1.87	8 (16%)	66,82,82	1.47	9 (13%)
28	LMG	c	522	-	48,48,55	1.00	2 (4%)	56,56,63	1.25	6 (10%)
34	DMS	O	310	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
34	DMS	c	541	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
24	CLA	d	405	4	69,73,73	2.52	24 (34%)	83,113,113	2.47	29 (34%)
34	DMS	o	2610	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
29	LMT	J	102	-	24,24,36	0.51	0	29,29,47	1.05	2 (6%)
36	HTG	B	626	-	19,19,19	1.08	2 (10%)	23,24,24	1.57	3 (13%)
34	DMS	c	537	-	3,3,3	2.69	1 (33%)	3,3,3	0.63	0
24	CLA	B	602	44	69,73,73	2.48	25 (36%)	83,113,113	2.46	24 (28%)
28	LMG	c	521	-	49,49,55	0.93	2 (4%)	57,57,63	1.12	5 (8%)
34	DMS	C	528	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
24	CLA	b	606	2	69,73,73	2.51	23 (33%)	83,113,113	2.51	33 (39%)
28	LMG	A	412	-	51,51,55	0.97	2 (3%)	59,59,63	1.12	4 (6%)
24	CLA	c	503	3	69,73,73	2.43	23 (33%)	83,113,113	2.62	25 (30%)
34	DMS	A	423	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
36	HTG	B	625[B]	-	19,19,19	1.00	1 (5%)	23,24,24	1.47	4 (17%)
24	CLA	a	2113	1	69,73,73	2.26	22 (31%)	83,113,113	2.59	28 (33%)
26	BCR	B	619	-	41,41,41	0.85	1 (2%)	56,56,56	1.13	4 (7%)
34	DMS	v	206	-	3,3,3	2.70	1 (33%)	3,3,3	0.63	0
24	CLA	b	609	2	69,73,73	2.45	25 (36%)	83,113,113	2.39	25 (30%)
34	DMS	b	634	-	3,3,3	2.72	1 (33%)	3,3,3	0.63	0
34	DMS	c	533	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
24	CLA	A	405	1	69,73,73	2.40	23 (33%)	83,113,113	2.43	29 (34%)
24	CLA	c	504	3	69,73,73	2.38	23 (33%)	83,113,113	2.42	25 (30%)
34	DMS	C	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	c	530	-	3,3,3	2.62	1 (33%)	3,3,3	0.46	0
34	DMS	B	646	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
24	CLA	A	409	1	69,73,73	2.35	23 (33%)	83,113,113	2.56	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	b	641	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
34	DMS	A	426	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
34	DMS	O	313	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	v	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
31	PL9	A	417	-	38,38,55	0.52	0	45,45,69	1.67	9 (20%)
26	BCR	B	620	-	41,41,41	0.75	0	56,56,56	1.24	7 (12%)
34	DMS	O	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
24	CLA	B	603	2	69,73,73	2.46	23 (33%)	83,113,113	2.47	28 (33%)
39	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
25	PHO	a	2111	-	58,69,69	2.56	11 (18%)	56,99,99	2.79	12 (21%)
34	DMS	V	206	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
34	DMS	z	1802	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
26	BCR	c	516	-	41,41,41	0.75	0	56,56,56	1.56	9 (16%)
24	CLA	b	617	2	69,73,73	2.46	24 (34%)	83,113,113	2.53	29 (34%)
34	DMS	O	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.65	0
27	SQD	A	413	-	53,54,54	1.04	3 (5%)	62,65,65	1.29	6 (9%)
34	DMS	c	540	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
34	DMS	D	419	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
27	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.60	9 (14%)
29	LMT	f	101	-	24,24,36	0.55	1 (4%)	29,29,47	0.89	1 (3%)
24	CLA	a	2109	1	69,73,73	2.62	24 (34%)	83,113,113	2.50	27 (32%)
39	LHG	E	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.06	3 (5%)
26	BCR	C	515	-	41,41,41	0.75	0	56,56,56	1.45	7 (12%)
34	DMS	d	421	-	3,3,3	2.69	1 (33%)	3,3,3	0.66	0
34	DMS	c	539	-	3,3,3	2.69	1 (33%)	3,3,3	0.62	0
34	DMS	b	638	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
36	HTG	b	626	-	19,19,19	1.09	2 (10%)	23,24,24	1.33	2 (8%)
34	DMS	d	417	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
38	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.02	5 (6%)
24	CLA	c	506	44	69,73,73	2.35	22 (31%)	83,113,113	2.60	29 (34%)
24	CLA	c	512	3	69,73,73	2.43	23 (33%)	83,113,113	2.37	26 (31%)
24	CLA	B	610	2	69,73,73	2.59	23 (33%)	83,113,113	2.44	28 (33%)
24	CLA	c	514	3	69,73,73	2.63	24 (34%)	83,113,113	2.55	29 (34%)
34	DMS	v	212	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
27	SQD	f	102	-	35,36,54	1.65	3 (8%)	40,41,65	1.40	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LHG	d	409	-	48,48,48	0.80	2 (4%)	51,54,54	0.97	3 (5%)
29	LMT	B	637	-	24,24,36	0.51	0	29,29,47	0.71	0
24	CLA	c	508	3	69,73,73	2.49	24 (34%)	83,113,113	2.51	29 (34%)
34	DMS	D	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
36	HTG	i	103	-	19,19,19	0.97	2 (10%)	23,24,24	1.25	1 (4%)
34	DMS	j	1604	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
39	LHG	l	101	-	48,48,48	0.87	2 (4%)	51,54,54	1.13	3 (5%)
34	DMS	c	534	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
26	BCR	Y	302	-	41,41,41	0.77	0	56,56,56	1.62	10 (17%)
34	DMS	a	2121	-	3,3,3	2.51	1 (33%)	3,3,3	0.17	0
34	DMS	D	417	-	3,3,3	2.69	1 (33%)	3,3,3	0.48	0
38	DGD	c	520	-	63,63,67	0.84	3 (4%)	77,77,81	0.97	5 (6%)
26	BCR	b	620	-	41,41,41	0.78	0	56,56,56	1.38	4 (7%)
24	CLA	A	406	44	69,73,73	2.25	23 (33%)	83,113,113	2.50	31 (37%)
36	HTG	c	523	-	19,19,19	1.00	2 (10%)	23,24,24	1.68	4 (17%)
24	CLA	b	611	2	69,73,73	2.52	24 (34%)	83,113,113	2.49	29 (34%)
34	DMS	d	423	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0

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
32	K2I	A	419	-	-	-	0/1/1/1
24	CLA	b	612	2	-	3/39/115/115	-
36	HTG	C	521	-	-	3/10/30/30	0/1/1/1
24	CLA	B	604	2	-	3/39/115/115	-
24	CLA	b	618	2	-	6/39/115/115	-
36	HTG	C	522	-	-	3/10/30/30	0/1/1/1
28	LMG	B	622	-	-	12/46/66/70	0/1/1/1
24	CLA	B	616	2	-	11/39/115/115	-
26	BCR	b	621	-	-	1/29/63/63	0/2/2/2
28	LMG	i	101	-	-	12/46/66/70	0/1/1/1
26	BCR	k	2003	-	-	0/29/63/63	0/2/2/2
28	LMG	C	520	-	-	14/46/66/70	0/1/1/1
27	SQD	F	101	-	-	15/40/60/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LHG	D	410	-	-	9/53/53/53	-
29	LMT	a	2120	-	-	12/21/61/61	0/2/2/2
25	PHO	A	407	-	-	5/37/103/103	0/5/6/6
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
24	CLA	d	404	4	-	4/39/115/115	-
24	CLA	c	513	3	-	3/39/115/115	-
29	LMT	Z	101	-	-	10/21/61/61	0/2/2/2
26	BCR	d	406	-	-	6/29/63/63	0/2/2/2
24	CLA	B	614	2	-	3/39/115/115	-
37	GOL	k	2001	-	-	2/4/4/4	-
24	CLA	B	607	2	-	10/39/115/115	-
24	CLA	C	507	3	-	14/39/115/115	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
24	CLA	B	606	2	-	5/39/115/115	-
24	CLA	b	619	2	-	8/39/115/115	-
25	PHO	a	2112	-	-	2/37/103/103	0/5/6/6
38	DGD	c	519	-	-	19/51/91/95	0/2/2/2
28	LMG	c	522	-	-	9/43/63/70	0/1/1/1
40	HEM	F	102	6,5	-	3/14/54/54	-
24	CLA	c	511	3	-	8/39/115/115	-
24	CLA	d	405	4	-	4/39/115/115	-
24	CLA	C	513	3	-	7/39/115/115	-
24	CLA	d	401	44	-	4/39/115/115	-
24	CLA	B	608	44	-	3/39/115/115	-
29	LMT	m	103	-	-	1/21/61/61	0/2/2/2
24	CLA	B	611	44	-	9/39/115/115	-
24	CLA	b	616	2	-	4/39/115/115	-
28	LMG	b	623	-	-	12/46/66/70	0/1/1/1
29	LMT	A	414	-	-	6/20/60/61	0/2/2/2
36	HTG	B	625[A]	-	-	4/10/30/30	0/1/1/1
37	GOL	C	525	-	-	2/4/4/4	-
24	CLA	c	509	44	-	8/39/115/115	-
29	LMT	J	102	-	-	6/15/35/61	0/1/1/2
32	K2I	A	418[B]	-	-	-	0/1/1/1
29	LMT	E	105	-	-	7/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	B	626	-	-	4/10/30/30	0/1/1/1
24	CLA	B	602	44	-	12/39/115/115	-
37	GOL	O	303	-	-	4/4/4/4	-
29	LMT	B	623	-	-	10/21/61/61	0/2/2/2
28	LMG	c	521	-	-	13/44/64/70	0/1/1/1
24	CLA	C	508	44	-	7/39/115/115	-
28	LMG	d	411	42	-	7/43/63/70	0/1/1/1
24	CLA	C	511	3	-	6/39/115/115	-
37	GOL	a	2101	-	-	2/4/4/4	-
24	CLA	b	606	2	-	2/39/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
37	GOL	o	2601	-	-	3/4/4/4	-
24	CLA	a	2110	44	-	7/39/115/115	-
28	LMG	A	412	-	-	16/46/66/70	0/1/1/1
24	CLA	c	503	3	-	1/39/115/115	-
38	DGD	C	519	-	-	6/51/91/95	0/2/2/2
24	CLA	C	509	3	-	7/39/115/115	-
36	HTG	B	625[B]	-	-	3/10/30/30	0/1/1/1
24	CLA	B	609	2	-	1/39/115/115	-
37	GOL	C	524	-	-	0/4/4/4	-
37	GOL	U	501	-	-	2/4/4/4	-
24	CLA	a	2113	1	-	7/39/115/115	-
24	CLA	c	510	3	-	5/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
39	LHG	e	101	-	-	16/35/35/53	-
24	CLA	C	504	3	-	5/39/115/115	-
24	CLA	C	512	3	-	5/39/115/115	-
24	CLA	b	607	2	-	6/39/115/115	-
24	CLA	B	613	2	-	3/39/115/115	-
29	LMT	A	420	-	-	6/21/61/61	0/2/2/2
24	CLA	b	609	2	-	5/39/115/115	-
29	LMT	b	624	-	-	4/17/37/61	0/1/1/2
37	GOL	v	203	-	-	1/4/4/4	-
24	CLA	C	514	3	-	2/39/115/115	-
24	CLA	A	405	1	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	504	3	-	6/39/115/115	-
36	HTG	V	204	-	-	5/10/30/30	0/1/1/1
37	GOL	v	202	-	-	2/4/4/4	-
24	CLA	B	605	2	-	7/39/115/115	-
24	CLA	b	604	44	-	12/39/115/115	-
24	CLA	A	409	1	-	9/39/115/115	-
24	CLA	D	401	44	-	5/39/115/115	-
26	BCR	T	101	-	-	3/29/63/63	0/2/2/2
24	CLA	b	610	44	-	1/39/115/115	-
36	HTG	b	625	-	-	0/10/30/30	0/1/1/1
31	PL9	A	417	-	-	11/42/42/73	-
37	GOL	v	204	-	-	4/4/4/4	-
24	CLA	C	502	3	-	6/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
37	GOL	H	103	-	-	2/4/4/4	-
24	CLA	B	603	2	-	5/39/115/115	-
37	GOL	V	203	-	-	4/4/4/4	-
39	LHG	d	408	-	-	11/53/53/53	-
40	HEM	e	103	6,5	-	4/14/54/54	-
25	PHO	a	2111	-	-	4/37/103/103	0/5/6/6
26	BCR	C	516	-	-	2/29/63/63	0/2/2/2
29	LMT	i	104	-	-	11/15/35/61	0/1/1/2
31	PL9	D	407	-	-	3/53/73/73	0/1/1/1
37	GOL	b	631	-	-	2/4/4/4	-
26	BCR	c	516	-	-	2/29/63/63	0/2/2/2
32	K2I	a	2119	-	-	-	0/1/1/1
39	LHG	L	101	-	-	14/53/53/53	-
24	CLA	c	507	3	-	5/39/115/115	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
24	CLA	b	617	2	-	12/39/115/115	-
29	LMT	B	636	-	-	8/21/61/61	0/2/2/2
27	SQD	A	413	-	-	12/49/69/69	0/1/1/1
36	HTG	c	526	-	-	2/10/30/30	0/1/1/1
36	HTG	b	601	-	-	2/10/30/30	0/1/1/1
27	SQD	a	2102	-	-	12/48/68/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	B	627	-	-	3/10/30/30	0/1/1/1
27	SQD	L	102	-	-	22/49/69/69	0/1/1/1
29	LMT	f	101	-	-	6/15/35/61	0/1/1/2
38	DGD	h	703	-	-	8/51/91/95	0/2/2/2
24	CLA	D	404	4	-	3/39/115/115	-
24	CLA	a	2109	1	-	3/39/115/115	-
37	GOL	D	403	-	-	0/4/4/4	-
28	LMG	C	526	-	-	11/43/63/70	0/1/1/1
39	LHG	E	101	-	-	19/53/53/53	-
37	GOL	B	632	-	-	0/4/4/4	-
43	HEC	V	201	16	1/1/3/7	6/14/54/54	-
26	BCR	C	515	-	-	3/29/63/63	0/2/2/2
43	HEC	v	201	16	1/1/3/7	6/14/54/54	-
24	CLA	c	505	3	-	1/39/115/115	-
37	GOL	Z	102	-	-	2/4/4/4	-
24	CLA	b	614	2	-	3/39/115/115	-
36	HTG	c	524	-	-	0/10/30/30	0/1/1/1
24	CLA	D	405	4	-	6/39/115/115	-
36	HTG	D	413	-	-	2/10/30/30	0/1/1/1
24	CLA	C	503	3	-	5/39/115/115	-
31	PL9	x	801	-	-	9/42/42/73	-
36	HTG	d	403	-	-	4/10/30/30	0/1/1/1
24	CLA	C	505	44	-	6/39/115/115	-
24	CLA	C	506	3	-	4/39/115/115	-
24	CLA	b	613	44	-	6/39/115/115	-
36	HTG	b	626	-	-	5/10/30/30	0/1/1/1
37	GOL	d	415	-	-	2/4/4/4	-
26	BCR	A	410	-	-	1/29/63/63	0/2/2/2
29	LMT	I	1201	-	-	7/15/35/61	0/1/1/2
38	DGD	H	102	-	-	9/51/91/95	0/2/2/2
29	LMT	M	101	-	-	5/21/61/61	0/2/2/2
37	GOL	c	527	-	-	1/4/4/4	-
24	CLA	c	506	44	-	8/39/115/115	-
24	CLA	c	515	3	-	6/39/115/115	-
24	CLA	c	512	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	510	3	-	6/39/115/115	-
29	LMT	T	102	-	-	7/15/35/61	0/1/1/2
31	PL9	d	407	-	-	4/53/73/73	0/1/1/1
24	CLA	B	610	2	-	5/39/115/115	-
36	HTG	I	1202	-	-	3/10/30/30	0/1/1/1
29	LMT	j	1601	-	-	5/11/31/61	0/1/1/2
24	CLA	c	514	3	-	6/39/115/115	-
26	BCR	t	102	-	-	3/29/63/63	0/2/2/2
38	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	B	617	2	-	11/39/115/115	-
27	SQD	f	102	-	-	13/38/38/69	-
41	RRX	h	702	-	-	1/29/65/65	0/2/2/2
36	HTG	d	414	-	-	1/10/30/30	0/1/1/1
38	DGD	C	518	-	-	19/51/91/95	0/2/2/2
39	LHG	d	409	-	-	12/53/53/53	-
32	K2I	A	418[A]	-	-	-	0/1/1/1
32	K2I	a	2118[A]	-	-	-	0/1/1/1
29	LMT	B	637	-	-	9/15/35/61	0/1/1/2
24	CLA	c	508	3	-	8/39/115/115	-
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
27	SQD	A	411	-	-	9/44/64/69	0/1/1/1
27	SQD	a	2115	-	-	12/42/62/69	0/1/1/1
36	HTG	i	103	-	-	1/10/30/30	0/1/1/1
36	HTG	O	302	-	-	5/10/30/30	0/1/1/1
41	RRX	H	101	-	-	1/29/65/65	0/2/2/2
26	BCR	a	2114	-	-	2/29/63/63	0/2/2/2
39	LHG	D	411	-	-	11/48/48/53	-
37	GOL	o	2603	-	-	3/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
36	HTG	B	624	-	-	3/10/30/30	0/1/1/1
29	LMT	z	1801	-	-	8/16/56/61	0/2/2/2
39	LHG	l	101	-	-	16/53/53/53	-
24	CLA	B	615	2	-	12/39/115/115	-
24	CLA	b	608	2	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LHG	D	409	-	-	16/53/53/53	-
24	CLA	b	615	2	-	3/39/115/115	-
26	BCR	Y	302	-	-	4/29/63/63	0/2/2/2
24	CLA	b	605	2	-	1/39/115/115	-
26	BCR	c	517	-	-	2/29/63/63	0/2/2/2
38	DGD	c	520	-	-	10/51/91/95	0/2/2/2
26	BCR	b	620	-	-	2/29/63/63	0/2/2/2
24	CLA	A	406	44	-	7/39/115/115	-
38	DGD	c	518	-	-	17/51/91/95	0/2/2/2
39	LHG	d	410	-	-	6/40/40/53	-
36	HTG	c	523	-	-	2/10/30/30	0/1/1/1
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
37	GOL	B	635	-	-	0/4/4/4	-
32	K2I	a	2118[B]	-	-	-	0/1/1/1
24	CLA	B	612	2	-	5/39/115/115	-
38	DGD	D	408	-	-	17/40/61/95	0/1/1/2
37	GOL	U	502	-	-	2/4/4/4	-
29	LMT	a	2103	-	-	11/21/61/61	0/2/2/2
24	CLA	b	611	2	-	1/39/115/115	-
36	HTG	B	628	-	-	1/10/30/30	0/1/1/1
26	BCR	c	528	-	-	4/29/63/63	0/2/2/2
28	LMG	D	412	42	-	10/39/59/70	0/1/1/1

All (1999) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	MG-NA	11.53	2.33	2.06
24	C	512	CLA	MG-NA	11.41	2.33	2.06
24	C	508	CLA	MG-NA	10.32	2.30	2.06
24	C	506	CLA	MG-NA	9.69	2.29	2.06
24	C	504	CLA	MG-NA	9.53	2.28	2.06
24	a	2109	CLA	MG-ND	-9.47	1.87	2.05
24	B	607	CLA	MG-NA	9.40	2.28	2.06
24	b	607	CLA	MG-NA	9.38	2.28	2.06
24	b	607	CLA	MG-ND	-9.16	1.87	2.05
24	C	507	CLA	MG-ND	-9.13	1.87	2.05
24	c	513	CLA	MG-NA	9.13	2.27	2.06
24	b	607	CLA	MG-NC	9.11	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	MG-ND	-8.96	1.88	2.05
24	c	511	CLA	MG-NA	8.92	2.27	2.06
24	B	612	CLA	MG-NA	8.89	2.27	2.06
25	a	2112	PHO	C1D-C2D	8.88	1.49	1.39
24	C	503	CLA	MG-NA	8.79	2.27	2.06
25	A	408	PHO	C1B-C2B	8.77	1.49	1.39
25	a	2112	PHO	C1B-C2B	8.69	1.49	1.39
24	c	514	CLA	MG-ND	-8.66	1.88	2.05
25	A	407	PHO	C1D-C2D	8.65	1.49	1.39
24	b	612	CLA	MG-NA	8.52	2.26	2.06
25	a	2111	PHO	C1D-C2D	8.48	1.49	1.39
24	c	514	CLA	MG-NA	8.47	2.26	2.06
25	A	407	PHO	C1B-C2B	8.44	1.48	1.39
24	B	605	CLA	MG-NC	8.37	2.26	2.06
24	B	612	CLA	MG-ND	-8.36	1.89	2.05
24	C	503	CLA	MG-ND	-8.32	1.89	2.05
25	A	408	PHO	C1D-C2D	8.30	1.48	1.39
24	c	507	CLA	MG-NA	8.29	2.26	2.06
24	c	511	CLA	MG-ND	-8.29	1.89	2.05
24	c	509	CLA	MG-NA	8.28	2.25	2.06
24	B	608	CLA	MG-NA	8.25	2.25	2.06
24	C	513	CLA	MG-NA	8.20	2.25	2.06
24	c	506	CLA	MG-NA	8.20	2.25	2.06
24	C	512	CLA	MG-ND	-8.19	1.89	2.05
24	B	617	CLA	MG-NA	8.17	2.25	2.06
24	b	614	CLA	MG-ND	-8.15	1.89	2.05
24	b	611	CLA	MG-ND	-8.00	1.89	2.05
24	b	619	CLA	MG-NA	7.90	2.25	2.06
24	c	508	CLA	MG-ND	-7.89	1.90	2.05
24	C	507	CLA	MG-NC	7.87	2.25	2.06
40	e	103	HEM	C3D-C2D	7.84	1.53	1.36
24	b	618	CLA	MG-NA	7.83	2.24	2.06
24	C	505	CLA	MG-NC	7.79	2.24	2.06
43	v	201	HEC	C3D-C2D	7.79	1.53	1.36
24	C	510	CLA	MG-NA	7.76	2.24	2.06
24	C	507	CLA	MG-NA	7.74	2.24	2.06
43	V	201	HEC	C3D-C2D	7.70	1.53	1.36
24	C	509	CLA	MG-ND	-7.66	1.90	2.05
25	a	2111	PHO	C1B-C2B	7.65	1.48	1.39
24	B	610	CLA	MG-ND	-7.63	1.90	2.05
24	C	514	CLA	MG-ND	-7.61	1.90	2.05
24	c	505	CLA	MG-NC	7.60	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	MG-NA	7.57	2.24	2.06
24	B	602	CLA	MG-NA	7.57	2.24	2.06
24	c	515	CLA	MG-NC	7.57	2.24	2.06
24	d	405	CLA	MG-NA	7.55	2.24	2.06
40	F	102	HEM	C3D-C2D	7.55	1.52	1.36
24	b	605	CLA	MG-NA	7.48	2.24	2.06
24	d	404	CLA	MG-NC	7.46	2.24	2.06
24	B	615	CLA	MG-NA	7.38	2.23	2.06
24	B	610	CLA	MG-NA	7.36	2.23	2.06
25	A	408	PHO	C3B-C4B	7.33	1.49	1.41
24	C	509	CLA	MG-NC	7.28	2.23	2.06
25	a	2112	PHO	C3B-C4B	7.23	1.49	1.41
24	B	613	CLA	MG-NA	7.22	2.23	2.06
24	d	401	CLA	MG-ND	-7.19	1.91	2.05
24	b	604	CLA	MG-NC	7.18	2.23	2.06
24	B	603	CLA	MG-NA	7.12	2.23	2.06
24	C	502	CLA	MG-NC	7.12	2.23	2.06
24	B	609	CLA	MG-ND	-7.11	1.91	2.05
24	B	610	CLA	MG-NC	7.09	2.23	2.06
24	B	606	CLA	MG-NA	7.05	2.23	2.06
24	c	503	CLA	MG-ND	-7.03	1.91	2.05
24	B	616	CLA	MG-ND	-7.01	1.91	2.05
24	c	510	CLA	MG-NC	6.96	2.22	2.06
24	C	510	CLA	MG-ND	-6.92	1.92	2.05
24	B	604	CLA	MG-NA	6.92	2.22	2.06
24	c	503	CLA	MG-NA	6.90	2.22	2.06
27	f	102	SQD	C6-S	-6.90	1.67	1.77
24	B	616	CLA	MG-NA	6.88	2.22	2.06
24	a	2110	CLA	MG-NA	6.86	2.22	2.06
24	B	609	CLA	MG-NA	6.80	2.22	2.06
24	b	606	CLA	MG-NC	6.77	2.22	2.06
24	b	612	CLA	MG-NC	6.75	2.22	2.06
24	b	614	CLA	MG-NA	6.73	2.22	2.06
24	b	616	CLA	MG-ND	-6.73	1.92	2.05
24	B	605	CLA	MG-ND	-6.72	1.92	2.05
25	A	408	PHO	C3B-C2B	6.70	1.49	1.40
24	c	507	CLA	MG-ND	-6.70	1.92	2.05
24	b	619	CLA	MG-ND	-6.69	1.92	2.05
24	C	506	CLA	MG-ND	-6.69	1.92	2.05
24	c	507	CLA	MG-NC	6.68	2.22	2.06
24	b	616	CLA	MG-NA	6.67	2.22	2.06
25	a	2111	PHO	C3B-C2B	6.65	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C4D-CHA	6.65	1.50	1.39
24	d	404	CLA	MG-NA	6.65	2.22	2.06
24	C	511	CLA	MG-NA	6.65	2.22	2.06
24	C	504	CLA	MG-NC	6.63	2.22	2.06
24	a	2109	CLA	MG-NA	6.61	2.22	2.06
24	C	511	CLA	MG-NC	6.60	2.21	2.06
24	b	610	CLA	MG-NC	6.58	2.21	2.06
24	c	505	CLA	MG-ND	-6.56	1.92	2.05
24	B	604	CLA	MG-NC	6.53	2.21	2.06
25	A	407	PHO	C3B-C4B	6.53	1.49	1.41
24	C	511	CLA	MG-ND	-6.51	1.92	2.05
24	A	405	CLA	MG-ND	-6.49	1.92	2.05
24	b	607	CLA	C1D-ND	6.48	1.45	1.37
24	a	2110	CLA	MG-ND	-6.46	1.93	2.05
24	D	405	CLA	MG-NA	6.46	2.21	2.06
24	D	405	CLA	MG-NC	6.45	2.21	2.06
24	c	511	CLA	MG-NC	6.45	2.21	2.06
24	b	617	CLA	MG-ND	-6.45	1.93	2.05
24	b	609	CLA	MG-NC	6.43	2.21	2.06
24	C	505	CLA	MG-NA	6.43	2.21	2.06
24	b	616	CLA	MG-NC	6.39	2.21	2.06
24	C	503	CLA	C1D-ND	6.39	1.45	1.37
24	b	606	CLA	MG-ND	-6.37	1.93	2.05
24	C	506	CLA	MG-NC	6.37	2.21	2.06
24	b	610	CLA	MG-NA	6.34	2.21	2.06
24	c	510	CLA	MG-ND	-6.33	1.93	2.05
24	c	515	CLA	MG-NA	6.33	2.21	2.06
24	D	404	CLA	MG-NA	6.31	2.21	2.06
24	b	605	CLA	MG-NC	6.28	2.21	2.06
24	c	515	CLA	C1D-ND	6.26	1.45	1.37
24	b	609	CLA	MG-NA	6.23	2.21	2.06
24	C	507	CLA	C1D-ND	6.23	1.45	1.37
24	C	502	CLA	C1D-ND	6.22	1.45	1.37
24	B	610	CLA	C1D-ND	6.22	1.45	1.37
24	c	511	CLA	C1D-ND	6.22	1.45	1.37
24	B	605	CLA	MG-NA	6.18	2.21	2.06
25	a	2112	PHO	C4D-CHA	6.17	1.49	1.39
25	A	407	PHO	C3B-C2B	6.17	1.48	1.40
25	A	407	PHO	C4D-CHA	6.17	1.49	1.39
24	c	509	CLA	MG-NC	6.16	2.20	2.06
24	b	604	CLA	MG-NA	6.16	2.20	2.06
24	c	505	CLA	C1D-ND	6.15	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	405	CLA	C3C-C2C	6.15	1.49	1.36
24	b	613	CLA	MG-NA	6.12	2.20	2.06
24	b	617	CLA	MG-NA	6.12	2.20	2.06
24	b	606	CLA	MG-NA	6.10	2.20	2.06
24	c	515	CLA	MG-ND	-6.09	1.93	2.05
24	c	508	CLA	C1D-ND	6.09	1.45	1.37
24	B	603	CLA	MG-ND	-6.08	1.93	2.05
24	b	612	CLA	C1D-ND	6.07	1.45	1.37
24	A	409	CLA	MG-NC	6.07	2.20	2.06
24	B	611	CLA	MG-NC	6.06	2.20	2.06
24	B	612	CLA	MG-NC	6.01	2.20	2.06
24	C	504	CLA	C1D-ND	5.99	1.45	1.37
24	C	509	CLA	C3C-C2C	5.99	1.49	1.36
24	C	513	CLA	MG-ND	-5.99	1.93	2.05
24	C	514	CLA	C1D-ND	5.98	1.45	1.37
24	c	510	CLA	C3C-C2C	5.96	1.49	1.36
24	C	502	CLA	MG-NA	5.96	2.20	2.06
24	B	604	CLA	C3C-C2C	5.93	1.49	1.36
24	b	611	CLA	MG-NC	5.93	2.20	2.06
24	a	2113	CLA	C3C-C2C	5.92	1.49	1.36
24	B	611	CLA	C3C-C2C	5.90	1.49	1.36
24	c	514	CLA	C1D-ND	5.89	1.45	1.37
24	b	613	CLA	C3C-C2C	5.89	1.49	1.36
25	a	2111	PHO	C4D-CHA	5.89	1.49	1.39
24	c	512	CLA	MG-NC	5.88	2.20	2.06
24	A	405	CLA	MG-NA	5.87	2.20	2.06
24	d	401	CLA	C3C-C2C	5.87	1.49	1.36
24	C	510	CLA	C3C-C2C	5.86	1.49	1.36
24	C	510	CLA	MG-NC	5.86	2.20	2.06
24	c	515	CLA	C3C-C2C	5.86	1.49	1.36
24	b	604	CLA	C3C-C2C	5.85	1.49	1.36
24	b	615	CLA	MG-NA	5.82	2.20	2.06
24	C	508	CLA	MG-ND	-5.81	1.94	2.05
24	C	510	CLA	C1D-ND	5.80	1.44	1.37
24	b	609	CLA	C1D-ND	5.80	1.44	1.37
24	c	512	CLA	C3C-C2C	5.80	1.49	1.36
24	C	514	CLA	C3C-C2C	5.79	1.49	1.36
40	e	103	HEM	FE-ND	5.79	2.12	1.94
24	b	606	CLA	C3C-C2C	5.79	1.49	1.36
24	b	616	CLA	C1D-ND	5.78	1.44	1.37
24	B	608	CLA	MG-NC	5.78	2.20	2.06
24	B	612	CLA	C1D-ND	5.78	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	C1D-ND	5.78	1.44	1.37
24	B	609	CLA	C1D-ND	5.78	1.44	1.37
24	d	401	CLA	C1D-ND	5.77	1.44	1.37
24	B	603	CLA	C3C-C2C	5.77	1.49	1.36
24	A	405	CLA	C3C-C2C	5.76	1.49	1.36
24	C	508	CLA	C1D-ND	5.76	1.44	1.37
24	B	602	CLA	C3C-C2C	5.75	1.49	1.36
24	b	617	CLA	C1D-ND	5.75	1.44	1.37
24	c	514	CLA	C3C-C2C	5.75	1.48	1.36
24	c	507	CLA	C1D-ND	5.74	1.44	1.37
24	B	602	CLA	C1D-ND	5.74	1.44	1.37
24	A	409	CLA	C1D-ND	5.73	1.44	1.37
24	c	504	CLA	C3C-C2C	5.73	1.48	1.36
24	b	611	CLA	C1D-ND	5.72	1.44	1.37
24	C	506	CLA	C3C-C2C	5.71	1.48	1.36
40	F	102	HEM	FE-ND	5.71	2.12	1.94
24	b	610	CLA	C3C-C2C	5.70	1.48	1.36
24	A	409	CLA	C3C-C2C	5.67	1.48	1.36
24	C	506	CLA	C1D-ND	5.67	1.44	1.37
24	b	613	CLA	C1D-ND	5.67	1.44	1.37
24	C	514	CLA	MG-NC	5.66	2.19	2.06
25	a	2112	PHO	C3B-C2B	5.66	1.48	1.40
24	c	508	CLA	MG-NC	5.66	2.19	2.06
24	b	614	CLA	C1D-ND	5.65	1.44	1.37
25	A	407	PHO	C3C-C2C	5.65	1.48	1.36
24	C	502	CLA	C3C-C2C	5.65	1.48	1.36
24	C	513	CLA	C3C-C2C	5.65	1.48	1.36
24	c	508	CLA	C3C-C2C	5.64	1.48	1.36
24	C	503	CLA	C3C-C2C	5.64	1.48	1.36
24	A	406	CLA	C3C-C2C	5.62	1.48	1.36
24	C	504	CLA	C3C-C2C	5.62	1.48	1.36
24	C	507	CLA	C3C-C2C	5.62	1.48	1.36
24	b	605	CLA	C3C-C2C	5.61	1.48	1.36
25	a	2112	PHO	C3C-C2C	5.61	1.48	1.36
24	C	505	CLA	C1D-ND	5.60	1.44	1.37
24	a	2113	CLA	MG-NC	5.59	2.19	2.06
24	b	612	CLA	C3C-C2C	5.59	1.48	1.36
24	B	607	CLA	C3C-C2C	5.59	1.48	1.36
24	C	511	CLA	C1D-ND	5.58	1.44	1.37
24	b	608	CLA	C3C-C2C	5.58	1.48	1.36
24	c	504	CLA	MG-NA	5.58	2.19	2.06
24	C	505	CLA	C3C-C2C	5.57	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	C3C-C2C	5.57	1.48	1.36
24	B	616	CLA	C1D-ND	5.57	1.44	1.37
24	c	511	CLA	C3C-C2C	5.57	1.48	1.36
24	B	614	CLA	C1D-ND	5.57	1.44	1.37
24	B	604	CLA	C1D-ND	5.55	1.44	1.37
24	c	509	CLA	C3C-C2C	5.55	1.48	1.36
24	B	614	CLA	C3C-C2C	5.54	1.48	1.36
24	b	616	CLA	C3C-C2C	5.54	1.48	1.36
24	D	401	CLA	C3C-C2C	5.54	1.48	1.36
24	c	512	CLA	C1D-ND	5.53	1.44	1.37
24	b	618	CLA	C3C-C2C	5.52	1.48	1.36
24	b	617	CLA	C3C-C2C	5.51	1.48	1.36
24	C	508	CLA	C3C-C2C	5.51	1.48	1.36
25	A	408	PHO	C3C-C2C	5.51	1.48	1.36
24	a	2109	CLA	C3C-C2C	5.51	1.48	1.36
24	b	606	CLA	C1D-ND	5.51	1.44	1.37
24	B	607	CLA	C1D-ND	5.51	1.44	1.37
24	C	511	CLA	C3C-C2C	5.50	1.48	1.36
24	c	513	CLA	C1D-ND	5.49	1.44	1.37
24	b	611	CLA	C3C-C2C	5.48	1.48	1.36
24	B	609	CLA	C3C-C2C	5.48	1.48	1.36
24	c	512	CLA	MG-ND	-5.48	1.94	2.05
24	b	614	CLA	MG-NC	5.48	2.19	2.06
24	B	613	CLA	CHC-C1C	5.47	1.49	1.38
24	b	617	CLA	MG-NC	5.47	2.19	2.06
24	B	608	CLA	C3C-C2C	5.47	1.48	1.36
24	c	504	CLA	C1D-ND	5.46	1.44	1.37
24	b	618	CLA	C1D-ND	5.46	1.44	1.37
24	b	614	CLA	MG-NB	5.46	2.16	2.05
24	d	405	CLA	C3C-C2C	5.45	1.48	1.36
24	B	605	CLA	C1D-ND	5.45	1.44	1.37
24	D	405	CLA	C1D-ND	5.44	1.44	1.37
24	B	610	CLA	C3C-C2C	5.44	1.48	1.36
24	c	513	CLA	C3C-C2C	5.41	1.48	1.36
24	b	609	CLA	C3C-C2C	5.40	1.48	1.36
24	B	611	CLA	C1D-ND	5.40	1.44	1.37
24	C	512	CLA	C3C-C2C	5.40	1.48	1.36
24	c	506	CLA	C3C-C2C	5.39	1.48	1.36
24	B	615	CLA	C3C-C2C	5.39	1.48	1.36
25	a	2111	PHO	C3B-C4B	5.38	1.47	1.41
24	d	405	CLA	MG-ND	-5.37	1.95	2.05
24	b	605	CLA	C1D-ND	5.37	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	2109	CLA	C1D-ND	5.37	1.44	1.37
24	C	507	CLA	O2D-CGD	5.37	1.46	1.33
24	d	404	CLA	C3C-C2C	5.37	1.48	1.36
24	D	401	CLA	MG-ND	-5.36	1.95	2.05
24	a	2110	CLA	C3C-C2C	5.35	1.48	1.36
24	D	404	CLA	C3C-C2C	5.35	1.48	1.36
24	c	508	CLA	MG-NA	5.34	2.19	2.06
24	C	512	CLA	C1D-ND	5.33	1.44	1.37
24	b	612	CLA	O2D-CGD	5.33	1.46	1.33
24	C	509	CLA	C1D-ND	5.33	1.44	1.37
24	c	504	CLA	MG-ND	-5.32	1.95	2.05
24	B	612	CLA	C3C-C2C	5.31	1.48	1.36
24	b	609	CLA	MG-ND	-5.31	1.95	2.05
24	B	605	CLA	C3C-C2C	5.30	1.48	1.36
24	B	613	CLA	C3C-C2C	5.30	1.48	1.36
24	c	506	CLA	O2D-CGD	5.30	1.46	1.33
24	c	503	CLA	C3C-C2C	5.29	1.48	1.36
24	B	617	CLA	C3C-C2C	5.29	1.48	1.36
24	B	602	CLA	CHC-C1C	5.29	1.49	1.38
24	b	619	CLA	C3C-C2C	5.28	1.48	1.36
24	b	607	CLA	C3C-C2C	5.28	1.48	1.36
24	B	616	CLA	C3C-C2C	5.27	1.47	1.36
24	C	513	CLA	C1D-ND	5.27	1.44	1.37
24	b	608	CLA	CHC-C1C	5.26	1.49	1.38
24	b	614	CLA	C3C-C2C	5.24	1.47	1.36
24	c	509	CLA	C1D-ND	5.23	1.44	1.37
25	a	2112	PHO	C3D-C2D	5.23	1.48	1.39
24	B	606	CLA	C1D-ND	5.23	1.44	1.37
24	b	615	CLA	C3C-C2C	5.23	1.47	1.36
25	A	407	PHO	C3D-C2D	5.23	1.48	1.39
24	d	405	CLA	C1D-ND	5.22	1.44	1.37
24	b	614	CLA	O2D-CGD	5.22	1.45	1.33
24	c	510	CLA	C1D-ND	5.21	1.44	1.37
24	B	616	CLA	O2D-CGD	5.21	1.45	1.33
24	b	615	CLA	MG-ND	-5.20	1.95	2.05
24	b	613	CLA	CHC-C1C	5.20	1.49	1.38
24	b	608	CLA	MG-NA	5.20	2.18	2.06
24	c	504	CLA	O2D-CGD	5.19	1.45	1.33
24	B	606	CLA	C3C-C2C	5.17	1.47	1.36
24	b	619	CLA	C1D-ND	5.17	1.44	1.37
24	B	614	CLA	MG-NA	5.17	2.18	2.06
25	a	2111	PHO	O2D-CGD	5.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	O2D-CGD	5.16	1.45	1.33
24	b	613	CLA	MG-ND	-5.16	1.95	2.05
24	b	611	CLA	O2D-CGD	5.16	1.45	1.33
24	B	608	CLA	MG-ND	-5.16	1.95	2.05
24	B	609	CLA	MG-NC	5.15	2.18	2.06
24	B	604	CLA	MG-ND	-5.14	1.95	2.05
24	D	401	CLA	C1D-ND	5.14	1.44	1.37
24	C	513	CLA	CHC-C1C	5.14	1.49	1.38
24	b	611	CLA	MG-NA	5.14	2.18	2.06
24	C	512	CLA	CHC-C1C	5.13	1.48	1.38
24	b	605	CLA	O2D-CGD	5.13	1.45	1.33
24	A	405	CLA	C1D-ND	5.12	1.44	1.37
25	A	408	PHO	C3D-C2D	5.12	1.48	1.39
24	b	617	CLA	CHC-C1C	5.11	1.48	1.38
24	C	506	CLA	CHD-C1D	5.11	1.48	1.38
24	B	607	CLA	MG-NC	5.10	2.18	2.06
24	c	512	CLA	MG-NA	5.10	2.18	2.06
24	b	619	CLA	O2D-CGD	5.10	1.45	1.33
24	c	508	CLA	O2D-CGD	5.09	1.45	1.33
24	D	401	CLA	O2D-CGD	5.08	1.45	1.33
25	a	2111	PHO	C3C-C2C	5.08	1.47	1.36
25	a	2111	PHO	C3D-C2D	5.08	1.48	1.39
24	b	610	CLA	O2D-CGD	5.07	1.45	1.33
24	B	617	CLA	C1D-ND	5.07	1.44	1.37
24	c	507	CLA	C3C-C2C	5.07	1.47	1.36
24	d	401	CLA	O2D-CGD	5.07	1.45	1.33
24	B	603	CLA	C1D-ND	5.07	1.44	1.37
24	C	511	CLA	CHC-C1C	5.07	1.48	1.38
24	b	610	CLA	C1D-ND	5.07	1.44	1.37
24	b	612	CLA	CHD-C1D	5.06	1.48	1.38
24	c	513	CLA	CHC-C1C	5.05	1.48	1.38
24	B	617	CLA	O2D-CGD	5.05	1.45	1.33
24	C	509	CLA	CHC-C1C	5.04	1.48	1.38
24	b	618	CLA	CHC-C1C	5.04	1.48	1.38
24	C	514	CLA	O2D-CGD	5.04	1.45	1.33
24	b	608	CLA	O2D-CGD	5.03	1.45	1.33
24	B	615	CLA	C1D-ND	5.03	1.44	1.37
24	b	615	CLA	C1D-ND	5.03	1.44	1.37
24	B	608	CLA	C1D-ND	5.03	1.44	1.37
24	c	510	CLA	CHC-C1C	5.02	1.48	1.38
24	b	610	CLA	CHC-C1C	5.02	1.48	1.38
24	a	2113	CLA	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	CHC-C1C	5.02	1.48	1.38
24	D	405	CLA	CHC-C1C	5.01	1.48	1.38
24	c	514	CLA	MG-NC	5.01	2.18	2.06
24	B	610	CLA	O2D-CGD	5.00	1.45	1.33
24	B	606	CLA	O2D-CGD	5.00	1.45	1.33
24	a	2113	CLA	C1D-ND	5.00	1.43	1.37
24	b	616	CLA	O2D-CGD	5.00	1.45	1.33
24	b	604	CLA	O2D-CGD	4.99	1.45	1.33
24	b	615	CLA	O2D-CGD	4.99	1.45	1.33
24	B	611	CLA	MG-NA	4.98	2.18	2.06
24	C	511	CLA	CHB-C1B	4.98	1.50	1.39
43	V	201	HEC	FE-NB	4.98	2.10	1.94
24	B	614	CLA	MG-NC	4.97	2.18	2.06
24	c	503	CLA	C1D-ND	4.97	1.43	1.37
24	B	603	CLA	CHC-C1C	4.97	1.48	1.38
24	B	617	CLA	MG-ND	-4.97	1.95	2.05
24	C	510	CLA	O2D-CGD	4.96	1.45	1.33
24	c	505	CLA	CHC-C1C	4.96	1.48	1.38
24	B	611	CLA	CHC-C1C	4.96	1.48	1.38
24	c	515	CLA	CHD-C1D	4.95	1.48	1.38
24	B	613	CLA	O2D-CGD	4.95	1.45	1.33
24	b	604	CLA	CHC-C1C	4.94	1.48	1.38
24	b	607	CLA	O2D-CGD	4.94	1.45	1.33
24	C	506	CLA	CHC-C1C	4.94	1.48	1.38
24	D	405	CLA	O2D-CGD	4.94	1.45	1.33
24	C	510	CLA	CHC-C1C	4.93	1.48	1.38
24	c	515	CLA	CHC-C1C	4.93	1.48	1.38
24	B	612	CLA	CHC-C1C	4.92	1.48	1.38
24	d	401	CLA	MG-NA	4.92	2.18	2.06
24	C	505	CLA	CHC-C1C	4.92	1.48	1.38
24	A	406	CLA	CHD-C1D	4.92	1.47	1.38
24	c	504	CLA	CHC-C1C	4.91	1.48	1.38
24	c	503	CLA	MG-NC	4.91	2.17	2.06
24	b	608	CLA	C1D-ND	4.90	1.43	1.37
24	c	513	CLA	CHD-C1D	4.90	1.47	1.38
24	B	609	CLA	CHD-C1D	4.90	1.47	1.38
24	a	2110	CLA	C1D-ND	4.90	1.43	1.37
24	C	509	CLA	O2D-CGD	4.89	1.45	1.33
25	A	408	PHO	O2D-CGD	4.89	1.45	1.33
24	B	608	CLA	CHC-C1C	4.89	1.48	1.38
24	B	614	CLA	O2D-CGD	4.89	1.45	1.33
24	d	405	CLA	CHC-C1C	4.89	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	CHC-C1C	4.88	1.48	1.38
24	C	505	CLA	MG-ND	-4.88	1.96	2.05
24	B	602	CLA	O2D-CGD	4.88	1.45	1.33
24	c	503	CLA	CHC-C1C	4.88	1.48	1.38
24	C	502	CLA	CHC-C1C	4.88	1.48	1.38
24	c	505	CLA	CHD-C1D	4.88	1.47	1.38
24	d	405	CLA	MG-NC	4.87	2.17	2.06
24	B	616	CLA	CHC-C1C	4.87	1.48	1.38
24	A	409	CLA	CHC-C1C	4.87	1.48	1.38
24	D	401	CLA	MG-NA	4.87	2.17	2.06
24	B	604	CLA	CHC-C1C	4.87	1.48	1.38
24	A	406	CLA	MG-NC	4.86	2.17	2.06
24	c	511	CLA	CHC-C1C	4.86	1.48	1.38
24	A	406	CLA	CHC-C1C	4.86	1.48	1.38
24	b	615	CLA	CHC-C1C	4.86	1.48	1.38
24	c	504	CLA	MG-NC	4.86	2.17	2.06
24	c	511	CLA	CHB-C1B	4.86	1.50	1.39
24	A	406	CLA	C1D-ND	4.84	1.43	1.37
24	b	616	CLA	CHC-C1C	4.84	1.48	1.38
24	C	502	CLA	CHD-C1D	4.84	1.47	1.38
24	A	405	CLA	O2D-CGD	4.84	1.45	1.33
24	c	511	CLA	O2D-CGD	4.83	1.45	1.33
24	C	514	CLA	CHC-C1C	4.83	1.48	1.38
24	b	607	CLA	CHC-C1C	4.83	1.48	1.38
24	B	609	CLA	CHC-C1C	4.82	1.48	1.38
24	b	604	CLA	CHD-C1D	4.82	1.47	1.38
24	b	610	CLA	CHD-C1D	4.82	1.47	1.38
24	B	606	CLA	CHC-C1C	4.81	1.48	1.38
24	b	609	CLA	CHC-C1C	4.81	1.48	1.38
24	b	605	CLA	CHC-C1C	4.81	1.48	1.38
24	b	617	CLA	O2D-CGD	4.81	1.44	1.33
24	C	508	CLA	CHD-C1D	4.80	1.47	1.38
24	B	607	CLA	CHC-C1C	4.80	1.48	1.38
24	b	607	CLA	CHD-C1D	4.80	1.47	1.38
24	b	618	CLA	O2D-CGD	4.80	1.44	1.33
25	A	407	PHO	O2D-CGD	4.79	1.44	1.33
24	b	605	CLA	CHD-C1D	4.78	1.47	1.38
24	b	618	CLA	MG-NC	4.78	2.17	2.06
24	b	606	CLA	CHD-C1D	4.78	1.47	1.38
24	C	505	CLA	O2D-CGD	4.78	1.44	1.33
24	c	507	CLA	CHD-C1D	4.78	1.47	1.38
24	C	504	CLA	CHC-C1C	4.78	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	CHC-C1C	4.78	1.48	1.38
24	a	2109	CLA	MG-NC	4.77	2.17	2.06
24	C	508	CLA	O2D-CGD	4.77	1.44	1.33
24	C	514	CLA	CHD-C1D	4.77	1.47	1.38
24	c	512	CLA	CHC-C1C	4.76	1.48	1.38
24	B	611	CLA	MG-ND	-4.76	1.96	2.05
24	c	514	CLA	O2D-CGD	4.76	1.44	1.33
24	B	611	CLA	O2D-CGD	4.76	1.44	1.33
40	e	103	HEM	FE-NB	4.75	2.09	1.94
24	B	612	CLA	O2D-CGD	4.75	1.44	1.33
24	B	607	CLA	O2D-CGD	4.75	1.44	1.33
24	C	503	CLA	O2D-CGD	4.75	1.44	1.33
24	C	506	CLA	O2D-CGD	4.74	1.44	1.33
24	B	604	CLA	O2D-CGD	4.74	1.44	1.33
24	B	603	CLA	MG-NC	4.74	2.17	2.06
24	c	512	CLA	O2D-CGD	4.74	1.44	1.33
24	b	609	CLA	O2D-CGD	4.73	1.44	1.33
24	C	503	CLA	CHC-C1C	4.73	1.48	1.38
24	c	515	CLA	O2D-CGD	4.73	1.44	1.33
24	c	511	CLA	CHD-C1D	4.73	1.47	1.38
24	d	405	CLA	O2D-CGD	4.73	1.44	1.33
24	c	509	CLA	MG-ND	-4.72	1.96	2.05
24	B	613	CLA	CHB-C1B	4.72	1.50	1.39
25	a	2112	PHO	O2D-CGD	4.72	1.44	1.33
24	C	513	CLA	MG-NB	4.71	2.15	2.05
24	A	409	CLA	O2D-CGD	4.71	1.44	1.33
24	c	506	CLA	C1D-ND	4.71	1.43	1.37
24	A	406	CLA	O2D-CGD	4.71	1.44	1.33
24	B	603	CLA	CHD-C1D	4.70	1.47	1.38
24	c	510	CLA	O2D-CGD	4.69	1.44	1.33
24	B	608	CLA	O2D-CGD	4.68	1.44	1.33
24	c	510	CLA	CHD-C1D	4.68	1.47	1.38
24	a	2110	CLA	O2D-CGD	4.68	1.44	1.33
24	C	509	CLA	MG-NB	4.68	2.15	2.05
24	a	2113	CLA	CHC-C1C	4.68	1.48	1.38
24	D	404	CLA	CHB-C1B	4.68	1.49	1.39
24	c	509	CLA	O2D-CGD	4.68	1.44	1.33
24	B	605	CLA	O2D-CGD	4.67	1.44	1.33
24	D	404	CLA	MG-NB	-4.67	1.96	2.05
24	B	610	CLA	CHC-C1C	4.67	1.48	1.38
24	C	513	CLA	O2D-CGD	4.67	1.44	1.33
24	a	2109	CLA	CHC-C1C	4.66	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	O2D-CGD	4.66	1.44	1.33
24	C	505	CLA	CHD-C1D	4.66	1.47	1.38
24	c	508	CLA	CHD-C1D	4.66	1.47	1.38
24	D	404	CLA	O2D-CGD	4.65	1.44	1.33
24	b	610	CLA	MG-NB	4.65	2.15	2.05
24	C	512	CLA	O2D-CGD	4.65	1.44	1.33
24	B	603	CLA	O2D-CGD	4.64	1.44	1.33
24	C	508	CLA	CHC-C1C	4.64	1.48	1.38
24	b	614	CLA	CHC-C1C	4.64	1.48	1.38
24	C	507	CLA	CHC-C1C	4.64	1.47	1.38
24	c	507	CLA	CHC-C1C	4.64	1.47	1.38
24	b	613	CLA	O2D-CGD	4.64	1.44	1.33
24	c	506	CLA	MG-ND	-4.63	1.96	2.05
24	c	503	CLA	O2D-CGD	4.63	1.44	1.33
24	C	502	CLA	O2D-CGD	4.63	1.44	1.33
24	b	611	CLA	CHC-C1C	4.63	1.47	1.38
24	B	614	CLA	MG-ND	-4.63	1.96	2.05
34	C	539	DMS	O-S	4.62	1.81	1.50
24	c	507	CLA	O2D-CGD	4.62	1.44	1.33
34	v	214	DMS	O-S	4.61	1.81	1.50
24	c	510	CLA	MG-NA	4.60	2.17	2.06
24	b	609	CLA	CHD-C1D	4.60	1.47	1.38
24	C	503	CLA	MG-NC	4.60	2.17	2.06
24	B	602	CLA	O2A-CGA	4.60	1.46	1.33
24	B	610	CLA	CHD-C1D	4.60	1.47	1.38
24	c	512	CLA	CHB-C1B	4.60	1.49	1.39
24	D	405	CLA	CHD-C1D	4.59	1.47	1.38
34	c	536	DMS	O-S	4.59	1.81	1.50
24	a	2109	CLA	MG-NB	4.59	2.14	2.05
34	b	636	DMS	O-S	4.59	1.81	1.50
24	c	505	CLA	CHB-C1B	4.58	1.49	1.39
27	B	621	SQD	O47-C7	4.58	1.47	1.34
24	C	509	CLA	MG-NA	4.57	2.17	2.06
34	d	417	DMS	O-S	4.57	1.81	1.50
24	C	511	CLA	CHD-C1D	4.57	1.47	1.38
34	u	204	DMS	O-S	4.56	1.81	1.50
24	b	605	CLA	MG-ND	-4.56	1.96	2.05
24	A	409	CLA	CHD-C1D	4.56	1.47	1.38
34	O	306	DMS	O-S	4.56	1.81	1.50
24	B	602	CLA	CHD-C1D	4.56	1.47	1.38
34	V	205	DMS	O-S	4.56	1.81	1.50
24	B	615	CLA	CHB-C1B	4.56	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	O2A-CGA	4.56	1.46	1.33
34	b	641	DMS	O-S	4.55	1.81	1.50
24	c	503	CLA	CHB-C1B	4.55	1.49	1.39
34	b	634	DMS	O-S	4.55	1.81	1.50
34	x	802	DMS	O-S	4.55	1.81	1.50
34	B	643	DMS	O-S	4.55	1.81	1.50
24	b	617	CLA	CHD-C1D	4.55	1.47	1.38
24	c	514	CLA	CHC-C1C	4.55	1.47	1.38
34	t	103	DMS	O-S	4.55	1.81	1.50
34	c	538	DMS	O-S	4.55	1.81	1.50
34	o	2612	DMS	O-S	4.55	1.80	1.50
24	B	610	CLA	CHB-C1B	4.54	1.49	1.39
34	b	642	DMS	O-S	4.54	1.80	1.50
24	C	509	CLA	CHD-C1D	4.54	1.47	1.38
43	V	201	HEC	FE-ND	4.54	2.08	1.94
34	C	538	DMS	O-S	4.54	1.80	1.50
24	d	405	CLA	CHB-C1B	4.54	1.49	1.39
24	B	606	CLA	CHD-C1D	4.54	1.47	1.38
24	c	505	CLA	O2D-CGD	4.54	1.44	1.33
34	v	206	DMS	O-S	4.53	1.80	1.50
24	A	409	CLA	MG-ND	-4.53	1.96	2.05
24	b	619	CLA	CHD-C1D	4.53	1.47	1.38
24	b	606	CLA	CHC-C1C	4.53	1.47	1.38
24	C	512	CLA	CHB-C1B	4.53	1.49	1.39
34	B	640	DMS	O-S	4.53	1.80	1.50
24	B	615	CLA	MG-ND	-4.53	1.96	2.05
24	C	504	CLA	CHD-C1D	4.53	1.47	1.38
34	d	420	DMS	O-S	4.52	1.80	1.50
34	a	2122	DMS	O-S	4.52	1.80	1.50
24	b	614	CLA	CHD-C1D	4.52	1.47	1.38
34	A	423	DMS	O-S	4.52	1.80	1.50
24	b	618	CLA	CHD-C1D	4.52	1.47	1.38
34	O	311	DMS	O-S	4.52	1.80	1.50
34	T	106	DMS	O-S	4.52	1.80	1.50
24	B	605	CLA	CHC-C1C	4.52	1.47	1.38
34	b	638	DMS	O-S	4.51	1.80	1.50
34	C	527	DMS	O-S	4.51	1.80	1.50
34	d	423	DMS	O-S	4.51	1.80	1.50
24	C	510	CLA	CHD-C1D	4.51	1.47	1.38
34	B	650	DMS	O-S	4.51	1.80	1.50
34	B	647	DMS	O-S	4.51	1.80	1.50
24	b	619	CLA	CHC-C1C	4.51	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	522	LMG	O7-C10	4.51	1.47	1.34
34	B	645	DMS	O-S	4.51	1.80	1.50
34	c	539	DMS	O-S	4.51	1.80	1.50
24	A	405	CLA	MG-NC	4.51	2.17	2.06
34	A	426	DMS	O-S	4.51	1.80	1.50
34	d	421	DMS	O-S	4.51	1.80	1.50
34	C	530	DMS	O-S	4.51	1.80	1.50
34	v	211	DMS	O-S	4.51	1.80	1.50
34	C	536	DMS	O-S	4.51	1.80	1.50
24	b	612	CLA	CHB-C1B	4.50	1.49	1.39
24	d	401	CLA	CHC-C1C	4.50	1.47	1.38
34	a	2124	DMS	O-S	4.50	1.80	1.50
27	f	102	SQD	O47-C7	4.50	1.47	1.34
34	D	417	DMS	O-S	4.50	1.80	1.50
34	V	206	DMS	O-S	4.50	1.80	1.50
34	E	108	DMS	O-S	4.50	1.80	1.50
24	C	510	CLA	O2A-CGA	4.50	1.46	1.33
34	A	425	DMS	O-S	4.50	1.80	1.50
34	o	2609	DMS	O-S	4.50	1.80	1.50
34	D	419	DMS	O-S	4.50	1.80	1.50
34	c	534	DMS	O-S	4.50	1.80	1.50
24	B	615	CLA	CHC-C1C	4.50	1.47	1.38
34	c	541	DMS	O-S	4.49	1.80	1.50
34	a	2123	DMS	O-S	4.49	1.80	1.50
24	b	615	CLA	CHB-C1B	4.49	1.49	1.39
24	B	611	CLA	CHD-C1D	4.49	1.47	1.38
34	e	104	DMS	O-S	4.49	1.80	1.50
34	v	208	DMS	O-S	4.49	1.80	1.50
34	O	309	DMS	O-S	4.49	1.80	1.50
34	O	310	DMS	O-S	4.49	1.80	1.50
34	b	637	DMS	O-S	4.49	1.80	1.50
34	c	535	DMS	O-S	4.49	1.80	1.50
24	d	404	CLA	O2D-CGD	4.49	1.44	1.33
24	C	504	CLA	O2D-CGD	4.49	1.44	1.33
34	D	416	DMS	O-S	4.49	1.80	1.50
34	c	537	DMS	O-S	4.49	1.80	1.50
34	O	313	DMS	O-S	4.49	1.80	1.50
34	O	314	DMS	O-S	4.49	1.80	1.50
34	b	643	DMS	O-S	4.49	1.80	1.50
34	v	213	DMS	O-S	4.49	1.80	1.50
34	z	1802	DMS	O-S	4.49	1.80	1.50
24	D	405	CLA	MG-ND	-4.49	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	638	DMS	O-S	4.48	1.80	1.50
34	C	535	DMS	O-S	4.48	1.80	1.50
34	c	533	DMS	O-S	4.48	1.80	1.50
28	C	526	LMG	O7-C10	4.48	1.46	1.34
34	B	646	DMS	O-S	4.48	1.80	1.50
24	d	404	CLA	O2A-CGA	4.48	1.46	1.33
34	v	210	DMS	O-S	4.48	1.80	1.50
34	d	418	DMS	O-S	4.48	1.80	1.50
34	C	537	DMS	O-S	4.48	1.80	1.50
24	b	607	CLA	CHB-C1B	4.48	1.49	1.39
34	v	209	DMS	O-S	4.48	1.80	1.50
34	T	104	DMS	O-S	4.48	1.80	1.50
34	d	422	DMS	O-S	4.48	1.80	1.50
34	D	420	DMS	O-S	4.48	1.80	1.50
34	F	103	DMS	O-S	4.48	1.80	1.50
34	O	304	DMS	O-S	4.48	1.80	1.50
34	C	529	DMS	O-S	4.48	1.80	1.50
34	B	649	DMS	O-S	4.48	1.80	1.50
34	O	308	DMS	O-S	4.48	1.80	1.50
34	k	2004	DMS	O-S	4.47	1.80	1.50
34	o	2604	DMS	O-S	4.47	1.80	1.50
24	c	513	CLA	O2D-CGD	4.47	1.44	1.33
34	V	208	DMS	O-S	4.47	1.80	1.50
34	U	503	DMS	O-S	4.47	1.80	1.50
34	o	2605	DMS	O-S	4.47	1.80	1.50
34	B	644	DMS	O-S	4.47	1.80	1.50
34	v	212	DMS	O-S	4.47	1.80	1.50
27	A	413	SQD	O48-C23	4.47	1.46	1.33
24	c	508	CLA	CHC-C1C	4.47	1.47	1.38
34	B	642	DMS	O-S	4.47	1.80	1.50
34	o	2607	DMS	O-S	4.47	1.80	1.50
34	u	202	DMS	O-S	4.47	1.80	1.50
34	o	2606	DMS	O-S	4.47	1.80	1.50
34	V	202	DMS	O-S	4.47	1.80	1.50
34	B	648	DMS	O-S	4.46	1.80	1.50
34	D	418	DMS	O-S	4.46	1.80	1.50
34	j	1604	DMS	O-S	4.46	1.80	1.50
34	C	534	DMS	O-S	4.46	1.80	1.50
34	o	2610	DMS	O-S	4.46	1.80	1.50
34	O	307	DMS	O-S	4.46	1.80	1.50
34	b	640	DMS	O-S	4.45	1.80	1.50
34	c	531	DMS	O-S	4.45	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	540	DMS	O-S	4.45	1.80	1.50
34	b	635	DMS	O-S	4.45	1.80	1.50
34	E	107	DMS	O-S	4.45	1.80	1.50
34	O	312	DMS	O-S	4.45	1.80	1.50
34	T	105	DMS	O-S	4.45	1.80	1.50
34	u	201	DMS	O-S	4.45	1.80	1.50
34	d	419	DMS	O-S	4.45	1.80	1.50
34	o	2608	DMS	O-S	4.45	1.80	1.50
24	c	512	CLA	CHD-C1D	4.45	1.47	1.38
24	B	608	CLA	CHB-C1B	4.45	1.49	1.39
34	C	533	DMS	O-S	4.45	1.80	1.50
24	b	619	CLA	CHB-C1B	4.45	1.49	1.39
24	a	2110	CLA	CHB-C1B	4.45	1.49	1.39
24	D	405	CLA	CHB-C1B	4.45	1.49	1.39
34	V	210	DMS	O-S	4.45	1.80	1.50
27	A	413	SQD	O47-C7	4.44	1.46	1.34
28	A	412	LMG	O7-C10	4.44	1.46	1.34
24	b	611	CLA	CHD-C1D	4.44	1.47	1.38
24	A	409	CLA	CHB-C1B	4.44	1.49	1.39
24	B	606	CLA	MG-ND	-4.44	1.97	2.05
24	C	503	CLA	CHB-C1B	4.44	1.49	1.39
34	o	2611	DMS	O-S	4.44	1.80	1.50
24	c	514	CLA	CHD-C1D	4.44	1.47	1.38
25	a	2112	PHO	OBD-CAD	4.44	1.28	1.22
34	b	633	DMS	O-S	4.43	1.80	1.50
34	c	542	DMS	O-S	4.43	1.80	1.50
34	C	532	DMS	O-S	4.43	1.80	1.50
24	C	506	CLA	CHB-C1B	4.43	1.49	1.39
34	i	106	DMS	O-S	4.43	1.80	1.50
34	V	209	DMS	O-S	4.43	1.80	1.50
34	v	207	DMS	O-S	4.43	1.80	1.50
24	b	604	CLA	CHC-C4B	4.43	1.49	1.39
34	V	207	DMS	O-S	4.42	1.80	1.50
24	D	401	CLA	O2A-CGA	4.42	1.46	1.33
38	D	408	DGD	O1G-C1A	4.42	1.46	1.33
24	C	512	CLA	CHD-C1D	4.42	1.47	1.38
24	a	2110	CLA	CHC-C1C	4.42	1.47	1.38
24	c	507	CLA	CHB-C1B	4.42	1.49	1.39
24	B	608	CLA	CHC-C4B	4.42	1.49	1.39
34	C	528	DMS	O-S	4.42	1.80	1.50
34	v	205	DMS	O-S	4.42	1.80	1.50
34	O	305	DMS	O-S	4.41	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NB	4.41	2.14	2.05
24	C	504	CLA	CHB-C1B	4.41	1.49	1.39
34	u	203	DMS	O-S	4.41	1.80	1.50
34	b	639	DMS	O-S	4.40	1.80	1.50
24	B	607	CLA	CHD-C1D	4.40	1.46	1.38
24	C	509	CLA	O2A-CGA	4.40	1.46	1.33
24	C	508	CLA	MG-NC	4.40	2.16	2.06
24	b	612	CLA	CHC-C1C	4.40	1.47	1.38
24	b	608	CLA	CHC-C4B	4.40	1.49	1.39
24	C	507	CLA	CHD-C1D	4.40	1.46	1.38
28	b	623	LMG	O8-C28	4.39	1.46	1.33
24	b	616	CLA	MG-NB	4.39	2.14	2.05
24	C	503	CLA	CHD-C1D	4.39	1.46	1.38
24	B	605	CLA	CHD-C1D	4.39	1.46	1.38
34	c	529	DMS	O-S	4.39	1.79	1.50
34	B	639	DMS	O-S	4.39	1.79	1.50
24	c	504	CLA	CHD-C1D	4.38	1.46	1.38
24	d	405	CLA	CHD-C1D	4.38	1.46	1.38
34	c	530	DMS	O-S	4.38	1.79	1.50
24	b	614	CLA	CHB-C1B	4.38	1.49	1.39
24	B	615	CLA	O2D-CGD	4.38	1.43	1.33
24	a	2109	CLA	O2D-CGD	4.38	1.43	1.33
24	D	404	CLA	C1D-ND	4.37	1.43	1.37
24	B	608	CLA	CHD-C1D	4.37	1.46	1.38
24	B	604	CLA	CHD-C1D	4.37	1.46	1.38
24	b	606	CLA	O2A-CGA	4.37	1.46	1.33
28	C	520	LMG	O8-C28	4.36	1.46	1.33
24	c	510	CLA	CHC-C4B	4.36	1.49	1.39
38	C	519	DGD	O1G-C1A	4.36	1.46	1.33
34	C	531	DMS	O-S	4.36	1.79	1.50
38	D	408	DGD	O2G-C1B	4.35	1.46	1.34
24	B	617	CLA	CHC-C1C	4.35	1.47	1.38
24	B	603	CLA	CHB-C1B	4.35	1.49	1.39
39	E	101	LHG	O8-C23	4.34	1.46	1.33
43	v	201	HEC	FE-ND	4.34	2.08	1.94
24	B	606	CLA	MG-NC	4.34	2.16	2.06
24	c	509	CLA	CHC-C1C	4.33	1.47	1.38
24	b	613	CLA	CHD-C1D	4.33	1.46	1.38
24	B	611	CLA	CHC-C4B	4.33	1.49	1.39
24	B	614	CLA	CHC-C4B	4.32	1.49	1.39
24	C	504	CLA	CHC-C4B	4.32	1.49	1.39
39	d	408	LHG	O8-C23	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	MG-ND	-4.32	1.97	2.05
24	C	502	CLA	CHB-C1B	4.32	1.49	1.39
34	c	532	DMS	O-S	4.32	1.79	1.50
24	d	401	CLA	CHD-C1D	4.32	1.46	1.38
24	d	404	CLA	CHD-C1D	4.32	1.46	1.38
24	a	2113	CLA	O2A-CGA	4.32	1.46	1.33
24	B	602	CLA	CHC-C4B	4.31	1.49	1.39
24	d	405	CLA	CHC-C4B	4.31	1.49	1.39
28	i	101	LMG	O8-C28	4.30	1.45	1.33
24	A	405	CLA	CHC-C1C	4.30	1.47	1.38
28	A	412	LMG	O8-C28	4.30	1.45	1.33
24	c	509	CLA	CHD-C1D	4.30	1.46	1.38
24	C	508	CLA	OBD-CAD	4.30	1.29	1.22
24	b	616	CLA	CHB-C1B	4.30	1.49	1.39
24	c	509	CLA	O2A-CGA	4.30	1.45	1.33
34	A	424	DMS	O-S	4.30	1.79	1.50
24	C	510	CLA	CHB-C1B	4.29	1.49	1.39
24	B	612	CLA	CHB-C1B	4.29	1.49	1.39
24	c	513	CLA	OBD-CAD	4.29	1.29	1.22
24	A	405	CLA	C1B-NB	-4.29	1.32	1.37
28	B	622	LMG	O8-C28	4.29	1.45	1.33
24	c	510	CLA	MG-NB	4.29	2.14	2.05
24	c	515	CLA	O2A-CGA	4.29	1.45	1.33
39	e	101	LHG	O7-C7	4.29	1.46	1.34
34	B	641	DMS	O-S	4.29	1.79	1.50
24	B	605	CLA	CHB-C1B	4.28	1.49	1.39
24	C	513	CLA	CHB-C1B	4.28	1.49	1.39
27	L	102	SQD	O47-C7	4.28	1.46	1.34
27	a	2102	SQD	O47-C7	4.28	1.46	1.34
27	a	2102	SQD	O48-C23	4.28	1.45	1.33
24	b	611	CLA	CHB-C1B	4.27	1.49	1.39
27	F	101	SQD	O47-C7	4.27	1.46	1.34
24	c	504	CLA	CHB-C1B	4.27	1.49	1.39
24	C	512	CLA	O2A-CGA	4.27	1.45	1.33
24	B	617	CLA	CHD-C1D	4.26	1.46	1.38
24	B	609	CLA	O2D-CGD	4.25	1.43	1.33
24	b	609	CLA	CHB-C1B	4.25	1.48	1.39
36	B	624	HTG	C1'-S1	-4.25	1.76	1.81
24	c	515	CLA	CHB-C1B	4.25	1.48	1.39
24	b	615	CLA	CHC-C4B	4.25	1.48	1.39
24	C	503	CLA	O2A-CGA	4.24	1.45	1.33
27	F	101	SQD	O48-C23	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	CHD-C1D	4.24	1.46	1.38
24	b	605	CLA	CHB-C1B	4.23	1.48	1.39
24	C	513	CLA	CHD-C1D	4.23	1.46	1.38
24	d	405	CLA	O2A-CGA	4.23	1.45	1.33
34	A	422	DMS	O-S	4.22	1.78	1.50
24	C	507	CLA	CHB-C1B	4.22	1.48	1.39
24	C	514	CLA	CHB-C1B	4.22	1.48	1.39
24	C	505	CLA	CHD-C4C	4.21	1.48	1.39
24	c	511	CLA	O2A-CGA	4.21	1.45	1.33
24	d	404	CLA	CHB-C1B	4.21	1.48	1.39
24	D	404	CLA	O2A-CGA	4.21	1.45	1.33
24	b	609	CLA	O2A-CGA	4.21	1.45	1.33
24	B	613	CLA	CHD-C1D	4.21	1.46	1.38
24	C	502	CLA	CHC-C4B	4.20	1.48	1.39
24	B	615	CLA	CHD-C1D	4.20	1.46	1.38
24	B	604	CLA	CHB-C1B	4.20	1.48	1.39
24	A	406	CLA	OBD-CAD	4.20	1.29	1.22
24	B	617	CLA	CHB-C1B	4.20	1.48	1.39
24	B	606	CLA	CHB-C1B	4.20	1.48	1.39
24	b	618	CLA	CHB-C1B	4.20	1.48	1.39
24	a	2109	CLA	CHB-C1B	4.20	1.48	1.39
24	b	605	CLA	O2A-CGA	4.20	1.45	1.33
38	h	703	DGD	O1G-C1A	4.19	1.45	1.33
24	C	502	CLA	CHD-C4C	4.19	1.48	1.39
24	D	405	CLA	CHC-C4B	4.19	1.48	1.39
34	a	2121	DMS	O-S	4.19	1.78	1.50
24	b	612	CLA	O2A-CGA	4.19	1.45	1.33
24	b	619	CLA	O2A-CGA	4.18	1.45	1.33
24	D	401	CLA	CHC-C1C	4.18	1.47	1.38
24	b	613	CLA	CHB-C1B	4.18	1.48	1.39
24	b	608	CLA	CHD-C1D	4.18	1.46	1.38
24	a	2109	CLA	CHD-C1D	4.17	1.46	1.38
24	d	401	CLA	CHB-C1B	4.17	1.48	1.39
24	B	602	CLA	MG-NC	4.17	2.16	2.06
24	B	612	CLA	CHC-C4B	4.17	1.48	1.39
39	E	101	LHG	O7-C7	4.17	1.46	1.34
24	a	2113	CLA	CHB-C1B	4.16	1.48	1.39
24	b	617	CLA	CHB-C1B	4.16	1.48	1.39
24	B	611	CLA	CHB-C1B	4.16	1.48	1.39
28	c	522	LMG	O8-C28	4.16	1.45	1.33
27	A	411	SQD	O48-C23	4.16	1.45	1.33
24	b	604	CLA	CHB-C1B	4.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	O2A-CGA	4.16	1.45	1.33
24	c	508	CLA	O2A-CGA	4.16	1.45	1.33
24	C	506	CLA	CHC-C4B	4.16	1.48	1.39
27	f	102	SQD	O48-C23	4.16	1.45	1.33
24	C	513	CLA	O2A-CGA	4.15	1.45	1.33
24	b	605	CLA	CHC-C4B	4.15	1.48	1.39
24	B	602	CLA	CHB-C1B	4.15	1.48	1.39
24	d	401	CLA	O2A-CGA	4.15	1.45	1.33
24	b	608	CLA	O2A-CGA	4.15	1.45	1.33
24	c	513	CLA	CHB-C1B	4.15	1.48	1.39
24	B	602	CLA	MG-ND	-4.15	1.97	2.05
24	b	607	CLA	CHC-C4B	4.14	1.48	1.39
28	d	411	LMG	O8-C28	4.13	1.45	1.33
39	d	410	LHG	O8-C23	4.13	1.45	1.33
24	B	604	CLA	CHC-C4B	4.13	1.48	1.39
24	c	506	CLA	CHD-C1D	4.13	1.46	1.38
24	b	613	CLA	CHC-C4B	4.13	1.48	1.39
24	B	605	CLA	CHC-C4B	4.13	1.48	1.39
24	C	511	CLA	CHC-C4B	4.13	1.48	1.39
38	H	102	DGD	O1G-C1A	4.13	1.45	1.33
24	b	616	CLA	O2A-CGA	4.13	1.45	1.33
24	a	2110	CLA	O2A-CGA	4.12	1.45	1.33
24	b	610	CLA	CHB-C1B	4.12	1.48	1.39
27	L	102	SQD	O48-C23	4.12	1.45	1.33
24	b	616	CLA	CHD-C1D	4.12	1.46	1.38
24	b	610	CLA	CHC-C4B	4.12	1.48	1.39
24	B	610	CLA	O2A-CGA	4.11	1.45	1.33
24	A	405	CLA	CHD-C1D	4.11	1.46	1.38
34	b	632	DMS	O-S	4.11	1.78	1.50
24	B	614	CLA	CHB-C1B	4.11	1.48	1.39
24	B	602	CLA	CHD-C4C	4.11	1.48	1.39
25	A	408	PHO	O2A-CGA	4.10	1.45	1.33
24	c	510	CLA	CHB-C1B	4.10	1.48	1.39
24	C	509	CLA	CHB-C1B	4.10	1.48	1.39
24	b	618	CLA	O2A-CGA	4.10	1.45	1.33
24	c	507	CLA	CHC-C4B	4.10	1.48	1.39
24	c	512	CLA	CHC-C4B	4.10	1.48	1.39
24	b	617	CLA	CHC-C4B	4.10	1.48	1.39
24	C	514	CLA	O2A-CGA	4.09	1.45	1.33
39	D	409	LHG	O8-C23	4.09	1.45	1.33
24	B	616	CLA	OBD-CAD	4.09	1.29	1.22
28	c	521	LMG	O8-C28	4.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	O2A-CGA	4.08	1.45	1.33
28	c	521	LMG	O7-C10	4.08	1.45	1.34
24	A	406	CLA	CHD-C4C	4.08	1.48	1.39
24	C	505	CLA	CHB-C1B	4.08	1.48	1.39
24	b	611	CLA	O2A-CGA	4.08	1.45	1.33
24	C	505	CLA	CHC-C4B	4.08	1.48	1.39
24	c	509	CLA	CHB-C1B	4.08	1.48	1.39
24	B	608	CLA	O2A-CGA	4.07	1.45	1.33
24	D	404	CLA	CHC-C1C	4.07	1.46	1.38
28	i	101	LMG	O7-C10	4.07	1.45	1.34
24	b	606	CLA	CHB-C1B	4.07	1.48	1.39
24	B	603	CLA	CHC-C4B	4.07	1.48	1.39
24	c	504	CLA	CHC-C4B	4.07	1.48	1.39
28	C	526	LMG	O8-C28	4.07	1.45	1.33
24	B	604	CLA	O2A-CGA	4.07	1.45	1.33
24	B	607	CLA	CHC-C4B	4.07	1.48	1.39
24	c	510	CLA	O2A-CGA	4.07	1.45	1.33
24	d	405	CLA	OBD-CAD	4.06	1.29	1.22
25	a	2111	PHO	OBD-CAD	4.06	1.28	1.22
24	b	604	CLA	CHD-C4C	4.06	1.48	1.39
24	B	603	CLA	O2A-CGA	4.06	1.45	1.33
24	b	604	CLA	C3D-C2D	4.06	1.50	1.39
38	C	517	DGD	O2G-C1B	4.06	1.45	1.34
24	a	2110	CLA	OBD-CAD	4.06	1.29	1.22
39	d	410	LHG	O7-C7	4.05	1.45	1.34
24	C	502	CLA	OBD-CAD	4.05	1.29	1.22
28	b	623	LMG	O7-C10	4.05	1.45	1.34
24	c	513	CLA	O2A-CGA	4.04	1.45	1.33
36	I	1202	HTG	C1'-S1	-4.04	1.76	1.81
25	A	407	PHO	O2A-CGA	4.04	1.45	1.33
24	a	2113	CLA	CHD-C1D	4.04	1.46	1.38
24	b	607	CLA	O2A-CGA	4.03	1.45	1.33
24	b	619	CLA	MG-NC	4.03	2.15	2.06
24	b	613	CLA	MG-NB	4.03	2.13	2.05
24	A	406	CLA	MG-NA	4.03	2.15	2.06
24	B	612	CLA	CHD-C1D	4.03	1.46	1.38
24	D	404	CLA	CHC-C4B	4.03	1.48	1.39
24	a	2109	CLA	CHC-C4B	4.03	1.48	1.39
24	A	409	CLA	CHC-C4B	4.03	1.48	1.39
24	B	606	CLA	CHC-C4B	4.03	1.48	1.39
24	b	613	CLA	C1B-NB	-4.03	1.32	1.37
24	c	510	CLA	OBD-CAD	4.02	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	OBD-CAD	4.02	1.29	1.22
24	c	503	CLA	O2A-CGA	4.02	1.45	1.33
24	C	503	CLA	C3D-C2D	4.02	1.50	1.39
24	b	605	CLA	CHD-C4C	4.02	1.48	1.39
24	C	507	CLA	O2A-CGA	4.02	1.45	1.33
24	b	608	CLA	MG-NC	4.01	2.15	2.06
24	b	618	CLA	C3D-C2D	4.01	1.50	1.39
24	C	509	CLA	CHC-C4B	4.01	1.48	1.39
24	C	508	CLA	CHB-C1B	4.01	1.48	1.39
24	c	509	CLA	OBD-CAD	4.01	1.29	1.22
24	C	508	CLA	O2A-CGA	4.01	1.45	1.33
24	c	504	CLA	C3D-C2D	4.01	1.50	1.39
24	b	613	CLA	CHD-C4C	4.00	1.48	1.39
24	b	613	CLA	MG-NC	4.00	2.15	2.06
24	B	616	CLA	CHD-C1D	4.00	1.46	1.38
24	C	505	CLA	C3D-C2D	4.00	1.50	1.39
27	B	621	SQD	O48-C23	4.00	1.45	1.33
24	B	610	CLA	CHC-C4B	4.00	1.48	1.39
39	L	101	LHG	O8-C23	4.00	1.45	1.33
24	B	617	CLA	MG-NC	4.00	2.15	2.06
24	C	513	CLA	CHC-C4B	3.99	1.48	1.39
28	B	622	LMG	O7-C10	3.99	1.45	1.34
24	B	607	CLA	CHB-C1B	3.99	1.48	1.39
28	C	520	LMG	O7-C10	3.99	1.45	1.34
24	B	613	CLA	C1B-NB	-3.99	1.32	1.37
24	c	514	CLA	CHB-C1B	3.99	1.48	1.39
24	C	502	CLA	O2A-CGA	3.99	1.45	1.33
24	b	615	CLA	MG-NC	3.99	2.15	2.06
24	c	503	CLA	CHC-C4B	3.98	1.48	1.39
24	D	405	CLA	CHD-C4C	3.98	1.48	1.39
24	a	2113	CLA	MG-ND	-3.98	1.97	2.05
24	C	509	CLA	OBD-CAD	3.98	1.29	1.22
24	b	618	CLA	CHD-C4C	3.98	1.48	1.39
24	B	609	CLA	CHB-C1B	3.98	1.48	1.39
24	d	405	CLA	CHD-C4C	3.98	1.48	1.39
24	c	513	CLA	MG-ND	-3.98	1.97	2.05
24	c	513	CLA	MG-NC	3.98	2.15	2.06
24	D	404	CLA	MG-NC	3.98	2.15	2.06
24	B	617	CLA	O2A-CGA	3.97	1.45	1.33
24	A	405	CLA	CHB-C1B	3.97	1.48	1.39
24	c	506	CLA	CHB-C1B	3.97	1.48	1.39
24	C	511	CLA	CHD-C4C	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	CHD-C1D	3.97	1.46	1.38
25	a	2112	PHO	O2A-CGA	3.96	1.44	1.33
24	C	510	CLA	CHC-C4B	3.96	1.48	1.39
24	B	605	CLA	O2A-CGA	3.96	1.44	1.33
24	B	603	CLA	OBD-CAD	3.96	1.29	1.22
24	b	610	CLA	O2A-CGA	3.96	1.44	1.33
24	C	507	CLA	CHC-C4B	3.96	1.48	1.39
24	b	608	CLA	CHB-C1B	3.95	1.48	1.39
24	C	502	CLA	MG-ND	-3.95	1.98	2.05
24	c	511	CLA	OBD-CAD	3.95	1.29	1.22
24	c	513	CLA	CHC-C4B	3.95	1.48	1.39
24	C	510	CLA	C3D-C2D	3.95	1.49	1.39
25	A	408	PHO	OBD-CAD	3.95	1.27	1.22
24	c	503	CLA	CHD-C1D	3.94	1.46	1.38
24	C	511	CLA	MG-NB	3.94	2.13	2.05
24	B	615	CLA	C3D-C2D	3.94	1.49	1.39
24	B	608	CLA	CHD-C4C	3.94	1.48	1.39
24	c	505	CLA	CHC-C4B	3.94	1.48	1.39
24	c	515	CLA	CHC-C4B	3.94	1.48	1.39
24	b	615	CLA	O2A-CGA	3.93	1.44	1.33
39	L	101	LHG	O7-C7	3.93	1.45	1.34
24	B	608	CLA	OBD-CAD	3.93	1.29	1.22
24	A	409	CLA	O2A-CGA	3.93	1.44	1.33
24	b	617	CLA	O2A-CGA	3.93	1.44	1.33
24	b	606	CLA	CHD-C4C	3.92	1.48	1.39
24	B	616	CLA	CHC-C4B	3.92	1.48	1.39
24	B	609	CLA	O2A-CGA	3.92	1.44	1.33
24	B	616	CLA	C3D-C2D	3.92	1.49	1.39
24	B	616	CLA	O2A-CGA	3.92	1.44	1.33
24	b	616	CLA	CHC-C4B	3.92	1.48	1.39
24	C	504	CLA	O2A-CGA	3.92	1.44	1.33
24	B	609	CLA	CHC-C4B	3.91	1.48	1.39
36	c	524	HTG	C1'-S1	-3.91	1.76	1.81
24	C	509	CLA	C3D-C2D	3.91	1.49	1.39
28	D	412	LMG	O8-C28	3.91	1.44	1.33
24	B	613	CLA	O2A-CGA	3.91	1.44	1.33
38	h	703	DGD	O2G-C1B	3.91	1.45	1.34
24	B	616	CLA	CHB-C1B	3.91	1.48	1.39
24	b	606	CLA	CHC-C4B	3.91	1.48	1.39
24	c	511	CLA	CHC-C4B	3.90	1.48	1.39
24	B	612	CLA	OBD-CAD	3.90	1.29	1.22
39	D	410	LHG	O8-C23	3.90	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	C3D-C2D	3.90	1.49	1.39
27	a	2115	SQD	O48-C23	3.90	1.44	1.33
24	b	610	CLA	C3D-C2D	3.90	1.49	1.39
36	b	626	HTG	C1'-S1	-3.90	1.76	1.81
24	C	506	CLA	O2A-CGA	3.89	1.44	1.33
24	B	603	CLA	CHD-C4C	3.89	1.48	1.39
24	C	503	CLA	CHC-C4B	3.89	1.48	1.39
24	A	406	CLA	CHB-C1B	3.89	1.48	1.39
24	A	409	CLA	CHD-C4C	3.89	1.48	1.39
39	l	101	LHG	O8-C23	3.89	1.44	1.33
24	B	612	CLA	O2A-CGA	3.89	1.44	1.33
24	c	509	CLA	CHD-C4C	3.88	1.48	1.39
24	B	615	CLA	CHC-C4B	3.88	1.48	1.39
27	a	2115	SQD	O47-C7	3.88	1.45	1.34
24	c	514	CLA	C3D-C2D	3.88	1.49	1.39
24	B	607	CLA	O2A-CGA	3.88	1.44	1.33
24	D	401	CLA	OBD-CAD	3.88	1.29	1.22
24	b	604	CLA	OBD-CAD	3.88	1.29	1.22
24	C	509	CLA	CHD-C4C	3.88	1.48	1.39
24	b	614	CLA	CHC-C4B	3.88	1.48	1.39
24	b	612	CLA	MG-ND	-3.88	1.98	2.05
24	A	405	CLA	C3D-C2D	3.87	1.49	1.39
24	c	509	CLA	CHC-C4B	3.87	1.48	1.39
38	c	520	DGD	O1G-C1A	3.87	1.44	1.33
24	C	508	CLA	CHC-C4B	3.87	1.48	1.39
36	B	625[B]	HTG	C1'-S1	-3.87	1.76	1.81
24	b	617	CLA	CHD-C4C	3.87	1.48	1.39
24	b	612	CLA	CHD-C4C	3.87	1.48	1.39
24	B	615	CLA	CHD-C4C	3.86	1.48	1.39
38	c	519	DGD	O2G-C1B	3.86	1.45	1.34
36	B	625[A]	HTG	C1'-S1	-3.86	1.76	1.81
24	c	510	CLA	CHD-C4C	3.86	1.48	1.39
25	a	2111	PHO	O2A-CGA	3.86	1.44	1.33
24	B	609	CLA	C3D-C2D	3.86	1.49	1.39
24	B	606	CLA	O2A-CGA	3.86	1.44	1.33
38	c	518	DGD	O2G-C1B	3.86	1.45	1.34
24	c	513	CLA	CHD-C4C	3.86	1.48	1.39
24	C	513	CLA	C3D-C2D	3.86	1.49	1.39
27	A	411	SQD	O47-C7	3.86	1.45	1.34
24	B	615	CLA	C4B-NB	-3.85	1.33	1.37
24	c	506	CLA	C3D-C2D	3.85	1.49	1.39
24	c	505	CLA	O2A-CGA	3.85	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	OBD-CAD	3.85	1.29	1.22
24	b	611	CLA	OBD-CAD	3.85	1.29	1.22
24	C	503	CLA	OBD-CAD	3.85	1.29	1.22
24	C	506	CLA	OBD-CAD	3.85	1.29	1.22
24	c	503	CLA	OBD-CAD	3.85	1.29	1.22
24	D	405	CLA	O2A-CGA	3.84	1.44	1.33
24	C	512	CLA	C4B-NB	-3.84	1.33	1.37
24	d	404	CLA	CHC-C4B	3.84	1.48	1.39
36	b	602	HTG	C1'-S1	-3.84	1.76	1.81
24	b	616	CLA	CHD-C4C	3.84	1.48	1.39
24	c	508	CLA	CHD-C4C	3.84	1.48	1.39
24	A	406	CLA	O2A-CGA	3.84	1.44	1.33
24	B	608	CLA	C3D-C2D	3.83	1.49	1.39
38	c	519	DGD	O1G-C1A	3.83	1.44	1.33
24	d	405	CLA	C3D-C2D	3.83	1.49	1.39
24	B	610	CLA	C3D-C2D	3.83	1.49	1.39
24	C	502	CLA	C3D-C2D	3.83	1.49	1.39
24	C	514	CLA	CHD-C4C	3.83	1.48	1.39
24	B	612	CLA	CHD-C4C	3.83	1.48	1.39
24	d	404	CLA	C1D-ND	3.83	1.42	1.37
24	c	507	CLA	O2A-CGA	3.83	1.44	1.33
24	A	406	CLA	CHC-C4B	3.82	1.48	1.39
24	c	509	CLA	C3D-C2D	3.82	1.49	1.39
24	A	405	CLA	CHC-C4B	3.82	1.48	1.39
24	B	614	CLA	CHD-C4C	3.82	1.48	1.39
24	B	610	CLA	OBD-CAD	3.82	1.29	1.22
24	B	613	CLA	OBD-CAD	3.82	1.29	1.22
24	b	605	CLA	C3D-C2D	3.82	1.49	1.39
25	A	407	PHO	OBD-CAD	3.81	1.27	1.22
24	d	401	CLA	OBD-CAD	3.81	1.29	1.22
24	c	509	CLA	MG-NB	-3.81	1.98	2.05
24	A	409	CLA	C3D-C2D	3.81	1.49	1.39
39	D	411	LHG	O8-C23	3.81	1.44	1.33
24	a	2110	CLA	C3D-C2D	3.81	1.49	1.39
24	B	613	CLA	C1D-ND	3.81	1.42	1.37
24	C	512	CLA	CHC-C4B	3.81	1.47	1.39
24	b	618	CLA	CHC-C4B	3.81	1.47	1.39
24	d	401	CLA	C3D-C2D	3.81	1.49	1.39
24	c	511	CLA	C3D-C2D	3.80	1.49	1.39
24	b	609	CLA	CHC-C4B	3.80	1.47	1.39
24	B	607	CLA	CHD-C4C	3.80	1.47	1.39
24	D	401	CLA	CHC-C4B	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	CHB-C1B	3.80	1.47	1.39
24	C	514	CLA	CHC-C4B	3.80	1.47	1.39
36	B	626	HTG	C1'-S1	-3.80	1.76	1.81
24	C	512	CLA	CHD-C4C	3.80	1.47	1.39
24	a	2109	CLA	OBD-CAD	3.80	1.29	1.22
36	O	302	HTG	C1'-S1	-3.79	1.76	1.81
24	C	505	CLA	O2A-CGA	3.79	1.44	1.33
24	c	504	CLA	CHD-C4C	3.79	1.47	1.39
24	d	401	CLA	CHC-C4B	3.79	1.47	1.39
24	c	514	CLA	CHD-C4C	3.79	1.47	1.39
24	B	611	CLA	C3D-C2D	3.78	1.49	1.39
38	C	519	DGD	O2G-C1B	3.78	1.45	1.34
38	C	518	DGD	O1G-C1A	3.78	1.44	1.33
36	D	413	HTG	C1'-S1	-3.78	1.76	1.81
28	d	411	LMG	O7-C10	3.77	1.44	1.34
24	b	613	CLA	O2A-CGA	3.77	1.44	1.33
24	c	515	CLA	CHD-C4C	3.77	1.47	1.39
24	C	513	CLA	CHD-C4C	3.77	1.47	1.39
24	c	504	CLA	O2A-CGA	3.76	1.44	1.33
43	v	201	HEC	CBC-CAC	-3.76	1.34	1.51
24	A	405	CLA	OBD-CAD	3.76	1.29	1.22
24	C	512	CLA	C3D-C2D	3.76	1.49	1.39
24	D	401	CLA	C3D-C2D	3.75	1.49	1.39
24	A	409	CLA	OBD-CAD	3.75	1.28	1.22
24	c	506	CLA	CHC-C4B	3.75	1.47	1.39
39	D	411	LHG	O7-C7	3.75	1.44	1.34
24	c	512	CLA	CHD-C4C	3.75	1.47	1.39
24	d	404	CLA	CHD-C4C	3.75	1.47	1.39
24	c	512	CLA	OBD-CAD	3.75	1.28	1.22
24	a	2113	CLA	CHC-C4B	3.74	1.47	1.39
24	c	514	CLA	OBD-CAD	3.74	1.28	1.22
24	b	615	CLA	C3D-C2D	3.74	1.49	1.39
24	B	615	CLA	O2A-CGA	3.74	1.44	1.33
24	C	506	CLA	CHD-C4C	3.73	1.47	1.39
24	B	616	CLA	MG-NB	3.73	2.13	2.05
24	D	401	CLA	CHD-C1D	3.73	1.45	1.38
43	v	201	HEC	FE-NB	3.73	2.06	1.94
24	d	401	CLA	CHD-C4C	3.73	1.47	1.39
24	C	511	CLA	C3D-C2D	3.73	1.49	1.39
40	F	102	HEM	FE-NC	3.73	2.07	1.95
24	c	513	CLA	C3D-C2D	3.73	1.49	1.39
24	D	405	CLA	C3D-C2D	3.73	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	c	518	DGD	O1G-C1A	3.73	1.44	1.33
24	C	504	CLA	CHD-C4C	3.73	1.47	1.39
24	C	510	CLA	CHD-C4C	3.72	1.47	1.39
24	B	615	CLA	OBD-CAD	3.72	1.28	1.22
38	C	518	DGD	O2G-C1B	3.72	1.44	1.34
24	c	515	CLA	OBD-CAD	3.72	1.28	1.22
24	c	515	CLA	C3D-C2D	3.72	1.49	1.39
24	c	511	CLA	CHD-C4C	3.72	1.47	1.39
24	a	2110	CLA	CHD-C4C	3.72	1.47	1.39
24	B	617	CLA	C3D-C2D	3.72	1.49	1.39
24	b	614	CLA	CHD-C4C	3.71	1.47	1.39
24	a	2113	CLA	C3D-C2D	3.71	1.49	1.39
24	B	617	CLA	CHC-C4B	3.71	1.47	1.39
24	D	401	CLA	CHB-C1B	3.71	1.47	1.39
38	H	102	DGD	O2G-C1B	3.71	1.44	1.34
24	c	504	CLA	OBD-CAD	3.71	1.28	1.22
24	A	405	CLA	CHD-C4C	3.71	1.47	1.39
24	b	611	CLA	CHC-C4B	3.70	1.47	1.39
24	B	605	CLA	CHD-C4C	3.69	1.47	1.39
38	c	520	DGD	O2G-C1B	3.69	1.44	1.34
24	d	404	CLA	C3D-C2D	3.69	1.49	1.39
24	d	405	CLA	MG-NB	3.69	2.13	2.05
24	c	507	CLA	CHD-C4C	3.69	1.47	1.39
24	D	405	CLA	OBD-CAD	3.69	1.28	1.22
24	b	605	CLA	OBD-CAD	3.68	1.28	1.22
24	b	613	CLA	C3D-C2D	3.68	1.49	1.39
25	A	408	PHO	CHA-CBD	-3.68	1.47	1.51
24	c	505	CLA	C3D-C2D	3.68	1.49	1.39
24	d	401	CLA	C1B-NB	-3.68	1.33	1.37
24	C	508	CLA	C3D-C2D	3.68	1.49	1.39
24	A	406	CLA	C1B-NB	-3.68	1.33	1.37
24	b	618	CLA	OBD-CAD	3.68	1.28	1.22
24	C	513	CLA	MG-NC	3.68	2.15	2.06
24	b	612	CLA	CHC-C4B	3.68	1.47	1.39
24	C	503	CLA	CHD-C4C	3.67	1.47	1.39
24	A	405	CLA	O2A-CGA	3.67	1.44	1.33
24	B	603	CLA	C3D-C2D	3.67	1.49	1.39
38	C	517	DGD	O1G-C1A	3.67	1.44	1.33
24	c	506	CLA	CHD-C4C	3.67	1.47	1.39
24	b	610	CLA	CHD-C4C	3.67	1.47	1.39
24	c	505	CLA	CHD-C4C	3.66	1.47	1.39
39	D	410	LHG	O7-C7	3.66	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	2110	CLA	CHD-C1D	3.66	1.45	1.38
36	c	526	HTG	C1'-S1	-3.66	1.76	1.81
24	C	504	CLA	C3D-C2D	3.66	1.49	1.39
24	b	616	CLA	C3D-C2D	3.66	1.49	1.39
36	d	403	HTG	C1'-S1	-3.66	1.76	1.81
24	B	614	CLA	O2A-CGA	3.66	1.44	1.33
43	V	201	HEC	CBC-CAC	-3.66	1.35	1.51
24	B	612	CLA	C3D-C2D	3.66	1.49	1.39
24	c	510	CLA	C3D-C2D	3.65	1.49	1.39
24	b	612	CLA	OBD-CAD	3.65	1.28	1.22
24	c	505	CLA	OBD-CAD	3.65	1.28	1.22
24	B	602	CLA	C3D-C2D	3.65	1.49	1.39
24	a	2109	CLA	CHD-C4C	3.65	1.47	1.39
24	c	514	CLA	CHC-C4B	3.64	1.47	1.39
24	c	512	CLA	O2A-CGA	3.64	1.44	1.33
24	b	608	CLA	CHD-C4C	3.64	1.47	1.39
24	C	507	CLA	CHD-C4C	3.64	1.47	1.39
24	c	508	CLA	CHC-C4B	3.63	1.47	1.39
24	B	606	CLA	C3D-C2D	3.63	1.49	1.39
43	v	201	HEC	CBB-CAB	-3.62	1.35	1.51
24	b	617	CLA	C3D-C2D	3.62	1.49	1.39
24	B	616	CLA	C1B-NB	-3.62	1.33	1.37
24	c	506	CLA	O2A-CGA	3.62	1.43	1.33
24	b	609	CLA	CHD-C4C	3.62	1.47	1.39
24	b	619	CLA	CHC-C4B	3.61	1.47	1.39
36	b	601	HTG	C1'-S1	-3.61	1.76	1.81
24	B	602	CLA	OBD-CAD	3.61	1.28	1.22
24	c	508	CLA	OBD-CAD	3.61	1.28	1.22
24	A	406	CLA	C3D-C2D	3.60	1.49	1.39
24	B	613	CLA	MG-ND	-3.60	1.98	2.05
39	l	101	LHG	O7-C7	3.60	1.44	1.34
24	D	401	CLA	CHD-C4C	3.59	1.47	1.39
24	D	404	CLA	CHD-C4C	3.59	1.47	1.39
24	b	614	CLA	C3D-C2D	3.58	1.48	1.39
24	C	511	CLA	O2A-CGA	3.58	1.43	1.33
24	c	508	CLA	C3D-C2D	3.58	1.48	1.39
24	B	604	CLA	C3D-C2D	3.57	1.48	1.39
24	b	612	CLA	C3D-C2D	3.57	1.48	1.39
24	b	609	CLA	C3D-C2D	3.56	1.48	1.39
36	B	628	HTG	C1'-S1	-3.56	1.76	1.81
24	C	514	CLA	C3D-C2D	3.56	1.48	1.39
24	C	507	CLA	OBD-CAD	3.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	OBD-CAD	3.56	1.28	1.22
24	B	606	CLA	CHD-C4C	3.56	1.47	1.39
24	C	507	CLA	C3D-C2D	3.56	1.48	1.39
24	B	604	CLA	CHD-C4C	3.55	1.47	1.39
36	b	625	HTG	C1'-S1	-3.55	1.76	1.81
36	B	627	HTG	C1'-S1	-3.54	1.76	1.81
24	b	611	CLA	C3D-C2D	3.54	1.48	1.39
24	B	614	CLA	C3D-C2D	3.54	1.48	1.39
24	b	611	CLA	CHD-C4C	3.53	1.47	1.39
24	a	2109	CLA	O2A-CGA	3.53	1.43	1.33
24	b	613	CLA	OBD-CAD	3.53	1.28	1.22
24	B	616	CLA	CHD-C4C	3.53	1.47	1.39
24	B	613	CLA	C3D-C2D	3.52	1.48	1.39
24	C	508	CLA	CHD-C4C	3.52	1.47	1.39
24	C	513	CLA	OBD-CAD	3.52	1.28	1.22
24	B	611	CLA	O2A-CGA	3.52	1.43	1.33
24	B	605	CLA	OBD-CAD	3.52	1.28	1.22
24	a	2109	CLA	C1B-NB	-3.51	1.33	1.37
24	c	503	CLA	C3D-C2D	3.51	1.48	1.39
24	C	511	CLA	OBD-CAD	3.51	1.28	1.22
24	b	615	CLA	OBD-CAD	3.51	1.28	1.22
24	a	2113	CLA	CHD-C4C	3.51	1.47	1.39
24	D	404	CLA	C3D-C2D	3.50	1.48	1.39
24	b	607	CLA	CHD-C4C	3.50	1.47	1.39
24	B	605	CLA	C3D-C2D	3.50	1.48	1.39
36	C	521	HTG	C1'-S1	-3.50	1.77	1.81
36	d	414	HTG	C1'-S1	-3.49	1.77	1.81
24	B	613	CLA	MG-NC	3.49	2.14	2.06
24	B	611	CLA	OBD-CAD	3.49	1.28	1.22
24	B	611	CLA	C1B-NB	-3.49	1.33	1.37
39	d	408	LHG	O7-C7	3.48	1.44	1.34
24	B	610	CLA	CHD-C4C	3.48	1.47	1.39
36	c	523	HTG	C1'-S1	-3.48	1.77	1.81
24	B	607	CLA	C3D-C2D	3.47	1.48	1.39
24	c	503	CLA	CHD-C4C	3.47	1.47	1.39
24	B	611	CLA	CHD-C4C	3.46	1.47	1.39
24	C	514	CLA	OBD-CAD	3.46	1.28	1.22
24	b	607	CLA	C3D-C2D	3.46	1.48	1.39
24	D	401	CLA	C4B-NB	-3.46	1.33	1.37
24	b	619	CLA	C4B-NB	-3.46	1.33	1.37
24	c	506	CLA	OBD-CAD	3.45	1.28	1.22
24	B	613	CLA	CHD-C4C	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	412	LMG	O7-C10	3.45	1.44	1.34
24	C	512	CLA	OBD-CAD	3.44	1.28	1.22
24	B	609	CLA	CHD-C4C	3.44	1.47	1.39
36	V	204	HTG	C1'-S1	-3.44	1.77	1.81
24	B	613	CLA	CHC-C4B	3.44	1.47	1.39
24	b	619	CLA	C3D-C2D	3.44	1.48	1.39
24	b	614	CLA	OBD-CAD	3.43	1.28	1.22
24	b	616	CLA	OBD-CAD	3.43	1.28	1.22
24	b	615	CLA	C1B-NB	-3.42	1.33	1.37
24	b	608	CLA	C3B-C4B	3.42	1.50	1.42
24	B	606	CLA	OBD-CAD	3.42	1.28	1.22
24	b	619	CLA	OBD-CAD	3.42	1.28	1.22
24	C	505	CLA	OBD-CAD	3.41	1.28	1.22
24	b	608	CLA	C3D-C2D	3.41	1.48	1.39
24	B	609	CLA	OBD-CAD	3.40	1.28	1.22
24	a	2113	CLA	MG-NA	3.39	2.14	2.06
24	b	611	CLA	C1B-NB	-3.38	1.33	1.37
24	B	616	CLA	C4B-NB	-3.37	1.33	1.37
24	c	510	CLA	C1B-NB	-3.37	1.33	1.37
24	B	607	CLA	OBD-CAD	3.37	1.28	1.22
24	b	606	CLA	C3D-C2D	3.36	1.48	1.39
24	d	405	CLA	C1B-NB	-3.36	1.33	1.37
39	d	409	LHG	O7-C7	3.35	1.43	1.34
24	c	505	CLA	C4D-CHA	3.35	1.50	1.38
24	c	507	CLA	OBD-CAD	3.35	1.28	1.22
24	d	404	CLA	OBD-CAD	3.35	1.28	1.22
36	i	103	HTG	C1'-S1	-3.34	1.77	1.81
24	C	508	CLA	C4D-CHA	3.34	1.50	1.38
24	D	401	CLA	C1B-NB	-3.33	1.33	1.37
36	C	522	HTG	C1'-S1	-3.33	1.77	1.81
24	c	507	CLA	C3D-C2D	3.33	1.48	1.39
24	C	504	CLA	MG-ND	-3.33	1.99	2.05
24	a	2110	CLA	C4B-NB	-3.32	1.33	1.37
24	a	2109	CLA	C3D-C2D	3.32	1.48	1.39
24	C	510	CLA	C4B-NB	-3.31	1.33	1.37
24	B	617	CLA	CHD-C4C	3.31	1.46	1.39
24	d	401	CLA	MG-NB	3.31	2.12	2.05
24	B	604	CLA	OBD-CAD	3.31	1.28	1.22
43	V	201	HEC	FE-NC	3.31	2.06	1.95
39	d	409	LHG	O8-C23	3.30	1.43	1.33
43	V	201	HEC	CBB-CAB	-3.30	1.36	1.51
24	d	401	CLA	MG-NC	3.30	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C4D-CHA	3.29	1.50	1.38
24	C	504	CLA	OBD-CAD	3.29	1.28	1.22
24	D	404	CLA	CHD-C1D	3.29	1.44	1.38
24	C	506	CLA	C3D-C2D	3.29	1.48	1.39
24	b	607	CLA	OBD-CAD	3.29	1.28	1.22
24	C	508	CLA	MG-NB	-3.28	1.99	2.05
24	b	610	CLA	C1B-NB	-3.27	1.33	1.37
39	D	409	LHG	O7-C7	3.27	1.43	1.34
24	B	603	CLA	C1B-NB	-3.26	1.33	1.37
24	c	508	CLA	C1B-NB	-3.25	1.33	1.37
24	b	617	CLA	C1B-NB	-3.24	1.33	1.37
24	c	512	CLA	C1B-NB	-3.24	1.33	1.37
24	b	615	CLA	C4B-NB	-3.23	1.33	1.37
24	C	509	CLA	C3B-C4B	3.23	1.50	1.42
24	D	404	CLA	MG-ND	-3.21	1.99	2.05
24	a	2113	CLA	C1B-NB	-3.21	1.33	1.37
24	C	512	CLA	C4D-CHA	3.21	1.49	1.38
24	b	610	CLA	C1B-C2B	3.21	1.50	1.43
24	C	506	CLA	C1B-NB	-3.21	1.33	1.37
24	b	608	CLA	OBD-CAD	3.21	1.28	1.22
24	B	608	CLA	C4D-CHA	3.19	1.49	1.38
43	v	201	HEC	FE-NC	3.19	2.05	1.95
24	B	609	CLA	C1B-NB	-3.19	1.33	1.37
24	B	606	CLA	C3B-C4B	3.18	1.50	1.42
24	C	511	CLA	C1B-NB	-3.17	1.33	1.37
24	b	617	CLA	MG-NB	3.16	2.12	2.05
24	c	509	CLA	C4D-CHA	3.15	1.49	1.38
24	b	619	CLA	C1B-C2B	3.15	1.50	1.43
24	d	404	CLA	C1C-NC	-3.15	1.33	1.37
24	b	619	CLA	CHD-C4C	3.14	1.46	1.39
24	B	605	CLA	C4D-CHA	3.14	1.49	1.38
24	C	505	CLA	C1B-NB	-3.13	1.33	1.37
24	c	511	CLA	C4D-CHA	3.13	1.49	1.38
24	b	612	CLA	C1C-NC	-3.12	1.33	1.37
24	B	609	CLA	C4B-NB	-3.12	1.34	1.37
24	b	615	CLA	CHD-C4C	3.10	1.46	1.39
24	b	610	CLA	OBD-CAD	3.10	1.27	1.22
24	b	607	CLA	C1B-C2B	3.10	1.50	1.43
24	C	510	CLA	C1B-NB	-3.10	1.34	1.37
24	A	409	CLA	C1B-C2B	3.10	1.50	1.43
24	B	617	CLA	C4D-CHA	3.09	1.49	1.38
24	b	619	CLA	C1B-NB	-3.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C4D-CHA	3.09	1.49	1.38
24	a	2110	CLA	CHC-C4B	3.08	1.46	1.39
24	d	404	CLA	C1B-NB	-3.08	1.34	1.37
24	a	2110	CLA	C1B-C2B	3.08	1.50	1.43
24	B	607	CLA	C4D-CHA	3.07	1.49	1.38
24	b	619	CLA	C1C-NC	-3.07	1.33	1.37
24	B	605	CLA	C1B-C2B	3.07	1.50	1.43
24	B	617	CLA	C4B-NB	-3.06	1.34	1.37
24	C	506	CLA	C4D-CHA	3.06	1.49	1.38
24	b	604	CLA	C3B-C4B	3.06	1.49	1.42
24	a	2110	CLA	C1B-NB	-3.06	1.34	1.37
24	a	2113	CLA	C3B-C4B	3.06	1.49	1.42
24	c	506	CLA	C4D-CHA	3.06	1.49	1.38
24	b	618	CLA	C3B-C4B	3.06	1.49	1.42
24	A	406	CLA	C3B-C4B	3.06	1.49	1.42
24	c	509	CLA	C4B-NB	-3.05	1.34	1.37
24	b	609	CLA	C4D-CHA	3.05	1.49	1.38
24	B	608	CLA	C1B-NB	-3.05	1.34	1.37
24	a	2113	CLA	C4B-NB	-3.05	1.34	1.37
24	c	513	CLA	C1B-NB	-3.05	1.34	1.37
24	d	405	CLA	C4B-NB	-3.04	1.34	1.37
24	c	504	CLA	C1B-NB	-3.04	1.34	1.37
24	c	510	CLA	C3B-C4B	3.04	1.49	1.42
24	b	618	CLA	C4D-CHA	3.03	1.49	1.38
24	C	510	CLA	C4D-CHA	3.03	1.49	1.38
24	b	611	CLA	MG-NB	3.02	2.11	2.05
24	B	611	CLA	C4D-CHA	3.02	1.49	1.38
24	D	405	CLA	C1B-C2B	3.02	1.50	1.43
24	B	617	CLA	OBD-CAD	3.02	1.27	1.22
24	B	608	CLA	C1B-C2B	3.02	1.50	1.43
24	c	512	CLA	C4B-NB	-3.02	1.34	1.37
24	a	2113	CLA	C1B-C2B	3.02	1.50	1.43
24	b	613	CLA	C4D-CHA	3.01	1.49	1.38
24	C	511	CLA	C4D-CHA	3.01	1.49	1.38
24	D	401	CLA	MG-NC	3.01	2.13	2.06
24	c	507	CLA	C4B-NB	-3.01	1.34	1.37
24	C	503	CLA	C4D-CHA	3.01	1.49	1.38
24	B	614	CLA	C4D-CHA	3.01	1.49	1.38
24	C	506	CLA	C1B-C2B	3.01	1.50	1.43
40	F	102	HEM	CAB-C3B	3.00	1.55	1.47
43	v	201	HEC	FE-NA	3.00	2.05	1.95
24	c	514	CLA	C4D-CHA	3.00	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	CLA	C1B-C2B	3.00	1.50	1.43
24	B	615	CLA	C4D-CHA	2.99	1.49	1.38
24	C	507	CLA	C4D-CHA	2.99	1.49	1.38
24	B	611	CLA	C3B-C4B	2.99	1.49	1.42
24	c	507	CLA	C1B-C2B	2.99	1.50	1.43
24	B	609	CLA	C4D-CHA	2.99	1.49	1.38
24	b	610	CLA	C3B-C4B	2.98	1.49	1.42
24	B	602	CLA	C4D-CHA	2.98	1.49	1.38
24	c	503	CLA	C1B-NB	-2.98	1.34	1.37
24	B	612	CLA	C4D-CHA	2.98	1.49	1.38
24	c	507	CLA	C4D-CHA	2.98	1.49	1.38
24	b	618	CLA	C1B-C2B	2.98	1.50	1.43
24	C	502	CLA	C1B-NB	-2.98	1.34	1.37
24	C	503	CLA	C4B-NB	-2.97	1.34	1.37
24	C	513	CLA	C4B-NB	-2.97	1.34	1.37
24	C	511	CLA	C1C-C2C	2.97	1.50	1.44
24	c	506	CLA	C4B-NB	-2.97	1.34	1.37
24	B	602	CLA	C3B-C4B	2.97	1.49	1.42
24	b	608	CLA	MG-ND	-2.96	1.99	2.05
24	d	404	CLA	C1B-C2B	2.96	1.50	1.43
40	e	103	HEM	CAB-C3B	2.96	1.55	1.47
24	B	607	CLA	MG-NB	-2.96	1.99	2.05
24	b	616	CLA	C1B-C2B	2.95	1.50	1.43
24	A	409	CLA	MG-NA	2.95	2.13	2.06
24	b	617	CLA	OBD-CAD	2.95	1.27	1.22
24	D	404	CLA	C1B-C2B	2.95	1.50	1.43
24	D	404	CLA	OBD-CAD	2.94	1.27	1.22
24	C	502	CLA	C4D-CHA	2.94	1.48	1.38
24	b	611	CLA	C4B-NB	-2.94	1.34	1.37
24	C	505	CLA	C4B-NB	-2.94	1.34	1.37
24	C	507	CLA	C1C-NC	-2.94	1.33	1.37
24	c	505	CLA	C1C-NC	-2.94	1.33	1.37
24	B	615	CLA	C1B-C2B	2.94	1.50	1.43
24	C	504	CLA	C4D-CHA	2.94	1.48	1.38
24	c	505	CLA	C4B-NB	-2.93	1.34	1.37
24	c	512	CLA	C4D-CHA	2.93	1.48	1.38
24	c	511	CLA	C1B-C2B	2.93	1.50	1.43
24	b	605	CLA	C4D-CHA	2.93	1.48	1.38
24	a	2109	CLA	C4B-NB	-2.93	1.34	1.37
24	a	2113	CLA	OBD-CAD	2.93	1.27	1.22
24	b	607	CLA	C1C-NC	-2.92	1.33	1.37
40	F	102	HEM	CAC-C3C	2.92	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C4B-NB	-2.92	1.34	1.37
24	C	505	CLA	C4D-CHA	2.92	1.48	1.38
24	B	605	CLA	C3B-C4B	2.91	1.49	1.42
24	A	409	CLA	MG-NB	2.91	2.11	2.05
24	b	619	CLA	C4D-CHA	2.91	1.48	1.38
24	B	606	CLA	C1B-C2B	2.91	1.50	1.43
24	b	616	CLA	C4D-CHA	2.90	1.48	1.38
24	c	515	CLA	C4D-CHA	2.90	1.48	1.38
24	b	604	CLA	C4D-CHA	2.90	1.48	1.38
24	b	615	CLA	C1C-NC	-2.90	1.33	1.37
24	b	617	CLA	C1B-C2B	2.90	1.50	1.43
36	d	403	HTG	C1-S1	-2.89	1.76	1.80
40	e	103	HEM	CAC-C3C	2.89	1.55	1.47
24	b	609	CLA	C1B-NB	-2.89	1.34	1.37
24	b	616	CLA	C1B-NB	-2.89	1.34	1.37
24	d	405	CLA	C1B-C2B	2.89	1.50	1.43
24	B	616	CLA	MG-NC	2.89	2.13	2.06
24	c	505	CLA	C1B-C2B	2.88	1.50	1.43
24	b	605	CLA	C3B-C4B	2.88	1.49	1.42
24	b	612	CLA	C1B-C2B	2.88	1.50	1.43
24	b	609	CLA	OBD-CAD	2.88	1.27	1.22
24	b	608	CLA	C1B-NB	-2.88	1.34	1.37
24	B	604	CLA	C1B-C2B	2.88	1.50	1.43
24	c	509	CLA	C1B-C2B	2.88	1.50	1.43
24	D	401	CLA	C4D-CHA	2.87	1.48	1.38
24	c	512	CLA	C1B-C2B	2.87	1.50	1.43
27	A	413	SQD	C6-S	-2.87	1.66	1.77
24	D	405	CLA	C4D-CHA	2.87	1.48	1.38
24	b	612	CLA	C4D-CHA	2.86	1.48	1.38
24	a	2110	CLA	C4D-CHA	2.86	1.48	1.38
24	C	504	CLA	C1C-C2C	2.86	1.50	1.44
24	B	607	CLA	C1B-NB	-2.86	1.34	1.37
24	B	616	CLA	C1B-C2B	2.86	1.50	1.43
24	b	614	CLA	C4D-CHA	2.86	1.48	1.38
27	A	411	SQD	C6-S	-2.86	1.66	1.77
24	b	606	CLA	C4B-NB	-2.85	1.34	1.37
24	b	611	CLA	C4D-CHA	2.85	1.48	1.38
24	B	615	CLA	C1B-NB	-2.85	1.34	1.37
24	c	504	CLA	C1B-C2B	2.85	1.50	1.43
24	d	404	CLA	C4D-CHA	2.84	1.48	1.38
24	B	612	CLA	C1B-C2B	2.84	1.50	1.43
24	B	602	CLA	C4B-NB	-2.84	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C3B-C4B	2.84	1.49	1.42
24	b	610	CLA	C4D-CHA	2.84	1.48	1.38
24	B	613	CLA	C1B-C2B	2.84	1.49	1.43
24	b	615	CLA	C1B-C2B	2.84	1.49	1.43
24	B	604	CLA	C1C-C2C	2.84	1.50	1.44
24	B	614	CLA	C1B-NB	-2.83	1.34	1.37
24	C	514	CLA	C3B-C4B	2.83	1.49	1.42
24	B	610	CLA	C4D-CHA	2.83	1.48	1.38
24	C	502	CLA	C3B-C4B	2.83	1.49	1.42
24	d	401	CLA	C4B-NB	-2.83	1.34	1.37
24	b	614	CLA	C3B-C4B	2.83	1.49	1.42
24	b	614	CLA	C1B-NB	-2.83	1.34	1.37
24	C	513	CLA	C3B-C4B	2.82	1.49	1.42
24	B	606	CLA	C4D-CHA	2.82	1.48	1.38
24	C	514	CLA	C4D-CHA	2.82	1.48	1.38
24	A	409	CLA	C4D-CHA	2.81	1.48	1.38
24	A	409	CLA	C1B-NB	-2.81	1.34	1.37
24	c	513	CLA	C4D-CHA	2.81	1.48	1.38
24	C	505	CLA	C1C-NC	-2.81	1.33	1.37
24	b	614	CLA	C4B-NB	-2.81	1.34	1.37
24	b	615	CLA	C4D-CHA	2.80	1.48	1.38
24	D	405	CLA	C4B-NB	-2.80	1.34	1.37
24	B	604	CLA	C4D-CHA	2.80	1.48	1.38
24	C	506	CLA	C1C-NC	-2.80	1.33	1.37
24	a	2109	CLA	C4D-CHA	2.79	1.48	1.38
24	c	514	CLA	C1B-NB	-2.79	1.34	1.37
24	C	514	CLA	C1B-C2B	2.79	1.49	1.43
24	c	506	CLA	C1B-NB	-2.79	1.34	1.37
24	b	609	CLA	C1B-C2B	2.78	1.49	1.43
24	C	513	CLA	C1C-C2C	2.78	1.50	1.44
24	c	504	CLA	C4D-CHA	2.78	1.48	1.38
24	C	513	CLA	C1B-NB	-2.78	1.34	1.37
40	F	102	HEM	FE-NB	2.78	2.03	1.94
24	b	609	CLA	C3B-C4B	2.78	1.49	1.42
24	C	504	CLA	C1B-C2B	2.77	1.49	1.43
24	c	504	CLA	C3B-C4B	2.77	1.49	1.42
24	c	505	CLA	C1C-C2C	2.77	1.49	1.44
24	B	602	CLA	MG-NB	2.76	2.11	2.05
24	A	405	CLA	C4D-CHA	2.76	1.48	1.38
24	B	603	CLA	C4D-CHA	2.76	1.48	1.38
24	C	502	CLA	C1B-C2B	2.76	1.49	1.43
24	b	605	CLA	C4B-NB	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C1B-C2B	2.76	1.49	1.43
24	b	606	CLA	C3B-C4B	2.76	1.49	1.42
24	B	603	CLA	C1B-C2B	2.76	1.49	1.43
24	b	611	CLA	C3B-C4B	2.75	1.49	1.42
24	D	404	CLA	C4D-CHA	2.75	1.48	1.38
24	a	2113	CLA	C4D-CHA	2.75	1.48	1.38
24	C	511	CLA	C4B-NB	-2.75	1.34	1.37
24	b	606	CLA	C4D-CHA	2.75	1.48	1.38
24	A	409	CLA	C4B-NB	-2.75	1.34	1.37
24	c	515	CLA	C1B-C2B	2.74	1.49	1.43
24	B	612	CLA	C3B-C4B	2.74	1.49	1.42
24	c	507	CLA	C1C-C2C	2.74	1.49	1.44
24	C	509	CLA	C1B-NB	-2.74	1.34	1.37
24	d	404	CLA	MG-ND	-2.74	2.00	2.05
24	B	612	CLA	C4B-NB	-2.74	1.34	1.37
24	b	616	CLA	C4B-NB	-2.74	1.34	1.37
24	c	512	CLA	C3B-C4B	2.74	1.49	1.42
24	B	616	CLA	C4D-CHA	2.74	1.48	1.38
24	b	617	CLA	C4D-CHA	2.74	1.48	1.38
24	d	401	CLA	C4D-CHA	2.74	1.48	1.38
24	c	511	CLA	C1C-NC	-2.73	1.33	1.37
24	B	602	CLA	C1C-C2C	2.73	1.49	1.44
24	B	606	CLA	C1B-NB	-2.73	1.34	1.37
24	C	503	CLA	C1B-C2B	2.73	1.49	1.43
24	d	405	CLA	C4D-CHA	2.73	1.48	1.38
24	b	605	CLA	C1B-C2B	2.73	1.49	1.43
24	D	405	CLA	C3B-C4B	2.73	1.49	1.42
24	b	604	CLA	C1B-NB	-2.72	1.34	1.37
24	b	609	CLA	C4B-NB	-2.72	1.34	1.37
24	B	617	CLA	C1C-NC	-2.72	1.33	1.37
24	B	604	CLA	C3B-C4B	2.72	1.49	1.42
24	C	512	CLA	C3B-C4B	2.72	1.49	1.42
24	b	614	CLA	C1B-C2B	2.72	1.49	1.43
24	c	504	CLA	C4B-NB	-2.72	1.34	1.37
24	c	508	CLA	C3B-C4B	2.71	1.49	1.42
24	B	610	CLA	C1B-C2B	2.71	1.49	1.43
36	c	526	HTG	C1-S1	-2.71	1.76	1.80
24	B	617	CLA	C1B-C2B	2.71	1.49	1.43
24	C	508	CLA	C1B-C2B	2.71	1.49	1.43
24	c	513	CLA	C4B-NB	-2.70	1.34	1.37
24	b	613	CLA	C4B-NB	-2.70	1.34	1.37
24	c	514	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	621	SQD	C6-S	-2.70	1.67	1.77
27	a	2102	SQD	C6-S	-2.70	1.67	1.77
24	B	602	CLA	C1B-C2B	2.70	1.49	1.43
40	e	103	HEM	FE-NA	2.69	2.04	1.95
24	C	507	CLA	C1B-NB	-2.69	1.34	1.37
24	A	409	CLA	C4C-C3C	2.69	1.49	1.45
24	c	503	CLA	C4D-CHA	2.69	1.48	1.38
24	C	510	CLA	C1B-C2B	2.69	1.49	1.43
25	A	407	PHO	C4B-NB	-2.69	1.33	1.38
24	D	401	CLA	C1B-C2B	2.69	1.49	1.43
24	C	514	CLA	C1C-NC	-2.69	1.33	1.37
24	A	406	CLA	MG-ND	-2.69	2.00	2.05
24	C	504	CLA	C1C-NC	-2.68	1.33	1.37
25	a	2112	PHO	C4B-NB	-2.68	1.33	1.38
24	c	511	CLA	C1C-C2C	2.68	1.49	1.44
24	b	605	CLA	C1B-NB	-2.68	1.34	1.37
24	a	2109	CLA	C1B-C2B	2.68	1.49	1.43
24	b	608	CLA	C4D-CHA	2.67	1.47	1.38
24	c	513	CLA	C3B-C4B	2.67	1.49	1.42
24	b	612	CLA	MG-NB	-2.67	2.00	2.05
24	c	515	CLA	C4B-NB	-2.67	1.34	1.37
24	d	405	CLA	C4C-C3C	2.67	1.49	1.45
24	C	507	CLA	C4B-NB	-2.67	1.34	1.37
24	C	513	CLA	C1B-C2B	2.67	1.49	1.43
27	a	2115	SQD	C6-S	-2.67	1.67	1.77
24	c	508	CLA	C4D-CHA	2.66	1.47	1.38
24	C	510	CLA	C4D-ND	2.66	1.41	1.37
24	b	604	CLA	C1C-C2C	2.66	1.49	1.44
24	D	405	CLA	C1B-NB	-2.66	1.34	1.37
24	b	605	CLA	C4C-C3C	2.66	1.49	1.45
24	a	2113	CLA	C1C-NC	-2.66	1.33	1.37
24	b	609	CLA	MG-NB	2.65	2.11	2.05
24	c	509	CLA	C1C-NC	-2.65	1.33	1.37
24	B	611	CLA	C4B-NB	-2.65	1.34	1.37
24	C	509	CLA	C4B-NB	-2.65	1.34	1.37
24	D	401	CLA	C1C-C2C	2.65	1.49	1.44
24	B	609	CLA	C1C-C2C	2.65	1.49	1.44
24	c	513	CLA	C1B-C2B	2.65	1.49	1.43
24	c	515	CLA	C1C-C2C	2.64	1.49	1.44
24	B	607	CLA	C1B-C2B	2.64	1.49	1.43
24	c	506	CLA	C1B-C2B	2.64	1.49	1.43
24	D	401	CLA	C3B-C4B	2.64	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C4D-CHA	2.64	1.47	1.38
24	c	511	CLA	C1B-NB	-2.63	1.34	1.37
24	A	406	CLA	C4D-CHA	2.63	1.47	1.38
24	c	507	CLA	C3B-C4B	2.63	1.48	1.42
24	B	608	CLA	C3B-C4B	2.63	1.48	1.42
24	a	2110	CLA	C1C-NC	-2.63	1.33	1.37
24	B	613	CLA	C1C-C2C	2.63	1.49	1.44
24	b	608	CLA	C1C-C2C	2.63	1.49	1.44
24	c	510	CLA	C1C-C2C	2.63	1.49	1.44
24	b	604	CLA	C1B-C2B	2.63	1.49	1.43
24	b	610	CLA	C4B-NB	-2.63	1.34	1.37
24	C	511	CLA	C1B-C2B	2.63	1.49	1.43
24	c	507	CLA	C1C-NC	-2.62	1.33	1.37
24	b	618	CLA	C1B-NB	-2.62	1.34	1.37
24	b	612	CLA	C4B-NB	-2.62	1.34	1.37
24	B	614	CLA	C4B-NB	-2.62	1.34	1.37
24	B	611	CLA	C1C-C2C	2.61	1.49	1.44
24	C	509	CLA	C4D-CHA	2.61	1.47	1.38
24	B	609	CLA	C3B-C4B	2.61	1.48	1.42
24	B	604	CLA	C1B-NB	-2.61	1.34	1.37
38	h	703	DGD	O5D-C1E	2.61	1.44	1.40
24	C	505	CLA	C1B-C2B	2.61	1.49	1.43
24	A	405	CLA	C1C-C2C	2.60	1.49	1.44
24	B	609	CLA	C4C-C3C	2.60	1.49	1.45
24	d	405	CLA	C1C-C2C	2.60	1.49	1.44
24	B	606	CLA	C1C-C2C	2.60	1.49	1.44
26	b	622	BCR	C30-C25	-2.60	1.50	1.53
24	B	616	CLA	C3B-C4B	2.60	1.48	1.42
24	b	605	CLA	C1C-C2C	2.60	1.49	1.44
24	C	503	CLA	C3B-C4B	2.59	1.48	1.42
24	C	511	CLA	C3B-C4B	2.59	1.48	1.42
24	d	404	CLA	C3D-C4D	-2.59	1.38	1.44
31	d	407	PL9	C6-C5	2.59	1.48	1.35
24	C	503	CLA	C1C-C2C	2.59	1.49	1.44
24	C	505	CLA	C3B-C4B	2.58	1.48	1.42
24	b	606	CLA	C1B-C2B	2.58	1.49	1.43
24	B	603	CLA	C4C-C3C	2.58	1.49	1.45
24	b	616	CLA	C1C-NC	-2.58	1.34	1.37
24	C	510	CLA	C3B-C4B	2.58	1.48	1.42
24	A	409	CLA	C3B-C4B	2.58	1.48	1.42
24	C	512	CLA	C1B-NB	-2.58	1.34	1.37
24	c	515	CLA	C3B-C4B	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	C4C-C3C	2.57	1.49	1.45
24	b	615	CLA	C1C-C2C	2.57	1.49	1.44
24	b	616	CLA	C1C-C2C	2.57	1.49	1.44
24	c	509	CLA	C4C-C3C	2.57	1.49	1.45
24	B	609	CLA	C1B-C2B	2.57	1.49	1.43
24	b	605	CLA	C1C-NC	-2.57	1.34	1.37
36	B	627	HTG	C1-S1	-2.57	1.76	1.80
24	b	607	CLA	C4B-NB	-2.57	1.34	1.37
24	B	603	CLA	C3B-C4B	2.56	1.48	1.42
24	C	507	CLA	C1C-C2C	2.55	1.49	1.44
24	b	617	CLA	C1C-C2C	2.55	1.49	1.44
24	C	504	CLA	C4B-NB	-2.55	1.34	1.37
24	b	608	CLA	C1B-C2B	2.55	1.49	1.43
24	b	608	CLA	MG-NB	2.55	2.10	2.05
24	b	606	CLA	C1C-C2C	2.55	1.49	1.44
24	C	506	CLA	C4C-C3C	2.54	1.49	1.45
24	C	503	CLA	C3B-C2B	2.54	1.49	1.41
24	c	503	CLA	C4B-NB	-2.54	1.34	1.37
24	c	508	CLA	C1C-NC	-2.54	1.34	1.37
24	b	604	CLA	C1C-NC	-2.54	1.34	1.37
24	b	610	CLA	C1C-C2C	2.54	1.49	1.44
24	C	502	CLA	C1C-C2C	2.54	1.49	1.44
24	B	613	CLA	C3B-C4B	2.54	1.48	1.42
24	B	613	CLA	C4B-NB	-2.53	1.34	1.37
24	B	604	CLA	C4B-NB	-2.53	1.34	1.37
24	c	511	CLA	C3B-C2B	2.53	1.49	1.41
24	D	404	CLA	C3B-C4B	2.53	1.48	1.42
24	B	610	CLA	C1C-NC	-2.53	1.34	1.37
36	b	602	HTG	C1-S1	-2.53	1.76	1.80
24	c	511	CLA	C4B-NB	-2.53	1.34	1.37
43	V	201	HEC	CMC-C2C	2.52	1.56	1.50
24	d	404	CLA	C4B-NB	-2.52	1.34	1.37
25	A	408	PHO	C3D-C4D	-2.52	1.37	1.41
24	C	503	CLA	C4C-C3C	2.52	1.49	1.45
24	a	2109	CLA	C1C-C2C	2.52	1.49	1.44
24	b	613	CLA	C1B-C2B	2.51	1.49	1.43
24	c	511	CLA	C3B-C4B	2.51	1.48	1.42
25	A	408	PHO	C1D-ND	-2.51	1.33	1.38
24	D	404	CLA	C1C-C2C	2.51	1.49	1.44
24	C	502	CLA	C1C-NC	-2.51	1.34	1.37
24	b	618	CLA	C1C-C2C	2.51	1.49	1.44
24	b	616	CLA	C3B-C4B	2.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	MG-ND	-2.51	2.00	2.05
24	c	514	CLA	C4B-NB	-2.51	1.34	1.37
24	d	405	CLA	C3B-C4B	2.51	1.48	1.42
24	A	405	CLA	C4C-C3C	2.50	1.49	1.45
24	c	505	CLA	C1B-NB	-2.50	1.34	1.37
24	c	515	CLA	C1B-NB	-2.50	1.34	1.37
24	c	510	CLA	C1B-C2B	2.50	1.49	1.43
27	L	102	SQD	C6-S	-2.50	1.68	1.77
31	D	407	PL9	C6-C5	2.49	1.48	1.35
24	C	508	CLA	C1C-NC	-2.49	1.34	1.37
24	B	605	CLA	C4C-C3C	2.49	1.49	1.45
36	b	601	HTG	C1-S1	-2.48	1.76	1.80
24	C	506	CLA	C4B-NB	-2.48	1.34	1.37
25	a	2111	PHO	C4B-NB	-2.47	1.34	1.38
24	B	606	CLA	C4B-NB	-2.47	1.34	1.37
24	c	512	CLA	MG-NB	2.47	2.10	2.05
24	c	515	CLA	C1C-NC	-2.47	1.34	1.37
24	C	504	CLA	C3B-C4B	2.47	1.48	1.42
24	c	503	CLA	C1B-C2B	2.47	1.49	1.43
24	B	611	CLA	MG-NB	2.47	2.10	2.05
25	a	2112	PHO	C3A-C2A	-2.47	1.52	1.54
24	b	606	CLA	C4C-C3C	2.47	1.49	1.45
24	d	404	CLA	MG-NB	-2.46	2.00	2.05
24	C	505	CLA	C3B-C2B	2.46	1.49	1.41
24	c	508	CLA	C4B-NB	-2.45	1.34	1.37
24	b	611	CLA	C1B-C2B	2.45	1.49	1.43
31	D	407	PL9	C2-C3	2.45	1.41	1.34
24	C	514	CLA	C1C-C2C	2.45	1.49	1.44
24	A	405	CLA	C4B-NB	-2.45	1.34	1.37
24	b	617	CLA	C4B-NB	-2.45	1.34	1.37
24	B	609	CLA	C1C-NC	-2.45	1.34	1.37
24	c	506	CLA	C3B-C4B	2.44	1.48	1.42
24	C	508	CLA	C1C-C2C	2.44	1.49	1.44
24	b	614	CLA	C3B-C2B	2.44	1.49	1.41
24	c	510	CLA	C4D-CHA	2.44	1.47	1.38
24	B	611	CLA	C1B-C2B	2.44	1.49	1.43
27	B	621	SQD	O6-C1	2.44	1.44	1.40
24	c	507	CLA	C4C-C3C	2.44	1.49	1.45
24	c	508	CLA	C1B-C2B	2.44	1.49	1.43
24	a	2109	CLA	C1C-NC	-2.43	1.34	1.37
24	b	611	CLA	C1C-NC	-2.43	1.34	1.37
24	c	503	CLA	MG-NB	2.43	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C1C-C2C	2.43	1.49	1.44
24	b	609	CLA	C1C-C2C	2.43	1.49	1.44
24	B	612	CLA	C1B-NB	-2.43	1.34	1.37
24	B	603	CLA	C1C-C2C	2.43	1.49	1.44
24	B	607	CLA	C4B-NB	-2.43	1.34	1.37
24	B	610	CLA	C1B-NB	-2.43	1.34	1.37
24	b	605	CLA	C3B-C2B	2.43	1.49	1.41
24	B	602	CLA	C1C-NC	-2.42	1.34	1.37
24	b	616	CLA	C4C-C3C	2.42	1.49	1.45
24	C	507	CLA	C3B-C4B	2.42	1.48	1.42
24	C	512	CLA	C1C-C2C	2.42	1.49	1.44
24	B	606	CLA	C1C-NC	-2.42	1.34	1.37
24	C	514	CLA	C4B-NB	-2.42	1.34	1.37
24	C	510	CLA	C1C-NC	-2.41	1.34	1.37
36	b	626	HTG	C1-S1	-2.41	1.77	1.80
24	B	604	CLA	C1C-NC	-2.41	1.34	1.37
24	c	505	CLA	C4C-C3C	2.41	1.49	1.45
24	C	509	CLA	C1B-C2B	2.41	1.48	1.43
24	A	406	CLA	C4B-NB	-2.41	1.34	1.37
24	c	510	CLA	C3B-C2B	2.41	1.49	1.41
24	B	605	CLA	C1C-C2C	2.41	1.49	1.44
43	v	201	HEC	CMC-C2C	2.41	1.55	1.50
24	A	405	CLA	C3B-C2B	2.40	1.49	1.41
24	C	512	CLA	C3B-C2B	2.40	1.49	1.41
24	c	503	CLA	C1C-C2C	2.40	1.49	1.44
24	B	614	CLA	C1C-C2C	2.40	1.49	1.44
24	C	510	CLA	C1C-C2C	2.40	1.49	1.44
24	C	510	CLA	C4C-C3C	2.40	1.49	1.45
38	H	102	DGD	O5D-C1E	2.40	1.44	1.40
24	b	615	CLA	C3B-C2B	2.40	1.49	1.41
24	A	409	CLA	C3B-C2B	2.40	1.49	1.41
24	B	612	CLA	MG-NB	2.40	2.10	2.05
24	B	603	CLA	C4B-NB	-2.39	1.34	1.37
24	a	2109	CLA	C3B-C4B	2.39	1.48	1.42
24	c	512	CLA	C1C-NC	-2.39	1.34	1.37
24	D	405	CLA	C1C-NC	-2.39	1.34	1.37
24	B	609	CLA	MG-NB	2.39	2.10	2.05
24	b	619	CLA	C3B-C2B	2.38	1.49	1.41
24	c	511	CLA	C4D-ND	2.38	1.40	1.37
24	b	608	CLA	C4B-NB	-2.38	1.34	1.37
24	b	611	CLA	C1C-C2C	2.38	1.49	1.44
24	C	514	CLA	C3B-C2B	2.38	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C3B-C2B	2.38	1.49	1.41
24	c	507	CLA	C1B-NB	-2.38	1.34	1.37
24	c	506	CLA	MG-NC	2.38	2.11	2.06
24	b	612	CLA	C3B-C4B	2.38	1.48	1.42
24	B	614	CLA	C3B-C2B	2.37	1.49	1.41
24	b	606	CLA	C1C-NC	-2.37	1.34	1.37
24	B	602	CLA	C1B-NB	-2.37	1.34	1.37
24	c	515	CLA	C3B-C2B	2.37	1.49	1.41
24	C	508	CLA	C3B-C2B	2.37	1.49	1.41
24	C	506	CLA	C1C-C2C	2.37	1.49	1.44
25	A	408	PHO	C4B-NB	-2.36	1.34	1.38
24	b	609	CLA	C3B-C2B	2.36	1.49	1.41
24	c	509	CLA	C1C-C2C	2.36	1.49	1.44
24	B	614	CLA	C1B-C2B	2.36	1.48	1.43
24	c	506	CLA	C1C-C2C	2.36	1.49	1.44
24	C	509	CLA	C3B-C2B	2.36	1.49	1.41
24	b	613	CLA	C3B-C2B	2.36	1.49	1.41
24	C	506	CLA	C3B-C4B	2.36	1.48	1.42
24	c	514	CLA	C3B-C2B	2.36	1.49	1.41
36	C	521	HTG	C1-S1	-2.36	1.77	1.80
24	b	607	CLA	C4C-C3C	2.35	1.49	1.45
24	A	406	CLA	C1B-C2B	2.35	1.48	1.43
24	B	611	CLA	C4C-C3C	2.35	1.49	1.45
24	c	510	CLA	C4B-NB	-2.35	1.34	1.37
24	d	404	CLA	C3B-C4B	2.35	1.48	1.42
24	c	514	CLA	C3B-C4B	2.35	1.48	1.42
24	C	503	CLA	MG-NB	2.35	2.10	2.05
24	c	503	CLA	C1C-NC	-2.35	1.34	1.37
24	C	509	CLA	C1C-C2C	2.34	1.49	1.44
24	a	2109	CLA	C3B-C2B	2.34	1.49	1.41
24	B	604	CLA	C4C-C3C	2.34	1.49	1.45
24	b	613	CLA	C1C-C2C	2.34	1.49	1.44
24	C	504	CLA	C1B-NB	-2.34	1.34	1.37
24	B	616	CLA	C1C-NC	-2.34	1.34	1.37
24	A	409	CLA	C1C-C2C	2.34	1.49	1.44
24	b	617	CLA	C3B-C4B	2.34	1.48	1.42
24	b	614	CLA	C4C-C3C	2.33	1.49	1.45
24	c	514	CLA	C1C-C2C	2.33	1.49	1.44
24	A	406	CLA	C1C-C2C	2.33	1.49	1.44
24	D	404	CLA	C1B-NB	-2.32	1.34	1.37
24	B	607	CLA	C1C-C2C	2.32	1.49	1.44
24	a	2113	CLA	C3B-C2B	2.32	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	524	HTG	C1-S1	-2.32	1.77	1.80
24	c	508	CLA	C3D-C4D	-2.32	1.38	1.44
24	C	508	CLA	C3B-C4B	2.32	1.48	1.42
36	I	1202	HTG	C1-S1	-2.32	1.77	1.80
24	C	503	CLA	C1B-NB	-2.32	1.34	1.37
26	d	406	BCR	C30-C25	-2.32	1.50	1.53
43	v	201	HEC	CMD-C2D	2.32	1.55	1.50
27	F	101	SQD	C6-S	-2.31	1.68	1.77
29	j	1601	LMT	O1'-C1'	2.31	1.44	1.40
29	A	420	LMT	O1'-C1'	2.31	1.44	1.40
24	C	511	CLA	C1C-NC	-2.31	1.34	1.37
24	d	405	CLA	C3B-C2B	2.31	1.49	1.41
24	a	2110	CLA	C3B-C4B	2.31	1.48	1.42
24	b	615	CLA	C3B-C4B	2.31	1.48	1.42
24	d	404	CLA	C3B-C2B	2.31	1.49	1.41
24	B	613	CLA	C1C-NC	-2.30	1.34	1.37
24	b	612	CLA	C1B-NB	-2.30	1.35	1.37
24	c	508	CLA	C3B-C2B	2.30	1.49	1.41
24	B	617	CLA	C3B-C2B	2.30	1.49	1.41
24	a	2110	CLA	C4C-C3C	2.30	1.49	1.45
24	C	509	CLA	C4C-C3C	2.30	1.49	1.45
24	a	2109	CLA	C4C-C3C	2.30	1.49	1.45
24	C	509	CLA	C1C-NC	-2.30	1.34	1.37
24	b	610	CLA	C3D-C4D	-2.29	1.39	1.44
32	a	2119	K2I	C-C5	-2.29	1.38	1.44
24	C	505	CLA	C1C-C2C	2.29	1.49	1.44
24	b	614	CLA	C1C-C2C	2.29	1.49	1.44
24	c	504	CLA	C3D-C4D	-2.29	1.39	1.44
24	b	614	CLA	C3D-C4D	-2.29	1.39	1.44
24	C	502	CLA	C4B-NB	-2.28	1.35	1.37
24	c	507	CLA	C3B-C2B	2.28	1.48	1.41
24	C	512	CLA	C4D-ND	2.28	1.40	1.37
24	c	509	CLA	C3B-C2B	2.28	1.48	1.41
24	B	615	CLA	C3B-C4B	2.28	1.48	1.42
24	B	608	CLA	C4B-NB	-2.28	1.35	1.37
24	D	405	CLA	C1C-C2C	2.27	1.49	1.44
24	B	605	CLA	C1C-NC	-2.27	1.34	1.37
24	c	515	CLA	C4C-C3C	2.27	1.49	1.45
24	c	503	CLA	C3B-C2B	2.27	1.48	1.41
24	c	504	CLA	C1C-C2C	2.27	1.49	1.44
24	b	617	CLA	C4C-C3C	2.27	1.48	1.45
24	b	619	CLA	C3B-C4B	2.27	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	414	HTG	C1-S1	-2.26	1.77	1.80
24	c	513	CLA	C1C-C2C	2.26	1.48	1.44
24	A	406	CLA	C3D-C4D	-2.26	1.39	1.44
24	b	619	CLA	C3D-C4D	-2.26	1.39	1.44
24	d	405	CLA	C1D-C2D	2.26	1.49	1.45
36	D	413	HTG	C1-S1	-2.26	1.77	1.80
24	B	608	CLA	C3B-C2B	2.26	1.48	1.41
24	b	604	CLA	C4B-NB	-2.26	1.35	1.37
24	B	610	CLA	C1C-C2C	2.25	1.48	1.44
24	C	504	CLA	C3B-C2B	2.25	1.48	1.41
24	A	405	CLA	C1B-C2B	2.25	1.48	1.43
24	b	611	CLA	C3B-C2B	2.25	1.48	1.41
38	c	520	DGD	O2G-C2G	-2.25	1.41	1.46
40	e	103	HEM	CMC-C2C	2.24	1.55	1.50
24	c	509	CLA	C4D-ND	2.24	1.40	1.37
24	b	610	CLA	C3B-C2B	2.24	1.48	1.41
25	A	407	PHO	C1D-ND	-2.24	1.34	1.38
24	b	612	CLA	C1D-C2D	2.24	1.49	1.45
24	D	404	CLA	C3B-C2B	2.24	1.48	1.41
24	C	513	CLA	C3B-C2B	2.23	1.48	1.41
24	c	504	CLA	C1C-NC	-2.23	1.34	1.37
24	B	605	CLA	C1B-NB	-2.23	1.35	1.37
24	C	512	CLA	C4C-C3C	2.23	1.48	1.45
25	A	407	PHO	CBD-CGD	-2.23	1.49	1.52
24	b	618	CLA	C1C-NC	-2.23	1.34	1.37
24	D	404	CLA	C3D-C4D	-2.23	1.39	1.44
24	B	613	CLA	C3D-C4D	-2.23	1.39	1.44
24	B	604	CLA	C3D-C4D	-2.23	1.39	1.44
24	b	617	CLA	C3B-C2B	2.23	1.48	1.41
24	D	405	CLA	C3B-C2B	2.23	1.48	1.41
24	B	605	CLA	C4B-NB	-2.22	1.35	1.37
24	C	507	CLA	C1B-C2B	2.22	1.48	1.43
24	B	605	CLA	C3B-C2B	2.22	1.48	1.41
24	B	602	CLA	C3B-C2B	2.22	1.48	1.41
24	b	606	CLA	C3D-C4D	-2.22	1.39	1.44
24	C	511	CLA	C3B-C2B	2.22	1.48	1.41
24	B	612	CLA	C3B-C2B	2.22	1.48	1.41
24	a	2113	CLA	C1C-C2C	2.21	1.48	1.44
24	C	511	CLA	C4C-C3C	2.21	1.48	1.45
24	d	404	CLA	C4C-C3C	2.21	1.48	1.45
24	D	401	CLA	C3B-C2B	2.21	1.48	1.41
24	c	513	CLA	C3B-C2B	2.21	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C4C-C3C	2.21	1.48	1.45
24	C	508	CLA	C4D-ND	2.21	1.40	1.37
24	d	401	CLA	C3B-C2B	2.21	1.48	1.41
24	C	502	CLA	C3D-C4D	-2.21	1.39	1.44
24	c	505	CLA	C3B-C4B	2.21	1.47	1.42
24	C	510	CLA	C3D-C4D	-2.20	1.39	1.44
24	D	401	CLA	C4C-C3C	2.20	1.48	1.45
24	B	614	CLA	C4C-C3C	2.20	1.48	1.45
24	B	602	CLA	C4C-C3C	2.20	1.48	1.45
24	B	610	CLA	C3B-C4B	2.20	1.47	1.42
24	C	511	CLA	C3D-C4D	-2.20	1.39	1.44
24	B	611	CLA	C1C-NC	-2.20	1.34	1.37
24	b	607	CLA	C3B-C2B	2.20	1.48	1.41
24	C	506	CLA	C3B-C2B	2.19	1.48	1.41
24	d	401	CLA	C1C-C2C	2.18	1.48	1.44
24	b	617	CLA	C3D-C4D	-2.18	1.39	1.44
24	A	405	CLA	C1C-NC	-2.18	1.34	1.37
24	b	605	CLA	C3D-C4D	-2.18	1.39	1.44
24	b	604	CLA	C3B-C2B	2.18	1.48	1.41
24	B	615	CLA	MG-NC	2.18	2.11	2.06
24	B	606	CLA	C4C-C3C	2.18	1.48	1.45
24	c	509	CLA	C1B-NB	-2.18	1.35	1.37
29	f	101	LMT	O1'-C1'	2.18	1.43	1.40
36	B	626	HTG	C1-S1	-2.18	1.77	1.80
24	c	505	CLA	C3B-C2B	2.17	1.48	1.41
40	F	102	HEM	FE-NA	2.17	2.02	1.95
24	D	401	CLA	C1C-NC	-2.17	1.34	1.37
24	c	515	CLA	C3D-C4D	-2.17	1.39	1.44
24	c	503	CLA	C3B-C4B	2.17	1.47	1.42
24	B	616	CLA	C4D-ND	2.17	1.40	1.37
24	A	406	CLA	C1C-NC	-2.17	1.34	1.37
24	B	607	CLA	C3B-C4B	2.17	1.47	1.42
24	b	607	CLA	C3B-C4B	2.16	1.47	1.42
24	C	510	CLA	C3B-C2B	2.16	1.48	1.41
24	B	615	CLA	C3D-C4D	-2.16	1.39	1.44
24	b	613	CLA	C3D-C4D	-2.16	1.39	1.44
24	c	513	CLA	C1C-NC	-2.16	1.34	1.37
24	c	506	CLA	C3B-C2B	2.16	1.48	1.41
24	B	603	CLA	C3B-C2B	2.16	1.48	1.41
24	B	607	CLA	C3D-C4D	-2.16	1.39	1.44
24	b	608	CLA	C3B-C2B	2.16	1.48	1.41
24	C	512	CLA	C1C-NC	-2.15	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C3B-C2B	2.15	1.48	1.41
24	B	613	CLA	C4D-ND	2.15	1.40	1.37
24	b	607	CLA	C4D-ND	2.15	1.40	1.37
24	c	514	CLA	C3D-C4D	-2.15	1.39	1.44
26	D	406	BCR	C30-C25	-2.15	1.50	1.53
24	b	606	CLA	C3B-C2B	2.15	1.48	1.41
24	b	618	CLA	MG-ND	-2.14	2.01	2.05
24	b	609	CLA	C4C-C3C	2.14	1.48	1.45
24	c	504	CLA	C3B-C2B	2.14	1.48	1.41
24	C	507	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	617	CLA	C3D-C4D	-2.13	1.39	1.44
32	a	2118[B]	K2I	C3-C2	-2.13	1.38	1.44
24	b	610	CLA	C4C-C3C	2.13	1.48	1.45
24	B	617	CLA	C3B-C4B	2.13	1.47	1.42
36	c	523	HTG	C1-S1	-2.13	1.77	1.80
24	c	506	CLA	C1C-NC	-2.13	1.34	1.37
24	B	612	CLA	C3D-C4D	-2.13	1.39	1.44
24	b	604	CLA	C3D-C4D	-2.13	1.39	1.44
24	c	508	CLA	C1C-C2C	2.13	1.48	1.44
24	b	609	CLA	C1C-NC	-2.12	1.34	1.37
24	b	618	CLA	C3B-C2B	2.12	1.48	1.41
24	a	2110	CLA	C3B-C2B	2.12	1.48	1.41
24	C	506	CLA	C3D-C4D	-2.12	1.39	1.44
32	A	418[B]	K2I	C3-C2	-2.12	1.39	1.44
24	B	615	CLA	C4C-C3C	2.12	1.48	1.45
24	C	505	CLA	C3D-C4D	-2.12	1.39	1.44
24	B	608	CLA	C1C-C2C	2.11	1.48	1.44
24	C	512	CLA	MG-NC	2.11	2.11	2.06
24	c	507	CLA	C4D-ND	2.11	1.40	1.37
24	B	607	CLA	C4C-C3C	2.11	1.48	1.45
24	C	514	CLA	C4D-ND	2.11	1.40	1.37
24	C	514	CLA	C3D-C4D	-2.11	1.39	1.44
24	c	512	CLA	C3B-C2B	2.11	1.48	1.41
24	B	617	CLA	C1C-C2C	2.11	1.48	1.44
24	B	607	CLA	C3B-C2B	2.11	1.48	1.41
32	a	2119	K2I	C3-C2	-2.11	1.39	1.44
24	B	612	CLA	C4C-C3C	2.11	1.48	1.45
24	c	508	CLA	C4C-C3C	2.11	1.48	1.45
24	B	609	CLA	C3B-C2B	2.10	1.48	1.41
24	C	502	CLA	C4C-C3C	2.10	1.48	1.45
24	c	511	CLA	C4C-C3C	2.10	1.48	1.45
24	A	405	CLA	C3B-C4B	2.09	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C3B-C2B	2.09	1.48	1.41
36	B	628	HTG	C1-S1	-2.09	1.77	1.80
24	D	405	CLA	C4C-C3C	2.09	1.48	1.45
40	e	103	HEM	FE-NC	2.09	2.02	1.95
24	B	612	CLA	C4D-ND	2.09	1.40	1.37
24	b	608	CLA	C1C-NC	-2.09	1.34	1.37
24	b	614	CLA	C1C-NC	-2.09	1.34	1.37
24	b	612	CLA	C3D-C4D	-2.09	1.39	1.44
24	C	503	CLA	C1C-NC	-2.09	1.34	1.37
24	B	603	CLA	C3D-C4D	-2.08	1.39	1.44
24	C	514	CLA	C1B-NB	-2.07	1.35	1.37
24	b	619	CLA	C1C-C2C	2.07	1.48	1.44
24	B	602	CLA	C3D-C4D	-2.07	1.39	1.44
24	c	514	CLA	C1C-NC	-2.07	1.34	1.37
24	B	610	CLA	C3D-C4D	-2.07	1.39	1.44
24	B	614	CLA	C1C-NC	-2.07	1.34	1.37
38	C	517	DGD	O5D-C1E	2.06	1.43	1.40
24	b	612	CLA	C4C-C3C	2.06	1.48	1.45
29	i	104	LMT	O1'-C1'	2.06	1.43	1.40
24	C	508	CLA	C4C-C3C	2.06	1.48	1.45
24	B	610	CLA	C4D-ND	2.06	1.40	1.37
24	a	2110	CLA	C1C-C2C	2.06	1.48	1.44
24	B	609	CLA	C3D-C4D	-2.06	1.39	1.44
24	c	515	CLA	C4D-ND	2.05	1.40	1.37
24	B	614	CLA	C3B-C4B	2.05	1.47	1.42
24	b	604	CLA	C4C-C3C	2.05	1.48	1.45
24	b	607	CLA	C1B-NB	-2.04	1.35	1.37
40	F	102	HEM	CMB-C2B	2.04	1.55	1.50
24	B	610	CLA	C3B-C2B	2.04	1.48	1.41
24	B	611	CLA	C3B-C2B	2.04	1.48	1.41
25	a	2112	PHO	CHA-CBD	-2.04	1.49	1.51
29	E	105	LMT	O1'-C1'	2.04	1.43	1.40
24	C	505	CLA	C4C-C3C	2.04	1.48	1.45
24	c	512	CLA	C1C-C2C	2.03	1.48	1.44
43	v	201	HEC	CMB-C2B	2.03	1.55	1.50
24	b	611	CLA	C3D-C4D	-2.03	1.39	1.44
24	B	615	CLA	C3B-C2B	2.03	1.48	1.41
36	V	204	HTG	C1-S1	-2.03	1.77	1.80
40	e	103	HEM	CMA-C3A	2.03	1.55	1.50
32	a	2118[A]	K2I	C-C5	-2.03	1.39	1.44
24	b	609	CLA	C3D-C4D	-2.03	1.39	1.44
24	B	608	CLA	C1C-NC	-2.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	C4C-C3C	2.03	1.48	1.45
32	A	419	K2I	C-C5	-2.02	1.39	1.44
24	b	604	CLA	C4D-ND	2.02	1.40	1.37
26	B	619	BCR	C19-C18	2.02	1.50	1.45
36	i	103	HTG	C1-S1	-2.02	1.77	1.80
24	D	405	CLA	C3D-C4D	-2.02	1.39	1.44
24	C	502	CLA	C3B-C2B	2.02	1.48	1.41
24	b	608	CLA	C3D-C4D	-2.02	1.39	1.44
40	e	103	HEM	CMB-C2B	2.02	1.55	1.50
24	D	405	CLA	C4D-ND	2.02	1.40	1.37
24	b	613	CLA	C1C-NC	-2.01	1.34	1.37
24	B	617	CLA	C1B-NB	-2.01	1.35	1.37
24	c	510	CLA	C1C-NC	-2.00	1.34	1.37

All (2600) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	407	PHO	C2D-C1D-ND	12.52	118.17	109.53
25	A	408	PHO	C2D-C1D-ND	12.48	118.14	109.53
25	a	2111	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	c	503	CLA	C1D-ND-C4D	-10.88	98.61	106.33
24	D	404	CLA	C1D-ND-C4D	-10.56	98.83	106.33
24	a	2110	CLA	C1D-ND-C4D	-10.44	98.92	106.33
25	a	2112	PHO	C2D-C1D-ND	10.43	116.72	109.53
24	b	615	CLA	C1D-ND-C4D	-10.13	99.14	106.33
24	c	510	CLA	C1D-ND-C4D	-10.01	99.23	106.33
24	a	2109	CLA	C1D-ND-C4D	-9.98	99.24	106.33
24	b	608	CLA	C1D-ND-C4D	-9.90	99.30	106.33
24	B	612	CLA	C1D-ND-C4D	-9.84	99.34	106.33
24	D	401	CLA	C1D-ND-C4D	-9.84	99.35	106.33
24	d	401	CLA	C1D-ND-C4D	-9.79	99.38	106.33
24	B	613	CLA	C1D-ND-C4D	-9.78	99.38	106.33
24	B	606	CLA	C1D-ND-C4D	-9.78	99.39	106.33
24	b	611	CLA	C1D-ND-C4D	-9.68	99.46	106.33
24	D	404	CLA	C2D-C1D-ND	9.59	117.17	110.10
24	c	503	CLA	C2D-C1D-ND	9.53	117.13	110.10
24	a	2113	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	D	401	CLA	C2D-C1D-ND	9.47	117.08	110.10
24	B	616	CLA	C1D-ND-C4D	-9.47	99.61	106.33
24	C	509	CLA	C1D-ND-C4D	-9.42	99.64	106.33
24	a	2110	CLA	C2D-C1D-ND	9.40	117.03	110.10
24	C	514	CLA	C1D-ND-C4D	-9.38	99.67	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	614	CLA	C1D-ND-C4D	-9.36	99.69	106.33
24	B	610	CLA	C1D-ND-C4D	-9.34	99.70	106.33
24	b	615	CLA	C2D-C1D-ND	9.31	116.97	110.10
24	B	604	CLA	C1D-ND-C4D	-9.28	99.74	106.33
24	c	504	CLA	C1D-ND-C4D	-9.28	99.74	106.33
24	B	615	CLA	C1D-ND-C4D	-9.25	99.76	106.33
24	d	405	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	c	506	CLA	C1D-ND-C4D	-9.23	99.78	106.33
24	c	508	CLA	C1D-ND-C4D	-9.23	99.78	106.33
24	A	409	CLA	C1D-ND-C4D	-9.21	99.79	106.33
24	b	614	CLA	C1D-ND-C4D	-9.15	99.84	106.33
24	B	609	CLA	C1D-ND-C4D	-9.12	99.86	106.33
24	b	619	CLA	C1D-ND-C4D	-9.09	99.88	106.33
24	C	511	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	C	507	CLA	C1D-ND-C4D	-9.04	99.91	106.33
24	A	406	CLA	C1D-ND-C4D	-9.04	99.91	106.33
24	b	617	CLA	C1D-ND-C4D	-8.99	99.95	106.33
24	b	616	CLA	C1D-ND-C4D	-8.94	99.98	106.33
24	c	512	CLA	C1D-ND-C4D	-8.94	99.99	106.33
24	a	2113	CLA	C2D-C1D-ND	8.92	116.67	110.10
24	C	503	CLA	C1D-ND-C4D	-8.90	100.01	106.33
24	D	405	CLA	C1D-ND-C4D	-8.90	100.02	106.33
24	A	405	CLA	C1D-ND-C4D	-8.87	100.04	106.33
24	B	617	CLA	C1D-ND-C4D	-8.85	100.05	106.33
24	B	603	CLA	C1D-ND-C4D	-8.84	100.05	106.33
24	c	507	CLA	C1D-ND-C4D	-8.84	100.06	106.33
24	C	513	CLA	C1D-ND-C4D	-8.81	100.08	106.33
24	b	606	CLA	C1D-ND-C4D	-8.79	100.09	106.33
24	b	610	CLA	C1D-ND-C4D	-8.76	100.11	106.33
24	B	607	CLA	C1D-ND-C4D	-8.75	100.12	106.33
24	C	502	CLA	C1D-ND-C4D	-8.74	100.13	106.33
24	c	511	CLA	C1D-ND-C4D	-8.74	100.13	106.33
24	C	512	CLA	C1D-ND-C4D	-8.73	100.13	106.33
24	C	510	CLA	C1D-ND-C4D	-8.71	100.15	106.33
24	b	613	CLA	C1D-ND-C4D	-8.69	100.16	106.33
24	c	515	CLA	C1D-ND-C4D	-8.69	100.16	106.33
24	c	506	CLA	C2D-C1D-ND	8.68	116.50	110.10
24	B	612	CLA	C2D-C1D-ND	8.62	116.46	110.10
24	B	605	CLA	C1D-ND-C4D	-8.62	100.21	106.33
24	c	514	CLA	C1D-ND-C4D	-8.62	100.21	106.33
24	d	401	CLA	C2D-C1D-ND	8.61	116.45	110.10
24	B	617	CLA	C2D-C1D-ND	8.60	116.44	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	608	CLA	C2D-C1D-ND	8.60	116.44	110.10
24	b	607	CLA	C1D-ND-C4D	-8.58	100.24	106.33
24	B	615	CLA	C2D-C1D-ND	8.57	116.42	110.10
24	b	612	CLA	C1D-ND-C4D	-8.57	100.25	106.33
24	A	409	CLA	C2D-C1D-ND	8.53	116.39	110.10
24	B	602	CLA	C1D-ND-C4D	-8.49	100.30	106.33
24	c	509	CLA	C1D-ND-C4D	-8.49	100.30	106.33
24	C	505	CLA	C1D-ND-C4D	-8.44	100.34	106.33
24	B	616	CLA	C2D-C1D-ND	8.43	116.32	110.10
24	B	606	CLA	C2D-C1D-ND	8.43	116.31	110.10
24	B	608	CLA	C1D-ND-C4D	-8.37	100.39	106.33
24	B	613	CLA	C2D-C1D-ND	8.33	116.24	110.10
24	C	513	CLA	C2D-C1D-ND	8.32	116.24	110.10
24	b	609	CLA	C1D-ND-C4D	-8.31	100.43	106.33
24	C	512	CLA	C2D-C1D-ND	8.27	116.20	110.10
24	b	618	CLA	C1D-ND-C4D	-8.27	100.46	106.33
24	b	611	CLA	C2D-C1D-ND	8.25	116.19	110.10
24	B	614	CLA	C2D-C1D-ND	8.25	116.18	110.10
24	c	513	CLA	C1D-ND-C4D	-8.23	100.49	106.33
24	a	2109	CLA	C2D-C1D-ND	8.23	116.17	110.10
24	b	605	CLA	C1D-ND-C4D	-8.23	100.49	106.33
24	d	404	CLA	C1D-ND-C4D	-8.21	100.50	106.33
24	C	503	CLA	C2D-C1D-ND	8.19	116.14	110.10
24	b	604	CLA	C1D-ND-C4D	-8.19	100.52	106.33
24	c	510	CLA	C2D-C1D-ND	8.18	116.13	110.10
24	b	616	CLA	C2D-C1D-ND	8.17	116.13	110.10
24	b	619	CLA	C2D-C1D-ND	8.12	116.09	110.10
24	d	405	CLA	C2D-C1D-ND	8.08	116.06	110.10
24	b	614	CLA	C2D-C1D-ND	8.07	116.05	110.10
24	b	613	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	B	608	CLA	C2D-C1D-ND	8.02	116.02	110.10
24	B	611	CLA	C1D-ND-C4D	-8.02	100.64	106.33
24	b	610	CLA	C2D-C1D-ND	8.01	116.01	110.10
24	B	609	CLA	C2D-C1D-ND	7.92	115.94	110.10
24	B	607	CLA	C2D-C1D-ND	7.92	115.94	110.10
24	C	504	CLA	C1D-ND-C4D	-7.90	100.73	106.33
24	c	505	CLA	C1D-ND-C4D	-7.84	100.76	106.33
24	B	610	CLA	C2D-C1D-ND	7.82	115.87	110.10
24	C	508	CLA	C1D-ND-C4D	-7.78	100.81	106.33
24	C	509	CLA	C2D-C1D-ND	7.77	115.83	110.10
24	b	618	CLA	C2D-C1D-ND	7.77	115.83	110.10
25	a	2112	PHO	C2B-C1B-NB	7.77	114.89	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	2112	PHO	O2D-CGD-CBD	7.75	120.82	111.00
24	C	506	CLA	C1D-ND-C4D	-7.74	100.83	106.33
24	c	505	CLA	C2D-C1D-ND	7.73	115.80	110.10
24	b	617	CLA	C2D-C1D-ND	7.68	115.77	110.10
24	B	604	CLA	C2D-C1D-ND	7.68	115.76	110.10
24	c	509	CLA	C2D-C1D-ND	7.64	115.74	110.10
25	a	2111	PHO	O2D-CGD-CBD	7.64	120.68	111.00
24	b	607	CLA	C2D-C1D-ND	7.64	115.73	110.10
24	c	504	CLA	C2D-C1D-ND	7.62	115.72	110.10
24	c	511	CLA	C2D-C1D-ND	7.57	115.69	110.10
24	c	514	CLA	C2D-C1D-ND	7.55	115.67	110.10
24	B	611	CLA	C2D-C1D-ND	7.52	115.64	110.10
24	C	507	CLA	C2D-C1D-ND	7.51	115.64	110.10
24	C	504	CLA	C2D-C1D-ND	7.43	115.58	110.10
24	A	405	CLA	C2D-C1D-ND	7.37	115.54	110.10
24	C	514	CLA	C2D-C1D-ND	7.34	115.52	110.10
24	B	603	CLA	C2D-C1D-ND	7.31	115.49	110.10
24	D	405	CLA	C2D-C1D-ND	7.30	115.48	110.10
25	A	407	PHO	C1C-C2C-C3C	-7.24	102.59	108.61
24	b	609	CLA	C2D-C1D-ND	7.24	115.44	110.10
24	C	511	CLA	C2D-C1D-ND	7.21	115.42	110.10
24	C	510	CLA	C2D-C1D-ND	7.20	115.41	110.10
24	C	508	CLA	C2D-C1D-ND	7.18	115.40	110.10
24	c	508	CLA	C2D-C1D-ND	7.15	115.38	110.10
25	A	407	PHO	C4D-ND-C1D	-7.13	101.58	108.83
24	c	509	CLA	O2D-CGD-CBD	7.13	123.93	111.27
25	A	408	PHO	C4D-ND-C1D	-7.11	101.59	108.83
24	A	406	CLA	C2D-C1D-ND	7.11	115.34	110.10
24	B	602	CLA	C2D-C1D-ND	7.09	115.33	110.10
24	c	513	CLA	C2D-C1D-ND	7.08	115.32	110.10
24	c	512	CLA	C2D-C1D-ND	7.07	115.31	110.10
24	B	605	CLA	C2D-C1D-ND	7.02	115.28	110.10
25	A	407	PHO	C2B-C1B-NB	7.02	114.37	109.53
24	C	505	CLA	C2D-C1D-ND	6.99	115.26	110.10
25	a	2111	PHO	C4D-ND-C1D	-6.99	101.72	108.83
25	A	408	PHO	C2B-C1B-NB	6.93	114.31	109.53
36	I	1202	HTG	C1'-S1-C1	6.92	113.03	100.09
24	b	612	CLA	C2D-C1D-ND	6.87	115.17	110.10
24	C	502	CLA	C2D-C1D-ND	6.86	115.16	110.10
24	c	507	CLA	C2D-C1D-ND	6.83	115.14	110.10
24	b	608	CLA	CMD-C2D-C1D	6.82	136.73	124.71
43	V	201	HEC	C1D-ND-C4D	6.81	112.11	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	C1-C2-C3	-6.80	114.28	126.04
24	c	515	CLA	C2D-C1D-ND	6.77	115.09	110.10
24	b	605	CLA	C2D-C1D-ND	6.76	115.08	110.10
24	B	602	CLA	CMD-C2D-C1D	6.75	136.60	124.71
24	B	605	CLA	CMD-C2D-C1D	6.72	136.56	124.71
24	b	612	CLA	CMD-C2D-C1D	6.72	136.56	124.71
24	b	604	CLA	C2D-C1D-ND	6.71	115.05	110.10
24	B	607	CLA	CMD-C2D-C1D	6.69	136.50	124.71
24	b	606	CLA	C2D-C1D-ND	6.68	115.03	110.10
24	c	514	CLA	O2D-CGD-CBD	6.68	123.15	111.27
24	c	508	CLA	CMD-C2D-C1D	6.60	136.34	124.71
25	a	2112	PHO	C4D-ND-C1D	-6.59	102.12	108.83
43	v	201	HEC	C1D-ND-C4D	6.59	111.88	105.07
24	A	406	CLA	C2B-C1B-NB	6.58	114.64	110.23
25	a	2111	PHO	C2B-C1B-NB	6.55	114.05	109.53
25	A	408	PHO	O2D-CGD-CBD	6.55	119.29	111.00
24	b	617	CLA	CMD-C2D-C1D	6.53	136.23	124.71
24	d	404	CLA	C2D-C1D-ND	6.52	114.91	110.10
24	C	504	CLA	CMD-C2D-C1D	6.46	136.09	124.71
24	b	613	CLA	CMD-C2D-C1D	6.45	136.07	124.71
24	b	616	CLA	CMD-C2D-C1D	6.42	136.03	124.71
24	C	507	CLA	CMD-C2D-C1D	6.39	135.98	124.71
24	d	404	CLA	CMD-C2D-C1D	6.37	135.94	124.71
24	D	401	CLA	C2B-C1B-NB	6.37	114.50	110.23
24	c	515	CLA	CMD-C2D-C1D	6.37	135.94	124.71
24	B	614	CLA	CMD-C2D-C1D	6.35	135.90	124.71
36	c	523	HTG	C1'-S1-C1	6.35	111.97	100.09
25	a	2112	PHO	C1C-C2C-C3C	-6.31	103.37	108.61
24	B	612	CLA	CMD-C2D-C1D	6.27	135.77	124.71
24	b	604	CLA	O2D-CGD-CBD	6.26	122.40	111.27
24	d	401	CLA	C2B-C1B-NB	6.26	114.43	110.23
24	B	602	CLA	O2D-CGD-CBD	6.24	122.35	111.27
24	B	615	CLA	O2D-CGD-CBD	6.19	122.27	111.27
24	A	406	CLA	CMD-C2D-C1D	6.18	135.60	124.71
24	b	608	CLA	C2B-C1B-NB	6.17	114.37	110.23
24	C	502	CLA	CMD-C2D-C1D	6.14	135.54	124.71
24	C	506	CLA	CMD-C2D-C1D	6.14	135.54	124.71
24	b	606	CLA	CMD-C2D-C1D	6.14	135.54	124.71
24	b	607	CLA	CMD-C2D-C1D	6.11	135.48	124.71
24	C	510	CLA	CMD-C2D-C1D	6.06	135.39	124.71
24	B	616	CLA	C2B-C1B-NB	6.05	114.29	110.23
24	b	608	CLA	CHD-C1D-ND	-6.02	118.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	C2B-C1B-NB	6.00	114.25	110.23
24	D	404	CLA	CMD-C2D-C1D	6.00	135.28	124.71
24	B	613	CLA	O2D-CGD-CBD	6.00	121.92	111.27
24	C	512	CLA	CMD-C2D-C1D	5.99	135.28	124.71
24	C	505	CLA	CMD-C2D-C1D	5.98	135.25	124.71
24	b	604	CLA	C2B-C1B-NB	5.98	114.24	110.23
24	b	609	CLA	CMD-C2D-C1D	5.97	135.24	124.71
36	c	524	HTG	C1'-S1-C1	5.97	111.25	100.09
24	C	510	CLA	O2D-CGD-CBD	5.96	121.87	111.27
24	C	511	CLA	O2D-CGD-CBD	5.95	121.85	111.27
24	C	514	CLA	CMD-C2D-C1D	5.93	135.16	124.71
24	c	510	CLA	C2B-C1B-NB	5.92	114.20	110.23
27	a	2115	SQD	O6-C1-C2	5.92	117.54	108.30
24	B	617	CLA	O2D-CGD-CBD	5.92	121.78	111.27
24	c	507	CLA	CMD-C2D-C1D	5.91	135.13	124.71
24	b	605	CLA	C2B-C1B-NB	5.89	114.18	110.23
24	C	506	CLA	C2D-C1D-ND	5.88	114.44	110.10
24	D	405	CLA	CMD-C2D-C1D	5.88	135.08	124.71
24	B	610	CLA	CMD-C2D-C1D	5.87	135.06	124.71
24	b	605	CLA	O2D-CGD-CBD	5.87	121.70	111.27
24	b	614	CLA	CMD-C2D-C1D	5.86	135.04	124.71
24	C	503	CLA	O2D-CGD-CBD	5.85	121.66	111.27
24	C	514	CLA	C2B-C1B-NB	5.85	114.15	110.23
24	b	606	CLA	C2B-C1B-NB	5.85	114.15	110.23
24	c	513	CLA	CMD-C2D-C1D	5.83	135.00	124.71
24	B	611	CLA	CMD-C2D-C1D	5.83	134.99	124.71
24	d	405	CLA	CMD-C2D-C1D	5.83	134.99	124.71
24	C	508	CLA	O2D-CGD-CBD	5.83	121.62	111.27
24	b	605	CLA	CMD-C2D-C1D	5.82	134.97	124.71
24	D	405	CLA	O2D-CGD-CBD	5.81	121.58	111.27
24	c	508	CLA	C2B-C1B-NB	5.80	114.12	110.23
24	C	509	CLA	C2B-C1B-NB	5.80	114.12	110.23
24	C	508	CLA	CMD-C2D-C1D	5.80	134.93	124.71
24	A	409	CLA	C2B-C1B-NB	5.79	114.11	110.23
24	d	401	CLA	CMD-C2D-C1D	5.79	134.91	124.71
24	c	504	CLA	C2B-C1B-NB	5.78	114.11	110.23
24	B	604	CLA	CMD-C2D-C1D	5.77	134.88	124.71
24	b	604	CLA	CMD-C2D-C1D	5.77	134.88	124.71
24	D	401	CLA	CMD-C2D-C1D	5.76	134.86	124.71
24	b	619	CLA	CMD-C2D-C1D	5.75	134.84	124.71
25	a	2111	PHO	C1C-C2C-C3C	-5.74	103.84	108.61
24	a	2109	CLA	CMD-C2D-C1D	5.73	134.81	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	511	CLA	CMD-C2D-C1D	5.72	134.80	124.71
24	b	611	CLA	CMD-C2D-C1D	5.72	134.79	124.71
24	B	604	CLA	O2D-CGD-CBD	5.72	121.42	111.27
24	C	510	CLA	C2B-C1B-NB	5.70	114.06	110.23
24	c	507	CLA	O2D-CGD-CBD	5.68	121.37	111.27
40	e	103	HEM	C4D-ND-C1D	5.67	110.93	105.07
25	A	407	PHO	O2D-CGD-CBD	5.66	118.17	111.00
36	C	522	HTG	C1'-S1-C1	5.66	110.68	100.09
24	C	513	CLA	O2D-CGD-CBD	5.66	121.33	111.27
40	F	102	HEM	C4D-ND-C1D	5.66	110.92	105.07
24	c	506	CLA	CMD-C2D-C1D	5.66	134.68	124.71
24	B	617	CLA	CMD-C2D-C1D	5.64	134.66	124.71
24	b	619	CLA	O2D-CGD-CBD	5.63	121.28	111.27
24	a	2110	CLA	C2B-C1B-NB	5.61	113.99	110.23
26	D	406	BCR	C7-C8-C9	-5.60	117.78	126.23
24	C	513	CLA	C2B-C1B-NB	5.60	113.98	110.23
24	C	511	CLA	CMD-C2D-C1D	5.60	134.57	124.71
24	A	405	CLA	CMD-C2D-C1D	5.59	134.56	124.71
24	a	2113	CLA	C2B-C1B-NB	5.58	113.97	110.23
24	b	613	CLA	C2B-C1B-NB	5.57	113.97	110.23
24	B	603	CLA	CMD-C2D-C1D	5.56	134.51	124.71
24	b	609	CLA	O2D-CGD-CBD	5.56	121.14	111.27
24	C	502	CLA	O2D-CGD-CBD	5.55	121.14	111.27
24	A	409	CLA	CMD-C2D-C1D	5.55	134.50	124.71
24	B	608	CLA	CMD-C2D-C1D	5.55	134.50	124.71
24	c	515	CLA	C2B-C1B-NB	5.55	113.95	110.23
24	B	606	CLA	CMD-C2D-C1D	5.54	134.47	124.71
24	b	611	CLA	C2B-C1B-NB	5.52	113.93	110.23
24	b	613	CLA	O2D-CGD-CBD	5.48	121.00	111.27
24	B	613	CLA	C2B-C1B-NB	5.46	113.89	110.23
24	C	509	CLA	O2D-CGD-CBD	5.46	120.98	111.27
24	c	506	CLA	O2D-CGD-CBD	5.45	120.96	111.27
36	B	627	HTG	C1'-S1-C1	5.44	110.27	100.09
24	b	618	CLA	CMD-C2D-C1D	5.44	134.29	124.71
24	c	503	CLA	CMD-C2D-C1D	5.43	134.28	124.71
24	B	609	CLA	C2B-C1B-NB	5.42	113.87	110.23
24	c	513	CLA	C2B-C1B-NB	5.42	113.87	110.23
24	B	615	CLA	C2B-C1B-NB	5.42	113.86	110.23
24	b	617	CLA	C2B-C1B-NB	5.42	113.86	110.23
24	D	405	CLA	C2B-C1B-NB	5.41	113.86	110.23
24	c	503	CLA	O2D-CGD-CBD	5.40	120.87	111.27
24	b	614	CLA	O2D-CGD-CBD	5.40	120.86	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	404	CLA	C2C-C1C-NC	5.39	115.02	109.97
24	c	514	CLA	C2B-C1B-NB	5.39	113.84	110.23
24	c	514	CLA	CMD-C2D-C1D	5.38	134.20	124.71
24	B	615	CLA	CMD-C2D-C1D	5.38	134.19	124.71
24	B	613	CLA	CMD-C2D-C1D	5.37	134.18	124.71
24	C	505	CLA	C2B-C1B-NB	5.37	113.83	110.23
24	B	616	CLA	CMD-C2D-C1D	5.36	134.16	124.71
24	C	513	CLA	CMD-C2D-C1D	5.36	134.16	124.71
24	B	607	CLA	C2B-C1B-NB	5.36	113.82	110.23
24	b	609	CLA	C2B-C1B-NB	5.35	113.82	110.23
24	b	618	CLA	C2B-C1B-NB	5.35	113.82	110.23
24	c	509	CLA	C2B-C1B-NB	5.35	113.82	110.23
24	B	614	CLA	C2B-C1B-NB	5.34	113.81	110.23
24	c	507	CLA	C2B-C1B-NB	5.34	113.81	110.23
24	b	608	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
28	C	526	LMG	O7-C10-C11	5.30	122.93	111.50
24	b	606	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	B	602	CLA	C2B-C1B-NB	5.30	113.79	110.23
24	B	611	CLA	C1-C2-C3	-5.30	116.88	126.04
27	A	411	SQD	O6-C1-C2	5.29	116.57	108.30
24	b	610	CLA	CMD-C2D-C1D	5.27	134.00	124.71
24	c	506	CLA	C2B-C1B-NB	5.26	113.76	110.23
24	B	606	CLA	C2B-C1B-NB	5.25	113.75	110.23
24	b	615	CLA	O2D-CGD-CBD	5.25	120.60	111.27
24	B	603	CLA	C2B-C1B-NB	5.25	113.75	110.23
25	A	407	PHO	C3D-C4D-ND	5.25	114.87	107.72
25	A	408	PHO	C1-C2-C3	-5.24	116.98	126.04
24	C	503	CLA	CMD-C2D-C1D	5.22	133.91	124.71
24	c	505	CLA	CMD-C2D-C1D	5.21	133.90	124.71
25	a	2111	PHO	C3D-C4D-ND	5.21	114.82	107.72
26	d	406	BCR	C38-C26-C25	-5.21	118.68	124.53
24	B	603	CLA	O2D-CGD-CBD	5.20	120.52	111.27
24	c	509	CLA	C2C-C1C-NC	5.18	114.83	109.97
24	D	404	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
24	B	612	CLA	O2D-CGD-CBD	5.17	120.45	111.27
24	c	512	CLA	C2B-C1B-NB	5.17	113.69	110.23
24	B	611	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	c	509	CLA	CMD-C2D-C1D	5.15	133.79	124.71
24	D	401	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
24	b	612	CLA	C2B-C1B-NB	5.15	113.68	110.23
24	a	2110	CLA	CMD-C2D-C1D	5.14	133.78	124.71
24	b	619	CLA	C2B-C1B-NB	5.14	113.68	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	621	SQD	O47-C7-C8	5.13	122.55	111.50
24	D	401	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
29	A	420	LMT	C1'-O5'-C5'	5.12	123.74	113.69
24	A	405	CLA	C2B-C1B-NB	5.12	113.66	110.23
24	C	512	CLA	C2B-C1B-NB	5.12	113.66	110.23
24	a	2109	CLA	C2B-C1B-NB	5.12	113.66	110.23
24	C	510	CLA	C1-C2-C3	-5.12	117.19	126.04
24	b	617	CLA	O2D-CGD-CBD	5.11	120.34	111.27
24	d	404	CLA	O2D-CGD-CBD	5.10	120.33	111.27
25	a	2112	PHO	C3D-C4D-ND	5.09	114.66	107.72
24	B	617	CLA	C2B-C1B-NB	5.09	113.64	110.23
25	A	408	PHO	C3D-C4D-ND	5.08	114.65	107.72
24	C	505	CLA	O2D-CGD-CBD	5.08	120.30	111.27
24	b	615	CLA	CHD-C4C-C3C	-5.08	117.38	124.84
24	C	503	CLA	C2B-C1B-NB	5.08	113.64	110.23
24	C	508	CLA	C3B-C2B-C1B	-5.06	101.05	107.16
24	b	613	CLA	C3D-C2D-C1D	-5.05	98.95	105.83
24	D	401	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	B	604	CLA	C2B-C1B-NB	5.04	113.61	110.23
24	C	507	CLA	C2B-C1B-NB	5.04	113.61	110.23
36	d	414	HTG	C1'-S1-C1	5.03	109.51	100.09
24	B	607	CLA	O2D-CGD-CBD	5.03	120.21	111.27
24	d	405	CLA	CHD-C1D-ND	-5.02	119.84	124.45
24	b	610	CLA	C2B-C1B-NB	5.01	113.59	110.23
24	C	509	CLA	CMD-C2D-C1D	5.01	133.55	124.71
27	f	102	SQD	O47-C7-C8	5.01	122.30	111.50
27	L	102	SQD	O47-C7-C8	4.99	122.25	111.50
27	B	621	SQD	C1-O5-C5	4.99	123.48	113.69
24	a	2113	CLA	O2D-CGD-CBD	4.98	120.12	111.27
36	b	626	HTG	C1'-S1-C1	4.98	109.40	100.09
24	D	401	CLA	CHD-C1D-ND	-4.97	119.88	124.45
24	c	510	CLA	CMD-C2D-C1D	4.97	133.47	124.71
24	c	506	CLA	CHD-C1D-ND	-4.96	119.90	124.45
24	b	614	CLA	C2B-C1B-NB	4.92	113.53	110.23
24	B	609	CLA	CMD-C2D-C1D	4.92	133.38	124.71
24	d	405	CLA	C2B-C1B-NB	4.92	113.53	110.23
24	A	409	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	B	611	CLA	C2B-C1B-NB	4.90	113.52	110.23
24	B	605	CLA	O2D-CGD-CBD	4.88	119.95	111.27
38	c	518	DGD	O2G-C1B-C2B	4.88	122.03	111.50
24	d	401	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
24	c	512	CLA	CMD-C2D-C1D	4.88	133.31	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C2B-C1B-NB	4.87	113.50	110.23
36	b	602	HTG	C1'-S1-C1	4.87	109.21	100.09
24	B	612	CLA	C2B-C1B-NB	4.87	113.50	110.23
24	c	509	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
24	C	513	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
27	L	102	SQD	O6-C1-C2	4.86	115.89	108.30
24	a	2110	CLA	C2C-C1C-NC	4.86	114.52	109.97
24	B	615	CLA	C2C-C1C-NC	4.85	114.52	109.97
24	c	509	CLA	C1C-C2C-C3C	-4.85	101.86	106.96
24	D	404	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
31	d	407	PL9	C7-C8-C9	-4.83	118.75	126.79
24	b	616	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
24	B	608	CLA	O2D-CGD-CBD	4.83	119.85	111.27
24	b	610	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	B	617	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	a	2113	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
24	b	607	CLA	C1-C2-C3	-4.80	117.73	126.04
25	A	408	PHO	C1C-C2C-C3C	-4.80	104.62	108.61
24	b	608	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
36	B	626	HTG	C1'-S1-C1	4.79	109.06	100.09
24	d	401	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	c	504	CLA	O2D-CGD-CBD	4.79	119.78	111.27
24	B	612	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
28	c	522	LMG	O7-C10-C11	4.79	121.82	111.50
24	a	2110	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	B	616	CLA	CHD-C4C-C3C	-4.77	117.82	124.84
24	c	504	CLA	CHD-C4C-C3C	-4.76	117.84	124.84
36	b	601	HTG	C1'-S1-C1	4.74	108.96	100.09
24	b	607	CLA	O2D-CGD-CBD	4.74	119.68	111.27
29	i	104	LMT	C1'-O5'-C5'	4.73	122.98	113.69
27	A	411	SQD	C1-O5-C5	-4.72	104.42	113.69
24	c	503	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
24	B	611	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	A	409	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
27	A	413	SQD	O47-C7-C8	4.68	121.59	111.50
36	c	526	HTG	C1'-S1-C1	4.68	108.85	100.09
24	b	615	CLA	C2B-C1B-NB	4.68	113.37	110.23
24	c	505	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
24	B	614	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
24	b	614	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
24	B	616	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
24	C	513	CLA	C3D-C2D-C1D	-4.67	99.46	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	506	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	C	503	CLA	C1-C2-C3	-4.66	117.98	126.04
24	d	401	CLA	CHD-C4C-C3C	-4.66	117.99	124.84
24	D	401	CLA	O2D-CGD-CBD	4.65	119.52	111.27
24	b	616	CLA	C2B-C1B-NB	4.65	113.35	110.23
24	d	404	CLA	C2B-C1B-NB	4.64	113.34	110.23
24	c	504	CLA	CMD-C2D-C1D	4.64	132.89	124.71
24	D	404	CLA	CHD-C1D-ND	-4.64	120.19	124.45
24	a	2113	CLA	CMD-C2D-C1D	4.64	132.89	124.71
24	B	615	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
24	C	506	CLA	O2D-CGD-CBD	4.63	119.49	111.27
24	B	607	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
24	B	606	CLA	CHD-C4C-C3C	-4.62	118.04	124.84
26	k	2003	BCR	C24-C23-C22	-4.62	119.25	126.23
24	b	606	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
24	c	511	CLA	O2D-CGD-CBD	4.62	119.48	111.27
24	c	507	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
32	A	418[A]	K2I	C3-C4-C5	-4.60	119.22	123.61
24	d	401	CLA	C2C-C1C-NC	4.60	114.28	109.97
24	b	619	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
24	C	504	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
24	b	617	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
36	B	625[B]	HTG	C1'-S1-C1	4.59	108.68	100.09
24	C	506	CLA	C2B-C1B-NB	4.59	113.31	110.23
24	c	510	CLA	C3D-C4D-ND	4.59	117.66	110.24
24	d	404	CLA	C2C-C1C-NC	4.59	114.27	109.97
24	C	513	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
24	C	512	CLA	C3D-C2D-C1D	-4.58	99.57	105.83
24	b	607	CLA	C2B-C1B-NB	4.58	113.31	110.23
24	B	610	CLA	O2D-CGD-CBD	4.58	119.41	111.27
26	b	622	BCR	C24-C23-C22	-4.57	119.32	126.23
24	b	611	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
36	V	204	HTG	C1'-S1-C1	4.57	108.64	100.09
24	c	510	CLA	O2D-CGD-CBD	4.57	119.39	111.27
24	b	618	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	B	617	CLA	CHD-C4C-C3C	-4.56	118.14	124.84
24	C	514	CLA	C3B-C2B-C1B	-4.55	101.66	107.16
24	a	2110	CLA	CHD-C1D-ND	-4.55	120.27	124.45
25	a	2112	PHO	C1-C2-C3	-4.55	118.18	126.04
24	B	608	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
24	C	512	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
24	C	503	CLA	C3D-C2D-C1D	-4.53	99.65	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	504	CLA	C2B-C1B-NB	4.53	113.27	110.23
24	c	503	CLA	O2D-CGD-O1D	-4.52	114.99	123.84
24	B	615	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
24	D	405	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
24	b	615	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	B	617	CLA	C3B-C2B-C1B	-4.50	101.72	107.16
24	b	606	CLA	C2C-C1C-NC	4.50	114.19	109.97
24	b	607	CLA	CAC-C3C-C4C	4.50	130.65	124.81
24	c	504	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
29	B	623	LMT	C1-O1'-C1'	-4.50	106.39	113.84
24	B	615	CLA	CHD-C4C-C3C	-4.50	118.23	124.84
24	b	610	CLA	O2D-CGD-CBD	4.50	119.26	111.27
39	e	101	LHG	O7-C7-C8	4.49	121.19	111.50
24	b	617	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
24	B	608	CLA	C2B-C1B-NB	4.49	113.24	110.23
24	A	406	CLA	C3D-C4D-ND	4.49	117.50	110.24
24	b	615	CLA	CMD-C2D-C1D	4.48	132.61	124.71
24	c	515	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
24	b	612	CLA	C2C-C1C-NC	4.48	114.17	109.97
24	C	504	CLA	C1-C2-C3	-4.48	118.30	126.04
24	a	2110	CLA	C3D-C4D-ND	4.47	117.48	110.24
24	b	609	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	d	405	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	a	2113	CLA	CHD-C4C-C3C	-4.47	118.27	124.84
24	D	404	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
24	b	619	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
27	F	101	SQD	O47-C7-C8	4.46	121.12	111.50
24	B	616	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
24	D	401	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
24	B	606	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
24	C	509	CLA	C3D-C4D-ND	4.45	117.44	110.24
26	c	516	BCR	C15-C14-C13	-4.45	120.96	127.31
24	D	401	CLA	CBC-CAC-C3C	-4.45	100.16	112.43
24	b	608	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
24	c	503	CLA	C3D-C4D-ND	4.44	117.42	110.24
24	D	401	CLA	CHD-C4C-C3C	-4.44	118.31	124.84
24	c	507	CLA	C2C-C1C-NC	4.44	114.13	109.97
26	T	101	BCR	C33-C5-C6	-4.44	119.54	124.53
28	A	412	LMG	O7-C10-C11	4.43	121.06	111.50
24	B	609	CLA	O2D-CGD-CBD	4.42	119.13	111.27
24	C	510	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
24	b	611	CLA	O2D-CGD-CBD	4.42	119.12	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	503	CLA	CHD-C1D-ND	-4.41	120.40	124.45
32	a	2118[A]	K2I	C3-C4-C5	-4.40	119.41	123.61
36	i	103	HTG	C1'-S1-C1	4.40	108.33	100.09
24	C	507	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
24	c	508	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
24	c	506	CLA	CHD-C4C-C3C	-4.39	118.38	124.84
36	C	522	HTG	C1-O5-C5	4.39	120.68	112.58
24	B	613	CLA	CHD-C4C-C3C	-4.39	118.38	124.84
24	A	406	CLA	CHD-C1D-ND	-4.39	120.42	124.45
24	D	404	CLA	C3D-C4D-ND	4.39	117.34	110.24
39	E	101	LHG	O7-C7-C8	4.39	120.96	111.50
24	d	405	CLA	O2D-CGD-CBD	4.39	119.06	111.27
24	B	614	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
24	b	605	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
24	B	614	CLA	CHD-C4C-C3C	-4.38	118.40	124.84
24	B	606	CLA	O2D-CGD-CBD	4.38	119.05	111.27
24	c	515	CLA	O2D-CGD-CBD	4.38	119.05	111.27
24	b	612	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
24	d	401	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
24	B	613	CLA	CHD-C1D-ND	-4.37	120.44	124.45
26	d	406	BCR	C24-C23-C22	-4.37	119.64	126.23
24	C	503	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
26	C	516	BCR	C7-C8-C9	-4.37	119.64	126.23
24	a	2110	CLA	C3B-C4B-NB	4.37	114.56	110.52
24	B	615	CLA	O2D-CGD-O1D	-4.36	115.31	123.84
24	B	610	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	a	2109	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	b	607	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	B	613	CLA	C3D-C4D-ND	4.36	117.28	110.24
27	L	102	SQD	O7-S-C6	4.35	112.11	106.94
40	F	102	HEM	CBD-CAD-C3D	-4.35	100.53	112.63
24	C	511	CLA	C2B-C1B-NB	4.35	113.15	110.23
24	b	608	CLA	O2D-CGD-CBD	4.35	119.00	111.27
24	b	619	CLA	CHD-C4C-C3C	-4.35	118.45	124.84
24	B	609	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
32	a	2118[B]	K2I	BR-C4-C5	4.35	121.23	116.03
24	c	503	CLA	C2B-C1B-NB	4.35	113.14	110.23
24	A	405	CLA	CHD-C1D-ND	-4.34	120.46	124.45
24	c	514	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
27	L	102	SQD	C3-C4-C5	4.34	117.98	110.24
24	C	504	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
36	V	204	HTG	C1-C2-C3	-4.34	102.02	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	C3D-C4D-ND	4.34	117.26	110.24
24	C	504	CLA	CHD-C4C-C3C	-4.34	118.47	124.84
24	C	503	CLA	O2D-CGD-O1D	-4.34	115.36	123.84
24	c	505	CLA	C2B-C1B-NB	4.33	113.14	110.23
26	b	620	BCR	C7-C8-C9	-4.33	119.69	126.23
24	b	604	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
24	B	602	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
24	B	602	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
24	c	514	CLA	C2C-C1C-NC	4.33	114.03	109.97
26	C	515	BCR	C33-C5-C6	-4.33	119.67	124.53
24	C	502	CLA	C2B-C1B-NB	4.32	113.13	110.23
36	V	204	HTG	O5-C1-C2	-4.32	104.88	110.31
24	c	508	CLA	C2C-C1C-NC	4.32	114.02	109.97
24	b	608	CLA	C3D-C4D-ND	4.32	117.22	110.24
26	B	618	BCR	C33-C5-C6	-4.31	119.69	124.53
24	c	504	CLA	C3D-C4D-ND	4.31	117.20	110.24
24	c	512	CLA	C3D-C4D-ND	4.30	117.20	110.24
24	B	607	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
24	B	609	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
26	D	406	BCR	C24-C23-C22	-4.30	119.74	126.23
24	B	610	CLA	C2B-C1B-NB	4.29	113.11	110.23
38	C	519	DGD	O2G-C1B-C2B	4.29	120.75	111.50
24	b	606	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
24	c	514	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	b	610	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
24	d	405	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
24	b	607	CLA	C3B-C2B-C1B	-4.26	102.01	107.16
24	C	505	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
24	D	404	CLA	O2D-CGD-CBD	4.26	118.83	111.27
24	d	404	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
24	B	604	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	C	507	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	b	615	CLA	C3C-C4C-NC	4.25	115.34	110.57
26	D	406	BCR	C38-C26-C25	-4.25	119.76	124.53
24	B	602	CLA	CHD-C4C-C3C	-4.25	118.60	124.84
36	b	602	HTG	C1-O5-C5	4.24	120.41	112.58
24	c	513	CLA	C4-C3-C5	4.24	122.41	115.27
24	B	603	CLA	CAA-C2A-C3A	-4.24	101.16	112.78
24	B	616	CLA	O2D-CGD-CBD	4.24	118.80	111.27
28	i	101	LMG	O7-C10-C11	4.24	120.63	111.50
36	B	628	HTG	C1'-S1-C1	4.24	108.02	100.09
24	a	2113	CLA	C1-C2-C3	-4.24	118.72	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
24	B	615	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
26	t	102	BCR	C33-C5-C6	-4.23	119.78	124.53
24	c	505	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
24	c	511	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
24	b	618	CLA	CHD-C4C-C3C	-4.22	118.63	124.84
24	C	514	CLA	O2D-CGD-CBD	4.22	118.77	111.27
38	D	408	DGD	O2G-C1B-C2B	4.22	120.60	111.50
24	A	409	CLA	C2C-C1C-NC	4.22	113.93	109.97
24	b	609	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
24	a	2113	CLA	C2C-C1C-NC	4.21	113.92	109.97
24	B	607	CLA	CHD-C1D-ND	-4.21	120.59	124.45
24	b	613	CLA	CHD-C4C-C3C	-4.21	118.65	124.84
24	d	404	CLA	C3D-C4D-ND	4.20	117.04	110.24
24	B	617	CLA	C2C-C1C-NC	4.20	113.91	109.97
24	C	507	CLA	C2C-C1C-NC	4.20	113.91	109.97
36	b	625	HTG	C1'-S1-C1	4.20	107.95	100.09
24	C	505	CLA	CHD-C1D-ND	-4.20	120.60	124.45
24	C	508	CLA	C3D-C2D-C1D	-4.20	100.11	105.83
24	c	510	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
24	C	510	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
38	c	519	DGD	O2G-C1B-C2B	4.18	120.52	111.50
36	B	625[A]	HTG	C1'-S1-C1	4.18	107.91	100.09
24	d	401	CLA	C3D-C4D-ND	4.18	117.00	110.24
24	B	604	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
38	C	517	DGD	O2G-C1B-C2B	4.18	120.50	111.50
24	d	401	CLA	CBC-CAC-C3C	-4.18	100.92	112.43
24	c	513	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
24	c	511	CLA	C2B-C1B-NB	4.18	113.03	110.23
24	B	616	CLA	C1D-CHD-C4C	-4.17	117.05	126.06
24	a	2110	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
24	b	612	CLA	CBC-CAC-C3C	-4.17	100.93	112.43
24	b	615	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
27	F	101	SQD	O6-C1-C2	4.17	114.81	108.30
24	b	615	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	c	508	CLA	C3D-C4D-ND	4.16	116.97	110.24
24	A	406	CLA	O2D-CGD-CBD	4.16	118.66	111.27
26	c	528	BCR	C33-C5-C6	-4.16	119.86	124.53
24	b	617	CLA	C1-C2-C3	-4.16	118.85	126.04
27	a	2115	SQD	C1-C2-C3	-4.16	101.33	110.00
24	d	405	CLA	C3D-C4D-ND	4.16	116.97	110.24
24	C	508	CLA	C2C-C1C-NC	4.16	113.86	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	505	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
24	C	505	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
24	d	405	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
24	b	613	CLA	CHD-C1D-ND	-4.15	120.64	124.45
24	B	605	CLA	C2C-C1C-NC	4.15	113.86	109.97
24	a	2109	CLA	C3D-C4D-ND	4.15	116.95	110.24
24	b	613	CLA	C3B-C2B-C1B	-4.15	102.16	107.16
24	c	503	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
24	c	514	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
24	c	506	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
24	C	514	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
24	b	612	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
24	C	511	CLA	C3D-C4D-ND	4.14	116.93	110.24
24	c	505	CLA	C2C-C1C-NC	4.13	113.84	109.97
24	B	612	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
24	C	507	CLA	O2D-CGD-CBD	4.13	118.61	111.27
24	c	514	CLA	CBA-CAA-C2A	-4.13	101.66	113.86
28	C	520	LMG	O7-C10-C11	4.13	120.41	111.50
24	b	605	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
24	a	2110	CLA	O2D-CGD-CBD	4.13	118.61	111.27
24	A	405	CLA	C2C-C1C-NC	4.13	113.84	109.97
24	B	611	CLA	CHD-C4C-C3C	-4.13	118.77	124.84
24	C	509	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
24	B	602	CLA	CHD-C1D-ND	-4.13	120.66	124.45
24	A	405	CLA	C3D-C4D-ND	4.12	116.91	110.24
24	b	618	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
24	D	404	CLA	C3C-C4C-NC	4.12	115.19	110.57
27	f	102	SQD	O7-S-C6	4.12	111.87	106.92
24	a	2109	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
24	a	2113	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
24	b	611	CLA	C3D-C4D-ND	4.12	116.90	110.24
24	C	510	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
24	a	2109	CLA	C2C-C1C-NC	4.11	113.83	109.97
24	B	606	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
31	D	407	PL9	C40-C39-C41	4.11	122.18	115.27
24	B	613	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
24	b	614	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
24	c	510	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
24	c	504	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
24	C	506	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
26	Y	302	BCR	C33-C5-C6	-4.09	119.94	124.53
26	d	406	BCR	C33-C5-C6	-4.09	119.94	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	512	CLA	O2D-CGD-CBD	4.09	118.53	111.27
24	c	513	CLA	CHD-C4C-C3C	-4.08	118.84	124.84
24	c	509	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
24	B	608	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
24	C	508	CLA	CHD-C4C-C3C	-4.08	118.84	124.84
26	A	410	BCR	C33-C5-C6	-4.08	119.95	124.53
24	b	609	CLA	CHD-C4C-C3C	-4.07	118.86	124.84
24	B	603	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
24	c	506	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	B	603	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
24	D	405	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
32	A	418[A]	K2I	C-C1-C2	-4.06	119.74	123.61
24	b	607	CLA	C2C-C1C-NC	4.06	113.77	109.97
24	C	514	CLA	C3D-C4D-ND	4.05	116.79	110.24
24	c	515	CLA	C3D-C2D-C1D	-4.05	100.31	105.83
24	B	615	CLA	O2A-CGA-O1A	-4.05	113.38	123.59
24	B	615	CLA	CHD-C1D-ND	-4.05	120.73	124.45
24	b	618	CLA	CHD-C1D-ND	-4.04	120.74	124.45
24	a	2113	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	B	605	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	b	612	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	B	604	CLA	C2C-C1C-NC	4.02	113.74	109.97
24	B	603	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	b	606	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	C	505	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	b	619	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
24	a	2113	CLA	C3D-C4D-ND	4.01	116.73	110.24
24	b	612	CLA	O2D-CGD-CBD	4.00	118.38	111.27
36	B	626	HTG	O5-C1-C2	4.00	115.35	110.31
24	D	404	CLA	C2B-C1B-NB	4.00	112.92	110.23
24	C	510	CLA	C2C-C1C-NC	4.00	113.72	109.97
24	b	616	CLA	C1-C2-C3	-4.00	119.12	126.04
24	B	604	CLA	C3D-C4D-ND	4.00	116.71	110.24
24	C	502	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
24	b	610	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	D	405	CLA	C3D-C4D-ND	4.00	116.71	110.24
24	B	604	CLA	C3B-C2B-C1B	-4.00	102.34	107.16
24	b	604	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
32	A	418[A]	K2I	BR-C4-C5	3.99	120.81	116.03
24	D	401	CLA	C3D-C4D-ND	3.99	116.69	110.24
24	B	605	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
24	c	510	CLA	CHD-C4C-C3C	-3.99	118.98	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	C2C-C1C-NC	3.98	113.70	109.97
27	a	2102	SQD	O47-C7-C8	3.98	120.08	111.50
24	d	404	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
24	B	609	CLA	C3D-C4D-ND	3.98	116.67	110.24
24	a	2110	CLA	CHD-C4C-C3C	-3.97	119.00	124.84
27	a	2115	SQD	O47-C7-C8	3.97	120.07	111.50
24	A	409	CLA	CHD-C1D-ND	-3.97	120.80	124.45
24	C	502	CLA	C3D-C4D-ND	3.96	116.65	110.24
24	C	510	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
24	c	513	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
24	B	613	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
26	c	516	BCR	C33-C5-C6	-3.96	120.08	124.53
24	b	619	CLA	C3C-C4C-NC	3.96	115.01	110.57
24	d	404	CLA	C1-C2-C3	-3.96	119.20	126.04
24	C	504	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
24	b	610	CLA	C4-C3-C5	3.95	121.91	115.27
26	T	101	BCR	C15-C16-C17	-3.95	115.39	123.47
24	b	616	CLA	C3B-C2B-C1B	-3.95	102.40	107.16
24	A	406	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
24	a	2110	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
24	d	404	CLA	CHD-C1D-ND	-3.94	120.83	124.45
24	B	612	CLA	CAC-C3C-C4C	3.94	129.92	124.81
24	A	406	CLA	C3B-C2B-C1B	-3.94	102.41	107.16
24	c	515	CLA	C1-C2-C3	-3.93	119.25	126.04
24	B	614	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
24	c	506	CLA	C3D-C4D-ND	3.92	116.59	110.24
26	b	620	BCR	C33-C5-C6	-3.92	120.12	124.53
24	B	616	CLA	C3D-C4D-ND	3.92	116.58	110.24
39	d	408	LHG	O8-C23-C24	3.92	124.20	111.91
27	A	411	SQD	O9-S-C6	3.92	111.60	106.94
24	A	405	CLA	C3D-C2D-C1D	-3.92	100.48	105.83
24	B	614	CLA	C2C-C1C-NC	3.92	113.64	109.97
24	b	604	CLA	CHD-C4C-C3C	-3.91	119.09	124.84
24	d	401	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
27	a	2102	SQD	O8-S-C6	3.91	111.97	105.74
24	c	512	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
24	c	510	CLA	C1-C2-C3	-3.91	119.29	126.04
36	B	628	HTG	C1-O5-C5	3.91	119.78	112.58
24	c	510	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
24	C	508	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
24	c	507	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
24	b	616	CLA	C2C-C1C-NC	3.90	113.62	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	405	CLA	C2C-C1C-NC	3.90	113.62	109.97
24	B	610	CLA	C3D-C4D-ND	3.89	116.53	110.24
24	A	409	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
24	b	604	CLA	C4-C3-C5	3.89	121.81	115.27
24	c	503	CLA	CHD-C4C-C3C	-3.89	119.13	124.84
26	Y	302	BCR	C38-C26-C25	-3.88	120.17	124.53
24	b	604	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
24	b	619	CLA	C4C-C3C-C2C	-3.88	101.24	106.90
24	b	611	CLA	C3B-C2B-C1B	-3.88	102.48	107.16
24	b	604	CLA	C3D-C4D-ND	3.88	116.51	110.24
24	B	608	CLA	C2C-C1C-NC	3.88	113.60	109.97
24	c	506	CLA	C2C-C1C-NC	3.87	113.60	109.97
24	B	614	CLA	C3D-C4D-ND	3.87	116.50	110.24
24	B	612	CLA	C3D-C4D-ND	3.87	116.49	110.24
26	c	516	BCR	C16-C17-C18	-3.87	121.79	127.31
24	c	511	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
24	A	409	CLA	C3D-C4D-ND	3.86	116.49	110.24
24	b	606	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
24	c	515	CLA	C3D-C4D-ND	3.86	116.48	110.24
24	b	607	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
24	B	615	CLA	C4-C3-C5	3.85	121.75	115.27
24	B	605	CLA	C3B-C2B-C1B	-3.85	102.51	107.16
24	A	406	CLA	CHD-C4C-C3C	-3.85	119.18	124.84
24	b	617	CLA	C3D-C4D-ND	3.85	116.46	110.24
27	A	411	SQD	C1-C2-C3	-3.84	101.99	110.00
24	C	505	CLA	C2C-C1C-NC	3.84	113.57	109.97
24	B	603	CLA	C2C-C1C-NC	3.84	113.56	109.97
24	B	615	CLA	C3D-C4D-ND	3.83	116.44	110.24
36	b	602	HTG	O5-C1-C2	3.83	115.13	110.31
26	d	406	BCR	C7-C8-C9	-3.82	120.46	126.23
24	A	409	CLA	O2D-CGD-CBD	3.82	118.06	111.27
24	c	508	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
24	c	505	CLA	C4A-NA-C1A	3.82	108.42	106.71
24	C	511	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
24	B	607	CLA	CHD-C4C-C3C	-3.81	119.23	124.84
24	C	514	CLA	C1-C2-C3	-3.81	119.45	126.04
24	B	611	CLA	C3B-C2B-C1B	-3.81	102.56	107.16
24	c	508	CLA	C3B-C2B-C1B	-3.81	102.56	107.16
24	c	512	CLA	CHD-C4C-C3C	-3.81	119.25	124.84
24	c	511	CLA	C3B-C2B-C1B	-3.81	102.57	107.16
24	b	607	CLA	CHC-C4B-NB	3.80	128.28	124.26
24	B	605	CLA	C3D-C4D-ND	3.80	116.39	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	2109	CLA	CAA-C2A-C1A	-3.80	99.51	111.97
24	C	513	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
24	D	405	CLA	CHD-C1D-ND	-3.80	120.96	124.45
24	B	614	CLA	CHD-C1D-ND	-3.80	120.97	124.45
24	b	605	CLA	C3D-C4D-ND	3.79	116.38	110.24
24	b	616	CLA	O2D-CGD-CBD	3.79	118.01	111.27
24	A	405	CLA	CAA-C2A-C3A	-3.79	102.40	112.78
24	b	610	CLA	C3D-C4D-ND	3.79	116.36	110.24
24	B	608	CLA	C3B-C2B-C1B	-3.79	102.59	107.16
26	a	2114	BCR	C33-C5-C6	-3.78	120.28	124.53
24	b	611	CLA	C2C-C1C-NC	3.78	113.52	109.97
24	c	503	CLA	C3B-C2B-C1B	-3.78	102.60	107.16
24	B	617	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
24	C	507	CLA	C3B-C2B-C1B	-3.78	102.60	107.16
24	C	506	CLA	C2C-C1C-NC	3.78	113.51	109.97
28	b	623	LMG	O7-C10-C11	3.78	119.64	111.50
31	A	417	PL9	C27-C28-C29	-3.78	118.57	127.66
24	B	613	CLA	O2D-CGD-O1D	-3.77	116.46	123.84
24	d	401	CLA	O2D-CGD-CBD	3.77	117.97	111.27
29	A	420	LMT	O1B-C4'-C3'	3.77	117.32	107.28
24	B	608	CLA	CAA-C2A-C3A	-3.77	102.45	112.78
24	c	507	CLA	C3D-C4D-ND	3.77	116.34	110.24
26	t	102	BCR	C15-C16-C17	-3.77	115.75	123.47
24	b	612	CLA	C3D-C4D-ND	3.77	116.33	110.24
24	c	514	CLA	C1-O2A-CGA	3.77	126.33	116.44
24	B	606	CLA	C3C-C4C-NC	3.77	114.80	110.57
27	a	2115	SQD	O8-S-C6	3.77	111.74	105.74
41	H	101	RRX	C24-C23-C22	-3.76	120.55	126.23
24	C	510	CLA	C3D-C4D-ND	3.75	116.31	110.24
24	b	614	CLA	C3D-C4D-ND	3.75	116.31	110.24
24	b	611	CLA	CHD-C4C-C3C	-3.75	119.33	124.84
24	B	617	CLA	C1D-CHD-C4C	-3.75	117.98	126.06
24	B	607	CLA	C2C-C1C-NC	3.74	113.48	109.97
27	A	411	SQD	O47-C7-C8	3.74	119.56	111.50
24	c	509	CLA	CMB-C2B-C1B	3.74	131.06	125.37
24	b	605	CLA	C2C-C1C-NC	3.74	113.47	109.97
24	d	401	CLA	CHD-C1D-ND	-3.73	121.02	124.45
24	b	616	CLA	C3D-C4D-ND	3.73	116.28	110.24
24	C	513	CLA	CBC-CAC-C3C	-3.73	102.15	112.43
24	C	512	CLA	CHD-C1D-ND	-3.73	121.03	124.45
24	B	612	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
24	b	613	CLA	C3D-C4D-ND	3.73	116.27	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	CMA-C3A-C4A	-3.73	101.75	111.77
24	B	602	CLA	C3D-C4D-ND	3.73	116.27	110.24
24	A	406	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
24	C	513	CLA	C1-C2-C3	-3.73	119.60	126.04
24	b	614	CLA	C2C-C1C-NC	3.72	113.46	109.97
24	A	405	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
24	d	404	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
24	C	503	CLA	C3D-C4D-ND	3.72	116.25	110.24
24	a	2110	CLA	C3C-C4C-NC	3.71	114.74	110.57
24	B	608	CLA	CBC-CAC-C3C	-3.71	102.19	112.43
24	c	503	CLA	C2C-C1C-NC	3.71	113.45	109.97
24	A	409	CLA	CMA-C3A-C4A	-3.71	101.80	111.77
24	C	504	CLA	O2D-CGD-CBD	3.71	117.86	111.27
27	B	621	SQD	O7-S-C6	3.71	111.34	106.94
24	C	503	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
24	c	508	CLA	O2D-CGD-CBD	3.71	117.86	111.27
24	d	401	CLA	CAA-C2A-C3A	-3.71	102.63	112.78
24	C	507	CLA	C3D-C4D-ND	3.70	116.22	110.24
38	C	518	DGD	O2G-C1B-C2B	3.70	119.47	111.50
32	a	2118[B]	K2I	C3-C4-C5	-3.70	120.09	123.61
24	b	609	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
24	c	507	CLA	C3D-C2D-C1D	-3.69	100.79	105.83
24	a	2109	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
24	b	606	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
24	c	514	CLA	C3D-C4D-ND	3.69	116.20	110.24
24	B	611	CLA	C3C-C4C-NC	3.68	114.70	110.57
24	D	404	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
24	D	405	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
24	a	2113	CLA	C3C-C4C-NC	3.67	114.69	110.57
24	c	513	CLA	C3D-C4D-ND	3.67	116.17	110.24
24	A	406	CLA	C2C-C1C-NC	3.67	113.41	109.97
24	b	617	CLA	O2D-CGD-O1D	-3.66	116.67	123.84
24	b	612	CLA	CHD-C1D-ND	-3.66	121.09	124.45
32	a	2118[A]	K2I	C-C1-C2	-3.66	120.12	123.61
24	c	505	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	C	511	CLA	C3B-C2B-C1B	-3.66	102.74	107.16
28	C	520	LMG	O8-C28-C29	3.66	123.39	111.91
24	b	608	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
24	B	606	CLA	CHD-C1D-ND	-3.64	121.11	124.45
24	B	617	CLA	CBC-CAC-C3C	-3.64	102.40	112.43
24	D	404	CLA	C1-C2-C3	-3.64	119.75	126.04
24	c	509	CLA	CHC-C4B-NB	3.64	128.11	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	405	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	C	513	CLA	C3D-C4D-ND	3.63	116.12	110.24
24	A	405	CLA	C3B-C2B-C1B	-3.63	102.77	107.16
25	A	407	PHO	CBC-CAC-C3C	-3.63	107.56	112.88
24	B	602	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
24	c	514	CLA	CBC-CAC-C3C	-3.63	102.43	112.43
24	B	615	CLA	C1D-CHD-C4C	-3.63	118.24	126.06
24	a	2109	CLA	C3C-C4C-NC	3.62	114.64	110.57
24	c	509	CLA	C3D-C4D-ND	3.62	116.10	110.24
24	c	508	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
31	x	801	PL9	C27-C28-C29	-3.62	118.95	127.66
24	C	513	CLA	CHD-C1D-ND	-3.62	121.13	124.45
24	b	618	CLA	C3D-C4D-ND	3.62	116.09	110.24
25	a	2111	PHO	O1D-CGD-CBD	-3.62	118.72	124.74
24	b	619	CLA	C3B-C4B-NB	3.62	113.87	110.52
26	c	517	BCR	C33-C5-C6	-3.61	120.47	124.53
26	c	517	BCR	C38-C26-C25	-3.61	120.47	124.53
24	c	513	CLA	O2D-CGD-CBD	3.61	117.69	111.27
24	b	619	CLA	C3D-C4D-ND	3.61	116.08	110.24
24	B	612	CLA	C2C-C1C-NC	3.61	113.36	109.97
24	B	610	CLA	CHD-C4C-C3C	-3.61	119.53	124.84
24	b	616	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	c	507	CLA	C3C-C4C-NC	3.61	114.61	110.57
24	B	616	CLA	C2C-C1C-NC	3.60	113.34	109.97
25	a	2112	PHO	O2D-CGD-O1D	-3.60	116.80	123.84
24	c	505	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
24	c	505	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	A	405	CLA	O2D-CGD-CBD	3.59	117.65	111.27
24	A	406	CLA	C4-C3-C5	3.59	121.31	115.27
24	C	513	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
24	c	504	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
26	b	622	BCR	C38-C26-C25	-3.59	120.50	124.53
24	B	608	CLA	C3D-C4D-ND	3.59	116.04	110.24
32	A	418[B]	K2I	BR-C4-C5	3.58	120.32	116.03
24	B	612	CLA	CMC-C2C-C1C	3.58	130.49	125.04
38	h	703	DGD	O2G-C1B-C2B	3.58	119.22	111.50
24	b	618	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
29	b	624	LMT	O5'-C5'-C4'	3.58	117.29	109.75
24	c	507	CLA	C1-O2A-CGA	3.58	125.83	116.44
36	B	624	HTG	C1'-S1-C1	3.58	106.78	100.09
24	c	509	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
26	c	517	BCR	C7-C8-C9	-3.57	120.84	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
24	c	508	CLA	CBC-CAC-C3C	-3.57	102.59	112.43
24	c	513	CLA	C1-O2A-CGA	3.57	125.81	116.44
24	d	401	CLA	C3C-C4C-NC	3.56	114.57	110.57
24	a	2110	CLA	C4-C3-C5	3.56	121.26	115.27
24	b	605	CLA	CHD-C1D-ND	-3.56	121.18	124.45
24	c	512	CLA	C3D-C2D-C1D	-3.56	100.97	105.83
24	b	612	CLA	CMB-C2B-C1B	3.56	130.79	125.37
24	C	506	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
24	C	514	CLA	CHD-C4C-C3C	-3.55	119.62	124.84
26	C	515	BCR	C7-C8-C9	-3.55	120.87	126.23
24	C	511	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
24	B	610	CLA	C3B-C2B-C1B	-3.55	102.88	107.16
24	B	609	CLA	C2C-C1C-NC	3.55	113.30	109.97
24	b	611	CLA	C1D-CHD-C4C	-3.55	118.41	126.06
24	b	605	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
26	C	516	BCR	C33-C5-C6	-3.54	120.55	124.53
24	b	615	CLA	C1-C2-C3	-3.54	119.92	126.04
36	I	1202	HTG	C1-O5-C5	3.54	119.11	112.58
25	A	408	PHO	C1A-C2A-C3A	-3.54	99.47	102.84
24	B	607	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
24	b	610	CLA	CBC-CAC-C3C	-3.54	102.68	112.43
24	B	602	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
24	c	511	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
24	B	604	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
24	b	611	CLA	C3C-C4C-NC	3.53	114.53	110.57
24	C	502	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
24	c	514	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
24	b	616	CLA	CHD-C1D-ND	-3.53	121.21	124.45
24	C	507	CLA	CBC-CAC-C3C	-3.53	102.71	112.43
24	c	503	CLA	CMC-C2C-C1C	3.52	130.41	125.04
24	a	2109	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
24	C	514	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
28	c	521	LMG	O7-C10-C11	3.52	119.08	111.50
27	a	2115	SQD	O9-S-C6	3.51	111.12	106.94
26	T	101	BCR	C7-C8-C9	-3.51	120.93	126.23
24	C	502	CLA	C3B-C2B-C1B	-3.51	102.93	107.16
24	C	503	CLA	CHD-C4C-C3C	-3.51	119.69	124.84
24	B	611	CLA	C3D-C4D-ND	3.51	115.91	110.24
24	c	510	CLA	CAA-C2A-C3A	-3.51	103.18	112.78
24	c	504	CLA	C3C-C4C-NC	3.51	114.50	110.57
24	c	512	CLA	C2C-C1C-NC	3.50	113.25	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	508	CLA	CHD-C4C-C3C	-3.50	119.70	124.84
36	b	625	HTG	C6-C5-C4	-3.50	104.81	113.00
24	C	508	CLA	C1-C2-C3	-3.50	120.00	126.04
24	A	406	CLA	CMB-C2B-C1B	3.50	130.69	125.37
24	B	611	CLA	CMB-C2B-C1B	3.50	130.69	125.37
26	B	618	BCR	C24-C23-C22	-3.50	120.95	126.23
24	b	617	CLA	CHD-C4C-C3C	-3.50	119.70	124.84
27	a	2115	SQD	C1-O5-C5	-3.50	106.83	113.69
24	c	511	CLA	C2C-C1C-NC	3.49	113.24	109.97
24	B	609	CLA	CAC-C3C-C4C	3.49	129.34	124.81
24	c	503	CLA	CBC-CAC-C3C	-3.49	102.81	112.43
24	a	2113	CLA	CBC-CAC-C3C	-3.49	102.81	112.43
39	d	408	LHG	O8-C23-O10	-3.49	114.78	123.59
24	b	608	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
43	V	201	HEC	C4B-NB-C1B	3.49	108.67	105.07
24	b	618	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
24	B	609	CLA	C3C-C4C-NC	3.48	114.48	110.57
24	b	615	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
24	c	506	CLA	CBC-CAC-C3C	-3.48	102.84	112.43
24	c	513	CLA	CHD-C1D-ND	-3.48	121.26	124.45
24	b	604	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
25	A	407	PHO	C1A-C2A-C3A	-3.48	99.53	102.84
24	B	603	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
24	B	611	CLA	C2C-C1C-NC	3.48	113.23	109.97
24	c	504	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
24	b	617	CLA	CBC-CAC-C3C	-3.47	102.85	112.43
24	C	503	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
31	x	801	PL9	C32-C33-C34	-3.47	119.30	127.66
24	B	611	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
24	b	615	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
24	b	607	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
24	C	506	CLA	C3C-C4C-NC	3.47	114.46	110.57
24	c	511	CLA	C3D-C4D-ND	3.47	115.85	110.24
24	c	508	CLA	C4-C3-C5	3.47	121.10	115.27
24	B	610	CLA	C3C-C4C-NC	3.47	114.46	110.57
24	B	610	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
24	c	514	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
24	B	613	CLA	C4-C3-C5	3.46	121.09	115.27
24	b	609	CLA	C3D-C4D-ND	3.46	115.84	110.24
24	B	606	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
29	j	1601	LMT	C1'-C2'-C3'	3.46	117.20	110.00
24	D	401	CLA	C3B-C4B-NB	3.46	113.72	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	511	CLA	C3C-C4C-NC	3.46	114.45	110.57
24	b	616	CLA	C3C-C4C-NC	3.46	114.45	110.57
24	C	502	CLA	C2C-C1C-NC	3.45	113.21	109.97
24	b	617	CLA	CHD-C1D-ND	-3.45	121.28	124.45
28	d	411	LMG	O7-C10-C11	3.45	118.94	111.50
24	C	502	CLA	CMB-C2B-C1B	3.45	130.63	125.37
24	C	506	CLA	C3D-C2D-C1D	-3.45	101.12	105.83
24	b	614	CLA	CAC-C3C-C4C	3.45	129.29	124.81
24	B	611	CLA	O2A-C1-C2	3.45	117.69	108.64
24	C	506	CLA	CAC-C3C-C4C	3.45	129.28	124.81
24	c	510	CLA	C2C-C1C-NC	3.45	113.20	109.97
24	B	617	CLA	O2D-CGD-O1D	-3.44	117.10	123.84
24	B	617	CLA	C3D-C4D-ND	3.44	115.81	110.24
25	A	408	PHO	C4-C3-C5	3.44	121.06	115.27
27	F	101	SQD	O7-S-C6	3.44	111.03	106.94
24	b	606	CLA	O2A-CGA-O1A	-3.44	114.92	123.59
24	d	401	CLA	C3B-C4B-NB	3.44	113.70	110.52
24	C	505	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
24	C	502	CLA	C1D-CHD-C4C	-3.44	118.65	126.06
24	B	610	CLA	C1-C2-C3	-3.44	120.10	126.04
24	b	615	CLA	C2C-C1C-NC	3.44	113.19	109.97
24	C	502	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
24	c	513	CLA	C2C-C1C-NC	3.43	113.19	109.97
29	A	414	LMT	C1'-O5'-C5'	3.43	120.43	113.69
24	B	616	CLA	CMB-C2B-C1B	3.43	130.60	125.37
24	a	2109	CLA	CAA-C2A-C3A	-3.43	103.38	112.78
24	B	612	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
24	D	405	CLA	C4-C3-C5	3.42	121.03	115.27
24	b	619	CLA	C2C-C1C-NC	3.42	113.18	109.97
24	c	512	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
27	F	101	SQD	O9-S-C6	3.42	111.00	106.94
24	C	504	CLA	C2C-C1C-NC	3.42	113.17	109.97
24	C	512	CLA	C2C-C1C-NC	3.42	113.17	109.97
24	C	512	CLA	CAC-C3C-C4C	3.42	129.24	124.81
24	c	504	CLA	C2C-C1C-NC	3.41	113.17	109.97
29	a	2103	LMT	C1'-O5'-C5'	3.41	120.39	113.69
24	C	508	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
24	c	504	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
24	c	513	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
24	c	513	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
24	B	607	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	c	515	CLA	C2C-C1C-NC	3.40	113.16	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
24	B	603	CLA	CHD-C1D-ND	-3.40	121.33	124.45
24	c	511	CLA	CHD-C4C-C3C	-3.40	119.84	124.84
24	c	511	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
24	C	507	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	B	617	CLA	CMB-C2B-C1B	3.40	130.55	125.37
24	c	506	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	b	610	CLA	C2C-C1C-NC	3.40	113.15	109.97
24	b	611	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
24	b	618	CLA	O2D-CGD-CBD	3.39	117.30	111.27
24	b	605	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
24	B	610	CLA	CMB-C2B-C1B	3.39	130.53	125.37
24	B	603	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
24	B	607	CLA	C3D-C4D-ND	3.39	115.72	110.24
41	H	101	RRX	C16-C17-C18	-3.39	122.47	127.31
32	A	418[A]	K2I	BR1-C1-C2	3.39	120.08	116.03
24	B	606	CLA	CMB-C2B-C1B	3.39	130.53	125.37
24	B	611	CLA	CAA-C2A-C3A	-3.38	103.51	112.78
24	D	404	CLA	C3B-C2B-C1B	-3.38	103.08	107.16
24	B	617	CLA	C3C-C4C-NC	3.38	114.36	110.57
24	C	504	CLA	C4A-NA-C1A	3.38	108.23	106.71
24	b	606	CLA	O2A-CGA-CBA	3.38	122.52	111.91
24	b	617	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
24	C	508	CLA	C3C-C4C-NC	3.37	114.36	110.57
31	A	417	PL9	C12-C13-C14	-3.37	119.54	127.66
38	C	518	DGD	O1G-C1A-C2A	3.37	122.49	111.91
24	B	606	CLA	C4-C3-C5	3.37	120.94	115.27
24	B	616	CLA	C3C-C4C-NC	3.37	114.35	110.57
24	A	406	CLA	CBC-CAC-C3C	-3.37	103.15	112.43
24	c	507	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
24	B	603	CLA	CHD-C4C-C3C	-3.37	119.89	124.84
24	b	606	CLA	CHD-C4C-C3C	-3.36	119.89	124.84
24	c	511	CLA	C4A-NA-C1A	3.36	108.22	106.71
32	a	2118[B]	K2I	C-C1-C2	-3.36	120.41	123.61
24	C	512	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
24	A	409	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
24	c	512	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
24	A	405	CLA	C3C-C4C-NC	3.36	114.33	110.57
24	C	512	CLA	C3D-C4D-ND	3.35	115.66	110.24
31	x	801	PL9	C37-C38-C39	-3.35	119.59	127.66
24	b	617	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
39	l	101	LHG	O7-C7-C8	3.35	118.72	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	CHD-C4C-C3C	-3.35	119.92	124.84
24	c	505	CLA	CHA-C1A-NA	-3.35	118.73	126.40
24	C	507	CLA	C3C-C4C-NC	3.35	114.32	110.57
24	b	615	CLA	O2A-CGA-CBA	3.35	122.41	111.91
24	C	506	CLA	C3D-C4D-ND	3.34	115.65	110.24
24	b	609	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
24	a	2113	CLA	C1D-CHD-C4C	-3.34	118.84	126.06
24	b	617	CLA	C2C-C1C-NC	3.34	113.10	109.97
24	b	614	CLA	C3C-C4C-NC	3.34	114.32	110.57
24	c	515	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
24	C	504	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
24	B	609	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	c	515	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
24	B	606	CLA	CMC-C2C-C1C	3.33	130.11	125.04
24	b	618	CLA	C2C-C1C-NC	3.33	113.09	109.97
24	c	505	CLA	O2D-CGD-CBD	3.33	117.18	111.27
38	c	518	DGD	C2G-O2G-C1B	-3.32	109.61	117.79
24	C	506	CLA	CHA-C1A-NA	-3.32	118.79	126.40
24	c	508	CLA	CAA-C2A-C3A	-3.32	103.68	112.78
24	C	506	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
27	B	621	SQD	C4-C3-C2	-3.32	105.02	110.82
24	B	612	CLA	CHD-C1D-ND	-3.32	121.40	124.45
24	c	509	CLA	CHD-C4C-C3C	-3.32	119.96	124.84
24	B	616	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
24	A	409	CLA	C1-C2-C3	-3.32	120.31	126.04
27	A	413	SQD	O48-C23-C24	3.32	122.32	111.91
24	B	603	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
24	B	616	CLA	C11-C10-C8	-3.31	105.22	115.92
24	b	608	CLA	C3C-C4C-NC	3.31	114.28	110.57
39	D	409	LHG	C5-O7-C7	-3.31	109.65	117.79
32	A	418[B]	K2I	C-C1-C2	-3.31	120.46	123.61
24	C	509	CLA	CHD-C4C-C3C	-3.31	119.98	124.84
24	b	604	CLA	C2C-C1C-NC	3.30	113.07	109.97
24	b	609	CLA	C2C-C1C-NC	3.30	113.07	109.97
24	b	614	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
31	x	801	PL9	C22-C23-C24	-3.30	119.71	127.66
24	B	613	CLA	CMC-C2C-C1C	3.30	130.07	125.04
24	B	617	CLA	C4-C3-C5	3.30	120.83	115.27
24	B	608	CLA	CHD-C1D-ND	-3.30	121.42	124.45
24	b	619	CLA	O2A-CGA-CBA	3.30	122.27	111.91
31	D	407	PL9	C25-C24-C26	3.30	120.82	115.27
25	a	2112	PHO	CMB-C2B-C3B	3.30	130.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	m	103	LMT	C1'-O5'-C5'	3.30	120.16	113.69
24	c	510	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
24	B	604	CLA	O2A-CGA-CBA	3.29	122.25	111.91
32	A	418[B]	K2I	C3-C4-C5	-3.29	120.47	123.61
24	C	514	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
24	b	607	CLA	CMC-C2C-C1C	3.29	130.05	125.04
24	B	610	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
24	B	611	CLA	O2D-CGD-O1D	-3.29	117.42	123.84
24	b	619	CLA	CAC-C3C-C4C	3.28	129.07	124.81
24	B	604	CLA	CHD-C4C-C3C	-3.28	120.01	124.84
24	c	507	CLA	CHD-C4C-C3C	-3.28	120.01	124.84
24	b	604	CLA	C1-O2A-CGA	3.28	125.06	116.44
24	c	515	CLA	C3C-C4C-NC	3.28	114.25	110.57
26	C	515	BCR	C11-C10-C9	-3.28	122.63	127.31
24	C	512	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
24	C	512	CLA	C3C-C4C-NC	3.27	114.24	110.57
24	b	615	CLA	C4-C3-C5	3.27	120.77	115.27
24	c	514	CLA	CHD-C4C-C3C	-3.27	120.04	124.84
24	c	513	CLA	C4A-NA-C1A	3.27	108.17	106.71
24	C	502	CLA	CHD-C4C-C3C	-3.26	120.04	124.84
24	B	613	CLA	C3C-C4C-NC	3.26	114.23	110.57
27	a	2115	SQD	O48-C23-C24	3.26	122.14	111.91
36	b	625	HTG	C1-C2-C3	3.26	117.02	110.59
24	C	511	CLA	C1-C2-C3	-3.26	120.41	126.04
24	b	615	CLA	CMC-C2C-C1C	3.26	130.00	125.04
24	b	618	CLA	CMB-C2B-C1B	3.25	130.32	125.37
24	c	510	CLA	C4-C3-C5	3.25	120.74	115.27
39	d	409	LHG	O8-C23-O10	-3.25	115.38	123.59
43	v	201	HEC	CMD-C2D-C1D	3.25	129.99	125.04
24	D	401	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
24	B	613	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
26	C	515	BCR	C38-C26-C25	-3.25	120.88	124.53
24	b	614	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
27	a	2102	SQD	O48-C23-C24	3.24	122.09	111.91
32	a	2118[A]	K2I	BR-C4-C5	3.24	119.91	116.03
24	b	612	CLA	CHD-C4C-C3C	-3.24	120.08	124.84
24	C	509	CLA	C2C-C1C-NC	3.24	113.01	109.97
26	A	410	BCR	C38-C26-C25	-3.24	120.89	124.53
24	B	616	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
24	B	607	CLA	C3C-C4C-NC	3.24	114.20	110.57
24	c	505	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
24	D	405	CLA	CHD-C4C-C3C	-3.23	120.08	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	605	CLA	C1D-CHD-C4C	-3.23	119.08	126.06
24	B	614	CLA	CMA-C3A-C4A	-3.23	103.08	111.77
24	b	613	CLA	C1D-CHD-C4C	-3.23	119.08	126.06
24	B	606	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
24	B	609	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
27	a	2115	SQD	C44-O6-C1	-3.23	107.43	113.74
24	c	509	CLA	CBC-CAC-C3C	-3.23	103.53	112.43
24	A	405	CLA	CAA-C2A-C1A	-3.23	101.40	111.97
24	b	607	CLA	CMB-C2B-C1B	3.23	130.28	125.37
31	A	417	PL9	C17-C18-C19	-3.23	119.89	127.66
39	D	409	LHG	O7-C7-C8	3.22	118.45	111.50
24	A	406	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
24	B	615	CLA	C3B-C4B-NB	3.22	113.50	110.52
24	d	404	CLA	C3C-C4C-NC	3.22	114.18	110.57
25	a	2112	PHO	C1A-C2A-C3A	-3.22	99.78	102.84
24	a	2110	CLA	O2A-CGA-O1A	-3.22	115.47	123.59
24	c	511	CLA	C1-C2-C3	-3.22	120.48	126.04
31	d	407	PL9	C42-C43-C44	-3.22	119.92	127.66
24	b	614	CLA	CHD-C4C-C3C	-3.22	120.11	124.84
28	C	526	LMG	C9-C8-C7	-3.22	104.18	111.79
24	B	610	CLA	C2C-C1C-NC	3.21	112.98	109.97
24	b	604	CLA	C1D-CHD-C4C	-3.21	119.12	126.06
24	c	505	CLA	CMB-C2B-C1B	3.21	130.26	125.37
24	C	509	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
40	F	102	HEM	C4A-NA-C1A	3.21	108.49	105.35
24	C	503	CLA	C3C-C4C-NC	3.21	114.17	110.57
38	c	520	DGD	O3G-C3G-C2G	-3.20	103.17	110.90
24	C	514	CLA	C2C-C1C-NC	3.20	112.97	109.97
24	b	616	CLA	CHD-C4C-C3C	-3.20	120.14	124.84
24	B	604	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
24	C	511	CLA	CBC-CAC-C3C	-3.20	103.61	112.43
24	C	512	CLA	O2D-CGD-CBD	3.20	116.95	111.27
24	a	2113	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
36	d	403	HTG	C1'-S1-C1	3.20	106.07	100.09
24	b	606	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
31	A	417	PL9	C20-C19-C21	3.19	120.64	115.27
24	D	405	CLA	C2C-C1C-NC	3.19	112.96	109.97
38	C	518	DGD	O1G-C1A-O1A	-3.19	115.54	123.59
24	c	511	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
24	b	604	CLA	CHD-C1D-ND	-3.19	121.52	124.45
24	B	604	CLA	O2A-CGA-O1A	-3.19	115.54	123.59
27	F	101	SQD	C1-C2-C3	-3.19	103.35	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	504	CLA	CHD-C1D-ND	-3.19	121.52	124.45
24	B	603	CLA	C3C-C4C-NC	3.19	114.15	110.57
24	b	613	CLA	C2C-C1C-NC	3.19	112.96	109.97
24	B	609	CLA	CHD-C4C-C3C	-3.19	120.16	124.84
24	b	608	CLA	C4-C3-C5	3.18	120.63	115.27
26	K	101	BCR	C33-C5-C6	-3.18	120.95	124.53
24	C	504	CLA	CBC-CAC-C3C	-3.18	103.66	112.43
24	c	515	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	c	504	CLA	O2A-CGA-CBA	3.18	121.89	111.91
24	b	605	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
24	b	614	CLA	C1-C2-C3	-3.18	120.55	126.04
24	B	604	CLA	C3C-C4C-NC	3.18	114.13	110.57
29	a	2120	LMT	C1'-O5'-C5'	3.18	119.92	113.69
24	D	404	CLA	C1D-CHD-C4C	-3.17	119.21	126.06
24	c	512	CLA	CBC-CAC-C3C	-3.17	103.68	112.43
24	C	503	CLA	CBC-CAC-C3C	-3.17	103.69	112.43
24	b	615	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
41	h	702	RRX	C11-C10-C9	-3.17	122.78	127.31
24	b	610	CLA	CHD-C4C-C3C	-3.17	120.18	124.84
24	C	510	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
24	C	513	CLA	C3C-C4C-NC	3.17	114.12	110.57
24	B	607	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
29	J	102	LMT	C1'-O5'-C5'	3.16	119.90	113.69
24	a	2109	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
24	c	505	CLA	C1-C2-C3	-3.16	120.58	126.04
24	a	2109	CLA	O2A-CGA-CBA	3.16	121.82	111.91
24	B	606	CLA	C2C-C1C-NC	3.16	112.93	109.97
24	b	613	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
24	C	509	CLA	C3C-C4C-NC	3.15	114.11	110.57
24	b	614	CLA	CHD-C1D-ND	-3.15	121.56	124.45
24	C	512	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
24	b	616	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	B	611	CLA	O2A-CGA-CBA	3.15	121.79	111.91
24	C	502	CLA	CBC-CAC-C3C	-3.15	103.75	112.43
24	d	404	CLA	CHD-C4C-C3C	-3.14	120.23	124.84
24	b	607	CLA	C3D-C4D-ND	3.13	115.31	110.24
24	c	509	CLA	C4A-NA-C1A	3.13	108.11	106.71
24	A	406	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
24	a	2109	CLA	CHD-C1D-ND	-3.13	121.58	124.45
24	c	510	CLA	C3C-C4C-NC	3.13	114.08	110.57
24	b	607	CLA	C6-C5-C3	-3.13	105.25	113.45
24	c	503	CLA	C3C-C4C-NC	3.13	114.08	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	2110	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
26	Y	302	BCR	C15-C14-C13	-3.13	122.84	127.31
24	b	607	CLA	CHA-C1A-NA	-3.13	119.23	126.40
43	v	201	HEC	CBC-CAC-C3C	3.13	121.05	112.43
24	c	512	CLA	C6-C7-C8	-3.13	105.81	115.92
24	b	613	CLA	C3C-C4C-NC	3.13	114.08	110.57
24	B	616	CLA	CAC-C3C-C4C	3.12	128.86	124.81
24	C	513	CLA	C2C-C1C-NC	3.12	112.90	109.97
24	C	506	CLA	C1-C2-C3	-3.12	120.64	126.04
24	B	610	CLA	CAC-C3C-C4C	3.12	128.86	124.81
24	C	510	CLA	CHD-C4C-C3C	-3.12	120.25	124.84
36	C	521	HTG	C1'-S1-C1	3.12	105.93	100.09
24	b	611	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
39	L	101	LHG	O8-C23-C24	3.12	121.69	111.91
24	B	602	CLA	O2A-CGA-CBA	3.12	121.69	111.91
29	a	2103	LMT	C2'-C3'-C4'	-3.11	102.57	109.68
24	c	506	CLA	C4-C3-C5	3.11	120.50	115.27
24	C	502	CLA	CHD-C1D-ND	-3.11	121.59	124.45
26	K	101	BCR	C20-C21-C22	-3.11	122.87	127.31
24	c	508	CLA	C3C-C4C-NC	3.11	114.06	110.57
39	L	101	LHG	O7-C7-C8	3.11	118.20	111.50
24	B	611	CLA	CAA-CBA-CGA	-3.11	104.17	113.25
24	B	614	CLA	C3C-C4C-NC	3.11	114.06	110.57
27	A	413	SQD	O8-S-C6	3.10	110.68	105.74
24	A	405	CLA	CHD-C4C-C3C	-3.10	120.29	124.84
24	D	404	CLA	CMC-C2C-C1C	3.10	129.76	125.04
24	c	507	CLA	CMC-C2C-C1C	3.10	129.76	125.04
24	a	2109	CLA	CAC-C3C-C4C	3.10	128.83	124.81
24	C	506	CLA	CHD-C4C-C3C	-3.10	120.29	124.84
39	d	410	LHG	O7-C7-C8	3.10	118.17	111.50
24	c	509	CLA	C4-C3-C5	3.09	120.48	115.27
39	D	409	LHG	O8-C23-O10	-3.09	115.79	123.59
24	C	504	CLA	CHD-C1D-ND	-3.09	121.61	124.45
24	B	602	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
24	c	509	CLA	C3C-C4C-NC	3.09	114.03	110.57
24	a	2109	CLA	O2A-CGA-O1A	-3.09	115.80	123.59
24	B	604	CLA	CHD-C1D-ND	-3.09	121.62	124.45
29	m	102	LMT	O1'-C1'-C2'	3.09	113.12	108.30
38	D	408	DGD	O1G-C1A-C2A	3.08	121.59	111.91
24	d	405	CLA	CHD-C4C-C3C	-3.08	120.31	124.84
24	b	615	CLA	CHD-C1D-ND	-3.08	121.62	124.45
24	C	514	CLA	C4C-C3C-C2C	-3.08	102.41	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	406	CLA	C1-C2-C3	-3.08	120.71	126.04
27	A	411	SQD	O8-S-C6	3.08	110.65	105.74
38	C	517	DGD	O3G-C3G-C2G	-3.08	103.47	110.90
24	B	609	CLA	C1C-C2C-C3C	-3.07	103.72	106.96
26	b	620	BCR	C24-C23-C22	-3.07	121.59	126.23
24	c	504	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
26	k	2003	BCR	C33-C5-C6	-3.07	121.08	124.53
24	B	611	CLA	CAC-C3C-C4C	3.07	128.79	124.81
24	B	609	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	a	2110	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
24	C	504	CLA	C3D-C4D-ND	3.06	115.19	110.24
24	b	610	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
24	c	512	CLA	C3B-C4B-NB	3.06	113.36	110.52
24	B	613	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
24	C	512	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
29	a	2120	LMT	C1B-O5B-C5B	3.06	119.70	113.69
24	B	612	CLA	C3C-C4C-NC	3.06	114.00	110.57
24	C	507	CLA	CHD-C4C-C3C	-3.06	120.34	124.84
36	I	1202	HTG	O5-C1-C2	3.06	114.16	110.31
24	C	511	CLA	C4-C3-C5	3.06	120.42	115.27
24	B	614	CLA	CBC-CAC-C3C	-3.06	104.00	112.43
29	M	101	LMT	C1'-O5'-C5'	-3.06	107.68	113.69
24	b	611	CLA	O2A-CGA-CBA	3.06	121.50	111.91
24	B	606	CLA	CAC-C3C-C4C	3.06	128.78	124.81
24	b	605	CLA	CBC-CAC-C3C	-3.06	104.00	112.43
24	c	507	CLA	CHA-C1A-NA	-3.06	119.40	126.40
43	V	201	HEC	CBC-CAC-C3C	3.06	120.85	112.43
24	B	604	CLA	CMC-C2C-C1C	3.05	129.69	125.04
24	b	608	CLA	CMC-C2C-C1C	3.05	129.69	125.04
24	C	504	CLA	CMB-C2B-C1B	3.05	130.02	125.37
24	B	613	CLA	C2C-C1C-NC	3.05	112.83	109.97
24	C	512	CLA	C4-C3-C5	3.05	120.40	115.27
24	a	2110	CLA	C1-C2-C3	-3.05	120.77	126.04
24	A	405	CLA	C3B-C4B-NB	3.05	113.34	110.52
24	D	404	CLA	CHC-C4B-NB	3.05	127.48	124.26
36	B	627	HTG	C3-C4-C5	3.04	115.67	110.24
24	C	514	CLA	C3C-C4C-NC	3.04	113.98	110.57
38	C	519	DGD	O1G-C1A-C2A	3.04	121.45	111.91
24	d	401	CLA	CMA-C3A-C2A	-3.04	101.57	113.83
24	D	401	CLA	C3C-C4C-NC	3.04	113.98	110.57
24	C	511	CLA	C11-C10-C8	-3.04	106.09	115.92
24	B	611	CLA	C1D-CHD-C4C	-3.04	119.50	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	CMA-C3A-C4A	-3.04	103.61	111.77
24	a	2109	CLA	CHD-C4C-C3C	-3.04	120.37	124.84
40	e	103	HEM	C4C-NC-C1C	3.03	108.32	105.35
24	b	614	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	B	605	CLA	CAC-C3C-C4C	3.03	128.74	124.81
24	c	515	CLA	CHD-C4C-C3C	-3.03	120.39	124.84
24	B	611	CLA	CHD-C1D-ND	-3.03	121.67	124.45
24	b	610	CLA	C1D-CHD-C4C	-3.03	119.53	126.06
24	b	613	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
29	f	101	LMT	O1'-C1'-C2'	3.03	113.03	108.30
24	a	2113	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
24	a	2113	CLA	C3B-C4B-NB	3.02	113.32	110.52
24	D	401	CLA	C1D-CHD-C4C	-3.02	119.54	126.06
39	D	409	LHG	O8-C23-C24	3.02	121.39	111.91
24	B	603	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	C	509	CLA	CHD-C1D-ND	-3.02	121.68	124.45
24	d	405	CLA	CMC-C2C-C1C	3.02	129.63	125.04
24	A	409	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
24	C	511	CLA	CHD-C1D-ND	-3.01	121.69	124.45
24	C	506	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
38	c	519	DGD	C3B-C2B-C1B	-3.01	102.68	113.62
24	B	607	CLA	CHC-C4B-NB	3.01	127.44	124.26
24	b	607	CLA	C3C-C4C-NC	3.01	113.94	110.57
24	B	617	CLA	CHD-C1D-ND	-3.00	121.69	124.45
24	d	405	CLA	CAC-C3C-C4C	3.00	128.71	124.81
24	B	610	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
24	b	607	CLA	C4A-NA-C1A	3.00	108.05	106.71
24	b	618	CLA	C4-C3-C5	3.00	120.31	115.27
24	B	614	CLA	C1D-CHD-C4C	-3.00	119.59	126.06
24	d	404	CLA	C4-C3-C5	2.99	120.31	115.27
24	C	504	CLA	CMC-C2C-C1C	2.99	129.60	125.04
24	B	607	CLA	CBC-CAC-C3C	-2.99	104.18	112.43
24	c	510	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
24	C	508	CLA	C3D-C4D-ND	2.99	115.08	110.24
24	A	405	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
38	h	703	DGD	O1G-C1A-C2A	2.99	121.30	111.91
24	c	508	CLA	C3B-C4B-NB	2.99	113.29	110.52
41	H	101	RRX	C7-C8-C9	-2.99	121.72	126.23
24	B	605	CLA	O2A-CGA-CBA	2.99	121.29	111.91
29	T	102	LMT	C1-O1'-C1'	-2.99	108.88	113.84
24	b	616	CLA	C3B-C4B-NB	2.99	113.28	110.52
38	H	102	DGD	O1G-C1A-C2A	2.98	121.27	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	404	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	B	607	CLA	C4-C3-C5	2.98	120.29	115.27
24	c	507	CLA	CBC-CAC-C3C	-2.98	104.21	112.43
24	C	509	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	a	2112	PHO	C4-C3-C5	2.98	120.28	115.27
24	c	512	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
26	t	102	BCR	C3-C4-C5	-2.98	108.76	114.08
24	b	615	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
24	C	509	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
29	i	104	LMT	O5'-C1'-C2'	2.97	116.65	110.35
24	c	513	CLA	CBC-CAC-C3C	-2.97	104.23	112.43
24	c	504	CLA	O2A-CGA-O1A	-2.97	116.09	123.59
28	b	623	LMG	O8-C28-C29	2.97	121.23	111.91
24	b	617	CLA	C3C-C4C-NC	2.97	113.90	110.57
31	d	407	PL9	C40-C39-C41	2.97	120.26	115.27
24	c	513	CLA	O2A-CGA-CBA	2.97	121.22	111.91
24	b	612	CLA	C1-C2-C3	-2.97	120.91	126.04
24	c	508	CLA	CHD-C1D-ND	-2.97	121.73	124.45
24	B	605	CLA	C1D-CHD-C4C	-2.96	119.66	126.06
24	C	505	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
24	B	610	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
24	C	509	CLA	C1-C2-C3	-2.96	120.92	126.04
24	C	512	CLA	C1-C2-C3	-2.96	120.92	126.04
24	B	605	CLA	CMB-C2B-C1B	2.96	129.88	125.37
24	B	613	CLA	C3B-C4B-NB	2.96	113.26	110.52
24	B	608	CLA	CHD-C4C-C3C	-2.95	120.50	124.84
24	A	405	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
24	b	618	CLA	C1-O2A-CGA	2.95	124.19	116.44
24	B	606	CLA	O2A-CGA-O1A	-2.95	116.15	123.59
24	b	608	CLA	C1D-CHD-C4C	-2.94	119.71	126.06
24	b	607	CLA	C3B-C4B-NB	2.94	113.24	110.52
41	h	702	RRX	C16-C17-C18	-2.94	123.11	127.31
24	D	404	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	B	615	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	d	404	CLA	CMB-C2B-C1B	2.94	129.85	125.37
24	c	512	CLA	C3C-C4C-NC	2.94	113.87	110.57
24	b	605	CLA	CHD-C4C-C3C	-2.94	120.52	124.84
24	c	507	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
24	C	514	CLA	CBC-CAC-C3C	-2.93	104.34	112.43
24	b	614	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
24	B	602	CLA	CMB-C2B-C1B	2.93	129.84	125.37
39	D	411	LHG	O7-C7-C8	2.93	117.82	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	CLA	CAA-C2A-C3A	-2.93	104.75	112.78
24	b	609	CLA	C3C-C4C-NC	2.93	113.86	110.57
24	a	2110	CLA	CBC-CAC-C3C	-2.93	104.36	112.43
24	d	404	CLA	O2A-CGA-CBA	2.93	121.10	111.91
28	c	521	LMG	O8-C28-C29	2.93	121.10	111.91
27	F	101	SQD	C44-O6-C1	-2.93	108.02	113.74
24	b	612	CLA	C3B-C4B-NB	2.93	113.23	110.52
24	D	404	CLA	CBC-CAC-C3C	-2.93	104.37	112.43
24	C	512	CLA	CBC-CAC-C3C	-2.93	104.37	112.43
24	B	617	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	B	605	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
24	c	506	CLA	C3C-C4C-NC	2.92	113.85	110.57
38	C	518	DGD	O2G-C1B-O1B	-2.92	116.64	123.70
24	C	507	CLA	CMC-C2C-C1C	2.92	129.49	125.04
31	x	801	PL9	C35-C34-C36	2.92	120.19	115.27
26	K	101	BCR	C7-C8-C9	-2.92	121.82	126.23
31	D	407	PL9	C36-C37-C38	-2.92	102.29	111.88
26	D	406	BCR	C33-C5-C6	-2.92	121.25	124.53
24	b	607	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	A	405	CLA	CMA-C3A-C4A	-2.92	103.93	111.77
24	C	503	CLA	CHA-C1A-NA	-2.92	119.72	126.40
24	c	510	CLA	CHD-C1D-ND	-2.91	121.78	124.45
27	L	102	SQD	C4-C3-C2	2.91	115.91	110.82
24	C	512	CLA	CHA-C1A-NA	-2.91	119.73	126.40
24	b	609	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
31	D	407	PL9	C10-C9-C11	2.91	120.17	115.27
24	B	602	CLA	C3C-C4C-NC	2.91	113.83	110.57
24	C	505	CLA	CHD-C4C-C3C	-2.90	120.57	124.84
36	B	627	HTG	O5-C5-C4	2.90	114.97	109.69
24	B	611	CLA	C1C-C2C-C3C	-2.90	103.90	106.96
24	B	602	CLA	C1C-C2C-C3C	-2.90	103.90	106.96
26	Y	302	BCR	C37-C22-C23	2.90	122.65	118.08
24	D	405	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
32	a	2118[A]	K2I	BR1-C1-C2	2.90	119.50	116.03
31	d	407	PL9	C37-C38-C39	-2.90	120.68	127.66
24	B	617	CLA	C1-C2-C3	-2.90	121.03	126.04
24	C	503	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
24	B	615	CLA	C3C-C4C-NC	2.89	113.82	110.57
24	b	604	CLA	C3C-C4C-NC	2.89	113.82	110.57
24	C	508	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
24	b	605	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
24	b	609	CLA	O2A-CGA-O1A	-2.89	116.29	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
24	C	505	CLA	C4A-NA-C1A	2.89	108.00	106.71
26	T	101	BCR	C11-C10-C9	-2.89	123.19	127.31
24	C	507	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
24	b	604	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	c	508	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	d	404	CLA	C3B-C4B-NB	2.88	113.19	110.52
39	l	101	LHG	O8-C23-C24	2.88	120.95	111.91
24	b	612	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
24	C	513	CLA	O2A-CGA-CBA	2.88	120.94	111.91
24	B	615	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
31	d	407	PL9	C15-C14-C16	2.88	120.11	115.27
41	h	702	RRX	C24-C23-C22	-2.88	121.89	126.23
26	b	621	BCR	C8-C7-C6	-2.87	119.13	127.20
24	b	618	CLA	CED-O2D-CGD	2.87	122.44	115.94
26	k	2003	BCR	C38-C26-C25	-2.87	121.30	124.53
29	B	623	LMT	C1B-O5B-C5B	2.87	119.32	113.69
24	C	510	CLA	C3C-C4C-NC	2.87	113.79	110.57
26	c	517	BCR	C15-C14-C13	-2.87	123.22	127.31
24	c	507	CLA	CAC-C3C-C4C	2.87	128.53	124.81
24	d	404	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	b	616	CLA	C4A-NA-C1A	2.87	108.00	106.71
24	C	513	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	a	2113	CLA	CMB-C2B-C1B	2.87	129.73	125.37
24	b	609	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	b	608	CLA	CHD-C4C-NC	2.86	128.72	124.20
24	a	2113	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
31	D	407	PL9	C53-C6-C1	2.86	120.84	114.99
24	C	507	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
36	C	522	HTG	O5-C5-C4	2.86	114.89	109.69
24	B	612	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
24	B	612	CLA	CHD-C4C-C3C	-2.85	120.64	124.84
24	c	513	CLA	O2A-CGA-O1A	-2.85	116.39	123.59
24	c	505	CLA	C3D-C4D-ND	2.85	114.86	110.24
24	C	504	CLA	C1-O2A-CGA	2.85	123.93	116.44
24	C	507	CLA	O2A-CGA-CBA	2.85	120.85	111.91
43	V	201	HEC	CBD-CAD-C3D	-2.85	104.71	112.63
24	B	605	CLA	C1-C2-C3	-2.85	121.11	126.04
24	B	602	CLA	C2C-C1C-NC	2.85	112.64	109.97
24	b	615	CLA	C3B-C4B-NB	2.85	113.16	110.52
24	A	409	CLA	CMA-C3A-C2A	-2.84	102.35	113.83
24	C	511	CLA	C1D-CHD-C4C	-2.84	119.92	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	508	CLA	O2A-CGA-O1A	-2.84	116.41	123.59
24	C	511	CLA	C2C-C1C-NC	2.84	112.64	109.97
24	b	608	CLA	CMB-C2B-C1B	2.84	129.70	125.37
26	c	516	BCR	C11-C10-C9	-2.84	123.25	127.31
24	c	506	CLA	C3B-C4B-NB	2.84	113.15	110.52
24	B	616	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
24	a	2113	CLA	C4-C3-C5	2.84	120.04	115.27
24	a	2110	CLA	O2A-CGA-CBA	2.84	120.81	111.91
24	b	611	CLA	CMA-C3A-C4A	-2.84	104.15	111.77
31	d	407	PL9	C10-C9-C11	2.84	120.04	115.27
24	d	404	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
26	C	516	BCR	C37-C22-C23	2.84	122.55	118.08
24	c	507	CLA	CMB-C2B-C1B	2.83	129.69	125.37
24	B	607	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
26	K	101	BCR	C11-C10-C9	-2.83	123.27	127.31
29	a	2103	LMT	O1B-C4'-C3'	2.83	114.81	107.28
27	L	102	SQD	C44-O6-C1	-2.83	108.21	113.74
24	B	616	CLA	CHD-C1D-ND	-2.83	121.85	124.45
24	C	511	CLA	CMC-C2C-C1C	2.83	129.35	125.04
24	b	606	CLA	CMC-C2C-C1C	2.83	129.35	125.04
24	C	505	CLA	C1D-CHD-C4C	-2.83	119.95	126.06
29	A	420	LMT	O5'-C5'-C4'	2.83	115.72	109.75
24	C	508	CLA	CHA-C1A-NA	-2.83	119.92	126.40
24	c	508	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	B	617	CLA	C3B-C4B-NB	2.83	113.14	110.52
24	c	513	CLA	C3C-C4C-NC	2.83	113.74	110.57
24	B	608	CLA	C1D-CHD-C4C	-2.82	119.96	126.06
24	b	609	CLA	C4-C3-C5	2.82	120.02	115.27
24	B	603	CLA	C4-C3-C5	2.82	120.02	115.27
38	C	519	DGD	C2G-O2G-C1B	-2.82	110.85	117.79
24	b	618	CLA	CBC-CAC-C3C	-2.82	104.66	112.43
39	d	408	LHG	O7-C7-C8	2.82	117.58	111.50
24	B	613	CLA	CAC-C3C-C4C	2.82	128.47	124.81
24	c	504	CLA	CMB-C2B-C1B	2.82	129.66	125.37
24	B	605	CLA	C3C-C4C-NC	2.82	113.73	110.57
24	d	405	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
24	A	406	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
24	b	616	CLA	CMB-C2B-C1B	2.81	129.65	125.37
24	b	609	CLA	CBC-CAC-C3C	-2.81	104.67	112.43
24	C	513	CLA	CMA-C3A-C4A	-2.81	104.21	111.77
24	b	614	CLA	CMC-C2C-C1C	2.81	129.32	125.04
24	C	514	CLA	CHD-C1D-ND	-2.81	121.87	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	F	101	SQD	O48-C23-C24	2.81	120.71	111.91
24	b	609	CLA	CAC-C3C-C4C	2.80	128.45	124.81
24	c	515	CLA	CAC-C3C-C4C	2.80	128.45	124.81
24	B	603	CLA	CAC-C3C-C4C	2.80	128.45	124.81
24	b	605	CLA	CMA-C3A-C4A	-2.80	104.24	111.77
25	A	407	PHO	CMB-C2B-C3B	2.80	129.92	124.68
27	A	411	SQD	O48-C23-C24	2.80	120.69	111.91
24	B	608	CLA	C4-C3-C5	2.80	119.98	115.27
31	d	407	PL9	C25-C24-C26	2.80	119.98	115.27
38	H	102	DGD	O1G-C1A-O1A	-2.79	116.54	123.59
24	d	405	CLA	C4-C3-C5	2.79	119.97	115.27
36	b	625	HTG	C1-O5-C5	2.79	117.73	112.58
26	K	101	BCR	C24-C23-C22	-2.79	122.02	126.23
24	A	409	CLA	C4-C3-C5	2.79	119.96	115.27
24	b	612	CLA	C4-C3-C5	2.79	119.96	115.27
28	c	522	LMG	O8-C28-C29	2.79	120.66	111.91
41	h	702	RRX	C10-C11-C12	-2.79	114.52	123.22
24	C	504	CLA	C3C-C4C-NC	2.79	113.70	110.57
24	c	514	CLA	C3C-C4C-NC	2.79	113.70	110.57
36	c	524	HTG	C1-O5-C5	2.79	117.72	112.58
27	L	102	SQD	O48-C23-C24	2.79	120.65	111.91
24	C	505	CLA	C1-O2A-CGA	2.79	123.75	116.44
25	A	408	PHO	CMA-C3A-C4A	-2.78	108.28	114.38
24	C	506	CLA	CMB-C2B-C1B	2.78	129.61	125.37
24	B	608	CLA	CMC-C2C-C1C	2.78	129.28	125.04
36	b	625	HTG	C2'-C1'-S1	-2.78	103.41	112.40
26	C	515	BCR	C23-C24-C25	-2.78	119.38	127.20
24	B	604	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
24	B	610	CLA	CMA-C3A-C4A	-2.78	104.30	111.77
24	c	512	CLA	C1-C2-C3	-2.78	121.23	126.04
43	v	201	HEC	C4C-NC-C1C	2.78	108.07	105.35
36	b	601	HTG	C3-C4-C5	2.78	115.20	110.24
24	C	508	CLA	C4A-NA-C1A	2.78	107.96	106.71
26	B	618	BCR	C7-C8-C9	-2.78	122.03	126.23
24	A	409	CLA	C3B-C4B-NB	2.78	113.09	110.52
24	C	507	CLA	CHA-C1A-NA	-2.78	120.03	126.40
27	a	2115	SQD	O48-C23-O10	-2.78	116.58	123.59
24	D	401	CLA	CED-O2D-CGD	2.78	122.22	115.94
24	C	514	CLA	CMB-C2B-C1B	2.78	129.60	125.37
24	c	509	CLA	C3B-C4B-NB	2.77	113.09	110.52
24	b	615	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	b	612	CLA	C4C-C3C-C2C	-2.77	102.86	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C1D-CHD-C4C	-2.77	120.08	126.06
26	c	528	BCR	C15-C14-C13	-2.77	123.36	127.31
24	b	608	CLA	C2C-C1C-NC	2.77	112.57	109.97
24	b	608	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	b	606	CLA	C3B-C4B-NB	2.77	113.08	110.52
26	c	528	BCR	C24-C23-C22	-2.77	122.06	126.23
24	A	409	CLA	C3C-C4C-NC	2.77	113.67	110.57
24	C	510	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
24	b	611	CLA	C3B-C4B-NB	2.76	113.08	110.52
24	C	507	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
24	b	610	CLA	C3C-C4C-NC	2.76	113.66	110.57
24	b	614	CLA	O2A-CGA-CBA	2.76	120.56	111.91
24	b	613	CLA	CHA-C1A-NA	-2.76	120.08	126.40
24	B	606	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
24	B	610	CLA	CBC-CAC-C3C	-2.76	104.83	112.43
24	B	614	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
24	B	605	CLA	CMC-C2C-C1C	2.75	129.23	125.04
24	a	2109	CLA	C3B-C4B-NB	2.75	113.07	110.52
28	c	521	LMG	C8-O7-C10	-2.75	111.01	117.79
24	d	401	CLA	CAA-CBA-CGA	2.75	121.29	113.25
24	c	511	CLA	C3B-C4B-NB	2.75	113.07	110.52
24	c	515	CLA	O2A-CGA-CBA	2.75	120.53	111.91
24	b	611	CLA	CBC-CAC-C3C	-2.74	104.86	112.43
24	C	511	CLA	C4A-NA-C1A	2.74	107.94	106.71
24	b	608	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
24	b	618	CLA	C3C-C4C-NC	2.74	113.65	110.57
24	c	509	CLA	C1D-CHD-C4C	-2.74	120.14	126.06
24	b	605	CLA	C3C-C4C-NC	2.74	113.64	110.57
38	H	102	DGD	O2G-C1B-C2B	2.74	117.41	111.50
24	c	510	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
36	D	413	HTG	C3-C4-C5	2.74	115.13	110.24
24	B	612	CLA	C1D-CHD-C4C	-2.74	120.15	126.06
24	B	611	CLA	C4-C3-C5	2.74	119.87	115.27
24	c	506	CLA	O2A-CGA-O1A	-2.74	116.69	123.59
24	C	513	CLA	CBA-CAA-C2A	-2.73	105.79	113.86
26	C	516	BCR	C38-C26-C25	-2.73	121.46	124.53
24	b	604	CLA	O2A-C1-C2	-2.73	101.45	108.64
29	j	1601	LMT	O5'-C1'-C2'	2.73	116.13	110.35
24	a	2110	CLA	CED-O2D-CGD	2.73	122.11	115.94
24	C	509	CLA	O2A-CGA-CBA	2.73	120.47	111.91
31	D	407	PL9	C42-C43-C44	-2.73	121.09	127.66
24	C	508	CLA	CHC-C4B-NB	2.73	127.14	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	604	CLA	CAA-CBA-CGA	-2.73	105.28	113.25
26	c	517	BCR	C3-C4-C5	-2.73	109.21	114.08
24	C	502	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	c	511	CLA	CMC-C2C-C1C	2.72	129.19	125.04
24	C	510	CLA	C3B-C4B-NB	2.72	113.04	110.52
26	C	516	BCR	C15-C14-C13	-2.72	123.42	127.31
24	B	605	CLA	C3B-C4B-NB	2.72	113.04	110.52
24	b	612	CLA	C3C-C4C-NC	2.72	113.62	110.57
24	c	509	CLA	C1-C2-C3	-2.72	121.34	126.04
28	c	522	LMG	O6-C5-C4	2.72	114.63	109.69
24	A	409	CLA	CBC-CAC-C3C	-2.72	104.94	112.43
43	v	201	HEC	C4A-NA-C1A	2.72	108.01	105.35
24	D	404	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
24	B	613	CLA	O2A-CGA-CBA	2.72	120.43	111.91
24	B	611	CLA	CMA-C3A-C4A	-2.72	104.47	111.77
24	B	603	CLA	CMA-C3A-C4A	-2.71	104.48	111.77
24	b	617	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
24	b	608	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
24	c	513	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
24	c	514	CLA	CHA-C1A-NA	-2.71	120.19	126.40
39	d	410	LHG	O8-C23-C24	2.71	120.41	111.91
38	H	102	DGD	C3G-O3G-C1D	-2.71	108.45	113.74
31	d	407	PL9	C20-C19-C21	2.71	119.82	115.27
24	c	505	CLA	C4-C3-C5	2.70	119.82	115.27
24	C	511	CLA	C3C-C4C-NC	2.70	113.60	110.57
28	C	526	LMG	O8-C28-C29	2.70	120.38	111.91
24	c	509	CLA	CHD-C1D-ND	-2.70	121.97	124.45
24	B	616	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
40	e	103	HEM	CHC-C1C-NC	2.70	127.36	124.44
31	x	801	PL9	C20-C19-C21	2.70	119.81	115.27
26	c	517	BCR	C21-C20-C19	-2.70	114.80	123.22
27	B	621	SQD	O5-C1-C2	2.70	116.05	110.35
31	D	407	PL9	C7-C8-C9	-2.69	122.31	126.79
24	b	606	CLA	CBC-CAC-C3C	-2.69	105.01	112.43
24	b	611	CLA	O2A-CGA-O1A	-2.69	116.80	123.59
36	D	413	HTG	C4-C3-C2	2.69	115.52	110.82
24	c	514	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
24	b	613	CLA	O2A-CGA-CBA	2.69	120.34	111.91
31	A	417	PL9	C22-C23-C24	-2.69	121.19	127.66
39	L	101	LHG	O8-C23-O10	-2.68	116.82	123.59
26	b	621	BCR	C28-C27-C26	-2.68	109.29	114.08
24	D	405	CLA	C3C-C4C-NC	2.68	113.58	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	405	CLA	C3C-C4C-NC	2.68	113.58	110.57
24	b	613	CLA	CMA-C3A-C4A	-2.68	104.57	111.77
29	B	623	LMT	O1B-C4'-C5'	-2.68	102.11	109.45
40	e	103	HEM	CBD-CAD-C3D	-2.68	105.19	112.63
24	C	502	CLA	C3C-C4C-NC	2.67	113.57	110.57
24	B	608	CLA	CAC-C3C-C4C	2.67	128.28	124.81
24	B	611	CLA	O2A-CGA-O1A	-2.67	116.84	123.59
24	C	507	CLA	C4-C3-C5	2.67	119.77	115.27
41	H	101	RRX	C29-C28-C27	-2.67	106.65	110.30
24	B	604	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
25	A	408	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
24	a	2113	CLA	CHD-C1D-ND	-2.67	122.00	124.45
36	c	523	HTG	C1-O5-C5	2.67	117.50	112.58
24	c	515	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	B	608	CLA	C3B-C4B-NB	2.67	112.99	110.52
27	f	102	SQD	O48-C23-C24	2.67	120.28	111.91
24	a	2113	CLA	CMA-C3A-C2A	-2.67	103.06	113.83
38	C	517	DGD	C3G-C2G-C1G	-2.67	105.48	111.79
24	B	610	CLA	C3B-C4B-NB	2.67	112.99	110.52
28	B	622	LMG	O7-C10-C11	2.67	117.25	111.50
24	B	608	CLA	C3C-C4C-NC	2.67	113.56	110.57
24	B	612	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
26	T	101	BCR	C12-C13-C14	-2.66	114.85	118.94
24	A	405	CLA	C1D-CHD-C4C	-2.66	120.31	126.06
24	b	614	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
24	C	503	CLA	C1-O2A-CGA	2.66	123.42	116.44
24	b	610	CLA	CMC-C2C-C1C	2.66	129.09	125.04
24	b	608	CLA	O2A-CGA-CBA	2.66	120.25	111.91
39	D	410	LHG	O8-C23-C24	2.66	120.25	111.91
26	T	101	BCR	C35-C13-C12	2.66	122.26	118.08
24	D	404	CLA	C4-C3-C5	2.66	119.74	115.27
24	C	514	CLA	C4-C3-C5	2.66	119.74	115.27
24	b	604	CLA	CMB-C2B-C1B	2.65	129.41	125.37
36	b	601	HTG	O5-C5-C4	2.65	114.51	109.69
24	B	607	CLA	CMC-C2C-C1C	2.65	129.08	125.04
24	B	607	CLA	CHA-C1A-NA	-2.65	120.33	126.40
38	h	703	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
24	B	616	CLA	CBA-CAA-C2A	-2.65	106.04	113.86
36	B	625[B]	HTG	C6-C5-C4	-2.65	106.80	113.00
24	C	513	CLA	CMB-C2B-C1B	2.65	129.40	125.37
24	B	604	CLA	C3B-C4B-NB	2.65	112.97	110.52
24	C	509	CLA	O2A-CGA-O1A	-2.65	116.91	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	407	PL9	C22-C23-C24	-2.64	121.29	127.66
24	C	511	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
24	C	512	CLA	C4A-NA-C1A	2.64	107.89	106.71
32	A	419	K2I	C-C1-C2	-2.64	121.09	123.61
24	B	606	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
24	C	511	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
24	c	514	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
36	b	602	HTG	O5-C5-C4	2.64	114.48	109.69
24	B	609	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
24	C	510	CLA	CHD-C1D-ND	-2.64	122.03	124.45
24	b	614	CLA	CMB-C2B-C1B	2.64	129.38	125.37
24	c	507	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
24	d	401	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
24	A	409	CLA	C1D-CHD-C4C	-2.63	120.38	126.06
24	B	603	CLA	C1-C2-C3	-2.63	121.49	126.04
43	v	201	HEC	CBD-CAD-C3D	-2.63	105.32	112.63
24	C	510	CLA	O2A-CGA-CBA	2.63	120.16	111.91
24	C	508	CLA	C4-C3-C5	2.63	119.69	115.27
24	D	405	CLA	C1D-CHD-C4C	-2.63	120.39	126.06
24	C	507	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
38	c	518	DGD	O2G-C1B-O1B	-2.63	117.36	123.70
24	D	405	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
24	b	617	CLA	CAC-C3C-C4C	2.62	128.21	124.81
24	b	611	CLA	CHA-C1A-NA	-2.62	120.39	126.40
41	H	101	RRX	C10-C11-C12	-2.62	115.04	123.22
24	C	506	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
24	b	612	CLA	CED-O2D-CGD	2.62	121.86	115.94
24	A	405	CLA	O2A-CGA-CBA	2.62	120.13	111.91
24	b	616	CLA	O2A-CGA-CBA	2.62	120.13	111.91
24	c	512	CLA	C4-C3-C5	2.62	119.68	115.27
24	c	505	CLA	CHD-C4C-C3C	-2.62	120.99	124.84
24	c	511	CLA	CHA-C1A-NA	-2.62	120.41	126.40
24	D	405	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
24	c	511	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
25	a	2111	PHO	CMB-C2B-C3B	2.61	129.56	124.68
24	D	404	CLA	C3B-C4B-NB	2.61	112.94	110.52
28	C	520	LMG	C8-O7-C10	-2.61	111.36	117.79
24	C	504	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
24	B	616	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
24	c	513	CLA	CMC-C2C-C1C	2.61	129.01	125.04
24	b	617	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
32	a	2119	K2I	BR-C4-C5	2.61	119.15	116.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	607	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	A	409	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
39	D	410	LHG	O8-C23-O10	-2.61	117.01	123.59
24	C	508	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
36	B	628	HTG	O5-C5-C4	2.61	114.43	109.69
24	c	506	CLA	CMC-C2C-C1C	2.61	129.01	125.04
26	b	621	BCR	C37-C22-C21	-2.60	119.28	122.92
24	C	505	CLA	C3C-C4C-NC	2.60	113.49	110.57
24	B	615	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
24	B	617	CLA	C1-O2A-CGA	2.60	123.27	116.44
24	b	615	CLA	CMB-C2B-C1B	2.60	129.33	125.37
24	C	504	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
24	B	613	CLA	C1D-CHD-C4C	-2.60	120.45	126.06
24	c	505	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	b	619	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
24	B	614	CLA	O2D-CGD-CBD	2.60	115.88	111.27
24	b	616	CLA	C1D-CHD-C4C	-2.60	120.46	126.06
24	c	506	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
24	B	602	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
24	b	618	CLA	C4C-C3C-C2C	-2.59	103.11	106.90
24	c	503	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
24	B	611	CLA	CHA-C1A-NA	-2.59	120.46	126.40
24	c	512	CLA	CHD-C1D-ND	-2.59	122.07	124.45
24	C	505	CLA	C4-C3-C5	2.59	119.63	115.27
26	d	406	BCR	C21-C20-C19	-2.59	115.13	123.22
24	c	512	CLA	C11-C10-C8	-2.59	107.55	115.92
24	B	612	CLA	CHA-C1A-NA	-2.59	120.47	126.40
26	c	517	BCR	C31-C1-C6	-2.59	106.10	110.30
28	c	522	LMG	C3-C4-C5	2.59	114.85	110.24
24	c	509	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
31	x	801	PL9	C15-C14-C16	2.58	119.62	115.27
24	a	2113	CLA	O2A-CGA-CBA	2.58	120.02	111.91
26	T	101	BCR	C15-C14-C13	2.58	131.00	127.31
24	c	514	CLA	CMA-C3A-C4A	-2.58	104.83	111.77
26	k	2003	BCR	C20-C21-C22	-2.58	123.63	127.31
31	x	801	PL9	C12-C13-C14	-2.58	121.45	127.66
24	c	509	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
39	D	411	LHG	O8-C23-C24	2.58	120.00	111.91
24	C	505	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
26	A	410	BCR	C31-C1-C6	-2.58	106.12	110.30
24	B	610	CLA	CHA-C1A-NA	-2.58	120.50	126.40
24	B	603	CLA	CMA-C3A-C2A	-2.57	103.44	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	405	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
24	b	616	CLA	CHA-C1A-NA	-2.57	120.50	126.40
24	B	607	CLA	O2A-CGA-CBA	2.57	119.98	111.91
24	B	605	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
24	B	609	CLA	C1-C2-C3	-2.57	121.59	126.04
24	b	618	CLA	CMC-C2C-C1C	2.57	128.96	125.04
24	c	511	CLA	O2A-CGA-CBA	2.57	119.98	111.91
24	b	616	CLA	C4-C3-C5	2.57	119.60	115.27
24	C	513	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
24	D	404	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
24	d	405	CLA	C1-C2-C3	-2.57	121.60	126.04
24	c	514	CLA	C11-C12-C13	-2.57	107.62	115.92
24	b	611	CLA	C1-C2-C3	-2.57	121.60	126.04
24	C	504	CLA	O2A-CGA-CBA	2.57	119.97	111.91
43	v	201	HEC	CBB-CAB-C3B	2.57	119.51	112.43
24	B	612	CLA	C4-C3-C5	2.57	119.59	115.27
28	c	522	LMG	C8-O7-C10	-2.57	111.47	117.79
24	B	609	CLA	O2A-CGA-CBA	2.57	119.96	111.91
29	b	624	LMT	C1'-O5'-C5'	2.56	118.72	113.69
31	D	407	PL9	C37-C38-C39	-2.56	121.49	127.66
24	c	508	CLA	CHA-C1A-NA	-2.56	120.53	126.40
38	c	520	DGD	O1G-C1A-C2A	2.56	119.94	111.91
24	c	508	CLA	CGD-CBD-CAD	-2.56	102.45	110.73
24	B	616	CLA	CHA-C1A-NA	-2.56	120.54	126.40
24	D	401	CLA	CHC-C1C-C2C	-2.56	119.63	126.73
24	c	505	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
24	b	610	CLA	CAA-CBA-CGA	2.56	120.72	113.25
26	B	619	BCR	C38-C26-C25	-2.56	121.66	124.53
24	c	504	CLA	CMC-C2C-C1C	2.56	128.93	125.04
24	B	616	CLA	C3B-C4B-NB	2.55	112.89	110.52
26	t	102	BCR	C21-C20-C19	-2.55	115.25	123.22
24	c	514	CLA	C1-C2-C3	-2.55	121.63	126.04
24	C	512	CLA	C1-O2A-CGA	2.55	123.14	116.44
24	C	504	CLA	CHA-C1A-NA	-2.55	120.56	126.40
24	A	405	CLA	CMA-C3A-C2A	-2.55	103.55	113.83
24	C	513	CLA	C4A-NA-C1A	2.55	107.85	106.71
24	c	509	CLA	CHA-C1A-NA	-2.55	120.57	126.40
29	z	1801	LMT	C1B-O1B-C4'	-2.55	111.67	117.96
26	D	406	BCR	C10-C11-C12	-2.54	115.28	123.22
24	b	616	CLA	CAC-C3C-C4C	2.54	128.11	124.81
26	B	620	BCR	C38-C26-C25	-2.54	121.67	124.53
24	b	616	CLA	CED-O2D-CGD	2.54	121.69	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	CAC-C3C-C4C	2.54	128.11	124.81
24	b	610	CLA	CHD-C1D-ND	-2.54	122.12	124.45
24	B	614	CLA	C4-C3-C5	2.54	119.54	115.27
24	b	613	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
43	v	201	HEC	C4B-NB-C1B	2.54	107.69	105.07
24	b	619	CLA	CHA-C1A-NA	-2.54	120.59	126.40
26	t	102	BCR	C1-C6-C7	2.53	122.95	115.78
24	b	608	CLA	CED-O2D-CGD	2.53	121.67	115.94
36	B	628	HTG	C4-C3-C2	-2.53	106.40	110.82
24	C	506	CLA	C4A-NA-C1A	2.53	107.84	106.71
24	b	605	CLA	C3B-C4B-NB	2.53	112.86	110.52
31	A	417	PL9	C40-C39-C41	2.53	119.53	115.27
24	C	514	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
24	C	512	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
24	c	514	CLA	C3B-C4B-NB	2.53	112.86	110.52
24	B	605	CLA	CHD-C4C-C3C	-2.53	121.12	124.84
24	b	612	CLA	CMA-C3A-C4A	-2.53	104.98	111.77
24	B	605	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
27	A	413	SQD	C44-O6-C1	-2.53	108.80	113.74
24	C	513	CLA	CHA-C1A-NA	-2.53	120.61	126.40
24	C	508	CLA	CHB-C1B-C2B	-2.53	120.10	127.24
24	D	405	CLA	C1-C2-C3	-2.53	121.67	126.04
24	B	609	CLA	CMC-C2C-C1C	2.52	128.88	125.04
29	b	624	LMT	C3'-C4'-C5'	2.52	116.71	110.93
24	a	2110	CLA	CHC-C1C-C2C	-2.52	119.72	126.73
29	i	104	LMT	O5'-C5'-C4'	2.52	114.28	109.69
24	b	619	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
24	B	604	CLA	CAA-C2A-C1A	-2.52	103.72	111.97
24	b	617	CLA	CMC-C2C-C1C	2.52	128.88	125.04
29	B	623	LMT	O5B-C5B-C4B	2.52	114.27	109.69
27	A	413	SQD	O9-S-C6	2.52	109.93	106.94
26	C	515	BCR	C20-C21-C22	-2.52	123.72	127.31
24	b	613	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
24	b	609	CLA	CMC-C2C-C1C	2.51	128.87	125.04
24	B	615	CLA	CMB-C2B-C1B	2.51	129.20	125.37
24	d	401	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
24	A	409	CLA	CMB-C2B-C1B	2.51	129.20	125.37
24	D	401	CLA	CMA-C3A-C4A	-2.51	105.02	111.77
24	C	514	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
24	a	2110	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
24	B	605	CLA	CHA-C1A-NA	-2.51	120.65	126.40
28	D	412	LMG	O7-C10-C11	2.51	116.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	2109	CLA	O2D-CGD-CBD	2.51	115.72	111.27
26	T	101	BCR	C16-C17-C18	-2.51	123.73	127.31
26	C	516	BCR	C2-C1-C6	2.51	114.34	110.48
24	b	612	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
40	e	103	HEM	C4A-NA-C1A	2.50	107.80	105.35
24	C	505	CLA	C3B-C4B-NB	2.50	112.84	110.52
24	C	506	CLA	CMA-C3A-C4A	-2.50	105.05	111.77
24	b	609	CLA	O2A-CGA-CBA	2.50	119.75	111.91
24	c	503	CLA	C1D-CHD-C4C	-2.50	120.67	126.06
26	Y	302	BCR	C32-C1-C6	-2.50	106.25	110.30
31	A	417	PL9	C37-C38-C39	-2.49	121.65	127.66
24	B	613	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
24	b	619	CLA	CHD-C1D-ND	-2.49	122.16	124.45
38	C	517	DGD	O1G-C1A-O1A	-2.49	117.30	123.59
24	b	604	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
24	A	409	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	A	406	CLA	CMC-C2C-C1C	2.49	128.83	125.04
24	c	514	CLA	CMB-C2B-C1B	2.49	129.16	125.37
25	A	407	PHO	CMA-C3A-C4A	-2.49	108.93	114.38
40	e	103	HEM	C1B-NB-C4B	2.49	107.64	105.07
38	c	518	DGD	O6D-C1D-O3G	-2.49	104.08	109.97
24	B	607	CLA	C1-O2A-CGA	2.49	122.97	116.44
26	t	102	BCR	C7-C8-C9	-2.49	122.48	126.23
31	A	417	PL9	C25-C24-C26	2.48	119.45	115.27
24	B	607	CLA	C3B-C4B-NB	2.48	112.82	110.52
26	Y	302	BCR	C10-C11-C12	-2.48	115.47	123.22
24	C	511	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
31	x	801	PL9	C25-C24-C26	2.48	119.45	115.27
38	c	519	DGD	C5B-C4B-C3B	-2.48	101.82	114.42
24	b	607	CLA	CHD-C1D-C2D	-2.48	120.27	125.48
24	B	602	CLA	CMC-C2C-C1C	2.48	128.82	125.04
26	b	622	BCR	C15-C14-C13	-2.48	123.77	127.31
24	b	605	CLA	C4-C3-C5	2.48	119.44	115.27
27	A	411	SQD	O48-C23-O10	-2.48	117.33	123.59
24	B	610	CLA	C4-C3-C5	2.48	119.44	115.27
24	b	610	CLA	C4C-C3C-C2C	-2.48	103.29	106.90
24	a	2109	CLA	CMA-C3A-C2A	-2.48	103.84	113.83
26	k	2003	BCR	C15-C14-C13	-2.48	123.78	127.31
24	B	605	CLA	CHD-C1D-ND	-2.47	122.18	124.45
41	h	702	RRX	C7-C8-C9	-2.47	122.50	126.23
24	C	511	CLA	C1-O2A-CGA	2.47	122.94	116.44
24	B	604	CLA	C4-C3-C5	2.47	119.43	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	407	PL9	O1-C4-C3	-2.47	118.00	120.72
24	A	406	CLA	C3C-C4C-NC	2.47	113.34	110.57
24	b	617	CLA	O2A-CGA-CBA	2.47	119.66	111.91
31	d	407	PL9	C12-C13-C14	-2.47	121.72	127.66
24	C	510	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
24	d	405	CLA	C3B-C4B-NB	2.47	112.80	110.52
24	B	604	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
24	C	508	CLA	CMB-C2B-C1B	2.46	129.12	125.37
31	d	407	PL9	C36-C37-C38	-2.46	103.79	111.88
24	C	514	CLA	O2A-CGA-CBA	2.46	119.63	111.91
24	B	614	CLA	CMA-C3A-C2A	-2.46	103.90	113.83
24	A	406	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
24	C	513	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	b	613	CLA	C4-C3-C5	2.46	119.41	115.27
24	C	506	CLA	C3B-C4B-NB	2.46	112.80	110.52
26	t	102	BCR	C15-C14-C13	2.46	130.82	127.31
31	D	407	PL9	C40-C39-C38	-2.46	117.38	123.68
43	V	201	HEC	C4A-NA-C1A	2.46	107.75	105.35
24	B	604	CLA	CAC-C3C-C4C	2.46	128.00	124.81
24	C	505	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
29	I	1201	LMT	C1'-O5'-C5'	2.45	118.50	113.69
24	D	404	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
24	B	612	CLA	C7-C6-C5	-2.45	106.70	113.36
24	C	512	CLA	C3B-C4B-NB	2.45	112.79	110.52
24	c	505	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
26	c	528	BCR	C38-C26-C25	-2.45	121.78	124.53
40	F	102	HEM	C1B-NB-C4B	2.45	107.60	105.07
24	c	510	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
39	D	409	LHG	O7-C7-O9	-2.44	117.80	123.70
24	B	603	CLA	CHA-C1A-NA	-2.44	120.80	126.40
24	c	506	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
25	A	407	PHO	C1-C2-C3	-2.44	121.82	126.04
24	b	607	CLA	CHD-C4C-C3C	-2.44	121.25	124.84
24	c	503	CLA	CAC-C3C-C4C	2.44	127.98	124.81
24	b	606	CLA	C1-O2A-CGA	2.44	122.84	116.44
24	b	605	CLA	CAC-C3C-C4C	2.44	127.97	124.81
24	c	513	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
24	C	503	CLA	C3B-C4B-NB	2.44	112.78	110.52
24	b	612	CLA	CHC-C4B-NB	2.44	126.84	124.26
24	b	606	CLA	C3C-C4C-NC	2.44	113.31	110.57
24	A	406	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
28	C	520	LMG	O8-C28-O10	-2.43	117.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	c	516	BCR	C7-C8-C9	-2.43	122.56	126.23
28	i	101	LMG	C8-O7-C10	-2.43	111.80	117.79
31	D	407	PL9	C20-C19-C21	2.43	119.36	115.27
24	A	406	CLA	CAC-C3C-C4C	2.43	127.97	124.81
26	D	406	BCR	C15-C14-C13	-2.43	123.84	127.31
24	B	617	CLA	CHC-C4B-NB	2.43	126.83	124.26
24	C	503	CLA	O2A-C1-C2	2.43	115.03	108.64
24	B	604	CLA	CMB-C2B-C1B	2.43	129.07	125.37
27	L	102	SQD	O47-C7-O49	-2.43	117.83	123.70
28	B	622	LMG	O8-C28-C29	2.43	119.53	111.91
29	B	636	LMT	O5'-C5'-C4'	2.43	114.87	109.75
24	b	605	CLA	C1-C2-C3	-2.43	121.84	126.04
26	c	528	BCR	C10-C11-C12	-2.43	115.64	123.22
26	T	101	BCR	C29-C28-C27	-2.43	105.95	111.38
41	H	101	RRX	C38-C26-C25	-2.43	121.80	124.53
24	d	405	CLA	CAA-C2A-C3A	-2.43	106.14	112.78
26	C	516	BCR	C21-C20-C19	-2.43	115.65	123.22
24	d	405	CLA	C4C-C3C-C2C	-2.42	103.36	106.90
25	A	407	PHO	O1D-CGD-CBD	-2.42	120.70	124.74
24	c	505	CLA	CHC-C4B-NB	2.42	126.82	124.26
24	B	608	CLA	O2A-CGA-CBA	2.42	119.51	111.91
28	D	412	LMG	O8-C28-O10	-2.42	117.48	123.59
24	B	605	CLA	CHC-C4B-NB	2.42	126.82	124.26
24	b	619	CLA	C4-C3-C5	2.42	119.34	115.27
40	e	103	HEM	CBA-CAA-C2A	-2.42	105.90	112.63
24	b	609	CLA	C3B-C4B-NB	2.42	112.76	110.52
27	A	411	SQD	C45-O47-C7	-2.42	111.84	117.79
24	B	603	CLA	C3B-C4B-NB	2.42	112.76	110.52
24	A	409	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
26	B	618	BCR	C34-C9-C10	-2.41	119.54	122.92
24	C	512	CLA	CMC-C2C-C1C	2.41	128.71	125.04
26	b	621	BCR	C29-C28-C27	-2.41	105.99	111.38
25	a	2111	PHO	C1A-C2A-C3A	-2.41	100.54	102.84
29	m	102	LMT	C1B-O5B-C5B	2.41	118.42	113.69
24	b	606	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
24	b	605	CLA	CHB-C1B-C2B	-2.41	120.43	127.24
27	a	2102	SQD	O48-C23-O10	-2.41	117.51	123.59
40	F	102	HEM	C3B-C2B-C1B	2.41	108.27	106.49
24	b	610	CLA	CED-O2D-CGD	2.41	121.38	115.94
26	K	101	BCR	C38-C26-C25	-2.41	121.83	124.53
26	C	516	BCR	C20-C21-C22	-2.41	123.88	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	CHA-C1A-NA	-2.40	120.89	126.40
38	C	519	DGD	C4A-C3A-C2A	-2.40	104.55	113.19
27	A	411	SQD	C44-O6-C1	-2.40	109.04	113.74
24	c	512	CLA	CMA-C3A-C4A	-2.40	105.31	111.77
24	b	607	CLA	C6-C7-C8	-2.40	108.15	115.92
24	b	618	CLA	CHA-C1A-NA	-2.40	120.90	126.40
24	B	610	CLA	C1-O2A-CGA	2.40	122.74	116.44
39	d	409	LHG	O7-C7-C8	2.40	116.67	111.50
24	c	508	CLA	O2A-CGA-CBA	2.40	119.43	111.91
24	c	505	CLA	C3B-C4B-NB	2.40	112.74	110.52
24	b	606	CLA	CMA-C3A-C2A	-2.40	104.16	113.83
24	b	614	CLA	CBC-CAC-C3C	-2.39	105.83	112.43
24	b	605	CLA	O2A-CGA-CBA	2.39	119.42	111.91
26	B	618	BCR	C21-C20-C19	-2.39	115.75	123.22
24	C	512	CLA	O2A-CGA-CBA	2.39	119.42	111.91
24	a	2110	CLA	CHA-C1A-NA	-2.39	120.92	126.40
24	C	511	CLA	C3B-C4B-NB	2.39	112.73	110.52
24	b	611	CLA	CMC-C2C-C1C	2.39	128.68	125.04
24	C	510	CLA	CHA-C1A-NA	-2.39	120.93	126.40
24	C	513	CLA	CMC-C2C-C1C	2.39	128.68	125.04
25	a	2111	PHO	CBA-CAA-C2A	-2.39	106.84	113.81
24	b	605	CLA	CMA-C3A-C2A	-2.39	104.20	113.83
24	D	405	CLA	CMB-C2B-C1B	2.39	129.00	125.37
24	b	616	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
24	B	612	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
24	B	608	CLA	C4C-C3C-C2C	-2.38	103.42	106.90
24	C	507	CLA	CHB-C1B-C2B	-2.38	120.51	127.24
24	D	405	CLA	O2A-CGA-CBA	2.38	119.38	111.91
24	c	503	CLA	C3B-C4B-NB	2.38	112.72	110.52
26	Y	302	BCR	C1-C6-C7	2.38	122.52	115.78
24	b	618	CLA	C11-C10-C8	-2.38	108.22	115.92
26	c	516	BCR	C38-C26-C25	-2.38	121.86	124.53
26	T	101	BCR	C21-C20-C19	-2.38	115.79	123.22
24	a	2110	CLA	C11-C10-C8	-2.38	108.23	115.92
26	c	516	BCR	C20-C21-C22	-2.38	123.92	127.31
24	c	515	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	c	505	CLA	CMC-C2C-C1C	2.38	128.66	125.04
24	B	609	CLA	CHD-C1D-ND	-2.37	122.27	124.45
24	c	507	CLA	C3B-C4B-NB	2.37	112.72	110.52
24	B	615	CLA	CHD-C4C-NC	2.37	127.94	124.20
43	V	201	HEC	C3B-C4B-NB	-2.37	107.53	110.17
24	C	503	CLA	O2A-CGA-O1A	-2.37	117.61	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	CAC-C3C-C4C	2.37	127.89	124.81
24	c	514	CLA	CHC-C1C-C2C	-2.37	120.15	126.73
26	c	528	BCR	C1-C6-C7	2.37	122.48	115.78
24	b	612	CLA	CHA-C1A-NA	-2.37	120.97	126.40
24	b	614	CLA	CHA-C1A-NA	-2.37	120.97	126.40
24	c	515	CLA	C3B-C4B-NB	2.37	112.71	110.52
24	b	617	CLA	C4-C3-C5	2.37	119.25	115.27
26	C	515	BCR	C8-C7-C6	-2.37	120.55	127.20
26	t	102	BCR	C28-C27-C26	-2.37	109.85	114.08
26	A	410	BCR	C7-C8-C9	-2.36	122.66	126.23
24	B	607	CLA	CAC-C3C-C4C	2.36	127.88	124.81
24	B	610	CLA	CMC-C2C-C1C	2.36	128.64	125.04
24	b	610	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	A	409	CLA	C7-C6-C5	-2.36	106.95	113.36
24	b	610	CLA	CMB-C2B-C1B	2.36	128.96	125.37
24	C	506	CLA	C4-C3-C5	2.36	119.24	115.27
26	c	528	BCR	C21-C20-C19	-2.36	115.86	123.22
24	d	405	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
38	c	518	DGD	O4D-C4D-C3D	-2.36	104.90	110.35
24	c	514	CLA	CHD-C1D-ND	-2.35	122.29	124.45
24	b	617	CLA	C3B-C4B-NB	2.35	112.70	110.52
24	c	513	CLA	CMB-C2B-C1B	2.35	128.95	125.37
24	C	502	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
24	b	613	CLA	C1-C2-C3	-2.35	121.98	126.04
24	B	615	CLA	CMC-C2C-C1C	2.34	128.61	125.04
24	B	614	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
24	b	612	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
24	b	611	CLA	CAC-C3C-C4C	2.34	127.85	124.81
32	A	418[B]	K2I	BR1-C1-C2	2.34	118.83	116.03
24	C	513	CLA	CAC-C3C-C2C	2.34	131.53	127.53
24	A	405	CLA	CMC-C2C-C1C	2.34	128.60	125.04
24	C	503	CLA	O2A-CGA-CBA	2.34	119.25	111.91
38	C	517	DGD	C2G-O2G-C1B	-2.34	112.03	117.79
24	a	2109	CLA	CMA-C3A-C4A	-2.34	105.49	111.77
24	B	614	CLA	CMB-C2B-C1B	2.34	128.93	125.37
24	A	405	CLA	CMB-C2B-C3B	2.34	132.25	126.59
38	c	519	DGD	O2G-C1B-O1B	-2.34	118.06	123.70
24	c	503	CLA	C4-C3-C5	2.34	119.20	115.27
24	c	508	CLA	CHC-C1C-C2C	-2.34	120.24	126.73
24	c	515	CLA	CMB-C2B-C1B	2.34	128.93	125.37
26	c	516	BCR	C35-C13-C14	-2.34	119.65	122.92
24	a	2109	CLA	CHC-C1C-C2C	-2.33	120.24	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	614	CLA	C3B-C4B-NB	2.33	112.68	110.52
24	D	405	CLA	C3B-C4B-NB	2.33	112.68	110.52
24	b	606	CLA	C4C-C3C-C2C	-2.33	103.50	106.90
24	A	406	CLA	C3B-C4B-NB	2.33	112.68	110.52
39	d	409	LHG	O8-C23-C24	2.33	119.23	111.91
24	A	409	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
24	b	606	CLA	CAC-C3C-C4C	2.33	127.83	124.81
24	b	606	CLA	CHB-C1B-C2B	-2.33	120.65	127.24
24	c	513	CLA	CHA-C1A-NA	-2.33	121.06	126.40
24	c	515	CLA	C4-C3-C5	2.33	119.19	115.27
24	B	610	CLA	CHC-C4B-NB	2.33	126.72	124.26
25	a	2112	PHO	C4A-C3A-C2A	-2.33	100.62	102.84
26	a	2114	BCR	C15-C14-C13	-2.33	123.99	127.31
24	B	602	CLA	CAC-C3C-C4C	2.32	127.83	124.81
24	b	619	CLA	OBD-CAD-C3D	-2.32	122.93	128.52
26	B	620	BCR	C23-C24-C25	-2.32	120.68	127.20
24	B	615	CLA	C4C-C3C-C2C	-2.32	103.51	106.90
24	d	401	CLA	CHB-C1B-NB	-2.32	121.80	124.26
29	A	420	LMT	O5'-C1'-C2'	2.32	115.26	110.35
28	A	412	LMG	O6-C5-C4	2.32	113.91	109.69
24	B	606	CLA	CED-O2D-CGD	2.32	121.18	115.94
24	B	608	CLA	C1-O2A-CGA	2.32	122.53	116.44
24	C	511	CLA	C6-C7-C8	-2.32	108.43	115.92
26	c	528	BCR	C34-C9-C8	2.32	121.73	118.08
26	t	102	BCR	C2-C1-C6	2.32	114.05	110.48
43	v	201	HEC	C3D-C4D-ND	-2.32	108.11	110.36
26	k	2003	BCR	C16-C17-C18	-2.32	124.00	127.31
24	C	505	CLA	CMA-C3A-C4A	-2.32	105.55	111.77
38	h	703	DGD	C3G-O3G-C1D	-2.32	109.22	113.74
24	B	606	CLA	O2A-CGA-CBA	2.31	119.17	111.91
24	c	512	CLA	CMB-C2B-C1B	2.31	128.89	125.37
24	b	606	CLA	CHC-C4B-NB	2.31	126.71	124.26
28	d	411	LMG	O8-C28-O10	-2.31	117.75	123.59
24	b	619	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
40	F	102	HEM	C2A-C1A-NA	-2.31	107.56	110.15
24	d	401	CLA	CMB-C2B-C1B	2.31	128.89	125.37
24	a	2113	CLA	OBD-CAD-C3D	-2.31	122.96	128.52
24	c	513	CLA	C3B-C4B-NB	2.31	112.66	110.52
29	I	1201	LMT	C1-O1'-C1'	-2.31	110.01	113.84
24	C	504	CLA	CHC-C4B-NB	2.31	126.70	124.26
26	t	102	BCR	C11-C10-C9	-2.31	124.01	127.31
24	C	503	CLA	CHD-C1D-ND	-2.31	122.33	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	i	101	LMG	C7-O1-C1	-2.31	109.23	113.74
24	B	615	CLA	OBD-CAD-C3D	-2.31	122.96	128.52
24	C	512	CLA	CHC-C1C-C2C	-2.31	120.32	126.73
24	b	606	CLA	CHD-C1D-ND	-2.31	122.33	124.45
43	V	201	HEC	C3D-C4D-ND	-2.31	108.12	110.36
24	B	607	CLA	CHB-C1B-C2B	-2.31	120.72	127.24
24	b	617	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
24	C	511	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
36	b	625	HTG	O6-C6-C5	-2.31	103.38	111.29
24	c	510	CLA	CAC-C3C-C2C	2.31	131.47	127.53
26	C	516	BCR	C23-C24-C25	-2.31	120.73	127.20
24	b	619	CLA	C1C-C2C-C3C	-2.30	104.53	106.96
36	c	523	HTG	O5-C5-C4	2.30	113.88	109.69
26	t	102	BCR	C7-C6-C5	-2.30	115.88	121.46
39	E	101	LHG	C5-O7-C7	-2.30	112.12	117.79
29	a	2103	LMT	O5'-C1'-O1'	-2.30	104.53	109.97
24	c	506	CLA	CHC-C1C-C2C	-2.30	120.34	126.73
26	T	101	BCR	C23-C24-C25	-2.30	120.75	127.20
38	C	519	DGD	O2G-C1B-O1B	-2.30	118.15	123.70
25	A	407	PHO	CBA-CAA-C2A	-2.30	107.10	113.81
24	c	514	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
24	C	508	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
24	A	405	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
24	d	404	CLA	CHC-C4B-NB	2.30	126.69	124.26
24	C	514	CLA	C11-C10-C8	-2.30	108.50	115.92
24	A	405	CLA	C4-C3-C5	2.30	119.13	115.27
36	O	302	HTG	C1'-S1-C1	2.29	104.38	100.09
26	A	410	BCR	C20-C21-C22	-2.29	124.03	127.31
31	D	407	PL9	C27-C28-C29	-2.29	122.14	127.66
39	E	101	LHG	O8-C23-C24	2.29	119.09	111.91
31	D	407	PL9	C51-C49-C50	2.29	119.66	114.60
31	d	407	PL9	C53-C6-C1	2.29	119.67	114.99
26	t	102	BCR	C23-C24-C25	-2.29	120.78	127.20
36	b	601	HTG	C1-O5-C5	2.29	116.80	112.58
24	C	507	CLA	C3B-C4B-NB	2.29	112.64	110.52
29	a	2120	LMT	C1-O1'-C1'	-2.29	110.05	113.84
24	D	405	CLA	CMA-C3A-C2A	-2.29	104.61	113.83
24	C	503	CLA	CMB-C2B-C1B	2.29	128.85	125.37
26	a	2114	BCR	C31-C1-C6	-2.28	106.59	110.30
26	d	406	BCR	C15-C14-C13	-2.28	124.05	127.31
24	a	2110	CLA	CAA-CBA-CGA	2.28	119.93	113.25
24	b	614	CLA	CHC-C1C-C2C	-2.28	120.39	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	619	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
24	d	401	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
24	B	612	CLA	C4A-NA-C1A	2.28	107.73	106.71
40	e	103	HEM	CHD-C4C-NC	2.28	126.90	124.44
24	d	404	CLA	C1D-CHD-C4C	-2.28	121.15	126.06
36	I	1202	HTG	C3-C4-C5	2.28	114.30	110.24
24	D	401	CLA	CMC-C2C-C1C	2.28	128.50	125.04
28	B	622	LMG	O1-C7-C8	-2.28	105.41	110.90
26	c	517	BCR	C2-C1-C6	2.28	113.98	110.48
24	C	514	CLA	CMC-C2C-C1C	2.28	128.50	125.04
27	A	413	SQD	O48-C23-O10	-2.27	117.86	123.59
24	C	511	CLA	CAC-C3C-C4C	2.27	127.76	124.81
24	c	513	CLA	CAC-C3C-C4C	2.27	127.76	124.81
27	B	621	SQD	O47-C7-O49	-2.27	118.21	123.70
26	b	621	BCR	C20-C21-C22	-2.27	124.07	127.31
24	B	607	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
24	B	608	CLA	CAA-C2A-C1A	-2.27	104.54	111.97
24	C	510	CLA	CMC-C2C-C1C	2.27	128.50	125.04
24	D	405	CLA	CMC-C2C-C1C	2.27	128.49	125.04
24	B	613	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
25	A	408	PHO	C4A-C3A-C2A	-2.27	100.68	102.84
24	b	605	CLA	CHA-C1A-NA	-2.27	121.21	126.40
24	C	508	CLA	CHD-C1D-ND	-2.27	122.37	124.45
24	c	513	CLA	C6-C5-C3	-2.26	107.52	113.45
24	c	503	CLA	CMB-C2B-C1B	2.26	128.82	125.37
24	B	611	CLA	CMC-C2C-C1C	2.26	128.48	125.04
24	B	612	CLA	C1-C2-C3	-2.26	122.13	126.04
24	C	505	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
24	d	405	CLA	C1D-CHD-C4C	-2.26	121.18	126.06
24	A	405	CLA	CHC-C1C-C2C	-2.26	120.45	126.73
24	A	406	CLA	O2A-CGA-CBA	2.26	119.00	111.91
24	c	507	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
24	d	401	CLA	CED-O2D-CGD	2.26	121.04	115.94
24	c	506	CLA	C11-C10-C8	-2.25	108.63	115.92
28	C	520	LMG	O7-C10-O9	-2.25	118.26	123.70
41	h	702	RRX	C20-C21-C22	-2.25	124.09	127.31
31	D	407	PL9	C12-C13-C14	-2.25	122.24	127.66
24	b	607	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
24	D	401	CLA	CMA-C3A-C2A	-2.25	104.75	113.83
24	B	617	CLA	CHC-C1C-C2C	-2.25	120.48	126.73
39	d	410	LHG	O8-C23-O10	-2.25	117.91	123.59
26	T	101	BCR	C1-C6-C7	2.25	122.14	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	521	LMG	O1-C7-C8	-2.25	105.47	110.90
31	x	801	PL9	C46-C44-C45	2.25	119.56	114.60
25	A	408	PHO	CMB-C2B-C3B	2.25	128.88	124.68
36	c	523	HTG	C6-C5-C4	-2.25	107.74	113.00
24	B	612	CLA	C3B-C4B-NB	2.25	112.60	110.52
24	c	509	CLA	CMC-C2C-C1C	2.25	128.46	125.04
39	D	410	LHG	O7-C7-C8	2.24	116.34	111.50
24	B	609	CLA	CMA-C3A-C2A	-2.24	104.78	113.83
32	a	2119	K2I	C3-C4-C5	-2.24	121.47	123.61
31	x	801	PL9	C17-C18-C19	-2.24	122.26	127.66
24	C	508	CLA	C1-O2A-CGA	2.24	122.32	116.44
24	c	504	CLA	O2A-C1-C2	2.24	114.52	108.64
24	B	603	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
29	A	414	LMT	O5'-C1'-O1'	-2.24	104.67	109.97
24	b	613	CLA	CMC-C2C-C1C	2.24	128.45	125.04
25	A	407	PHO	C4-C3-C5	2.24	119.03	115.27
27	a	2115	SQD	O47-C7-O49	-2.24	118.30	123.70
29	m	102	LMT	C1-O1'-C1'	-2.24	110.13	113.84
24	d	404	CLA	CAC-C3C-C4C	2.24	127.71	124.81
43	V	201	HEC	C2A-C1A-NA	-2.24	108.15	110.32
29	M	101	LMT	O5B-C5B-C4B	2.23	113.75	109.69
24	b	611	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
29	B	636	LMT	C1B-C2B-C3B	2.23	114.65	110.00
24	b	618	CLA	CHD-C4C-NC	2.23	127.72	124.20
27	a	2102	SQD	C44-O6-C1	-2.23	109.38	113.74
27	B	621	SQD	O9-S-C6	2.23	109.59	106.94
24	B	608	CLA	CHA-C1A-NA	-2.23	121.29	126.40
24	B	616	CLA	C11-C12-C13	-2.23	108.71	115.92
24	c	512	CLA	CHC-C1C-C2C	-2.23	120.54	126.73
38	h	703	DGD	C2G-O2G-C1B	-2.23	112.31	117.79
24	d	405	CLA	CHA-C1A-NA	-2.23	121.30	126.40
24	b	618	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
24	C	510	CLA	C1-O2A-CGA	2.22	122.28	116.44
26	T	101	BCR	C3-C4-C5	-2.22	110.11	114.08
24	d	405	CLA	O2A-CGA-CBA	2.22	118.88	111.91
24	d	404	CLA	CMC-C2C-C1C	2.22	128.42	125.04
24	C	508	CLA	CBA-CAA-C2A	-2.22	107.30	113.86
24	D	401	CLA	CHD-C4C-NC	2.22	127.70	124.20
24	D	401	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
24	B	612	CLA	O2A-CGA-CBA	2.22	118.87	111.91
24	B	612	CLA	CMB-C2B-C1B	2.22	128.75	125.37
38	c	520	DGD	O2G-C1B-C2B	2.22	116.28	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	T	101	BCR	C7-C6-C5	-2.22	116.09	121.46
24	b	614	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	t	102	BCR	C35-C13-C12	2.22	121.57	118.08
26	B	619	BCR	C29-C28-C27	-2.22	106.42	111.38
31	d	407	PL9	C22-C23-C24	-2.22	122.33	127.66
28	c	522	LMG	O7-C10-O9	-2.21	118.36	123.70
29	I	1201	LMT	C3'-C4'-C5'	2.21	114.18	110.24
24	A	409	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
24	c	506	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	d	405	CLA	CMB-C2B-C1B	2.21	128.73	125.37
24	a	2110	CLA	CAC-C3C-C4C	2.21	127.68	124.81
24	C	508	CLA	CAC-C3C-C2C	2.21	131.31	127.53
24	C	508	CLA	C3B-C4B-NB	2.21	112.56	110.52
24	b	606	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
28	D	412	LMG	O8-C28-C29	2.21	118.84	111.91
24	B	616	CLA	C1-O2A-CGA	2.21	122.24	116.44
24	B	603	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
27	a	2115	SQD	C45-O47-C7	-2.21	112.36	117.79
24	C	507	CLA	CHC-C4B-NB	2.21	126.59	124.26
40	F	102	HEM	CBA-CAA-C2A	-2.21	106.50	112.63
24	b	613	CLA	CAC-C3C-C4C	2.21	127.67	124.81
39	D	411	LHG	O8-C23-O10	-2.20	118.03	123.59
24	b	618	CLA	C6-C7-C8	-2.20	108.80	115.92
24	b	609	CLA	CHD-C1D-ND	-2.20	122.43	124.45
41	H	101	RRX	C11-C10-C9	-2.20	124.17	127.31
26	a	2114	BCR	C7-C8-C9	-2.20	122.91	126.23
25	A	408	PHO	C4-C3-C2	-2.20	118.03	123.68
24	c	515	CLA	CMC-C2C-C1C	2.20	128.39	125.04
27	f	102	SQD	O47-C7-O49	-2.20	118.39	123.70
24	d	404	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
26	c	528	BCR	C16-C17-C18	-2.20	124.18	127.31
24	D	401	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
31	x	801	PL9	C30-C29-C31	2.20	118.96	115.27
24	B	609	CLA	C11-C12-C13	-2.20	108.82	115.92
43	v	201	HEC	C2A-C1A-NA	-2.19	108.19	110.32
24	B	609	CLA	C3B-C4B-NB	2.19	112.55	110.52
24	B	608	CLA	C4A-NA-C1A	2.19	107.69	106.71
29	a	2120	LMT	O5B-C5B-C4B	2.19	113.67	109.69
38	C	518	DGD	O6E-C5E-C6E	2.19	111.88	106.44
24	b	616	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
26	b	622	BCR	C3-C4-C5	-2.19	110.17	114.08
24	C	506	CLA	O2A-CGA-O1A	-2.19	118.07	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	BCR	C21-C20-C19	-2.19	116.39	123.22
24	C	506	CLA	O2A-CGA-CBA	2.19	118.77	111.91
27	L	102	SQD	O9-S-C6	2.19	109.54	106.94
24	c	511	CLA	CAC-C3C-C4C	2.19	127.65	124.81
25	a	2111	PHO	O2A-CGA-CBA	2.18	118.76	111.91
36	D	413	HTG	C1'-S1-C1	2.18	104.18	100.09
24	D	405	CLA	C11-C10-C8	-2.18	108.86	115.92
26	b	622	BCR	C2-C3-C4	-2.18	106.50	111.38
24	B	603	CLA	O2A-CGA-CBA	2.18	118.75	111.91
29	B	636	LMT	O5B-C5B-C6B	2.18	111.86	106.44
24	B	610	CLA	O2A-CGA-CBA	2.18	118.75	111.91
24	a	2109	CLA	CHA-C1A-NA	-2.18	121.41	126.40
24	b	606	CLA	CMB-C2B-C1B	2.18	128.69	125.37
24	b	606	CLA	CAA-C2A-C1A	-2.18	104.83	111.97
26	b	620	BCR	C15-C14-C13	-2.18	124.20	127.31
24	C	502	CLA	C1-O2A-CGA	2.18	122.15	116.44
26	B	619	BCR	C15-C16-C17	-2.18	119.02	123.47
24	b	612	CLA	O2A-CGA-CBA	2.18	118.73	111.91
24	b	616	CLA	CHC-C1C-C2C	-2.18	120.69	126.73
24	c	510	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	E	105	LMT	O2'-C2'-C3'	-2.17	105.32	110.35
32	A	419	K2I	C3-C4-C5	-2.17	121.54	123.61
26	c	517	BCR	C16-C17-C18	-2.17	124.21	127.31
24	b	606	CLA	C4-C3-C5	2.17	118.93	115.27
24	b	617	CLA	CMB-C2B-C1B	2.17	128.68	125.37
26	Y	302	BCR	C21-C20-C19	-2.17	116.44	123.22
24	c	512	CLA	O2A-CGA-CBA	2.17	118.72	111.91
27	B	621	SQD	O5-C5-C4	2.17	113.64	109.69
24	D	401	CLA	CAA-CBA-CGA	2.17	119.59	113.25
24	C	510	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
24	c	509	CLA	C1-O2A-CGA	2.17	122.13	116.44
24	c	508	CLA	CHB-C1B-C2B	-2.17	121.12	127.24
24	b	617	CLA	CED-O2D-CGD	2.17	120.84	115.94
24	b	613	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
36	C	521	HTG	O5-C1-C2	2.16	113.03	110.31
31	A	417	PL9	C30-C29-C28	-2.16	118.13	123.68
26	B	620	BCR	C16-C17-C18	-2.16	124.22	127.31
26	A	410	BCR	C15-C16-C17	-2.16	119.05	123.47
31	d	407	PL9	C47-C48-C49	-2.16	120.36	127.75
29	B	636	LMT	C1-O1'-C1'	-2.16	110.26	113.84
24	D	405	CLA	C6-C7-C8	-2.16	108.94	115.92
24	d	404	CLA	CHA-C1A-NA	-2.16	121.45	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	514	CLA	CAC-C3C-C4C	2.16	127.61	124.81
24	c	506	CLA	CMB-C2B-C1B	2.16	128.66	125.37
24	b	608	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
24	c	504	CLA	C3B-C4B-NB	2.16	112.52	110.52
24	B	614	CLA	CMC-C2C-C1C	2.16	128.32	125.04
24	c	505	CLA	O2A-CGA-CBA	2.16	118.68	111.91
24	b	610	CLA	CHC-C1C-C2C	-2.16	120.74	126.73
26	t	102	BCR	C12-C13-C14	-2.16	115.63	118.94
24	B	614	CLA	CHB-C4A-NA	2.15	127.49	124.51
29	A	420	LMT	C2'-C3'-C4'	-2.15	104.77	109.68
24	C	505	CLA	CMC-C2C-C1C	2.15	128.32	125.04
24	C	504	CLA	CHD-C4C-NC	2.15	127.59	124.20
26	k	2003	BCR	C3-C4-C5	-2.15	110.24	114.08
24	C	514	CLA	CHA-C1A-NA	-2.15	121.48	126.40
24	D	401	CLA	C4C-C3C-C2C	-2.15	103.77	106.90
24	d	405	CLA	C6-C7-C8	-2.15	108.98	115.92
24	b	605	CLA	CED-O2D-CGD	2.15	120.79	115.94
24	C	513	CLA	C6-C7-C8	-2.15	108.98	115.92
41	h	702	RRX	C15-C16-C17	-2.15	119.08	123.47
28	A	412	LMG	O8-C28-C29	2.15	118.64	111.91
24	c	513	CLA	CHC-C1C-C2C	-2.14	120.77	126.73
24	d	401	CLA	CHA-C1A-NA	-2.14	121.49	126.40
24	c	508	CLA	C11-C12-C13	-2.14	108.99	115.92
24	C	503	CLA	CAC-C3C-C4C	2.14	127.59	124.81
24	a	2109	CLA	CMC-C2C-C1C	2.14	128.30	125.04
24	b	617	CLA	CHC-C1C-C2C	-2.14	120.78	126.73
24	b	615	CLA	CED-O2D-CGD	2.14	120.78	115.94
24	C	507	CLA	CMB-C2B-C1B	2.14	128.63	125.37
29	m	102	LMT	O5'-C1'-O1'	-2.14	104.91	109.97
24	D	404	CLA	CHD-C4C-NC	2.14	127.57	124.20
24	c	508	CLA	CAC-C3C-C4C	2.14	127.58	124.81
24	D	404	CLA	CMA-C3A-C2A	-2.14	105.20	113.83
24	D	401	CLA	CHB-C4A-NA	2.14	127.47	124.51
28	B	622	LMG	C9-C8-C7	-2.14	106.73	111.79
29	A	414	LMT	O1B-C4'-C3'	2.14	112.97	107.28
24	C	514	CLA	C3B-C4B-NB	2.14	112.50	110.52
29	M	101	LMT	C3'-C4'-C5'	-2.14	106.03	110.93
24	B	602	CLA	CHD-C4C-NC	2.13	127.57	124.20
24	C	512	CLA	CMB-C2B-C1B	2.13	128.62	125.37
27	F	101	SQD	O47-C7-O49	-2.13	118.55	123.70
24	B	617	CLA	CMA-C3A-C4A	-2.13	106.04	111.77
24	B	615	CLA	CHA-C1A-NA	-2.13	121.51	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	522	HTG	O5-C1-C2	2.13	113.00	110.31
31	x	801	PL9	C40-C39-C41	2.13	118.86	115.27
24	C	513	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	b	613	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	c	505	CLA	CHD-C1D-C2D	-2.13	121.01	125.48
24	d	401	CLA	O2A-CGA-CBA	2.13	118.59	111.91
24	B	609	CLA	CHA-C1A-NA	-2.13	121.52	126.40
24	B	604	CLA	CMA-C3A-C2A	-2.13	105.24	113.83
24	B	609	CLA	CHB-C4A-NA	2.13	127.45	124.51
24	A	405	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
24	c	512	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	b	622	BCR	C21-C20-C19	-2.12	116.59	123.22
32	a	2119	K2I	C5-C-C1	-2.12	118.30	121.24
24	b	610	CLA	C3B-C4B-NB	2.12	112.49	110.52
24	b	614	CLA	C3B-C4B-NB	2.12	112.49	110.52
43	v	201	HEC	CHA-C4D-ND	2.12	126.73	124.42
41	h	702	RRX	C38-C26-C25	-2.12	122.14	124.53
24	b	614	CLA	C7-C6-C5	-2.12	107.59	113.36
24	b	604	CLA	CMC-C2C-C1C	2.12	128.27	125.04
24	b	606	CLA	C7-C6-C5	-2.12	107.60	113.36
29	z	1801	LMT	C1'-O5'-C5'	2.12	117.85	113.69
24	c	508	CLA	CAA-CBA-CGA	2.12	119.45	113.25
36	B	624	HTG	O5-C1-C2	2.12	112.98	110.31
38	C	519	DGD	O6E-C1E-O5D	-2.12	104.95	109.97
24	c	507	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	b	619	CLA	CHC-C1C-C2C	-2.12	120.84	126.73
24	c	506	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
26	b	621	BCR	C38-C26-C25	-2.12	122.15	124.53
24	C	513	CLA	CHC-C1C-C2C	-2.12	120.85	126.73
26	k	2003	BCR	C8-C7-C6	-2.12	121.25	127.20
24	d	405	CLA	CHC-C1C-C2C	-2.12	120.85	126.73
24	A	406	CLA	CMA-C3A-C2A	-2.12	105.29	113.83
24	A	406	CLA	CHB-C1B-C2B	-2.12	121.26	127.24
24	b	609	CLA	CHC-C1C-C2C	-2.12	120.85	126.73
29	B	623	LMT	O5'-C5'-C4'	2.12	114.21	109.75
26	B	619	BCR	C33-C5-C6	-2.11	122.15	124.53
29	m	103	LMT	O5'-C5'-C6'	2.11	111.69	106.44
24	B	608	CLA	CMB-C2B-C1B	2.11	128.59	125.37
24	b	617	CLA	OBD-CAD-C3D	-2.11	123.44	128.52
24	B	613	CLA	C11-C10-C8	-2.11	109.09	115.92
26	A	410	BCR	C8-C7-C6	-2.11	121.27	127.20
24	C	503	CLA	CHC-C1C-C2C	-2.11	120.87	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	x	801	PL9	C27-C26-C24	-2.11	106.04	112.98
39	d	408	LHG	O7-C7-O9	-2.11	118.60	123.70
26	k	2003	BCR	C11-C10-C9	-2.11	124.30	127.31
24	c	515	CLA	CHA-C1A-NA	-2.11	121.57	126.40
24	C	512	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
26	d	406	BCR	C3-C4-C5	-2.11	110.31	114.08
26	c	516	BCR	C37-C22-C23	2.11	121.40	118.08
24	c	503	CLA	C1-C2-C3	-2.11	122.40	126.04
38	D	408	DGD	O2G-C1B-O1B	-2.11	118.61	123.70
24	B	616	CLA	C4-C3-C5	2.11	118.82	115.27
24	B	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
26	a	2114	BCR	C33-C5-C4	2.11	117.66	113.62
24	c	506	CLA	CED-O2D-CGD	2.11	120.70	115.94
36	O	302	HTG	O2-C2-C3	-2.11	105.48	110.35
28	A	412	LMG	O1-C1-C2	2.11	111.59	108.30
26	Y	302	BCR	C3-C4-C5	-2.11	110.32	114.08
41	h	702	RRX	C29-C28-C27	-2.10	107.42	110.30
24	c	506	CLA	CAA-C2A-C1A	-2.10	105.08	111.97
38	c	518	DGD	O6D-C5D-C6D	2.10	110.91	106.67
24	d	401	CLA	C1-O2A-CGA	2.10	121.96	116.44
26	B	620	BCR	C10-C11-C12	-2.10	116.66	123.22
36	B	625[B]	HTG	C1-C2-C3	2.10	114.74	110.59
24	b	611	CLA	CHC-C1C-C2C	-2.10	120.89	126.73
38	C	519	DGD	O6D-C1D-O3G	-2.10	105.00	109.97
24	B	608	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
26	t	102	BCR	C29-C28-C27	-2.10	106.69	111.38
39	l	101	LHG	C9-C8-C7	-2.10	105.98	113.62
29	m	103	LMT	C1B-O1B-C4'	-2.10	112.77	117.96
24	c	504	CLA	CHD-C4C-NC	2.10	127.51	124.20
27	F	101	SQD	O48-C23-O10	-2.10	118.30	123.59
37	v	203	GOL	C3-C2-C1	-2.10	103.55	111.70
29	B	623	LMT	O5B-C1B-C2B	2.10	114.79	110.35
24	C	507	CLA	CAC-C3C-C4C	2.10	127.53	124.81
24	d	401	CLA	CHC-C4B-NB	2.10	126.48	124.26
24	C	510	CLA	CAC-C3C-C4C	2.10	127.53	124.81
29	m	102	LMT	O5B-C5B-C4B	2.09	113.50	109.69
24	d	401	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
28	D	412	LMG	C9-C8-C7	-2.09	106.83	111.79
24	B	614	CLA	O2A-CGA-CBA	2.09	118.48	111.91
25	A	407	PHO	C4A-C3A-C2A	-2.09	100.85	102.84
24	D	404	CLA	CAC-C3C-C2C	2.09	131.11	127.53
24	C	502	CLA	C3B-C4B-NB	2.09	112.45	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	C4-C3-C5	2.09	118.79	115.27
24	d	401	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
25	a	2111	PHO	C4A-C3A-C2A	-2.09	100.85	102.84
24	c	511	CLA	C4-C3-C5	2.09	118.78	115.27
24	b	605	CLA	CMC-C2C-C1C	2.09	128.22	125.04
24	D	404	CLA	CMB-C2B-C1B	2.09	128.55	125.37
26	B	620	BCR	C15-C14-C13	-2.09	124.33	127.31
25	A	407	PHO	CMD-C2D-C3D	2.09	128.58	124.68
24	b	610	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
24	B	602	CLA	CHA-C1A-NA	-2.09	121.62	126.40
24	C	511	CLA	CHA-C1A-NA	-2.09	121.62	126.40
28	c	521	LMG	O8-C28-O10	-2.09	118.33	123.59
40	F	102	HEM	C1D-C2D-C3D	-2.08	104.77	106.96
41	H	101	RRX	C40-C30-C25	-2.08	106.92	110.30
29	A	414	LMT	O5B-C5B-C6B	2.08	111.61	106.44
24	b	607	CLA	CHC-C4B-C3B	-2.08	118.45	127.71
26	Y	302	BCR	C16-C17-C18	-2.08	124.34	127.31
25	a	2112	PHO	C4D-CHA-CBD	2.08	109.46	108.52
24	a	2110	CLA	CMA-C3A-C2A	-2.08	105.44	113.83
24	a	2113	CLA	CHC-C1C-C2C	-2.08	120.95	126.73
24	C	510	CLA	CMB-C2B-C1B	2.08	128.53	125.37
24	b	611	CLA	C4-C3-C5	2.08	118.77	115.27
39	D	409	LHG	C25-C24-C23	-2.08	106.07	113.62
24	A	406	CLA	CHD-C4C-NC	2.08	127.47	124.20
29	a	2103	LMT	O5B-C5B-C6B	2.08	111.59	106.44
26	D	406	BCR	C16-C17-C18	-2.07	124.35	127.31
38	h	703	DGD	C6D-C5D-C4D	2.07	116.42	112.09
36	V	204	HTG	O5-C1-S1	2.07	114.78	109.82
36	b	626	HTG	O5-C1-C2	2.07	112.92	110.31
28	C	526	LMG	C12-C11-C10	-2.07	106.08	113.62
24	c	503	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
24	A	406	CLA	CHC-C1C-C2C	-2.07	120.97	126.73
24	b	613	CLA	CHC-C1C-C2C	-2.07	120.97	126.73
24	B	610	CLA	CED-O2D-CGD	2.07	120.62	115.94
24	b	618	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
24	d	404	CLA	CMA-C3A-C2A	-2.07	105.48	113.83
24	b	607	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
24	a	2110	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
24	b	612	CLA	C4A-NA-C1A	2.07	107.64	106.71
24	c	505	CLA	CBC-CAC-C3C	-2.07	106.74	112.43
36	B	626	HTG	C1-C2-C3	2.07	114.67	110.59
24	b	610	CLA	CAA-C2A-C1A	-2.06	105.21	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	516	BCR	C11-C10-C9	-2.06	124.37	127.31
24	C	502	CLA	CMC-C2C-C1C	2.06	128.18	125.04
24	C	506	CLA	CMC-C2C-C1C	2.06	128.18	125.04
26	K	101	BCR	C2-C3-C4	-2.06	106.77	111.38
24	B	611	CLA	CHC-C1C-C2C	-2.06	121.01	126.73
24	c	511	CLA	CMB-C2B-C1B	2.06	128.50	125.37
38	D	408	DGD	O6D-C5D-C6D	2.06	110.82	106.67
24	A	406	CLA	CAA-CBA-CGA	2.06	119.27	113.25
24	b	610	CLA	CHA-C1A-NA	-2.06	121.69	126.40
24	d	401	CLA	CHD-C4C-NC	2.06	127.44	124.20
24	b	611	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
24	c	513	CLA	C1-C2-C3	-2.06	122.49	126.04
24	c	509	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
31	D	407	PL9	O2-C1-C6	-2.05	117.04	120.59
24	b	607	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
24	c	505	CLA	C6-C7-C8	-2.05	109.28	115.92
38	c	520	DGD	O1G-C1A-O1A	-2.05	118.41	123.59
24	a	2113	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
24	c	509	CLA	O2A-CGA-CBA	2.05	118.34	111.91
24	b	613	CLA	C11-C12-C13	-2.05	109.29	115.92
24	b	606	CLA	CHC-C1C-C2C	-2.05	121.03	126.73
24	C	510	CLA	C4-C3-C2	-2.05	118.42	123.68
24	D	404	CLA	CHA-C1A-NA	-2.05	121.71	126.40
38	H	102	DGD	C6D-C5D-C4D	2.05	116.37	112.09
24	B	616	CLA	CMC-C2C-C1C	2.05	128.16	125.04
24	b	614	CLA	C11-C12-C13	-2.05	109.31	115.92
36	V	204	HTG	C4-C3-C2	-2.05	107.25	110.82
29	J	102	LMT	O5'-C5'-C4'	2.05	113.41	109.69
24	C	509	CLA	CMC-C2C-C1C	2.05	128.15	125.04
24	D	401	CLA	C4-C3-C5	2.04	118.71	115.27
29	a	2120	LMT	O5'-C5'-C6'	2.04	111.52	106.44
26	d	406	BCR	C10-C11-C12	-2.04	116.84	123.22
29	a	2120	LMT	O5'-C5'-C4'	2.04	114.06	109.75
38	C	517	DGD	O6D-C5D-C6D	2.04	110.79	106.67
43	v	201	HEC	C1D-C2D-C3D	-2.04	104.81	106.96
24	b	616	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	k	2003	BCR	C21-C20-C19	-2.04	116.85	123.22
24	A	409	CLA	CAC-C3C-C4C	2.04	127.46	124.81
31	x	801	PL9	C11-C12-C13	-2.04	105.17	111.88
24	B	608	CLA	CHC-C4B-NB	2.04	126.42	124.26
24	c	510	CLA	CHC-C1C-C2C	-2.04	121.06	126.73
29	m	103	LMT	O5'-C5'-C4'	2.04	114.05	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	2112	PHO	O2A-CGA-CBA	2.04	118.30	111.91
43	V	201	HEC	C4C-NC-C1C	2.04	107.34	105.35
24	d	405	CLA	C4A-NA-C1A	2.04	107.62	106.71
26	B	618	BCR	C28-C27-C26	-2.04	110.44	114.08
27	f	102	SQD	O48-C23-O10	-2.04	118.45	123.59
24	c	510	CLA	C3B-C4B-NB	2.04	112.40	110.52
24	a	2113	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	B	614	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
24	c	504	CLA	CHA-C1A-NA	-2.03	121.74	126.40
26	K	101	BCR	C10-C11-C12	-2.03	116.87	123.22
24	b	609	CLA	C1-O2A-CGA	2.03	121.78	116.44
24	B	614	CLA	CHC-C4B-NB	2.03	126.41	124.26
26	A	410	BCR	C33-C5-C4	2.03	117.52	113.62
27	F	101	SQD	O8-S-C6	2.03	108.97	105.74
24	B	616	CLA	CED-O2D-CGD	2.03	120.53	115.94
24	b	612	CLA	C7-C6-C5	-2.03	107.85	113.36
31	d	407	PL9	C35-C34-C36	2.03	118.68	115.27
24	b	612	CLA	CHC-C1C-C2C	-2.03	121.10	126.73
26	B	620	BCR	C15-C16-C17	-2.03	119.32	123.47
26	t	102	BCR	C16-C15-C14	2.03	127.62	123.47
29	M	101	LMT	O1B-C1B-O5B	-2.03	105.02	110.67
26	k	2003	BCR	C34-C9-C8	2.02	121.27	118.08
38	C	519	DGD	O5D-C6D-C5D	-2.02	105.30	109.05
36	d	403	HTG	O5-C5-C4	2.02	113.37	109.69
24	c	511	CLA	CHD-C1D-C2D	-2.02	121.24	125.48
40	F	102	HEM	CMB-C2B-C1B	-2.02	121.96	125.04
24	B	602	CLA	C4-C3-C5	2.02	118.67	115.27
24	B	603	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
24	B	616	CLA	C7-C6-C5	-2.02	107.87	113.36
24	b	611	CLA	C11-C10-C8	-2.02	109.39	115.92
24	c	504	CLA	CHC-C1C-C2C	-2.02	121.12	126.73
32	A	419	K2I	C2-C3-C4	-2.02	118.44	121.24
24	b	610	CLA	CAC-C3C-C4C	2.02	127.43	124.81
26	t	102	BCR	C33-C5-C4	2.02	117.49	113.62
36	B	625[B]	HTG	O5-C1-C2	2.02	112.85	110.31
24	B	606	CLA	CHA-C1A-NA	-2.02	121.78	126.40
24	c	513	CLA	CHD-C4C-NC	2.02	127.38	124.20
24	c	503	CLA	O2A-CGA-CBA	2.01	118.23	111.91
29	B	623	LMT	O1B-C4'-C3'	2.01	112.63	107.28
24	A	409	CLA	CHB-C1B-NB	-2.01	122.13	124.26
24	b	604	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
24	A	409	CLA	O2A-CGA-CBA	2.01	118.21	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	506	CLA	O2A-CGA-CBA	2.01	118.21	111.91
24	B	614	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	a	2109	CLA	C7-C6-C5	-2.01	107.91	113.36
28	C	526	LMG	O7-C10-O9	-2.01	118.86	123.70
24	c	509	CLA	CHC-C4B-C3B	-2.01	118.79	127.71
24	b	618	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
24	b	616	CLA	CHB-C4A-NA	2.00	127.28	124.51
26	a	2114	BCR	C8-C7-C6	-2.00	121.57	127.20
26	B	620	BCR	C7-C8-C9	-2.00	123.21	126.23
38	c	520	DGD	C2G-O2G-C1B	-2.00	112.86	117.79
26	c	517	BCR	C33-C5-C4	2.00	117.46	113.62
28	i	101	LMG	O8-C28-C29	2.00	118.19	111.91
24	c	507	CLA	CMA-C3A-C4A	-2.00	106.40	111.77

All (2) chirality outliers are listed below:

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

All (1230) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CHA-CBD-CGD-O1D
24	b	609	CLA	CHA-CBD-CGD-O2D
24	b	617	CLA	CHA-CBD-CGD-O1D
24	b	617	CLA	CHA-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O1D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	C4-C3-C5-C6
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
26	B	618	BCR	C1-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	D	406	BCR	C21-C22-C23-C24
26	D	406	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	T	101	BCR	C13-C14-C15-C16
26	b	620	BCR	C1-C6-C7-C8
26	c	517	BCR	C1-C6-C7-C8
26	d	406	BCR	C21-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
26	t	102	BCR	C13-C14-C15-C16
27	A	413	SQD	O6-C44-C45-O47
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	B	621	SQD	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O8
27	B	621	SQD	C5-C6-S-O9
27	F	101	SQD	C8-C7-O47-C45
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
27	L	102	SQD	C5-C6-S-O7
27	a	2102	SQD	O5-C5-C6-S
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
28	C	526	LMG	O9-C10-O7-C8
28	C	526	LMG	C11-C10-O7-C8
28	i	101	LMG	C11-C10-O7-C8
29	A	420	LMT	O5'-C1'-O1'-C1
29	B	637	LMT	C2'-C1'-O1'-C1
29	B	637	LMT	O5'-C1'-O1'-C1
29	E	105	LMT	O5'-C1'-O1'-C1
29	I	1201	LMT	C2'-C1'-O1'-C1
29	I	1201	LMT	O5'-C1'-O1'-C1
29	Z	101	LMT	C2'-C1'-O1'-C1
29	Z	101	LMT	O5'-C1'-O1'-C1
29	Z	101	LMT	C2-C1-O1'-C1'
29	a	2120	LMT	C2'-C1'-O1'-C1
29	f	101	LMT	O5'-C1'-O1'-C1
29	i	104	LMT	O5'-C1'-O1'-C1
29	j	1601	LMT	O5'-C1'-O1'-C1
29	z	1801	LMT	C2'-C1'-O1'-C1
29	z	1801	LMT	O5'-C1'-O1'-C1
31	A	417	PL9	C33-C34-C36-C37
31	A	417	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
36	B	626	HTG	O5-C1-S1-C1'
36	I	1202	HTG	O5-C1-S1-C1'
36	O	302	HTG	C2'-C1'-S1-C1
36	V	204	HTG	C2-C1-S1-C1'
36	V	204	HTG	O5-C1-S1-C1'
36	b	626	HTG	O5-C1-S1-C1'
36	b	626	HTG	C2'-C1'-S1-C1
37	C	525	GOL	C1-C2-C3-O3
37	C	525	GOL	O2-C2-C3-O3
37	H	103	GOL	C1-C2-C3-O3
37	U	501	GOL	C1-C2-C3-O3
37	Z	102	GOL	O2-C2-C3-O3
37	b	631	GOL	C1-C2-C3-O3
37	k	2001	GOL	O1-C1-C2-C3
37	o	2603	GOL	C1-C2-C3-O3
37	v	202	GOL	C1-C2-C3-O3
38	D	408	DGD	O1B-C1B-O2G-C2G
38	D	408	DGD	C2D-C1D-O3G-C3G
38	D	408	DGD	O6D-C1D-O3G-C3G
39	D	410	LHG	C4-O6-P-O4
39	E	101	LHG	O2-C2-C3-O3
39	E	101	LHG	C3-O3-P-O4
39	E	101	LHG	C3-O3-P-O5
39	E	101	LHG	C3-O3-P-O6
39	L	101	LHG	C4-O6-P-O4
39	L	101	LHG	C4-O6-P-O5
39	d	408	LHG	C1-C2-C3-O3
39	d	409	LHG	O1-C1-C2-C3
39	d	409	LHG	C1-C2-C3-O3
39	d	409	LHG	C3-O3-P-O4
39	d	409	LHG	C3-O3-P-O5
39	d	409	LHG	C3-O3-P-O6
39	e	101	LHG	O2-C2-C3-O3
39	e	101	LHG	C4-O6-P-O5
39	l	101	LHG	C4-O6-P-O4
39	l	101	LHG	C4-O6-P-O5
29	A	420	LMT	C3'-C4'-O1B-C1B
27	F	101	SQD	O10-C23-O48-C46
27	F	101	SQD	O49-C7-O47-C45
27	f	102	SQD	O49-C7-O47-C45
28	A	412	LMG	O9-C10-O7-C8
28	i	101	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C3-C5-C6-C7
24	b	619	CLA	C3-C5-C6-C7
27	L	102	SQD	C8-C7-O47-C45
38	D	408	DGD	C2B-C1B-O2G-C2G
24	B	606	CLA	C2-C3-C5-C6
24	c	509	CLA	C2-C3-C5-C6
27	F	101	SQD	C24-C23-O48-C46
36	O	302	HTG	S1-C1'-C2'-C3'
29	i	104	LMT	C4'-C5'-C6'-O6'
29	Z	101	LMT	O5B-C1B-O1B-C4'
43	V	201	HEC	C2B-C3B-CAB-CBB
39	d	408	LHG	O2-C2-C3-O3
39	d	409	LHG	O2-C2-C3-O3
24	B	615	CLA	C3-C5-C6-C7
43	v	201	HEC	C2C-C3C-CAC-CBC
28	A	412	LMG	C11-C10-O7-C8
43	v	201	HEC	C2B-C3B-CAB-CBB
24	C	504	CLA	CBD-CGD-O2D-CED
29	m	102	LMT	O5B-C5B-C6B-O6B
43	V	201	HEC	C2C-C3C-CAC-CBC
38	C	518	DGD	CAA-CBA-CCA-CDA
29	T	102	LMT	O5'-C5'-C6'-O6'
36	B	626	HTG	O5-C5-C6-O6
24	B	602	CLA	C3-C5-C6-C7
36	C	522	HTG	S1-C1'-C2'-C3'
29	B	637	LMT	O5'-C5'-C6'-O6'
29	a	2120	LMT	O5B-C5B-C6B-O6B
29	z	1801	LMT	O5B-C5B-C6B-O6B
24	B	612	CLA	C8-C10-C11-C12
24	c	508	CLA	C13-C15-C16-C17
24	B	615	CLA	C4-C3-C5-C6
24	b	608	CLA	C4-C3-C5-C6
24	b	617	CLA	C4-C3-C5-C6
24	B	615	CLA	C2-C3-C5-C6
24	b	608	CLA	C2-C3-C5-C6
24	b	617	CLA	C2-C3-C5-C6
24	B	607	CLA	C2A-CAA-CBA-CGA
39	D	409	LHG	C28-C29-C30-C31
29	i	104	LMT	O5'-C5'-C6'-O6'
36	b	602	HTG	O5-C5-C6-O6
36	b	626	HTG	O5-C5-C6-O6
31	A	417	PL9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
31	A	417	PL9	C29-C31-C32-C33
38	C	518	DGD	C3A-C4A-C5A-C6A
28	C	526	LMG	C29-C28-O8-C9
36	b	626	HTG	C4-C5-C6-O6
38	c	518	DGD	CAA-CBA-CCA-CDA
29	Z	101	LMT	C2B-C1B-O1B-C4'
29	B	637	LMT	C4'-C5'-C6'-O6'
24	B	611	CLA	C15-C16-C17-C18
24	b	609	CLA	C10-C11-C12-C13
29	A	420	LMT	C2'-C1'-O1'-C1
29	E	105	LMT	C2'-C1'-O1'-C1
29	f	101	LMT	C2'-C1'-O1'-C1
27	a	2102	SQD	O6-C44-C45-O47
38	C	518	DGD	C7A-C8A-C9A-CAA
24	B	602	CLA	C11-C10-C8-C9
24	B	611	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	C	510	CLA	C11-C10-C8-C9
24	b	604	CLA	C14-C13-C15-C16
24	b	613	CLA	C11-C12-C13-C14
24	c	506	CLA	C14-C13-C15-C16
24	B	605	CLA	CBD-CGD-O2D-CED
29	a	2103	LMT	C3'-C4'-O1B-C1B
29	b	624	LMT	C3'-C4'-O1B-C1B
26	D	406	BCR	C7-C8-C9-C34
26	Y	302	BCR	C37-C22-C23-C24
28	C	526	LMG	O6-C5-C6-O5
24	a	2109	CLA	C15-C16-C17-C18
29	z	1801	LMT	C4B-C5B-C6B-O6B
24	B	602	CLA	C10-C11-C12-C13
24	B	614	CLA	C15-C16-C17-C18
24	C	505	CLA	C15-C16-C17-C18
24	D	405	CLA	C8-C10-C11-C12
24	b	604	CLA	C10-C11-C12-C13
24	c	514	CLA	C15-C16-C17-C18
24	d	405	CLA	C8-C10-C11-C12
27	L	102	SQD	C31-C32-C33-C34
38	D	408	DGD	C1B-C2B-C3B-C4B
36	I	1202	HTG	C1'-C2'-C3'-C4'
24	b	604	CLA	C15-C16-C17-C18
37	d	415	GOL	O2-C2-C3-O3
27	F	101	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
39	e	101	LHG	C7-C8-C9-C10
24	b	607	CLA	C15-C16-C17-C18
29	i	104	LMT	O1'-C1-C2-C3
39	e	101	LHG	C11-C10-C9-C8
24	C	507	CLA	C8-C10-C11-C12
24	C	502	CLA	CBD-CGD-O2D-CED
36	b	602	HTG	C4-C5-C6-O6
24	b	616	CLA	C11-C12-C13-C15
24	A	406	CLA	C13-C15-C16-C17
24	B	615	CLA	C5-C6-C7-C8
28	C	526	LMG	O10-C28-O8-C9
29	m	102	LMT	C4B-C5B-C6B-O6B
29	a	2120	LMT	O5'-C1'-O1'-C1
29	b	624	LMT	O5'-C1'-O1'-C1
31	A	417	PL9	C14-C16-C17-C18
31	D	407	PL9	C39-C41-C42-C43
31	d	407	PL9	C39-C41-C42-C43
31	x	801	PL9	C14-C16-C17-C18
27	B	621	SQD	C23-C24-C25-C26
28	b	623	LMG	C10-C11-C12-C13
24	a	2113	CLA	C5-C6-C7-C8
24	b	618	CLA	C10-C11-C12-C13
29	T	102	LMT	C4'-C5'-C6'-O6'
24	c	515	CLA	C10-C11-C12-C13
36	B	626	HTG	C4-C5-C6-O6
43	v	201	HEC	C4C-C3C-CAC-CBC
38	c	519	DGD	CBB-CCB-CDB-CEB
24	B	617	CLA	C5-C6-C7-C8
24	C	507	CLA	C5-C6-C7-C8
24	b	619	CLA	C8-C10-C11-C12
39	L	101	LHG	C4-O6-P-O3
39	e	101	LHG	C3-O3-P-O6
39	l	101	LHG	C4-O6-P-O3
39	E	101	LHG	C17-C18-C19-C20
24	B	602	CLA	CBA-CGA-O2A-C1
27	B	621	SQD	C24-C23-O48-C46
29	b	624	LMT	O1'-C1-C2-C3
39	E	101	LHG	C1-C2-C3-O3
39	e	101	LHG	C1-C2-C3-O3
24	b	619	CLA	C13-C15-C16-C17
24	c	512	CLA	C8-C10-C11-C12
28	d	411	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
36	d	403	HTG	C4-C5-C6-O6
29	A	420	LMT	O1'-C1-C2-C3
29	B	623	LMT	O1'-C1-C2-C3
28	C	526	LMG	C28-C29-C30-C31
38	C	518	DGD	C1B-C2B-C3B-C4B
29	J	102	LMT	C7-C8-C9-C10
29	J	102	LMT	C11-C10-C9-C8
29	Z	101	LMT	C4-C5-C6-C7
39	D	409	LHG	C29-C30-C31-C32
24	b	606	CLA	C5-C6-C7-C8
27	a	2102	SQD	C32-C33-C34-C35
29	J	102	LMT	C5-C6-C7-C8
38	D	408	DGD	C8A-C9A-CAA-CBA
29	a	2103	LMT	C2-C3-C4-C5
28	C	526	LMG	C11-C12-C13-C14
28	C	526	LMG	C29-C30-C31-C32
29	z	1801	LMT	C7-C8-C9-C10
36	B	627	HTG	C2'-C3'-C4'-C5'
43	V	201	HEC	C4C-C3C-CAC-CBC
29	B	637	LMT	C6-C7-C8-C9
28	c	521	LMG	C33-C34-C35-C36
28	c	522	LMG	C35-C36-C37-C38
38	C	517	DGD	C4B-C5B-C6B-C7B
29	J	102	LMT	O5'-C5'-C6'-O6'
27	A	413	SQD	C2-C1-O6-C44
29	J	102	LMT	C2'-C1'-O1'-C1
29	a	2103	LMT	C2'-C1'-O1'-C1
29	b	624	LMT	C2'-C1'-O1'-C1
29	m	102	LMT	C2'-C1'-O1'-C1
27	F	101	SQD	C26-C27-C28-C29
28	C	520	LMG	C21-C22-C23-C24
28	b	623	LMG	C35-C36-C37-C38
28	c	521	LMG	C32-C33-C34-C35
28	i	101	LMG	C11-C12-C13-C14
39	D	409	LHG	C25-C26-C27-C28
28	c	522	LMG	O6-C5-C6-O5
28	D	412	LMG	C12-C13-C14-C15
28	b	623	LMG	C20-C21-C22-C23
28	c	521	LMG	C18-C19-C20-C21
39	E	101	LHG	C26-C27-C28-C29
25	A	407	PHO	C2-C3-C5-C6
24	A	409	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	612	CLA	C11-C10-C8-C9
24	C	507	CLA	C11-C12-C13-C14
24	D	405	CLA	C11-C10-C8-C9
24	a	2110	CLA	C6-C7-C8-C9
24	c	512	CLA	C11-C12-C13-C14
39	l	101	LHG	C7-C8-C9-C10
38	C	517	DGD	CCA-CDA-CEA-CFA
39	E	101	LHG	C18-C19-C20-C21
24	a	2113	CLA	C10-C11-C12-C13
24	B	602	CLA	O1A-CGA-O2A-C1
27	B	621	SQD	O10-C23-O48-C46
36	b	626	HTG	C1'-C2'-C3'-C4'
37	O	303	GOL	C1-C2-C3-O3
37	U	502	GOL	O1-C1-C2-C3
37	V	203	GOL	O1-C1-C2-C3
37	V	203	GOL	C1-C2-C3-O3
37	Z	102	GOL	C1-C2-C3-O3
37	d	415	GOL	C1-C2-C3-O3
37	o	2601	GOL	C1-C2-C3-O3
37	v	204	GOL	O1-C1-C2-C3
39	D	411	LHG	O1-C1-C2-C3
39	d	408	LHG	O1-C1-C2-C3
24	b	607	CLA	C13-C15-C16-C17
27	L	102	SQD	C29-C30-C31-C32
28	c	522	LMG	C36-C37-C38-C39
38	c	520	DGD	C8B-C9B-CAB-CBB
28	c	522	LMG	C10-C11-C12-C13
39	L	101	LHG	C7-C8-C9-C10
27	A	411	SQD	C11-C12-C13-C14
27	A	413	SQD	C33-C34-C35-C36
28	A	412	LMG	C12-C13-C14-C15
39	D	409	LHG	C32-C33-C34-C35
39	D	411	LHG	C27-C28-C29-C30
39	E	101	LHG	C25-C26-C27-C28
36	C	522	HTG	O5-C5-C6-O6
24	B	616	CLA	C4B-C3B-CAB-CBB
24	C	514	CLA	C4B-C3B-CAB-CBB
24	c	514	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	C16-C17-C18-C20
29	a	2120	LMT	C4B-C5B-C6B-O6B
27	A	413	SQD	O5-C1-O6-C44
29	B	636	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
29	J	102	LMT	O5'-C1'-O1'-C1
29	m	102	LMT	O5'-C1'-O1'-C1
31	x	801	PL9	C19-C21-C22-C23
28	A	412	LMG	C15-C16-C17-C18
29	A	414	LMT	C5'-C4'-O1B-C1B
38	C	518	DGD	C9A-CAA-CBA-CCA
38	C	518	DGD	C4B-C5B-C6B-C7B
39	E	101	LHG	C9-C10-C11-C12
27	L	102	SQD	C27-C28-C29-C30
28	A	412	LMG	C36-C37-C38-C39
29	i	104	LMT	C2-C3-C4-C5
39	d	408	LHG	C29-C30-C31-C32
39	E	101	LHG	C7-C8-C9-C10
24	c	508	CLA	C15-C16-C17-C18
28	b	623	LMG	C19-C20-C21-C22
39	d	408	LHG	C27-C28-C29-C30
24	C	513	CLA	CBA-CGA-O2A-C1
28	c	521	LMG	C16-C17-C18-C19
24	b	619	CLA	C5-C6-C7-C8
29	E	105	LMT	O5'-C5'-C6'-O6'
29	I	1201	LMT	C2-C1-O1'-C1'
28	C	520	LMG	C14-C15-C16-C17
29	i	104	LMT	C7-C8-C9-C10
38	c	520	DGD	CBA-CCA-CDA-CEA
39	e	101	LHG	C17-C18-C19-C20
28	B	622	LMG	C28-C29-C30-C31
24	b	618	CLA	C16-C17-C18-C19
24	b	618	CLA	C16-C17-C18-C20
27	B	621	SQD	C11-C10-C9-C8
27	f	102	SQD	C25-C26-C27-C28
28	C	520	LMG	C31-C32-C33-C34
28	D	412	LMG	C35-C36-C37-C38
28	b	623	LMG	C21-C22-C23-C24
36	V	204	HTG	C2'-C3'-C4'-C5'
38	C	517	DGD	C5B-C6B-C7B-C8B
38	c	518	DGD	C4B-C5B-C6B-C7B
25	A	407	PHO	C4-C3-C5-C6
25	a	2111	PHO	C4-C3-C5-C6
24	c	512	CLA	C2-C3-C5-C6
28	B	622	LMG	C37-C38-C39-C40
29	A	414	LMT	C3'-C4'-O1B-C1B
37	H	103	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
37	U	501	GOL	O2-C2-C3-O3
37	o	2601	GOL	O2-C2-C3-O3
37	o	2603	GOL	O2-C2-C3-O3
37	v	204	GOL	O1-C1-C2-O2
27	L	102	SQD	C28-C29-C30-C31
38	H	102	DGD	C7A-C8A-C9A-CAA
24	C	513	CLA	O1A-CGA-O2A-C1
39	l	101	LHG	C11-C10-C9-C8
24	B	610	CLA	C2B-C3B-CAB-CBB
24	B	616	CLA	C2B-C3B-CAB-CBB
24	C	514	CLA	C2B-C3B-CAB-CBB
24	c	514	CLA	C2B-C3B-CAB-CBB
28	c	521	LMG	C15-C16-C17-C18
29	f	101	LMT	C5-C6-C7-C8
27	F	101	SQD	C33-C34-C35-C36
28	A	412	LMG	C19-C20-C21-C22
38	h	703	DGD	C7A-C8A-C9A-CAA
43	V	201	HEC	C4B-C3B-CAB-CBB
24	B	617	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C1-O2A-CGA
24	b	604	CLA	C2-C1-O2A-CGA
29	Z	101	LMT	O1'-C1-C2-C3
38	c	518	DGD	C9A-CAA-CBA-CCA
27	A	413	SQD	C19-C20-C21-C22
27	B	621	SQD	C27-C28-C29-C30
38	D	408	DGD	C5A-C6A-C7A-C8A
26	B	618	BCR	C5-C6-C7-C8
26	b	620	BCR	C5-C6-C7-C8
26	c	517	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
26	d	406	BCR	C23-C24-C25-C30
29	B	637	LMT	C9-C10-C11-C12
29	T	102	LMT	C4-C5-C6-C7
24	A	409	CLA	C15-C16-C17-C18
24	B	615	CLA	C10-C11-C12-C13
24	D	405	CLA	C13-C15-C16-C17
24	a	2113	CLA	C8-C10-C11-C12
28	i	101	LMG	C36-C37-C38-C39
39	L	101	LHG	C11-C10-C9-C8
28	c	522	LMG	C28-C29-C30-C31
28	B	622	LMG	C16-C17-C18-C19
24	a	2110	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	d	411	LMG	C12-C13-C14-C15
43	v	201	HEC	C4B-C3B-CAB-CBB
24	C	511	CLA	C4-C3-C5-C6
24	c	512	CLA	C4-C3-C5-C6
24	A	409	CLA	C6-C7-C8-C10
24	B	612	CLA	C11-C10-C8-C7
24	B	617	CLA	C12-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C15
24	C	506	CLA	C2-C3-C5-C6
24	C	511	CLA	C2-C3-C5-C6
24	D	405	CLA	C11-C10-C8-C7
24	a	2110	CLA	C6-C7-C8-C10
24	c	506	CLA	C12-C13-C15-C16
24	c	512	CLA	C11-C12-C13-C15
25	a	2111	PHO	C2-C3-C5-C6
28	A	412	LMG	C13-C14-C15-C16
29	m	102	LMT	C6-C7-C8-C9
24	b	619	CLA	C15-C16-C17-C18
28	C	520	LMG	C10-C11-C12-C13
27	f	102	SQD	C30-C31-C32-C33
38	C	517	DGD	C2A-C3A-C4A-C5A
38	c	519	DGD	CAB-CBB-CCB-CDB
39	E	101	LHG	C33-C34-C35-C36
24	a	2109	CLA	C2C-C3C-CAC-CBC
28	c	521	LMG	C14-C15-C16-C17
38	C	518	DGD	C3B-C4B-C5B-C6B
39	L	101	LHG	C33-C34-C35-C36
29	B	636	LMT	C5-C6-C7-C8
39	d	408	LHG	C32-C33-C34-C35
38	c	518	DGD	O6E-C5E-C6E-O5E
29	M	101	LMT	O5'-C1'-O1'-C1
29	a	2103	LMT	O5'-C1'-O1'-C1
24	d	405	CLA	C13-C15-C16-C17
27	F	101	SQD	C24-C25-C26-C27
39	E	101	LHG	C11-C10-C9-C8
39	d	409	LHG	C32-C33-C34-C35
28	C	520	LMG	C32-C33-C34-C35
24	b	616	CLA	C8-C10-C11-C12
28	A	412	LMG	C21-C22-C23-C24
38	C	517	DGD	C1B-C2B-C3B-C4B
39	l	101	LHG	C13-C14-C15-C16
29	B	636	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
28	D	412	LMG	C30-C31-C32-C33
29	a	2103	LMT	C4B-C5B-C6B-O6B
24	b	614	CLA	C16-C17-C18-C19
29	B	623	LMT	C5'-C4'-O1B-C1B
29	j	1601	LMT	C2-C3-C4-C5
39	L	101	LHG	C13-C14-C15-C16
38	C	517	DGD	O6E-C5E-C6E-O5E
24	B	617	CLA	C4-C3-C5-C6
24	B	615	CLA	C14-C13-C15-C16
29	B	623	LMT	C3'-C4'-O1B-C1B
38	c	520	DGD	CCB-CDB-CEB-CFB
27	f	102	SQD	C26-C27-C28-C29
28	B	622	LMG	C36-C37-C38-C39
38	c	519	DGD	C9A-CAA-CBA-CCA
36	B	627	HTG	O5-C5-C6-O6
24	B	609	CLA	C13-C15-C16-C17
27	A	411	SQD	C12-C13-C14-C15
24	c	510	CLA	C1A-C2A-CAA-CBA
24	c	511	CLA	C8-C10-C11-C12
27	A	413	SQD	C34-C35-C36-C37
38	c	518	DGD	C8A-C9A-CAA-CBA
39	D	410	LHG	C32-C33-C34-C35
38	c	519	DGD	C1A-C2A-C3A-C4A
29	f	101	LMT	C1-C2-C3-C4
24	B	616	CLA	C10-C11-C12-C13
38	c	519	DGD	C4B-C5B-C6B-C7B
29	m	103	LMT	O5'-C5'-C6'-O6'
29	I	1201	LMT	O5'-C5'-C6'-O6'
36	C	521	HTG	C2'-C3'-C4'-C5'
38	c	518	DGD	C3B-C4B-C5B-C6B
28	c	521	LMG	C11-C12-C13-C14
29	E	105	LMT	C6-C7-C8-C9
29	Z	101	LMT	C3-C4-C5-C6
29	B	623	LMT	C6-C7-C8-C9
39	D	409	LHG	C7-C8-C9-C10
38	D	408	DGD	C6B-C7B-C8B-C9B
36	B	628	HTG	O5-C5-C6-O6
29	M	101	LMT	C4B-C5B-C6B-O6B
27	A	411	SQD	O6-C44-C45-C46
27	A	413	SQD	O6-C44-C45-C46
27	a	2102	SQD	O6-C44-C45-C46
27	a	2115	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
39	D	411	LHG	C14-C15-C16-C17
39	e	101	LHG	C19-C20-C21-C22
29	A	420	LMT	O5B-C5B-C6B-O6B
36	b	601	HTG	O5-C5-C6-O6
38	h	703	DGD	C9A-CAA-CBA-CCA
39	d	410	LHG	C28-C29-C30-C31
28	C	526	LMG	C8-C7-O1-C1
28	c	522	LMG	C8-C7-O1-C1
38	C	518	DGD	C2G-C3G-O3G-C1D
38	C	518	DGD	C5D-C6D-O5D-C1E
38	c	519	DGD	C2G-C3G-O3G-C1D
38	c	519	DGD	C5D-C6D-O5D-C1E
24	D	401	CLA	C2C-C3C-CAC-CBC
38	C	518	DGD	CBB-CCB-CDB-CEB
29	z	1801	LMT	O5'-C5'-C6'-O6'
24	C	511	CLA	C8-C10-C11-C12
28	c	522	LMG	C4-C5-C6-O5
37	b	631	GOL	O2-C2-C3-O3
37	k	2001	GOL	O1-C1-C2-O2
29	B	636	LMT	C4B-C5B-C6B-O6B
28	D	412	LMG	O6-C5-C6-O5
36	I	1202	HTG	O5-C5-C6-O6
31	d	407	PL9	C15-C14-C16-C17
28	c	521	LMG	C28-C29-C30-C31
29	B	637	LMT	C3-C4-C5-C6
24	B	604	CLA	C5-C6-C7-C8
29	A	414	LMT	C1-C2-C3-C4
38	H	102	DGD	C9A-CAA-CBA-CCA
38	c	519	DGD	CAA-CBA-CCA-CDA
27	B	621	SQD	C46-C45-O47-C7
24	C	508	CLA	C2-C1-O2A-CGA
27	L	102	SQD	C12-C13-C14-C15
27	f	102	SQD	C24-C25-C26-C27
27	a	2115	SQD	C24-C25-C26-C27
28	B	622	LMG	C15-C16-C17-C18
28	d	411	LMG	C19-C20-C21-C22
29	A	414	LMT	O1'-C1-C2-C3
36	B	625[B]	HTG	C1'-C2'-C3'-C4'
29	i	104	LMT	C2'-C1'-O1'-C1
29	j	1601	LMT	C2'-C1'-O1'-C1
38	C	518	DGD	C2E-C1E-O5D-C6D
27	a	2115	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	O47-C45-C46-O48
28	i	101	LMG	C40-C41-C42-C43
39	D	409	LHG	C13-C14-C15-C16
24	C	507	CLA	C16-C17-C18-C19
29	I	1201	LMT	C9-C10-C11-C12
39	D	410	LHG	C16-C17-C18-C19
38	c	519	DGD	C5B-C6B-C7B-C8B
24	A	409	CLA	C11-C10-C8-C7
24	A	409	CLA	C11-C12-C13-C15
24	B	611	CLA	C12-C13-C15-C16
24	B	614	CLA	C11-C10-C8-C7
24	B	615	CLA	C12-C13-C15-C16
24	a	2110	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C12-C13-C15
24	B	605	CLA	C6-C7-C8-C9
24	B	607	CLA	C11-C12-C13-C14
24	C	509	CLA	C11-C10-C8-C9
24	b	604	CLA	C11-C10-C8-C9
28	c	522	LMG	C34-C35-C36-C37
38	C	519	DGD	C9A-CAA-CBA-CCA
27	L	102	SQD	C24-C23-O48-C46
24	C	512	CLA	C8-C10-C11-C12
28	C	520	LMG	C11-C12-C13-C14
28	C	520	LMG	C39-C40-C41-C42
29	E	105	LMT	C1-C2-C3-C4
26	Y	302	BCR	C21-C22-C23-C24
28	i	101	LMG	C30-C31-C32-C33
39	e	101	LHG	C8-C7-O7-C5
27	L	102	SQD	C30-C31-C32-C33
27	a	2102	SQD	C13-C14-C15-C16
28	A	412	LMG	C14-C15-C16-C17
39	e	101	LHG	C12-C13-C14-C15
27	a	2115	SQD	C28-C29-C30-C31
27	A	411	SQD	C30-C31-C32-C33
29	a	2103	LMT	C5'-C4'-O1B-C1B
39	d	408	LHG	C30-C31-C32-C33
29	a	2120	LMT	C1-C2-C3-C4
24	B	607	CLA	C4B-C3B-CAB-CBB
24	B	610	CLA	C4B-C3B-CAB-CBB
24	b	612	CLA	C4B-C3B-CAB-CBB
24	b	604	CLA	C8-C10-C11-C12
39	d	408	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	a	2120	LMT	C2B-C1B-O1B-C4'
29	B	637	LMT	C4-C5-C6-C7
31	x	801	PL9	C25-C24-C26-C27
38	c	518	DGD	C7A-C8A-C9A-CAA
24	a	2113	CLA	C16-C17-C18-C20
36	d	403	HTG	C3'-C4'-C5'-C6'
39	l	101	LHG	C33-C34-C35-C36
38	C	517	DGD	O6D-C5D-C6D-O5D
27	f	102	SQD	C34-C35-C36-C37
38	c	518	DGD	C8B-C9B-CAB-CBB
39	e	101	LHG	C2-C3-O3-P
24	B	610	CLA	C3A-C2A-CAA-CBA
29	B	623	LMT	C2-C1-O1'-C1'
29	T	102	LMT	C2-C1-O1'-C1'
27	L	102	SQD	C11-C10-C9-C8
36	D	413	HTG	C4'-C5'-C6'-C7'
27	B	621	SQD	C7-C8-C9-C10
27	a	2115	SQD	C12-C13-C14-C15
38	C	518	DGD	C8B-C9B-CAB-CBB
39	d	410	LHG	C29-C30-C31-C32
39	l	101	LHG	C27-C28-C29-C30
24	b	604	CLA	CAA-CBA-CGA-O2A
29	f	101	LMT	C6-C7-C8-C9
38	h	703	DGD	C5B-C6B-C7B-C8B
24	a	2113	CLA	C16-C17-C18-C19
24	b	614	CLA	C16-C17-C18-C20
38	H	102	DGD	C5B-C6B-C7B-C8B
24	c	515	CLA	C3-C5-C6-C7
36	B	624	HTG	C4-C5-C6-O6
27	f	102	SQD	O6-C1-O5-C5
37	U	502	GOL	O1-C1-C2-O2
37	V	203	GOL	O1-C1-C2-O2
37	v	202	GOL	O2-C2-C3-O3
39	D	411	LHG	C24-C23-O8-C6
24	b	617	CLA	C16-C17-C18-C19
38	h	703	DGD	O2G-C1B-C2B-C3B
24	B	607	CLA	C2B-C3B-CAB-CBB
27	L	102	SQD	O10-C23-O48-C46
28	B	622	LMG	C40-C41-C42-C43
24	C	502	CLA	O1D-CGD-O2D-CED
27	A	411	SQD	O6-C44-C45-O47
27	F	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
27	a	2115	SQD	O6-C44-C45-O47
28	A	412	LMG	O1-C7-C8-O7
24	c	511	CLA	C13-C15-C16-C17
27	A	411	SQD	C8-C7-O47-C45
24	A	406	CLA	C16-C17-C18-C20
29	A	414	LMT	C2-C3-C4-C5
38	C	518	DGD	O6E-C1E-O5D-C6D
24	B	611	CLA	C8-C10-C11-C12
39	D	409	LHG	C1-C2-C3-O3
27	a	2102	SQD	C26-C27-C28-C29
28	b	623	LMG	C37-C38-C39-C40
24	b	617	CLA	C2-C1-O2A-CGA
25	a	2112	PHO	C2C-C3C-CAC-CBC
28	B	622	LMG	C34-C35-C36-C37
36	d	403	HTG	O5-C5-C6-O6
24	A	409	CLA	C14-C13-C15-C16
24	C	507	CLA	C14-C13-C15-C16
24	a	2113	CLA	C11-C12-C13-C14
24	c	504	CLA	C14-C13-C15-C16
24	c	509	CLA	C11-C10-C8-C9
24	c	515	CLA	C6-C7-C8-C9
28	D	412	LMG	C36-C37-C38-C39
28	D	412	LMG	C34-C35-C36-C37
38	c	520	DGD	CBB-CCB-CDB-CEB
24	B	606	CLA	C8-C10-C11-C12
24	C	507	CLA	C15-C16-C17-C18
39	D	411	LHG	C2-C3-O3-P
24	d	401	CLA	C2C-C3C-CAC-CBC
28	i	101	LMG	C34-C35-C36-C37
39	D	409	LHG	C17-C18-C19-C20
24	C	503	CLA	C16-C17-C18-C20
24	c	504	CLA	C16-C17-C18-C20
26	D	406	BCR	C23-C24-C25-C26
26	D	406	BCR	C23-C24-C25-C30
26	Y	302	BCR	C5-C6-C7-C8
26	c	528	BCR	C5-C6-C7-C8
24	A	409	CLA	C8-C10-C11-C12
27	F	101	SQD	C25-C26-C27-C28
27	L	102	SQD	C24-C25-C26-C27
29	a	2120	LMT	O1'-C1-C2-C3
24	A	405	CLA	C13-C15-C16-C17
24	B	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
38	C	519	DGD	C1B-C2B-C3B-C4B
29	B	636	LMT	O5'-C5'-C6'-O6'
27	A	411	SQD	O49-C7-O47-C45
28	C	520	LMG	C37-C38-C39-C40
29	B	623	LMT	C7-C8-C9-C10
24	c	508	CLA	C5-C6-C7-C8
27	a	2115	SQD	C30-C31-C32-C33
38	C	518	DGD	CAB-CBB-CCB-CDB
38	D	408	DGD	C2B-C3B-C4B-C5B
29	z	1801	LMT	C2-C1-O1'-C1'
24	B	602	CLA	C11-C10-C8-C7
24	B	605	CLA	C6-C7-C8-C10
24	B	607	CLA	C11-C12-C13-C15
24	C	507	CLA	C11-C12-C13-C15
24	C	509	CLA	C11-C10-C8-C7
24	C	510	CLA	C11-C10-C8-C7
24	a	2113	CLA	C11-C12-C13-C15
24	c	509	CLA	C11-C10-C8-C7
24	c	515	CLA	C12-C13-C15-C16
24	d	405	CLA	C6-C7-C8-C10
31	d	407	PL9	C13-C14-C16-C17
39	D	411	LHG	O10-C23-O8-C6
29	A	414	LMT	C7-C8-C9-C10
39	e	101	LHG	O9-C7-O7-C5
29	A	420	LMT	C3-C4-C5-C6
27	f	102	SQD	C28-C29-C30-C31
36	b	602	HTG	O5-C1-S1-C1'
36	c	523	HTG	O5-C1-S1-C1'
36	D	413	HTG	C1'-C2'-C3'-C4'
38	D	408	DGD	C3B-C4B-C5B-C6B
28	c	521	LMG	C39-C40-C41-C42
38	c	520	DGD	CDB-CEB-CFB-CGB
29	a	2120	LMT	O5B-C1B-O1B-C4'
24	B	605	CLA	O1D-CGD-O2D-CED
24	b	613	CLA	C15-C16-C17-C18
24	C	511	CLA	CAD-CBD-CGD-O2D
24	b	607	CLA	CAD-CBD-CGD-O2D
24	b	613	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	c	514	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D
24	B	617	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
39	l	101	LHG	C9-C10-C11-C12
38	H	102	DGD	O2G-C1B-C2B-C3B
24	b	619	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	CBA-CGA-O2A-C1
24	B	611	CLA	C16-C17-C18-C20
24	B	617	CLA	C2-C3-C5-C6
36	d	403	HTG	C4'-C5'-C6'-C7'
28	A	412	LMG	O1-C7-C8-C9
39	d	410	LHG	C2-C3-O3-P
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	617	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	608	CLA	CHA-CBD-CGD-O1D
24	c	504	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
36	O	302	HTG	C4-C5-C6-O6
29	B	623	LMT	C1-C2-C3-C4
29	M	101	LMT	C2'-C1'-O1'-C1
24	a	2109	CLA	C4C-C3C-CAC-CBC
29	I	1201	LMT	C6-C7-C8-C9
38	D	408	DGD	O1G-C1G-C2G-O2G
24	B	614	CLA	C13-C15-C16-C17
37	V	203	GOL	O2-C2-C3-O3
37	a	2101	GOL	O2-C2-C3-O3
37	v	204	GOL	O2-C2-C3-O3
39	D	410	LHG	O1-C1-C2-O2
39	d	408	LHG	O1-C1-C2-O2
39	d	409	LHG	O1-C1-C2-O2
28	D	412	LMG	C32-C33-C34-C35
36	d	414	HTG	S1-C1'-C2'-C3'
39	L	101	LHG	C9-C10-C11-C12
24	c	513	CLA	O1A-CGA-O2A-C1
36	O	302	HTG	O5-C5-C6-O6
24	c	511	CLA	C6-C7-C8-C9
24	d	405	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
39	d	410	LHG	C10-C11-C12-C13
24	C	512	CLA	O1A-CGA-O2A-C1
38	C	517	DGD	C4A-C5A-C6A-C7A
24	C	508	CLA	C5-C6-C7-C8
27	a	2102	SQD	C4-C5-C6-S
24	c	510	CLA	C15-C16-C17-C18
26	c	528	BCR	C37-C22-C23-C24
26	d	406	BCR	C7-C8-C9-C34
36	B	625[A]	HTG	C1'-C2'-C3'-C4'
37	O	303	GOL	O1-C1-C2-C3
36	V	204	HTG	C3'-C4'-C5'-C6'
26	c	528	BCR	C21-C22-C23-C24
24	C	509	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
24	c	515	CLA	C1A-C2A-CAA-CBA
24	b	604	CLA	C16-C17-C18-C20
24	C	504	CLA	C15-C16-C17-C18
39	L	101	LHG	C16-C17-C18-C19
27	a	2115	SQD	C25-C26-C27-C28
39	D	410	LHG	C3-O3-P-O6
39	D	410	LHG	C4-O6-P-O3
39	e	101	LHG	C4-O6-P-O3
31	D	407	PL9	C15-C14-C16-C17
38	C	517	DGD	C4D-C5D-C6D-O5D
27	L	102	SQD	C11-C12-C13-C14
39	e	101	LHG	C3-O3-P-O4
39	e	101	LHG	C3-O3-P-O5
39	D	411	LHG	C30-C31-C32-C33
28	A	412	LMG	O6-C1-O1-C7
24	b	618	CLA	C13-C15-C16-C17
38	C	518	DGD	CDA-CEA-CFA-CGA
24	b	610	CLA	C3-C5-C6-C7
39	l	101	LHG	C16-C17-C18-C19
24	b	613	CLA	C16-C17-C18-C19
29	a	2120	LMT	C4-C5-C6-C7
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	b	608	CLA	CAD-CBD-CGD-O1D
24	b	612	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	CAD-CBD-CGD-O1D
28	B	622	LMG	C10-C11-C12-C13
28	d	411	LMG	C29-C30-C31-C32
24	C	507	CLA	C3A-C2A-CAA-CBA
24	D	405	CLA	C6-C7-C8-C10
24	b	604	CLA	C12-C13-C15-C16
24	c	506	CLA	C11-C10-C8-C7
24	c	508	CLA	C11-C12-C13-C15
24	c	508	CLA	C12-C13-C15-C16
31	A	417	PL9	C13-C14-C16-C17
31	D	407	PL9	C13-C14-C16-C17
36	B	626	HTG	C2-C1-S1-C1'
36	C	522	HTG	C2-C1-S1-C1'
36	c	523	HTG	C2-C1-S1-C1'
39	L	101	LHG	C27-C28-C29-C30
29	z	1801	LMT	C6-C7-C8-C9
24	B	607	CLA	C13-C15-C16-C17
28	A	412	LMG	C10-C11-C12-C13
38	C	519	DGD	C8B-C9B-CAB-CBB
38	c	518	DGD	CAB-CBB-CCB-CDB
24	b	619	CLA	O1A-CGA-O2A-C1
39	D	409	LHG	O2-C2-C3-O3
27	B	621	SQD	C28-C29-C30-C31
27	L	102	SQD	C33-C34-C35-C36
27	L	102	SQD	C44-C45-C46-O48
38	D	408	DGD	O1G-C1G-C2G-C3G
27	a	2102	SQD	C24-C25-C26-C27
24	B	602	CLA	C8-C10-C11-C12
29	E	105	LMT	C9-C10-C11-C12
24	C	506	CLA	C4-C3-C5-C6
27	A	413	SQD	C24-C23-O48-C46
27	A	413	SQD	C32-C33-C34-C35
38	H	102	DGD	CCA-CDA-CEA-CFA
38	h	703	DGD	CCA-CDA-CEA-CFA
24	A	409	CLA	C11-C10-C8-C9
24	B	604	CLA	C6-C7-C8-C9
24	D	405	CLA	C6-C7-C8-C9
24	b	616	CLA	C11-C12-C13-C14
24	c	508	CLA	C14-C13-C15-C16
24	c	515	CLA	C14-C13-C15-C16
27	a	2102	SQD	C12-C13-C14-C15
24	b	613	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	a	2102	SQD	C14-C15-C16-C17
24	B	613	CLA	C8-C10-C11-C12
31	x	801	PL9	C9-C11-C12-C13
27	A	413	SQD	O10-C23-O48-C46
29	B	623	LMT	O5B-C1B-O1B-C4'
29	I	1201	LMT	C11-C10-C9-C8
28	c	521	LMG	C36-C37-C38-C39
24	b	612	CLA	C2B-C3B-CAB-CBB
24	c	506	CLA	C2B-C3B-CAB-CBB
24	d	404	CLA	C2B-C3B-CAB-CBB
24	b	617	CLA	C8-C10-C11-C12
36	C	521	HTG	C1'-C2'-C3'-C4'
31	A	417	PL9	C15-C14-C16-C17
31	x	801	PL9	C23-C24-C26-C27
24	b	611	CLA	C13-C15-C16-C17
28	B	622	LMG	C13-C14-C15-C16
29	f	101	LMT	C9-C10-C11-C12
38	c	519	DGD	C9B-CAB-CBB-CCB
24	B	612	CLA	C15-C16-C17-C18
24	c	506	CLA	C15-C16-C17-C18
27	B	621	SQD	C32-C33-C34-C35
38	C	519	DGD	C2A-C3A-C4A-C5A
27	L	102	SQD	C46-C45-O47-C7
39	l	101	LHG	O6-C4-C5-C6
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	609	CLA	C2A-CAA-CBA-CGA
24	B	611	CLA	C2-C1-O2A-CGA
38	c	520	DGD	O1A-C1A-O1G-C1G
38	H	102	DGD	C9B-CAB-CBB-CCB
39	D	409	LHG	C31-C32-C33-C34
38	c	518	DGD	C4D-C5D-C6D-O5D
24	c	512	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	C15-C16-C17-C18
26	C	515	BCR	C5-C6-C7-C8
26	a	2114	BCR	C1-C6-C7-C8
26	c	516	BCR	C1-C6-C7-C8
28	C	520	LMG	C33-C34-C35-C36
38	c	520	DGD	C2A-C1A-O1G-C1G
29	Z	101	LMT	C1-C2-C3-C4
24	B	607	CLA	C16-C17-C18-C20
27	F	101	SQD	C28-C29-C30-C31
24	b	617	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	b	618	CLA	C5-C6-C7-C8
25	a	2111	PHO	C8-C10-C11-C12
36	B	624	HTG	C3'-C4'-C5'-C6'
39	E	101	LHG	C4-O6-P-O3
27	F	101	SQD	C34-C35-C36-C37
27	F	101	SQD	C44-C45-C46-O48
28	B	622	LMG	C14-C15-C16-C17
24	B	603	CLA	C15-C16-C17-C18
24	A	409	CLA	C12-C13-C15-C16
24	B	604	CLA	C6-C7-C8-C10
24	c	507	CLA	C11-C12-C13-C15
39	D	411	LHG	C25-C26-C27-C28
24	B	617	CLA	C14-C13-C15-C16
24	a	2110	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C12-C13-C14
24	A	406	CLA	C16-C17-C18-C19
24	B	616	CLA	C16-C17-C18-C20
28	D	412	LMG	C10-C11-C12-C13
29	B	636	LMT	C3-C4-C5-C6
27	a	2102	SQD	C18-C19-C20-C21
26	T	101	BCR	C11-C12-C13-C35
26	b	622	BCR	C37-C22-C23-C24
26	t	102	BCR	C11-C12-C13-C35
24	c	507	CLA	C16-C17-C18-C19
27	B	621	SQD	C29-C30-C31-C32
39	d	409	LHG	C24-C23-O8-C6
37	o	2601	GOL	O1-C1-C2-C3
37	o	2603	GOL	O1-C1-C2-C3
26	D	406	BCR	C7-C8-C9-C10
29	i	104	LMT	C3-C4-C5-C6
28	b	623	LMG	O9-C10-O7-C8
28	b	623	LMG	C30-C31-C32-C33
29	B	636	LMT	O5B-C5B-C6B-O6B
38	D	408	DGD	CAB-CBB-CCB-CDB
24	B	616	CLA	C16-C17-C18-C19
24	c	512	CLA	CBA-CGA-O2A-C1
29	a	2120	LMT	C6-C7-C8-C9
29	a	2120	LMT	C9-C10-C11-C12
29	i	104	LMT	C6-C7-C8-C9
24	C	512	CLA	CBA-CGA-O2A-C1
24	D	404	CLA	C4B-C3B-CAB-CBB
24	c	506	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	d	404	CLA	C4B-C3B-CAB-CBB
38	c	518	DGD	O6E-C1E-O5D-C6D
39	L	101	LHG	O6-C4-C5-C6
38	c	518	DGD	O6D-C5D-C6D-O5D
27	a	2115	SQD	C13-C14-C15-C16
40	e	103	HEM	CAD-CBD-CGD-O1D
27	a	2115	SQD	C33-C34-C35-C36
24	C	503	CLA	C16-C17-C18-C19
24	b	617	CLA	C16-C17-C18-C20
27	L	102	SQD	C15-C16-C17-C18
38	C	517	DGD	C5A-C6A-C7A-C8A
36	B	627	HTG	C1'-C2'-C3'-C4'
36	V	204	HTG	C4-C5-C6-O6
24	B	613	CLA	C13-C15-C16-C17
27	a	2115	SQD	C11-C12-C13-C14
28	A	412	LMG	C2-C1-O1-C7
24	B	615	CLA	C2A-CAA-CBA-CGA
24	b	617	CLA	C2A-CAA-CBA-CGA
27	B	621	SQD	O47-C45-C46-O48
27	B	621	SQD	C26-C27-C28-C29
28	b	623	LMG	C16-C17-C18-C19
36	B	625[A]	HTG	C4'-C5'-C6'-C7'
38	h	703	DGD	C9B-CAB-CBB-CCB
36	i	103	HTG	O5-C5-C6-O6
24	c	504	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C20
29	a	2103	LMT	O1'-C1-C2-C3
28	c	521	LMG	C37-C38-C39-C40
38	C	517	DGD	C3B-C4B-C5B-C6B
36	B	624	HTG	O5-C5-C6-O6
38	c	519	DGD	C1B-C2B-C3B-C4B
24	B	617	CLA	C11-C10-C8-C9
24	c	506	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C12-C13-C14
38	c	518	DGD	C6A-C7A-C8A-C9A
40	F	102	HEM	CAD-CBD-CGD-O1D
28	C	526	LMG	O1-C7-C8-C9
24	c	514	CLA	O2A-C1-C2-C3
38	c	519	DGD	O6E-C1E-O5D-C6D
29	B	623	LMT	C9-C10-C11-C12
29	j	1601	LMT	C3-C4-C5-C6
39	l	101	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	a	2103	LMT	C1-C2-C3-C4
28	C	520	LMG	C40-C41-C42-C43
27	F	101	SQD	C46-C45-O47-C7
24	B	616	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	C	508	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C15
24	c	510	CLA	C12-C13-C15-C16
24	c	511	CLA	C12-C13-C15-C16
40	e	103	HEM	CAD-CBD-CGD-O2D
27	L	102	SQD	C9-C10-C11-C12
24	B	605	CLA	C13-C15-C16-C17
28	i	101	LMG	C33-C34-C35-C36
28	C	520	LMG	C16-C17-C18-C19
28	d	411	LMG	C30-C31-C32-C33
36	O	302	HTG	C4'-C5'-C6'-C7'
24	C	502	CLA	C13-C15-C16-C17
40	F	102	HEM	CAD-CBD-CGD-O2D
24	D	404	CLA	C2B-C3B-CAB-CBB
36	C	521	HTG	C4'-C5'-C6'-C7'
39	d	409	LHG	O10-C23-O8-C6
28	d	411	LMG	C10-C11-C12-C13
39	L	101	LHG	C10-C11-C12-C13
38	H	102	DGD	O1G-C1G-C2G-O2G
41	H	101	RRX	C9-C10-C11-C12
41	h	702	RRX	C9-C10-C11-C12
40	e	103	HEM	CAA-CBA-CGA-O1A
24	c	505	CLA	C10-C11-C12-C13
29	j	1601	LMT	O1'-C1-C2-C3
39	D	409	LHG	C30-C31-C32-C33
31	x	801	PL9	C34-C36-C37-C38
38	C	518	DGD	C6A-C7A-C8A-C9A
24	C	507	CLA	C4-C3-C5-C6
31	x	801	PL9	C15-C14-C16-C17
40	e	103	HEM	CAA-CBA-CGA-O2A
36	c	526	HTG	C1'-C2'-C3'-C4'
28	C	520	LMG	C17-C18-C19-C20
29	a	2103	LMT	C3-C4-C5-C6
24	C	504	CLA	C10-C11-C12-C13
24	C	509	CLA	C13-C15-C16-C17
24	b	613	CLA	C2A-CAA-CBA-CGA
24	c	503	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
39	D	411	LHG	C28-C29-C30-C31
26	A	410	BCR	C1-C6-C7-C8
26	C	515	BCR	C23-C24-C25-C30
26	C	516	BCR	C1-C6-C7-C8
26	Y	302	BCR	C1-C6-C7-C8
26	a	2114	BCR	C5-C6-C7-C8
26	b	621	BCR	C23-C24-C25-C30
26	c	528	BCR	C1-C6-C7-C8
29	Z	101	LMT	C5-C6-C7-C8
39	L	101	LHG	C17-C18-C19-C20
24	B	602	CLA	CAA-CBA-CGA-O2A
38	C	517	DGD	CAA-CBA-CCA-CDA
39	D	410	LHG	O1-C1-C2-C3
24	C	510	CLA	C13-C15-C16-C17
24	B	617	CLA	C10-C11-C12-C13
38	C	517	DGD	C5D-C6D-O5D-C1E
24	D	401	CLA	C4C-C3C-CAC-CBC
28	A	412	LMG	C30-C31-C32-C33
38	D	408	DGD	C7B-C8B-C9B-CAB
24	A	405	CLA	C16-C17-C18-C19
24	B	607	CLA	C16-C17-C18-C19
24	C	509	CLA	C5-C6-C7-C8
39	L	101	LHG	O6-C4-C5-O7
39	l	101	LHG	O6-C4-C5-O7
24	c	509	CLA	C2A-CAA-CBA-CGA
24	b	614	CLA	C8-C10-C11-C12
36	B	625[B]	HTG	C4'-C5'-C6'-C7'
24	C	506	CLA	C4B-C3B-CAB-CBB
31	A	417	PL9	C40-C39-C41-C42
31	A	417	PL9	C34-C36-C37-C38
24	A	406	CLA	C11-C10-C8-C7
24	a	2110	CLA	C12-C13-C15-C16
31	A	417	PL9	C12-C11-C9-C10
37	O	303	GOL	O1-C1-C2-O2
37	O	303	GOL	O2-C2-C3-O3
28	i	101	LMG	O8-C28-C29-C30
38	c	519	DGD	C2E-C1E-O5D-C6D
39	l	101	LHG	C17-C18-C19-C20
24	B	616	CLA	C5-C6-C7-C8
29	a	2103	LMT	O5B-C5B-C6B-O6B
36	B	625[A]	HTG	C2'-C1'-S1-C1
36	B	625[B]	HTG	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C4-C3-C5-C6
24	b	604	CLA	C4-C3-C5-C6
31	x	801	PL9	C40-C39-C41-C42
28	A	412	LMG	C29-C30-C31-C32
24	b	604	CLA	C2-C3-C5-C6
29	B	636	LMT	C6-C7-C8-C9
24	d	401	CLA	C4C-C3C-CAC-CBC
39	D	409	LHG	C33-C34-C35-C36
24	C	508	CLA	C14-C13-C15-C16
24	c	511	CLA	C14-C13-C15-C16
36	c	526	HTG	C2'-C3'-C4'-C5'
38	D	408	DGD	C7A-C8A-C9A-CAA
29	i	104	LMT	C5-C6-C7-C8
39	d	408	LHG	C34-C35-C36-C37
43	V	201	HEC	CAD-CBD-CGD-O2D
43	v	201	HEC	CAD-CBD-CGD-O2D
24	A	405	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	606	CLA	CAD-CBD-CGD-O2D
24	c	511	CLA	CAD-CBD-CGD-O2D
27	F	101	SQD	C44-C45-O47-C7
24	c	511	CLA	C3-C5-C6-C7
38	C	518	DGD	C5A-C6A-C7A-C8A
24	d	404	CLA	C2-C1-O2A-CGA
28	B	622	LMG	C30-C31-C32-C33
24	C	511	CLA	CAA-CBA-CGA-O2A
39	D	411	LHG	C16-C17-C18-C19
27	A	411	SQD	O47-C7-C8-C9
27	A	413	SQD	C28-C29-C30-C31
28	C	520	LMG	C30-C31-C32-C33
38	D	408	DGD	C2A-C3A-C4A-C5A
39	l	101	LHG	C25-C26-C27-C28
26	b	622	BCR	C21-C22-C23-C24
26	d	406	BCR	C7-C8-C9-C10
39	D	409	LHG	C11-C12-C13-C14
39	D	409	LHG	C15-C16-C17-C18
39	D	410	LHG	C14-C15-C16-C17
39	l	101	LHG	C30-C31-C32-C33
27	B	621	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
29	E	105	LMT	O1'-C1-C2-C3
38	C	518	DGD	O2G-C1B-C2B-C3B
29	M	101	LMT	O5B-C5B-C6B-O6B
43	V	201	HEC	CAD-CBD-CGD-O1D
24	D	404	CLA	O2A-C1-C2-C3
24	c	511	CLA	O2A-C1-C2-C3
24	d	404	CLA	O2A-C1-C2-C3
25	A	407	PHO	O2A-C1-C2-C3
38	c	520	DGD	C3B-C4B-C5B-C6B
24	b	615	CLA	C8-C10-C11-C12
43	v	201	HEC	CAD-CBD-CGD-O1D
27	f	102	SQD	C11-C10-C9-C8
27	a	2102	SQD	C31-C32-C33-C34
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	608	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	D	401	CLA	CHA-CBD-CGD-O1D
24	D	401	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O2D
39	E	101	LHG	O8-C23-C24-C25
31	x	801	PL9	C38-C39-C41-C42
39	d	409	LHG	C11-C10-C9-C8
39	e	101	LHG	C10-C11-C12-C13
38	c	519	DGD	C8A-C9A-CAA-CBA
39	D	409	LHG	O8-C23-C24-C25
28	c	522	LMG	O7-C8-C9-O8
38	h	703	DGD	O1G-C1G-C2G-O2G
38	c	518	DGD	C5A-C6A-C7A-C8A
24	C	504	CLA	O1D-CGD-O2D-CED
39	E	101	LHG	C10-C11-C12-C13
24	C	513	CLA	CAA-CBA-CGA-O2A
38	c	518	DGD	O2G-C1B-C2B-C3B
38	c	519	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
25	A	407	PHO	CHA-CBD-CGD-O1D
25	a	2111	PHO	CHA-CBD-CGD-O1D
39	d	408	LHG	C13-C14-C15-C16
28	b	623	LMG	C11-C10-O7-C8
29	T	102	LMT	C3-C4-C5-C6
24	C	507	CLA	C12-C13-C15-C16
24	b	609	CLA	C11-C10-C8-C7
38	C	517	DGD	O6E-C1E-O5D-C6D
24	B	616	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C14
24	C	504	CLA	C2B-C3B-CAB-CBB
24	A	405	CLA	C2C-C3C-CAC-CBC
29	B	637	LMT	C2-C3-C4-C5
29	a	2120	LMT	C3-C4-C5-C6
24	c	512	CLA	CAA-CBA-CGA-O2A
28	B	622	LMG	O8-C28-C29-C30
24	b	604	CLA	CAA-CBA-CGA-O1A
27	L	102	SQD	C5-C6-S-O8
31	A	417	PL9	C12-C11-C9-C8
29	M	101	LMT	C6-C7-C8-C9
39	E	101	LHG	C34-C35-C36-C37
37	a	2101	GOL	C1-C2-C3-O3
37	v	204	GOL	C1-C2-C3-O3
24	b	615	CLA	O1A-CGA-O2A-C1
26	T	101	BCR	C11-C12-C13-C14
26	t	102	BCR	C11-C12-C13-C14
28	i	101	LMG	C22-C23-C24-C25
24	B	610	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	CAA-CBA-CGA-O1A
27	A	411	SQD	O49-C7-C8-C9
38	h	703	DGD	O1B-C1B-C2B-C3B
29	m	102	LMT	C5-C6-C7-C8
38	C	519	DGD	C8A-C9A-CAA-CBA
29	B	623	LMT	C2B-C1B-O1B-C4'
40	F	102	HEM	CAA-CBA-CGA-O2A
38	H	102	DGD	O1G-C1G-C2G-C3G
24	b	605	CLA	C2A-CAA-CBA-CGA
24	c	512	CLA	CAA-CBA-CGA-O1A
24	A	405	CLA	C4C-C3C-CAC-CBC
28	i	101	LMG	C29-C30-C31-C32
38	D	408	DGD	C4A-C5A-C6A-C7A
28	C	520	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
31	d	407	PL9	C45-C44-C46-C47
29	T	102	LMT	C6-C7-C8-C9
24	B	602	CLA	C4B-C3B-CAB-CBB
24	B	603	CLA	C4B-C3B-CAB-CBB
24	C	502	CLA	C4B-C3B-CAB-CBB
39	D	410	LHG	C4-O6-P-O5
39	E	101	LHG	C4-O6-P-O5
39	d	409	LHG	C4-O6-P-O5
28	D	412	LMG	C18-C19-C20-C21
29	a	2103	LMT	C11-C10-C9-C8
24	C	511	CLA	CAA-CBA-CGA-O1A
28	b	623	LMG	C15-C16-C17-C18
38	c	519	DGD	CBA-CCA-CDA-CEA
26	C	516	BCR	C5-C6-C7-C8
26	c	516	BCR	C5-C6-C7-C8
24	c	509	CLA	C5-C6-C7-C8
38	C	518	DGD	O1B-C1B-C2B-C3B
39	E	101	LHG	O10-C23-C24-C25
28	c	521	LMG	C17-C18-C19-C20
38	c	519	DGD	C2A-C3A-C4A-C5A
24	b	615	CLA	CBA-CGA-O2A-C1
39	d	410	LHG	C11-C12-C13-C14
24	B	608	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	507	CLA	CAD-CBD-CGD-O1D
27	A	413	SQD	O5-C5-C6-S
38	c	519	DGD	CDA-CEA-CFA-CGA
24	B	613	CLA	CAA-CBA-CGA-O2A
24	A	406	CLA	C6-C7-C8-C9
24	C	505	CLA	C6-C7-C8-C9
24	C	513	CLA	C11-C10-C8-C9
24	a	2110	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C10-C8-C9
38	c	520	DGD	C9A-CAA-CBA-CCA
37	c	527	GOL	O2-C2-C3-O3
37	v	203	GOL	O2-C2-C3-O3
38	H	102	DGD	O1B-C1B-C2B-C3B
24	b	616	CLA	CAA-CBA-CGA-O2A
24	c	514	CLA	CAA-CBA-CGA-O2A
28	D	412	LMG	O7-C10-C11-C12
38	c	520	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
29	T	102	LMT	C2-C3-C4-C5
36	b	601	HTG	C2'-C3'-C4'-C5'
24	C	502	CLA	CAA-CBA-CGA-O2A
24	C	506	CLA	CAA-CBA-CGA-O2A
39	D	411	LHG	O8-C23-C24-C25
24	D	401	CLA	C15-C16-C17-C18
38	c	518	DGD	O1B-C1B-C2B-C3B
36	B	625[A]	HTG	C2'-C3'-C4'-C5'
38	c	518	DGD	CDA-CEA-CFA-CGA
24	A	406	CLA	C12-C13-C15-C16
24	B	612	CLA	C2-C3-C5-C6
24	C	505	CLA	C6-C7-C8-C10
24	C	507	CLA	C2-C3-C5-C6
24	C	512	CLA	C11-C12-C13-C15
27	B	621	SQD	C31-C32-C33-C34
24	A	405	CLA	C15-C16-C17-C18
39	D	409	LHG	O10-C23-C24-C25
28	d	411	LMG	O7-C10-C11-C12
28	C	526	LMG	C4-C5-C6-O5
24	B	611	CLA	C10-C11-C12-C13
24	C	513	CLA	C15-C16-C17-C18
24	C	502	CLA	CAA-CBA-CGA-O1A
38	c	519	DGD	O1B-C1B-C2B-C3B
28	i	101	LMG	C17-C18-C19-C20
38	C	519	DGD	CDA-CEA-CFA-CGA
25	a	2112	PHO	C8-C10-C11-C12
39	d	410	LHG	O8-C23-C24-C25
27	a	2115	SQD	C31-C32-C33-C34
24	b	618	CLA	C8-C10-C11-C12
24	b	608	CLA	C2A-CAA-CBA-CGA
24	B	616	CLA	C13-C15-C16-C17
24	C	508	CLA	C15-C16-C17-C18
28	b	623	LMG	C39-C40-C41-C42
29	i	104	LMT	C9-C10-C11-C12
28	c	521	LMG	C10-C11-C12-C13

There are no ring outliers.

170 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	604	CLA	1	0
27	F	101	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	d	406	BCR	1	0
24	B	606	CLA	4	0
29	A	414	LMT	2	0
28	b	623	LMG	1	0
36	B	625[A]	HTG	3	0
34	B	643	DMS	1	0
24	C	511	CLA	1	0
24	a	2110	CLA	2	0
38	C	519	DGD	1	0
24	c	510	CLA	3	0
24	C	504	CLA	5	0
24	b	607	CLA	3	0
24	B	613	CLA	1	0
24	B	605	CLA	3	0
24	b	604	CLA	4	0
24	D	401	CLA	2	0
26	T	101	BCR	5	0
24	b	610	CLA	1	0
36	b	625	HTG	3	0
34	U	503	DMS	2	0
29	i	104	LMT	1	0
24	c	507	CLA	2	0
29	B	636	LMT	1	0
36	b	601	HTG	1	0
24	D	404	CLA	2	0
36	D	413	HTG	3	0
34	b	633	DMS	1	0
24	C	506	CLA	1	0
29	M	101	LMT	2	0
24	C	510	CLA	4	0
38	C	518	DGD	6	0
34	c	532	DMS	1	0
27	A	411	SQD	2	0
27	a	2115	SQD	1	0
37	o	2603	GOL	1	0
24	B	615	CLA	2	0
24	b	608	CLA	6	0
26	c	517	BCR	2	0
32	a	2118[B]	K2I	2	0
26	c	528	BCR	1	0
28	C	520	LMG	1	0
29	a	2120	LMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	408	PHO	2	0
24	d	404	CLA	2	0
24	c	511	CLA	2	0
24	d	401	CLA	4	0
24	c	509	CLA	2	0
32	A	418[B]	K2I	2	0
24	C	509	CLA	2	0
24	C	512	CLA	2	0
24	C	514	CLA	6	0
34	B	647	DMS	1	0
34	o	2606	DMS	1	0
40	e	103	HEM	2	0
26	C	516	BCR	3	0
32	a	2119	K2I	1	0
26	K	101	BCR	1	0
38	h	703	DGD	1	0
37	D	403	GOL	1	0
24	b	614	CLA	1	0
24	C	505	CLA	1	0
26	A	410	BCR	1	0
31	d	407	PL9	1	0
26	t	102	BCR	6	0
38	C	517	DGD	2	0
34	C	534	DMS	1	0
24	B	617	CLA	3	0
36	O	302	HTG	1	0
41	H	101	RRX	3	0
39	D	411	LHG	2	0
26	B	618	BCR	2	0
36	b	602	HTG	3	0
39	D	409	LHG	3	0
24	b	605	CLA	1	0
37	B	635	GOL	2	0
24	B	612	CLA	1	0
29	a	2103	LMT	2	0
24	b	612	CLA	1	0
24	b	618	CLA	4	0
28	B	622	LMG	2	0
26	k	2003	BCR	1	0
24	B	614	CLA	1	0
24	B	607	CLA	1	0
27	B	621	SQD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	619	CLA	4	0
24	C	513	CLA	4	0
34	c	531	DMS	1	0
24	B	611	CLA	2	0
24	b	616	CLA	2	0
29	B	623	LMT	1	0
24	C	508	CLA	2	0
37	o	2601	GOL	1	0
39	e	101	LHG	1	0
29	A	420	LMT	1	0
34	b	643	DMS	1	0
24	C	502	CLA	4	0
39	L	101	LHG	2	0
27	a	2102	SQD	1	0
28	C	526	LMG	1	0
24	c	505	CLA	4	0
24	D	405	CLA	1	0
36	d	403	HTG	2	0
24	C	503	CLA	2	0
31	x	801	PL9	1	0
24	b	613	CLA	1	0
37	c	527	GOL	2	0
24	c	515	CLA	1	0
36	I	1202	HTG	1	0
41	h	702	RRX	3	0
26	b	622	BCR	2	0
26	a	2114	BCR	1	0
36	B	624	HTG	1	0
29	z	1801	LMT	2	0
38	c	518	DGD	1	0
29	m	102	LMT	2	0
34	v	205	DMS	1	0
36	B	628	HTG	1	0
32	A	419	K2I	1	0
24	B	616	CLA	2	0
26	b	621	BCR	3	0
28	i	101	LMG	2	0
24	c	513	CLA	4	0
24	C	507	CLA	1	0
25	a	2112	PHO	1	0
38	c	519	DGD	3	0
40	F	102	HEM	1	0

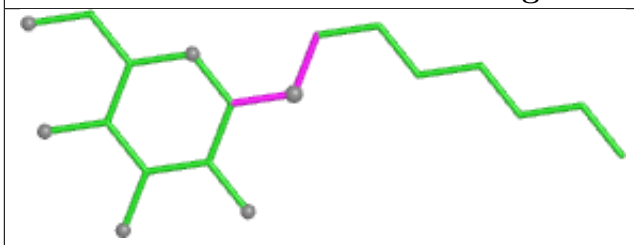
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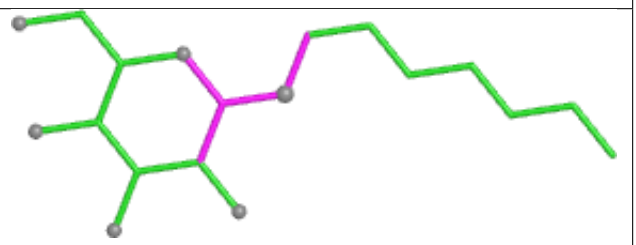
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	O	310	DMS	1	0
24	d	405	CLA	1	0
29	J	102	LMT	1	0
24	B	602	CLA	1	0
28	c	521	LMG	1	0
34	C	528	DMS	2	0
28	A	412	LMG	1	0
24	c	503	CLA	3	0
36	B	625[B]	HTG	3	0
24	a	2113	CLA	2	0
26	B	619	BCR	2	0
24	b	609	CLA	2	0
24	A	405	CLA	2	0
24	c	504	CLA	3	0
34	C	529	DMS	1	0
24	A	409	CLA	1	0
31	A	417	PL9	2	0
26	B	620	BCR	2	0
24	B	603	CLA	2	0
39	d	408	LHG	2	0
34	V	206	DMS	1	0
26	c	516	BCR	3	0
34	O	309	DMS	1	0
27	L	102	SQD	1	0
24	a	2109	CLA	2	0
39	E	101	LHG	5	0
26	C	515	BCR	4	0
36	b	626	HTG	1	0
34	d	417	DMS	2	0
24	c	506	CLA	5	0
24	c	512	CLA	1	0
24	B	610	CLA	4	0
24	c	514	CLA	4	0
27	f	102	SQD	1	0
39	d	409	LHG	1	0
24	c	508	CLA	2	0
39	l	101	LHG	1	0
26	Y	302	BCR	3	0
38	c	520	DGD	3	0
26	b	620	BCR	1	0
24	A	406	CLA	1	0
34	d	423	DMS	1	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.

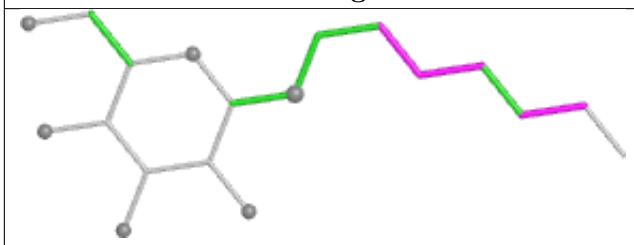
Ligand HTG C 521



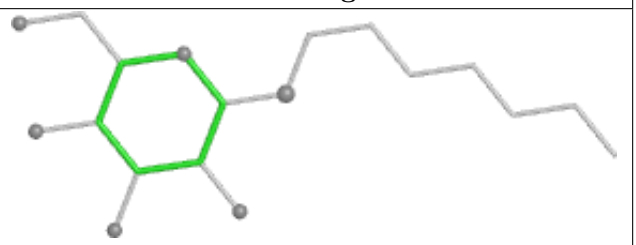
Bond lengths



Bond angles

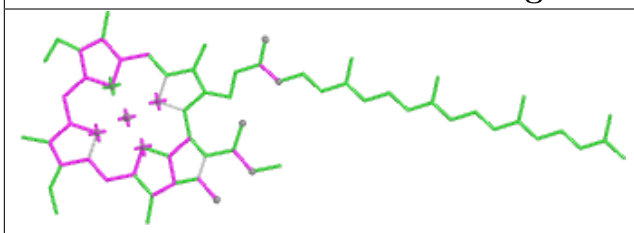


Torsions

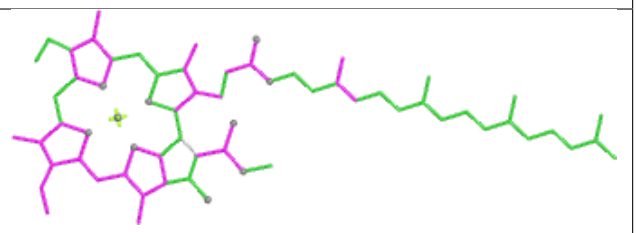


Rings

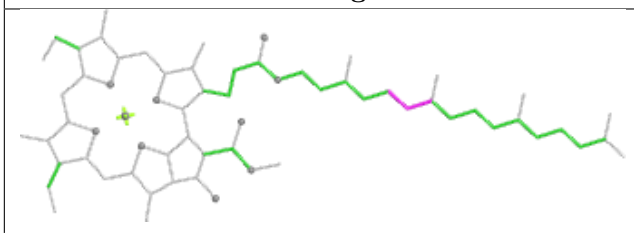
Ligand CLA B 604



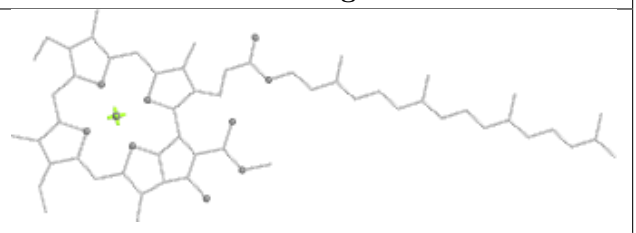
Bond lengths



Bond angles

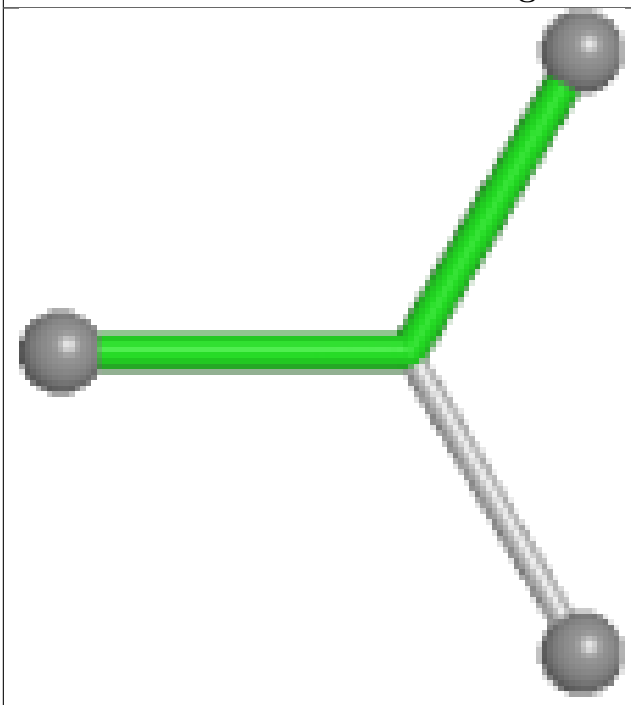


Torsions

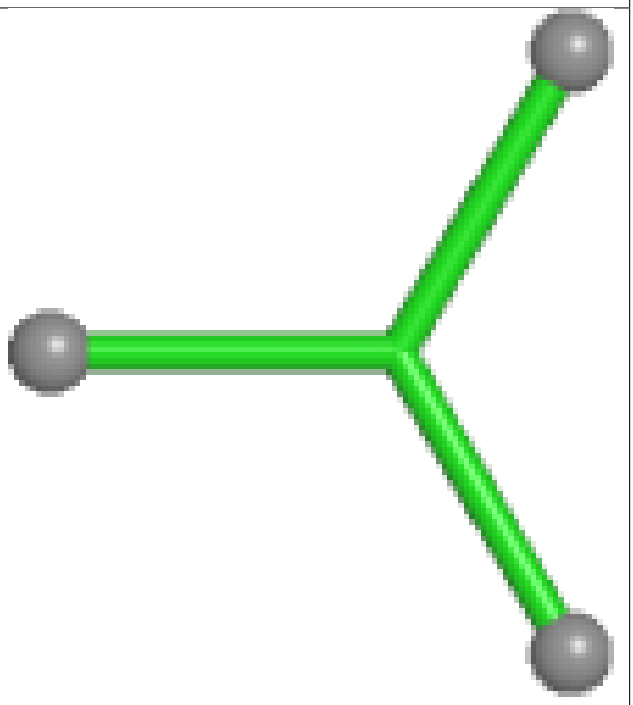


Rings

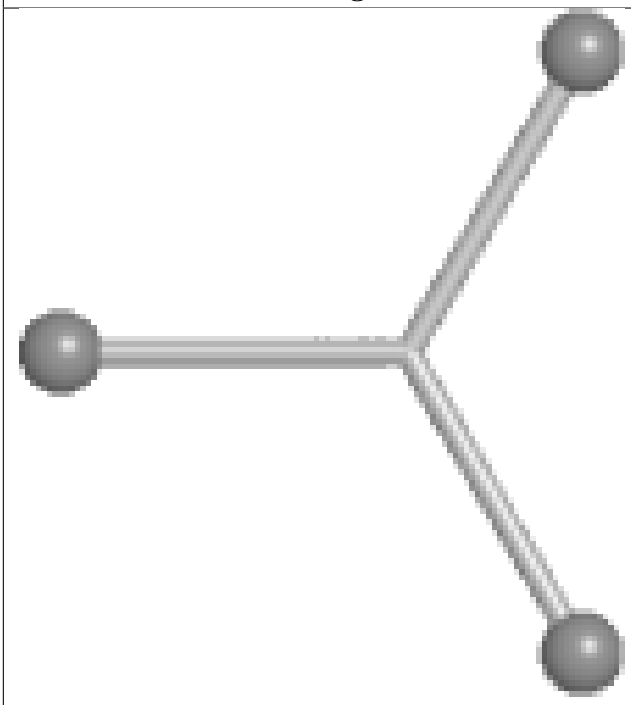
Ligand BCT a 2108



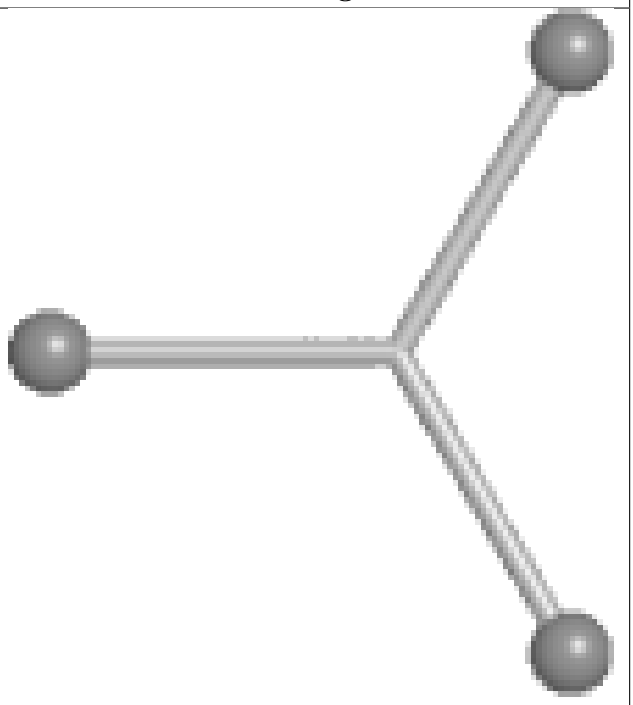
Bond lengths



Bond angles

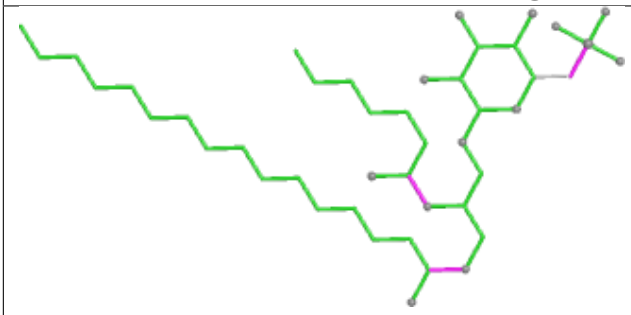


Torsions

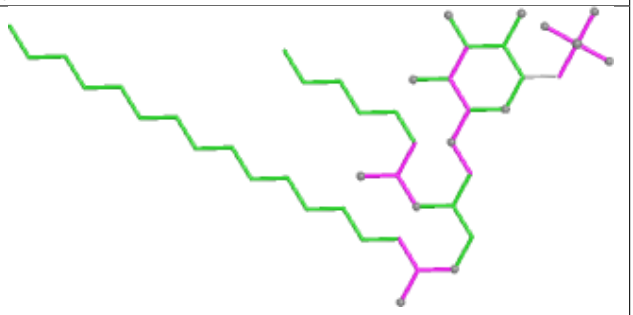


Rings

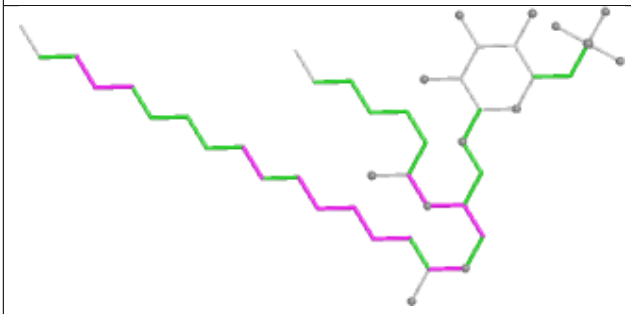
Ligand SQD F 101



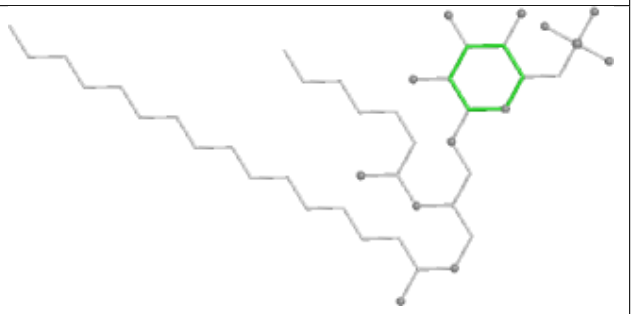
Bond lengths



Bond angles

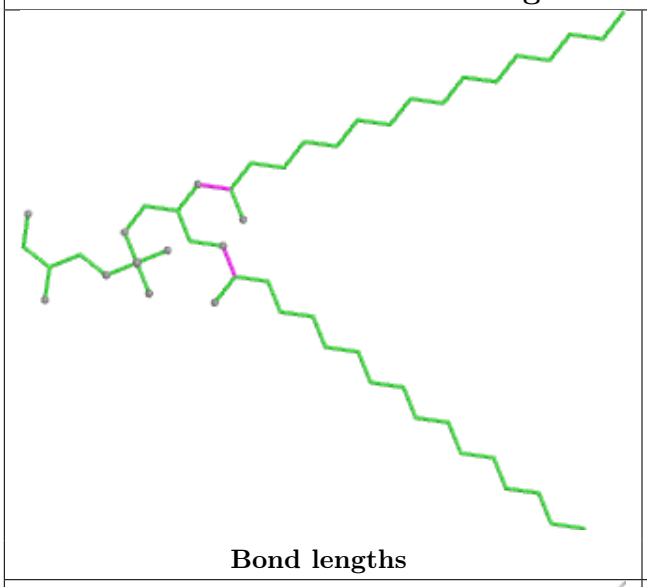


Torsions

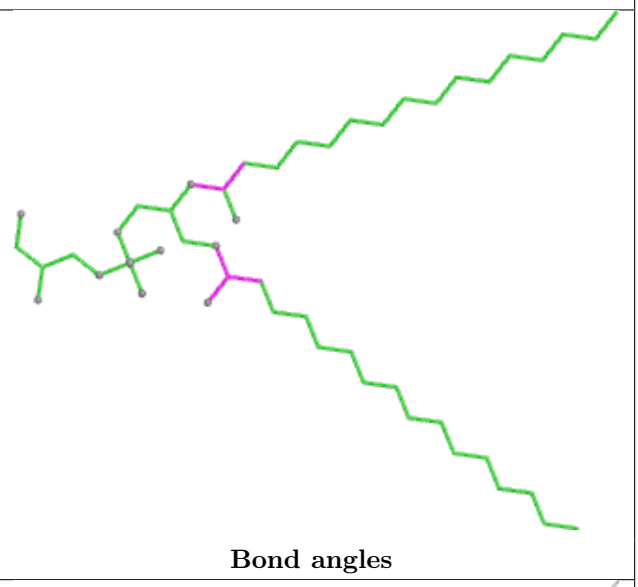


Rings

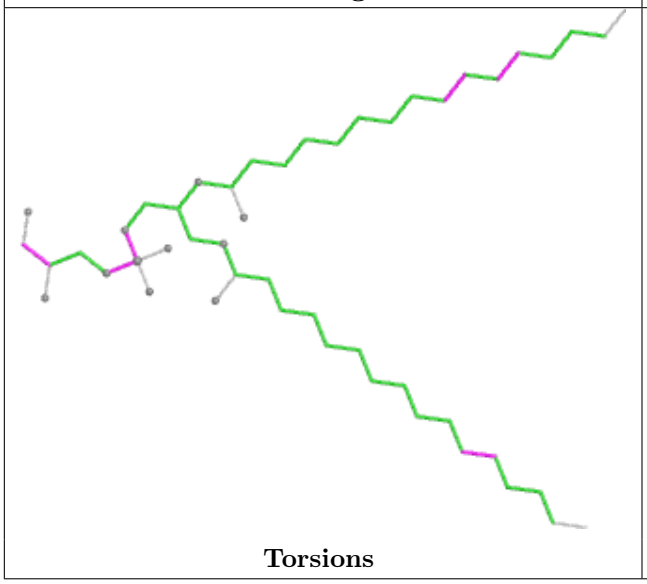
Ligand LHG D 410



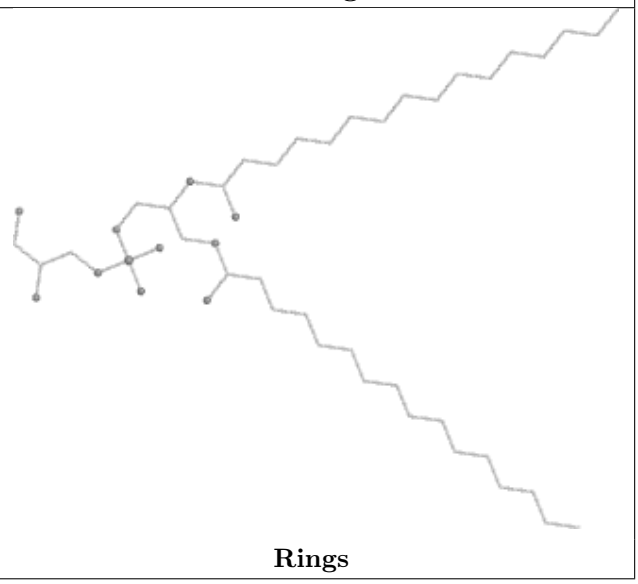
Bond lengths



Bond angles

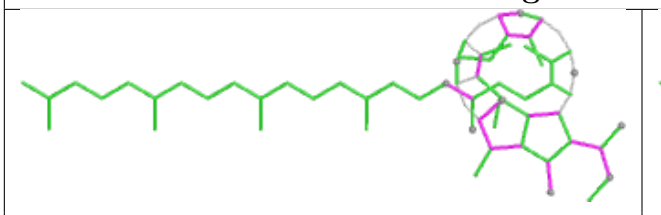


Torsions

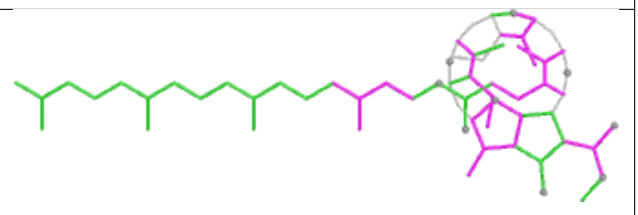


Rings

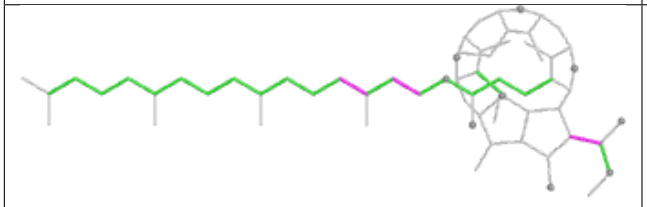
Ligand PHO A 407



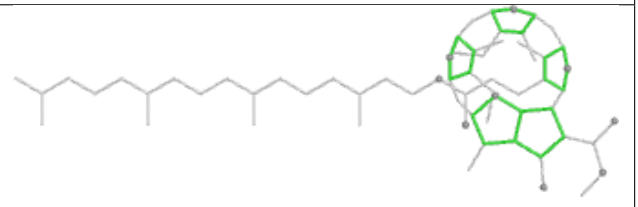
Bond lengths



Bond angles

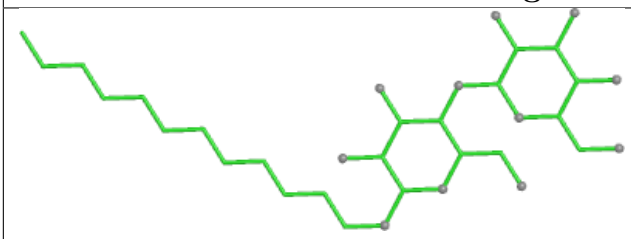


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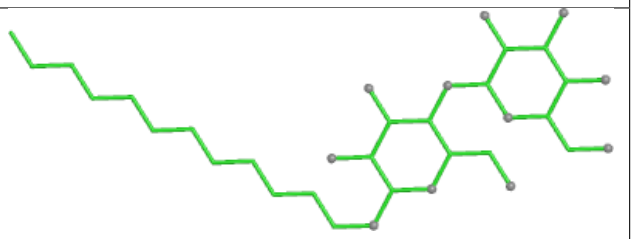


Rings

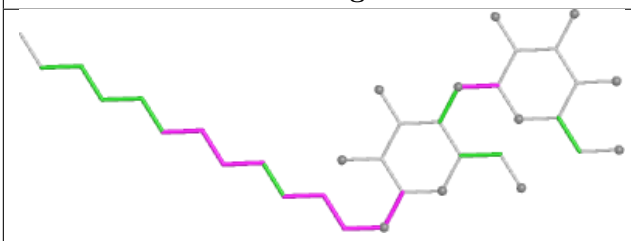
Ligand LMT Z 101



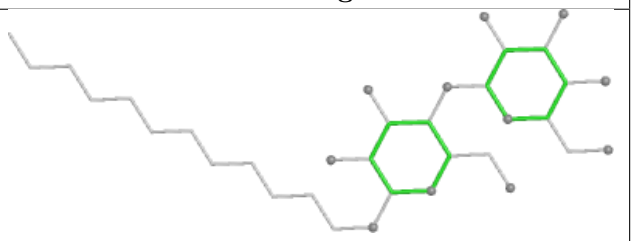
Bond lengths



Bond angles

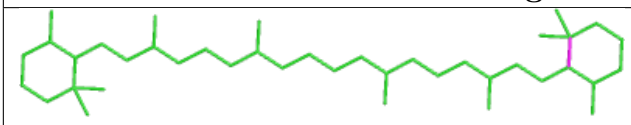


Torsions

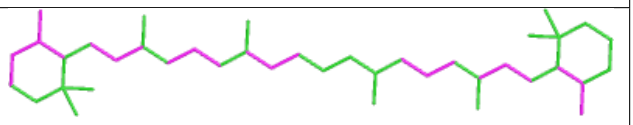


Rings

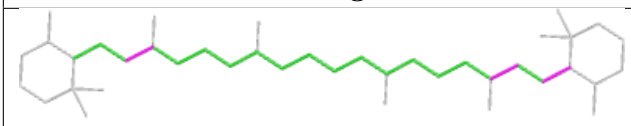
Ligand BCR d 406



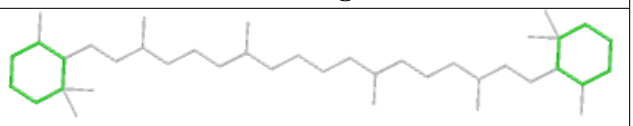
Bond lengths



Bond angles

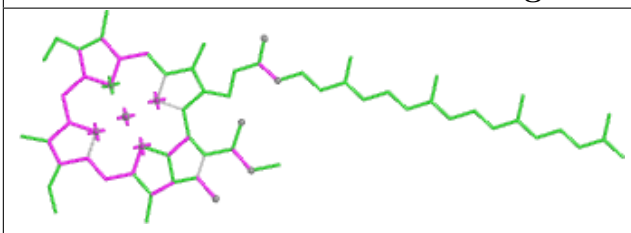


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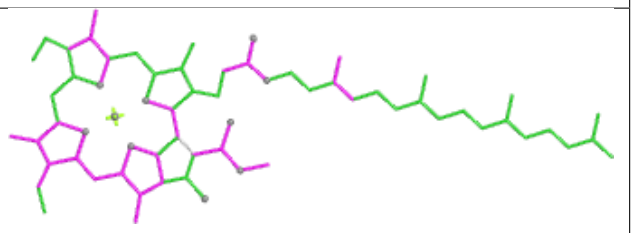


Rings

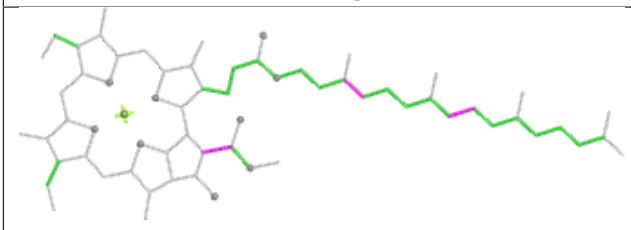
Ligand CLA B 606



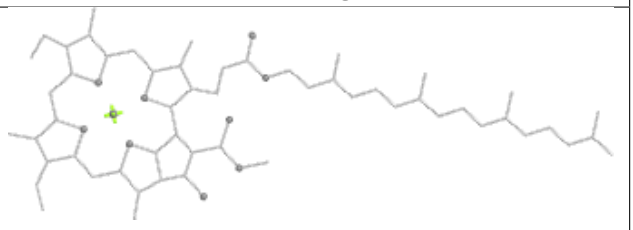
Bond lengths



Bond angles

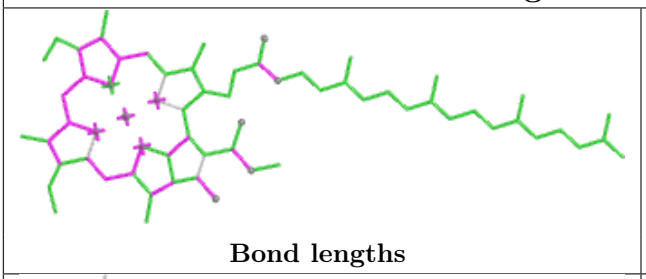


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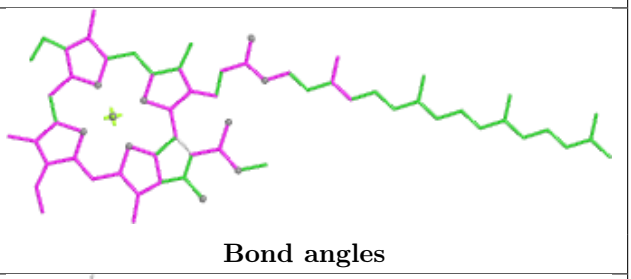


Rings

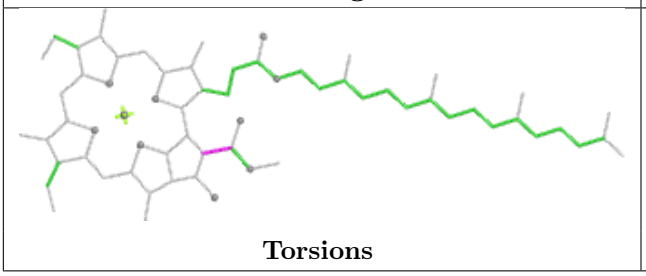
Ligand CLA B 608



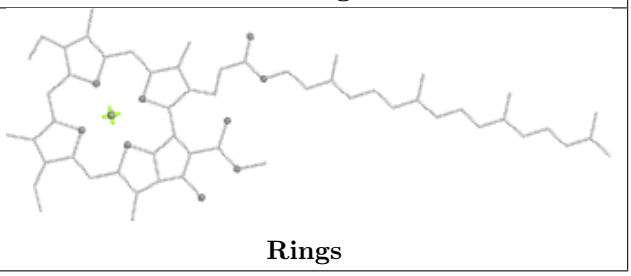
Bond lengths



Bond angles

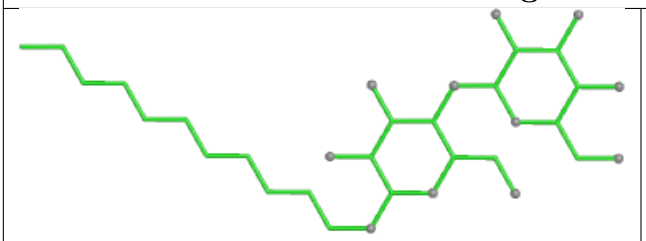


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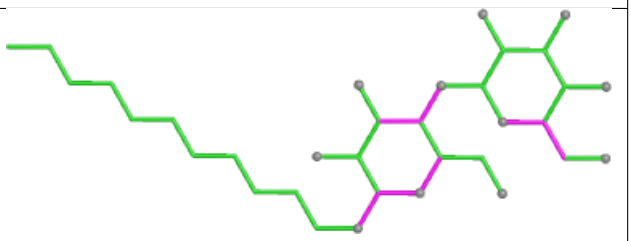


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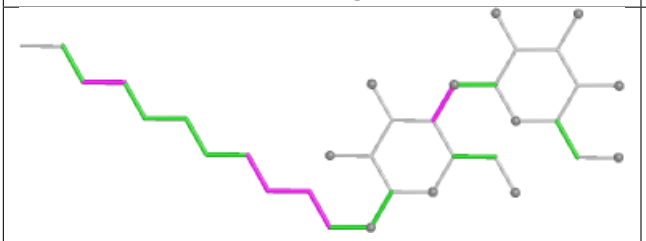
Ligand LMT A 414



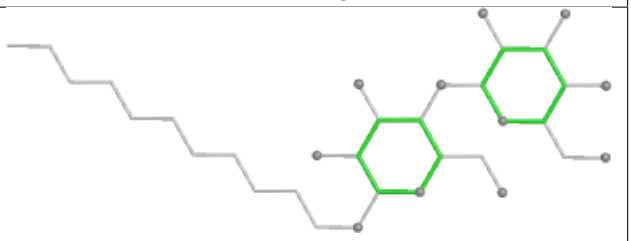
Bond lengths



Bond angles

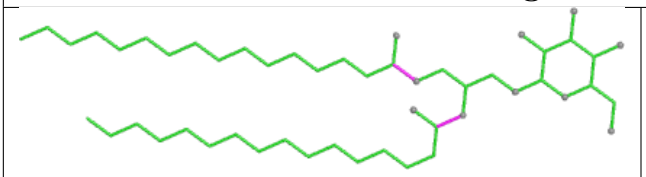


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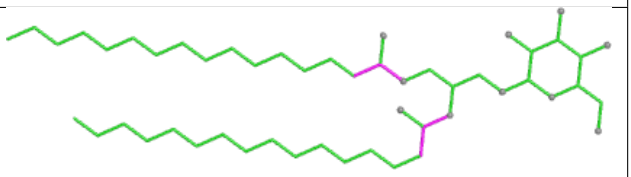


Rings

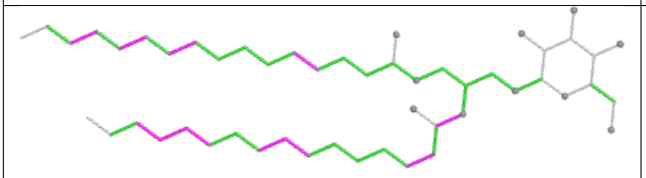
Ligand LMG b 623



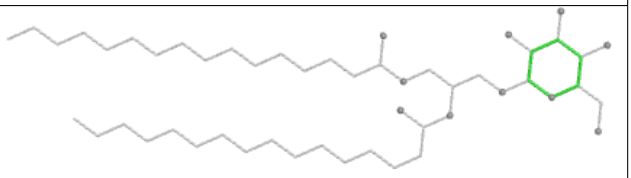
Bond lengths



Bond angles

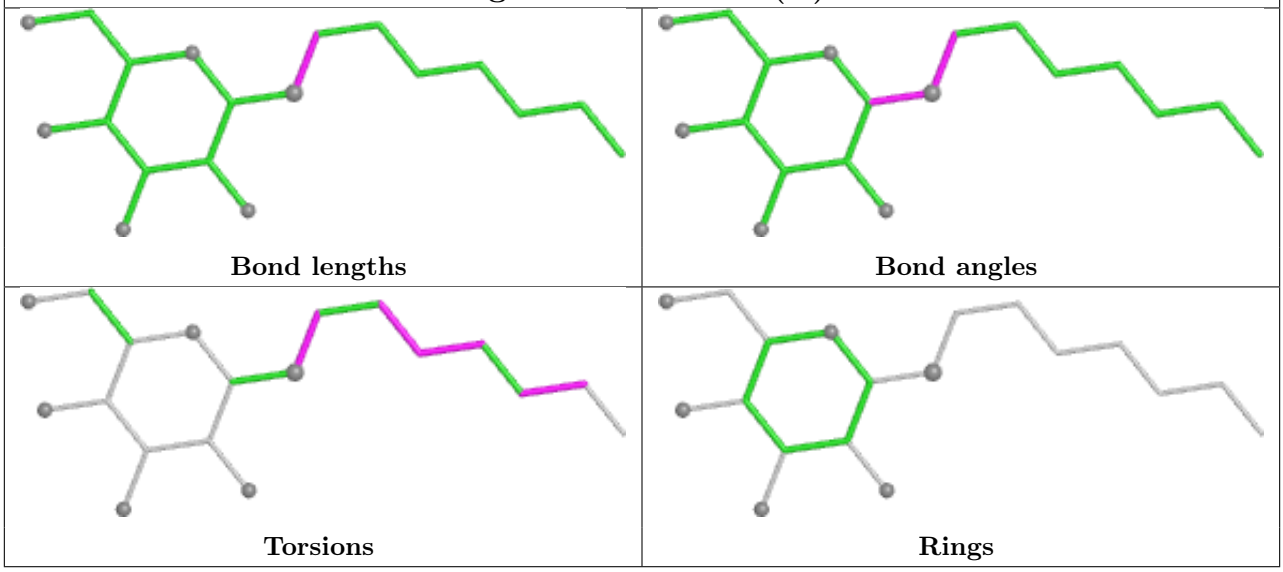


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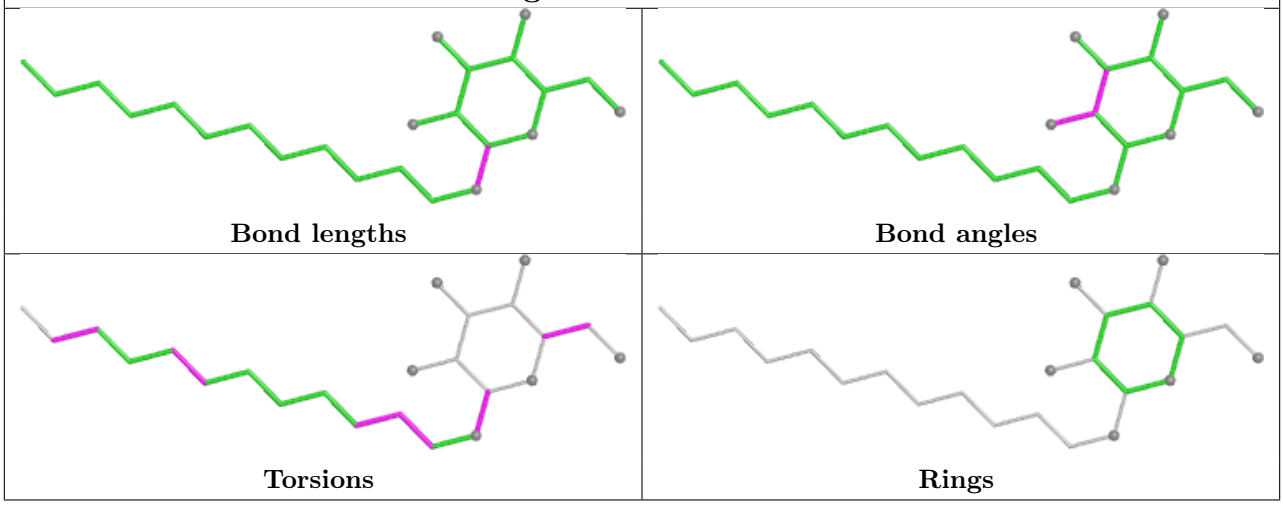


Rings

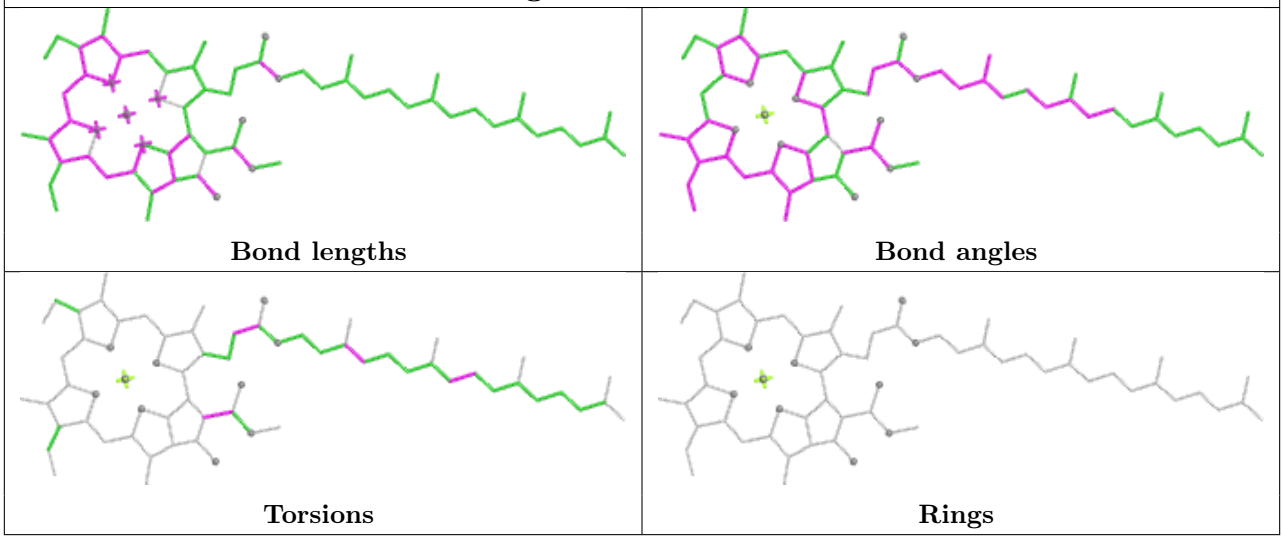
Ligand HTG B 625 (A)



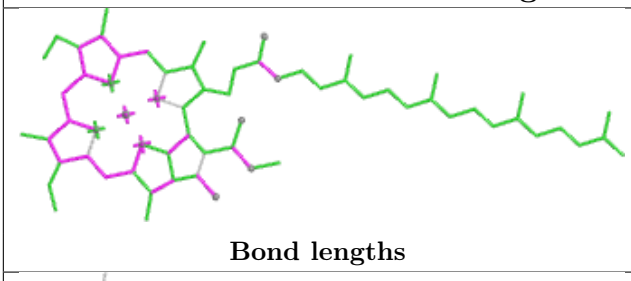
Ligand LMT E 105



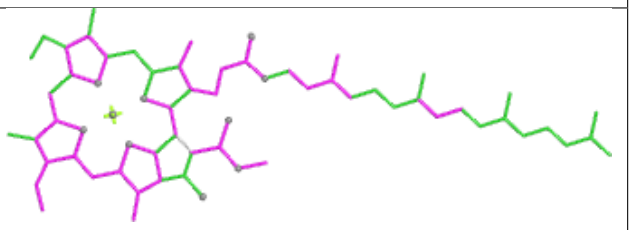
Ligand CLA C 511



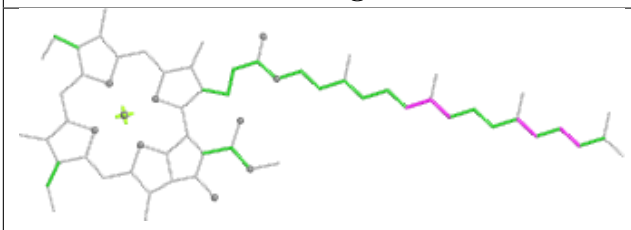
Ligand CLA a 2110



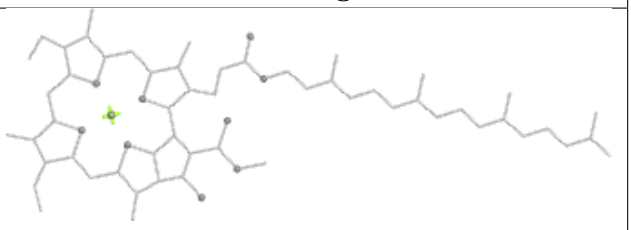
Bond lengths



Bond angles

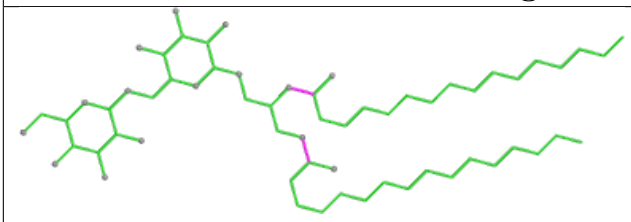


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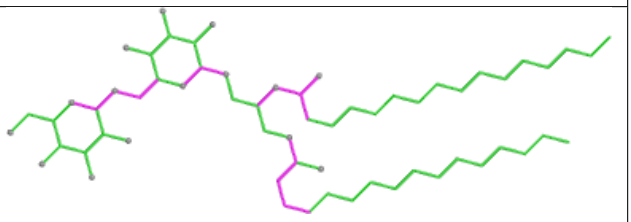


Rings

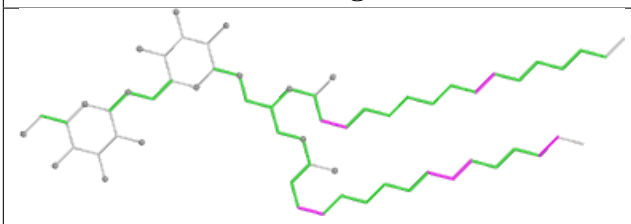
Ligand DGD C 519



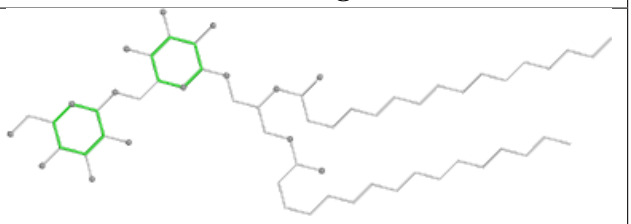
Bond lengths



Bond angles

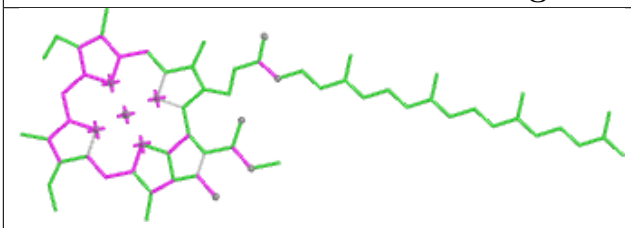


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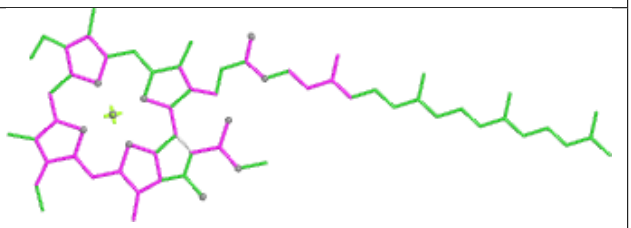


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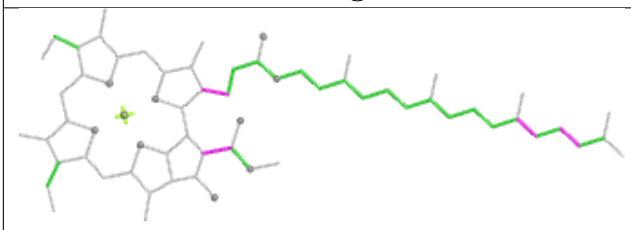
Ligand CLA c 510



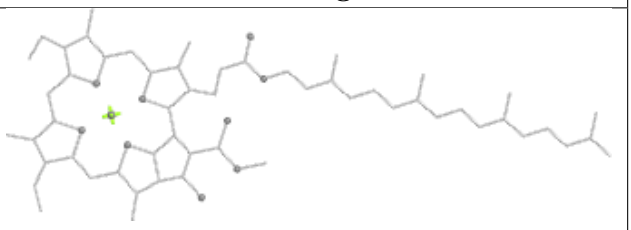
Bond lengths



Bond angles

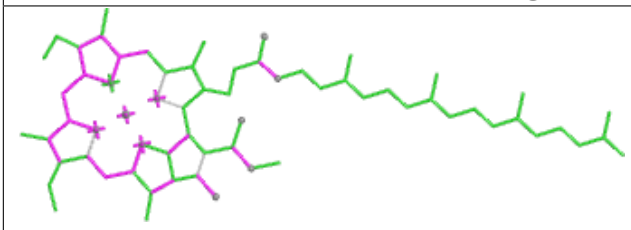


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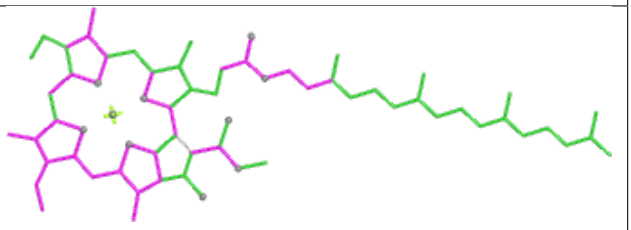


Rings

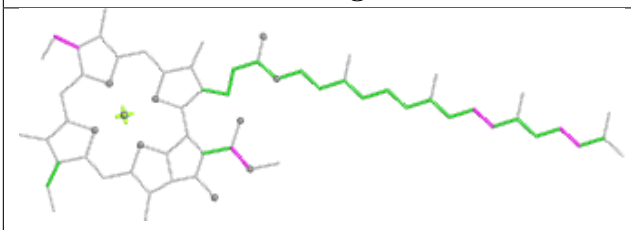
Ligand CLA C 504



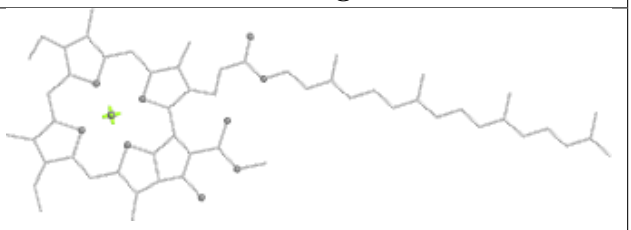
Bond lengths



Bond angles

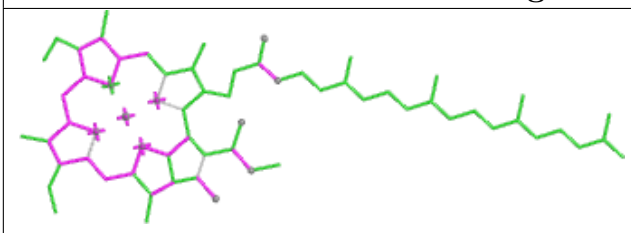


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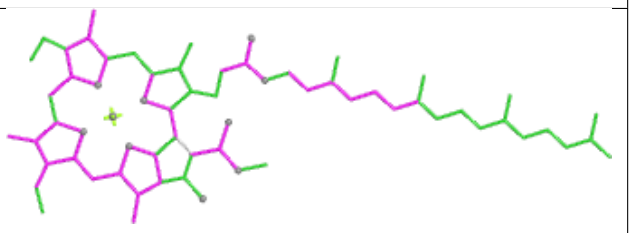


Rings

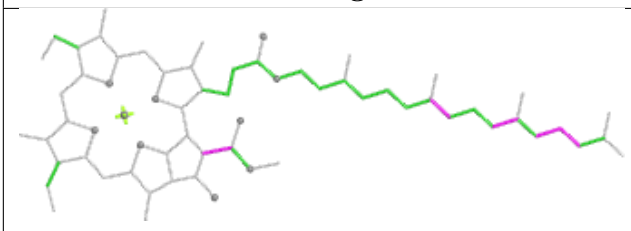
Ligand CLA b 607



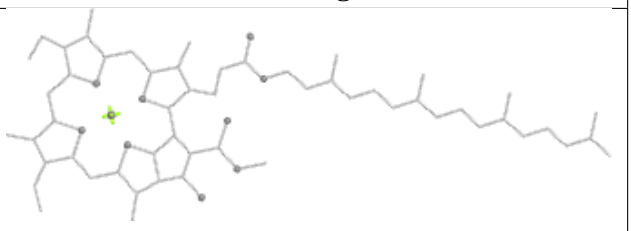
Bond lengths



Bond angles

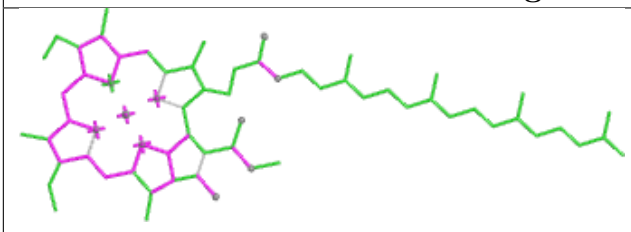


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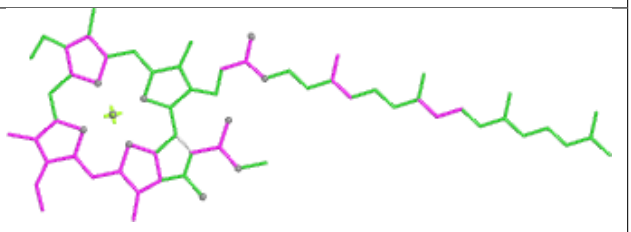


Rings

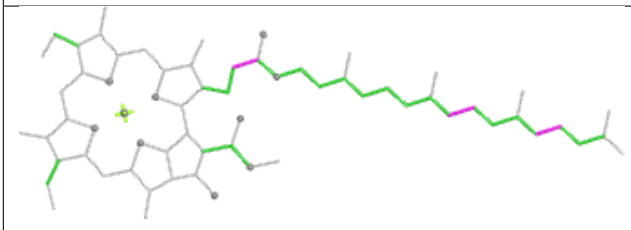
Ligand CLA B 613



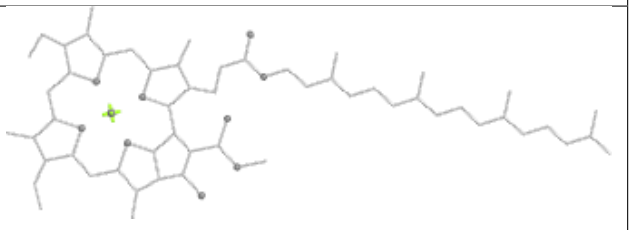
Bond lengths



Bond angles

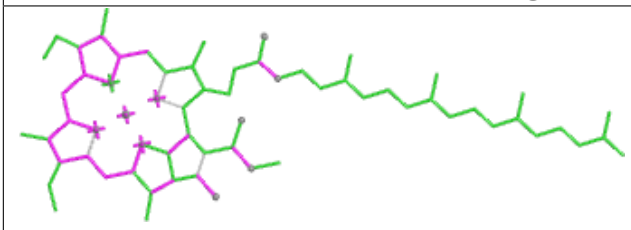


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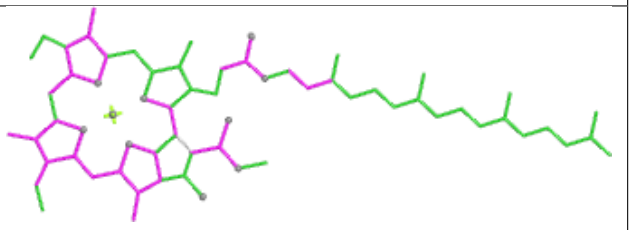


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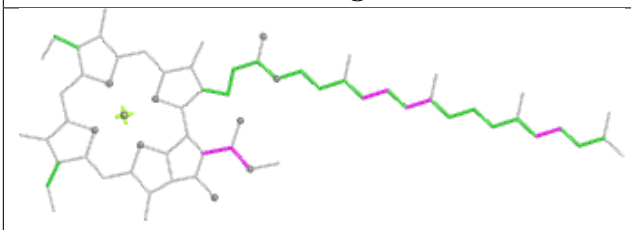
Ligand CLA B 605



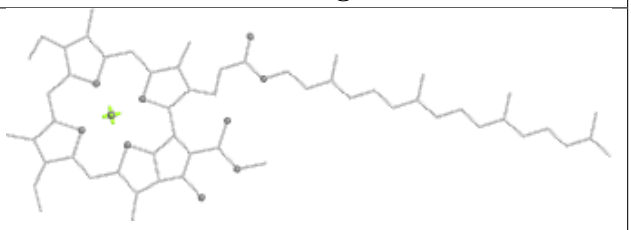
Bond lengths



Bond angles

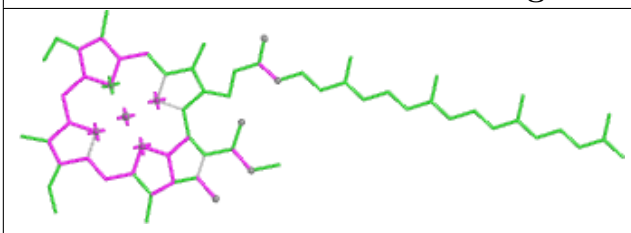


Torsions

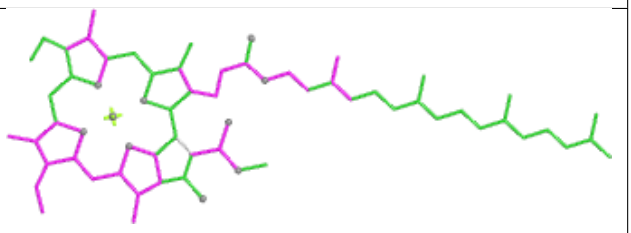


Rings

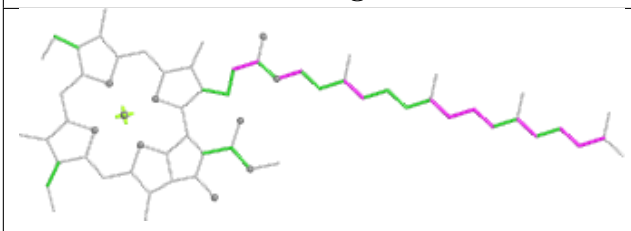
Ligand CLA b 604



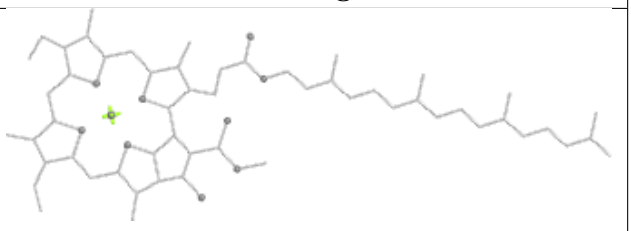
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Bond angles

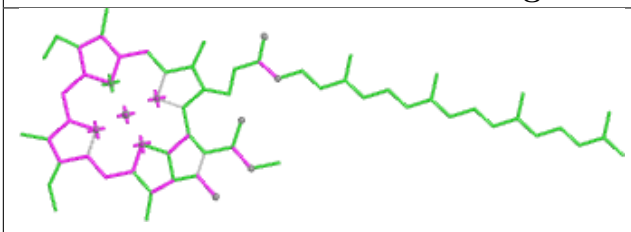


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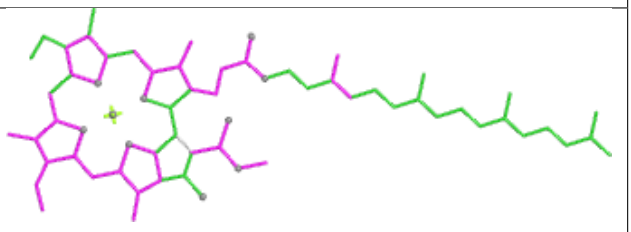


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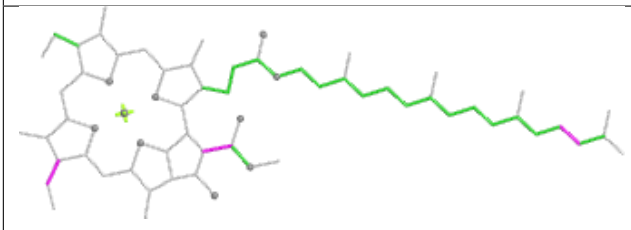
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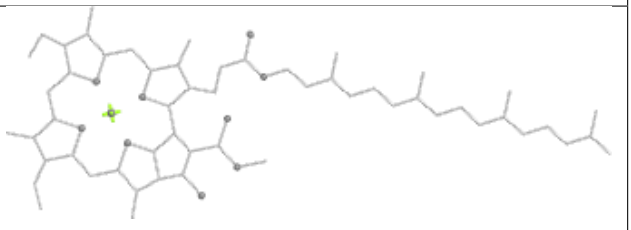
Bond lengths



Bond angles

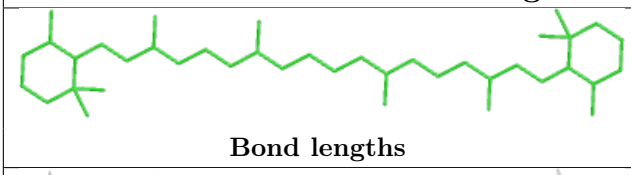


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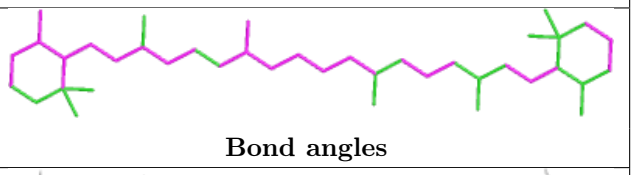


Rings

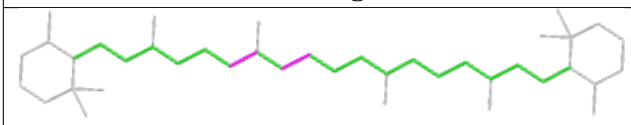
Ligand BCR T 101



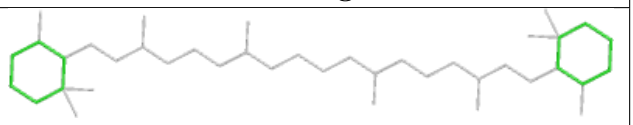
Bond lengths



Bond angles

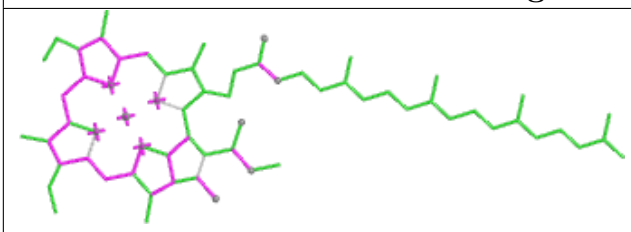


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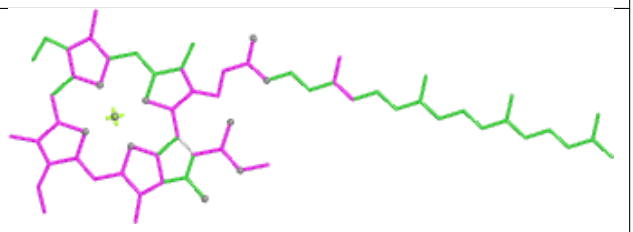


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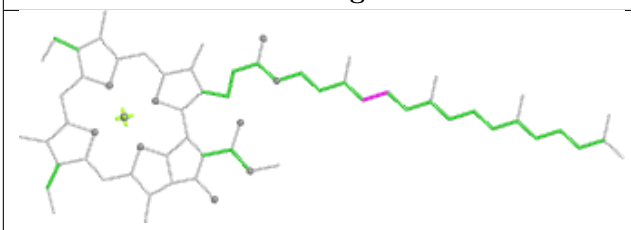
Ligand CLA b 610



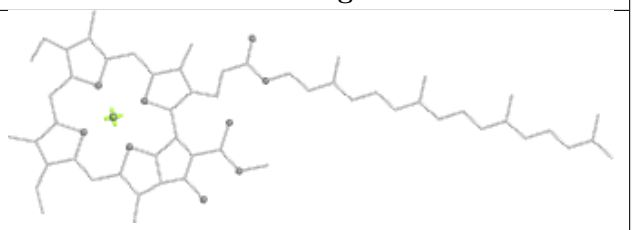
Bond lengths



Bond angles

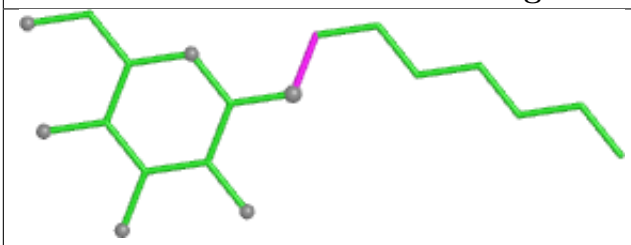


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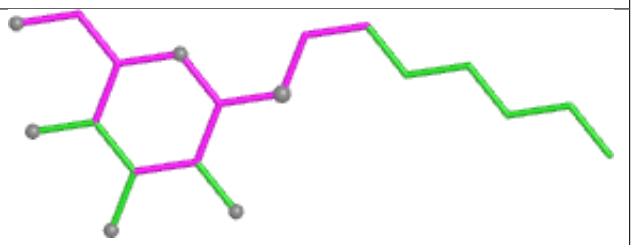


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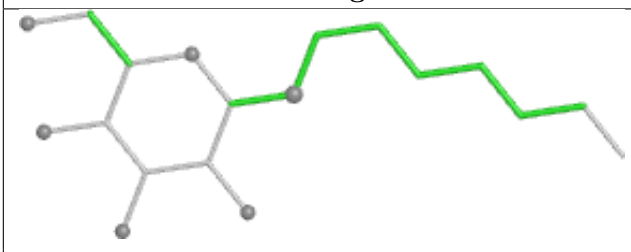
Ligand HTG b 625



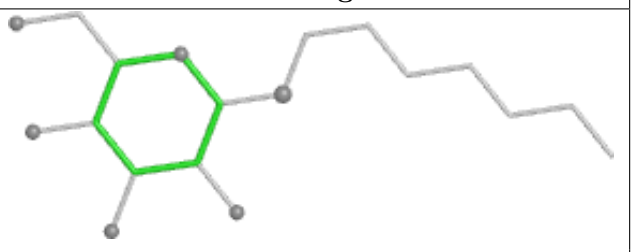
Bond lengths



Bond angles

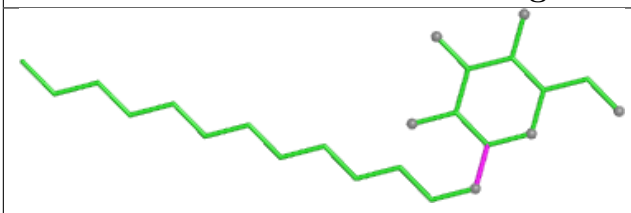


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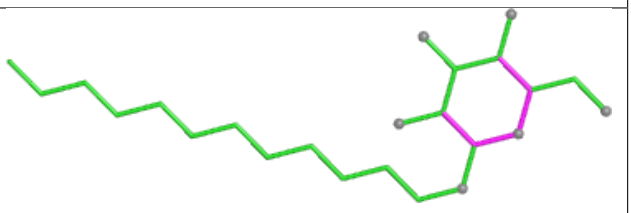


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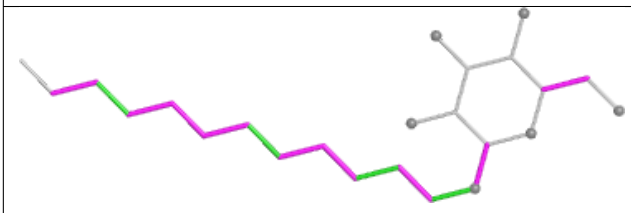
Ligand LMT i 104



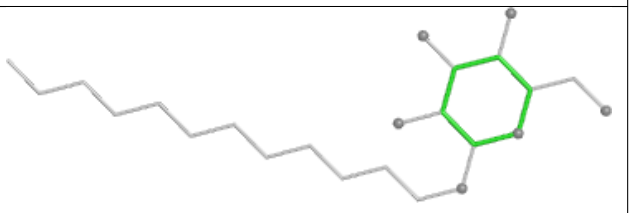
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Bond angles

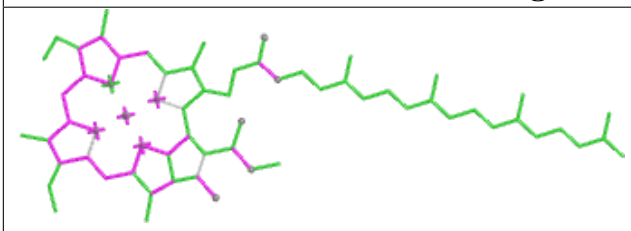


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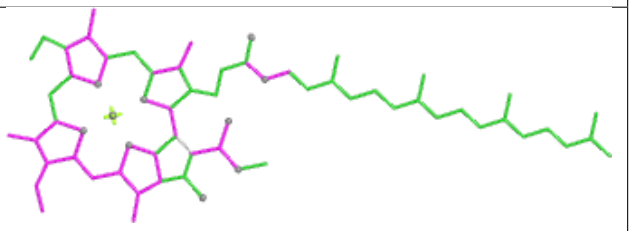


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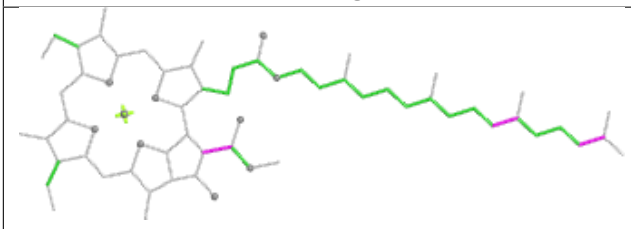
Ligand CLA c 507



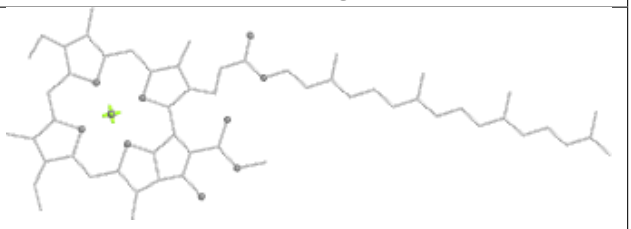
Bond lengths



Bond angles

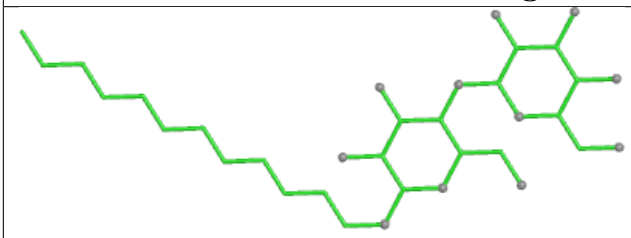


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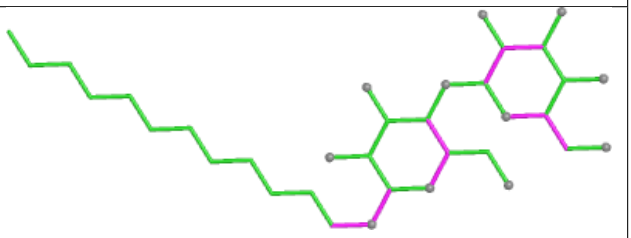


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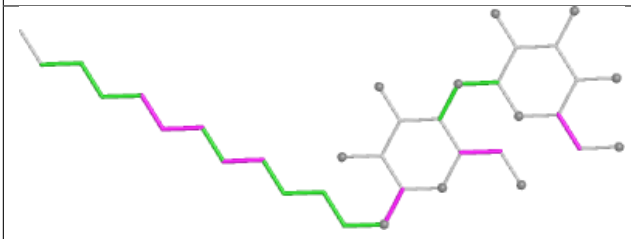
Ligand LMT B 636



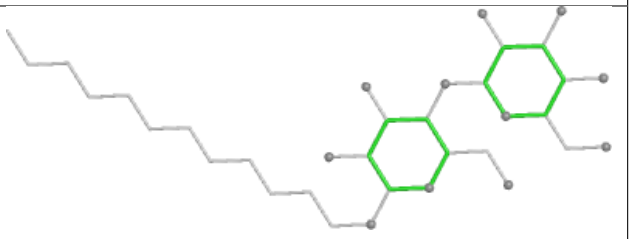
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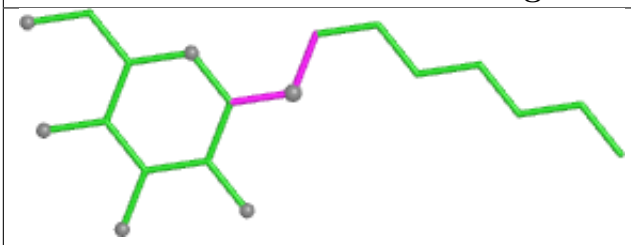


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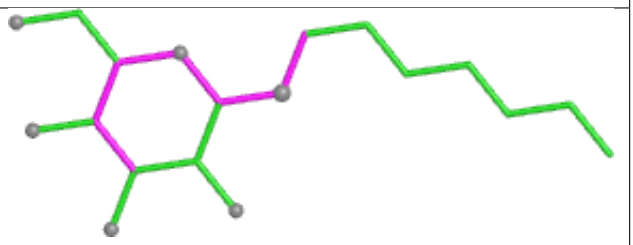


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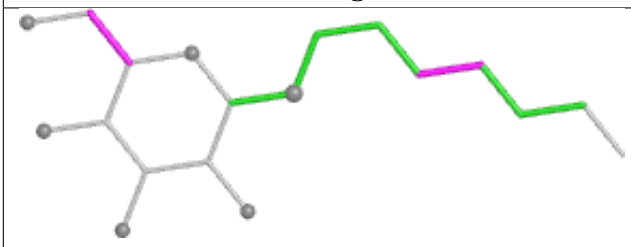
Ligand HTG b 601



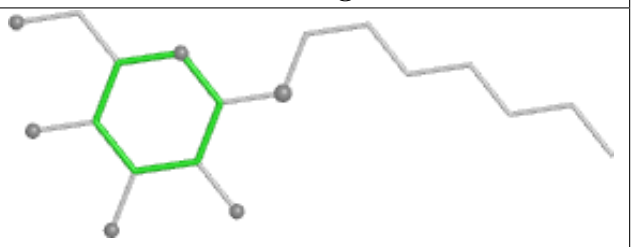
Bond lengths



Bond angles

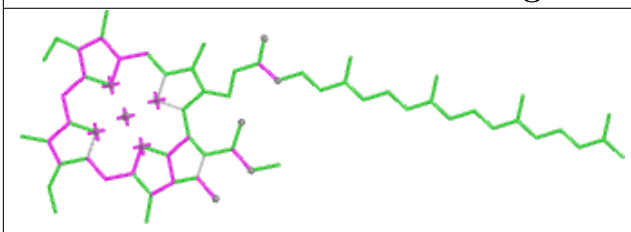


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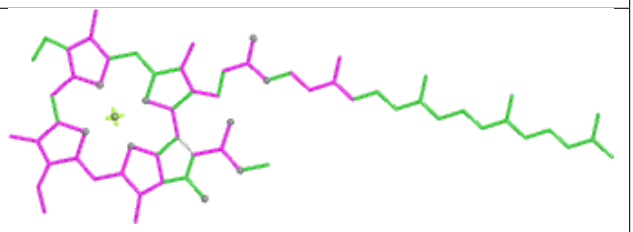


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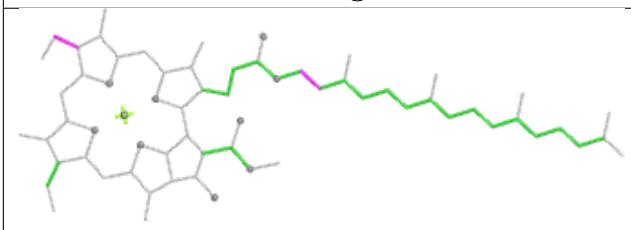
Ligand CLA D 404



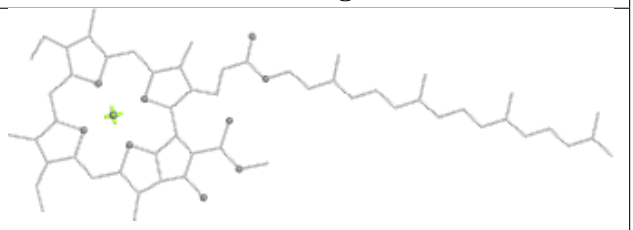
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Bond angles

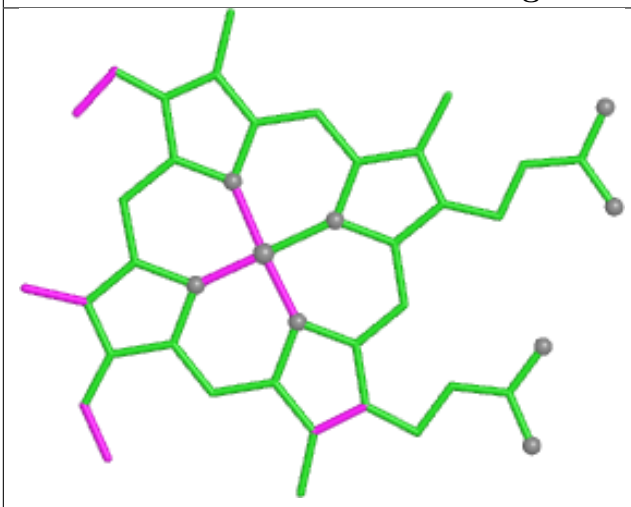


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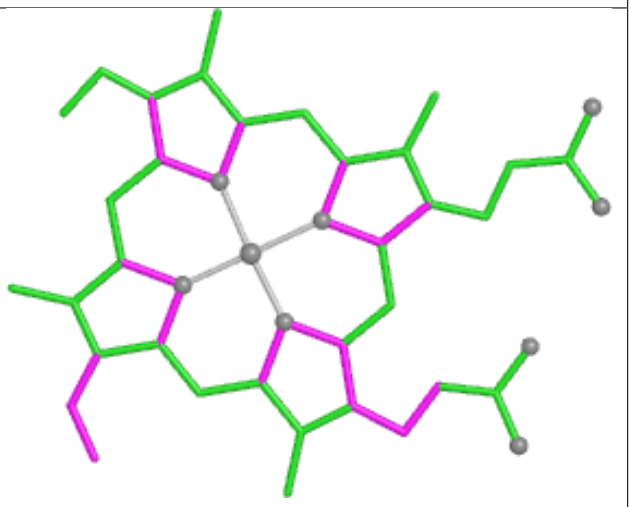


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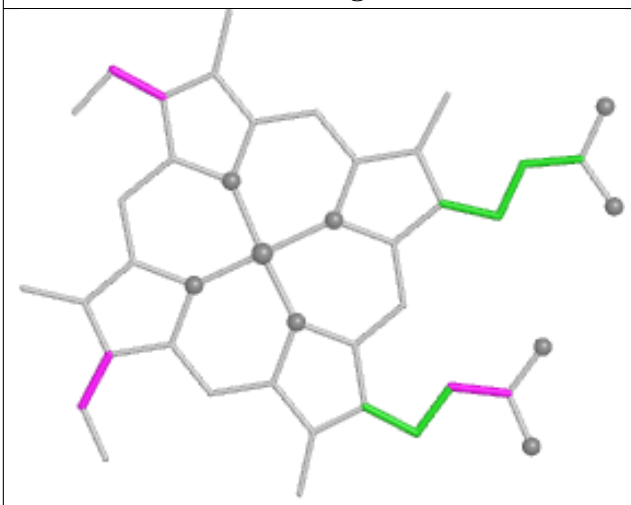
Ligand HEC V 201



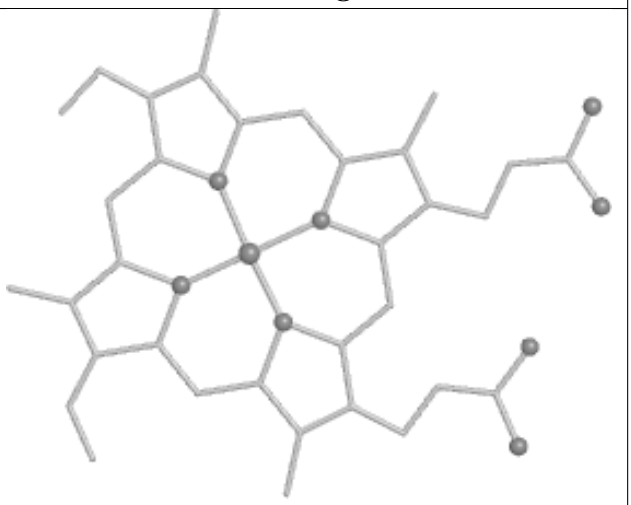
Bond lengths



Bond angles

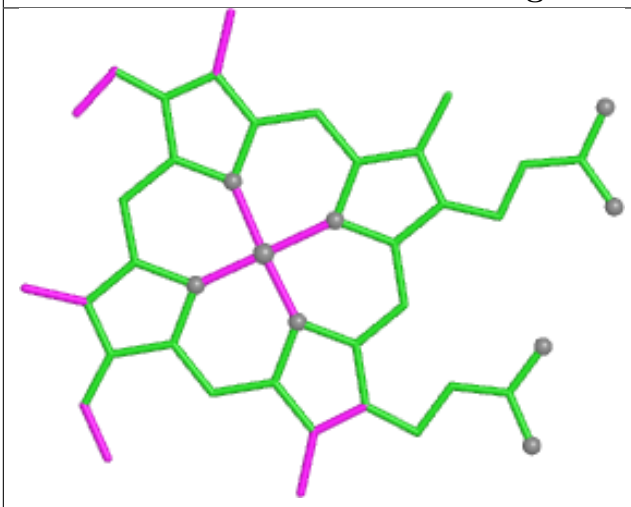


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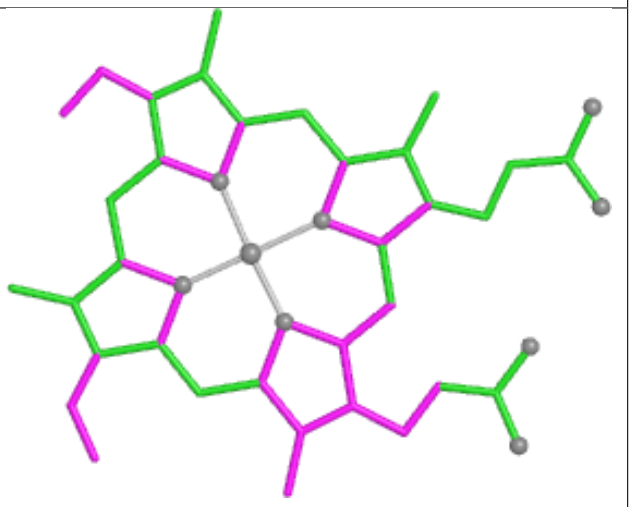


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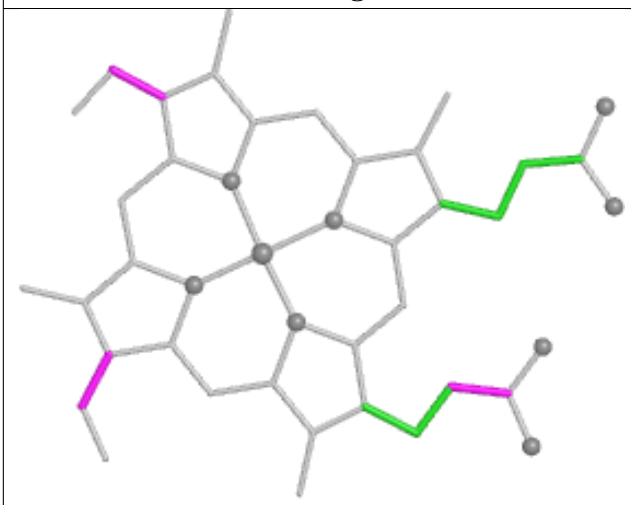
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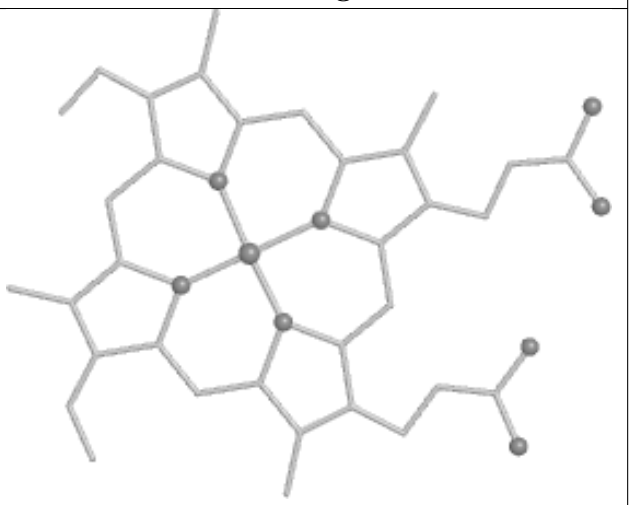
Bond lengths



Bond angles

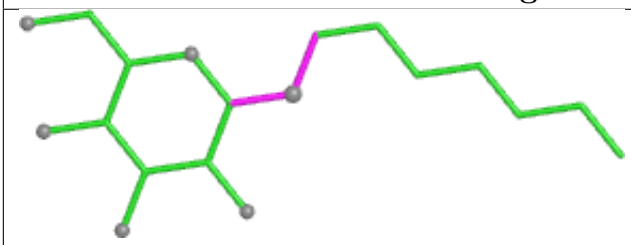


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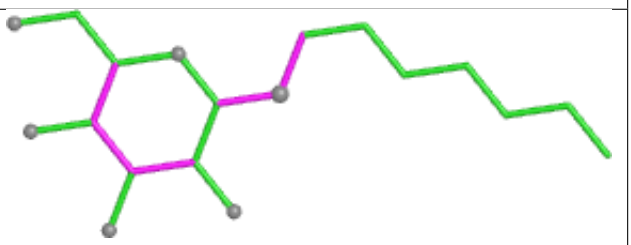


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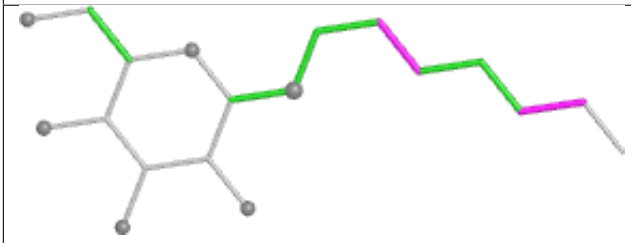
Ligand HTG D 413



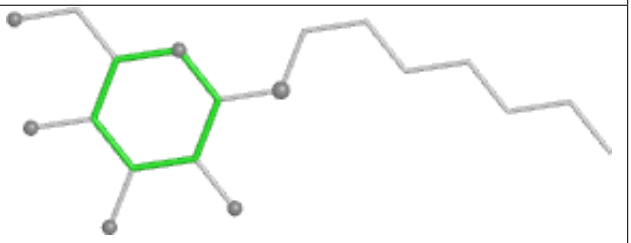
Bond lengths



Bond angles

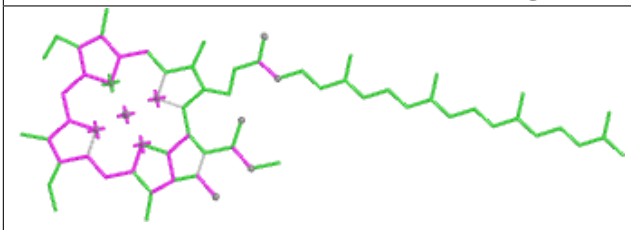


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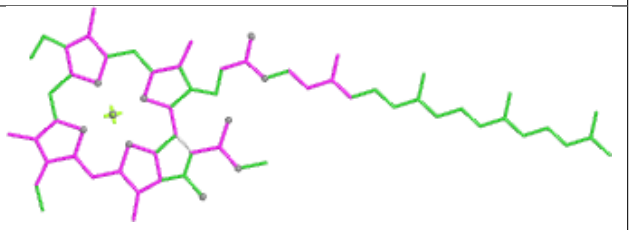


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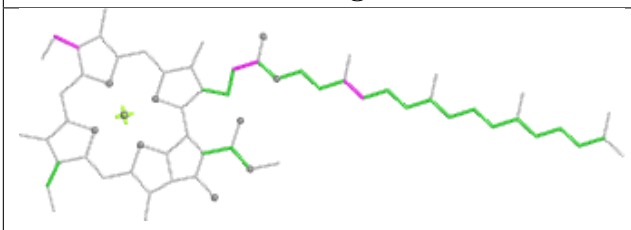
Ligand CLA C 506



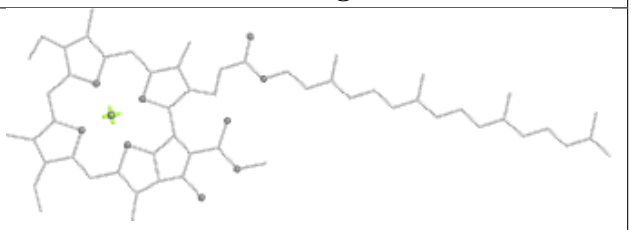
Bond lengths



Bond angles

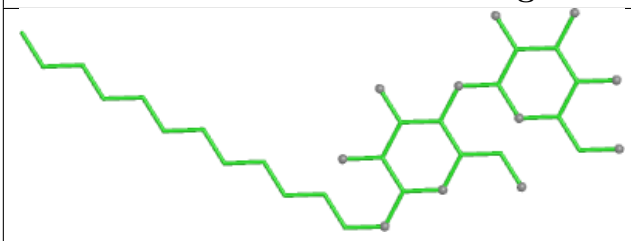


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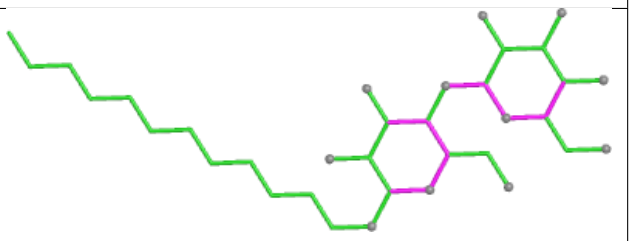


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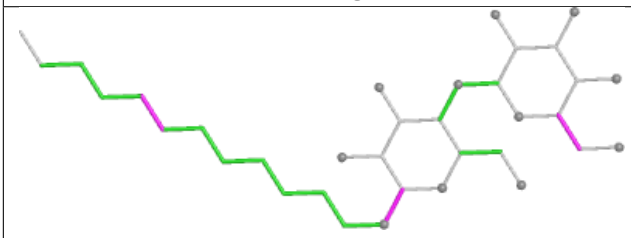
Ligand LMT M 101



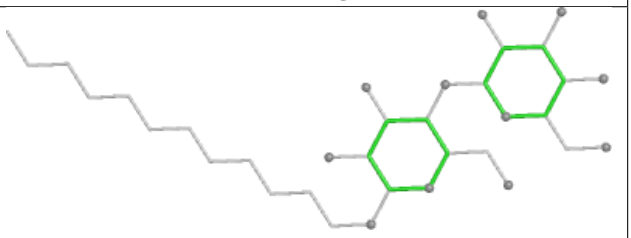
Bond lengths



Bond angles

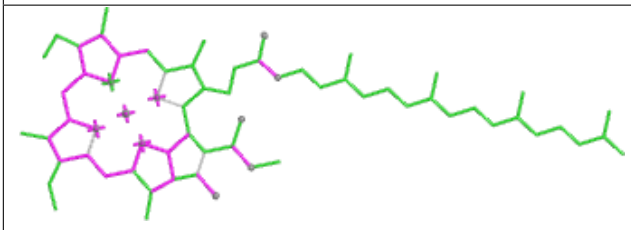


Torsions

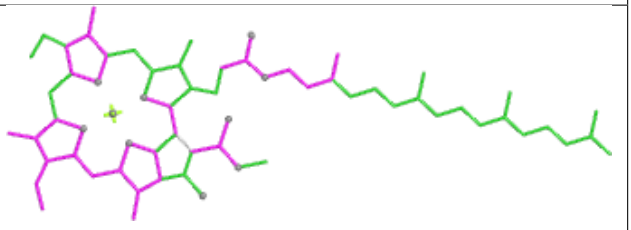


Rings

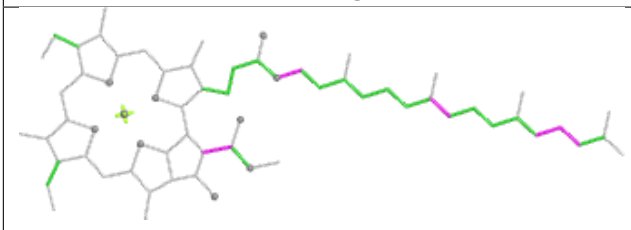
Ligand CLA C 510



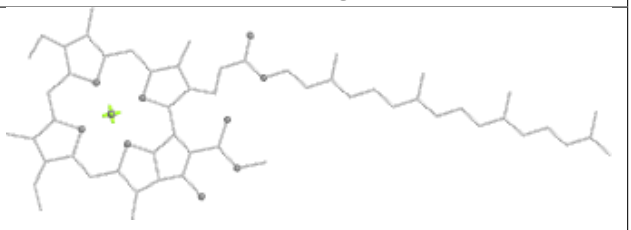
Bond lengths



Bond angles

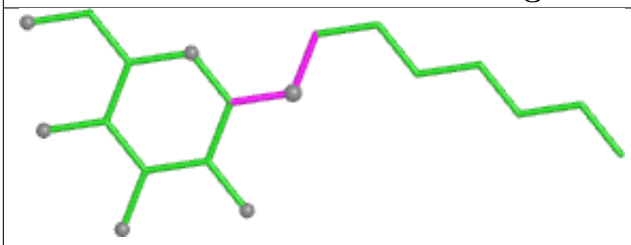


Torsions

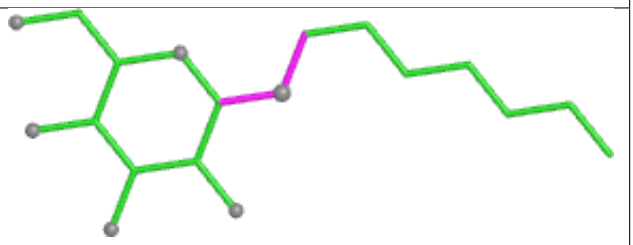


Rings

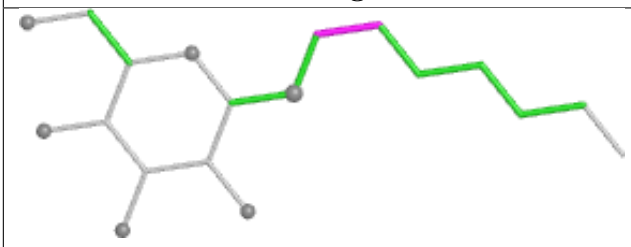
Ligand HTG d 414



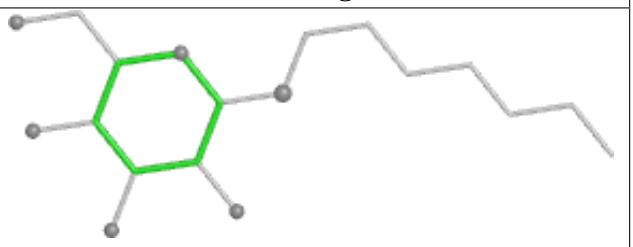
Bond lengths



Bond angles

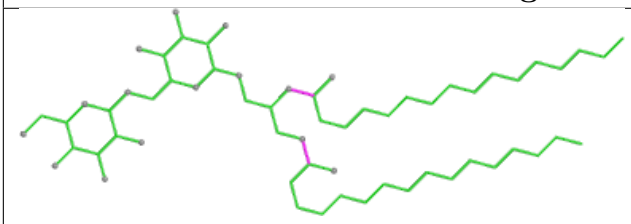


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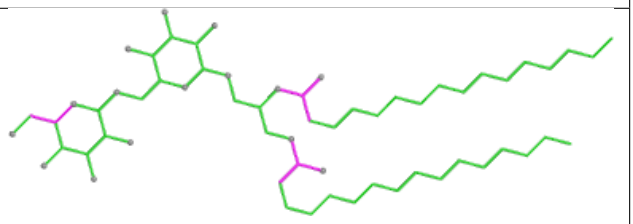


Rings

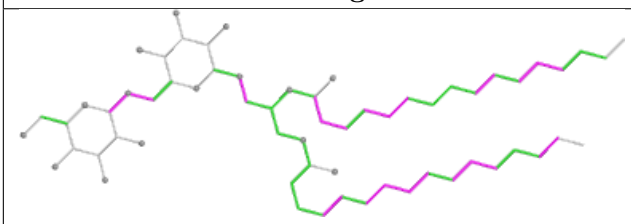
Ligand DGD C 518



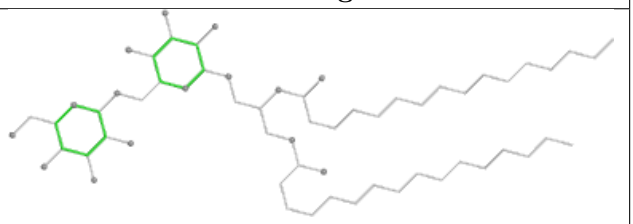
Bond lengths



Bond angles

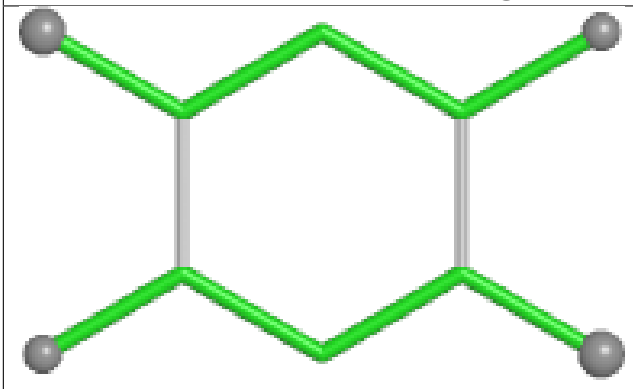


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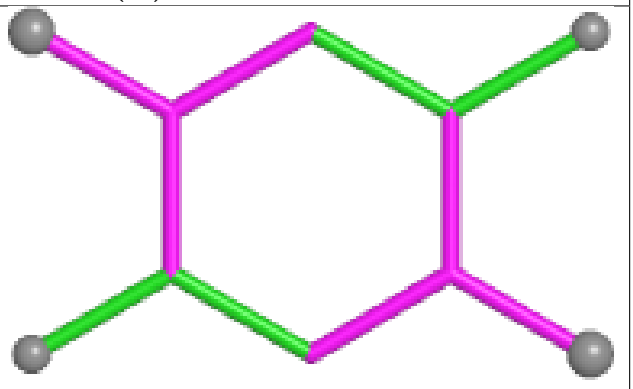


Rings

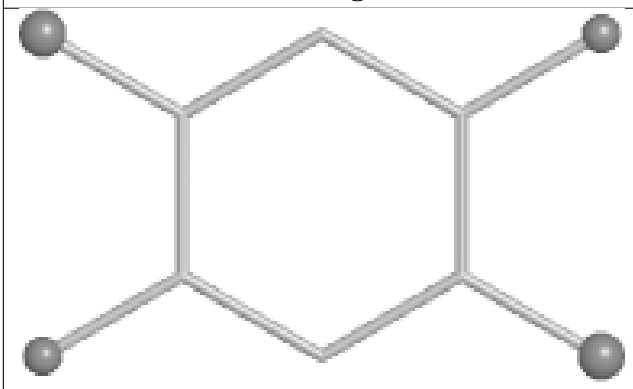
Ligand K2I A 418 (A)



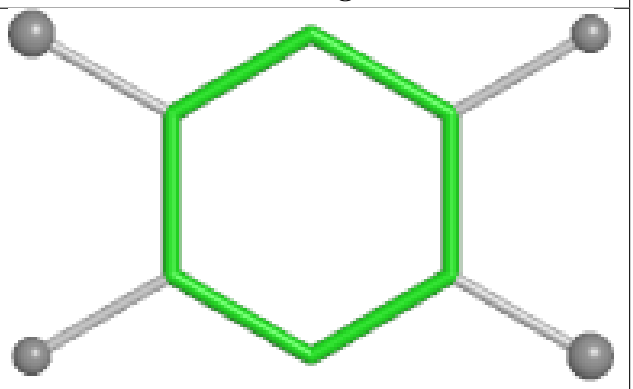
Bond lengths



Bond angles

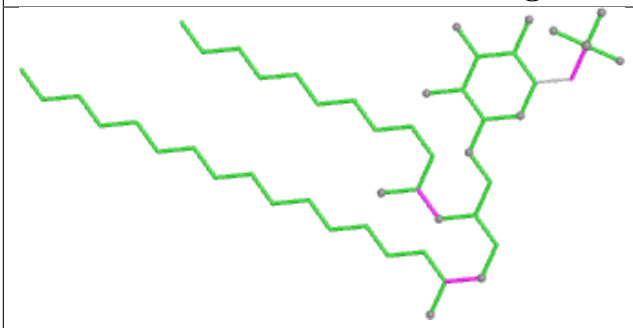


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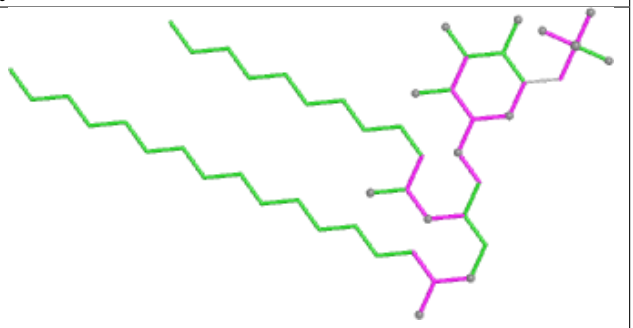


Rings

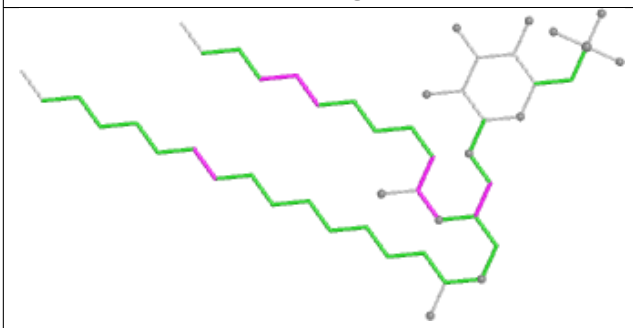
Ligand SQD A 411



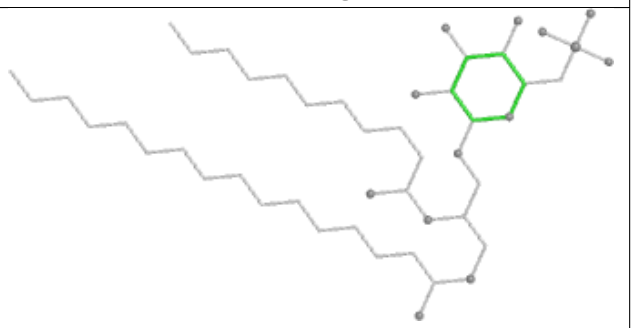
Bond lengths



Bond angles

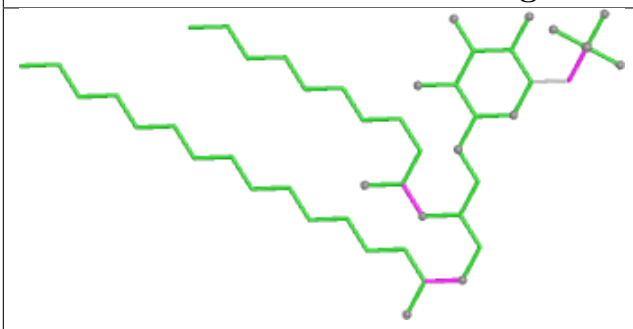


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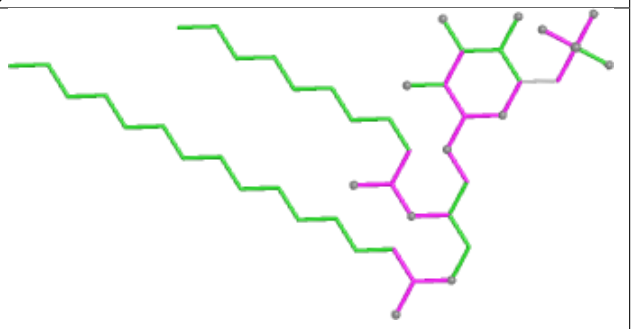


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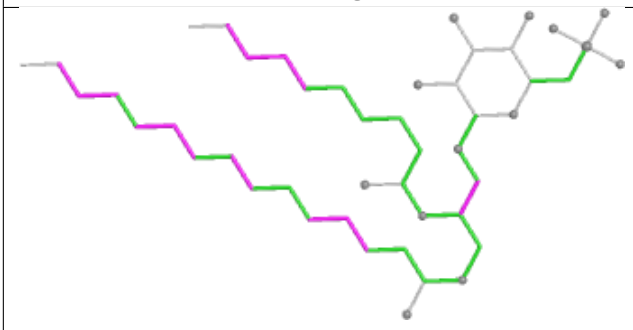
Ligand SQD a 2115



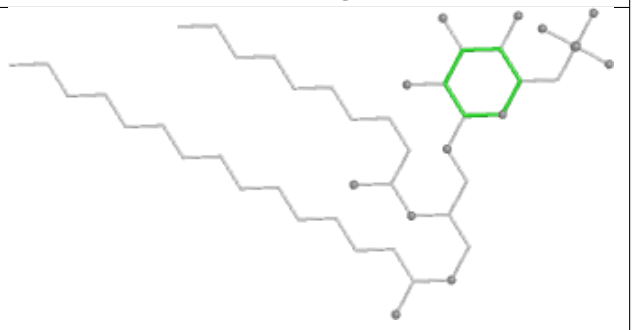
Bond lengths



Bond angles

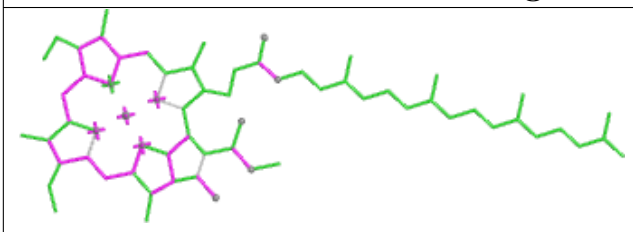


Torsions

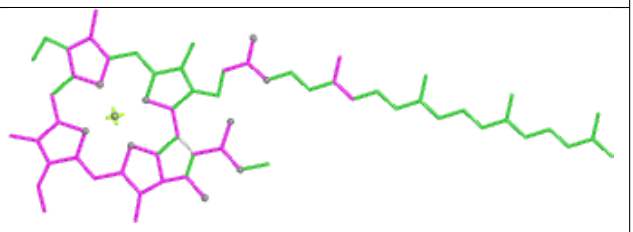


Rings

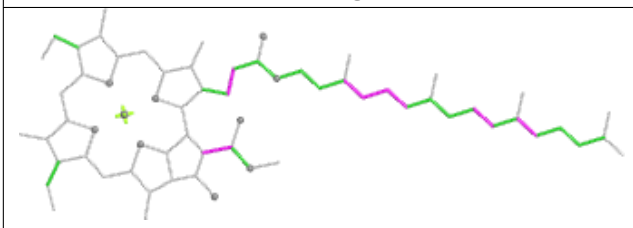
Ligand CLA B 615



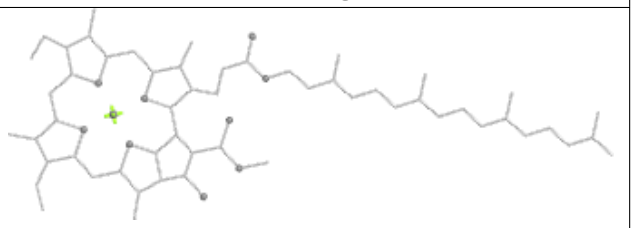
Bond lengths



Bond angles

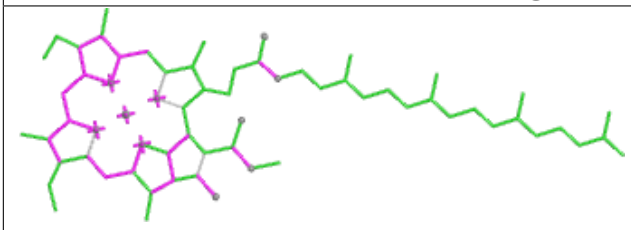


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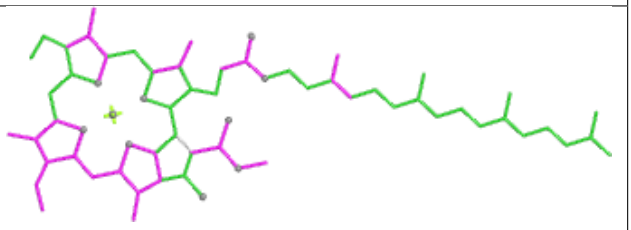


Rings

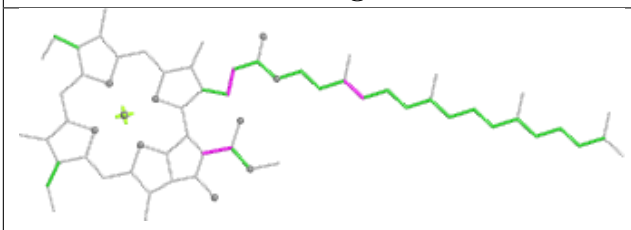
Ligand CLA b 608



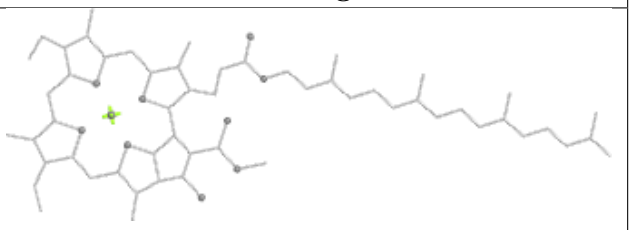
Bond lengths



Bond angles



Torsions

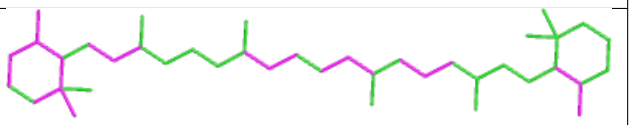


Rings

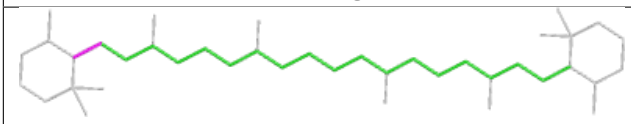
Ligand BCR c 517



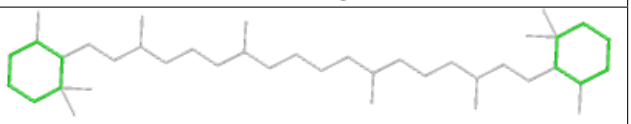
Bond lengths



Bond angles

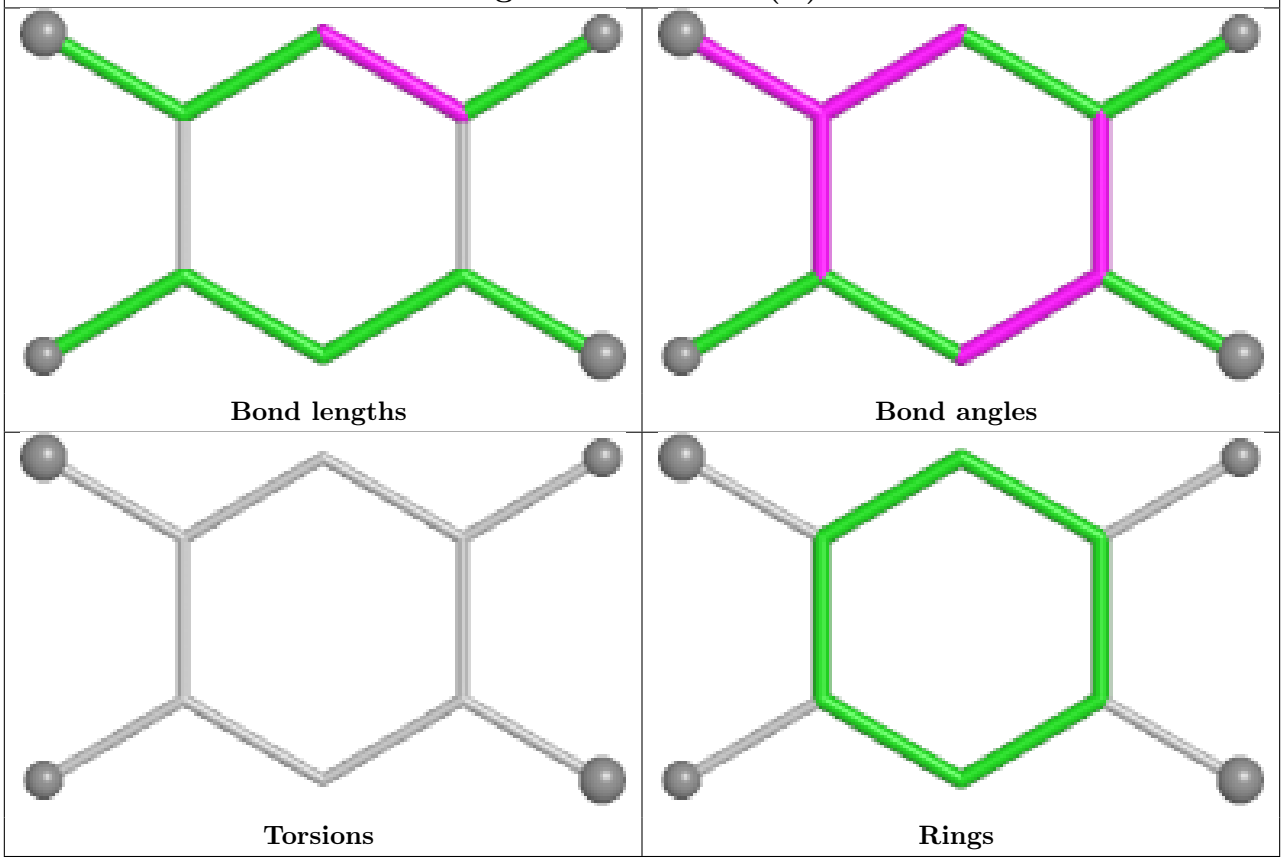


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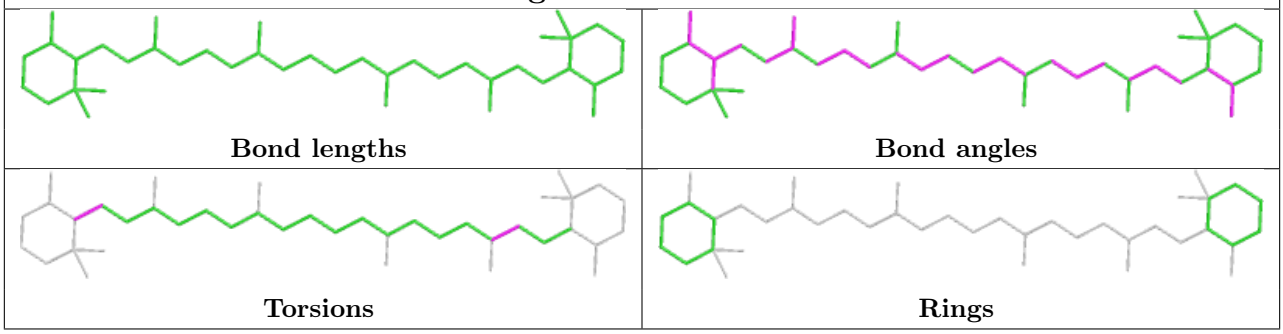


Rings

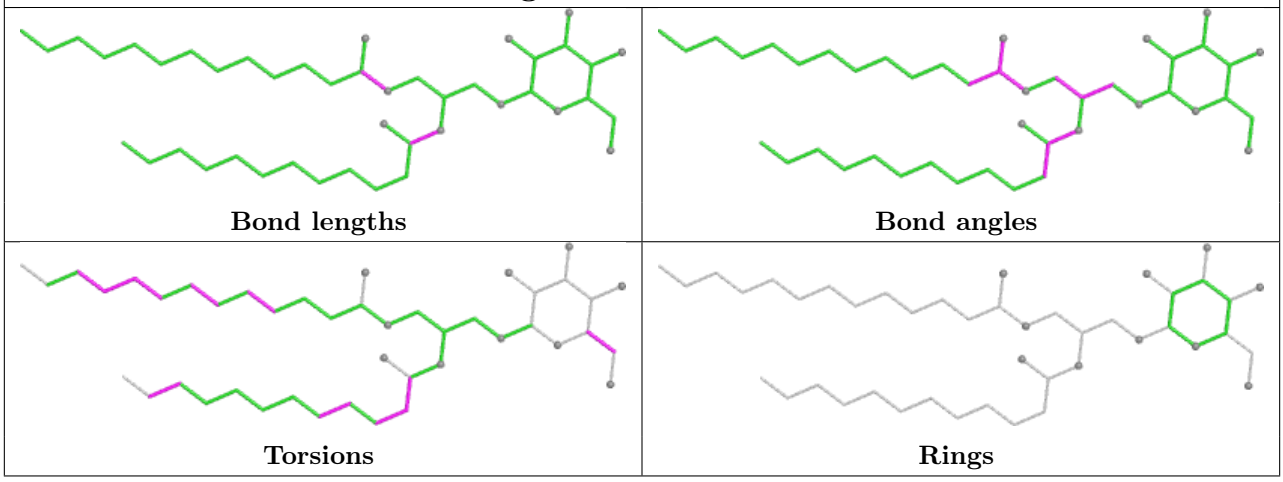
Ligand K2I a 2118 (B)



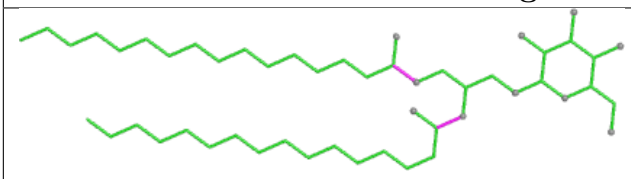
Ligand BCR c 528



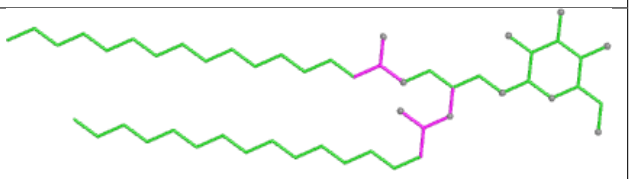
Ligand LMG D 412



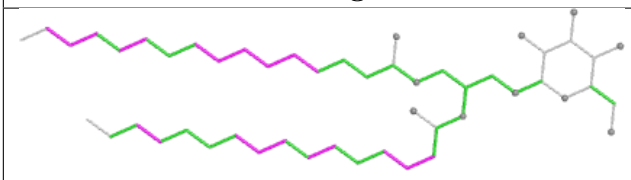
Ligand LMG C 520



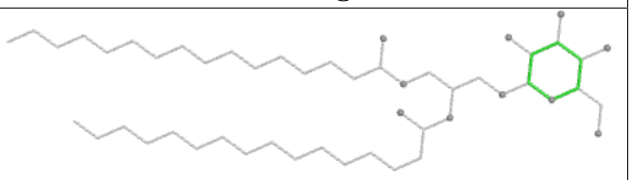
Bond lengths



Bond angles

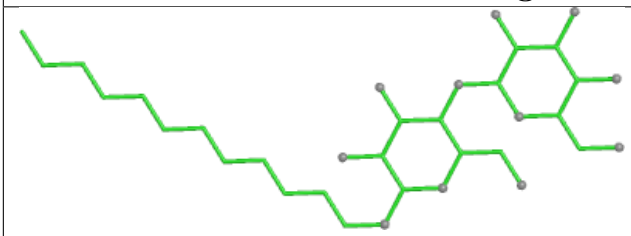


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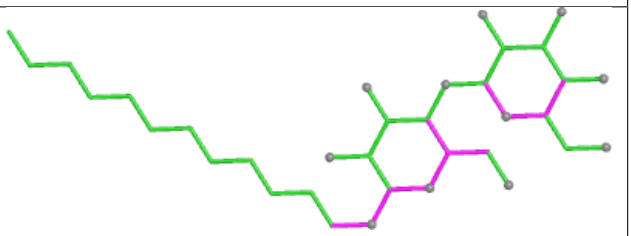


Rings

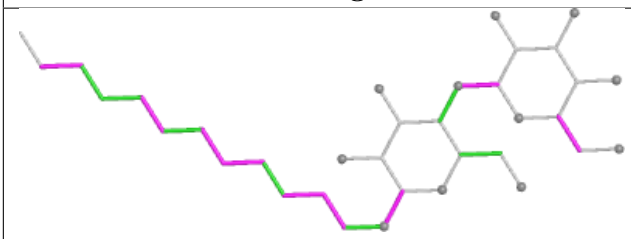
Ligand LMT a 2120



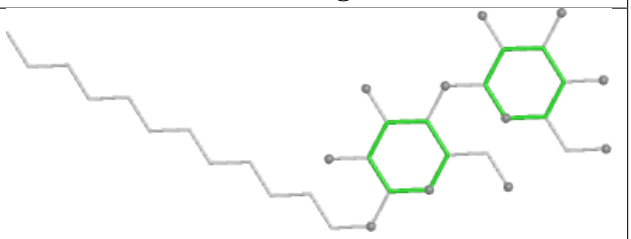
Bond lengths



Bond angles

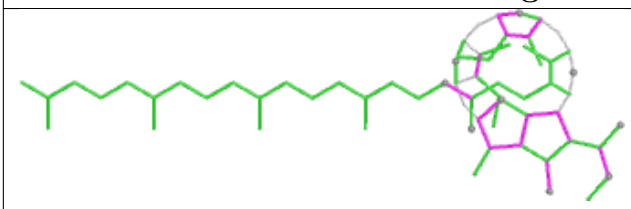


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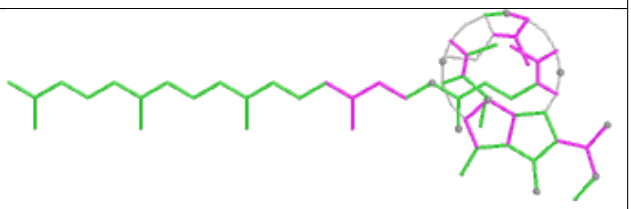


Rings

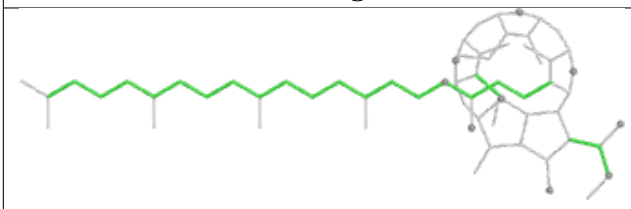
Ligand PHO A 408



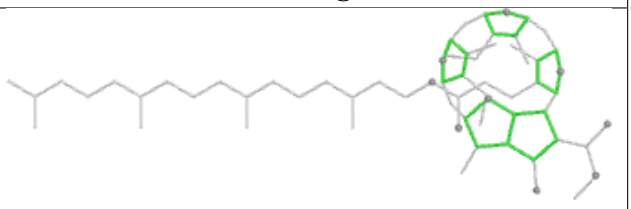
Bond lengths



Bond angles

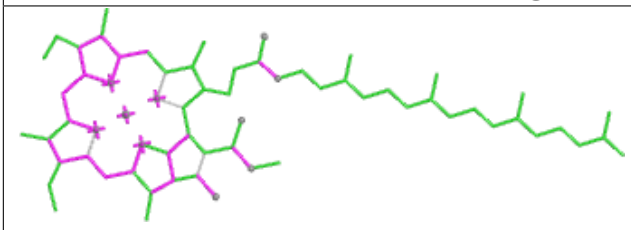


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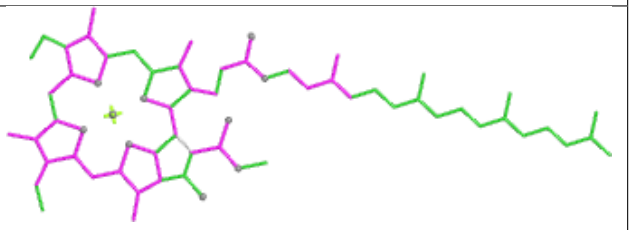


Rings

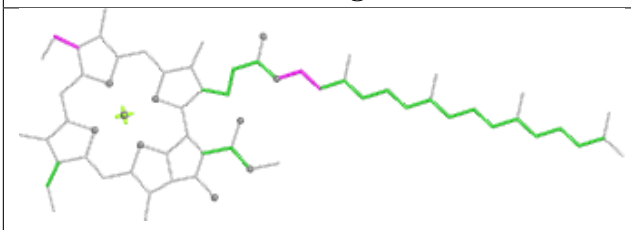
Ligand CLA d 404



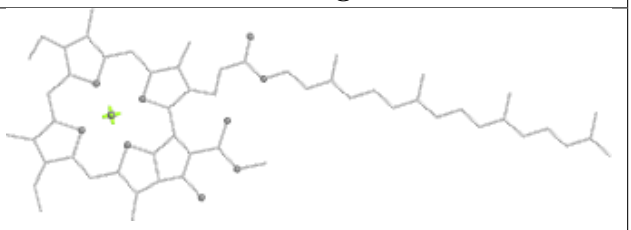
Bond lengths



Bond angles

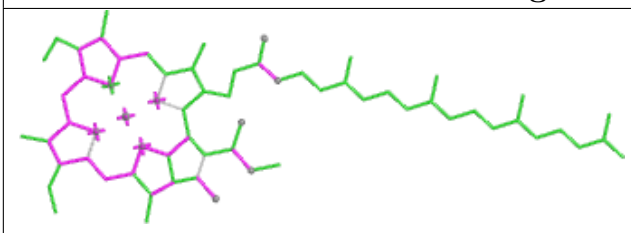


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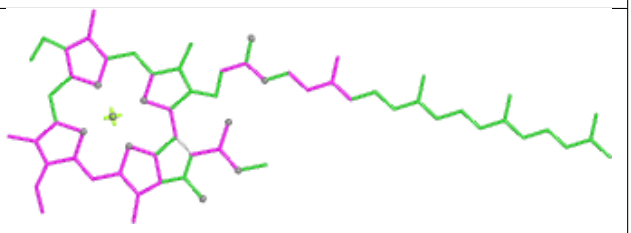


Rings

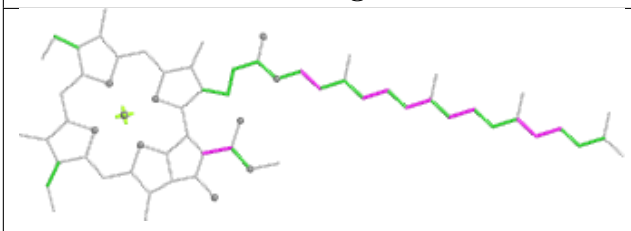
Ligand CLA c 511



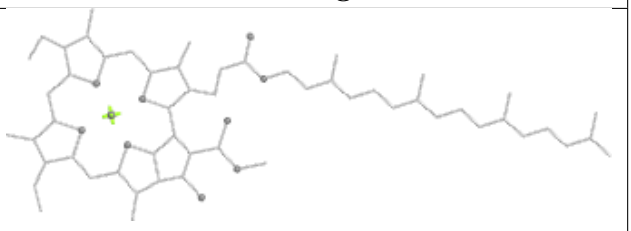
Bond lengths



Bond angles

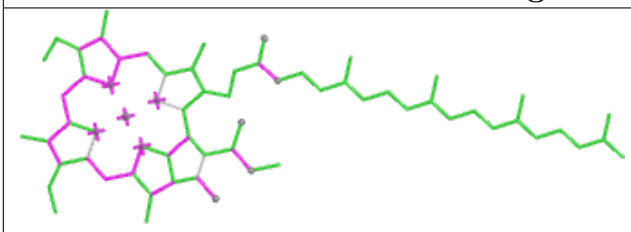


Torsions

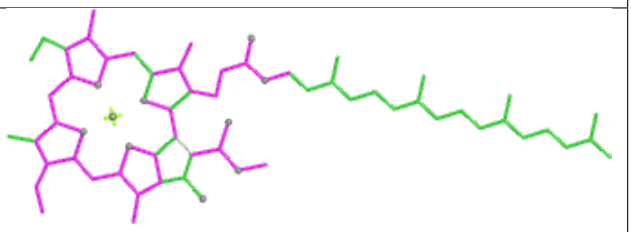


Rings

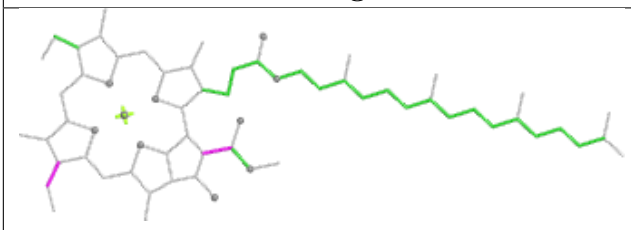
Ligand CLA d 401



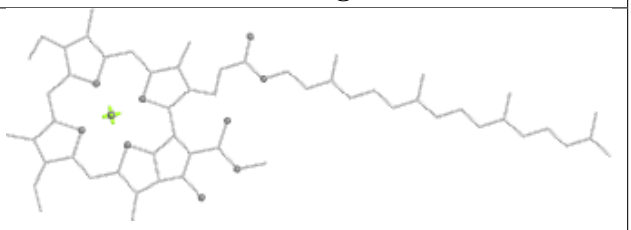
Bond lengths



Bond angles

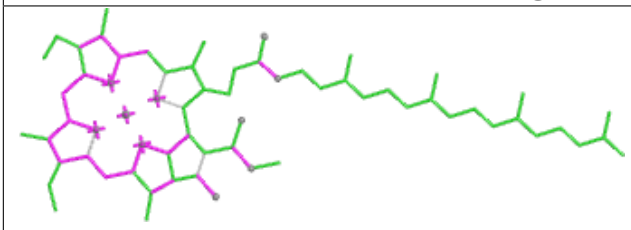


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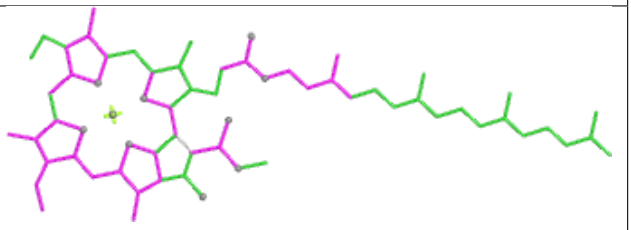


Rings

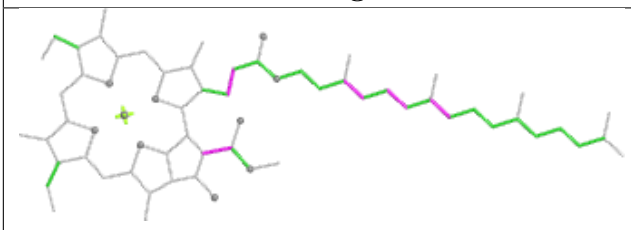
Ligand CLA c 509



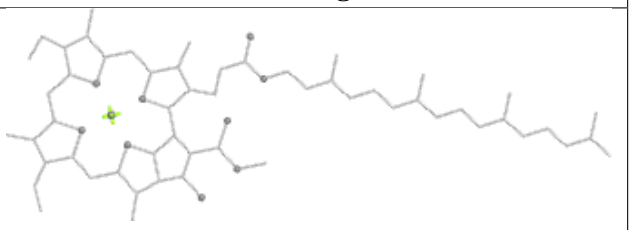
Bond lengths



Bond angles

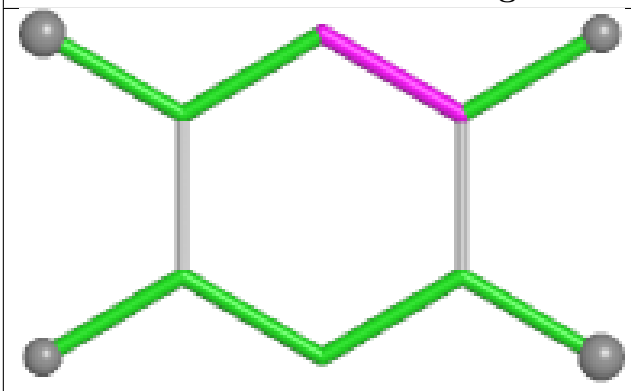


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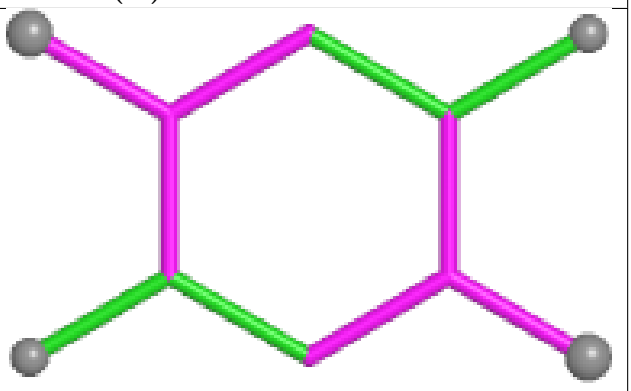


Rings

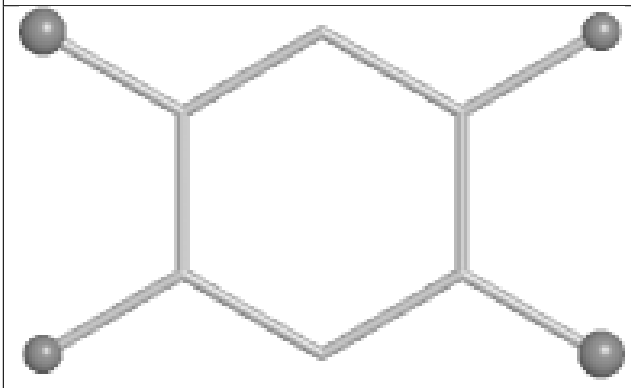
Ligand K2I A 418 (B)



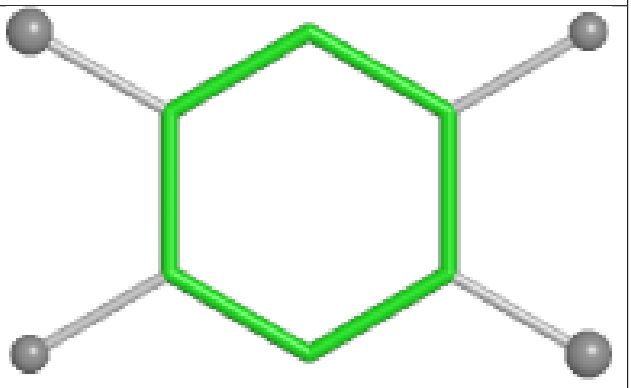
Bond lengths



Bond angles

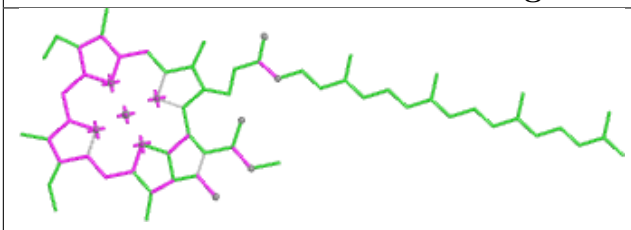


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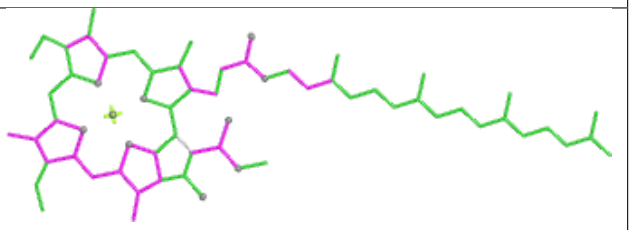


Rings

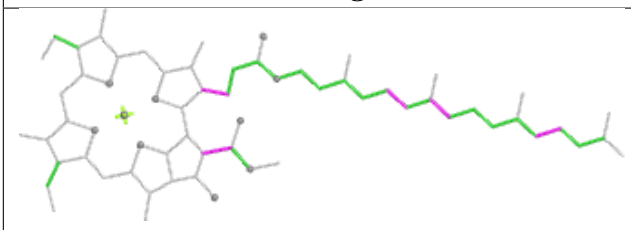
Ligand CLA C 509



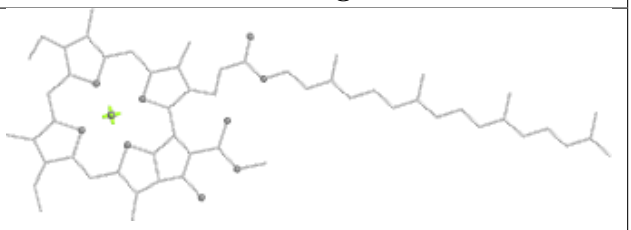
Bond lengths



Bond angles

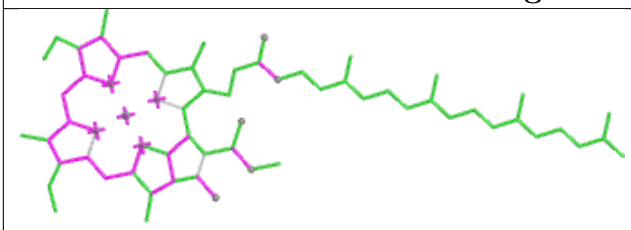


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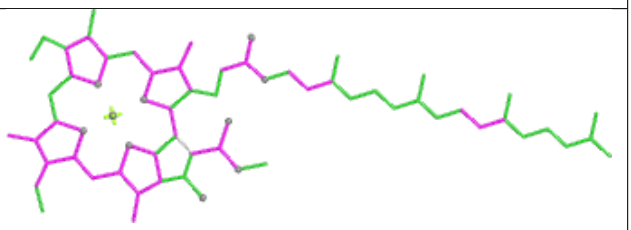


Rings

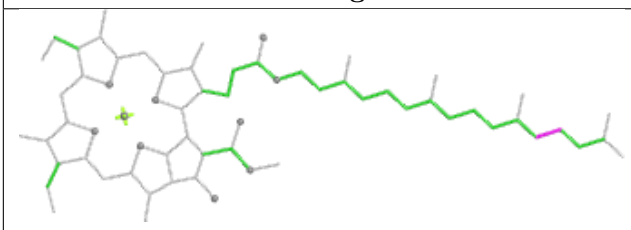
Ligand CLA B 609



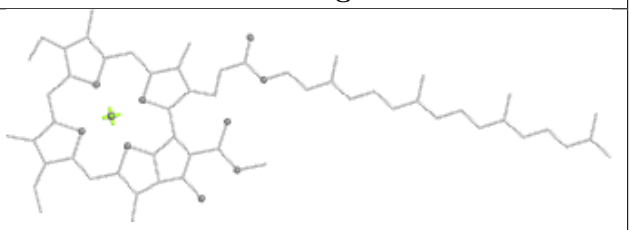
Bond lengths



Bond angles

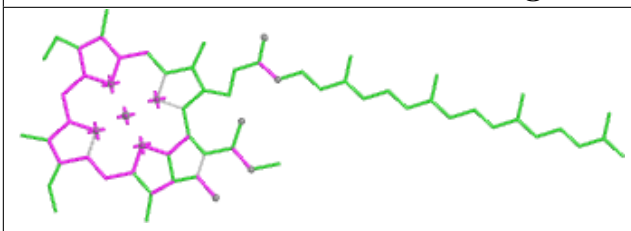


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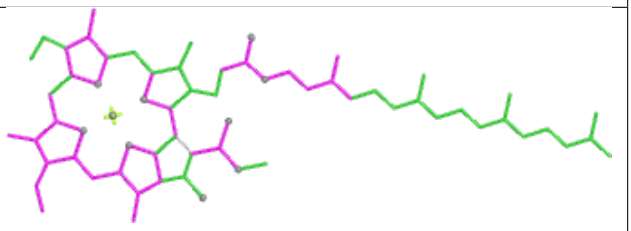


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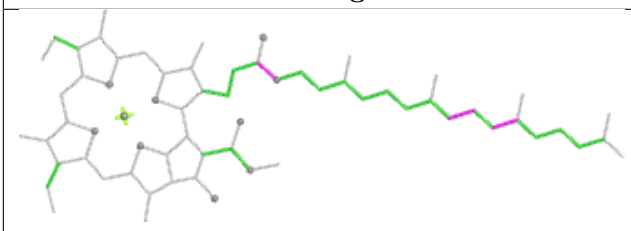
Ligand CLA C 512



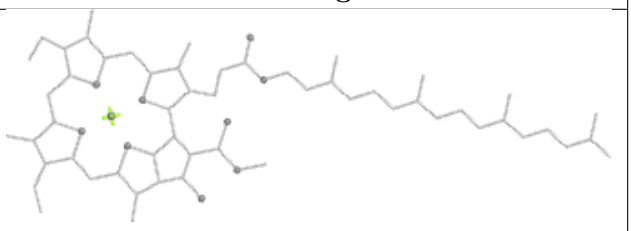
Bond lengths



Bond angles

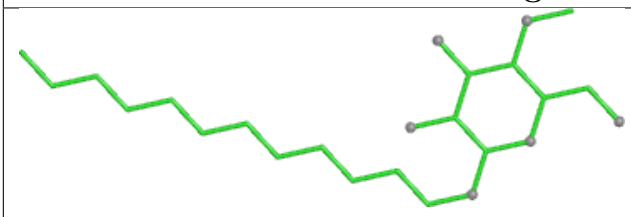


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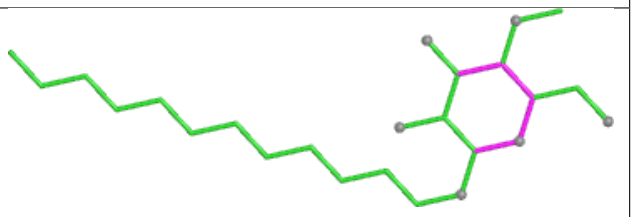


Rings

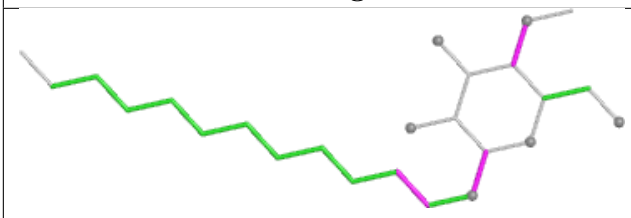
Ligand LMT b 624



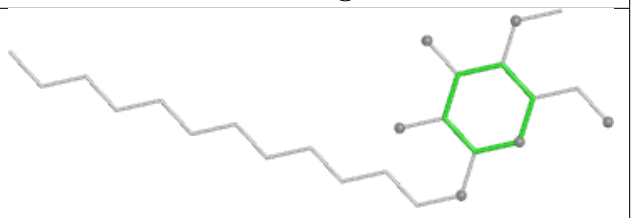
Bond lengths



Bond angles

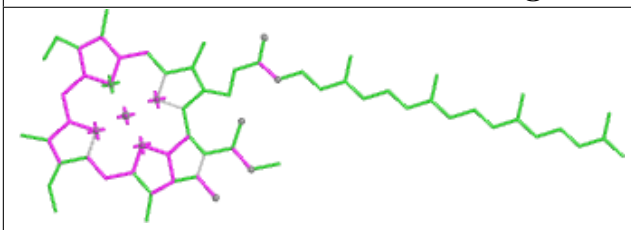


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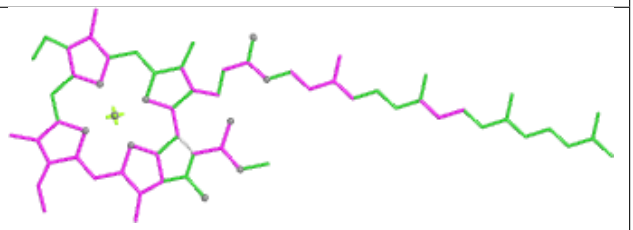


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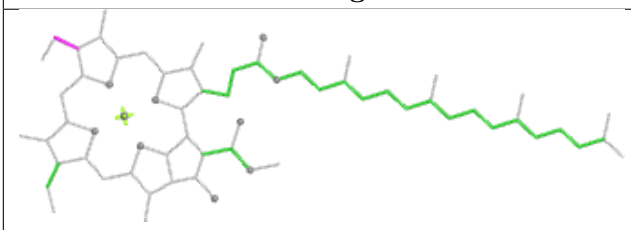
Ligand CLA C 514



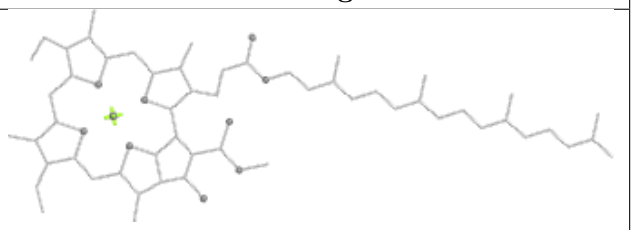
Bond lengths



Bond angles

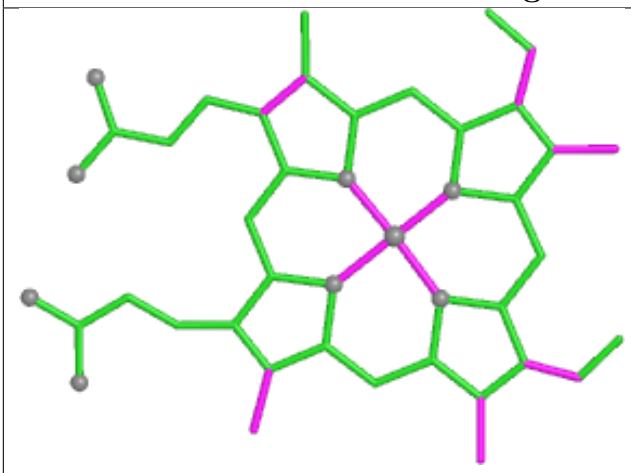


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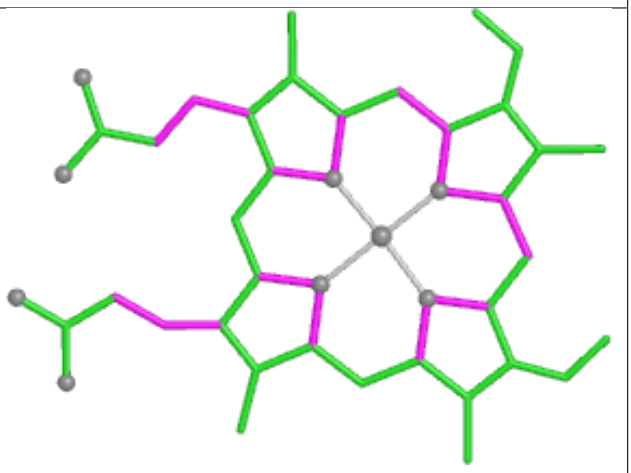


Rings

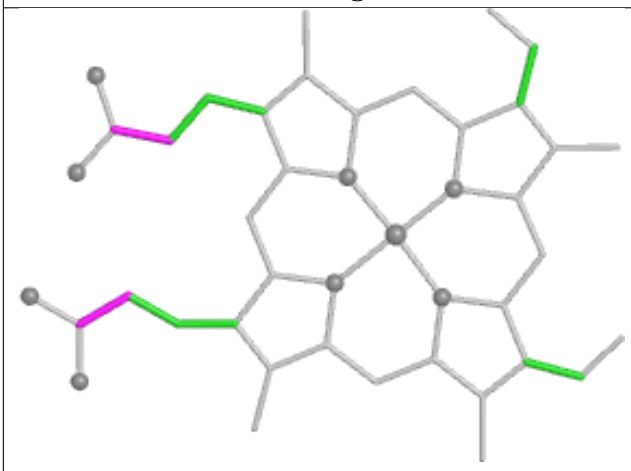
Ligand HEM e 103



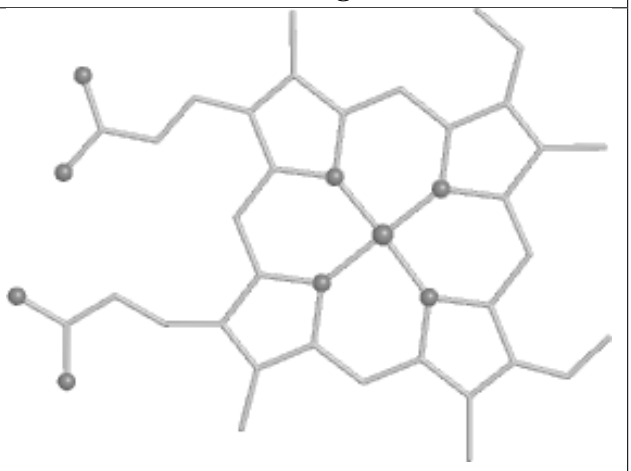
Bond lengths



Bond angles

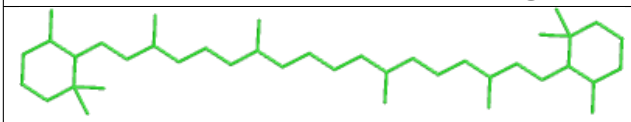


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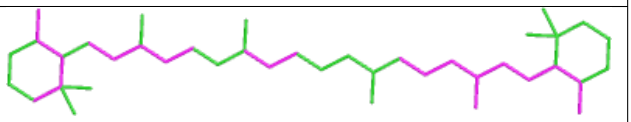


Rings

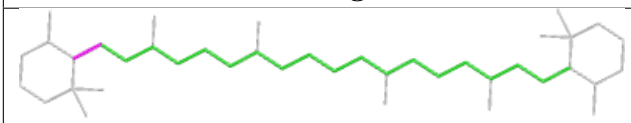
Ligand BCR C 516



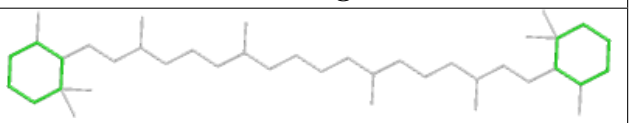
Bond lengths



Bond angles

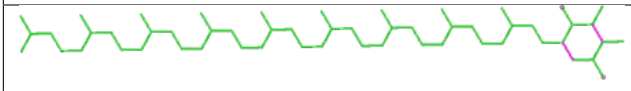


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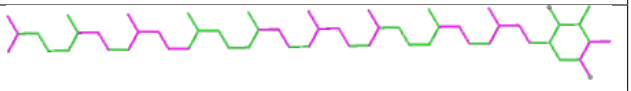


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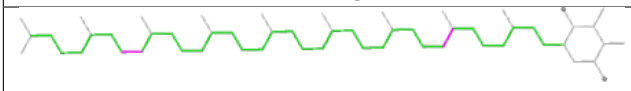
Ligand PL9 D 407



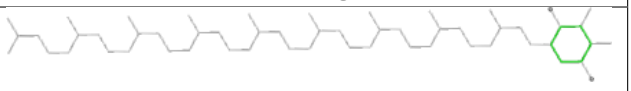
Bond lengths



Bond angles

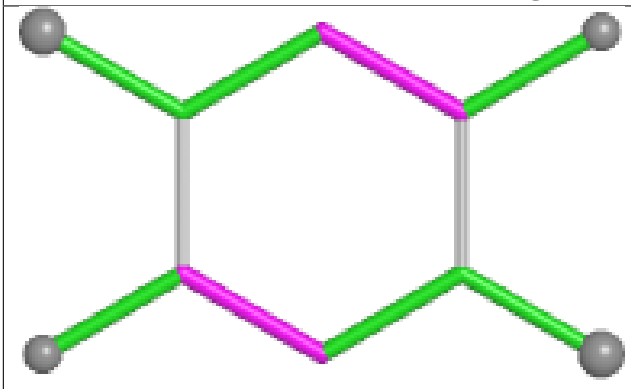


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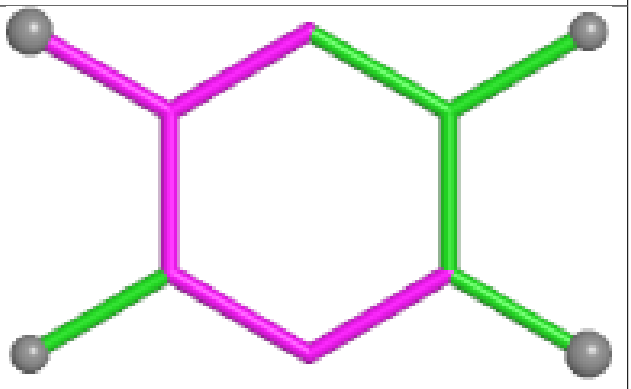


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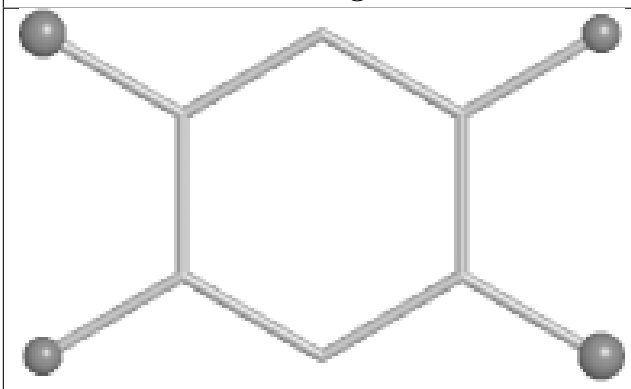
Ligand K2I a 2119



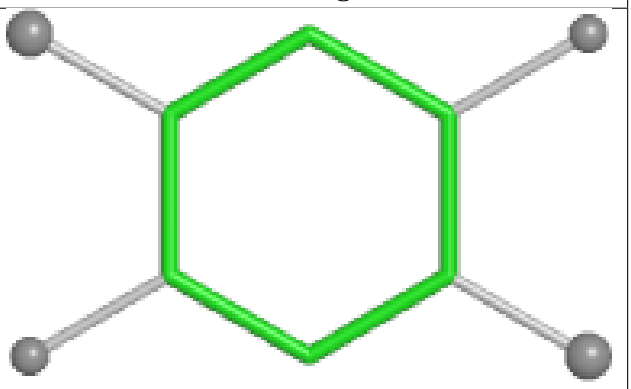
Bond lengths



Bond angles

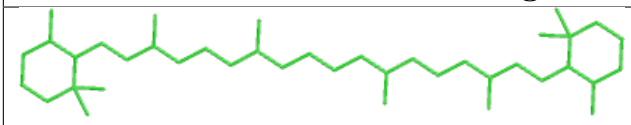


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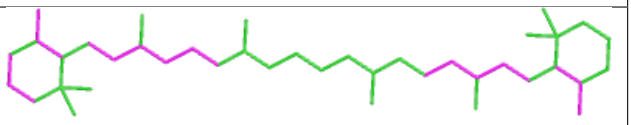


Rings

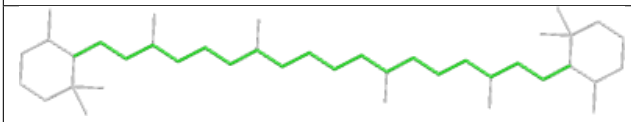
Ligand BCR K 101



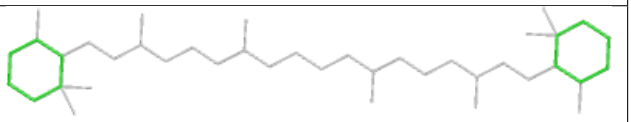
Bond lengths



Bond angles

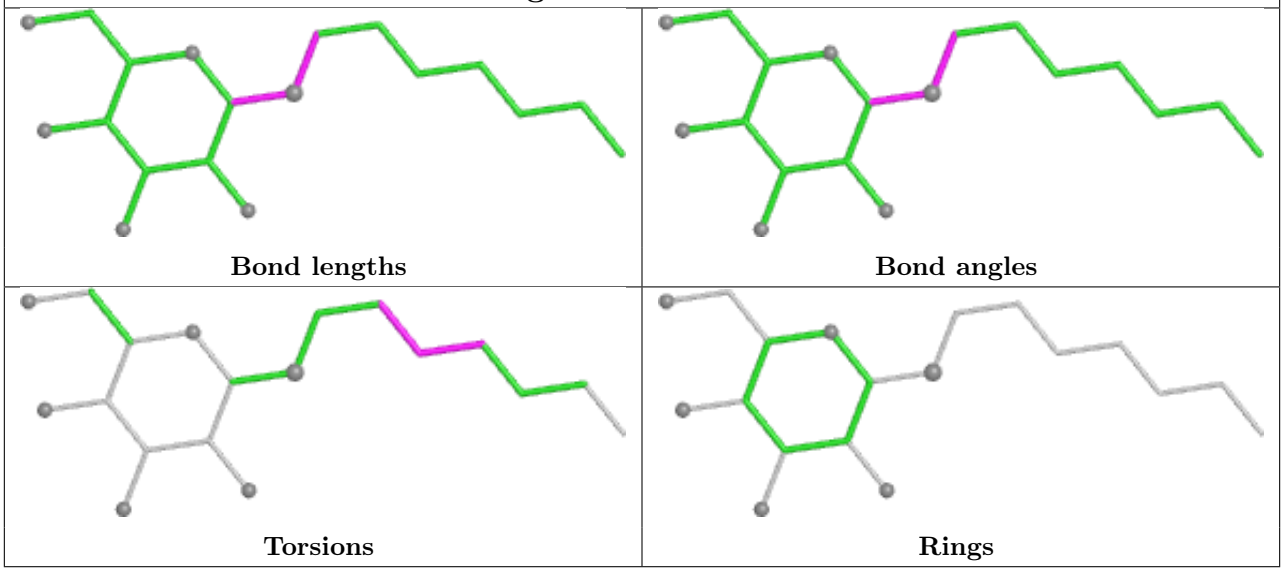


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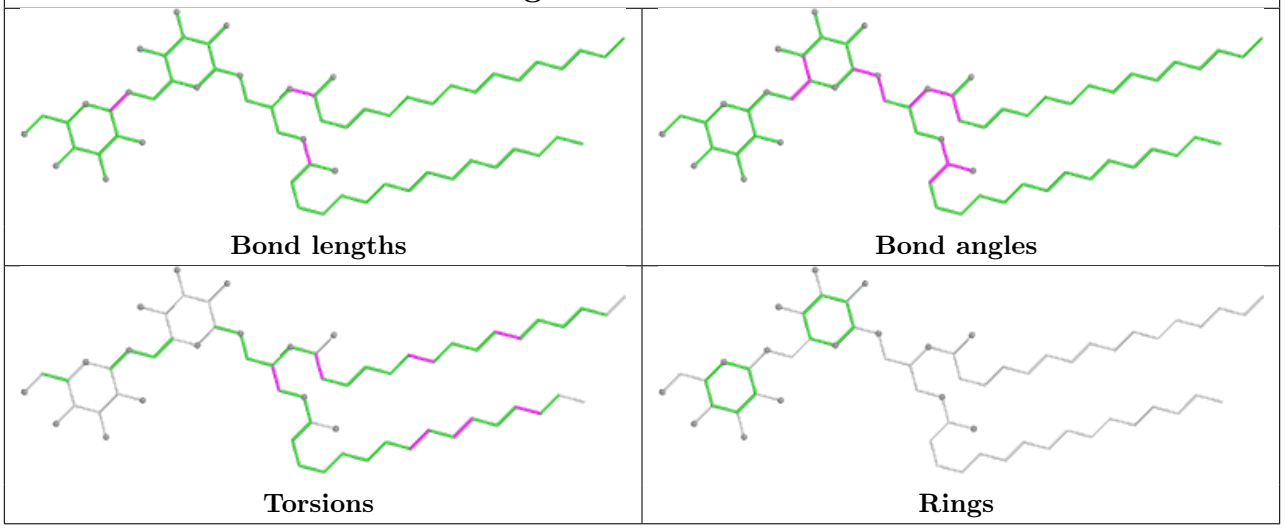


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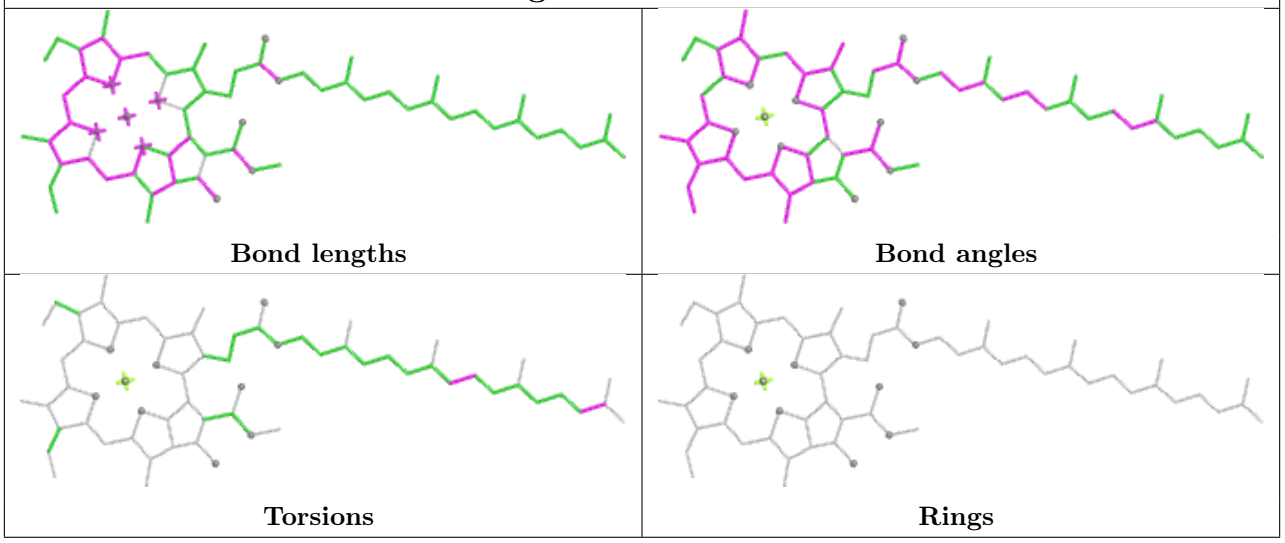
Ligand HTG c 526



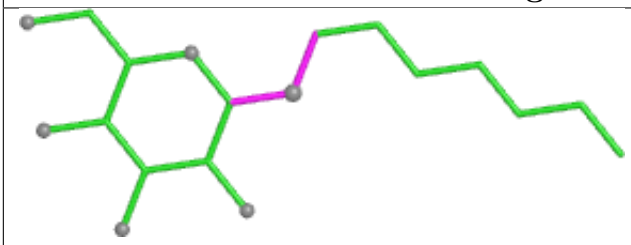
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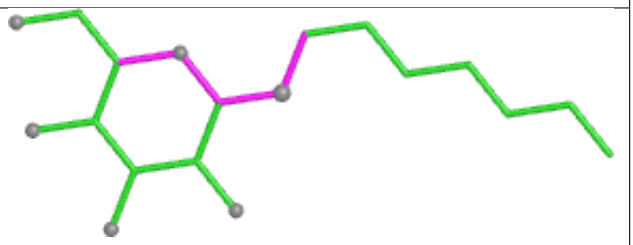
Ligand CLA b 614



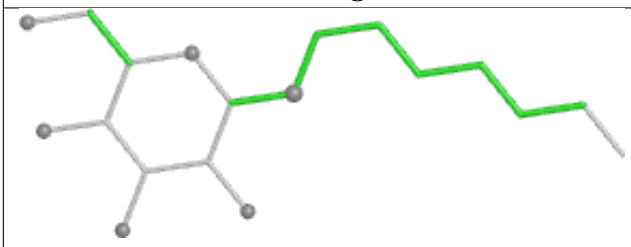
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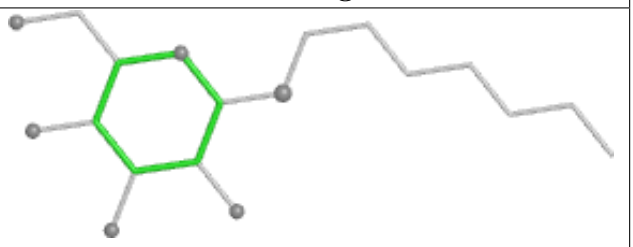
Bond lengths



Bond angles

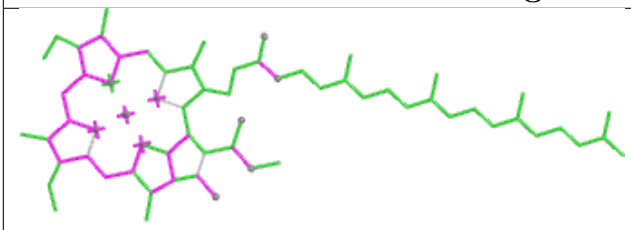


Torsions

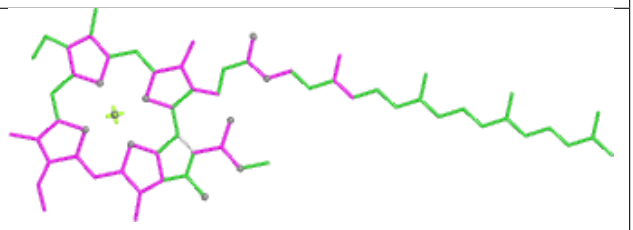


Rings

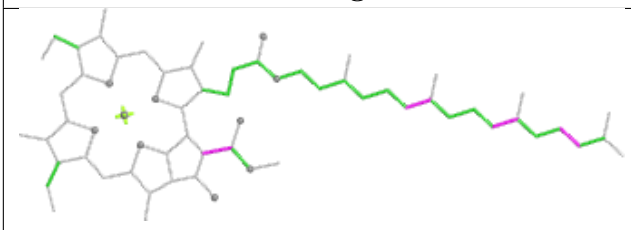
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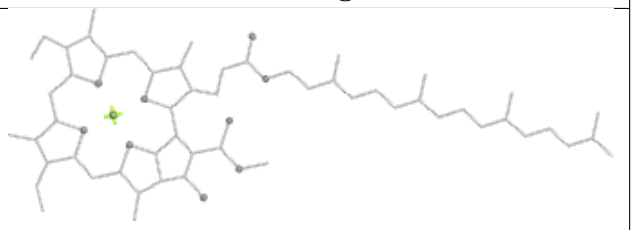
Bond lengths



Bond angles



Torsions

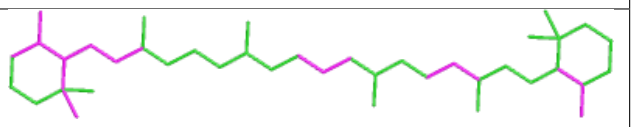


Rings

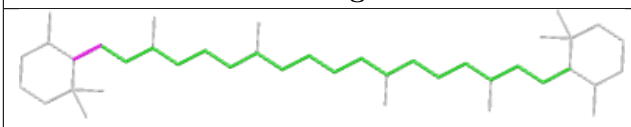
Ligand BCR A 410



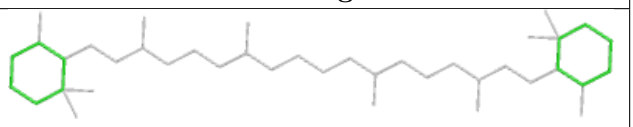
Bond lengths



Bond angles

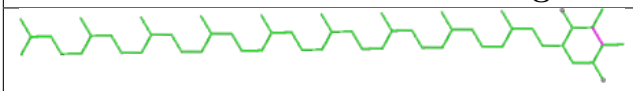


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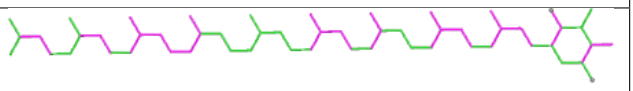


Rings

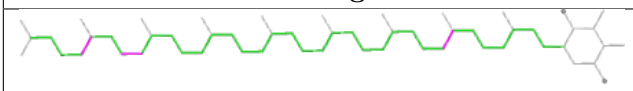
Ligand PL9 d 407



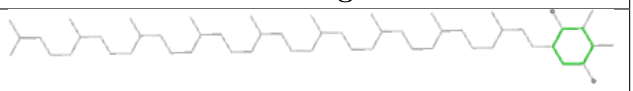
Bond lengths



Bond angles

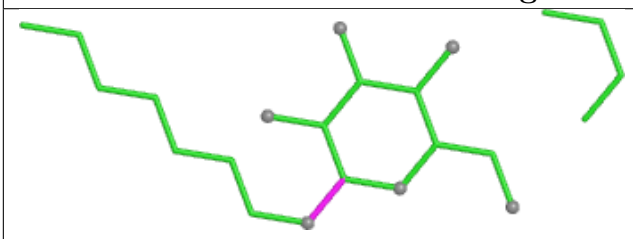


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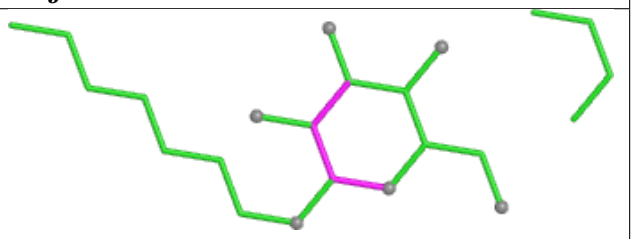


Rings

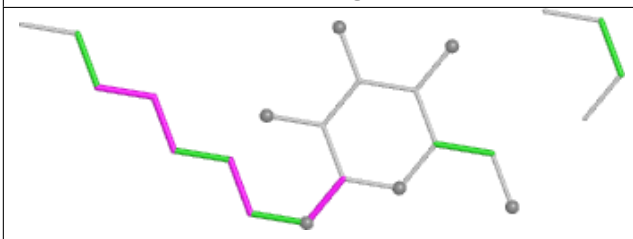
Ligand LMT j 1601



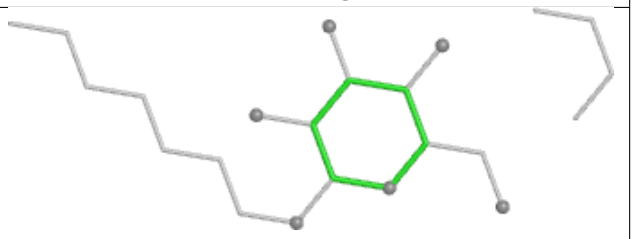
Bond lengths



Bond angles

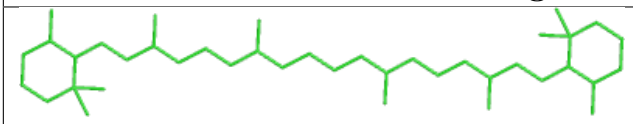


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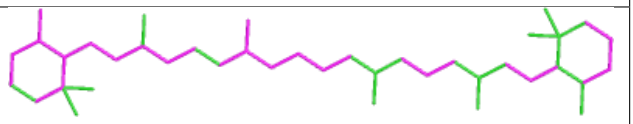


Rings

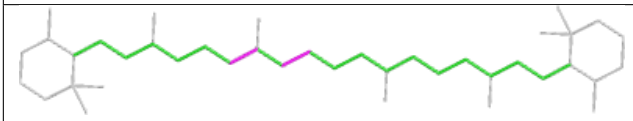
Ligand BCR t 102



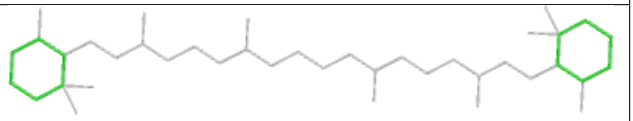
Bond lengths



Bond angles

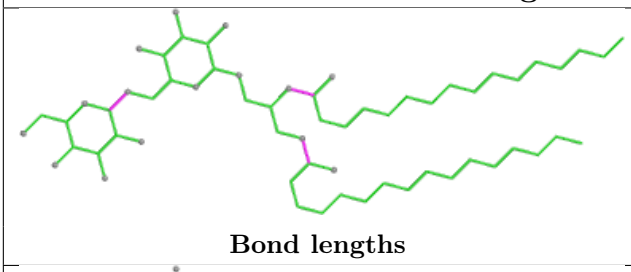


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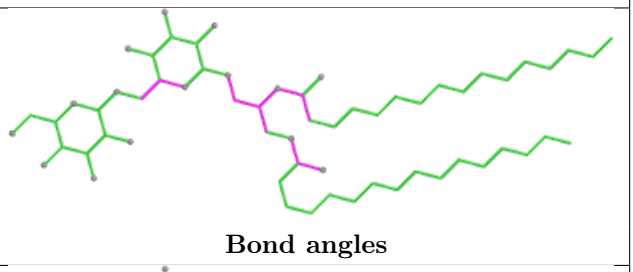


Rings

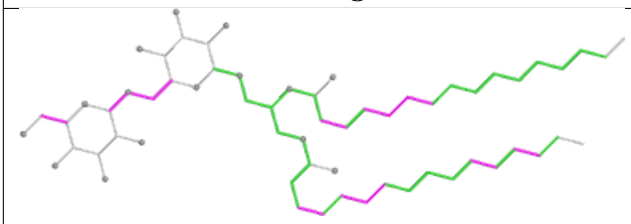
Ligand DGD C 517



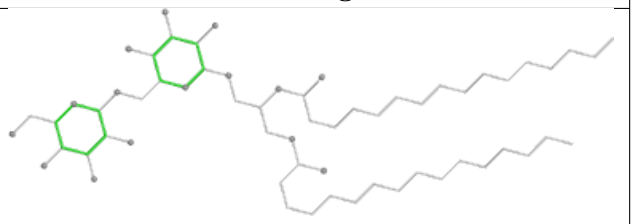
Bond lengths



Bond angles

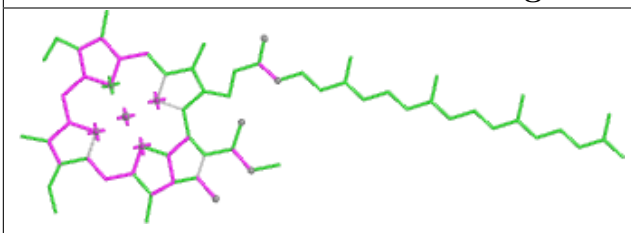


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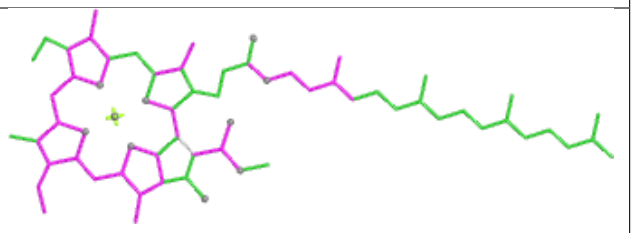


Rings

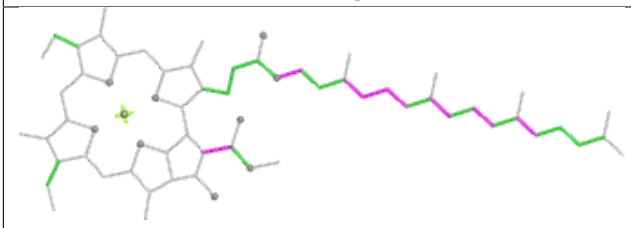
Ligand CLA B 617



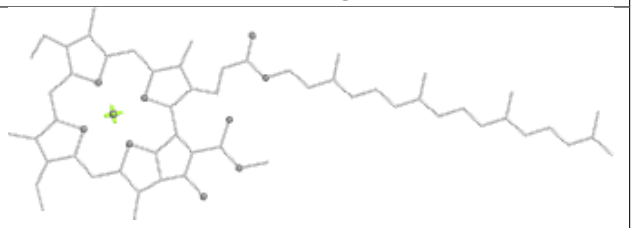
Bond lengths



Bond angles

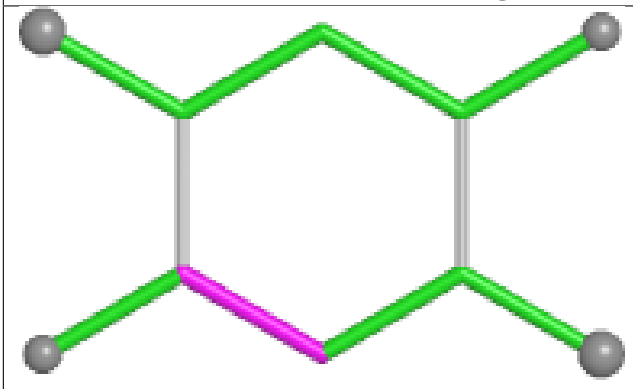


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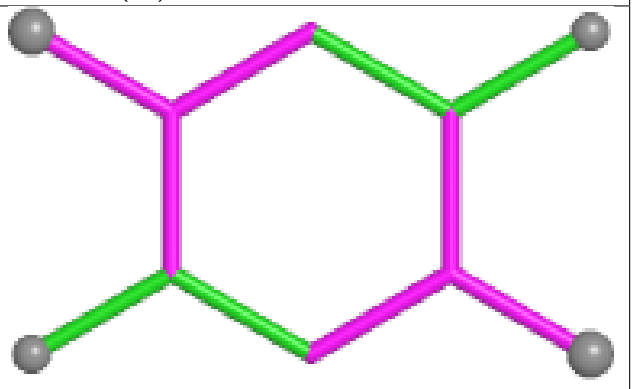


Rings

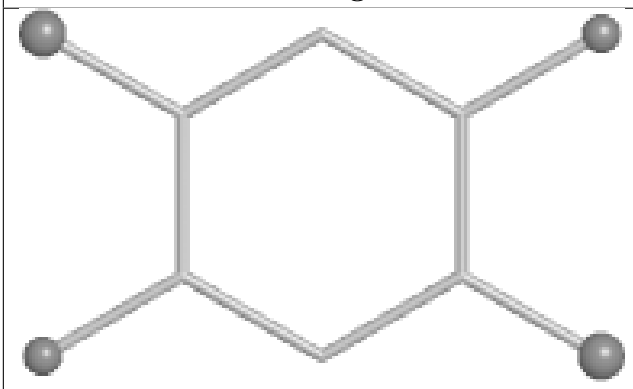
Ligand K2I a 2118 (A)



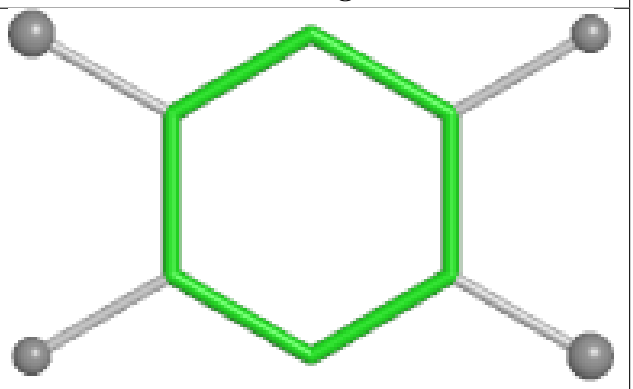
Bond lengths



Bond angles

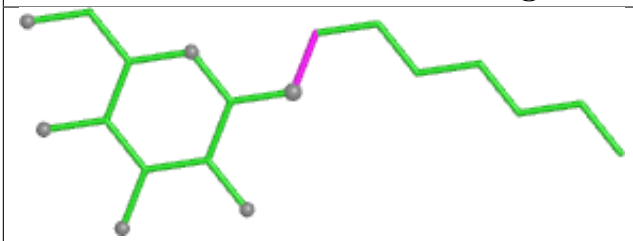


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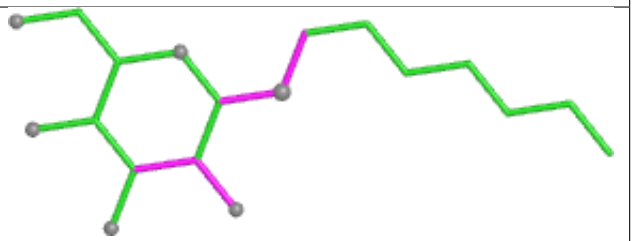


Rings

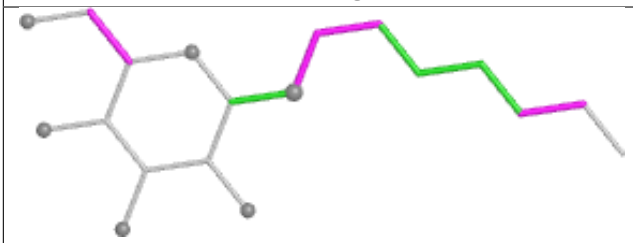
Ligand HTG O 302



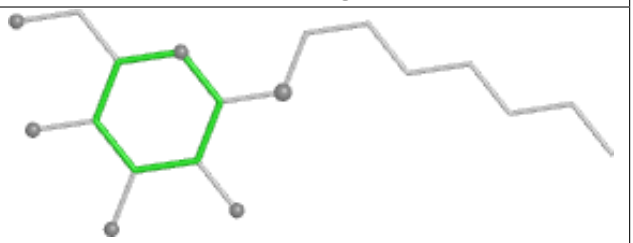
Bond lengths



Bond angles

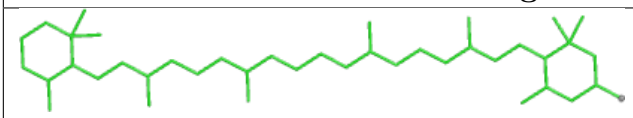


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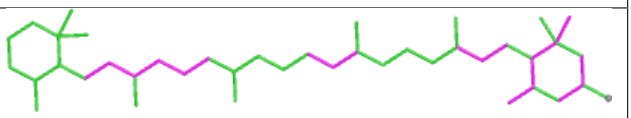


Rings

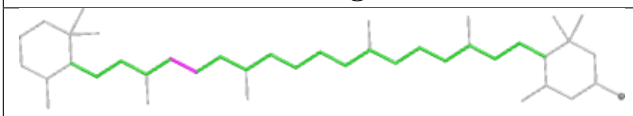
Ligand RRX H 101



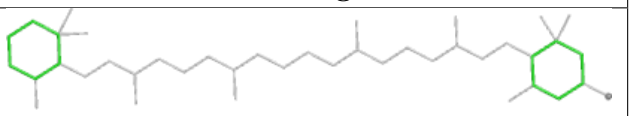
Bond lengths



Bond angles

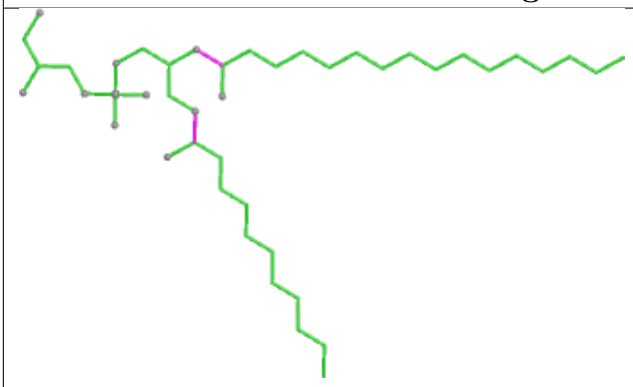


Torsions



Rings

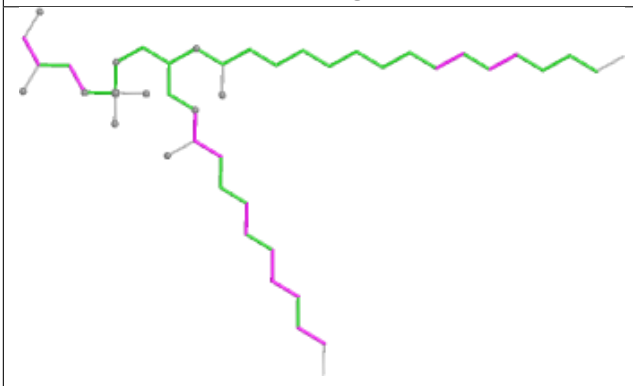
Ligand LHG D 411



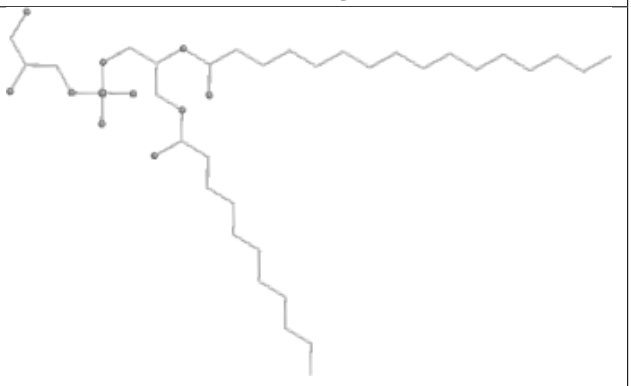
Bond lengths



Bond angles

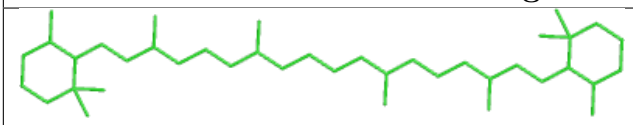


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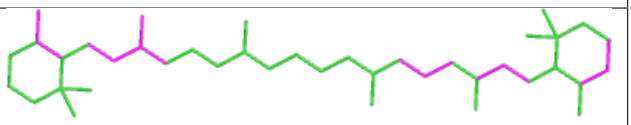


Rings

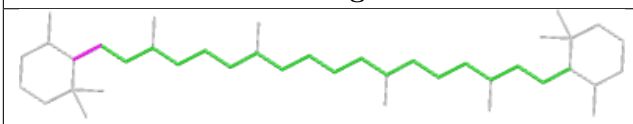
Ligand BCR B 618



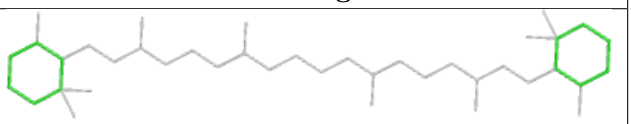
Bond lengths



Bond angles

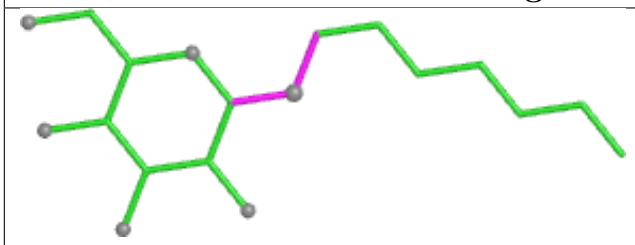


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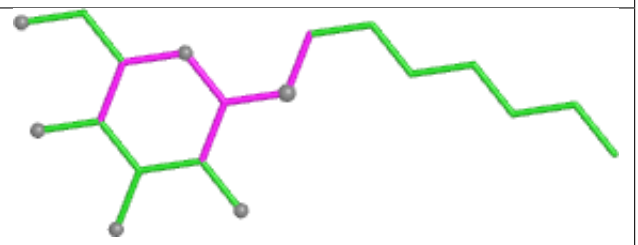


Rings

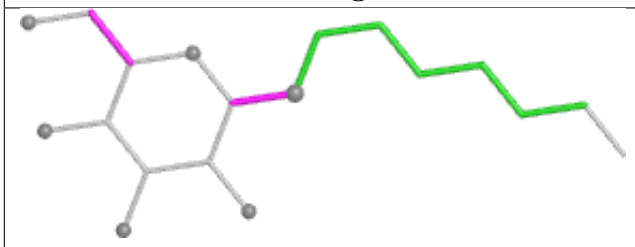
Ligand HTG b 602



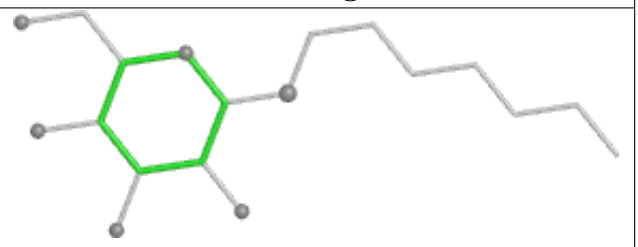
Bond lengths



Bond angles

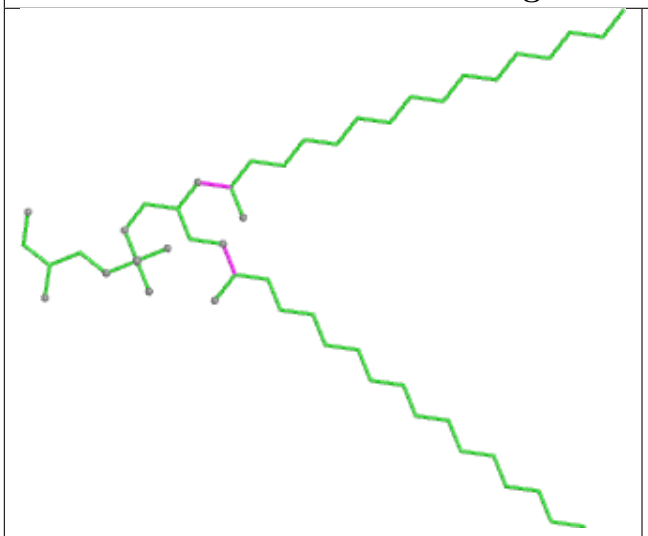


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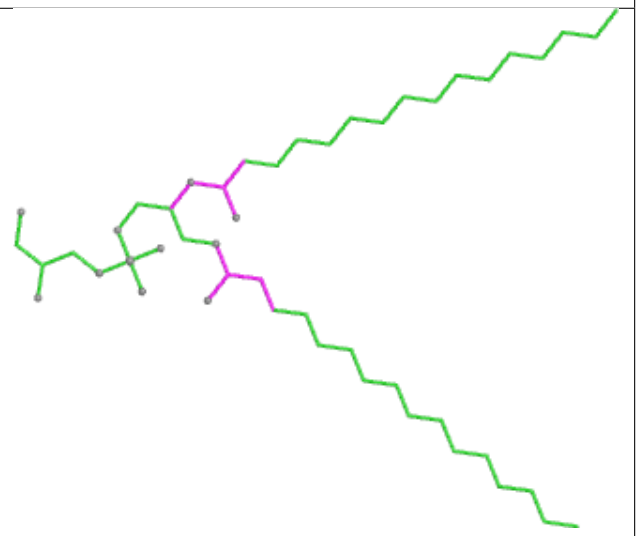


Rings

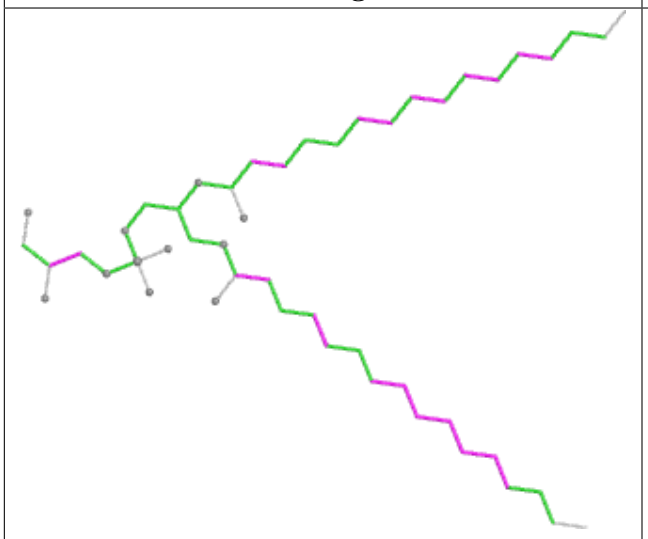
Ligand LHG D 409



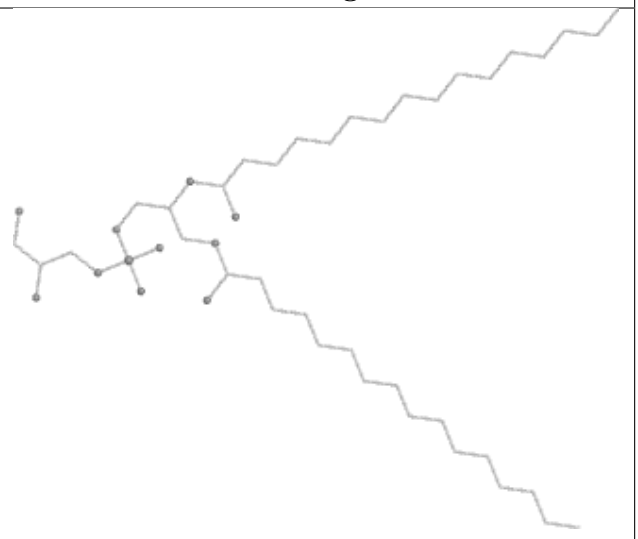
Bond lengths



Bond angles

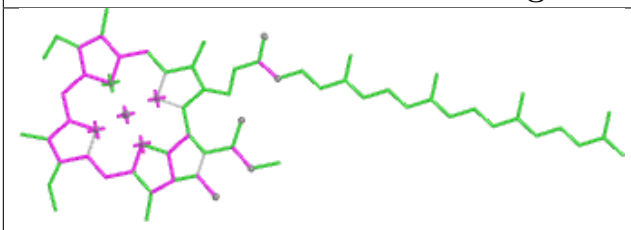


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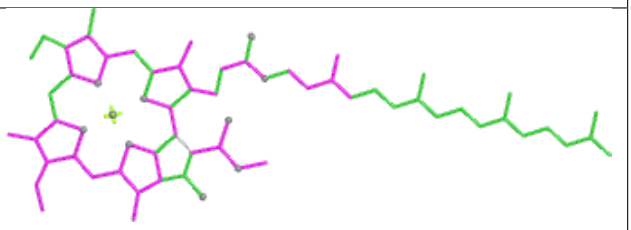


Rings

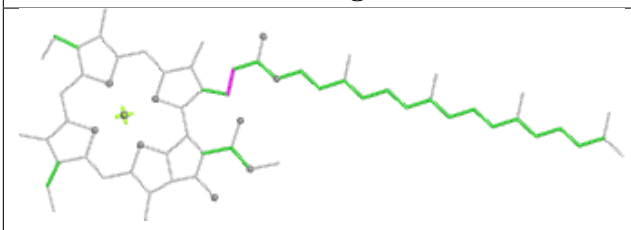
Ligand CLA b 605



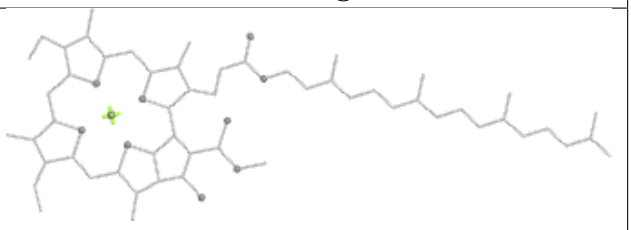
Bond lengths



Bond angles

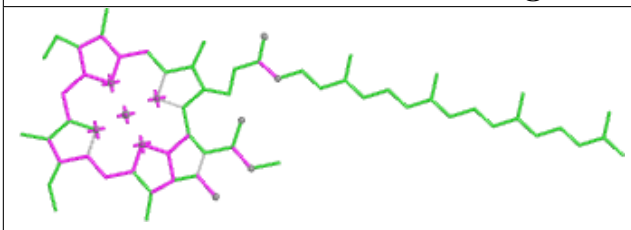


Torsions

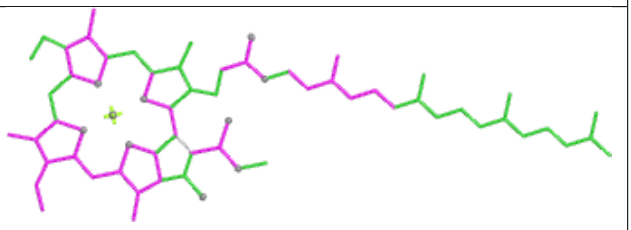


Rings

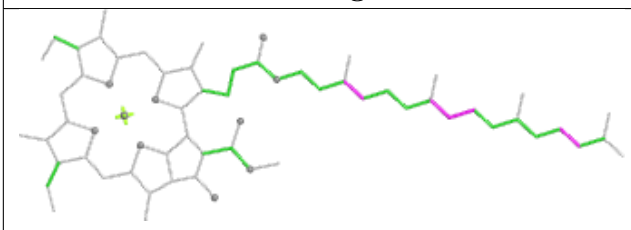
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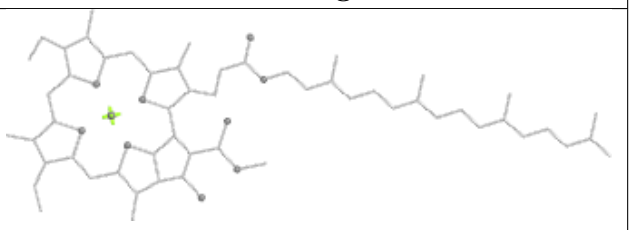
Bond lengths



Bond angles

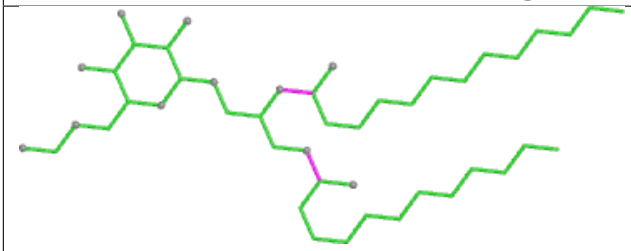


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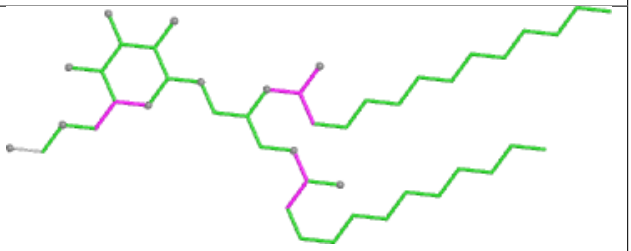


Rings

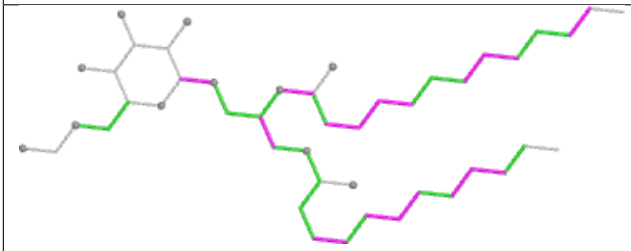
Ligand DGD D 408



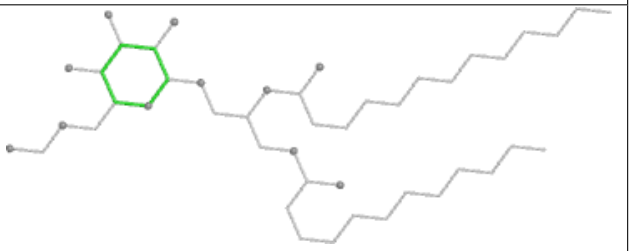
Bond lengths



Bond angles

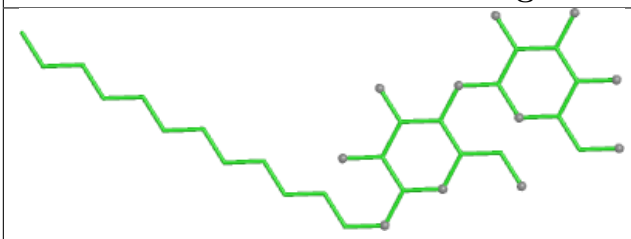


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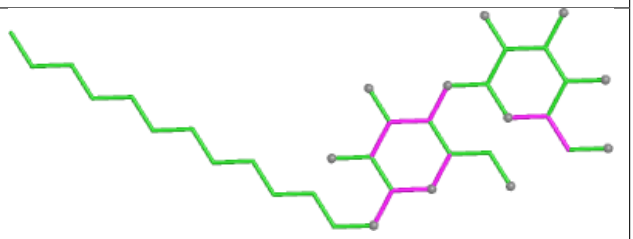


Rings

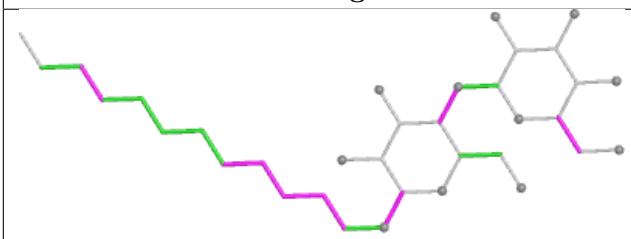
Ligand LMT a 2103



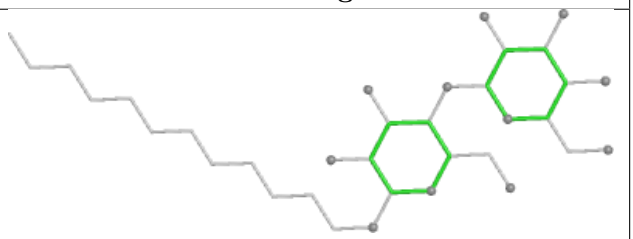
Bond lengths



Bond angles

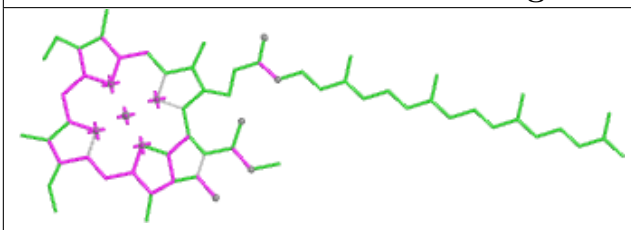


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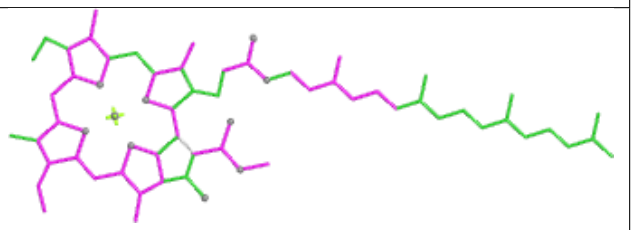


Rings

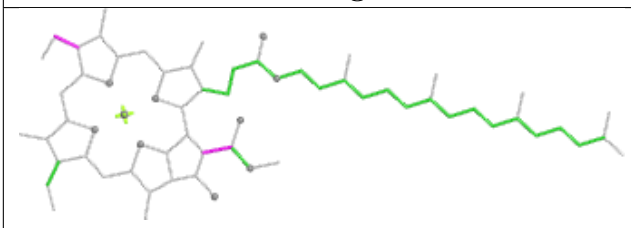
Ligand CLA b 612



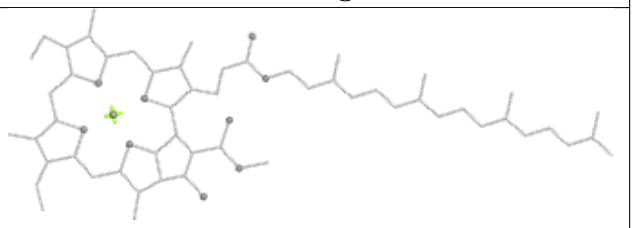
Bond lengths



Bond angles

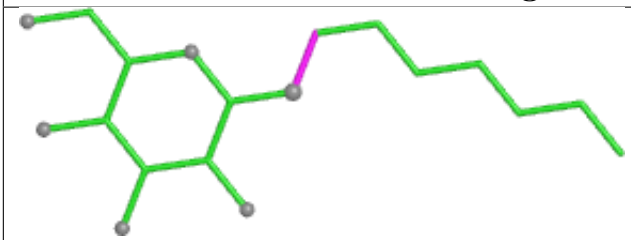


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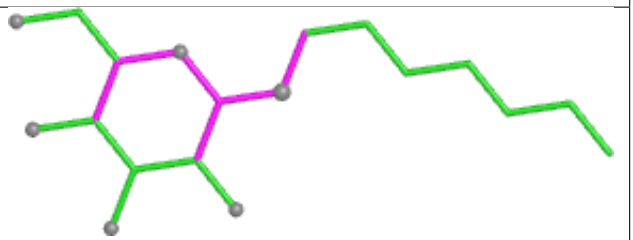


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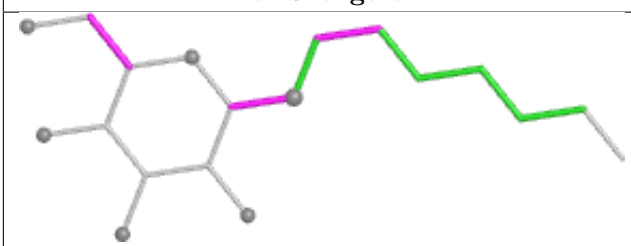
Ligand HTG C 522



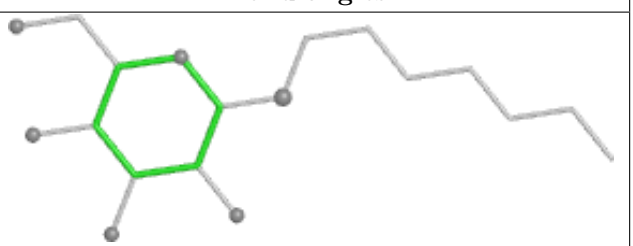
Bond lengths



Bond angles

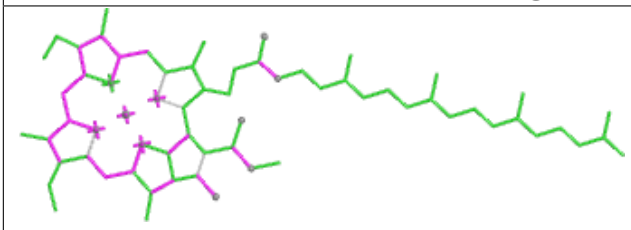


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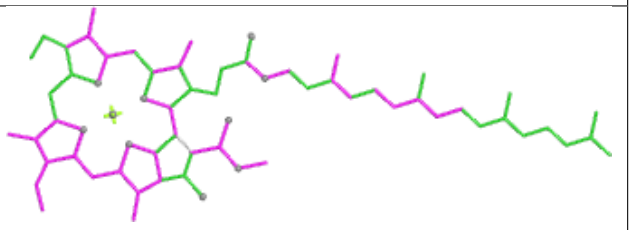


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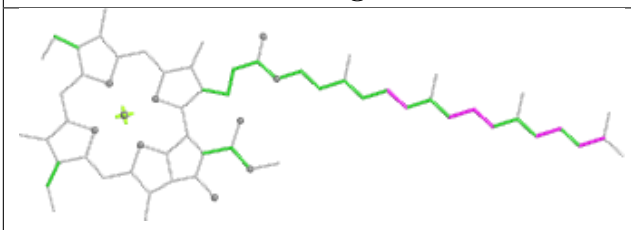
Ligand CLA b 618



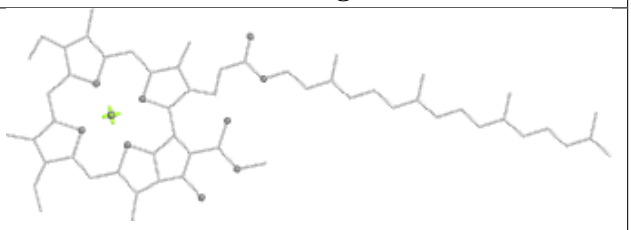
Bond lengths



Bond angles

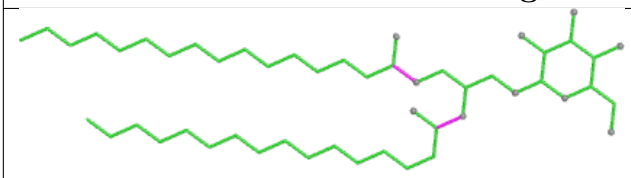


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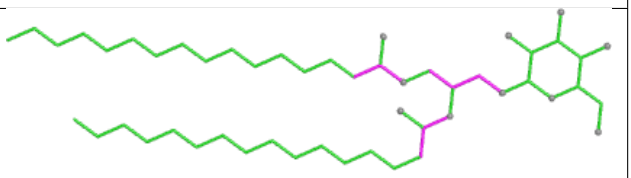


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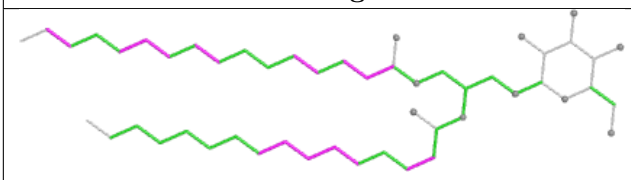
Ligand LMG B 622



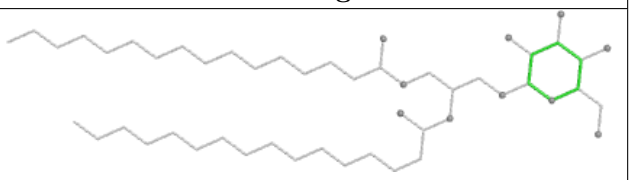
Bond lengths



Bond angles



Torsions

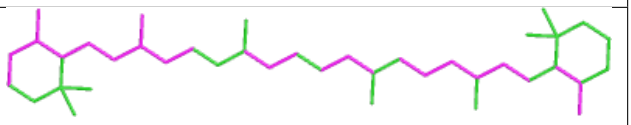


Rings

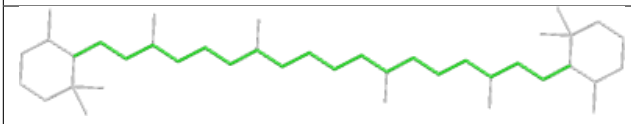
Ligand BCR k 2003



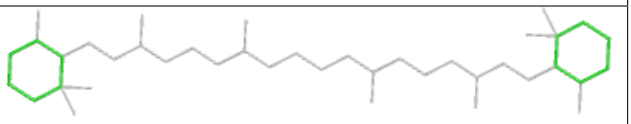
Bond lengths



Bond angles

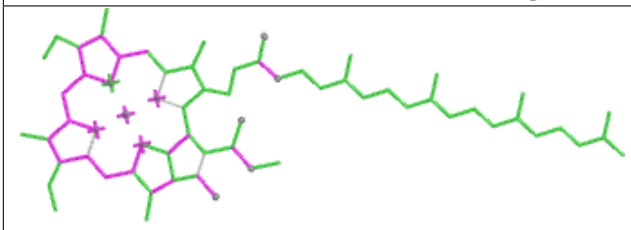


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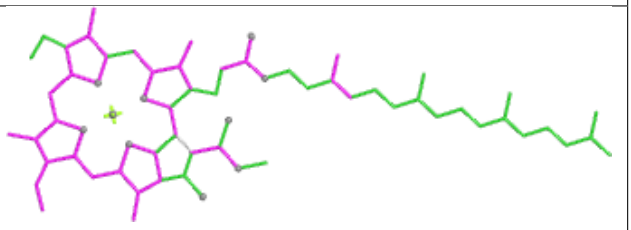


Rings

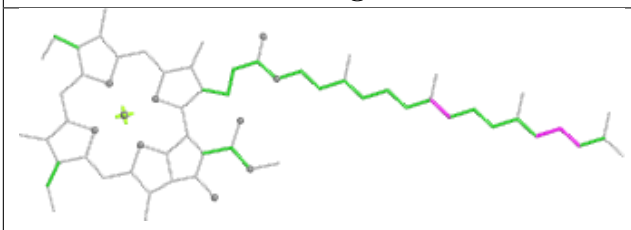
Ligand CLA B 614



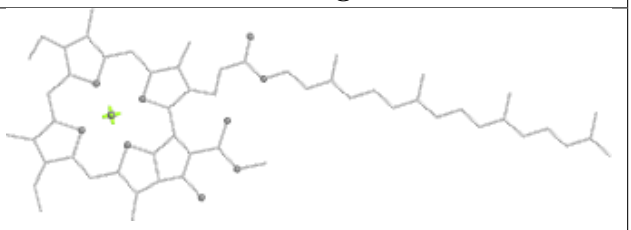
Bond lengths



Bond angles

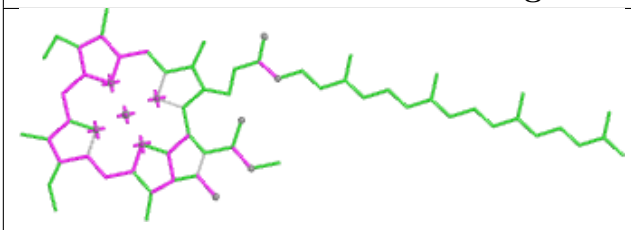


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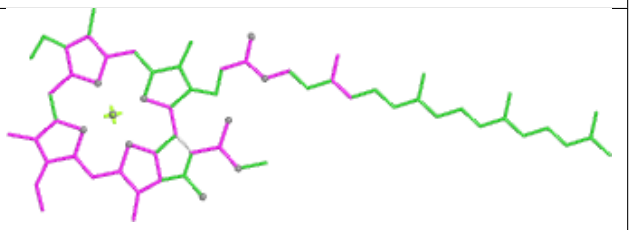


Rings

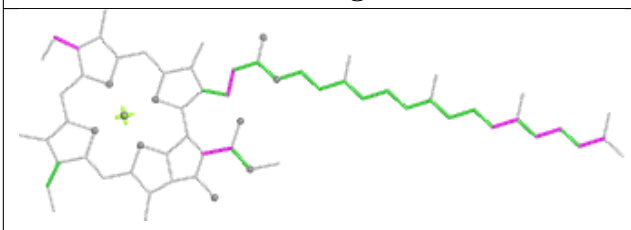
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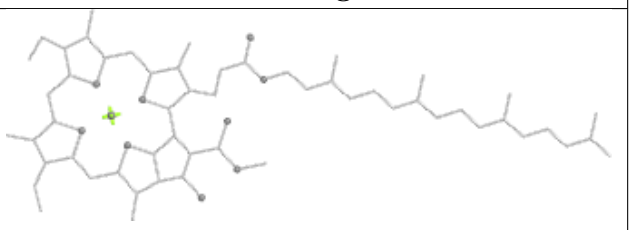
Bond lengths



Bond angles

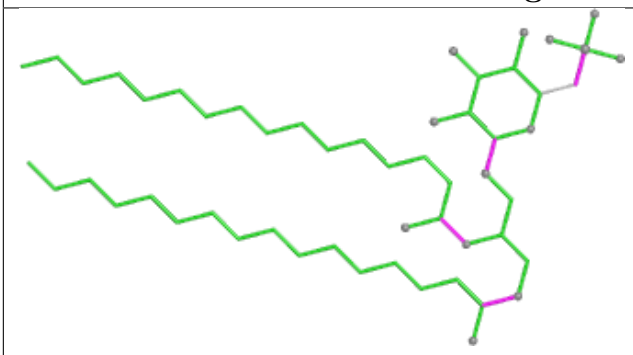


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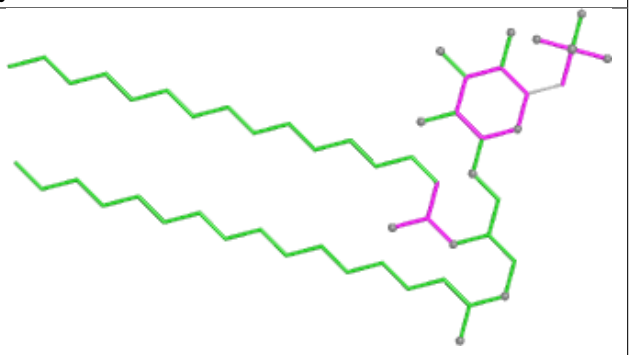


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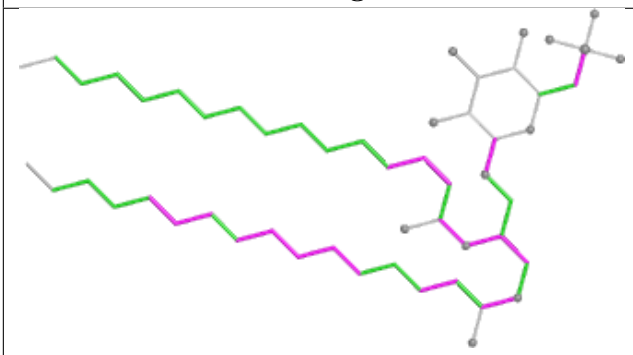
Ligand SQD B 621



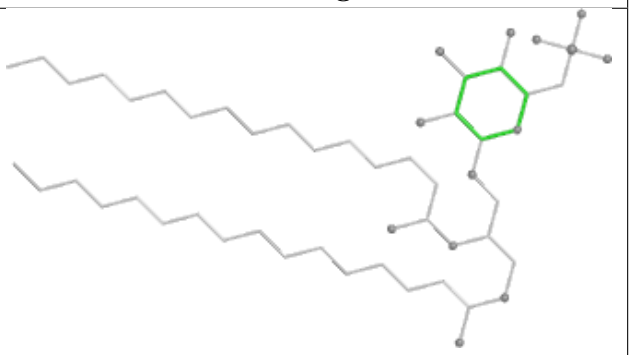
Bond lengths



Bond angles

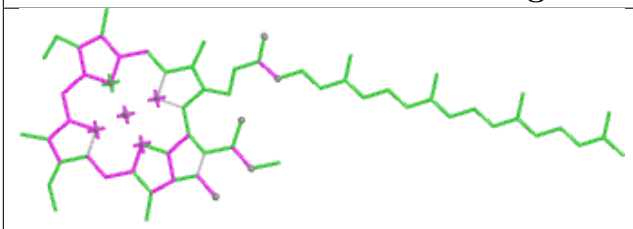


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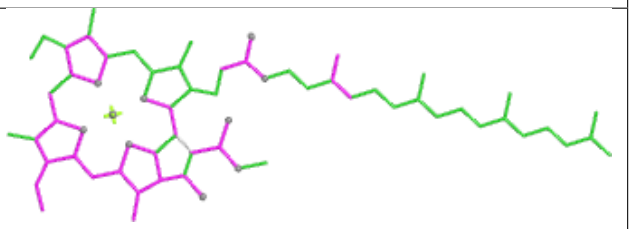


Rings

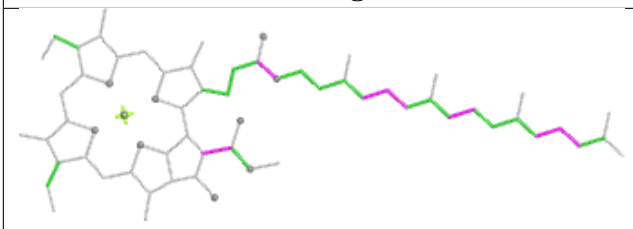
Ligand CLA b 619



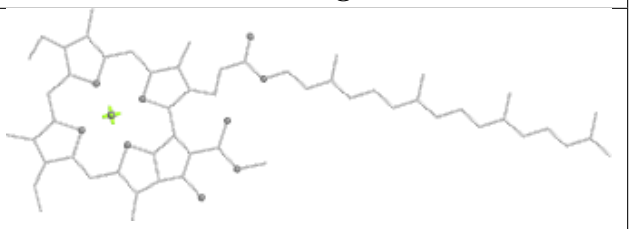
Bond lengths



Bond angles

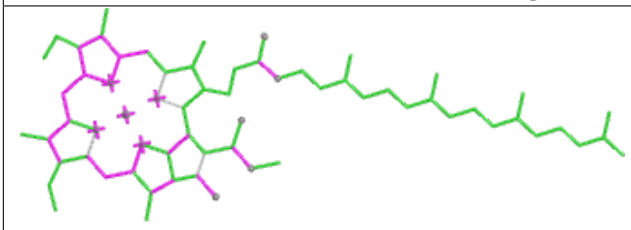


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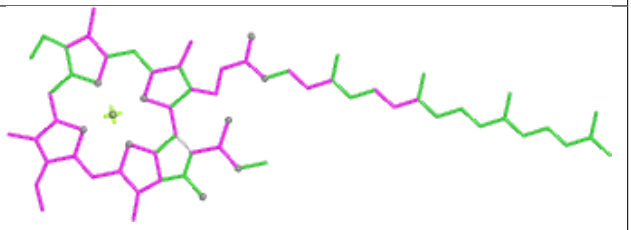


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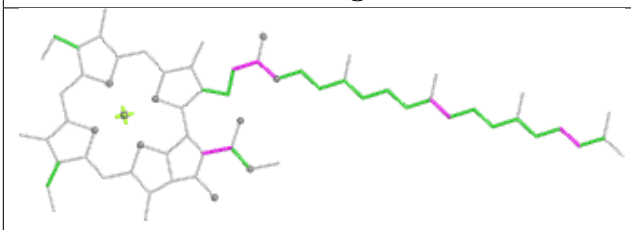
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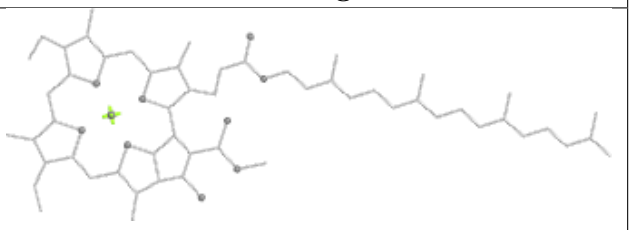
Bond lengths



Bond angles

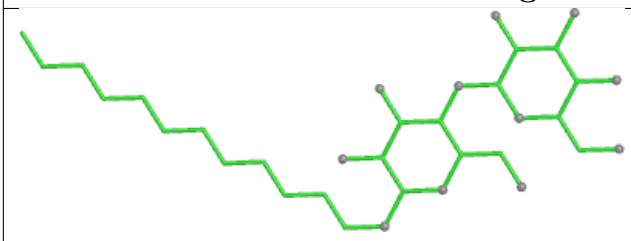


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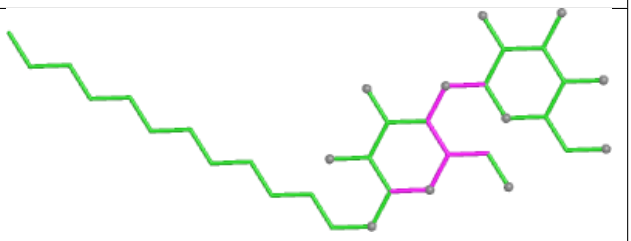


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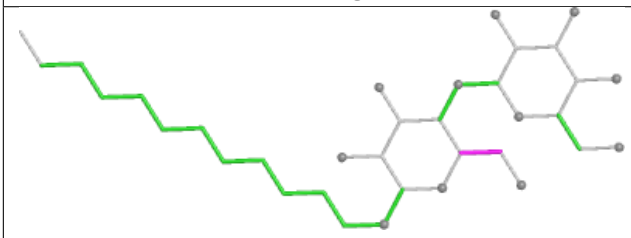
Ligand LMT m 103



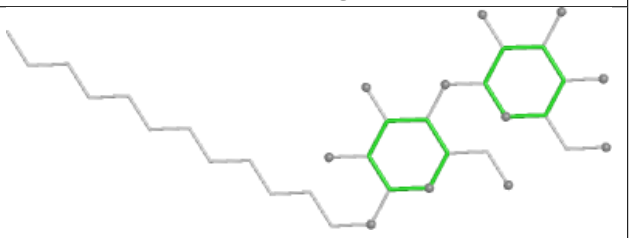
Bond lengths



Bond angles

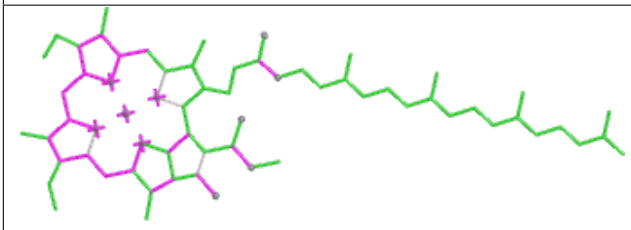


Torsions

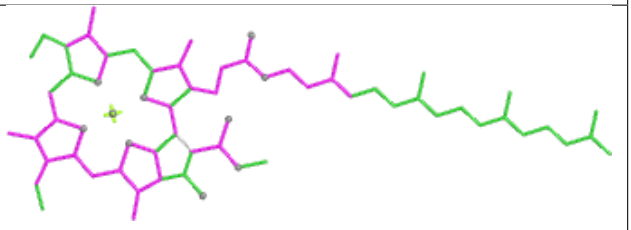


Rings

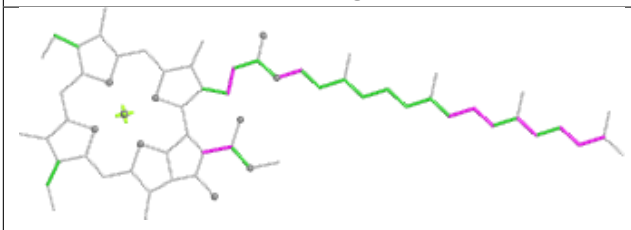
Ligand CLA B 611



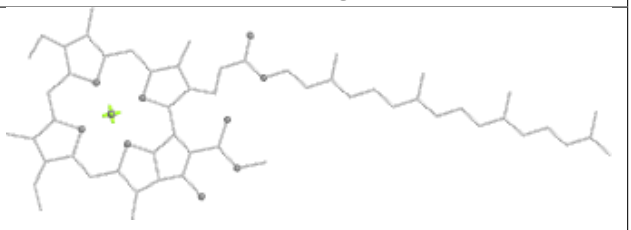
Bond lengths



Bond angles

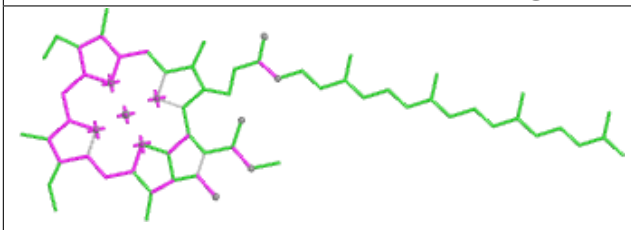


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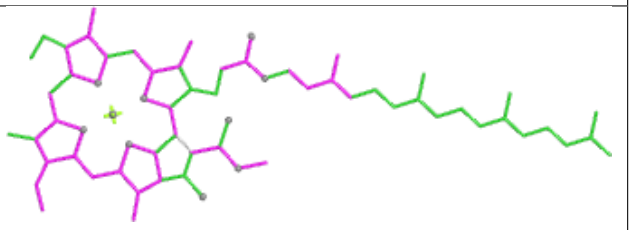


Rings

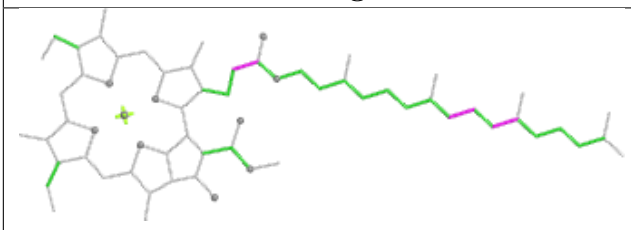
Ligand CLA b 616



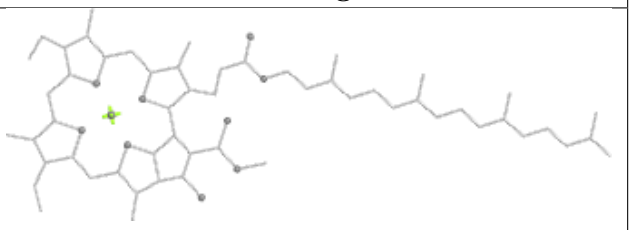
Bond lengths



Bond angles

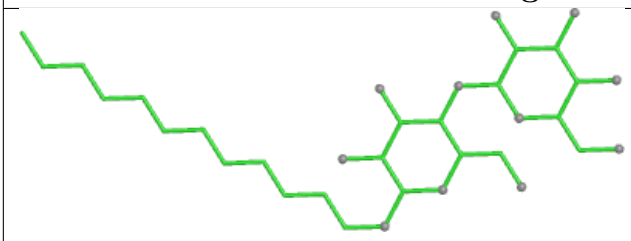


Torsions

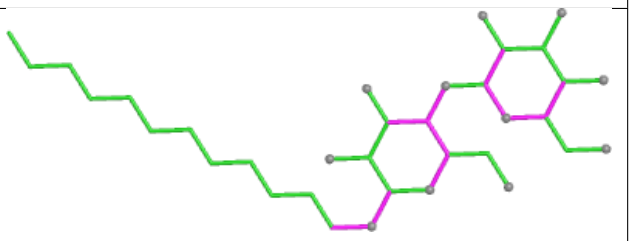


Rings

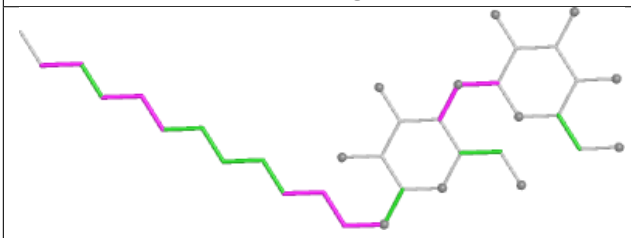
Ligand LMT B 623



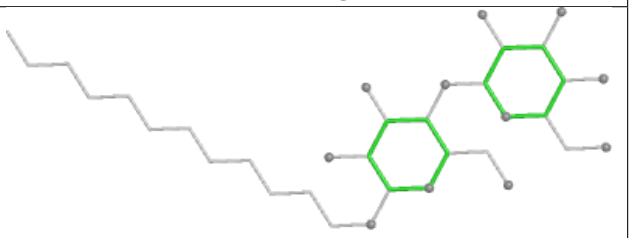
Bond lengths



Bond angles

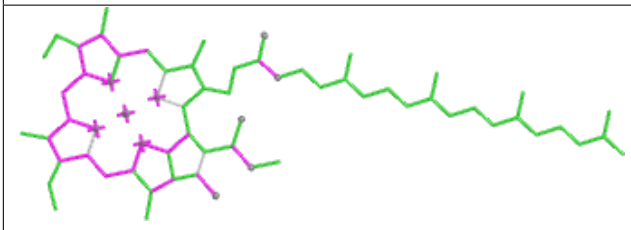


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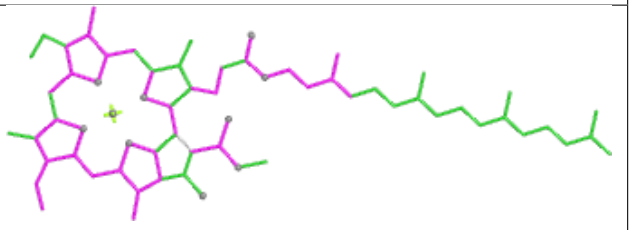


Rings

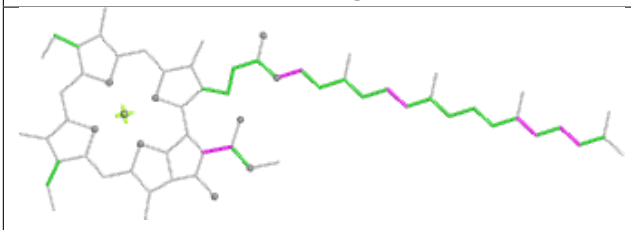
Ligand CLA C 508



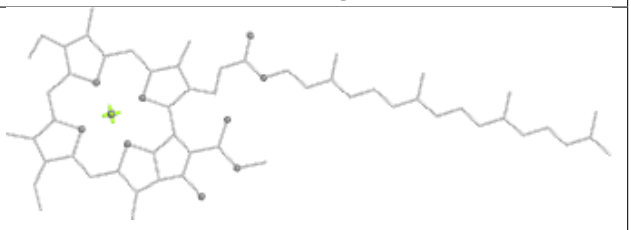
Bond lengths



Bond angles

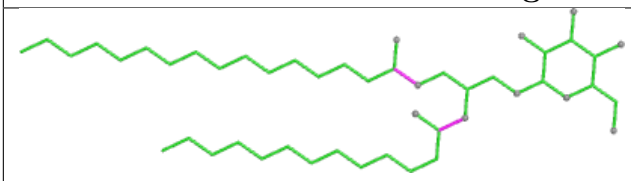


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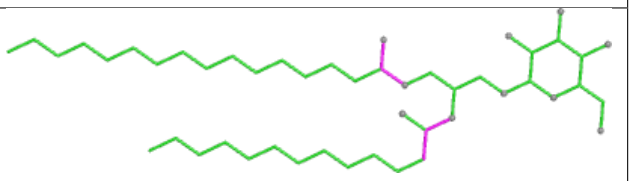


Rings

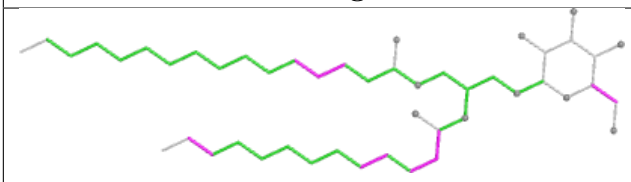
Ligand LMG d 411



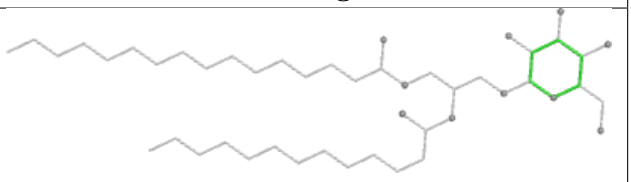
Bond lengths



Bond angles

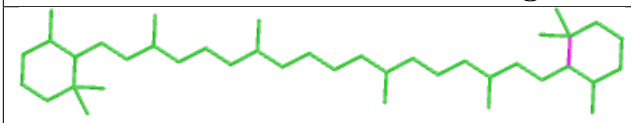


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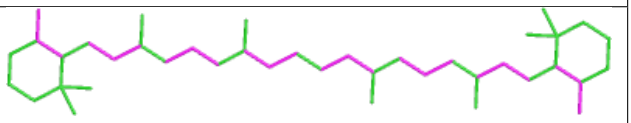


Rings

Ligand BCR D 406



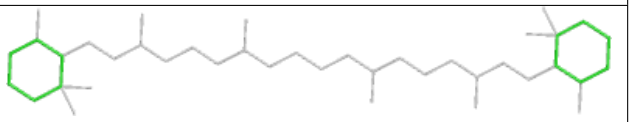
Bond lengths



Bond angles

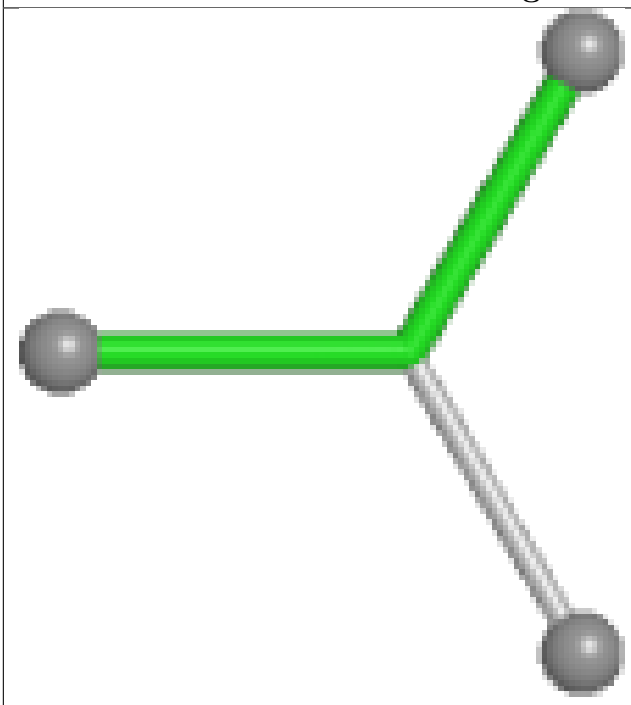


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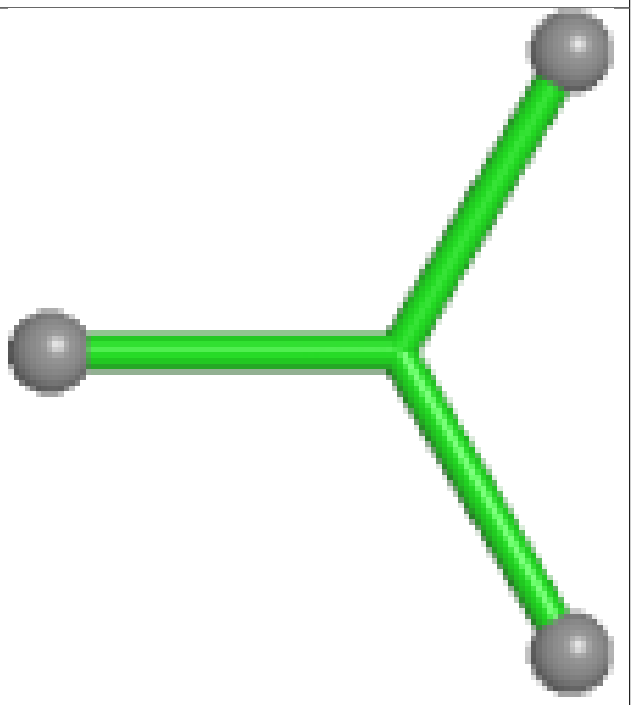


Rings

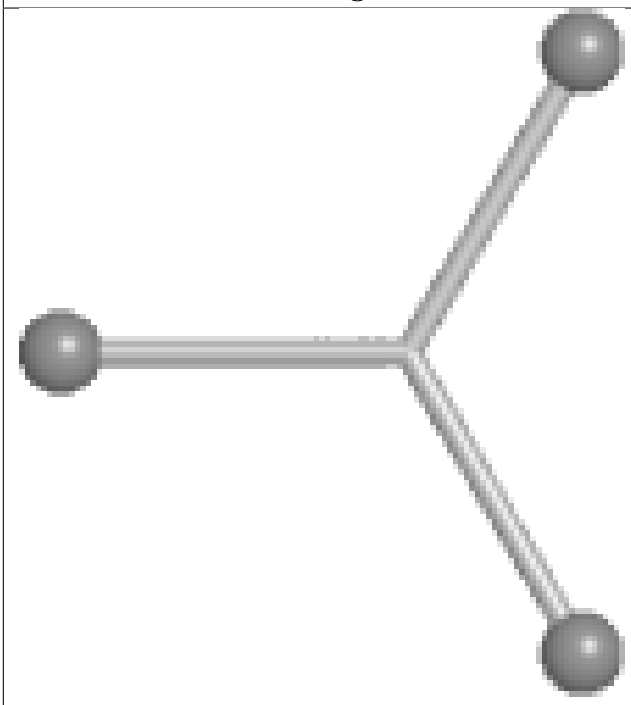
Ligand BCT A 421



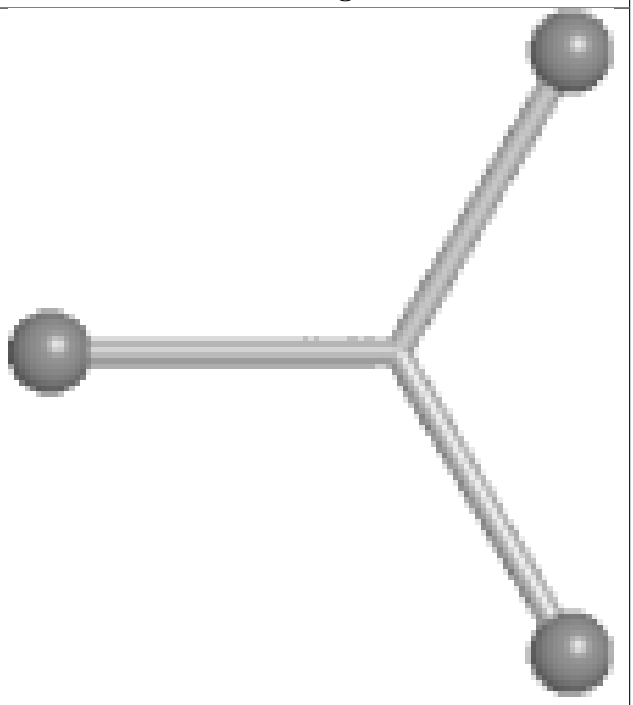
Bond lengths



Bond angles

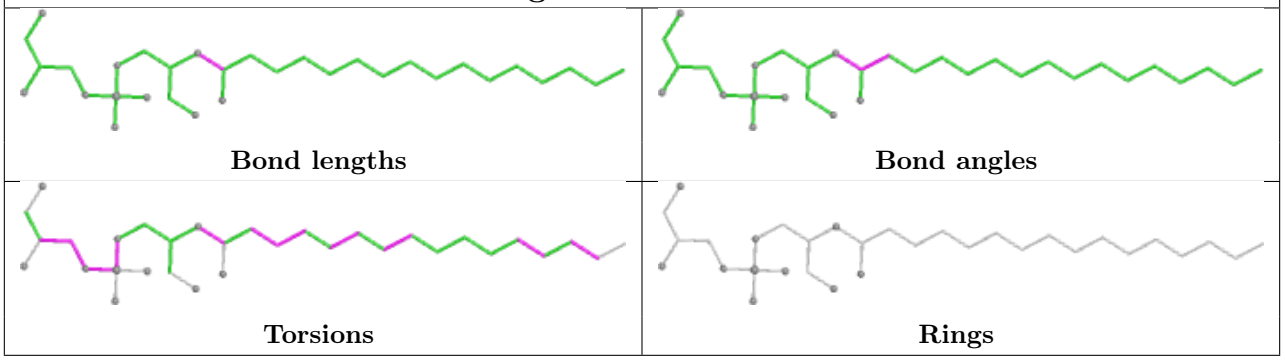


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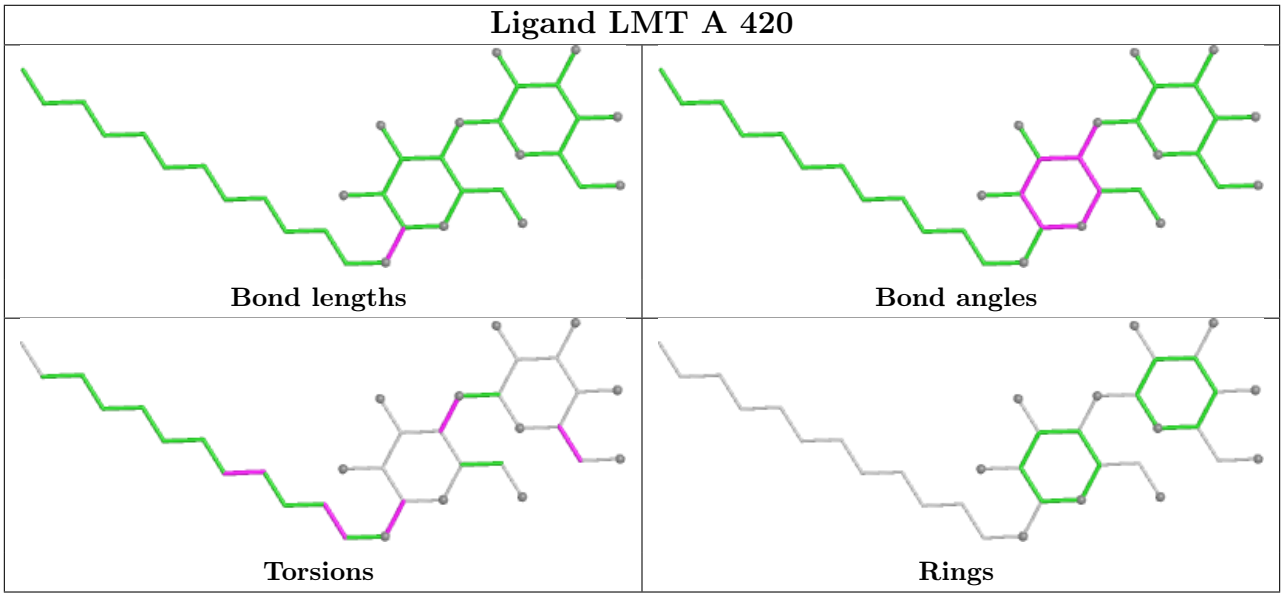


Rings

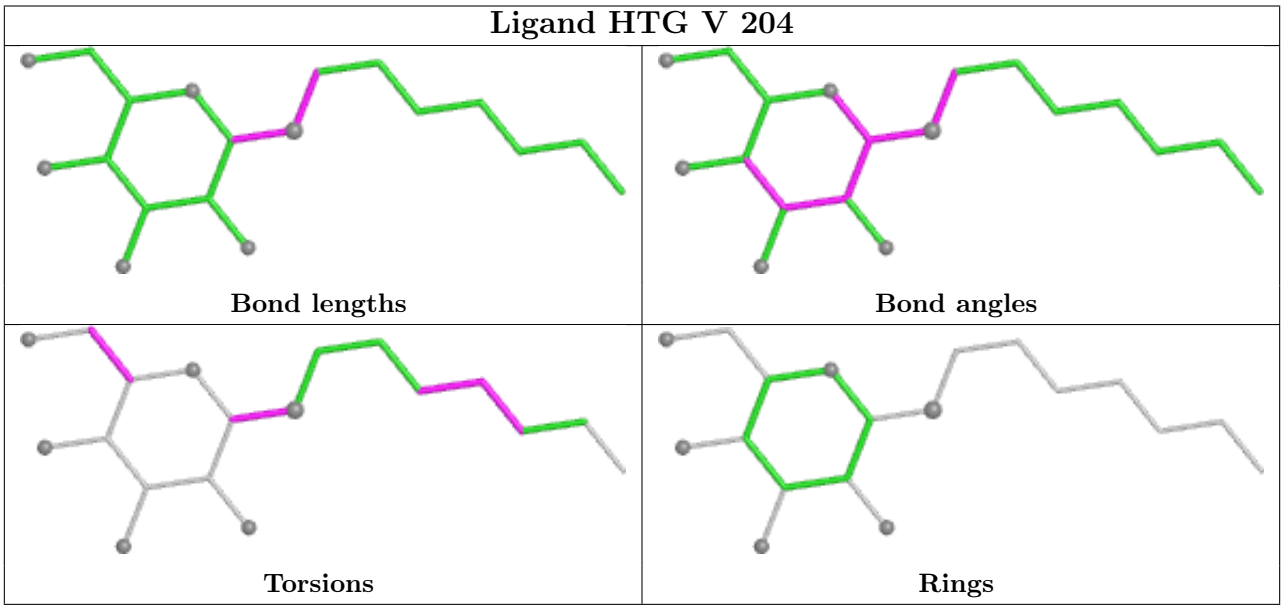
Ligand LHG e 101



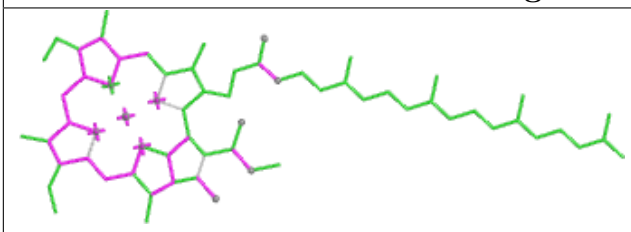
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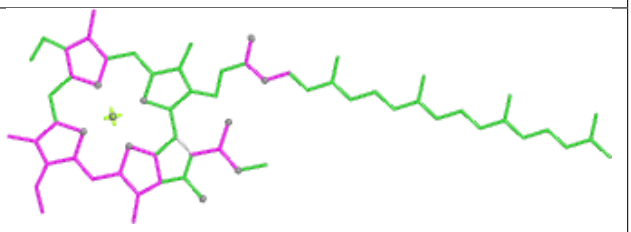
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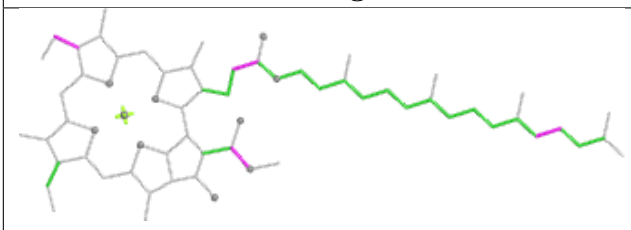
Ligand CLA C 502



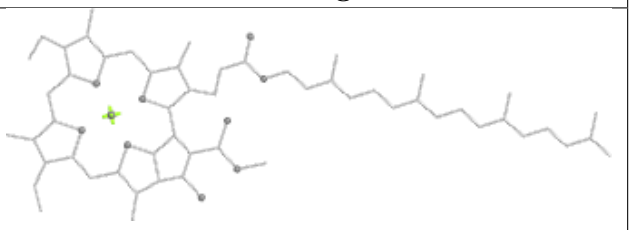
Bond lengths



Bond angles

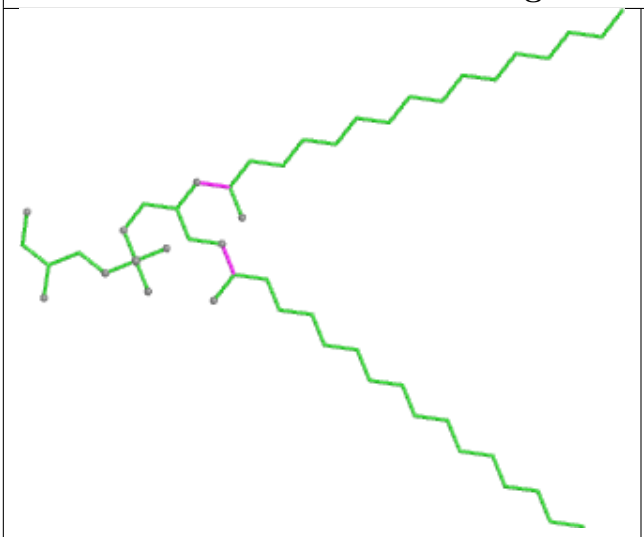


Torsions

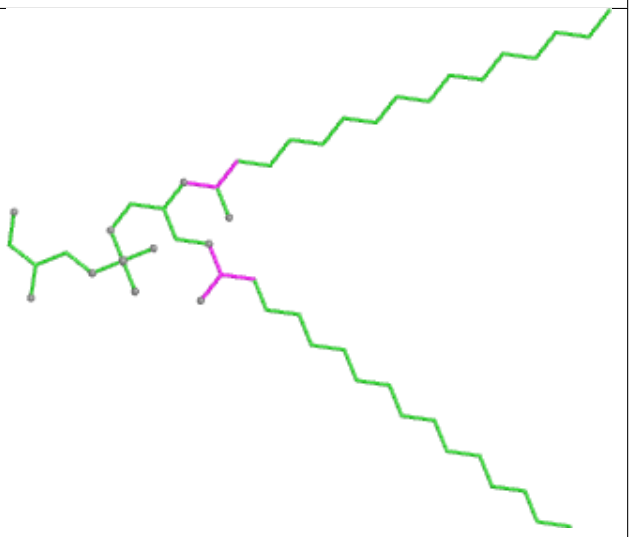


Rings

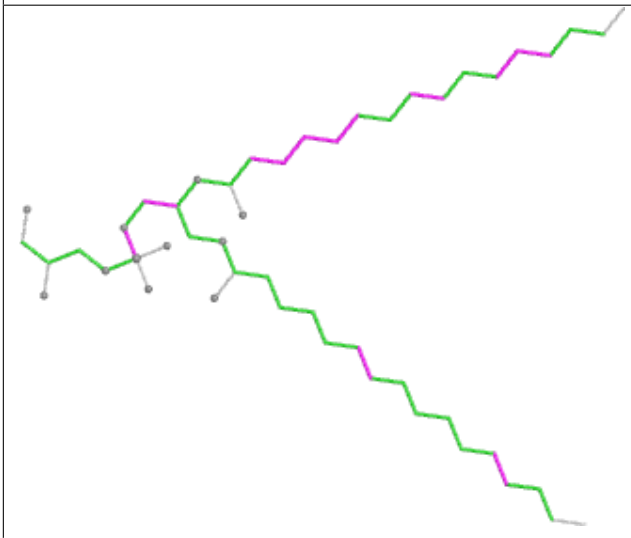
Ligand LHG L 101



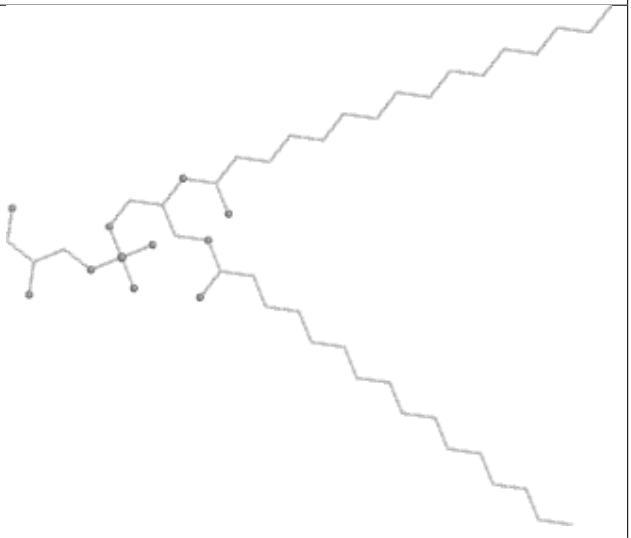
Bond lengths



Bond angles

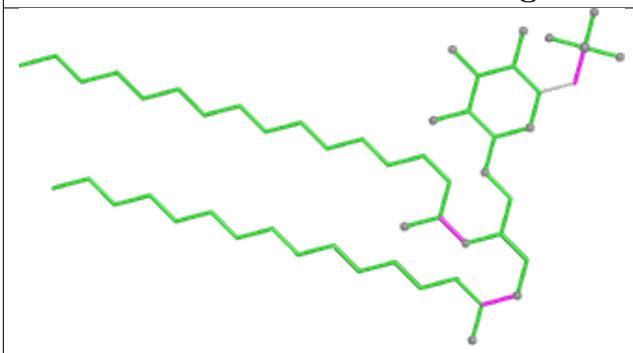


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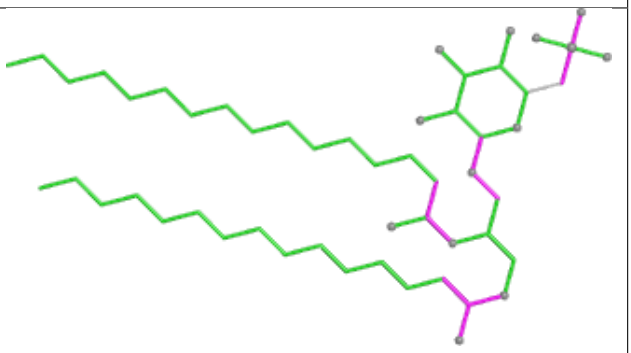


Rings

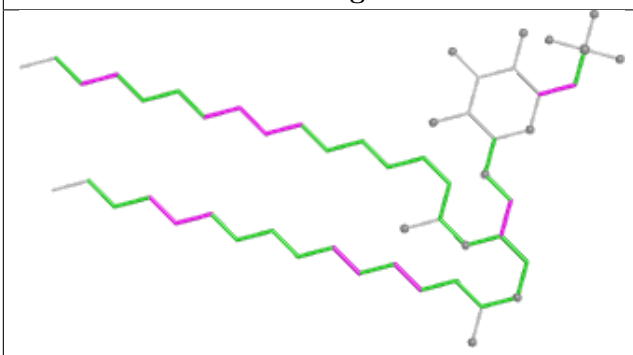
Ligand SQD a 2102



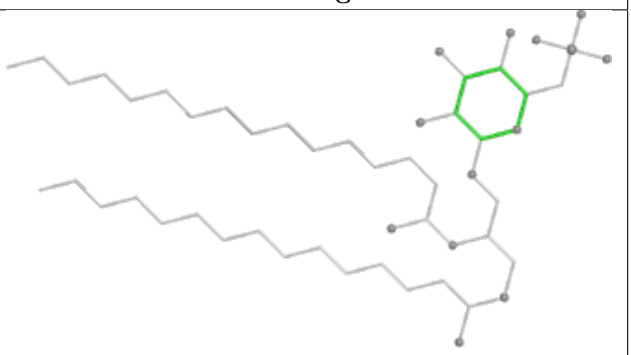
Bond lengths



Bond angles

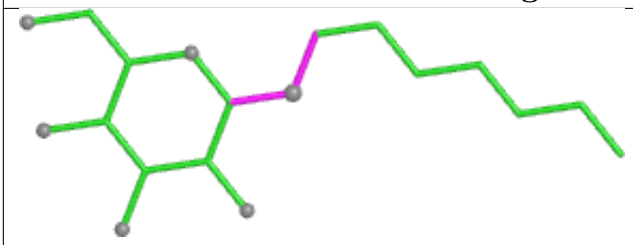


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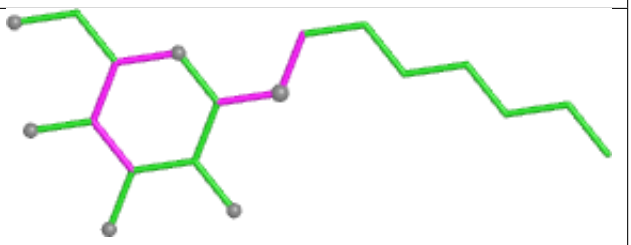


Rings

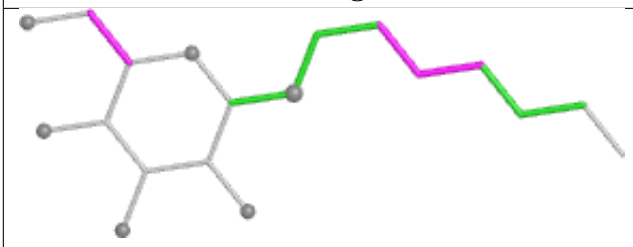
Ligand HTG B 627



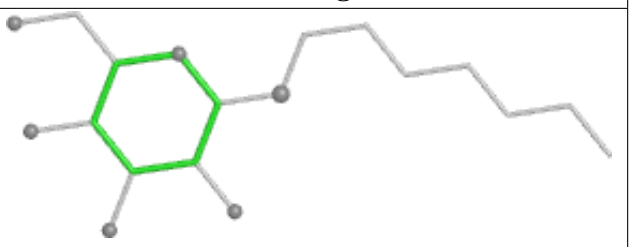
Bond lengths



Bond angles

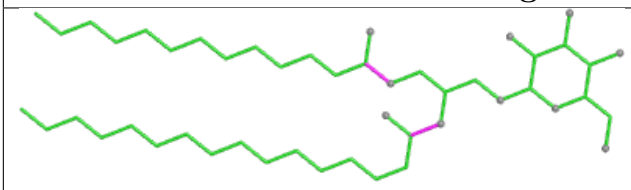


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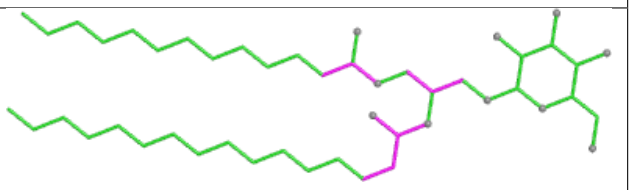


Rings

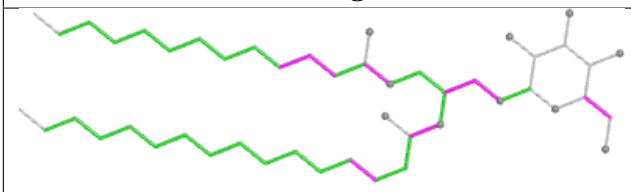
Ligand LMG C 526



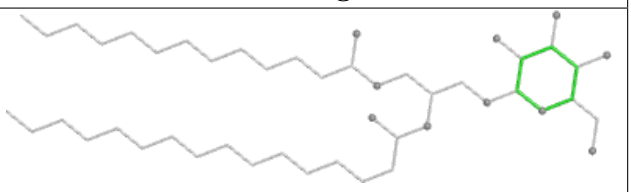
Bond lengths



Bond angles

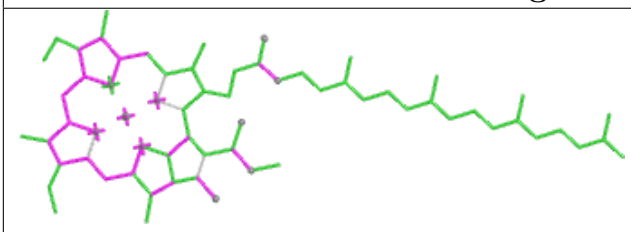


Torsions

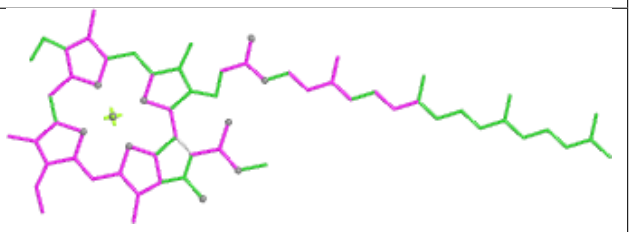


Rings

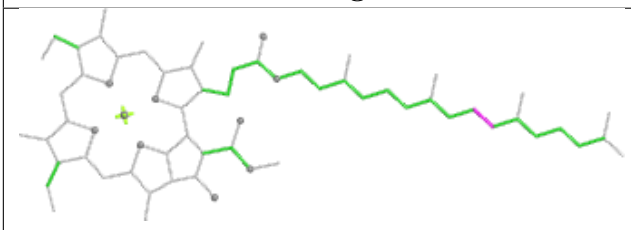
Ligand CLA c 505



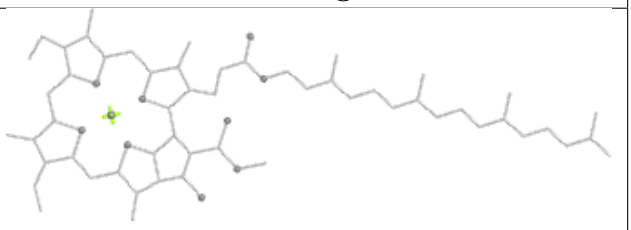
Bond lengths



Bond angles

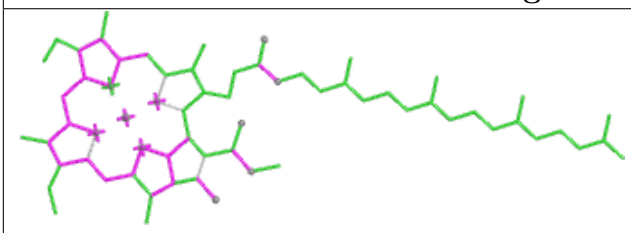


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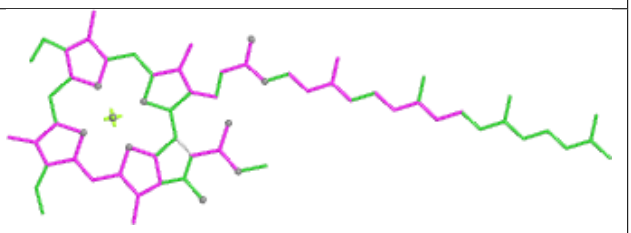


Rings

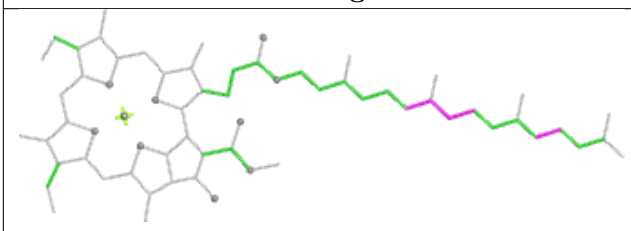
Ligand CLA D 405



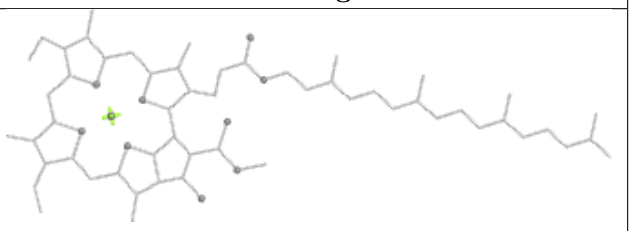
Bond lengths



Bond angles

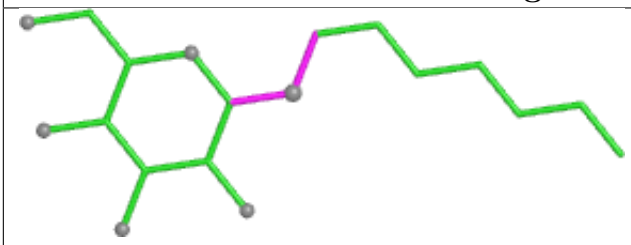


Torsions

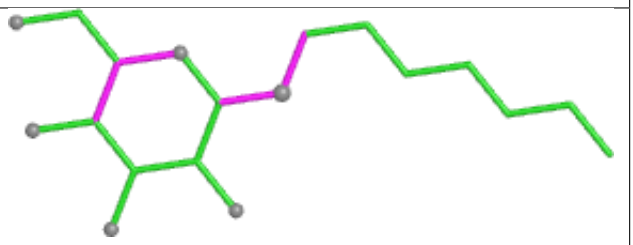


Rings

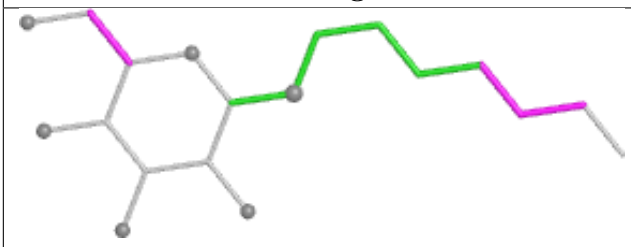
Ligand HTG d 403



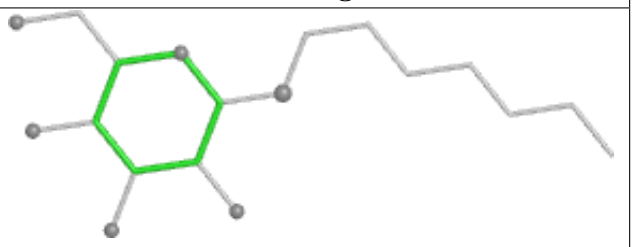
Bond lengths



Bond angles

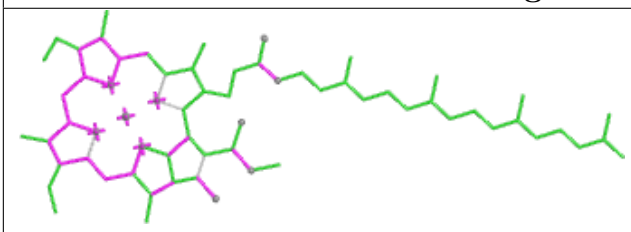


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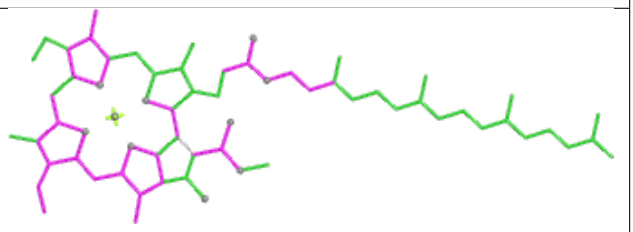


Rings

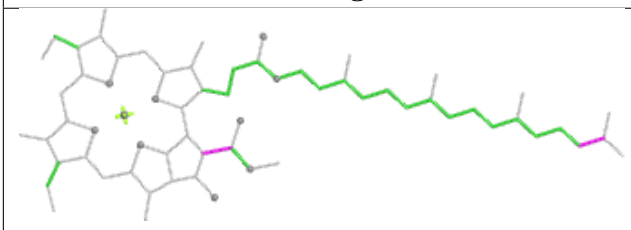
Ligand CLA C 503



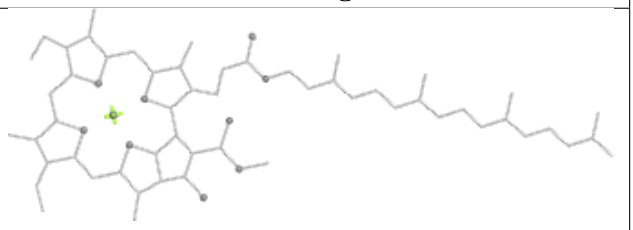
Bond lengths



Bond angles



Torsions



Rings

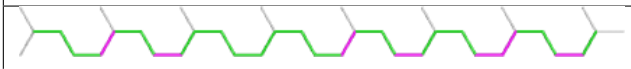
Ligand PL9 x 801



Bond lengths



Bond angles

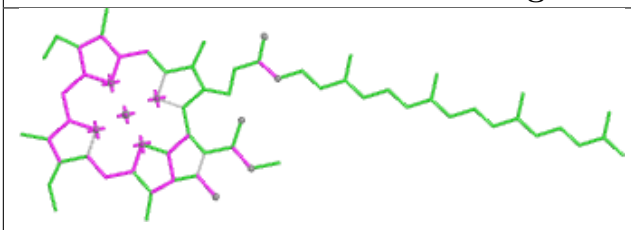


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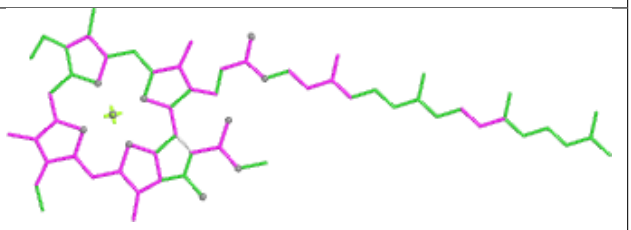


Rings

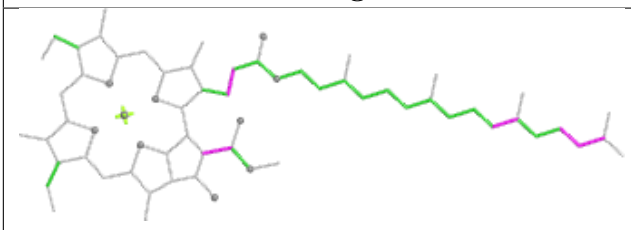
Ligand CLA b 613



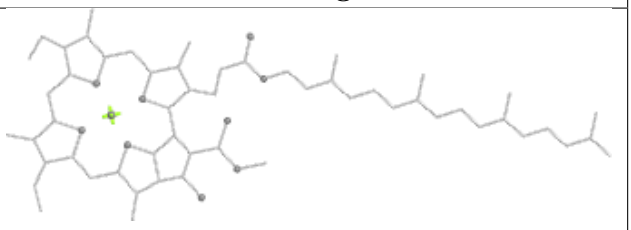
Bond lengths



Bond angles

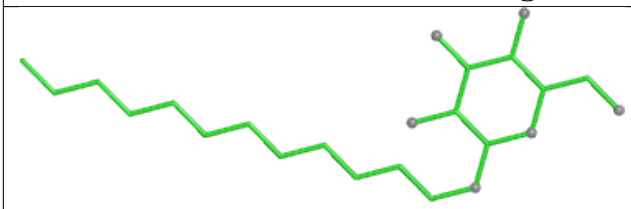


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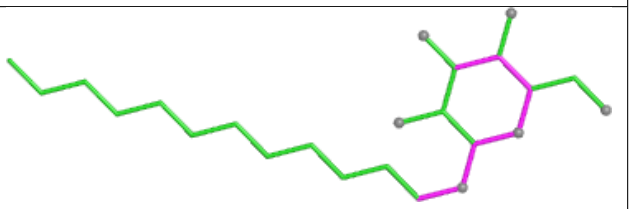


Rings

Ligand LMT I 1201



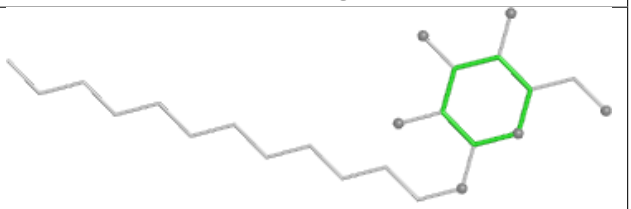
Bond lengths



Bond angles

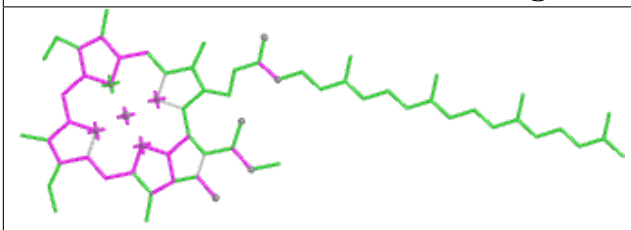


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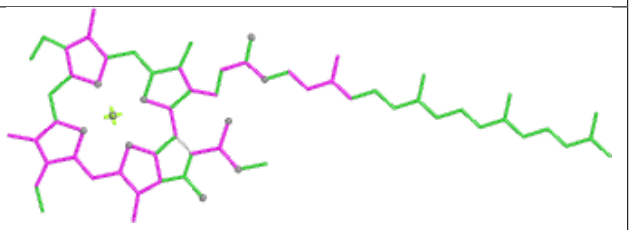


Rings

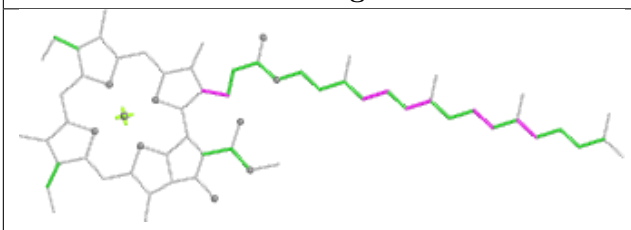
Ligand CLA c 515



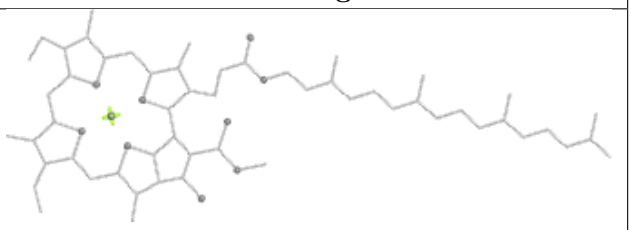
Bond lengths



Bond angles

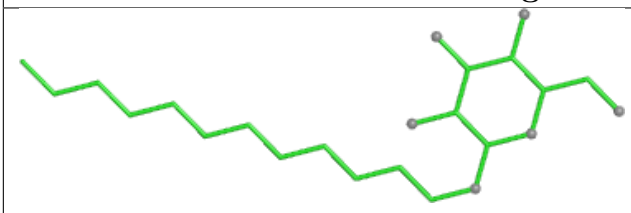


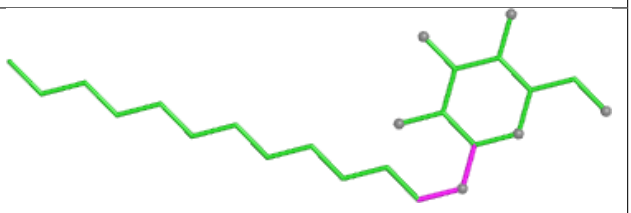
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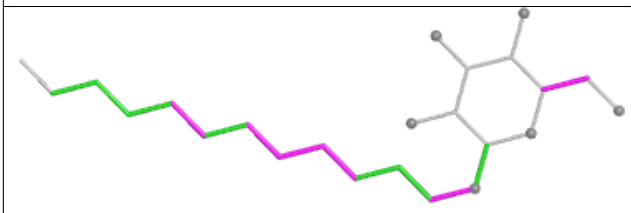


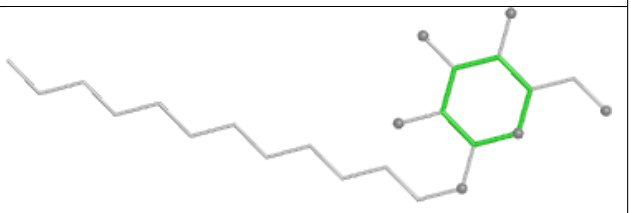
Rings

Ligand LMT T 102

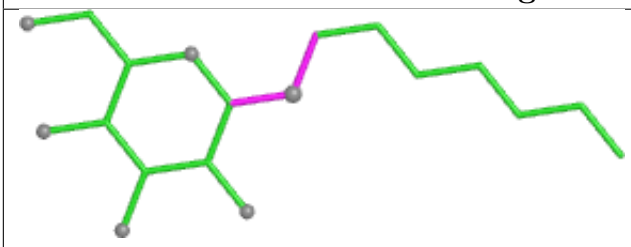

Bond lengths

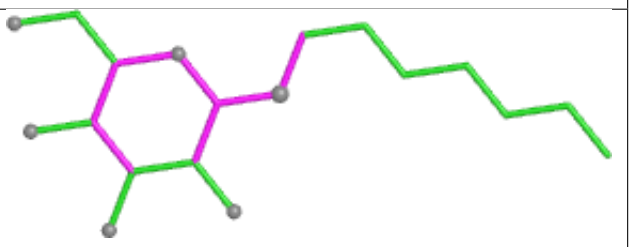

Bond angles

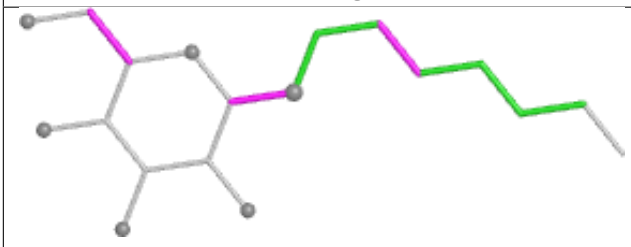

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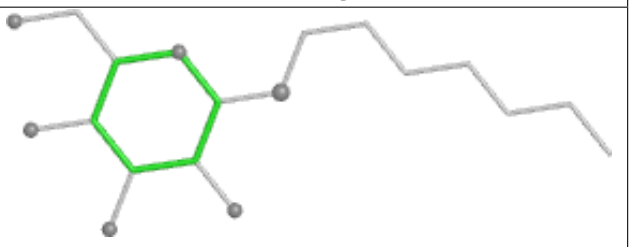

Rings

Ligand HTG I 1202

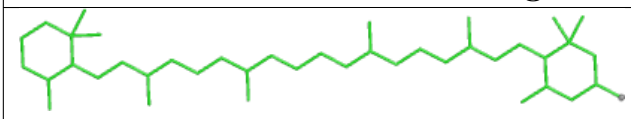

Bond lengths

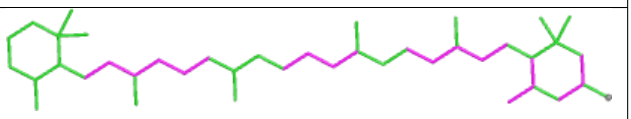

Bond angles


Torsions

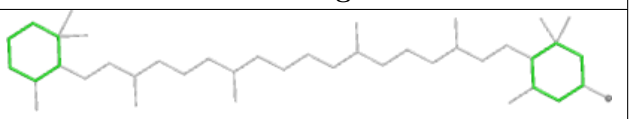

Rings

Ligand RRX h 702

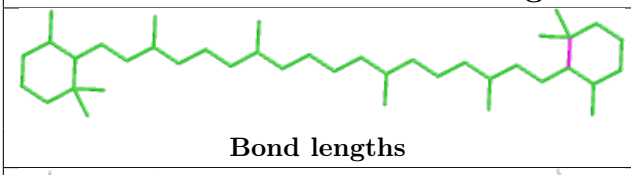

Bond lengths

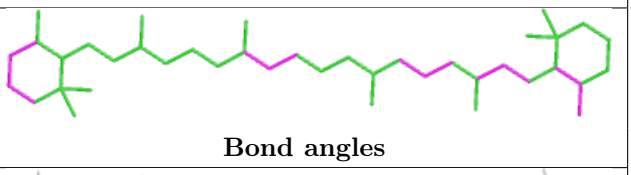

Bond angles

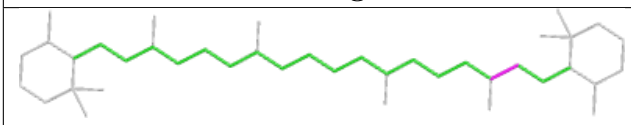

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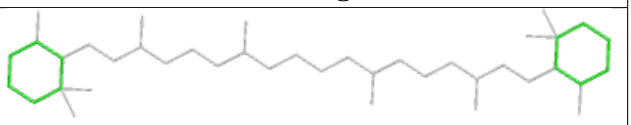

Rings

Ligand BCR b 622


Bond lengths

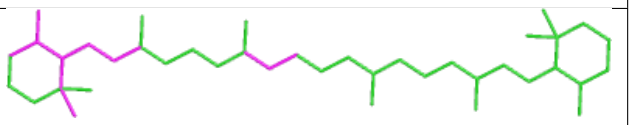

Bond angles

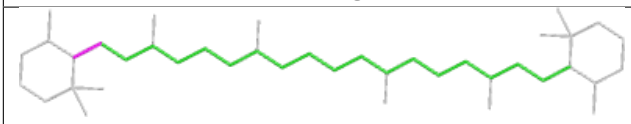

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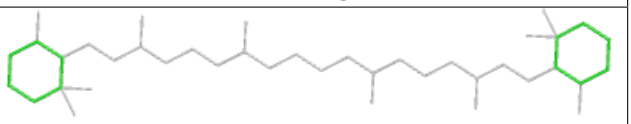

Rings

Ligand BCR a 2114

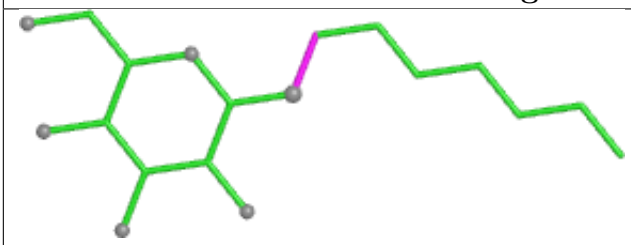

Bond lengths

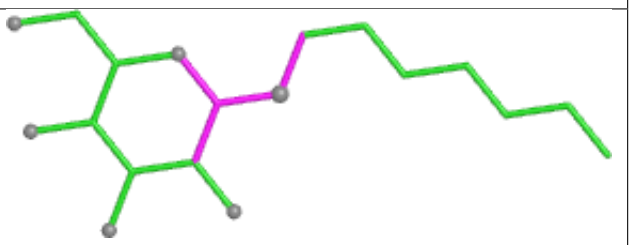

Bond angles

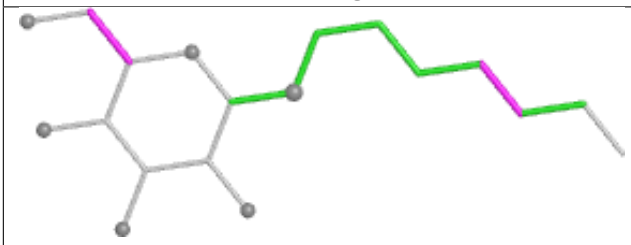

Torsions

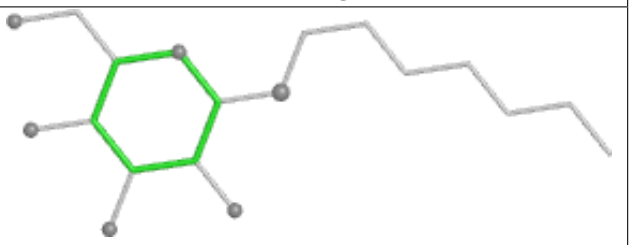

Rings

Ligand HTG B 624

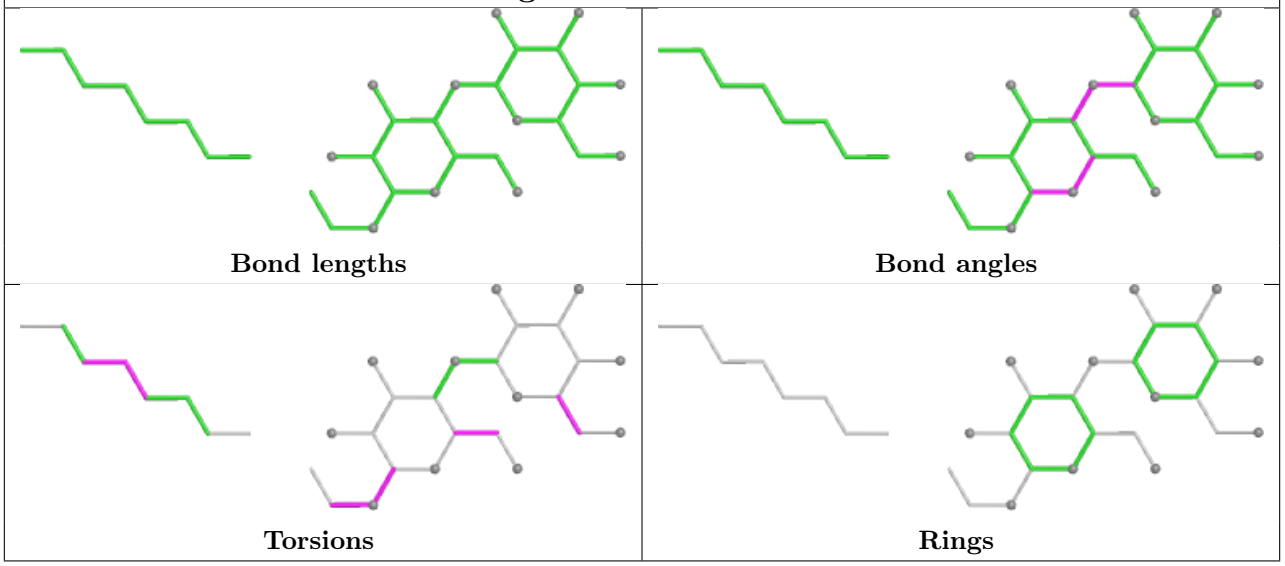

Bond lengths


Bond angles

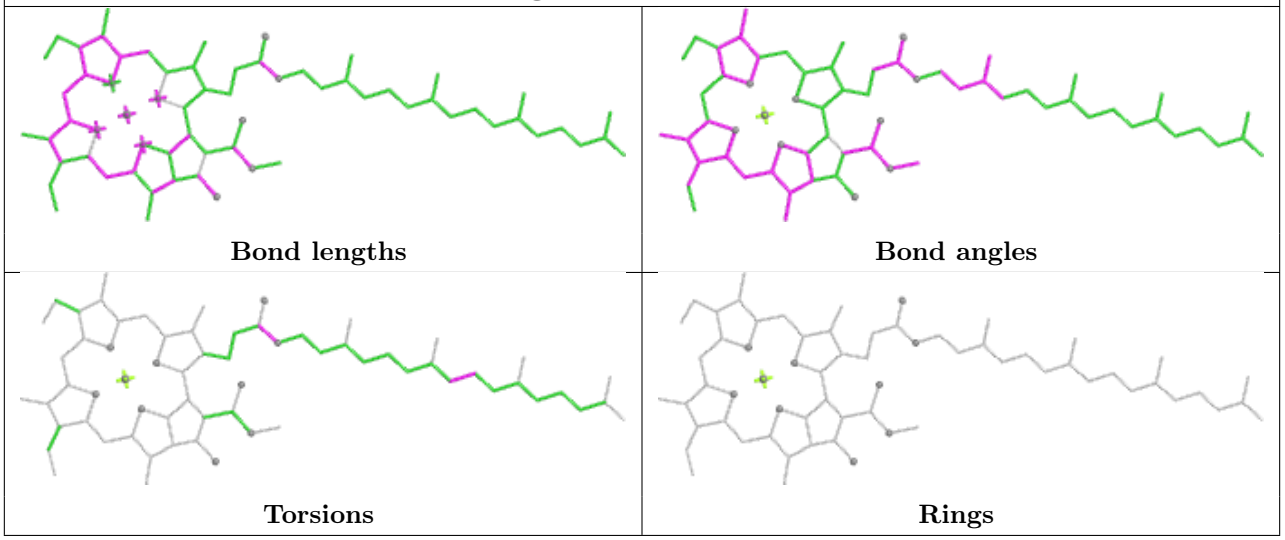

Torsions


Rings

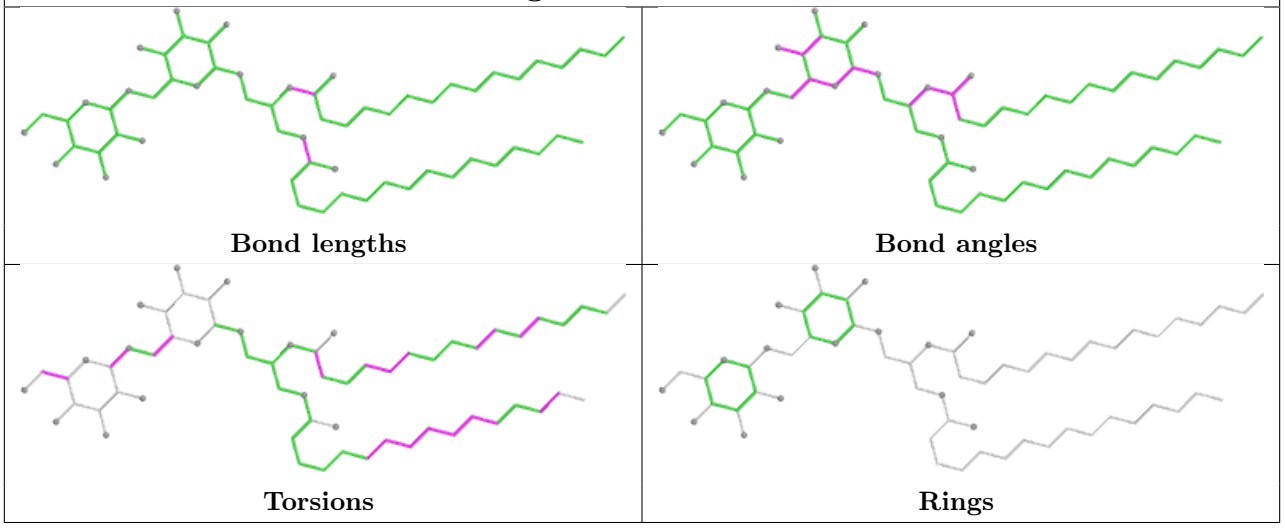
Ligand LMT z 1801



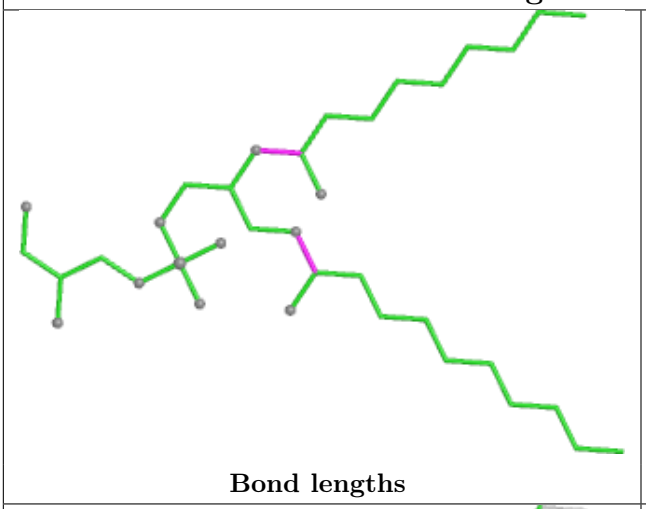
Ligand CLA b 615



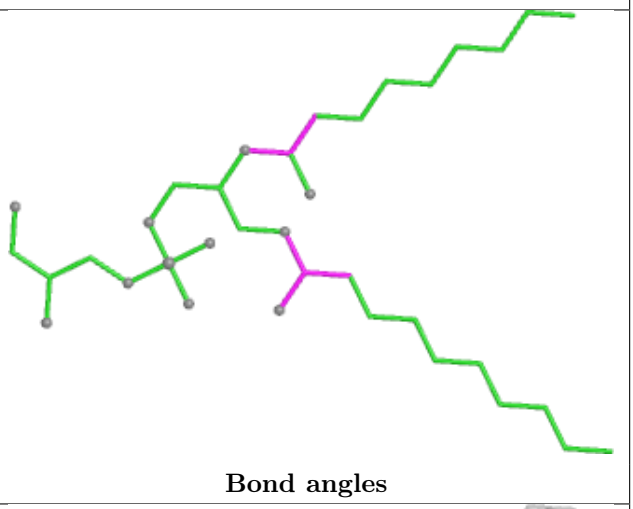
Ligand DGD c 518



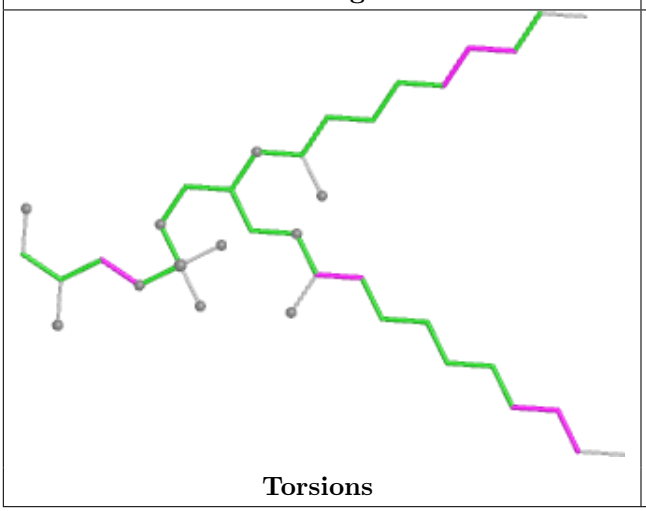
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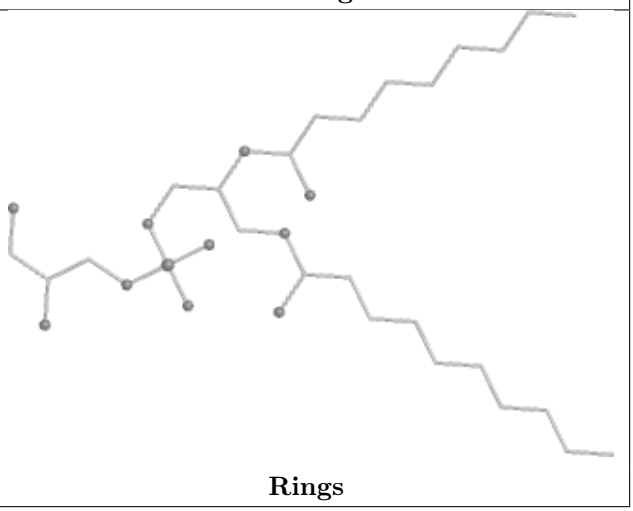
Bond lengths



Bond angles

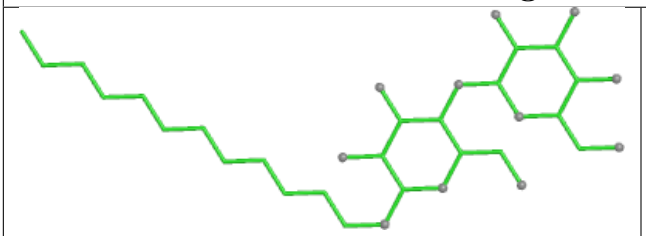


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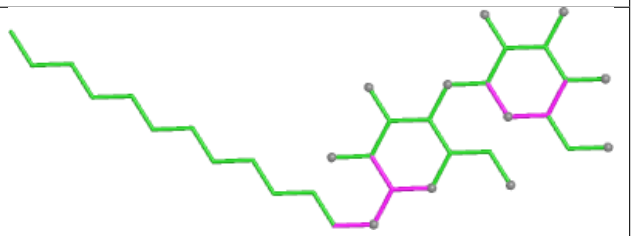


Rings

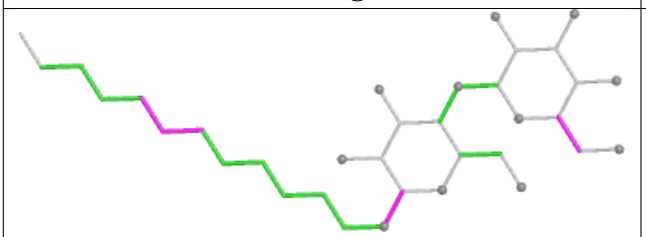
Ligand LMT m 102



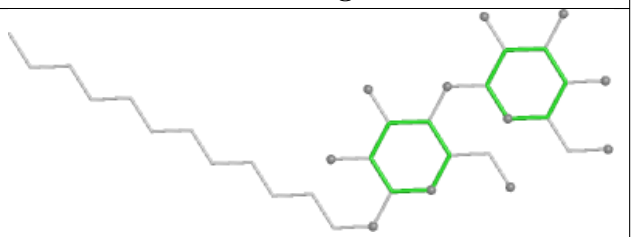
Bond lengths



Bond angles

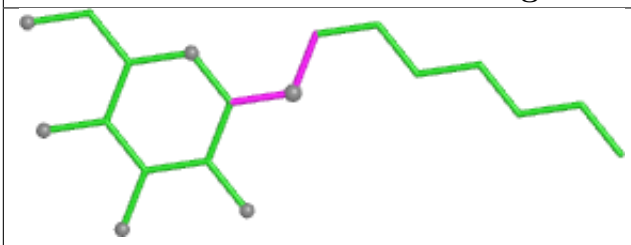


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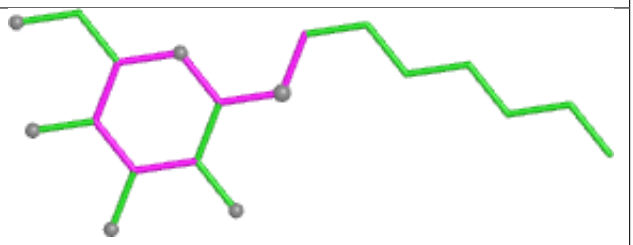


Rings

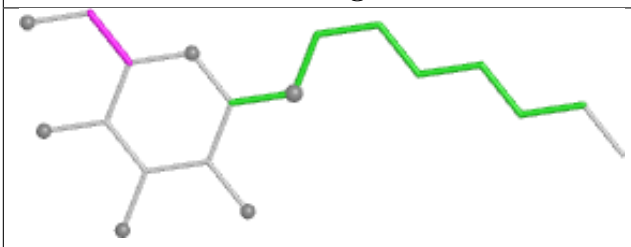
Ligand HTG B 628



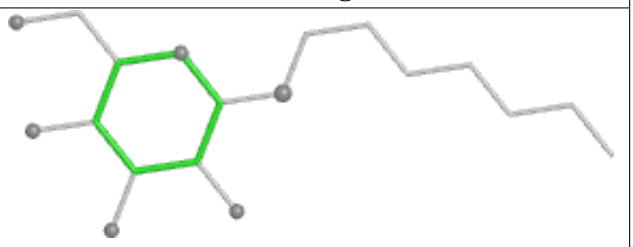
Bond lengths



Bond angles

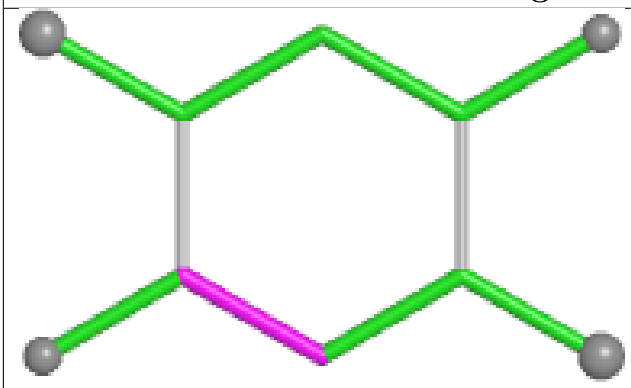


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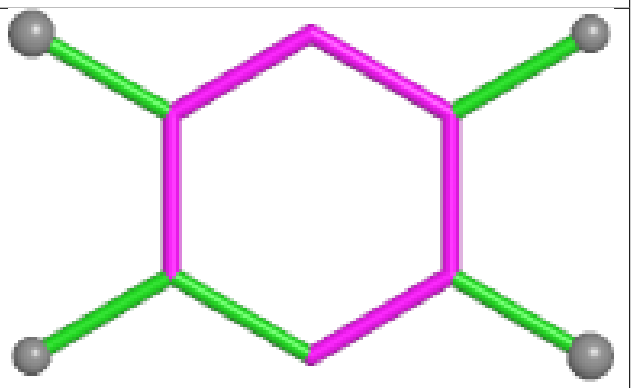


Rings

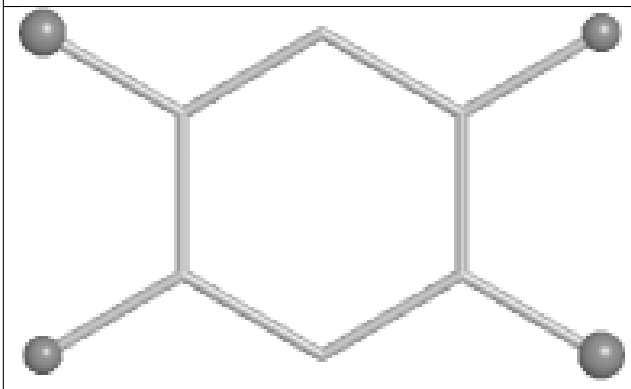
Ligand K2I A 419



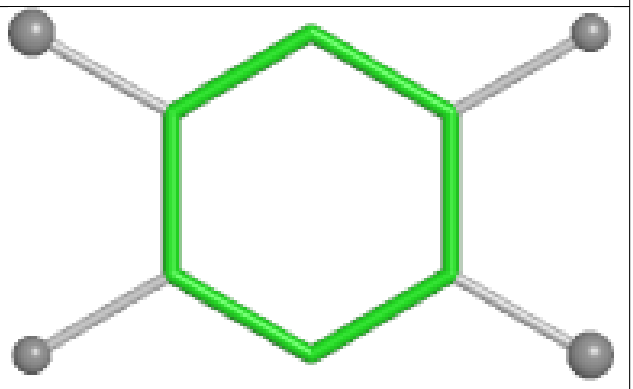
Bond lengths



Bond angles

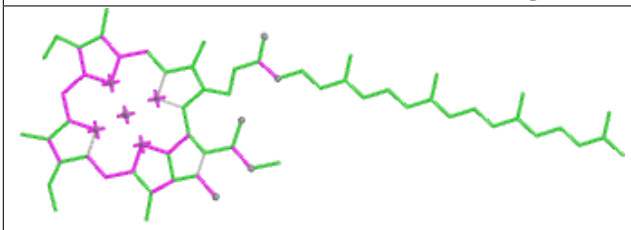


Torsions

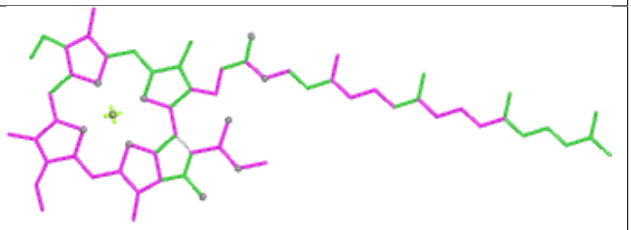


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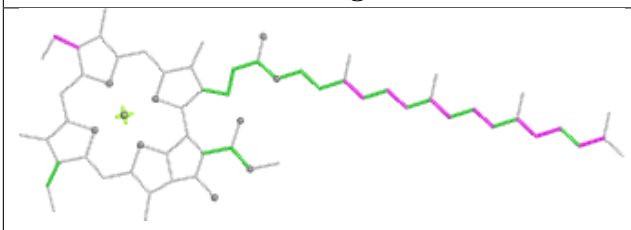
Ligand CLA B 616



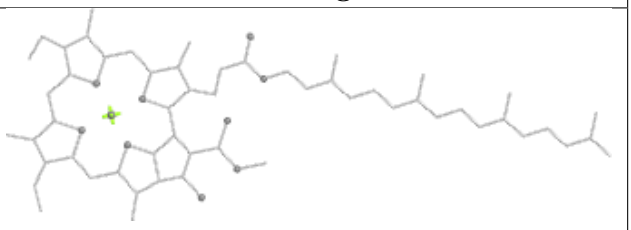
Bond lengths



Bond angles



Torsions

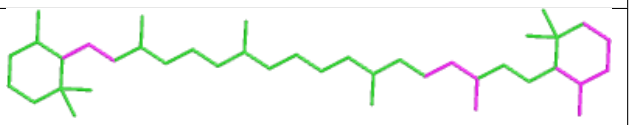


Rings

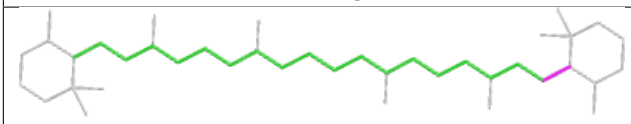
Ligand BCR b 621



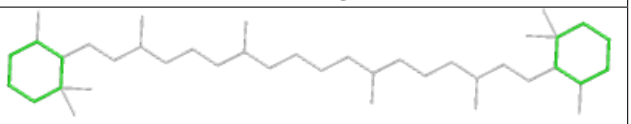
Bond lengths



Bond angles

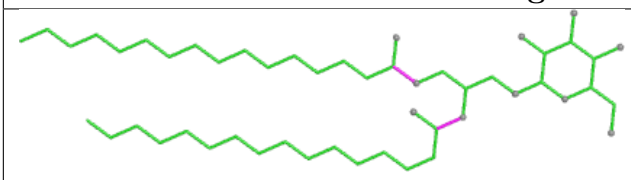


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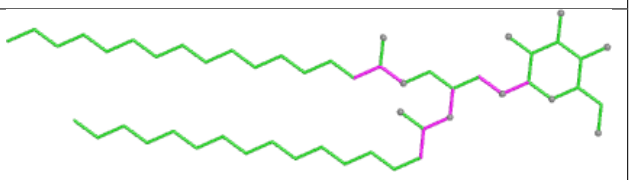


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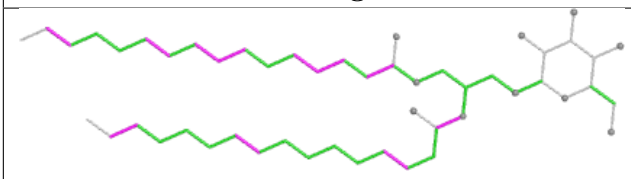
Ligand LMG i 101



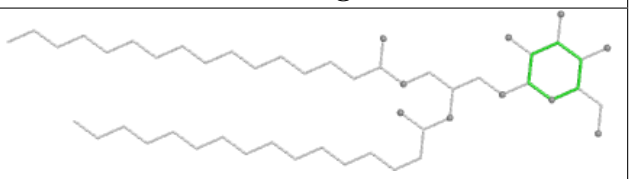
Bond lengths



Bond angles

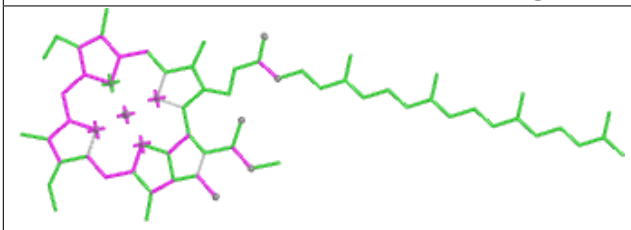


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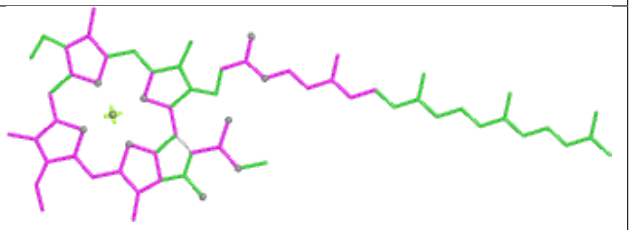


Rings

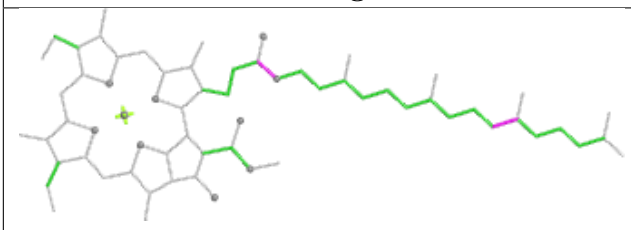
Ligand CLA c 513



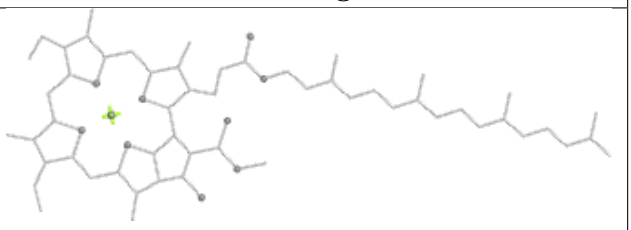
Bond lengths



Bond angles

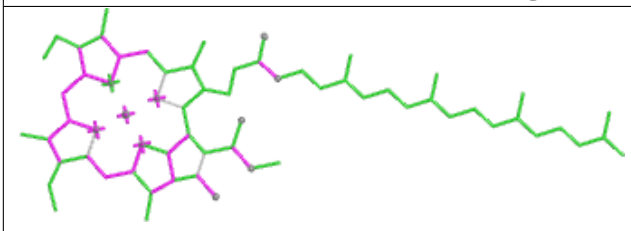


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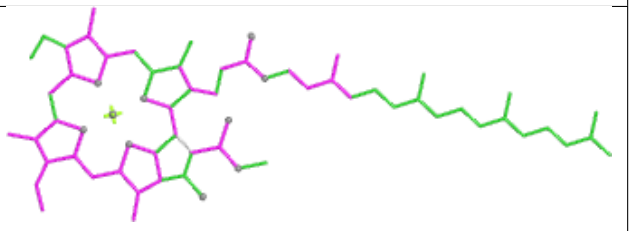


Rings

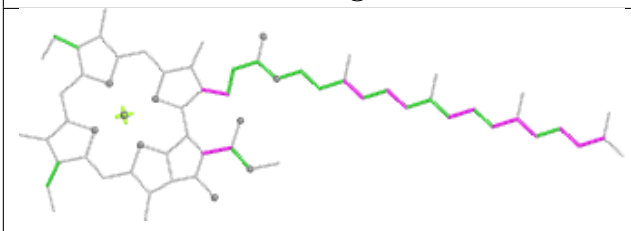
Ligand CLA C 507



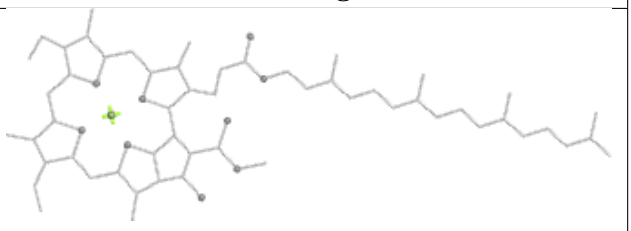
Bond lengths



Bond angles

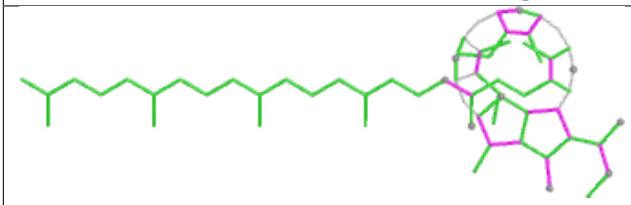


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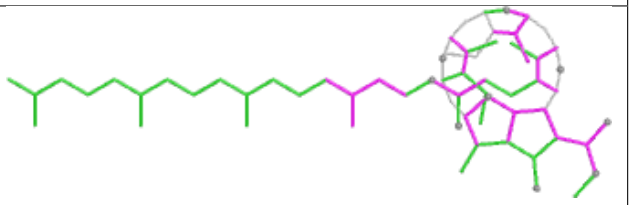


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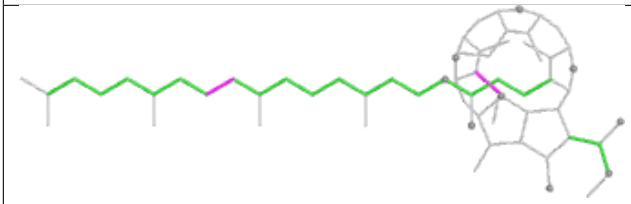
Ligand PHO a 2112



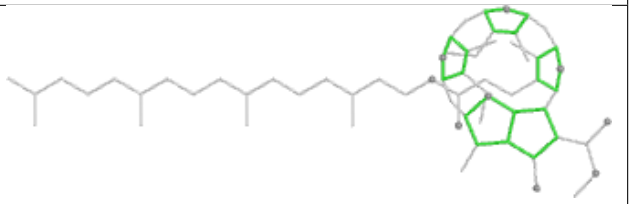
Bond lengths



Bond angles

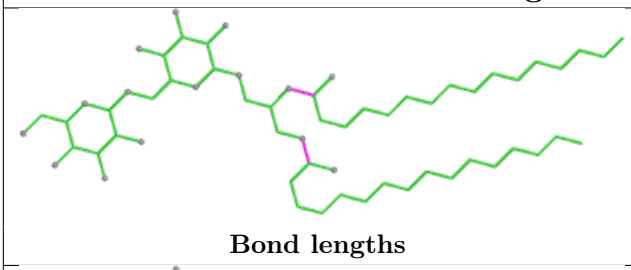


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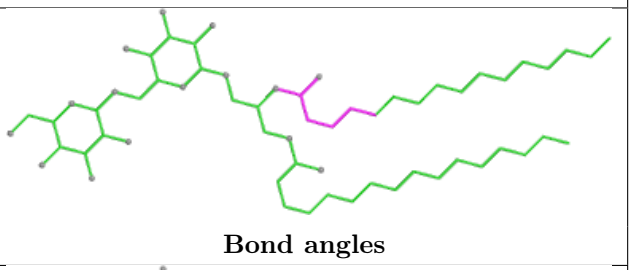


Rings

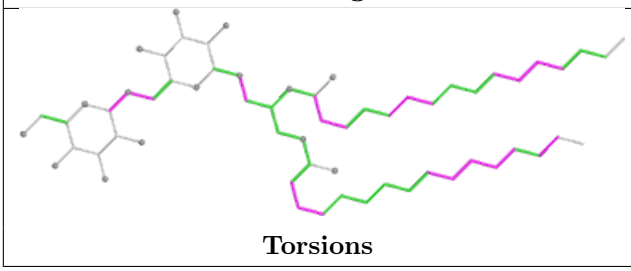
Ligand DGD c 519



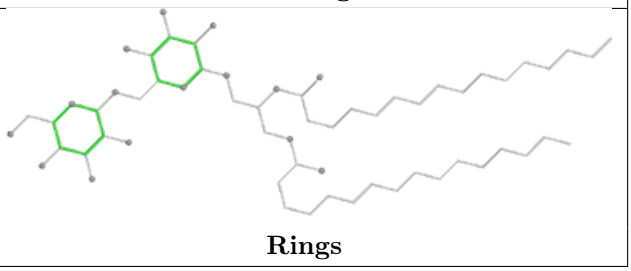
Bond lengths



Bond angles

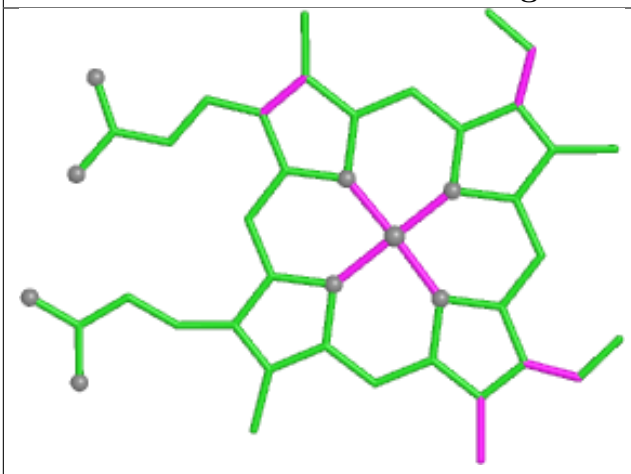


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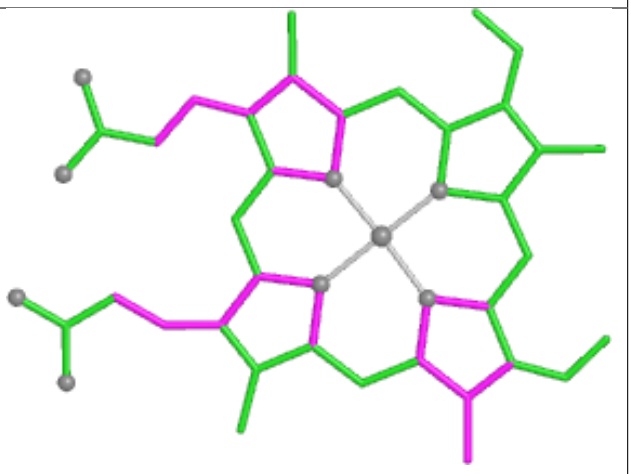


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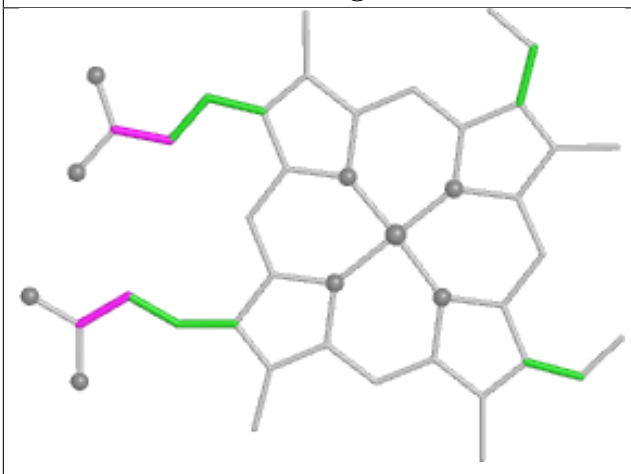
Ligand HEM F 102



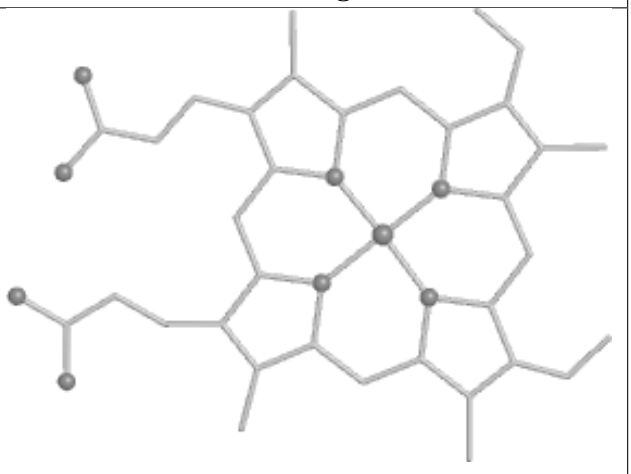
Bond lengths



Bond angles

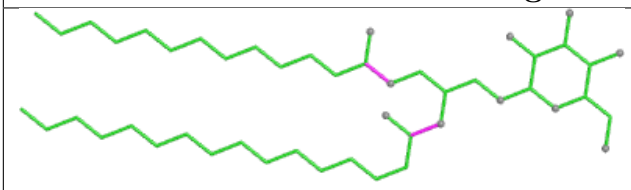


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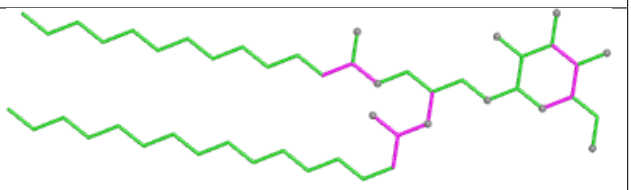


Rings

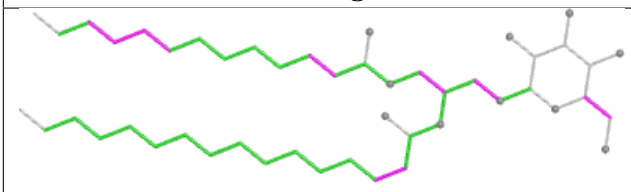
Ligand LMG c 522



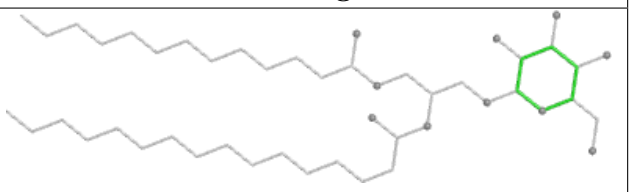
Bond lengths



Bond angles

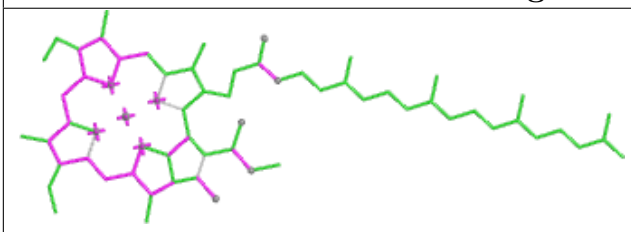


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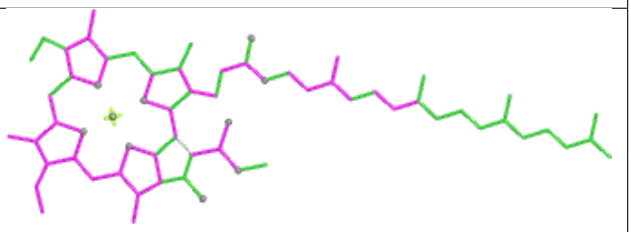


Rings

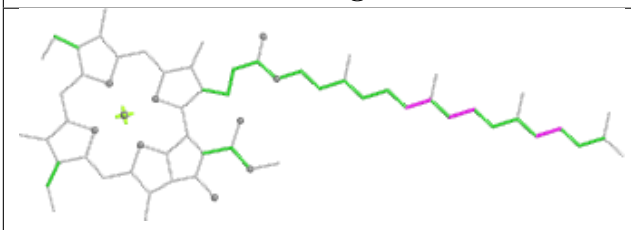
Ligand CLA d 405



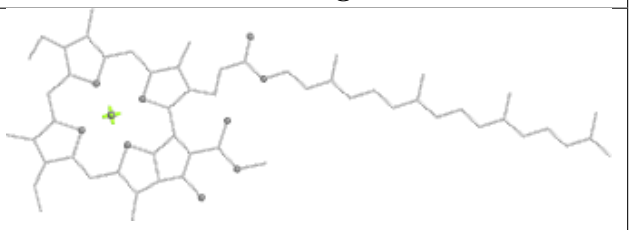
Bond lengths



Bond angles

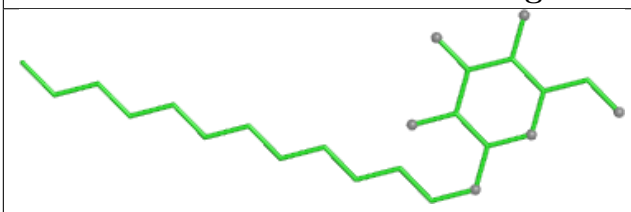


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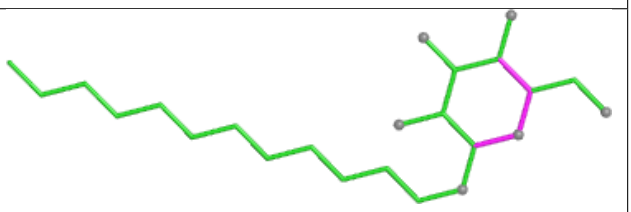


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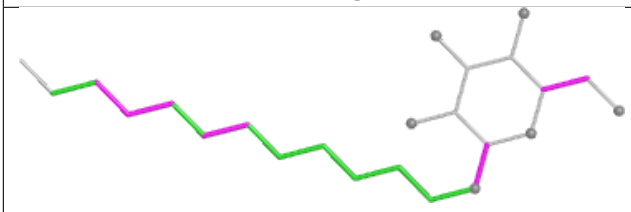
Ligand LMT J 102



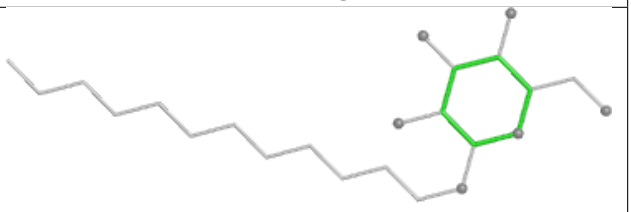
Bond lengths



Bond angles

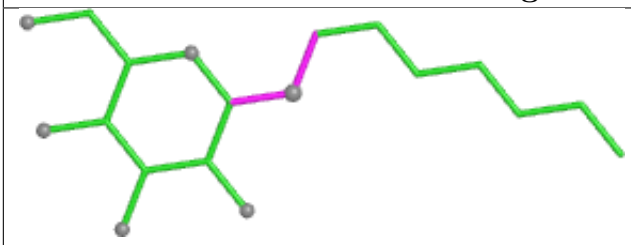


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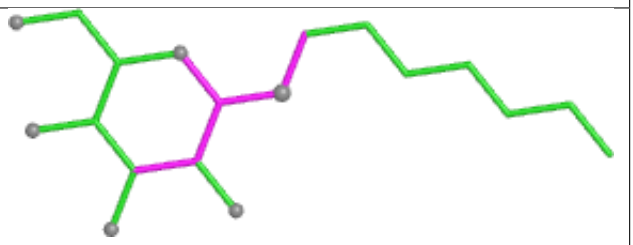


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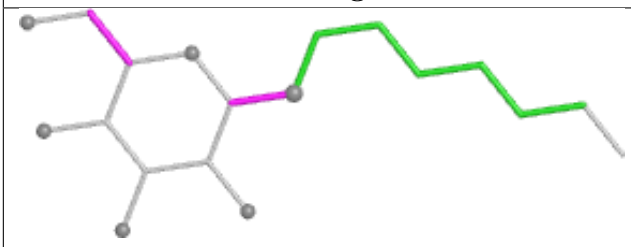
Ligand HTG B 626



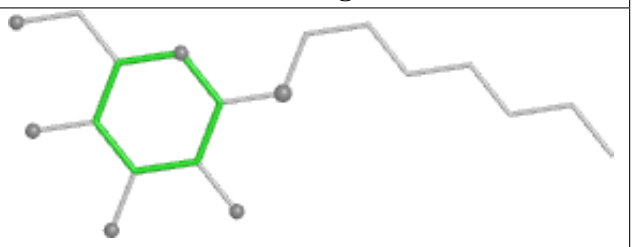
Bond lengths



Bond angles

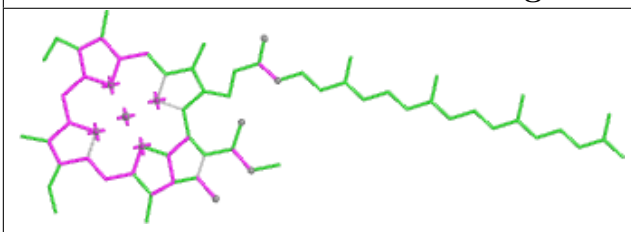


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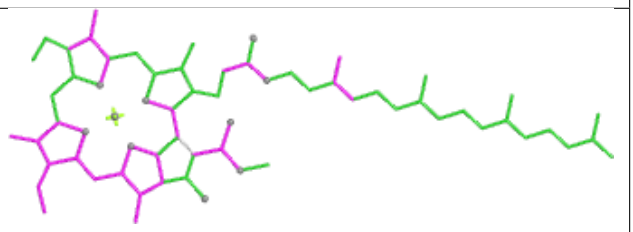


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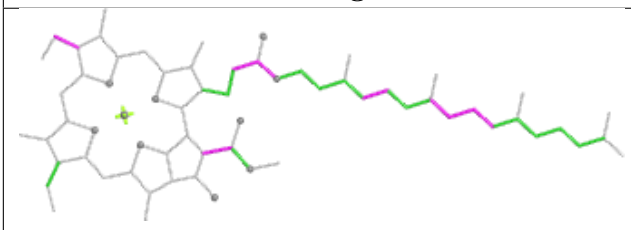
Ligand CLA B 602



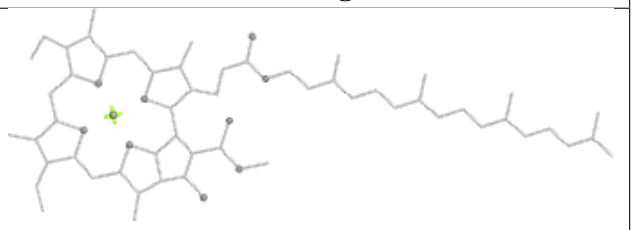
Bond lengths



Bond angles

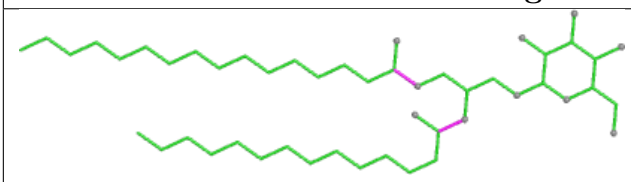


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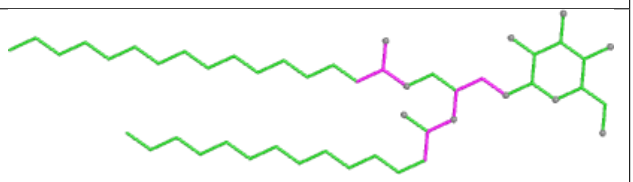


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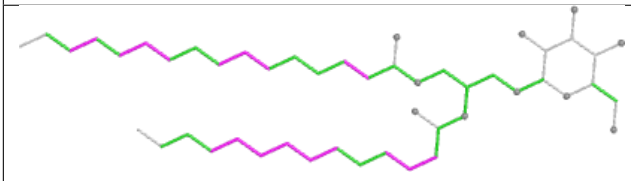
Ligand LMG c 521



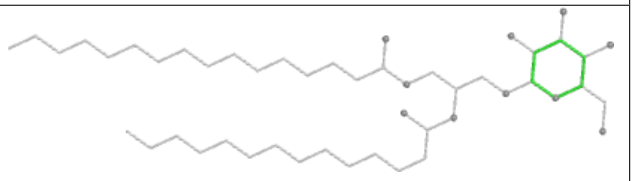
Bond lengths



Bond angles

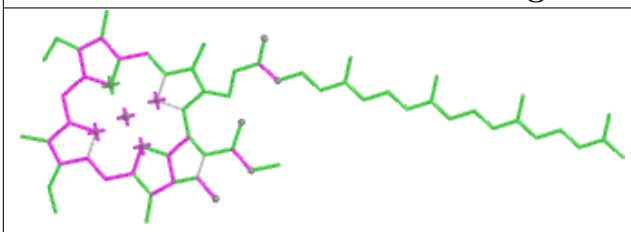


Torsions

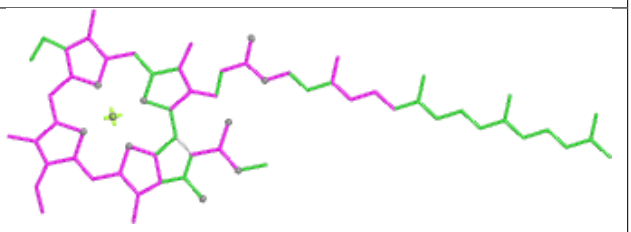


Rings

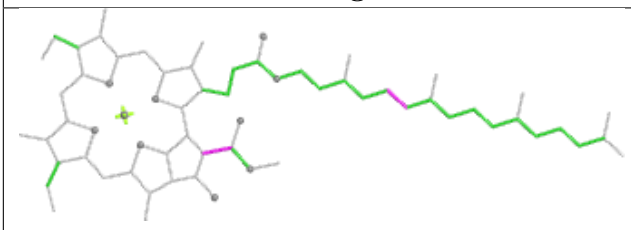
Ligand CLA b 606



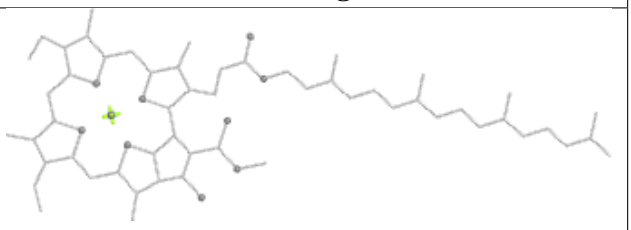
Bond lengths



Bond angles

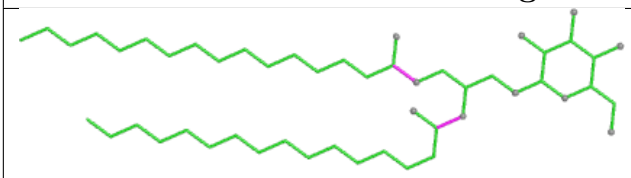


Torsions

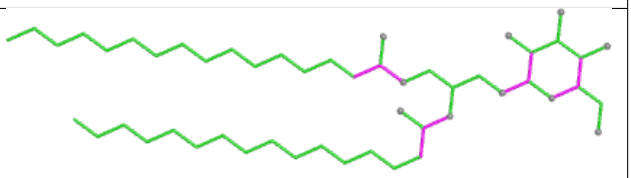


Rings

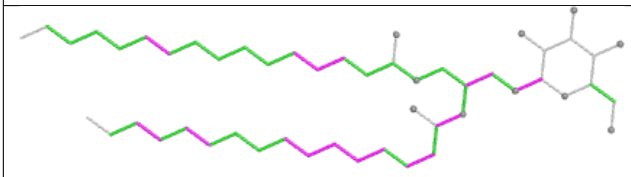
Ligand LMG A 412



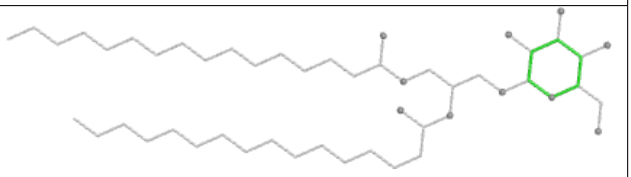
Bond lengths



Bond angles

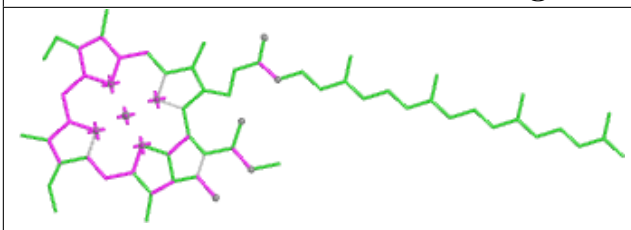


Torsions

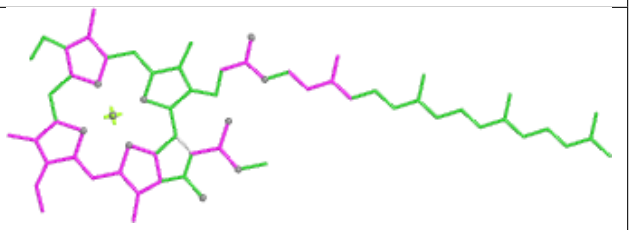


Rings

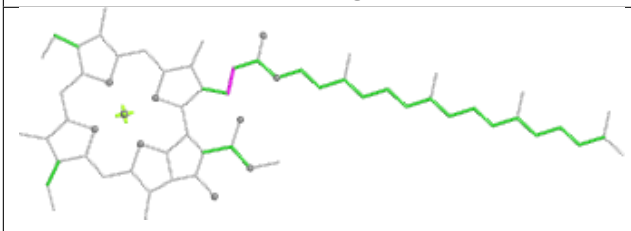
Ligand CLA c 503



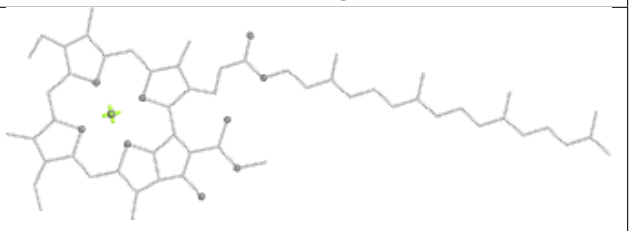
Bond lengths



Bond angles

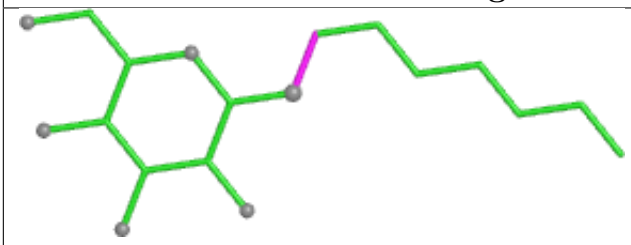


Torsions

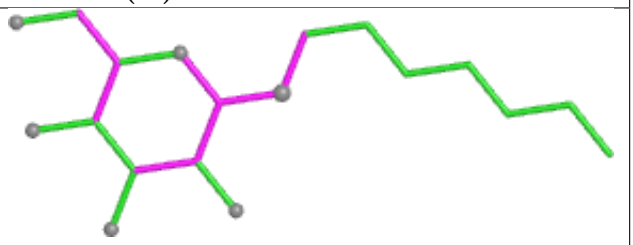


Rings

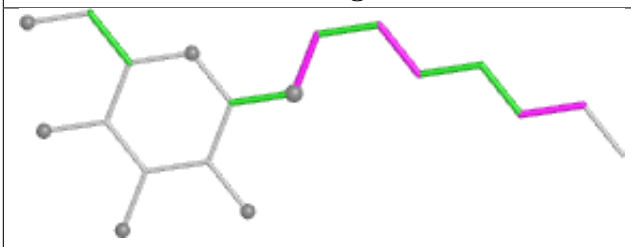
Ligand HTG B 625 (B)



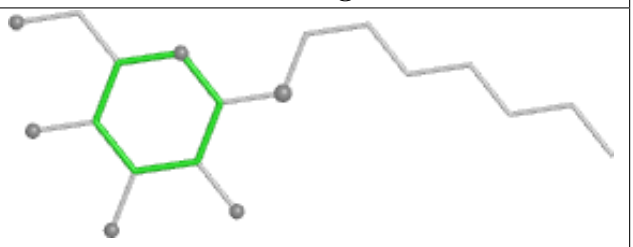
Bond lengths



Bond angles

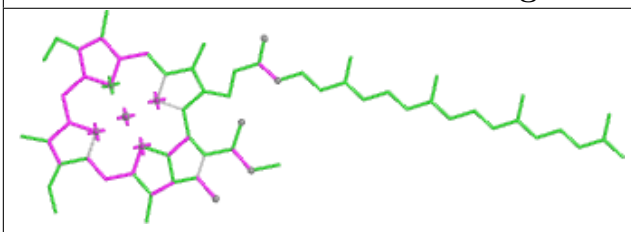


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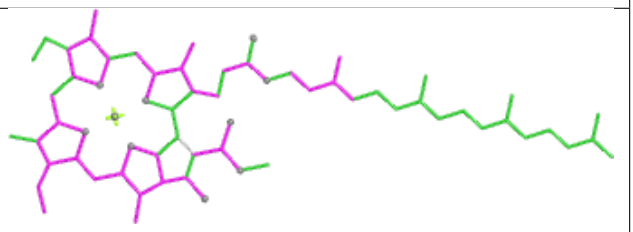


Rings

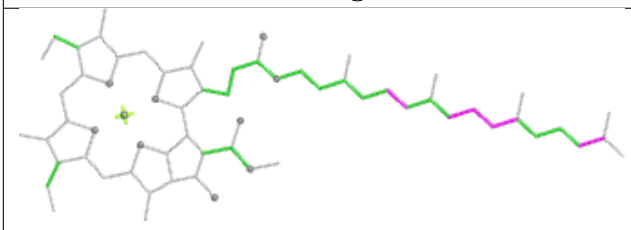
Ligand CLA a 2113



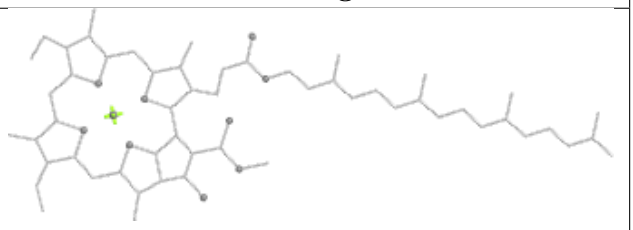
Bond lengths



Bond angles

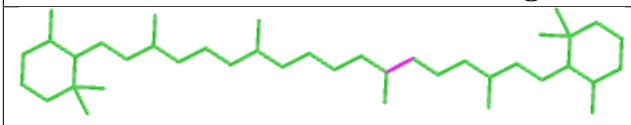


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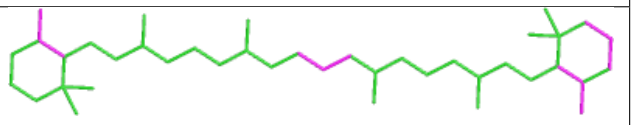


Rings

Ligand BCR B 619



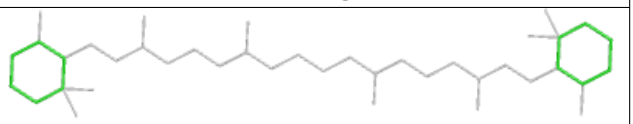
Bond lengths



Bond angles

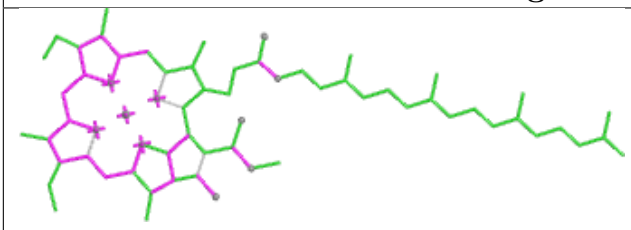


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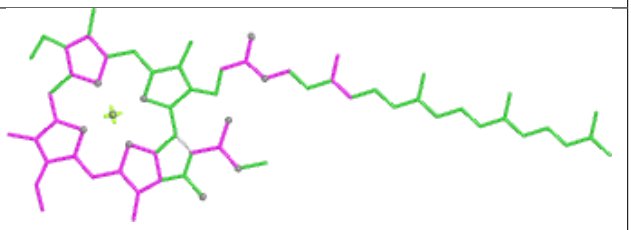


Rings

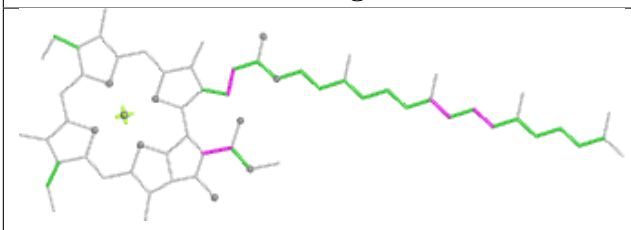
Ligand CLA b 609



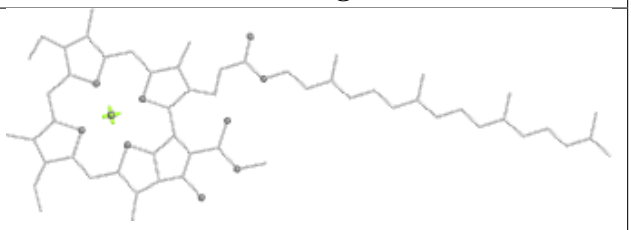
Bond lengths



Bond angles

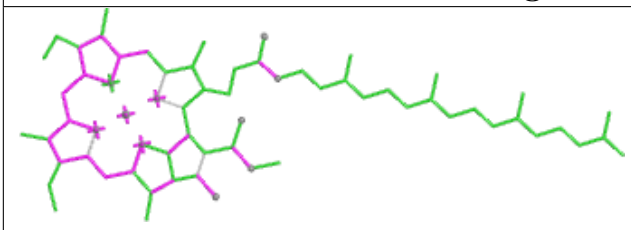


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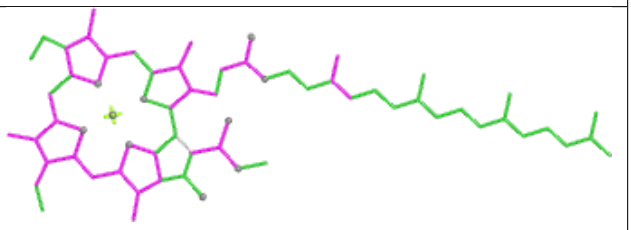


Rings

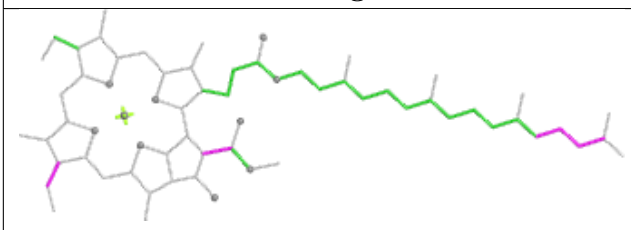
Ligand CLA A 405



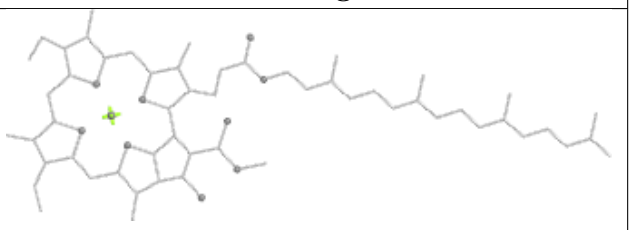
Bond lengths



Bond angles

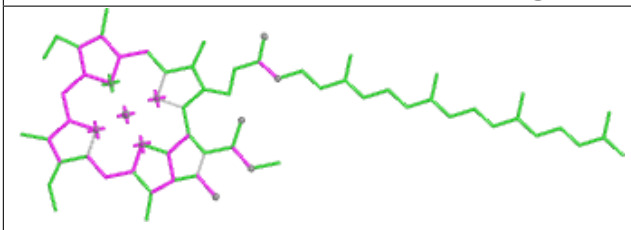


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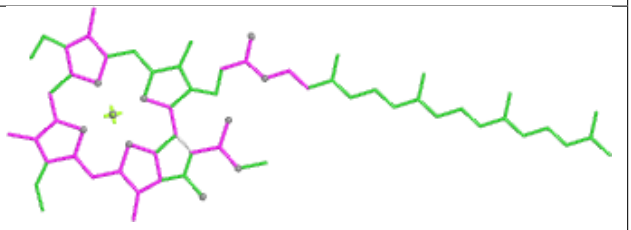


Rings

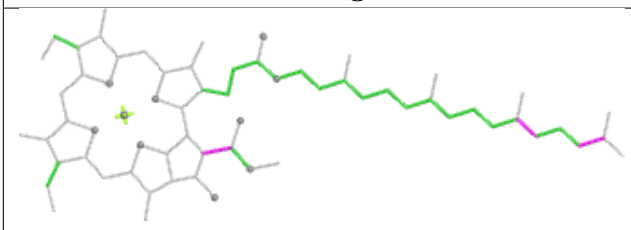
Ligand CLA c 504



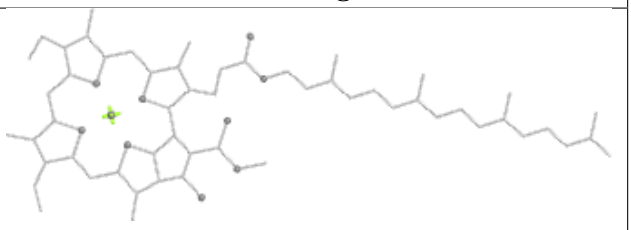
Bond lengths



Bond angles

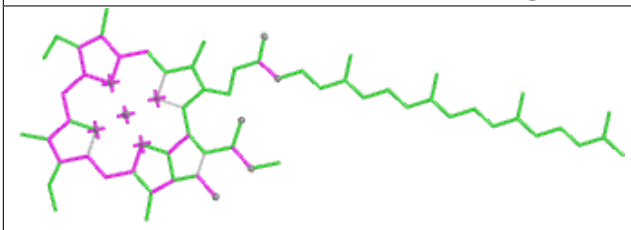


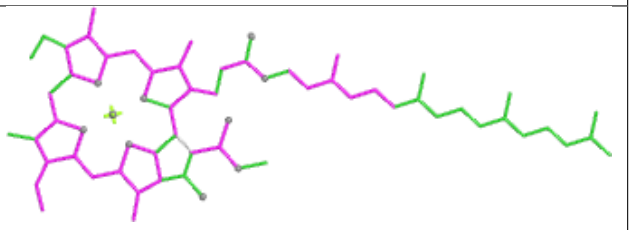
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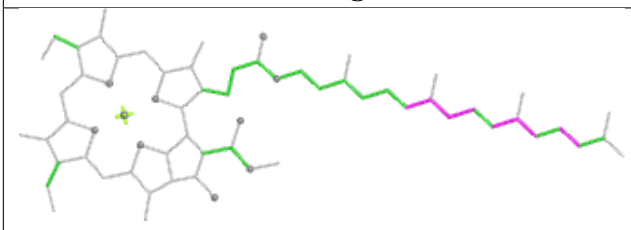


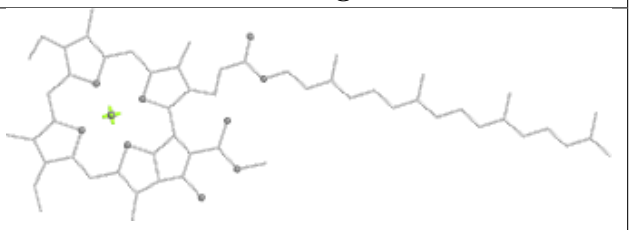
Rings

Ligand CLA A 409


Bond lengths


Bond angles


Torsions


Rings

Ligand PL9 A 417

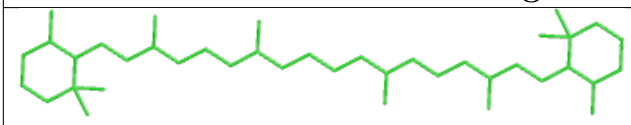

Bond lengths

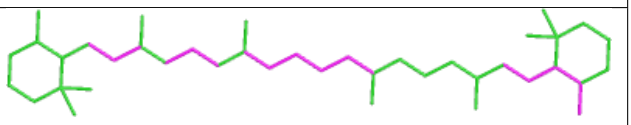

Bond angles


Torsions

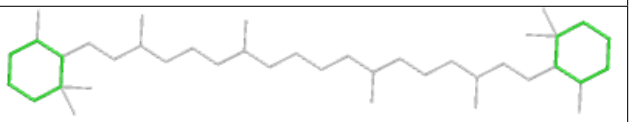

Rings

Ligand BCR B 620

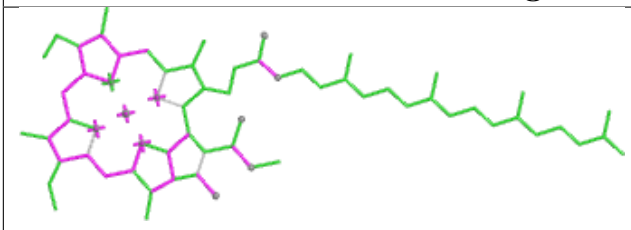

Bond lengths

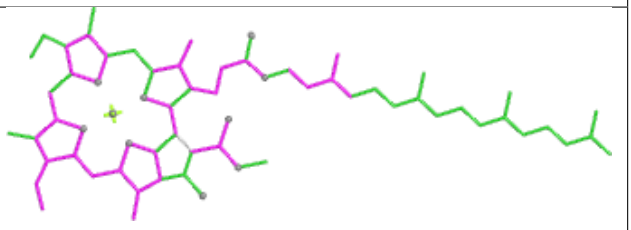

Bond angles

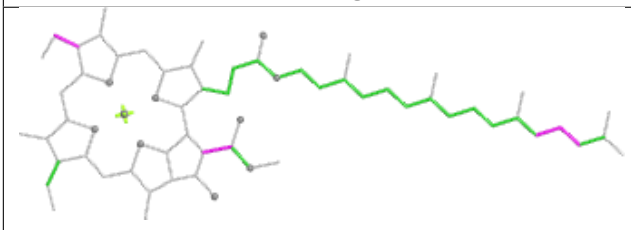

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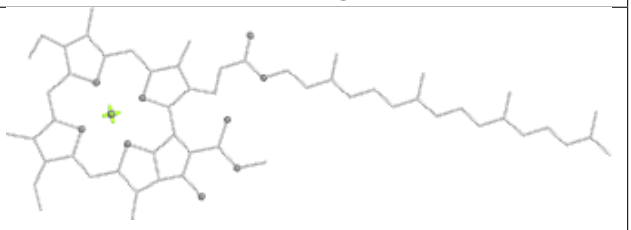

Rings

Ligand CLA B 603

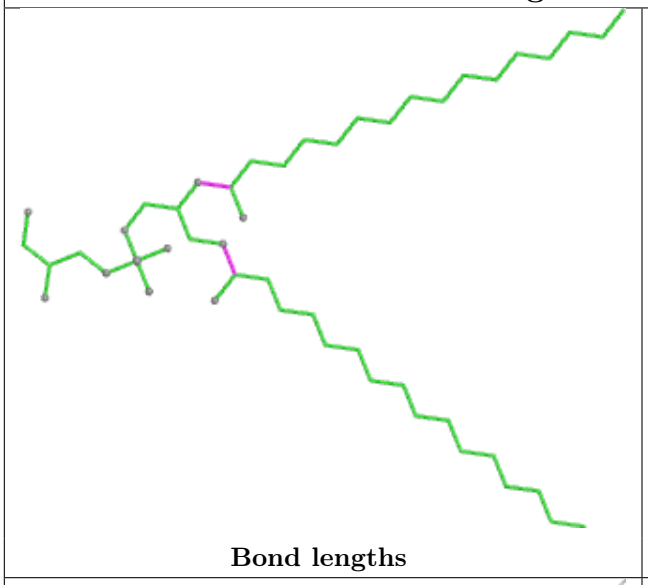

Bond lengths


Bond angles

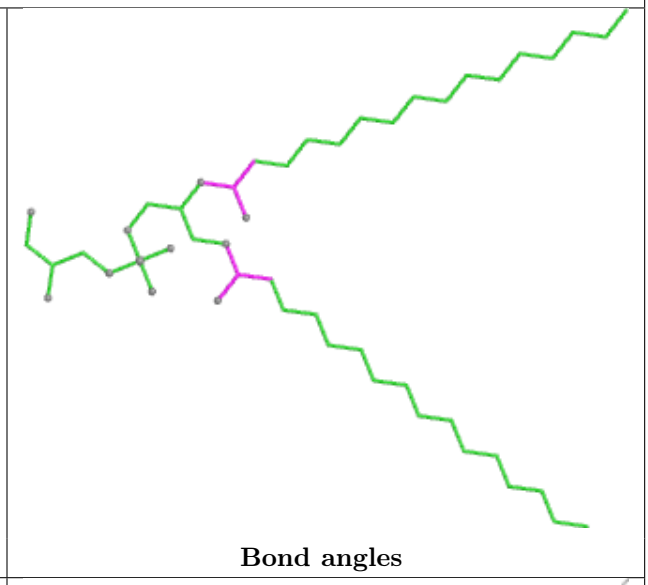

Torsions


Rings

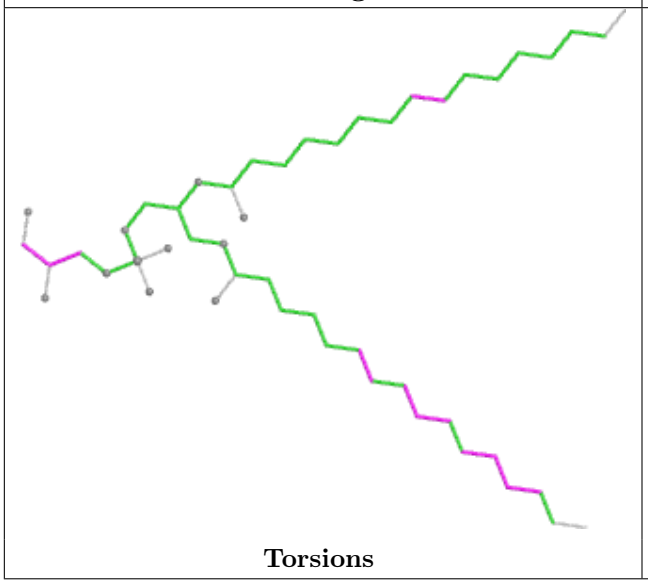
Ligand LHG d 408



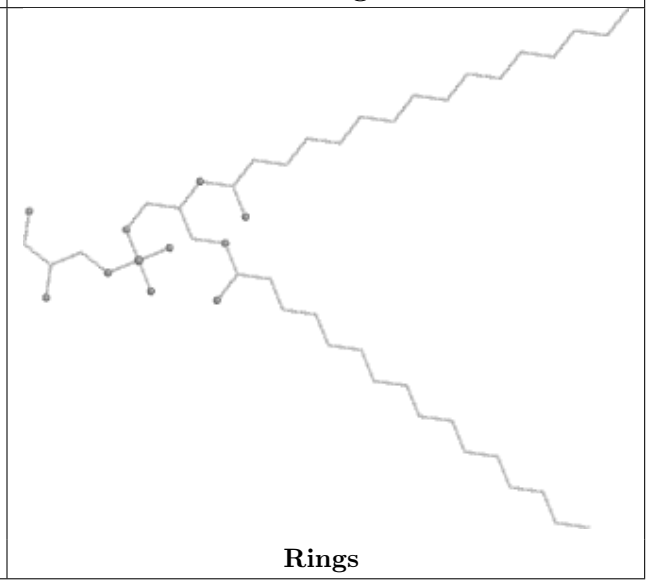
Bond lengths



Bond angles

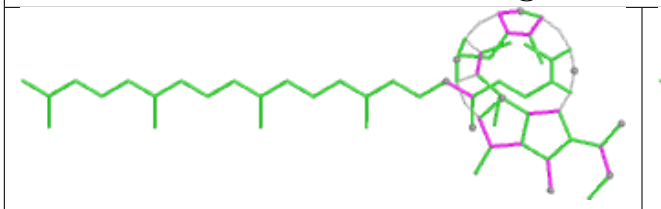


Torsions



Rings

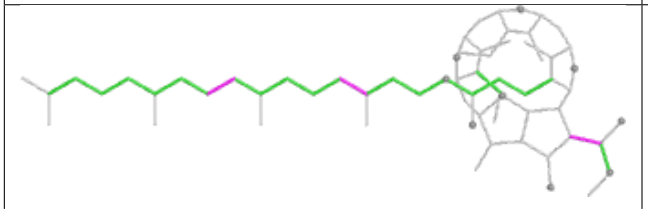
Ligand PHO a 2111



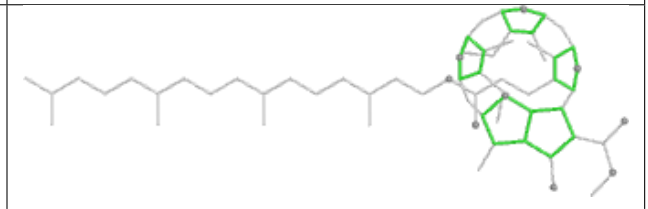
Bond lengths



Bond angles

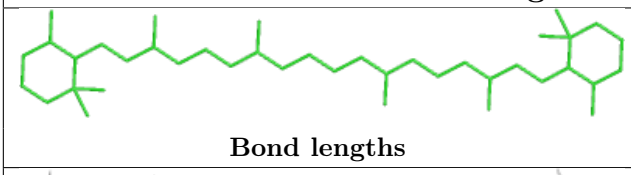


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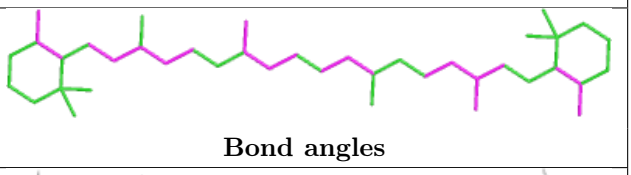


Rings

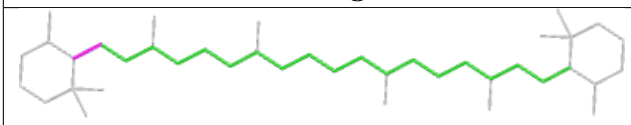
Ligand BCR c 516



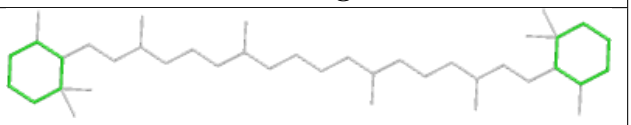
Bond lengths



Bond angles

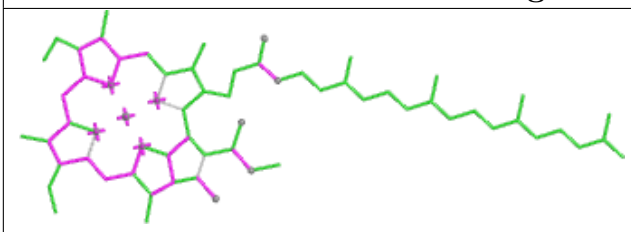


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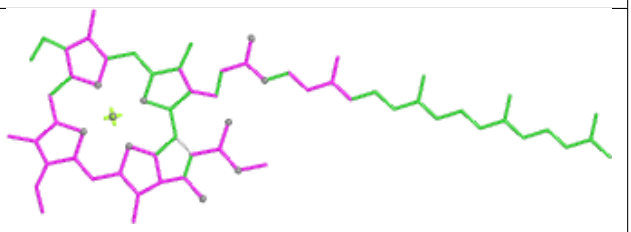


Rings

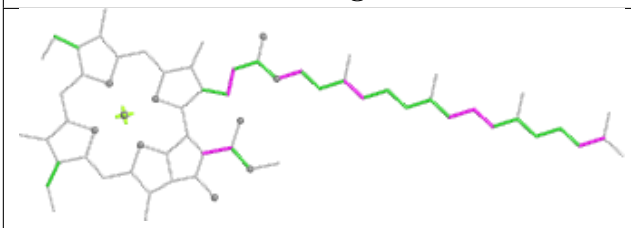
Ligand CLA b 617



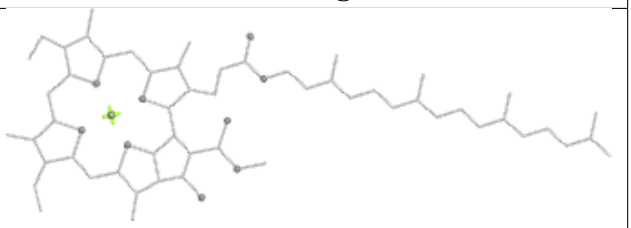
Bond lengths



Bond angles

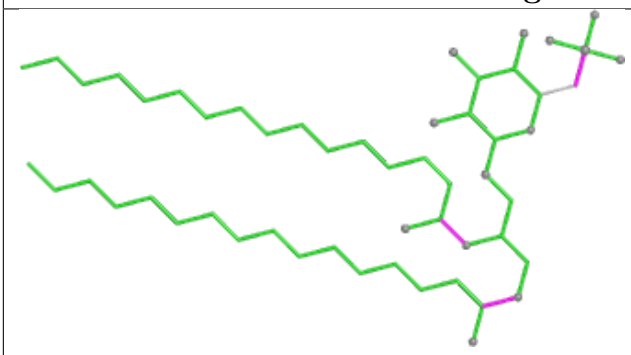


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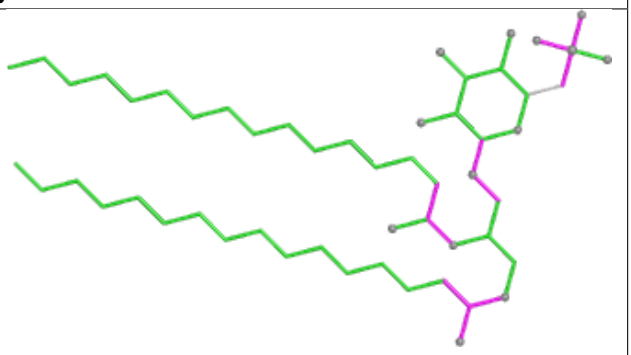


Rings

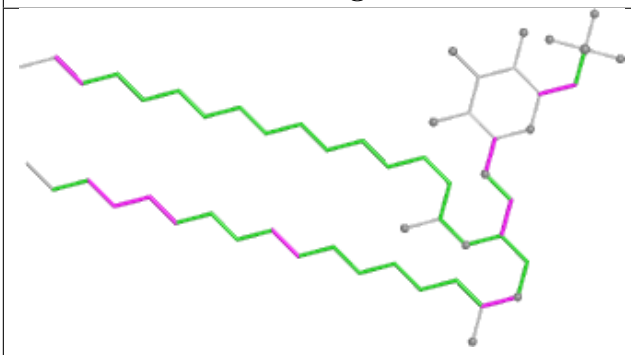
Ligand SQD A 413



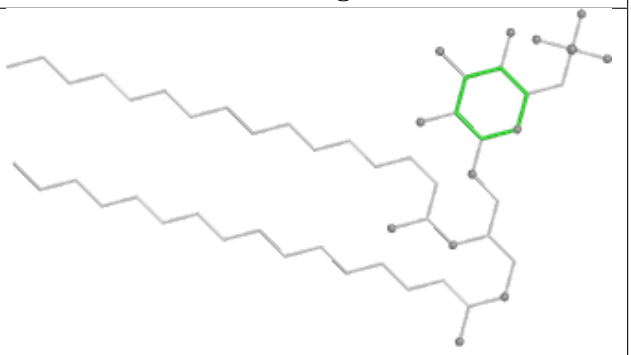
Bond lengths



Bond angles

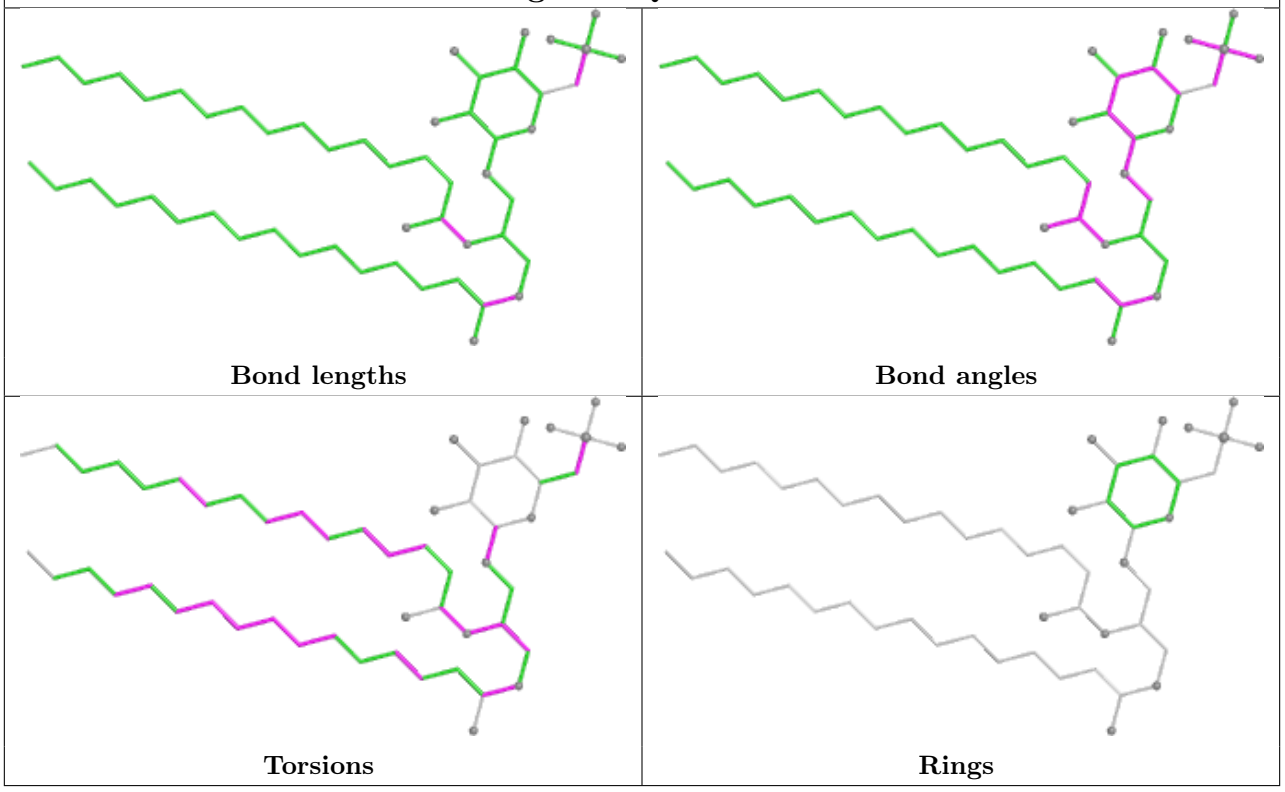


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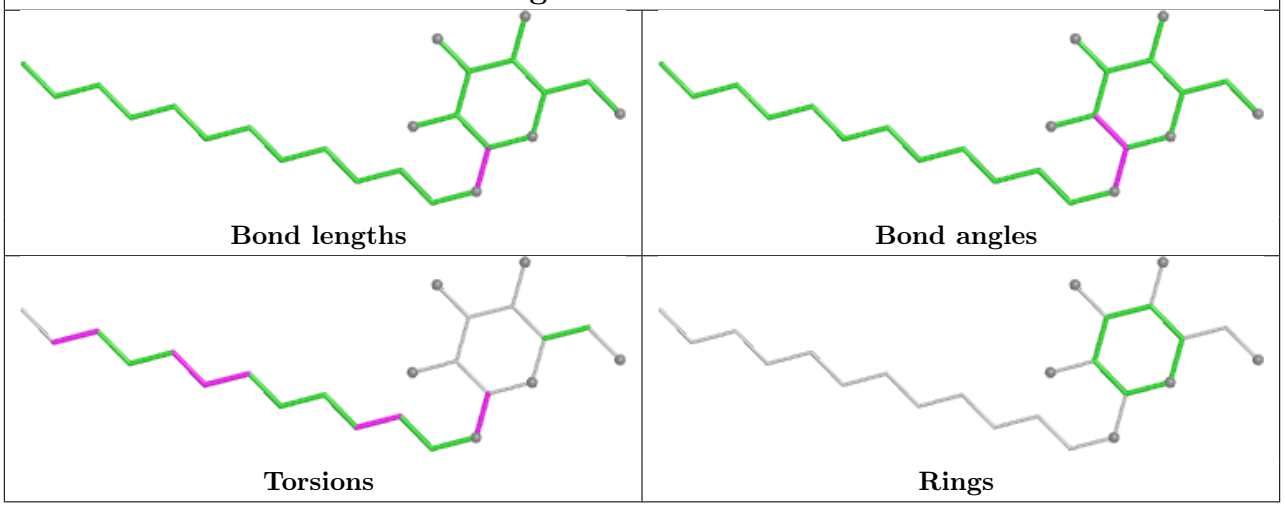


Rings

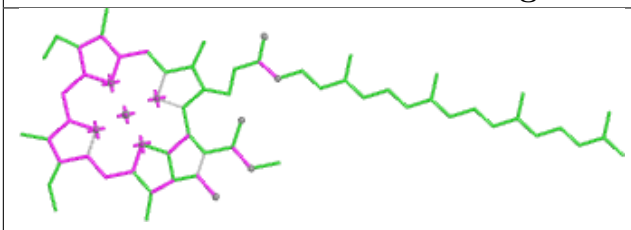
Ligand SQD L 102



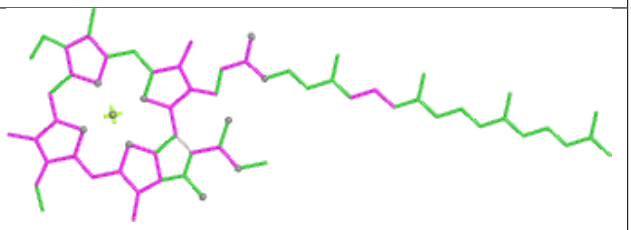
Ligand LMT f 101



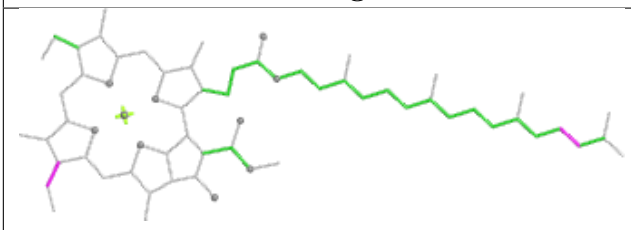
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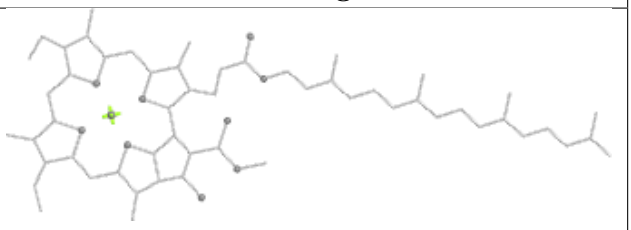
Bond lengths



Bond angles

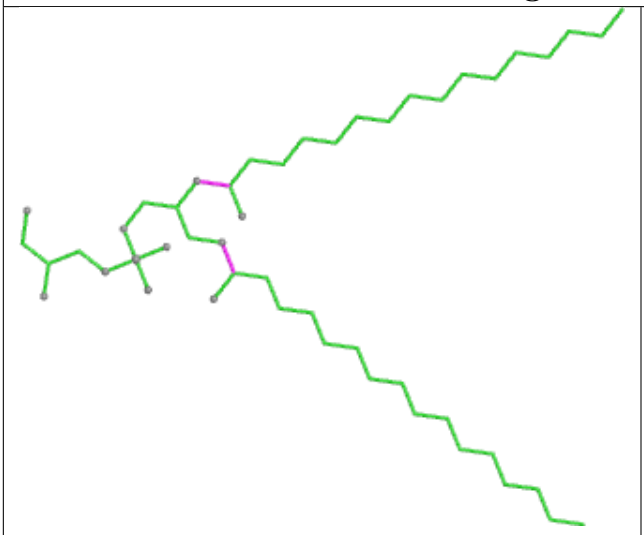


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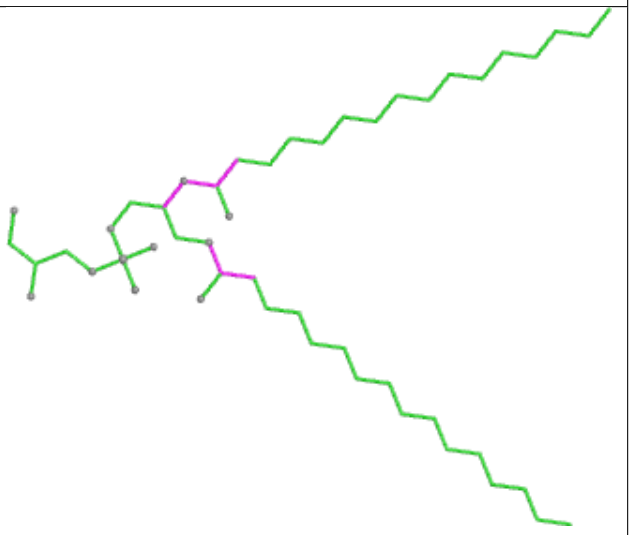


Rings

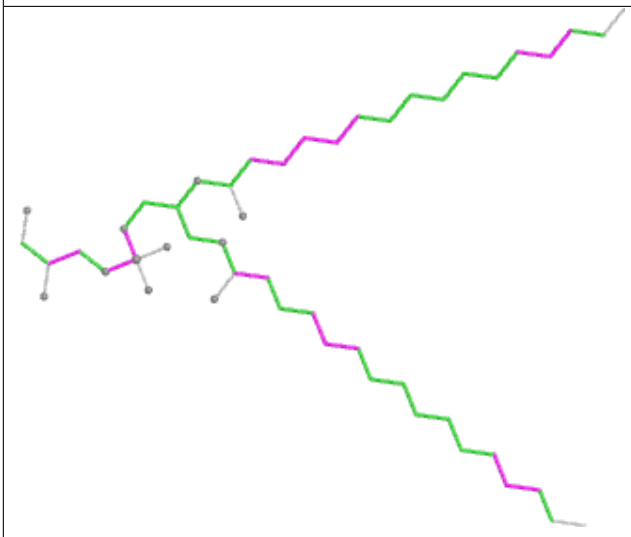
Ligand LHG E 101



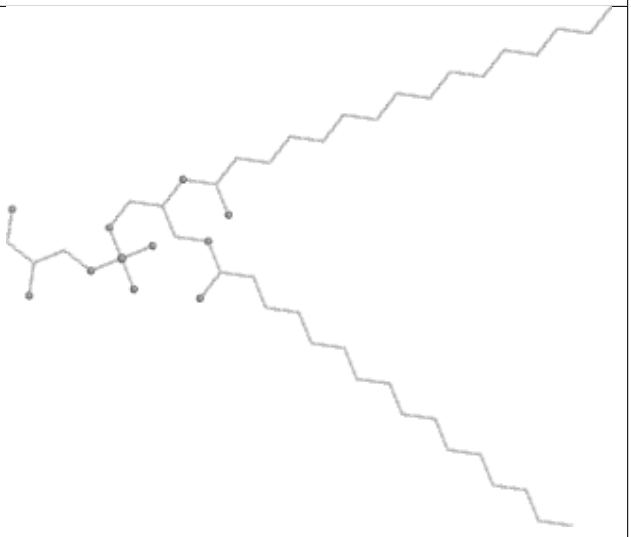
Bond lengths



Bond angles

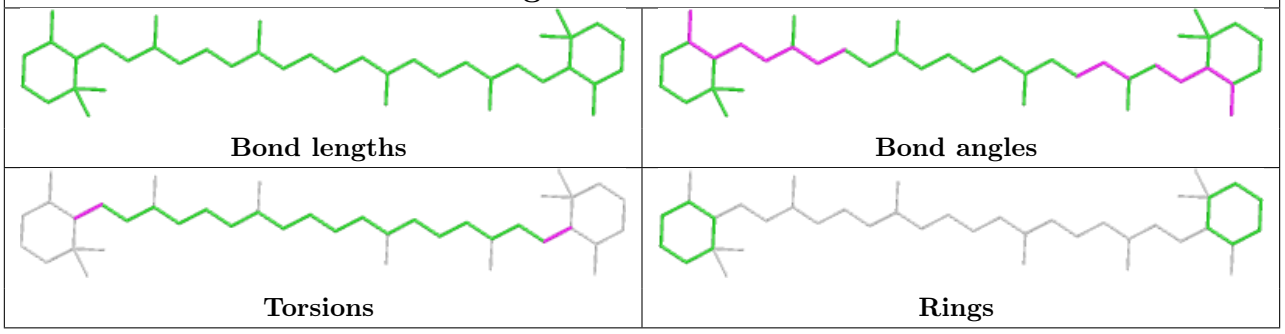


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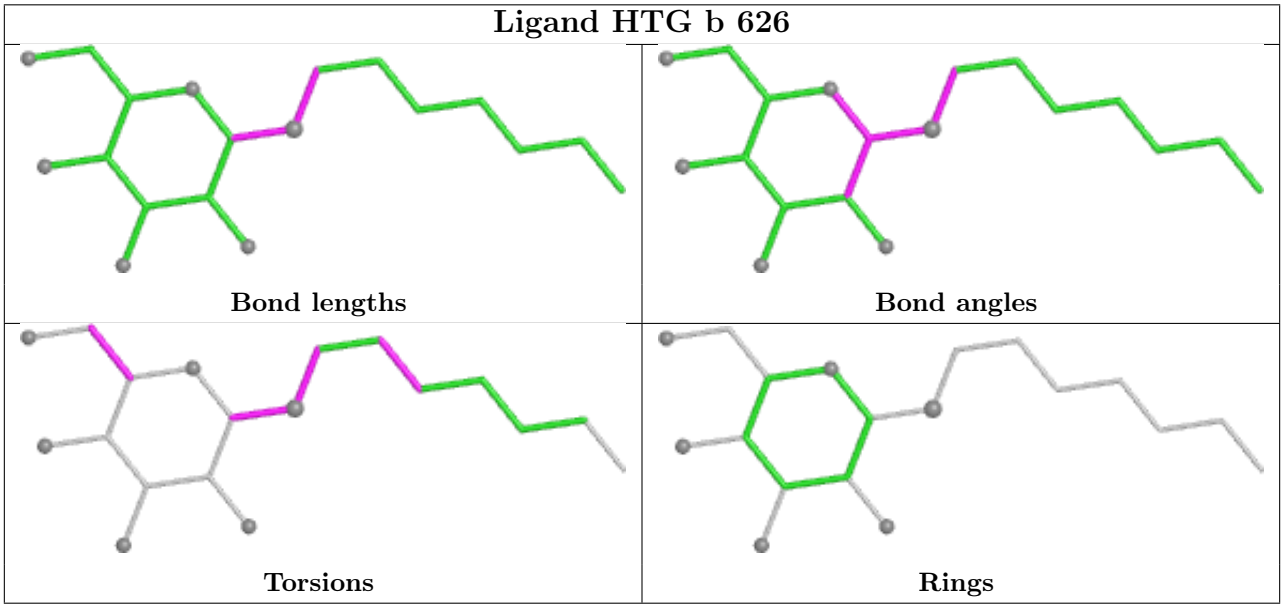


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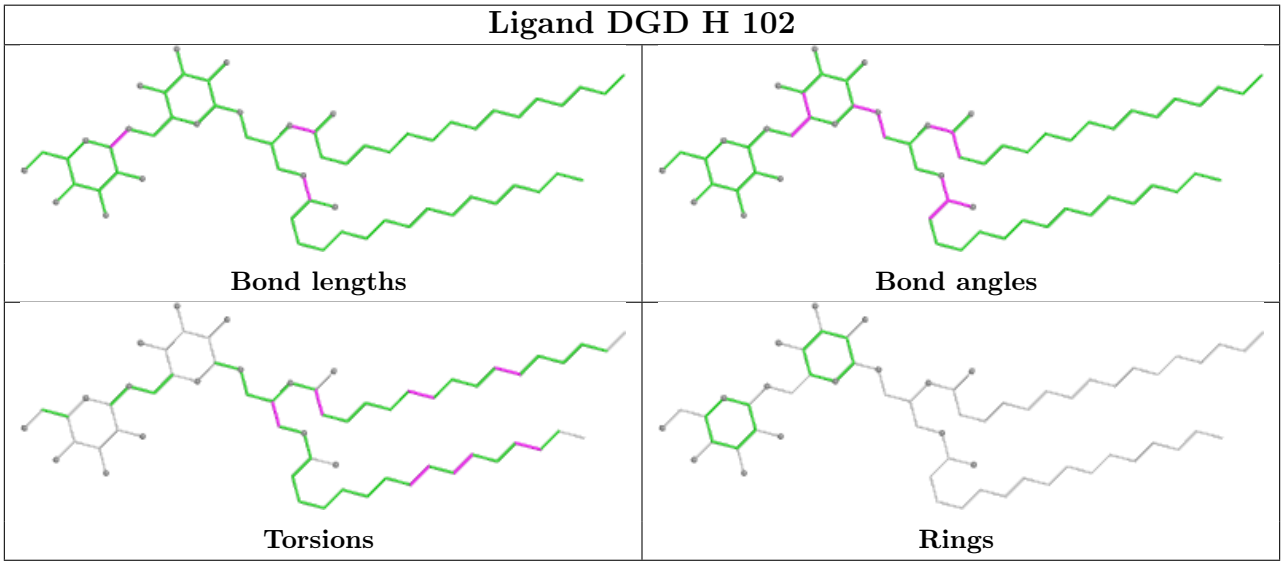
Ligand BCR C 515



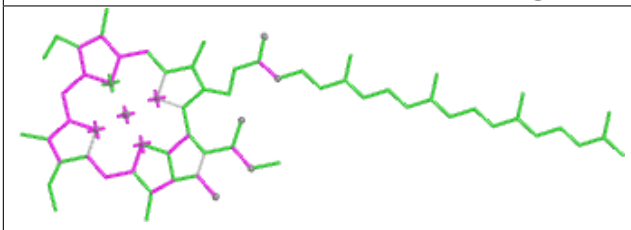
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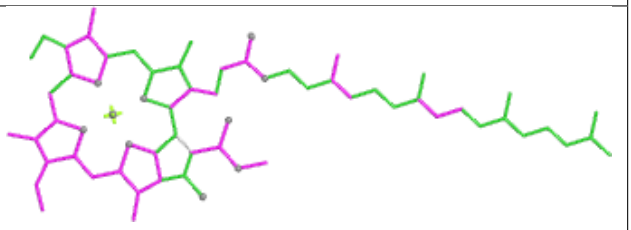
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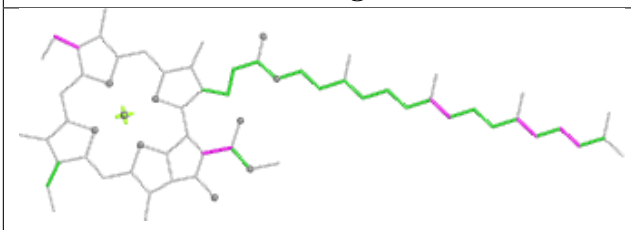
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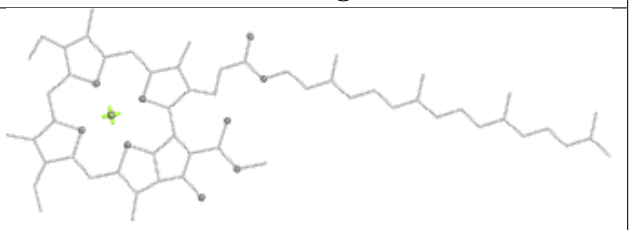
Bond lengths



Bond angles

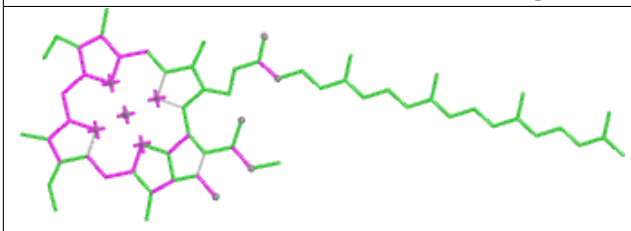


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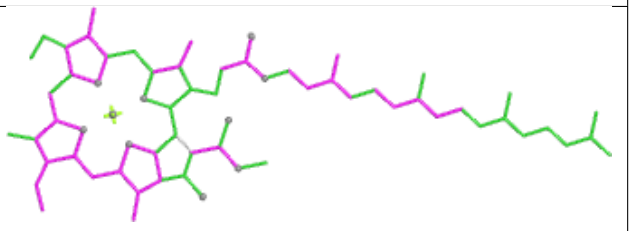


Rings

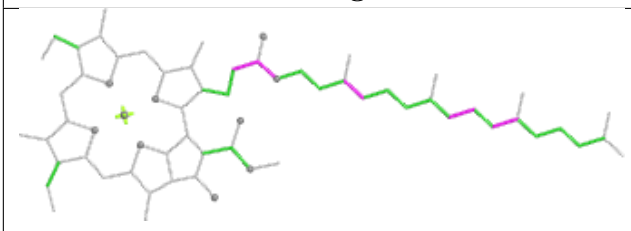
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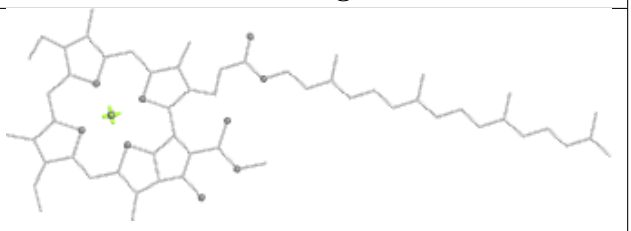
Bond lengths



Bond angles

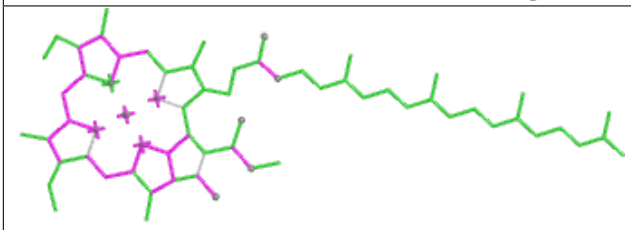


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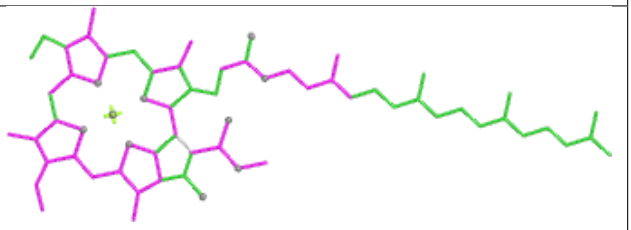


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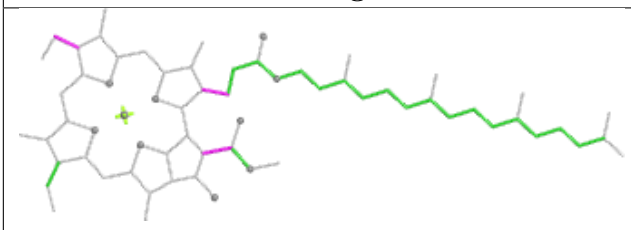
Ligand CLA B 610



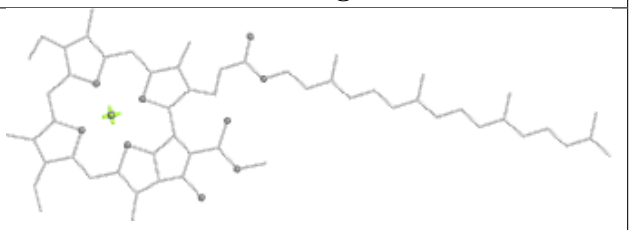
Bond lengths



Bond angles

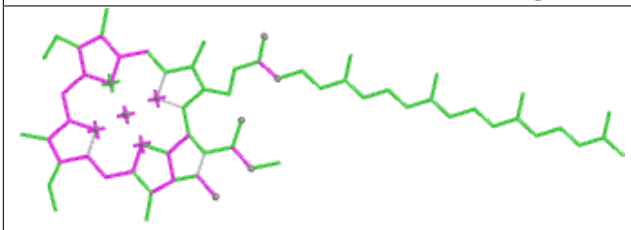


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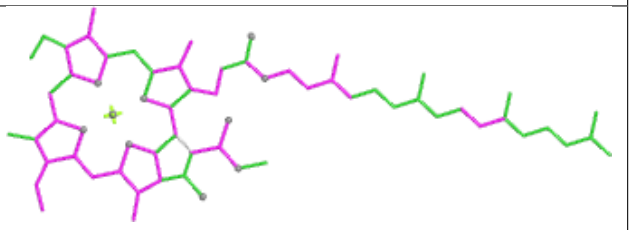


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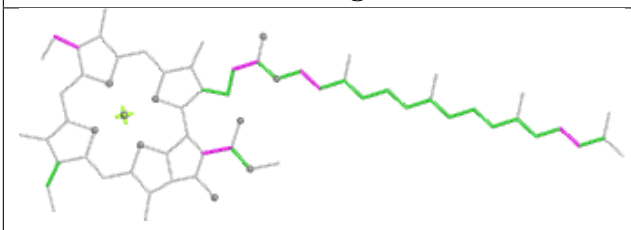
Ligand CLA c 514



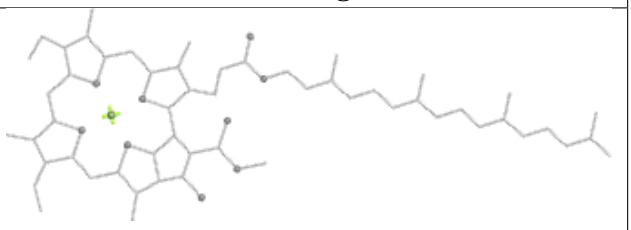
Bond lengths



Bond angles

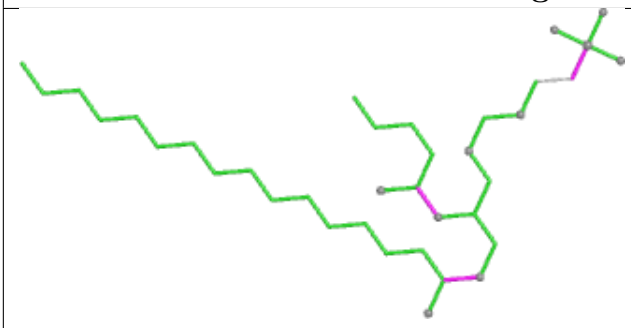


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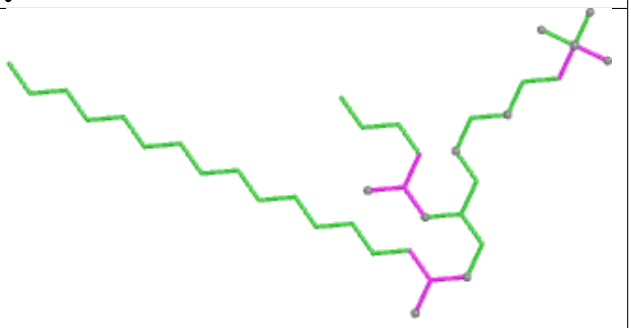


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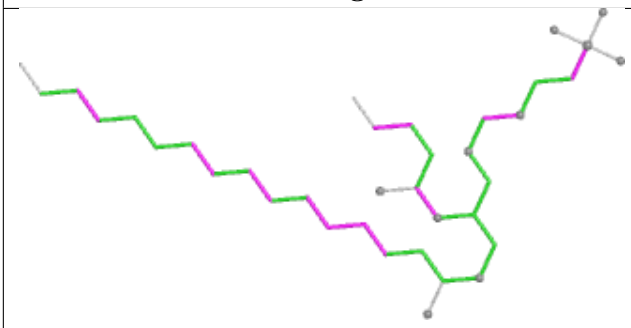
Ligand SQD f 102



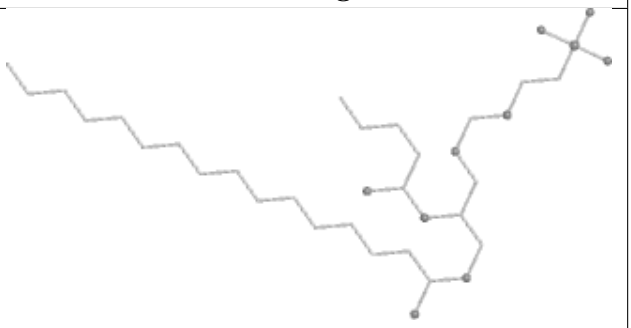
Bond lengths



Bond angles

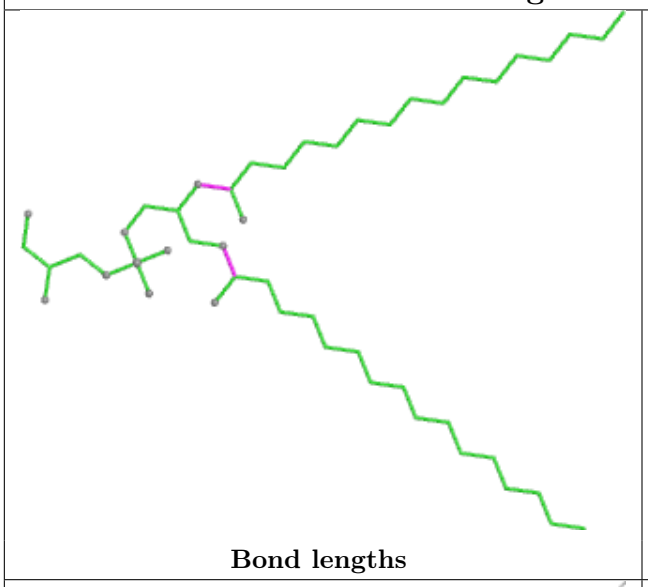


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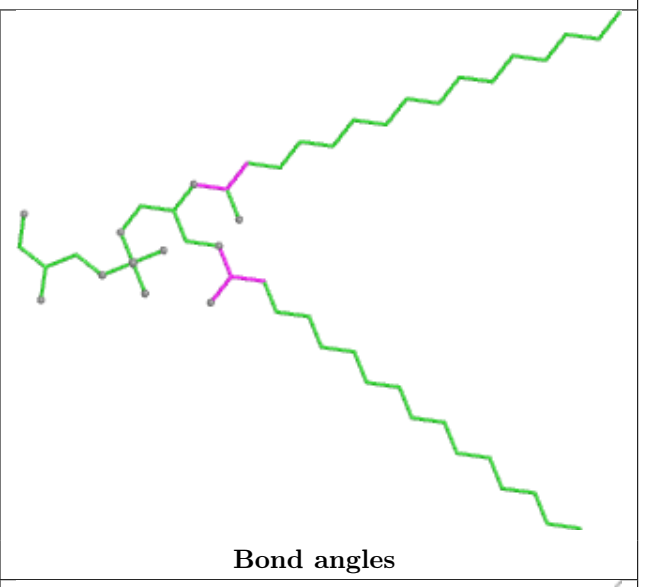


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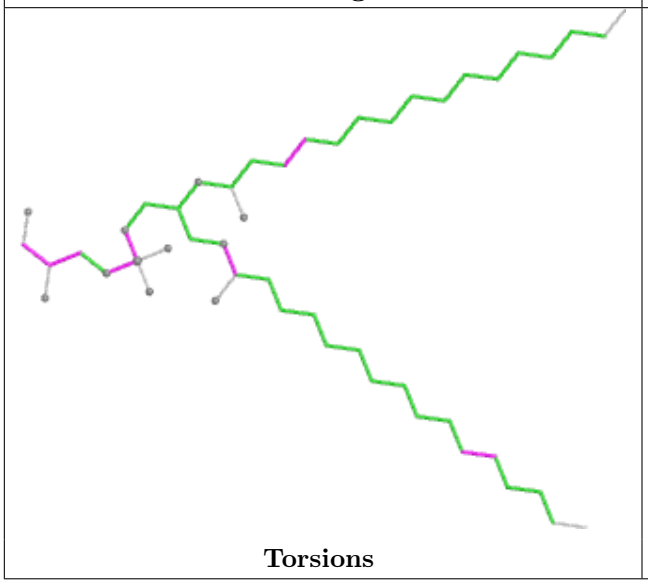
Ligand LHG d 409



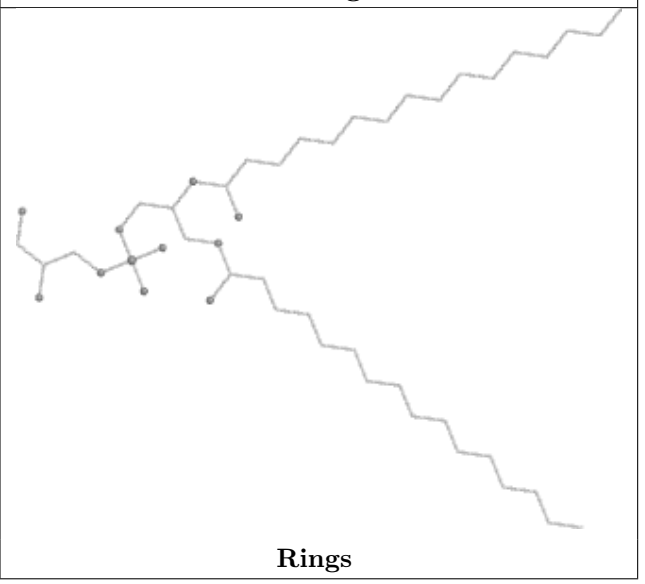
Bond lengths



Bond angles



Torsions



Rings

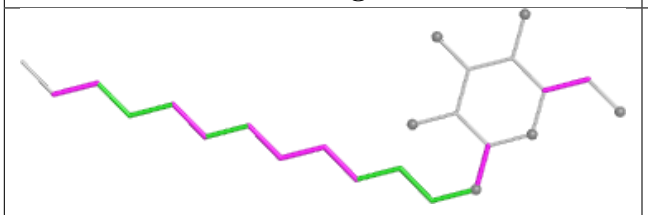
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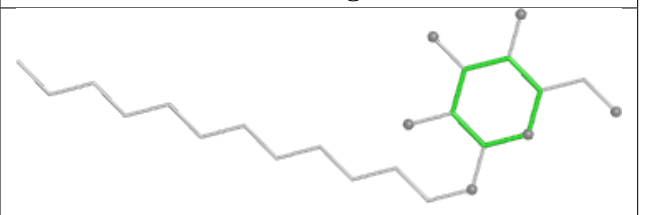
Bond lengths



Bond angles

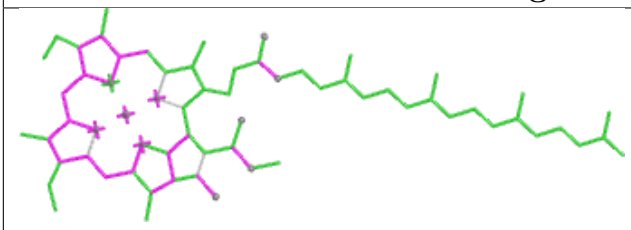


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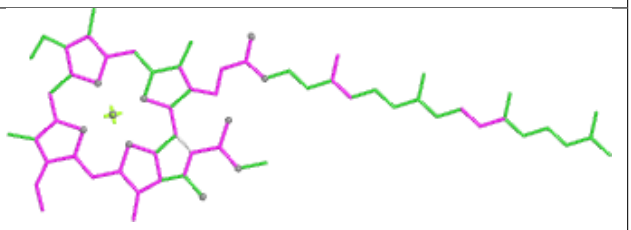


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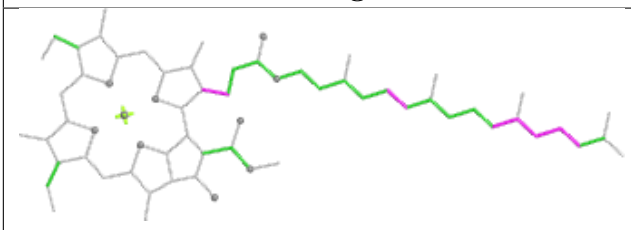
Ligand CLA c 508



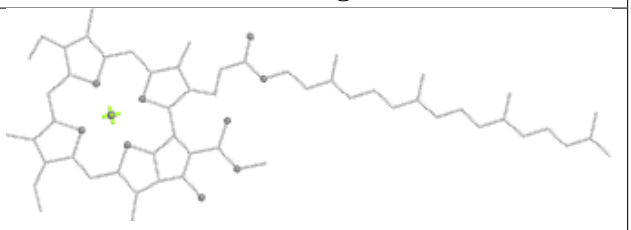
Bond lengths



Bond angles

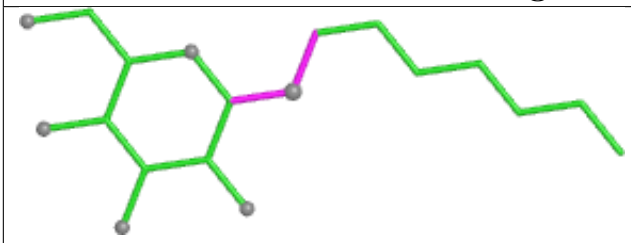


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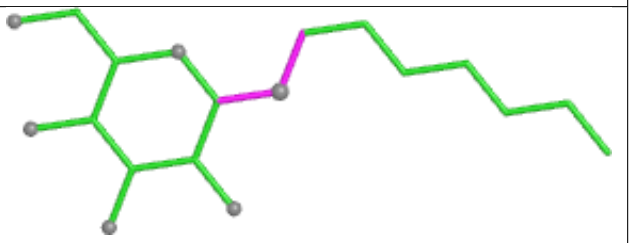


Rings

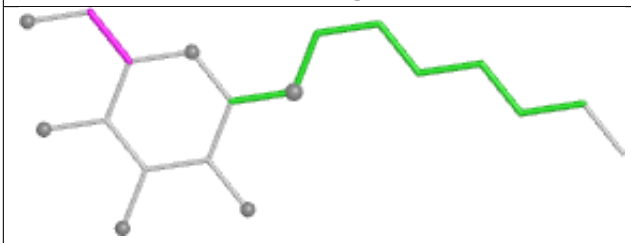
Ligand HTG i 103



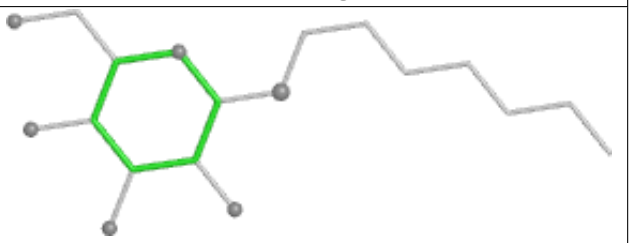
Bond lengths



Bond angles

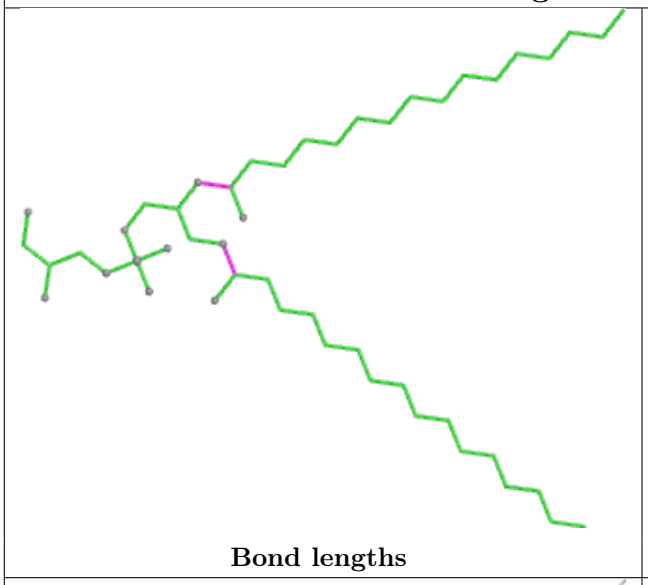


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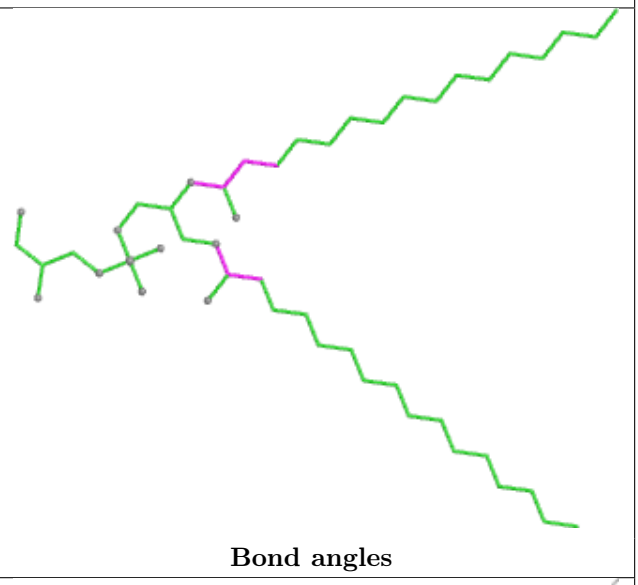


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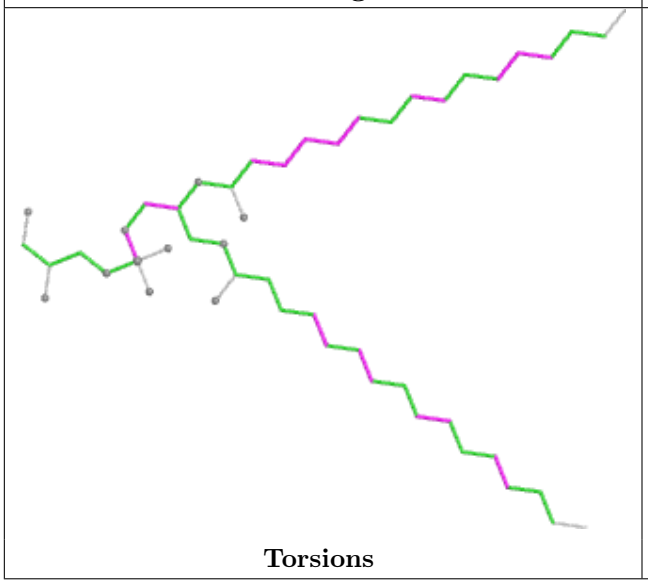
Ligand LHG l 101



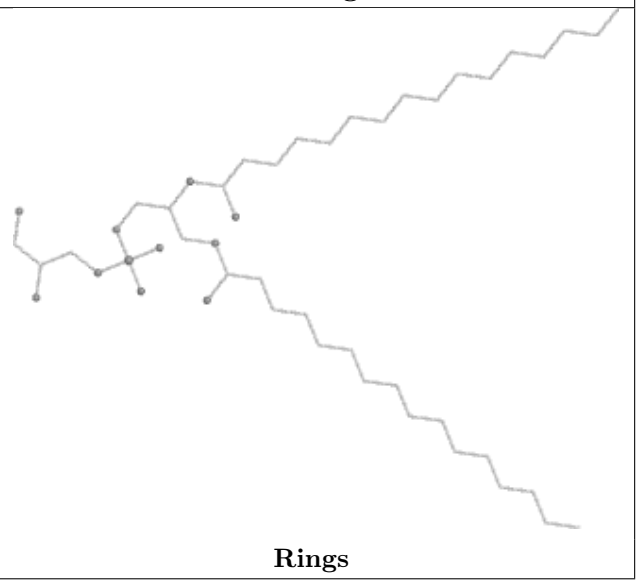
Bond lengths



Bond angles



Torsions

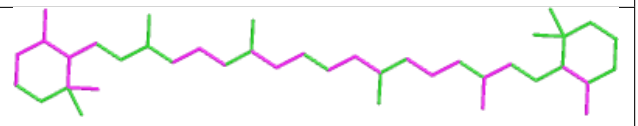


Rings

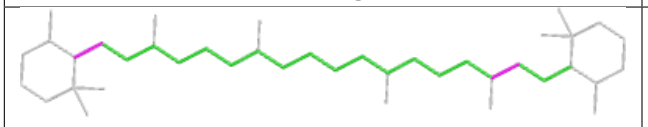
Ligand BCR Y 302



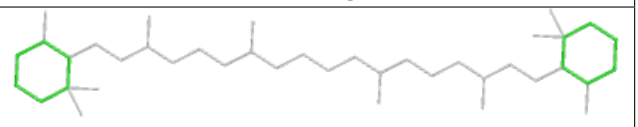
Bond lengths



Bond angles

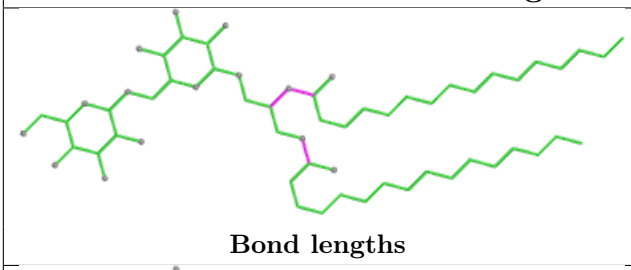


Torsions

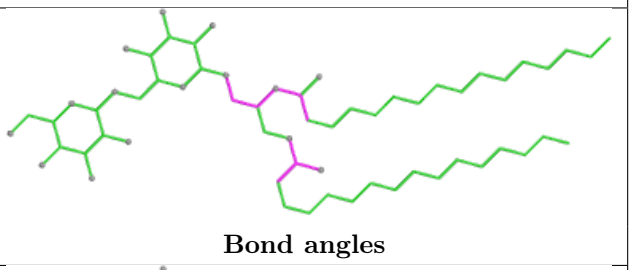


Rings

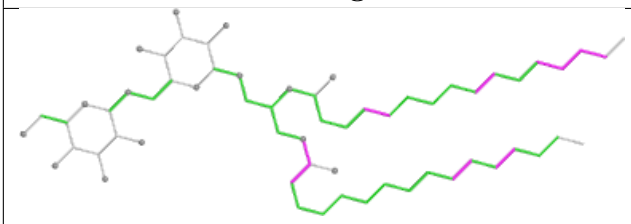
Ligand DGD c 520



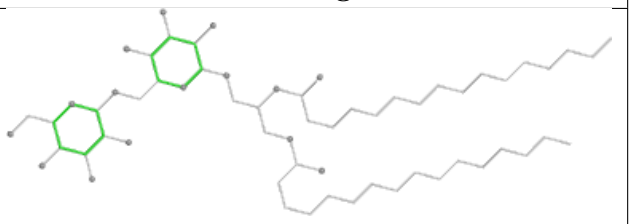
Bond lengths



Bond angles

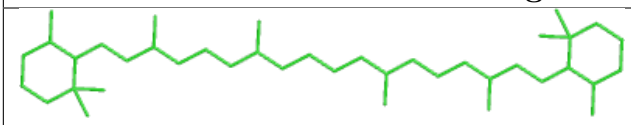


Torsions

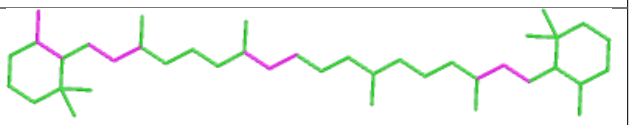


Rings

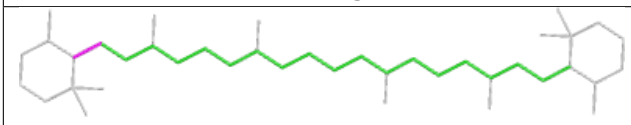
Ligand BCR b 620



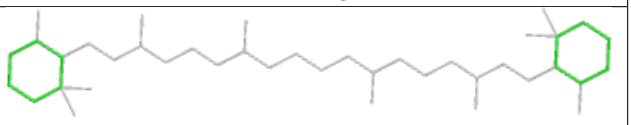
Bond lengths



Bond angles

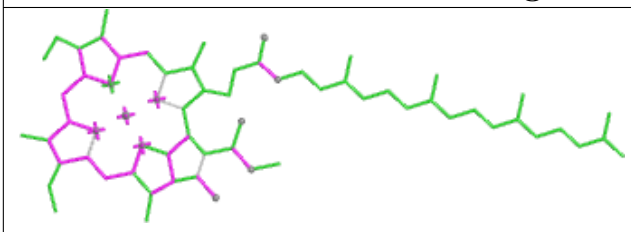


Torsions

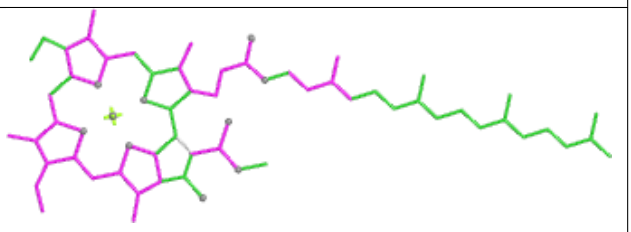


Rings

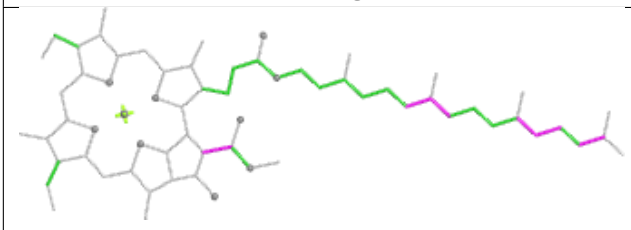
Ligand CLA A 406



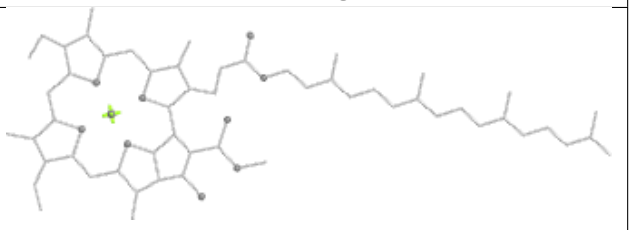
Bond lengths



Bond angles

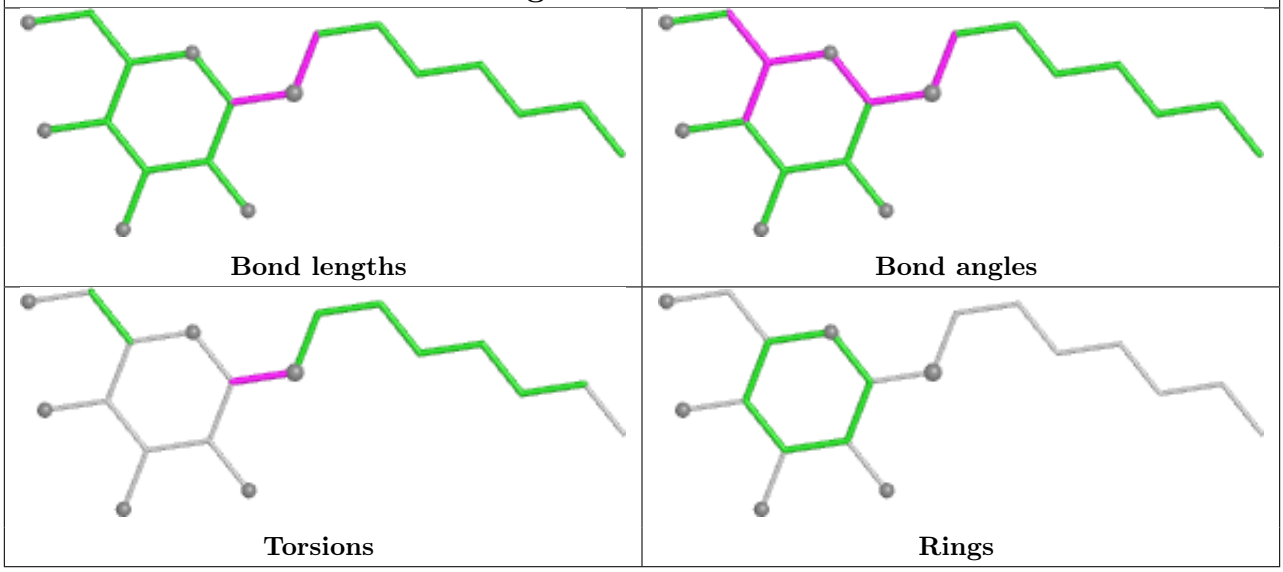


Torsions

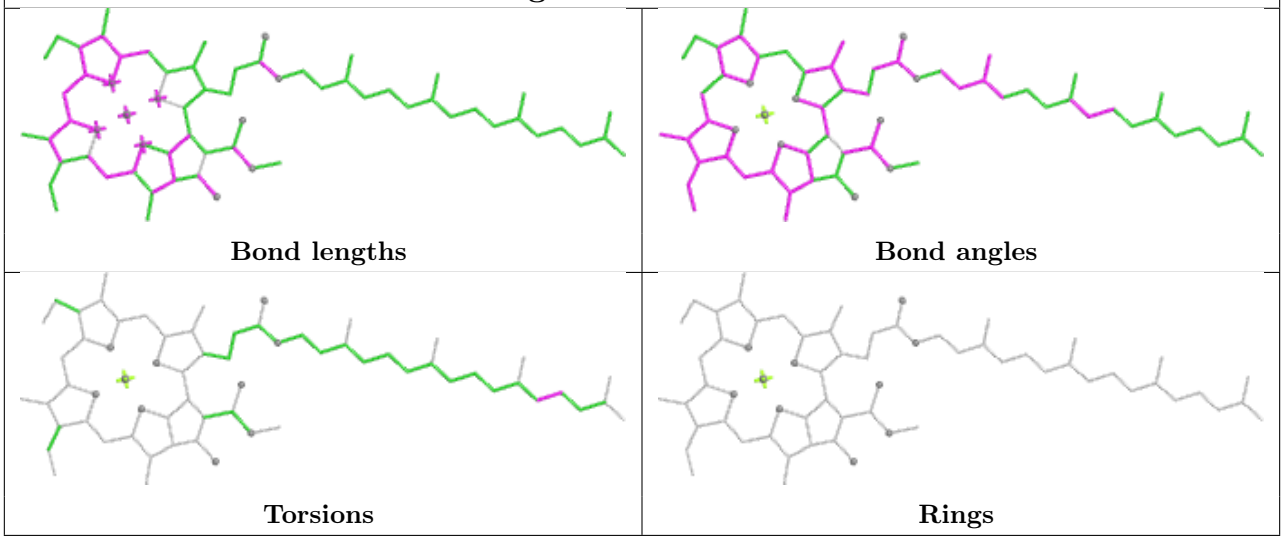


Rings

Ligand HTG c 523



Ligand CLA b 611



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/344 (97%)	-0.22	4 (1%) 76 78	27, 43, 72, 128	3 (0%)
1	a	334/344 (97%)	-0.07	7 (2%) 63 66	27, 45, 84, 116	3 (0%)
2	B	505/505 (100%)	-0.13	10 (1%) 65 67	27, 48, 79, 117	5 (0%)
2	b	503/505 (99%)	-0.05	17 (3%) 48 50	31, 50, 88, 168	8 (1%)
3	C	451/455 (99%)	-0.13	5 (1%) 78 80	35, 52, 71, 138	2 (0%)
3	c	455/455 (100%)	-0.00	4 (0%) 81 83	43, 57, 75, 119	0
4	D	340/342 (99%)	-0.25	1 (0%) 90 91	22, 44, 64, 107	1 (0%)
4	d	341/342 (99%)	-0.28	0 100 100	25, 46, 70, 114	3 (0%)
5	E	80/83 (96%)	0.28	4 (5%) 34 36	44, 66, 108, 118	1 (1%)
5	e	79/83 (95%)	0.29	3 (3%) 44 46	52, 67, 101, 124	0
6	F	34/44 (77%)	-0.20	1 (2%) 53 56	48, 56, 86, 104	0
6	f	32/44 (72%)	0.19	3 (9%) 14 14	49, 58, 104, 129	0
7	H	63/63 (100%)	0.15	1 (1%) 70 73	45, 57, 74, 103	0
7	h	63/63 (100%)	0.29	1 (1%) 70 73	46, 61, 80, 102	0
8	I	35/38 (92%)	0.61	1 (2%) 53 56	47, 63, 114, 124	0
8	i	35/38 (92%)	0.29	1 (2%) 53 56	47, 62, 109, 130	0
9	J	36/40 (90%)	-0.03	2 (5%) 30 32	45, 60, 95, 109	0
9	j	39/40 (97%)	-0.03	0 100 100	51, 62, 86, 108	0
10	K	37/37 (100%)	-0.07	0 100 100	38, 59, 73, 88	1 (2%)
10	k	37/37 (100%)	0.28	1 (2%) 56 59	54, 64, 85, 100	0
11	L	37/37 (100%)	-0.12	4 (10%) 11 11	22, 42, 94, 127	1 (2%)
11	l	36/37 (97%)	-0.24	1 (2%) 55 57	23, 43, 101, 128	2 (5%)
12	M	32/36 (88%)	-0.25	0 100 100	25, 44, 63, 86	1 (3%)
12	m	33/36 (91%)	-0.06	0 100 100	26, 45, 82, 105	1 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	0.02	3 (1%) 76 78	32, 55, 89, 169	2 (0%)
13	o	243/244 (99%)	0.00	4 (1%) 70 73	29, 57, 101, 138	3 (1%)
14	T	29/32 (90%)	-0.01	2 (6%) 23 24	36, 43, 72, 147	0
14	t	29/32 (90%)	-0.06	1 (3%) 48 50	37, 43, 76, 98	0
15	U	97/104 (93%)	-0.14	0 100 100	37, 52, 79, 92	1 (1%)
15	u	97/104 (93%)	-0.10	1 (1%) 79 81	46, 56, 75, 124	0
16	V	137/137 (100%)	-0.19	2 (1%) 72 74	32, 50, 68, 98	1 (0%)
16	v	137/137 (100%)	-0.13	0 100 100	48, 63, 87, 99	0
17	Y	30/30 (100%)	0.40	1 (3%) 49 51	59, 74, 114, 121	0
17	y	29/30 (96%)	0.51	1 (3%) 48 50	64, 78, 100, 113	0
18	X	38/40 (95%)	0.13	2 (5%) 32 34	53, 66, 85, 92	0
18	x	38/40 (95%)	0.34	2 (5%) 32 34	37, 66, 123, 143	1 (2%)
19	Z	61/62 (98%)	0.39	2 (3%) 49 51	58, 69, 110, 130	0
19	z	60/62 (96%)	0.64	8 (13%) 7 7	66, 79, 125, 142	0
20	R	34/41 (82%)	2.52	23 (67%) 0 0	99, 139, 163, 165	0
All	All	5274/5387 (97%)	-0.04	123 (2%) 61 64	22, 52, 89, 169	40 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	28	VAL	5.7
14	T	30	THR	5.3
20	R	26	TYR	4.8
7	H	64	ALA	4.7
1	a	260	PHE	4.7
18	x	37	VAL	4.5
2	b	495	PHE	4.4
2	b	499	VAL	4.2
7	h	64	ALA	3.9
2	b	493	TRP	3.6
2	b	487	SER	3.5
20	R	22	ASN	3.5
10	k	18	PHE	3.5
2	b	491	VAL	3.5
2	B	86	ILE	3.4
2	B	479	PHE	3.4
2	b	484	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	3.3
9	J	5	GLY	3.3
17	y	18	VAL	3.3
20	R	18	TRP	3.3
5	E	4	THR	3.3
3	c	183	GLY	3.3
20	R	35	LEU	3.3
14	t	30	THR	3.2
2	B	486	LEU	3.2
1	a	251	ALA	3.2
20	R	23	ILE	3.2
20	R	25	PRO	3.2
2	B	487	SER	3.1
20	R	31	VAL	3.1
20	R	6	LEU	3.1
20	R	34	LEU	3.1
20	R	3	TRP	3.0
2	b	486	LEU	3.0
1	A	229	GLU	3.0
1	a	11	ALA	3.0
19	z	61	VAL	3.0
8	i	36	ASP	2.9
2	B	495	PHE	2.9
13	O	58	ASN	2.8
2	b	485	GLU	2.8
2	b	479	PHE	2.8
20	R	2	ASP	2.8
20	R	10	LEU	2.8
20	R	24	LEU	2.8
18	x	2	THR	2.8
1	A	11	ALA	2.8
3	C	143	TYR	2.7
20	R	20	VAL	2.7
2	B	84	THR	2.7
13	o	61	GLN	2.6
11	l	2	GLU	2.6
13	o	58	ASN	2.6
20	R	13	LEU	2.6
4	D	12	ARG	2.6
5	E	61	ARG	2.6
2	B	85	GLY	2.6
1	a	19	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
19	z	2	THR	2.6
3	c	143	TYR	2.6
2	b	84	THR	2.6
6	f	14	PRO	2.6
11	L	2	GLU	2.5
17	Y	18	VAL	2.5
20	R	7	VAL	2.5
19	z	32	ASP	2.5
20	R	5	VAL	2.5
20	R	27	ALA	2.5
2	b	502	VAL	2.5
3	c	19	ASN	2.5
3	C	24	THR	2.4
13	o	62	GLU	2.4
5	E	72	ALA	2.4
1	a	229	GLU	2.4
2	b	489	GLU	2.4
11	L	10	VAL	2.3
2	B	496	TYR	2.3
5	e	61	ARG	2.3
3	c	147	PHE	2.3
18	X	31	ILE	2.3
5	e	84	LYS	2.3
13	O	65	PHE	2.3
15	u	70	ARG	2.3
1	A	230	THR	2.2
19	Z	32	ASP	2.2
3	C	260	ALA	2.2
1	A	14	TRP	2.2
2	b	497	GLN	2.2
13	o	4	THR	2.2
18	X	2	THR	2.2
2	B	502	VAL	2.2
20	R	12	VAL	2.2
11	L	1	MET	2.2
20	R	15	ALA	2.2
20	R	14	LEU	2.2
13	O	30	TYR	2.2
2	b	86	ILE	2.2
2	b	504	THR	2.2
19	z	13	VAL	2.2
19	z	4	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	262	ARG	2.2
16	V	106	ASN	2.2
20	R	11	PRO	2.1
19	Z	62	VAL	2.1
2	B	494	GLY	2.1
5	E	83	LEU	2.1
1	a	255	PHE	2.1
1	a	256	GLY	2.1
16	V	107	LEU	2.1
8	I	36	ASP	2.1
2	b	85	GLY	2.1
14	T	29	ILE	2.1
19	z	5	PHE	2.1
19	z	20	VAL	2.1
19	z	30	PRO	2.1
6	f	15	ILE	2.1
6	f	42	PHE	2.1
3	C	259	TRP	2.1
6	F	12	SER	2.1
11	L	3	PRO	2.0
5	e	79	PHE	2.0
9	J	30	TYR	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
19	FME	Z	1	10/11	0.87	0.13	86,100,112,113	0
19	FME	z	1	10/11	0.87	0.11	108,131,143,145	0
14	FME	T	1	10/11	0.94	0.09	45,52,78,79	0
14	FME	t	1	10/11	0.95	0.08	41,47,73,76	0
12	FME	M	1	10/11	0.95	0.09	42,48,82,86	0
4	HSK	d	336[A]	10/12	0.96	0.08	48,51,53,55	7
4	HSK	d	336[B]	11/12	0.96	0.08	48,51,55,59	8
12	FME	m	1	10/11	0.96	0.08	38,54,81,85	0
4	HSK	D	336[B]	11/12	0.96	0.08	45,48,49,50	8
4	HSK	D	336[A]	10/12	0.96	0.08	45,48,50,50	7
8	FME	I	1	10/11	0.97	0.06	45,54,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.98	0.07	41,53,56,56	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	O	314	4/4	0.56	0.17	133,135,136,138	0
34	DMS	k	2004	4/4	0.57	0.23	147,149,149,150	0
29	LMT	A	420	35/35	0.62	0.17	91,129,142,147	0
30	UNL	D	415	9/-	0.62	0.25	89,92,97,98	0
37	GOL	Z	102	6/6	0.62	0.16	105,121,124,124	0
30	UNL	B	630	9/-	0.63	0.35	80,89,103,103	0
37	GOL	v	202	6/6	0.63	0.13	100,106,107,107	0
37	GOL	o	2603	6/6	0.66	0.27	76,86,87,90	0
34	DMS	C	536	4/4	0.66	0.22	109,110,113,114	0
34	DMS	o	2604	4/4	0.67	0.28	124,124,125,126	0
34	DMS	E	108	4/4	0.67	0.21	115,118,120,120	0
34	DMS	b	643	4/4	0.68	0.17	149,150,151,151	0
37	GOL	k	2001	6/6	0.68	0.15	86,107,121,126	0
30	UNL	i	105	10/-	0.69	0.21	85,95,98,99	0
34	DMS	B	647	4/4	0.69	0.20	106,110,112,116	0
34	DMS	c	539	4/4	0.69	0.20	120,122,123,123	0
34	DMS	T	106	4/4	0.70	0.31	121,124,125,126	0
34	DMS	O	306	4/4	0.70	0.21	114,121,122,124	0
30	UNL	b	627	11/-	0.70	0.24	91,97,103,103	0
34	DMS	C	527	4/4	0.71	0.26	111,114,115,117	0
34	DMS	o	2610	4/4	0.71	0.20	131,131,131,133	0
34	DMS	z	1802	4/4	0.72	0.17	139,141,144,144	0
34	DMS	B	650	4/4	0.72	0.26	130,131,132,134	0
34	DMS	B	646	4/4	0.72	0.21	111,111,113,115	0
29	LMT	a	2120	35/35	0.72	0.15	101,133,144,145	0
34	DMS	v	214	4/4	0.72	0.21	127,132,134,135	0
34	DMS	C	535	4/4	0.73	0.29	121,122,124,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	o	2612	4/4	0.73	0.23	94,95,103,105	0
30	UNL	B	634	10/-	0.74	0.18	81,96,108,108	0
34	DMS	a	2124	4/4	0.74	0.20	128,130,130,131	0
34	DMS	B	649	4/4	0.74	0.15	124,124,125,126	0
34	DMS	D	420	4/4	0.74	0.24	124,124,126,126	0
30	UNL	A	415	40/-	0.74	0.20	80,111,132,143	0
30	UNL	E	102	15/-	0.74	0.24	96,102,109,111	0
34	DMS	C	533	4/4	0.74	0.18	120,121,121,122	0
34	DMS	o	2607	4/4	0.75	0.21	140,140,141,142	0
34	DMS	o	2609	4/4	0.75	0.24	110,119,119,121	0
30	UNL	h	701	11/-	0.75	0.23	85,89,97,98	0
34	DMS	O	309	4/4	0.75	0.26	98,101,104,109	0
30	UNL	e	102	15/-	0.75	0.20	76,82,95,98	0
30	UNL	E	104	6/-	0.76	0.24	67,78,88,89	0
34	DMS	b	640	4/4	0.76	0.21	103,108,109,111	0
30	UNL	a	2116	17/-	0.76	0.17	85,96,115,118	0
34	DMS	c	536	4/4	0.76	0.25	83,86,90,95	0
34	DMS	c	537	4/4	0.76	0.25	109,111,112,114	0
34	DMS	D	417	4/4	0.76	0.21	74,86,91,95	0
30	UNL	I	1203	16/-	0.77	0.20	88,99,102,103	0
34	DMS	C	539	4/4	0.77	0.25	75,90,91,96	0
30	UNL	j	1602	16/-	0.77	0.21	80,88,100,101	0
34	DMS	d	419	4/4	0.77	0.20	100,101,102,104	0
36	HTG	B	625[A]	19/19	0.77	0.19	57,70,80,83	19
36	HTG	B	625[B]	19/19	0.77	0.19	57,70,80,83	19
34	DMS	B	644	4/4	0.77	0.31	116,119,120,121	0
37	GOL	d	415	6/6	0.77	0.15	94,106,109,110	0
30	UNL	I	1204	13/-	0.77	0.18	80,87,94,95	0
37	GOL	o	2601	6/6	0.77	0.15	89,94,98,103	0
34	DMS	b	642	4/4	0.77	0.20	135,136,137,138	0
29	LMT	B	636	35/35	0.77	0.18	66,146,168,168	0
38	DGD	D	408	46/66	0.77	0.19	77,106,140,148	0
29	LMT	m	103	35/35	0.78	0.17	75,143,152,155	0
30	UNL	B	631	15/-	0.78	0.29	87,100,112,114	0
34	DMS	B	640	4/4	0.78	0.22	119,120,122,123	0
34	DMS	O	311	4/4	0.78	0.23	103,108,112,113	0
34	DMS	o	2605	4/4	0.78	0.28	111,114,114,122	0
34	DMS	b	639	4/4	0.79	0.19	93,94,94,99	0
30	UNL	B	629	18/-	0.79	0.17	78,85,103,105	0
34	DMS	d	422	4/4	0.79	0.19	113,118,118,121	0
34	DMS	O	312	4/4	0.79	0.23	112,116,117,118	0
30	UNL	E	106	16/-	0.79	0.27	93,104,113,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMT	f	101	24/35	0.79	0.15	93,112,125,126	0
30	UNL	b	628	15/-	0.79	0.22	85,97,105,106	0
34	DMS	x	802	4/4	0.80	0.21	110,115,116,118	0
34	DMS	O	304	4/4	0.80	0.28	129,133,136,141	0
34	DMS	b	635	4/4	0.80	0.19	102,104,106,108	0
30	UNL	c	525	12/-	0.80	0.24	88,97,118,118	0
36	HTG	B	626	19/19	0.80	0.15	53,114,123,126	19
36	HTG	B	628	19/19	0.80	0.14	56,128,134,137	0
36	HTG	I	1202	19/19	0.80	0.13	72,116,134,134	0
37	GOL	B	635	6/6	0.80	0.12	70,80,94,97	0
37	GOL	D	403	6/6	0.80	0.16	74,79,84,85	0
34	DMS	C	538	4/4	0.80	0.18	121,122,124,126	0
30	UNL	d	413	10/-	0.80	0.17	85,88,96,100	0
29	LMT	E	105	24/35	0.80	0.16	89,104,131,136	0
29	LMT	a	2103	35/35	0.80	0.18	60,100,116,118	0
34	DMS	T	104	4/4	0.80	0.24	118,127,127,129	0
34	DMS	c	538	4/4	0.80	0.18	111,113,114,116	0
30	UNL	J	103	15/-	0.80	0.24	86,93,99,99	0
29	LMT	j	1601	23/35	0.81	0.16	77,104,149,151	0
34	DMS	d	420	4/4	0.81	0.27	117,117,120,122	0
34	DMS	b	637	4/4	0.81	0.24	131,135,135,137	0
34	DMS	d	423	4/4	0.81	0.19	143,144,144,145	0
34	DMS	e	104	4/4	0.81	0.20	117,119,120,120	0
30	UNL	Y	301	10/-	0.81	0.21	93,101,108,109	0
36	HTG	d	414	19/19	0.81	0.17	76,99,110,110	19
30	UNL	k	2002	12/-	0.81	0.24	84,93,114,115	0
34	DMS	O	313	4/4	0.81	0.16	99,102,104,111	0
37	GOL	U	501	6/6	0.81	0.24	86,95,97,103	0
30	UNL	A	416	15/-	0.81	0.20	70,89,101,102	0
34	DMS	c	533	4/4	0.81	0.21	110,116,116,117	0
34	DMS	O	305	4/4	0.81	0.21	101,101,103,112	0
30	UNL	h	704	12/-	0.81	0.23	83,89,104,106	0
34	DMS	v	208	4/4	0.81	0.20	115,115,120,124	0
34	DMS	a	2122	4/4	0.81	0.16	128,128,129,129	0
37	GOL	v	204	6/6	0.81	0.15	85,89,93,97	0
34	DMS	O	307	4/4	0.81	0.20	119,120,120,120	0
39	LHG	e	101	32/49	0.81	0.17	77,130,154,158	0
30	UNL	i	102	19/-	0.82	0.16	86,96,114,114	0
30	UNL	C	501	40/-	0.82	0.19	75,102,126,129	0
34	DMS	c	534	4/4	0.82	0.15	120,120,122,123	0
37	GOL	b	631	6/6	0.82	0.15	94,99,103,109	0
36	HTG	C	522	19/19	0.82	0.13	66,115,134,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	HTG	D	413	19/19	0.82	0.15	74,106,124,127	0
34	DMS	V	206	4/4	0.82	0.16	88,96,102,105	0
36	HTG	b	626	19/19	0.82	0.14	96,137,142,142	0
36	HTG	d	403	19/19	0.82	0.14	83,114,127,128	0
30	UNL	C	523	10/-	0.82	0.21	81,88,98,100	0
37	GOL	B	632	6/6	0.82	0.18	95,101,103,106	0
39	LHG	E	101	49/49	0.82	0.17	77,108,122,123	0
29	LMT	A	414	34/35	0.82	0.17	68,107,122,131	0
30	UNL	b	629	9/-	0.83	0.20	76,90,96,96	0
37	GOL	H	103	6/6	0.83	0.17	85,97,100,102	0
30	UNL	E	103	6/-	0.83	0.16	82,82,84,85	0
37	GOL	V	203	6/6	0.83	0.15	84,103,106,107	0
34	DMS	j	1604	4/4	0.83	0.23	126,129,130,133	0
34	DMS	t	103	4/4	0.83	0.19	109,112,116,117	0
34	DMS	u	204	4/4	0.83	0.21	106,108,109,110	0
30	UNL	d	402	40/-	0.83	0.23	61,88,130,131	0
34	DMS	v	210	4/4	0.83	0.17	122,123,124,125	0
34	DMS	v	211	4/4	0.83	0.18	95,111,113,114	0
34	DMS	v	213	4/4	0.83	0.18	108,108,109,109	0
34	DMS	A	424	4/4	0.83	0.16	78,84,87,89	0
36	HTG	i	103	19/19	0.83	0.14	74,133,147,148	0
34	DMS	T	105	4/4	0.83	0.24	134,134,135,135	0
29	LMT	I	1201	24/35	0.83	0.17	56,96,144,148	0
34	DMS	c	540	4/4	0.84	0.15	118,124,125,128	0
34	DMS	A	423	4/4	0.84	0.22	113,115,117,121	0
34	DMS	C	537	4/4	0.84	0.17	112,114,116,118	0
36	HTG	b	602	19/19	0.84	0.14	68,120,134,138	0
34	DMS	o	2611	4/4	0.84	0.18	96,99,99,99	0
36	HTG	c	523	19/19	0.84	0.14	95,110,115,116	0
36	HTG	c	524	19/19	0.84	0.15	73,97,108,110	19
34	DMS	B	642	4/4	0.84	0.23	109,111,113,115	0
34	DMS	E	107	4/4	0.84	0.19	124,128,129,133	0
37	GOL	c	527	6/6	0.85	0.18	81,86,93,93	0
29	LMT	Z	101	35/35	0.85	0.15	60,125,151,156	0
27	SQD	L	102	54/54	0.85	0.17	55,78,119,123	0
34	DMS	B	638	4/4	0.85	0.20	124,124,126,126	0
29	LMT	J	102	24/35	0.85	0.16	76,101,135,137	0
37	GOL	O	303	6/6	0.85	0.12	91,94,95,96	0
37	GOL	v	203	6/6	0.85	0.14	78,80,83,87	0
30	UNL	b	630	21/-	0.85	0.14	61,79,105,107	0
34	DMS	C	534	4/4	0.85	0.22	119,119,120,121	0
30	UNL	c	501	36/-	0.85	0.19	80,98,127,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	m	101	13/-	0.85	0.21	70,75,95,99	0
34	DMS	v	212	4/4	0.86	0.17	119,121,122,124	0
29	LMT	z	1801	33/35	0.86	0.14	74,116,131,136	0
27	SQD	F	101	45/54	0.86	0.14	69,97,121,132	0
37	GOL	C	525	6/6	0.86	0.15	83,98,100,101	0
34	DMS	A	425	4/4	0.86	0.19	93,96,96,98	0
34	DMS	u	201	4/4	0.86	0.26	104,109,110,111	0
34	DMS	b	636	4/4	0.86	0.15	69,96,97,100	0
29	LMT	m	102	35/35	0.86	0.13	49,82,99,101	0
36	HTG	c	526	19/19	0.86	0.12	97,131,146,149	0
30	UNL	a	2117	9/-	0.86	0.17	72,79,83,84	0
28	LMG	C	526	48/55	0.86	0.16	63,111,128,134	0
36	HTG	V	204	19/19	0.87	0.13	67,84,115,118	0
34	DMS	B	645	4/4	0.87	0.13	86,91,92,93	0
29	LMT	b	624	25/35	0.87	0.17	80,110,138,139	0
29	LMT	B	623	35/35	0.87	0.13	74,104,121,122	0
34	DMS	C	529	4/4	0.87	0.24	123,124,124,127	0
30	UNL	D	402	40/-	0.88	0.18	60,82,118,122	0
29	LMT	M	101	35/35	0.88	0.12	57,89,104,107	0
27	SQD	B	621	54/54	0.88	0.14	48,87,130,133	0
34	DMS	c	535	4/4	0.88	0.17	95,103,106,106	0
36	HTG	b	625	19/19	0.88	0.16	46,69,88,89	19
27	SQD	f	102	37/54	0.88	0.15	73,101,129,134	0
30	UNL	M	102	15/-	0.88	0.17	58,68,108,113	0
30	UNL	T	103	9/-	0.88	0.21	78,85,93,95	0
29	LMT	i	104	24/35	0.88	0.15	64,103,141,147	0
34	DMS	V	208	4/4	0.88	0.14	81,91,94,96	0
34	DMS	c	541	4/4	0.88	0.14	104,106,106,106	0
31	PL9	A	417	39/55	0.89	0.18	73,85,102,105	0
34	DMS	b	641	4/4	0.89	0.14	67,70,72,74	0
34	DMS	V	207	4/4	0.89	0.14	92,93,99,100	0
34	DMS	C	530	4/4	0.89	0.15	88,93,97,99	0
34	DMS	c	530	4/4	0.89	0.20	121,122,122,126	0
31	PL9	x	801	39/55	0.89	0.19	71,91,119,122	0
28	LMG	i	101	51/55	0.89	0.15	65,82,94,101	0
34	DMS	b	634	4/4	0.89	0.17	96,98,98,104	0
37	GOL	C	524	6/6	0.89	0.12	91,98,103,105	0
27	SQD	A	413	54/54	0.89	0.13	62,81,122,128	0
30	UNL	B	633	22/-	0.89	0.13	61,84,112,113	0
34	DMS	O	310	4/4	0.89	0.15	102,103,103,107	0
34	DMS	o	2606	4/4	0.89	0.18	109,111,111,111	0
34	DMS	V	202	4/4	0.89	0.17	96,97,99,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	LMG	c	522	48/55	0.90	0.14	55,110,127,139	0
34	DMS	v	209	4/4	0.90	0.14	82,93,93,101	0
34	DMS	d	421	4/4	0.90	0.20	85,92,95,96	0
34	DMS	o	2608	4/4	0.90	0.12	102,107,110,114	0
34	DMS	V	209	4/4	0.90	0.16	87,103,104,110	0
24	CLA	B	602	65/65	0.90	0.10	45,68,113,120	0
29	LMT	B	637	24/35	0.90	0.13	50,77,118,128	0
34	DMS	U	503	4/4	0.90	0.20	95,109,110,112	0
34	DMS	B	648	4/4	0.90	0.14	63,65,67,80	0
28	LMG	C	520	51/55	0.90	0.15	48,81,101,108	0
34	DMS	u	203	4/4	0.90	0.14	76,85,86,89	0
27	SQD	a	2102	53/54	0.90	0.13	52,80,111,115	0
26	BCR	t	102	40/40	0.91	0.10	42,55,75,77	0
24	CLA	C	507	65/65	0.91	0.13	50,69,110,117	0
36	HTG	B	627	19/19	0.91	0.13	59,90,110,116	0
29	LMT	T	102	24/35	0.91	0.15	48,79,108,114	0
36	HTG	C	521	19/19	0.91	0.13	90,106,113,116	0
34	DMS	v	207	4/4	0.91	0.15	96,97,99,100	0
34	DMS	A	426	4/4	0.91	0.18	79,80,80,84	0
34	DMS	a	2123	4/4	0.91	0.19	113,115,118,123	0
36	HTG	B	624	19/19	0.91	0.13	60,69,74,76	0
34	DMS	d	417	4/4	0.91	0.22	84,87,87,90	0
30	UNL	D	414	16/-	0.92	0.16	55,70,85,89	0
28	LMG	B	622	51/55	0.92	0.13	51,70,83,92	0
34	DMS	b	633	4/4	0.92	0.16	79,80,81,92	0
32	K2I	A	418[A]	10/10	0.92	0.14	94,96,102,105	10
32	K2I	A	418[B]	10/10	0.92	0.14	74,95,100,112	10
26	BCR	C	516	40/40	0.92	0.11	48,56,69,72	0
34	DMS	u	202	4/4	0.92	0.14	79,80,89,90	0
26	BCR	T	101	40/40	0.92	0.09	39,52,71,75	0
34	DMS	D	419	4/4	0.92	0.15	88,95,95,104	0
28	LMG	b	623	51/55	0.92	0.13	56,70,83,100	0
36	HTG	b	601	19/19	0.92	0.11	63,84,94,98	0
30	UNL	X	801	18/-	0.92	0.12	65,71,96,98	0
34	DMS	C	528	4/4	0.92	0.17	88,96,97,98	0
34	DMS	i	106	4/4	0.92	0.15	95,96,97,98	0
34	DMS	F	103	4/4	0.92	0.13	77,78,79,88	0
24	CLA	b	604	65/65	0.92	0.11	52,73,118,121	0
28	LMG	A	412	51/55	0.92	0.13	57,79,100,104	0
30	UNL	t	101	8/-	0.92	0.16	75,81,88,89	0
34	DMS	B	643	4/4	0.92	0.17	81,85,90,91	0
34	DMS	V	210	4/4	0.92	0.15	87,96,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	O	308	4/4	0.92	0.18	102,105,106,108	0
32	K2I	a	2118[A]	10/10	0.93	0.10	103,106,111,114	10
37	GOL	a	2101	6/6	0.93	0.13	66,76,77,80	0
32	K2I	a	2118[B]	10/10	0.93	0.10	82,105,107,112	10
30	UNL	d	412	14/-	0.93	0.17	56,73,79,82	0
34	DMS	b	638	4/4	0.93	0.14	81,85,89,94	0
26	BCR	c	516	40/40	0.93	0.12	63,76,81,85	0
36	HTG	O	302	19/19	0.93	0.11	51,68,78,81	0
30	UNL	d	416	18/-	0.93	0.11	59,74,105,105	0
24	CLA	c	508	65/65	0.93	0.11	51,67,102,107	0
24	CLA	a	2113	65/65	0.93	0.11	40,46,116,121	0
34	DMS	c	542	4/4	0.93	0.11	113,114,117,118	0
27	SQD	a	2115	47/54	0.93	0.13	59,80,97,104	0
38	DGD	c	518	62/66	0.93	0.12	42,54,95,100	0
24	CLA	B	617	65/65	0.93	0.11	40,52,119,123	0
28	LMG	c	521	49/55	0.93	0.14	53,88,105,108	0
27	SQD	A	411	49/54	0.94	0.12	66,82,98,99	0
24	CLA	b	619	65/65	0.94	0.11	43,56,119,121	0
34	DMS	D	416	4/4	0.94	0.12	61,76,81,82	0
33	BCT	A	421	4/4	0.94	0.09	51,56,61,64	0
33	BCT	a	2108	4/4	0.94	0.10	55,57,63,68	0
24	CLA	C	514	65/65	0.94	0.09	54,65,95,98	0
24	CLA	c	514	65/65	0.94	0.10	56,64,100,102	0
24	CLA	c	515	65/65	0.94	0.10	55,68,98,106	0
34	DMS	d	418	4/4	0.94	0.14	69,73,81,88	0
24	CLA	d	405	65/65	0.94	0.09	46,55,105,115	0
24	CLA	B	615	65/65	0.94	0.10	35,45,99,107	0
34	DMS	C	531	4/4	0.94	0.14	63,70,77,78	0
24	CLA	C	513	65/65	0.94	0.10	51,65,107,110	0
26	BCR	a	2114	40/40	0.94	0.08	35,45,51,53	0
24	CLA	b	609	65/65	0.94	0.09	39,50,86,88	0
34	DMS	v	206	4/4	0.94	0.14	78,93,93,98	0
39	LHG	D	409	49/49	0.94	0.11	48,59,70,74	0
26	BCR	c	517	40/40	0.94	0.10	47,59,75,78	0
24	CLA	b	617	65/65	0.94	0.11	36,45,100,113	0
41	RRX	H	101	41/41	0.94	0.09	45,59,68,78	0
41	RRX	h	702	41/41	0.94	0.10	46,59,81,93	0
24	CLA	B	607	65/65	0.95	0.09	37,46,74,84	0
26	BCR	D	406	40/40	0.95	0.09	42,52,85,86	0
26	BCR	K	101	40/40	0.95	0.09	50,57,63,67	0
24	CLA	D	405	65/65	0.95	0.09	42,52,106,112	0
26	BCR	Y	302	40/40	0.95	0.07	48,56,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	c	505	65/65	0.95	0.09	43,57,63,70	0
26	BCR	b	622	40/40	0.95	0.09	45,57,71,76	0
24	CLA	c	506	65/65	0.95	0.10	44,52,86,90	0
24	CLA	B	611	65/65	0.95	0.08	41,49,57,68	0
28	LMG	d	411	48/55	0.95	0.10	47,56,86,95	0
26	BCR	c	528	40/40	0.95	0.09	48,58,68,69	0
26	BCR	d	406	40/40	0.95	0.09	47,55,75,82	0
24	CLA	c	510	65/65	0.95	0.09	41,51,114,126	0
24	CLA	C	511	65/65	0.95	0.09	37,51,59,70	0
34	DMS	c	531	4/4	0.95	0.14	97,99,101,106	0
38	DGD	C	517	62/66	0.95	0.10	40,51,93,96	0
38	DGD	C	518	62/66	0.95	0.10	41,54,109,119	0
38	DGD	C	519	62/66	0.95	0.10	39,51,92,103	0
24	CLA	A	409	65/65	0.95	0.11	35,45,117,121	0
38	DGD	H	102	62/66	0.95	0.10	45,54,66,70	0
24	CLA	b	610	65/65	0.95	0.08	31,43,58,62	0
38	DGD	c	519	62/66	0.95	0.10	47,59,107,117	0
38	DGD	h	703	62/66	0.95	0.10	46,57,74,79	0
26	BCR	B	618	40/40	0.95	0.08	38,47,54,55	0
26	BCR	B	620	40/40	0.95	0.08	42,52,63,67	0
39	LHG	d	408	49/49	0.95	0.10	45,58,73,78	0
26	BCR	C	515	40/40	0.95	0.08	47,65,74,79	0
39	LHG	l	101	49/49	0.95	0.10	43,52,71,79	0
31	PL9	D	407	55/55	0.95	0.08	34,43,50,55	0
31	PL9	d	407	55/55	0.95	0.09	33,44,55,60	0
24	CLA	A	406	65/65	0.96	0.09	34,42,100,104	0
24	CLA	c	507	65/65	0.96	0.08	42,52,66,74	0
24	CLA	C	508	65/65	0.96	0.09	47,56,73,77	0
24	CLA	c	509	65/65	0.96	0.09	45,56,77,79	0
24	CLA	C	509	65/65	0.96	0.08	38,50,106,117	0
24	CLA	c	511	65/65	0.96	0.09	43,55,79,90	0
24	CLA	c	513	65/65	0.96	0.08	45,59,70,79	0
24	CLA	C	510	65/65	0.96	0.09	46,54,74,77	0
28	LMG	D	412	44/55	0.96	0.09	44,53,80,83	0
24	CLA	B	608	65/65	0.96	0.08	33,42,57,67	0
24	CLA	C	512	65/65	0.96	0.07	41,56,65,69	0
34	DMS	v	205	4/4	0.96	0.13	75,76,84,85	0
25	PHO	A	407	64/64	0.96	0.07	33,39,48,49	0
37	GOL	U	502	6/6	0.96	0.09	69,78,90,95	0
25	PHO	A	408	64/64	0.96	0.07	34,45,52,55	0
24	CLA	B	610	65/65	0.96	0.07	42,49,58,60	0
34	DMS	c	532	4/4	0.96	0.11	72,72,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	B	619	40/40	0.96	0.07	40,50,62,67	0
24	CLA	B	603	65/65	0.96	0.08	41,48,57,58	0
24	CLA	B	614	65/65	0.96	0.07	34,41,79,93	0
24	CLA	a	2110	65/65	0.96	0.10	35,44,106,111	0
24	CLA	B	604	65/65	0.96	0.07	36,45,57,63	0
24	CLA	B	606	65/65	0.96	0.07	34,43,59,64	0
24	CLA	b	608	65/65	0.96	0.07	37,45,58,61	0
24	CLA	C	502	65/65	0.96	0.08	43,52,68,88	0
34	DMS	B	641	4/4	0.96	0.12	63,65,69,71	0
24	CLA	C	503	65/65	0.96	0.07	39,48,62,66	0
26	BCR	b	620	40/40	0.96	0.08	40,49,58,59	0
26	BCR	b	621	40/40	0.96	0.08	39,51,63,71	0
24	CLA	b	612	65/65	0.96	0.08	43,52,62,70	0
24	CLA	b	613	65/65	0.96	0.08	42,50,57,64	0
24	CLA	b	615	65/65	0.96	0.07	37,45,52,56	0
24	CLA	b	616	65/65	0.96	0.08	37,41,80,84	0
38	DGD	c	520	62/66	0.96	0.10	44,57,80,88	0
34	DMS	V	205	4/4	0.96	0.11	66,69,70,75	0
24	CLA	C	504	65/65	0.96	0.07	42,52,59,67	0
39	LHG	D	410	49/49	0.96	0.09	41,47,65,81	0
39	LHG	D	411	44/49	0.96	0.10	44,53,90,98	0
26	BCR	k	2003	40/40	0.96	0.09	50,60,69,71	0
24	CLA	b	618	65/65	0.96	0.09	41,51,70,78	0
39	LHG	d	409	49/49	0.96	0.09	40,46,72,84	0
39	LHG	d	410	36/49	0.96	0.08	46,54,79,85	0
24	CLA	C	505	65/65	0.96	0.09	41,49,81,86	0
24	CLA	c	503	65/65	0.96	0.09	44,55,68,73	0
24	CLA	c	504	65/65	0.96	0.08	40,50,64,81	0
24	CLA	C	506	65/65	0.96	0.09	45,52,70,76	0
25	PHO	a	2112	64/64	0.97	0.06	36,46,54,56	0
26	BCR	A	410	40/40	0.97	0.06	37,45,50,52	0
24	CLA	D	401	65/65	0.97	0.06	33,39,49,59	0
24	CLA	D	404	65/65	0.97	0.06	31,38,59,65	0
24	CLA	b	611	65/65	0.97	0.07	42,49,57,63	0
24	CLA	B	616	65/65	0.97	0.08	39,50,70,78	0
24	CLA	a	2109	65/65	0.97	0.07	33,40,51,74	0
24	CLA	b	614	65/65	0.97	0.07	34,44,61,64	0
24	CLA	B	612	65/65	0.97	0.07	35,44,57,68	0
24	CLA	c	512	65/65	0.97	0.08	42,52,62,74	0
34	DMS	D	418	4/4	0.97	0.11	77,82,88,90	0
24	CLA	B	613	65/65	0.97	0.06	34,43,50,53	0
34	DMS	c	529	4/4	0.97	0.15	57,60,62,63	0

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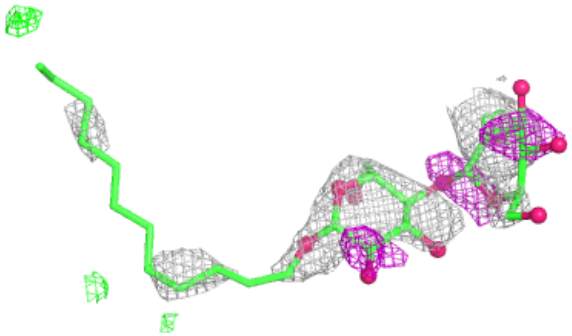
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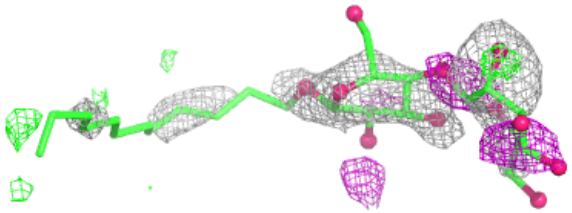
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	605	65/65	0.97	0.08	31,42,75,81	0
39	LHG	L	101	49/49	0.97	0.08	44,51,68,70	0
24	CLA	b	605	65/65	0.97	0.07	40,51,62,65	0
24	CLA	d	401	65/65	0.97	0.06	34,39,47,55	0
24	CLA	d	404	65/65	0.97	0.07	31,41,59,71	0
24	CLA	b	606	65/65	0.97	0.07	38,48,60,64	0
24	CLA	b	607	65/65	0.97	0.08	34,44,84,89	0
40	HEM	e	103	43/43	0.97	0.09	52,63,90,105	0
24	CLA	B	609	65/65	0.97	0.06	40,48,58,61	0
25	PHO	a	2111	64/64	0.97	0.06	33,41,47,55	0
35	CA	o	2602	1/1	0.98	0.04	71,71,71,71	0
34	DMS	b	632	4/4	0.98	0.07	47,48,54,58	0
24	CLA	A	405	65/65	0.98	0.06	30,38,50,72	0
34	DMS	C	532	4/4	0.98	0.07	62,63,63,67	0
32	K2I	A	419	10/10	0.98	0.09	43,52,58,64	10
34	DMS	A	422	4/4	0.98	0.08	45,48,53,55	0
32	K2I	a	2119	10/10	0.98	0.08	48,57,64,73	10
34	DMS	B	639	4/4	0.98	0.08	42,46,47,58	0
40	HEM	F	102	43/43	0.98	0.07	52,62,73,90	0
35	CA	B	601	1/1	0.98	0.05	64,64,64,64	0
35	CA	O	301	1/1	0.98	0.04	72,72,72,72	0
35	CA	b	603	1/1	0.98	0.04	72,72,72,72	0
42	MG	J	101	1/1	0.98	0.09	53,53,53,53	0
43	HEC	V	201	43/43	0.98	0.06	37,45,50,53	0
43	HEC	v	201	43/43	0.98	0.07	45,55,61,64	0
23	CL	A	404	1/1	0.99	0.03	41,41,41,41	0
23	CL	a	2106	1/1	0.99	0.07	47,47,47,47	0
34	DMS	a	2121	4/4	0.99	0.06	42,48,52,52	0
23	CL	a	2107	1/1	0.99	0.04	46,46,46,46	0
21	OEX	A	401	10/10	0.99	0.03	39,42,46,48	0
42	MG	j	1603	1/1	0.99	0.08	57,57,57,57	0
23	CL	A	403	1/1	0.99	0.08	42,42,42,42	0
35	CA	c	502	1/1	0.99	0.05	66,66,66,66	0
22	FE2	a	2105	1/1	1.00	0.02	47,47,47,47	0
21	OEX	a	2104	10/10	1.00	0.02	38,43,49,52	0
22	FE2	A	402	1/1	1.00	0.01	48,48,48,48	0

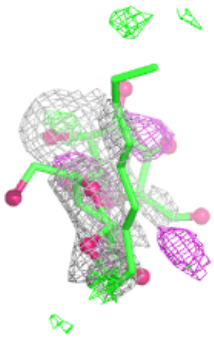
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 420:

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

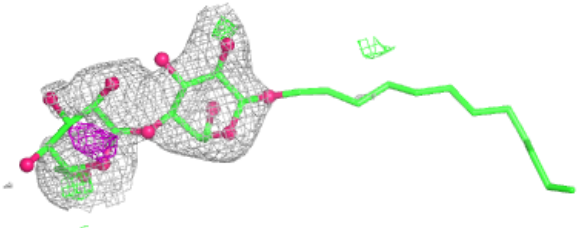


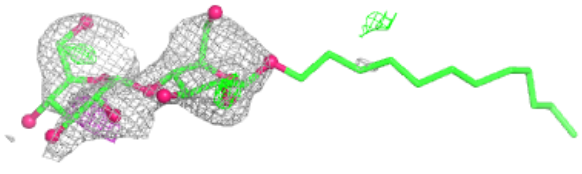


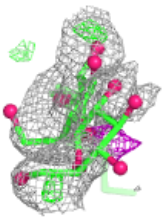


Electron density around LMT a 2120:

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

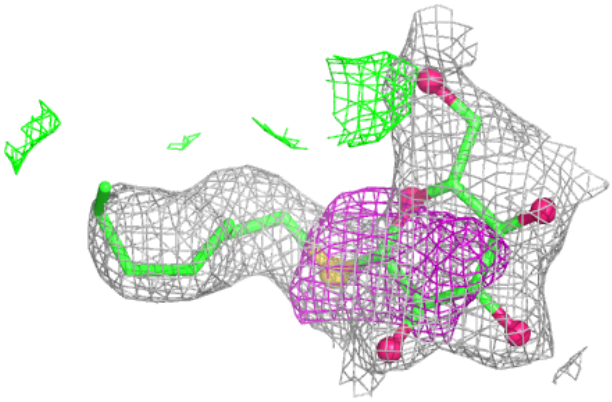


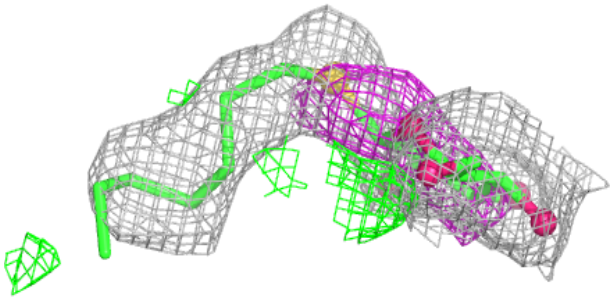


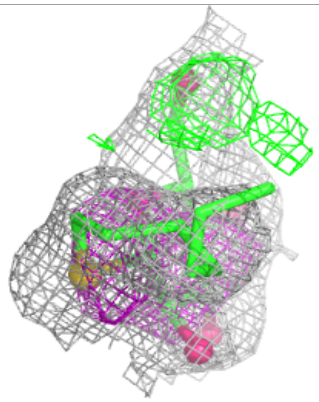


Electron density around HTG B 625 (A):

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

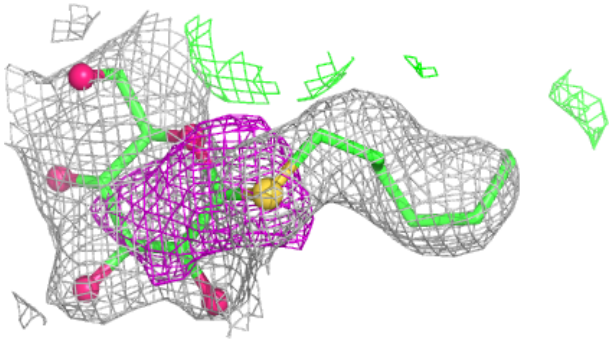


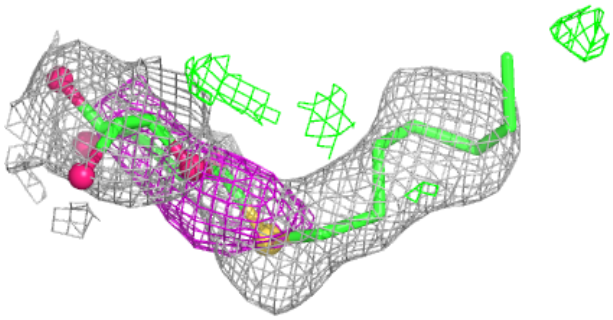


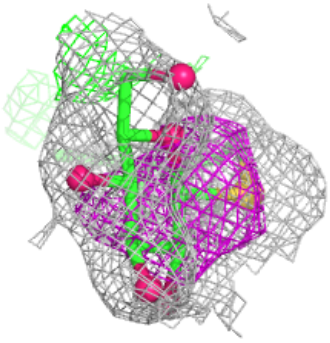


Electron density around HTG B 625 (B):

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

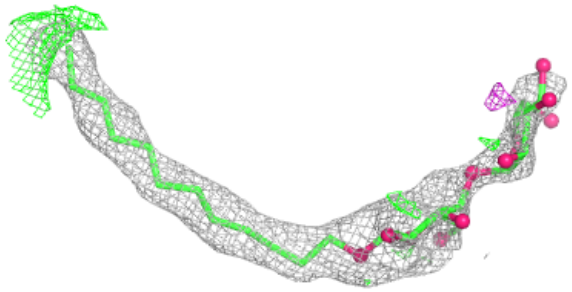


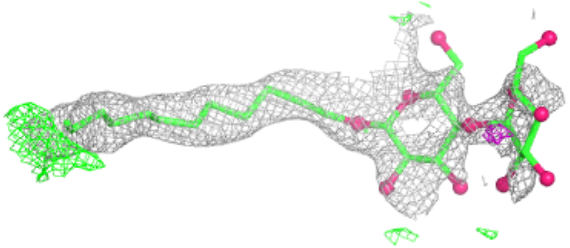




Electron density around LMT B 636:

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

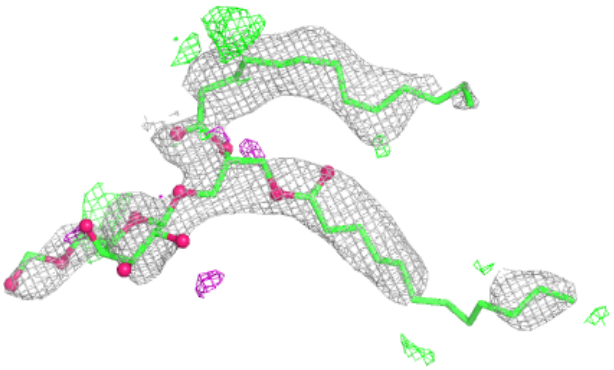


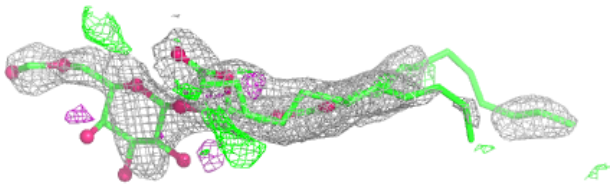


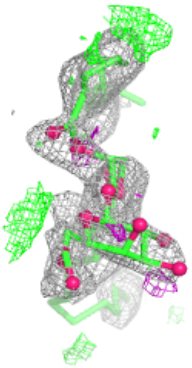


Electron density around DGD D 408:

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

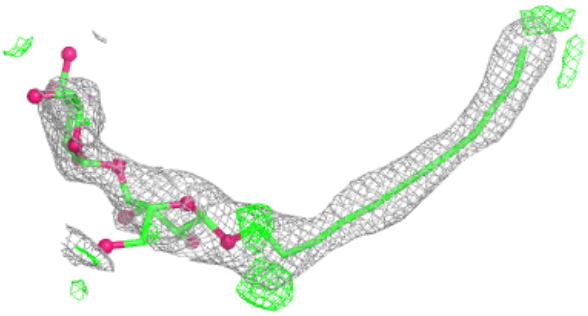


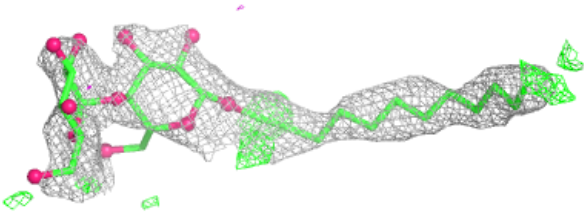


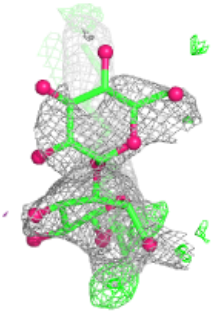


Electron density around LMT m 103:

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

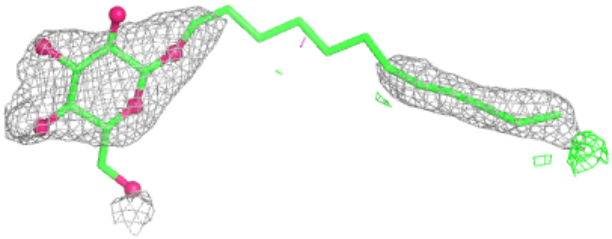


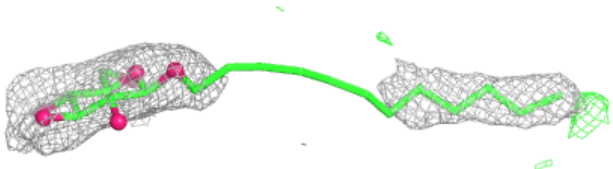


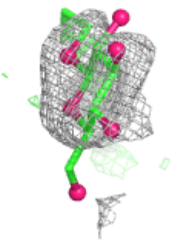


Electron density around LMT f 101:

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

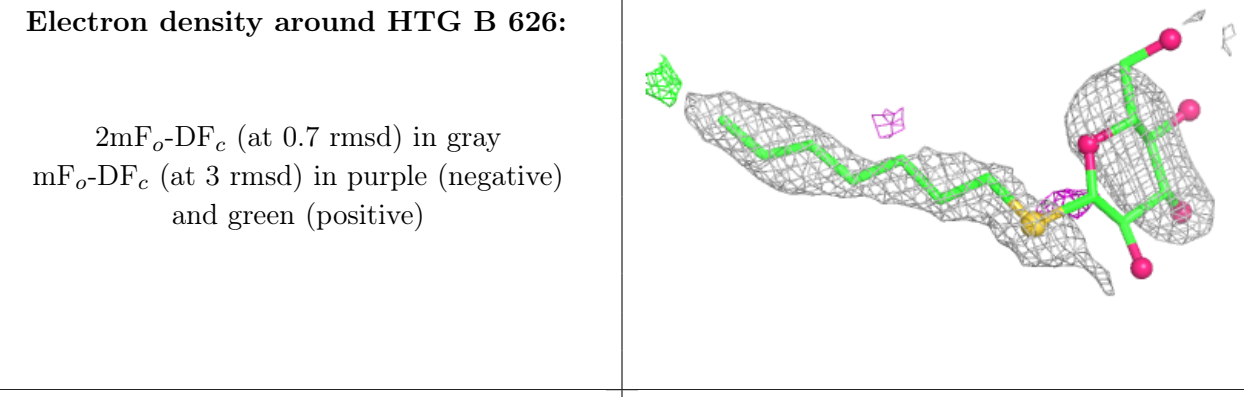






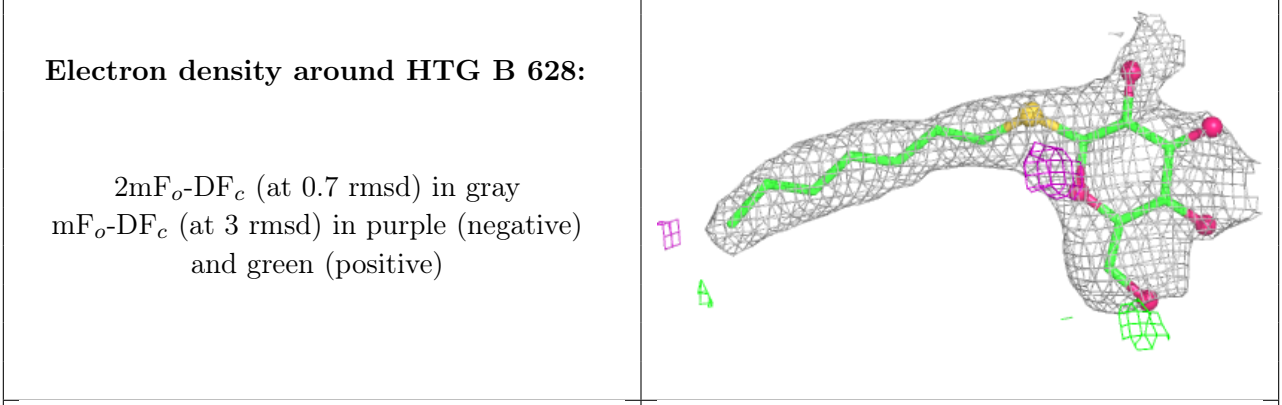
Electron density around HTG B 626:

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



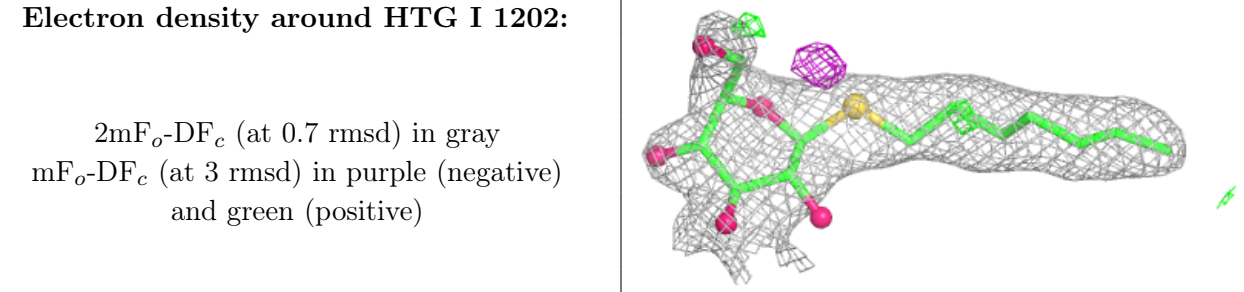
Electron density around HTG B 628:

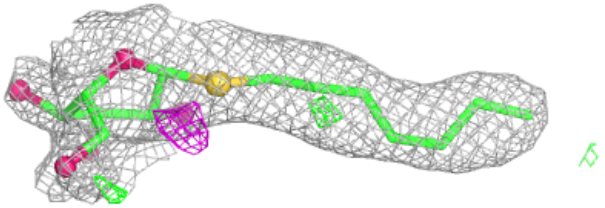
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

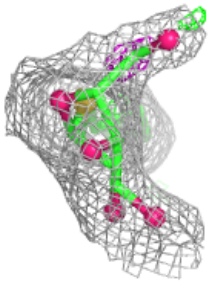


Electron density around HTG I 1202:

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

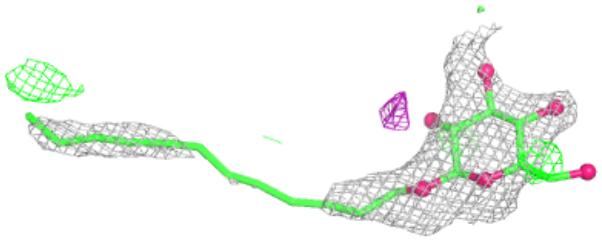


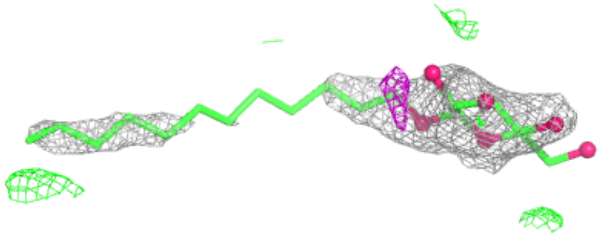


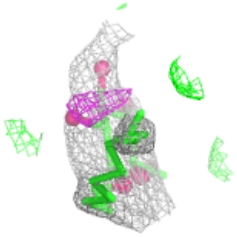


Electron density around LMT E 105:

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

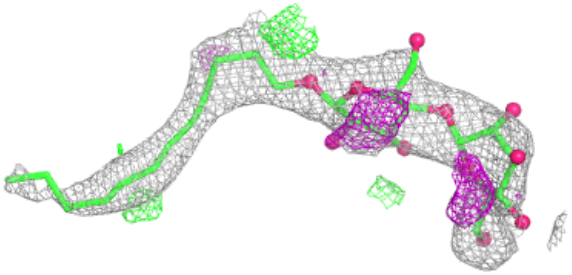


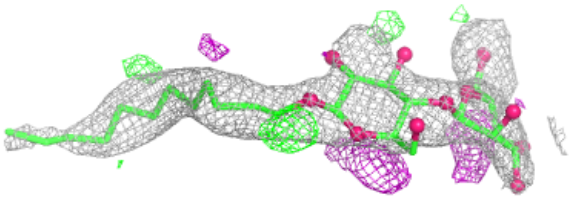


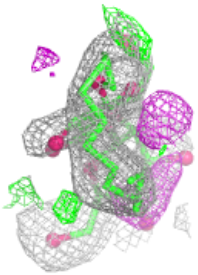


Electron density around LMT a 2103:

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

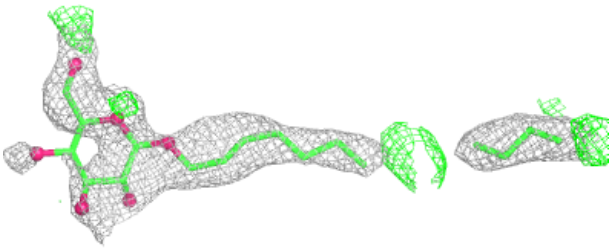


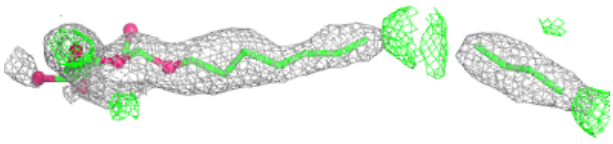


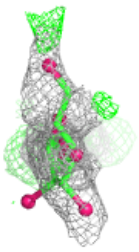


Electron density around LMT j 1601:

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

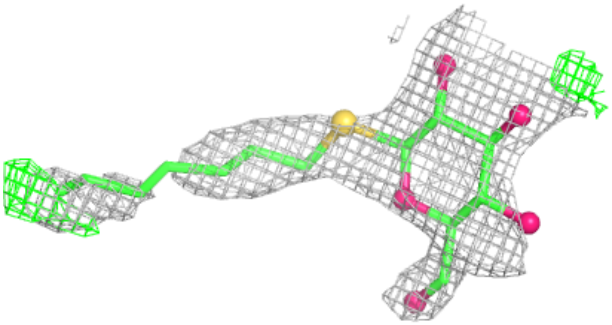


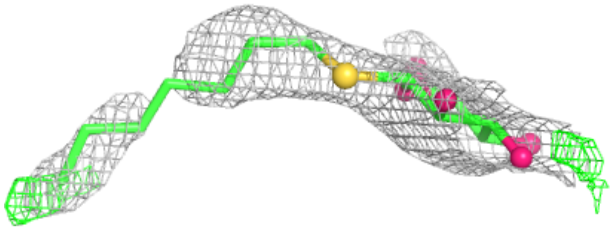


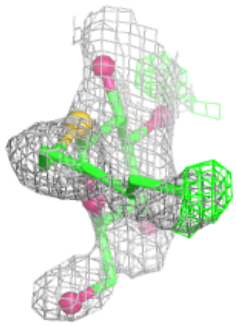


Electron density around HTG d 414:

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

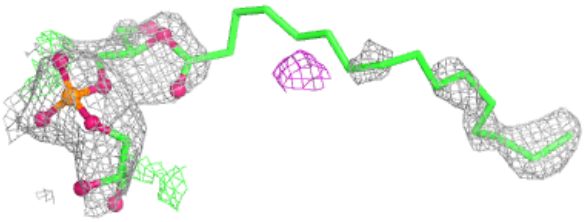


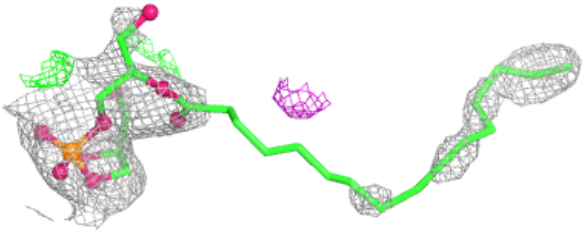


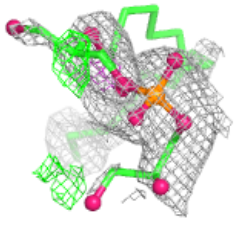


Electron density around LHG e 101:

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

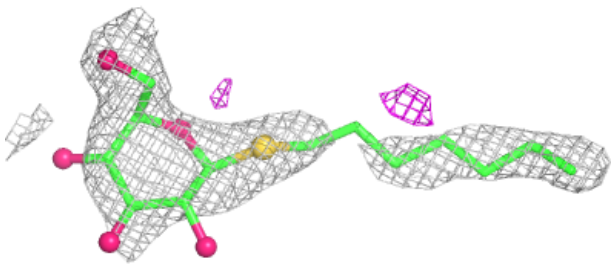


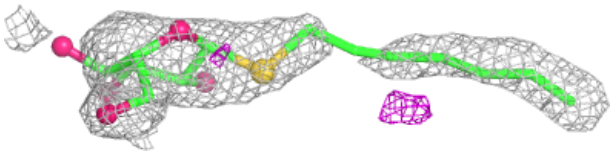


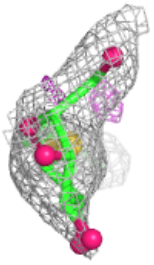


Electron density around HTG C 522:

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

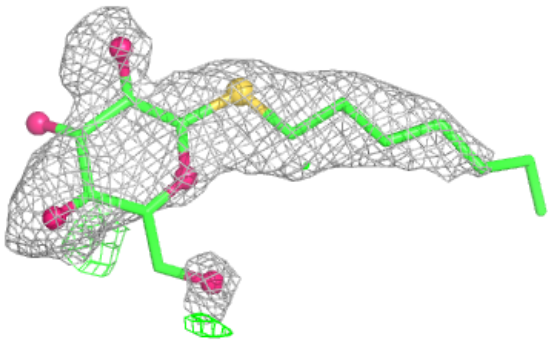


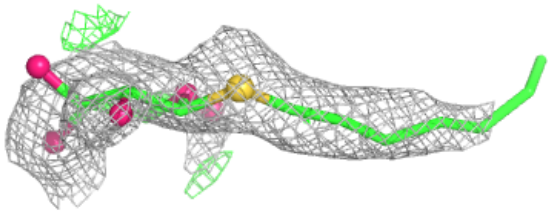


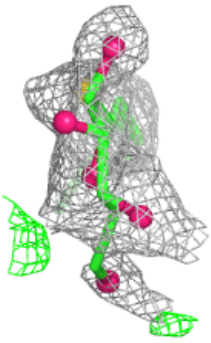


Electron density around HTG D 413:

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

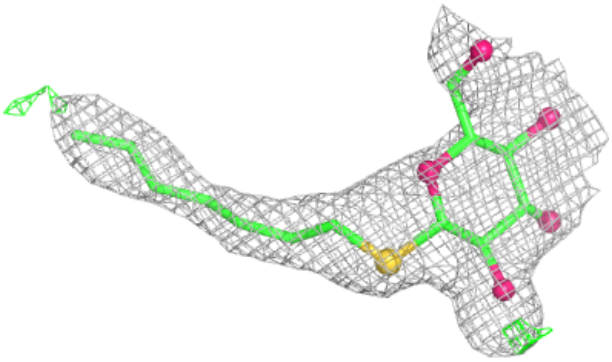


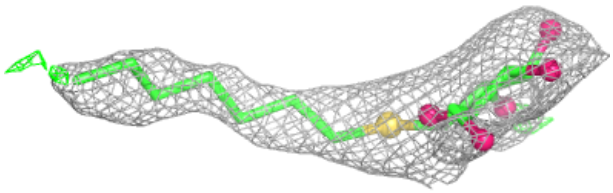


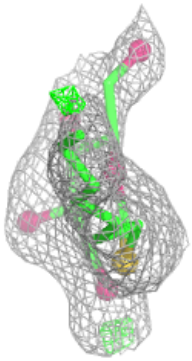


Electron density around HTG b 626:

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

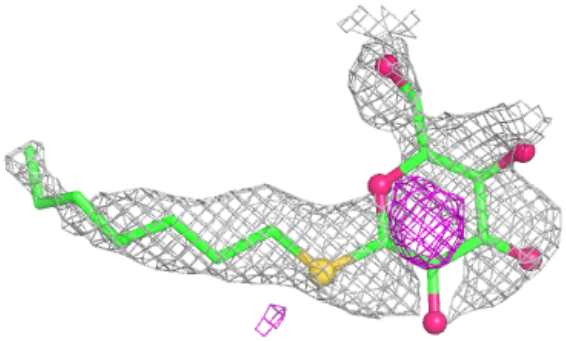


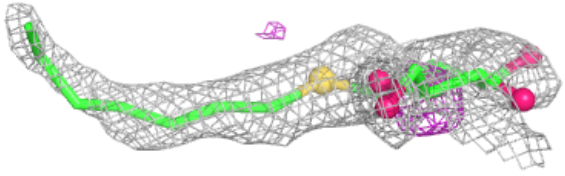


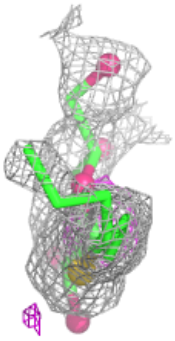


Electron density around HTG d 403:

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

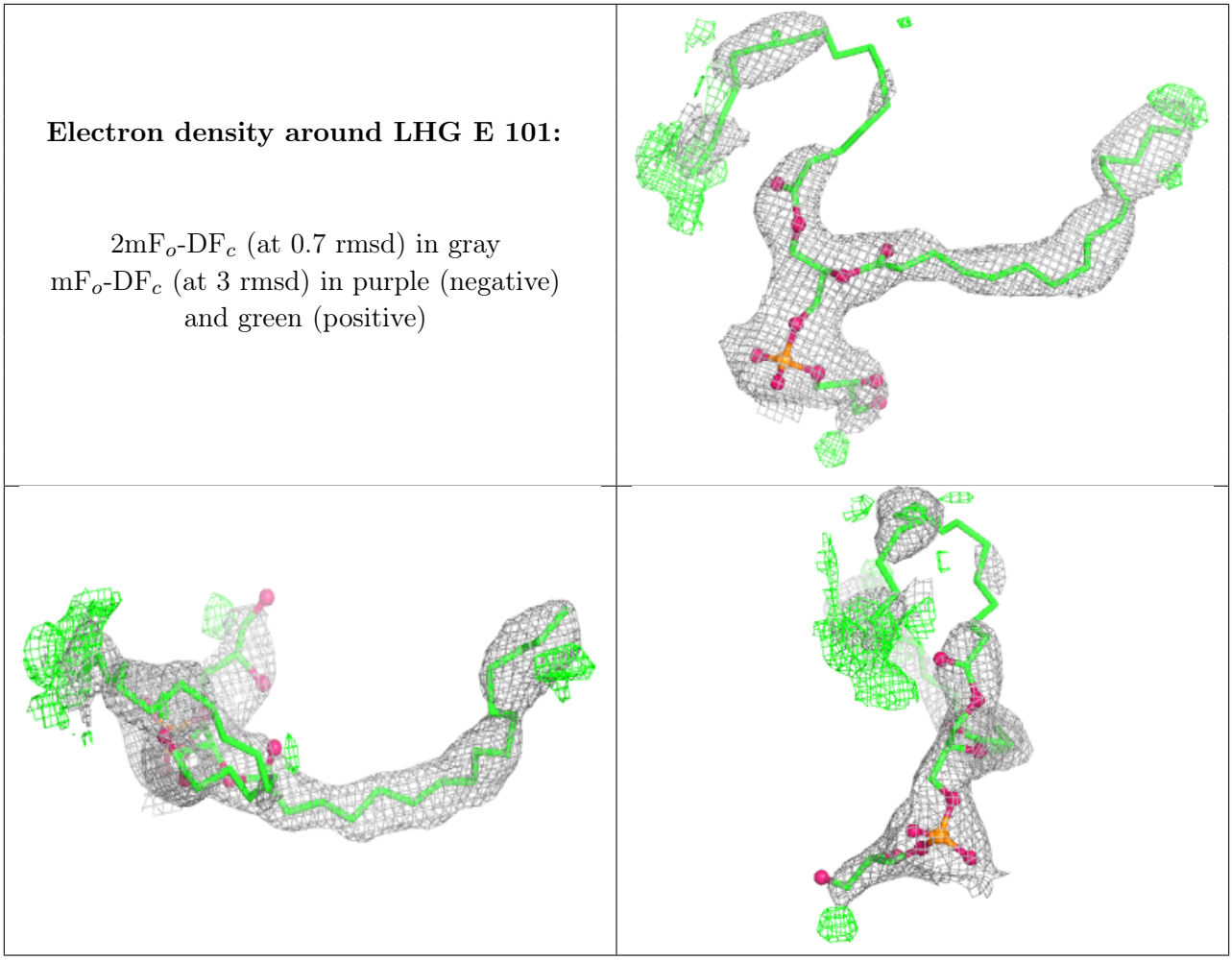






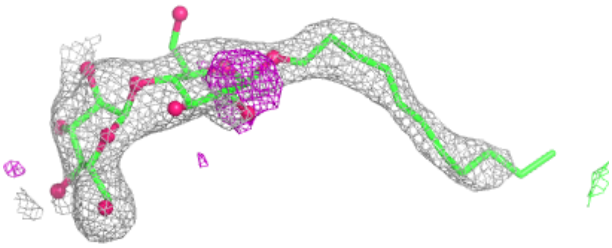
Electron density around LHG E 101:

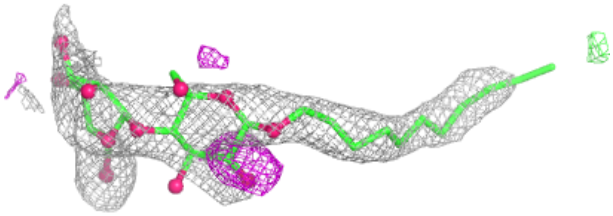
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

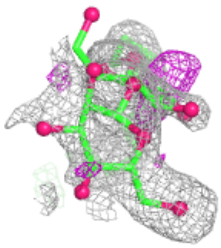


Electron density around LMT A 414:

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

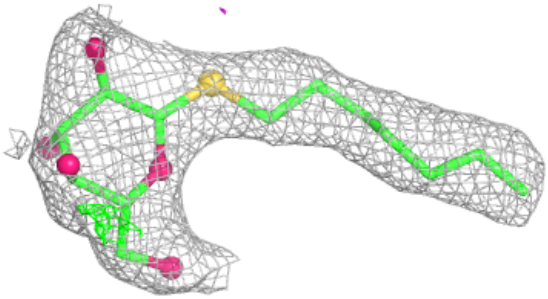


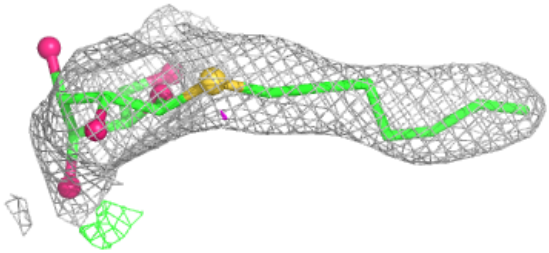


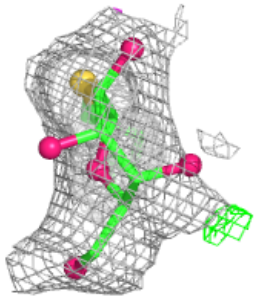


Electron density around HTG i 103:

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

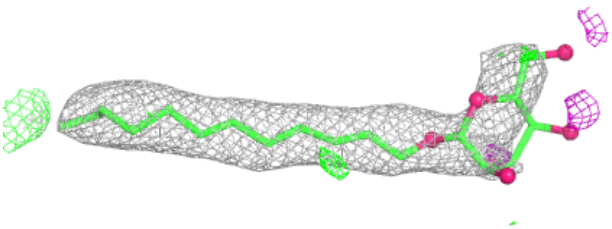


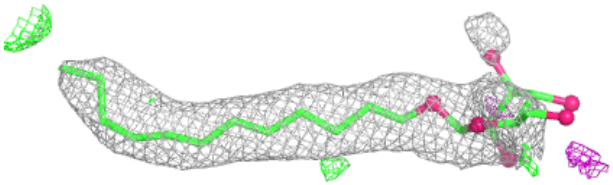


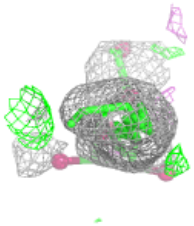


Electron density around LMT I 1201:

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

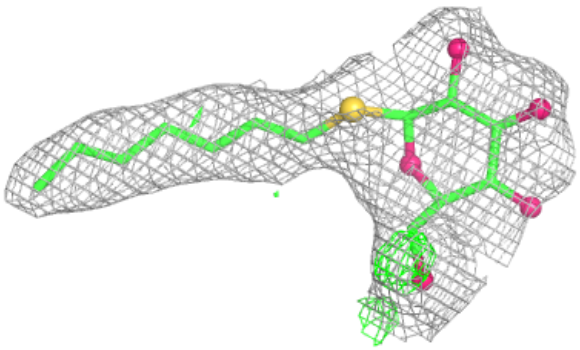


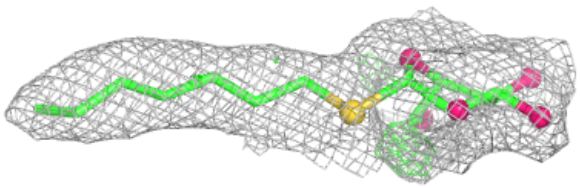


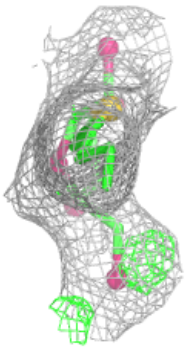


Electron density around HTG b 602:

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

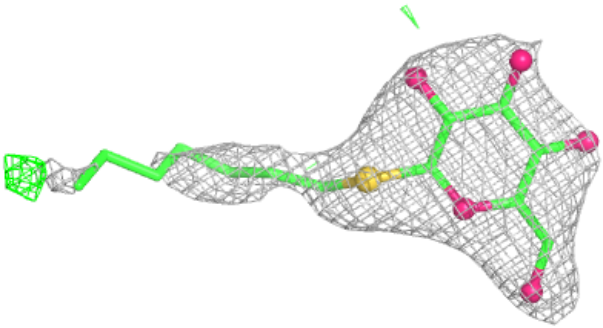


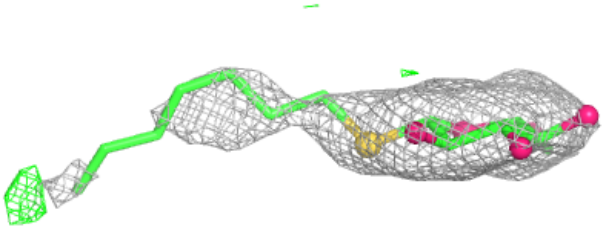


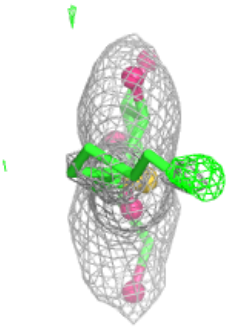


Electron density around HTG c 523:

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

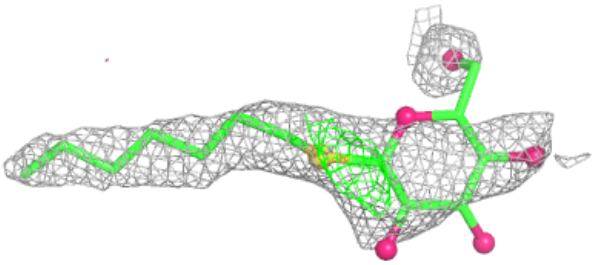


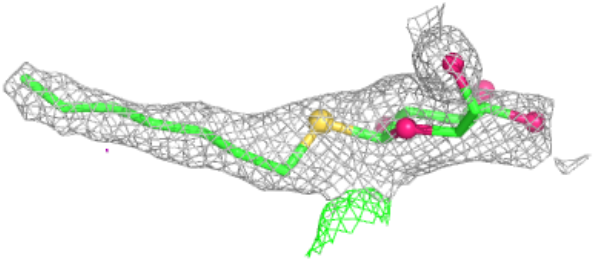


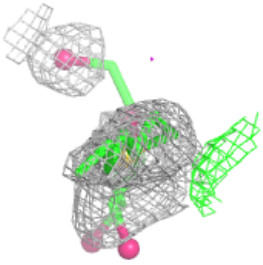


Electron density around HTG c 524:

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

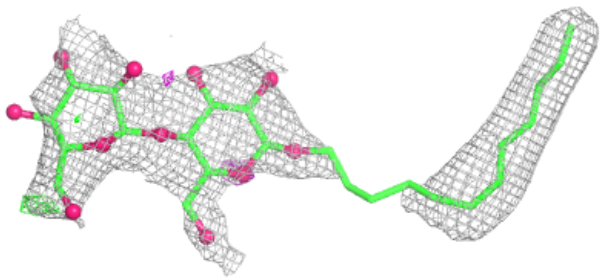


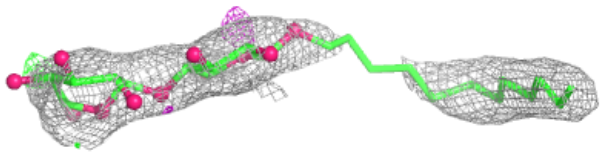


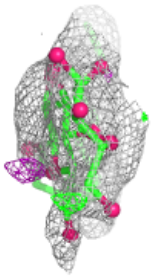


Electron density around LMT Z 101:

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

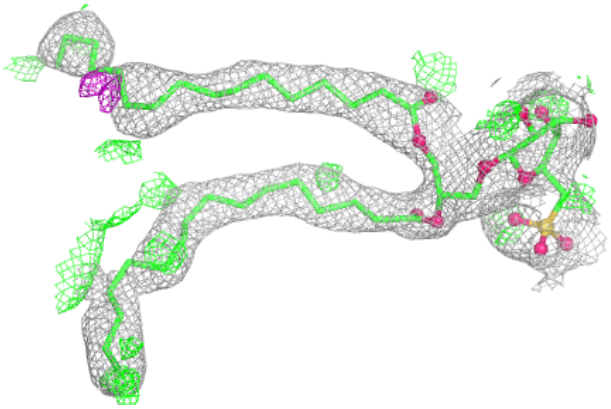


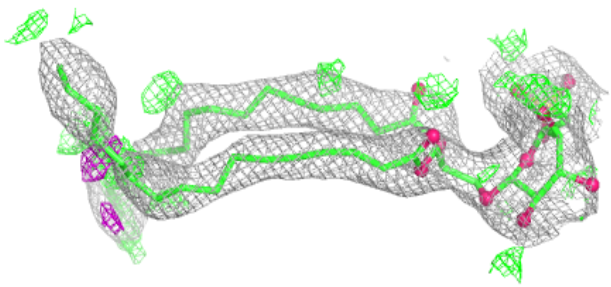


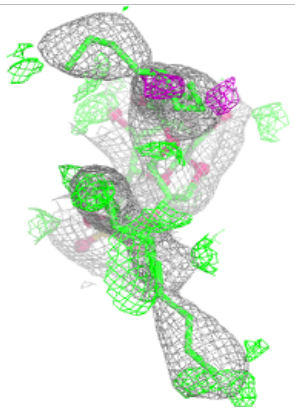


Electron density around SQD L 102:

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

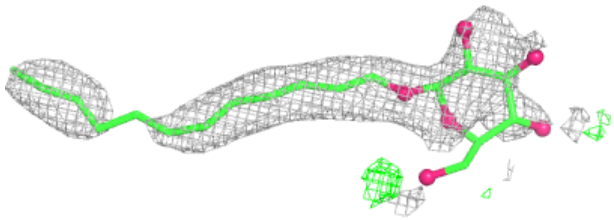


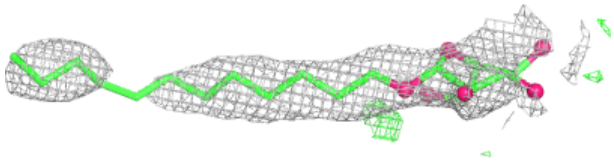


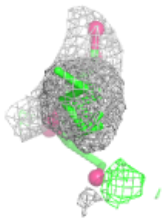


Electron density around LMT J 102:

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

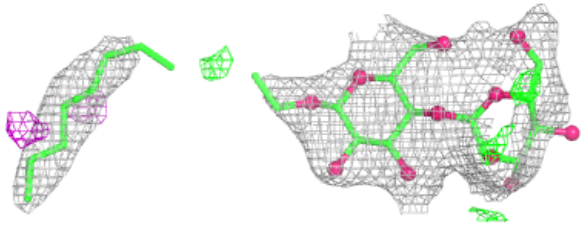


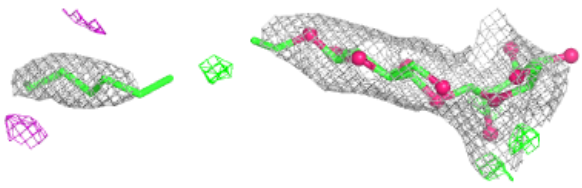


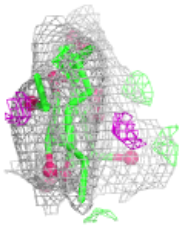


Electron density around LMT z 1801:

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

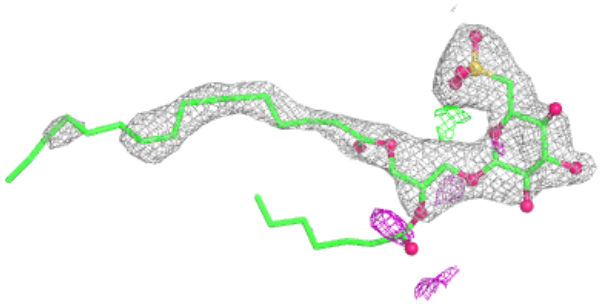


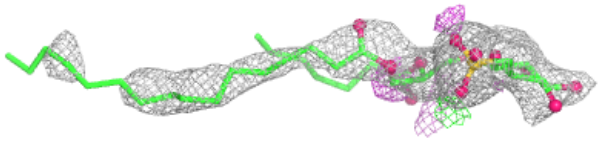


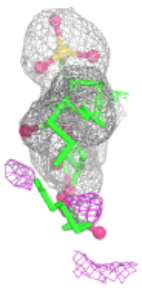


Electron density around SQD F 101:

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

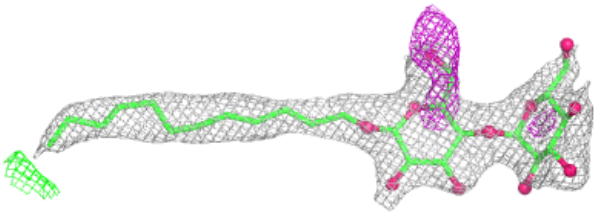


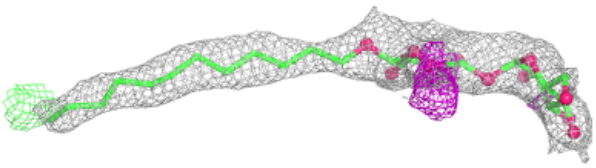




Electron density around LMT m 102:

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

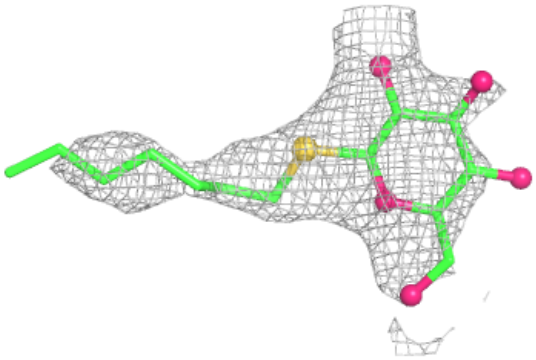


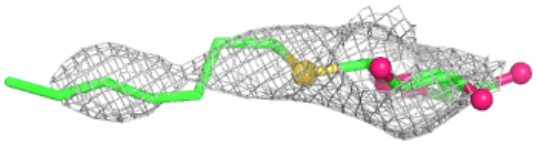


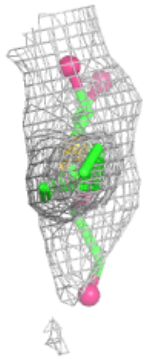


Electron density around HTG c 526:

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

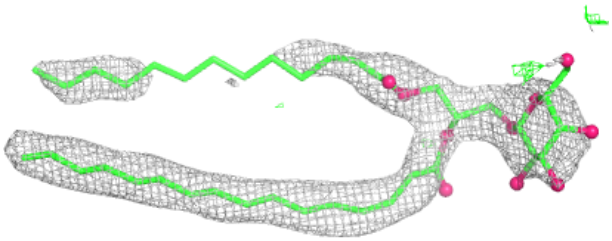


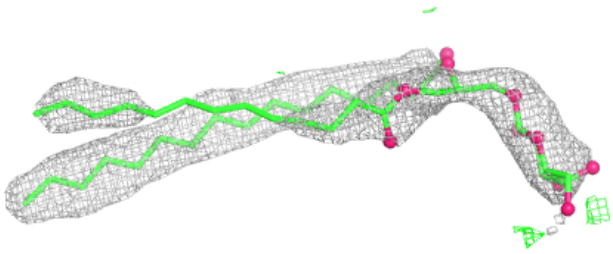


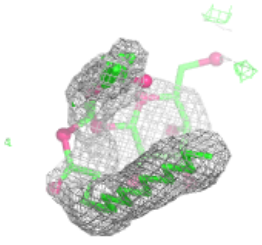


Electron density around LMG C 526:

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

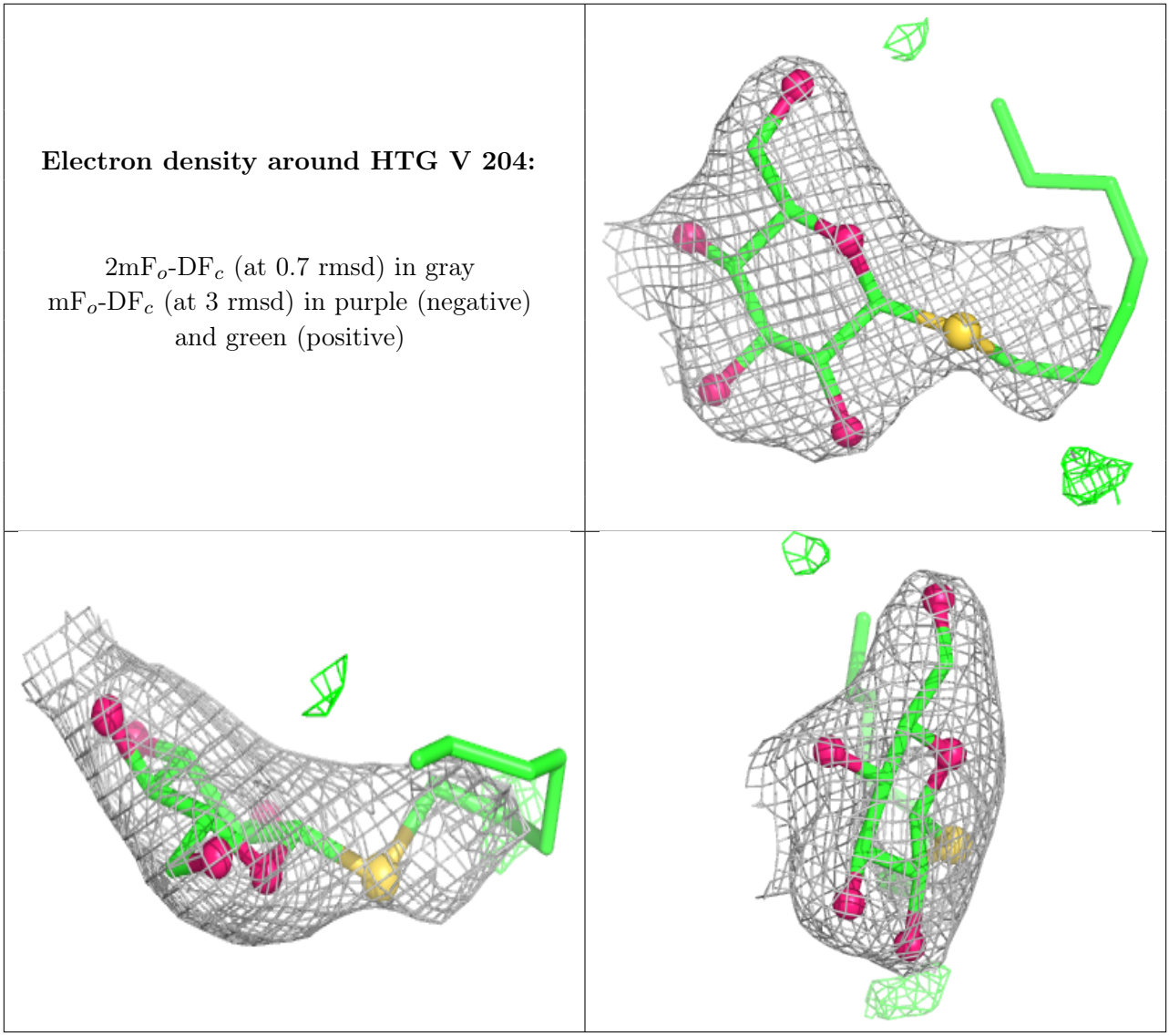






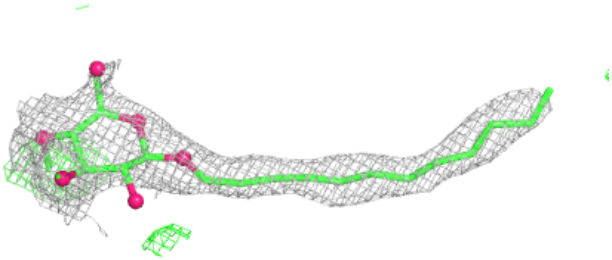
Electron density around HTG V 204:

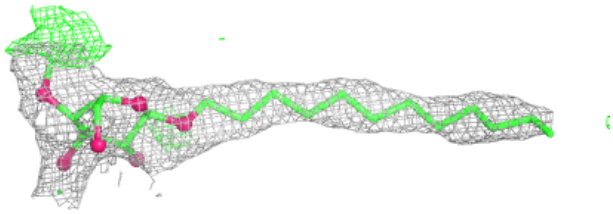
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

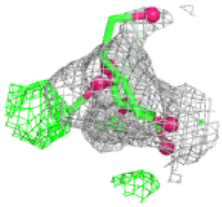


Electron density around LMT b 624:

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

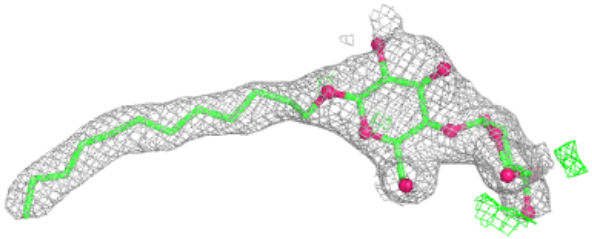


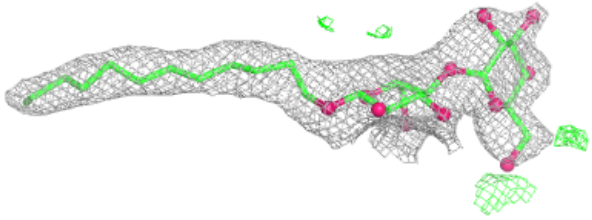


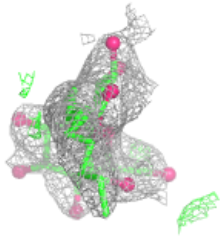


Electron density around LMT B 623:

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

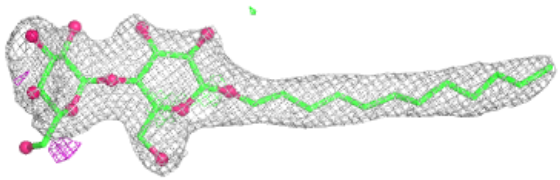


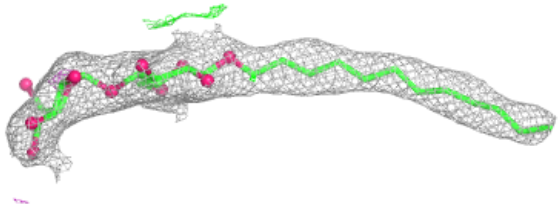


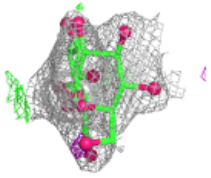


Electron density around LMT M 101:

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

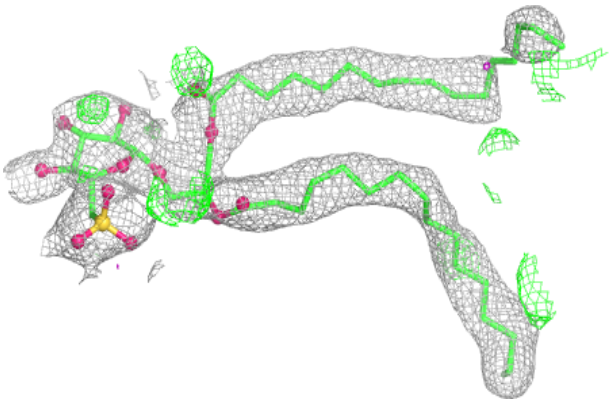


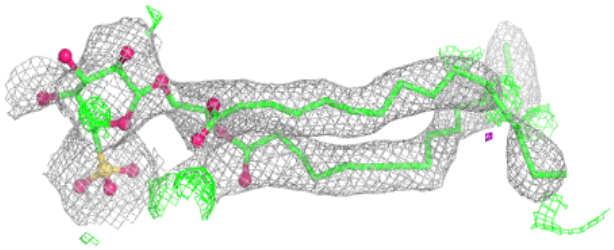


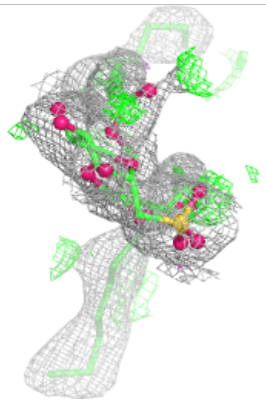


Electron density around SQD B 621:

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

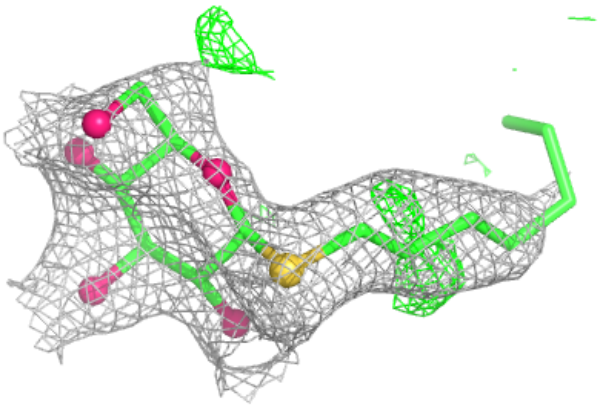


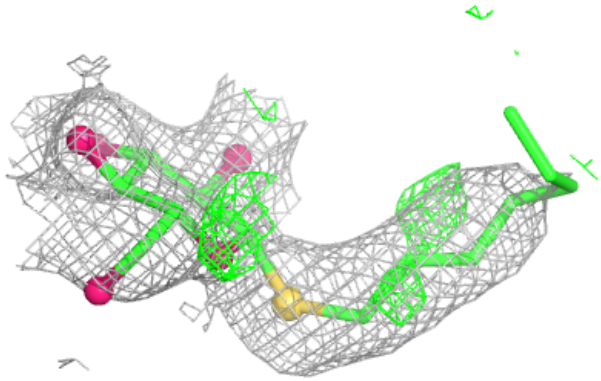


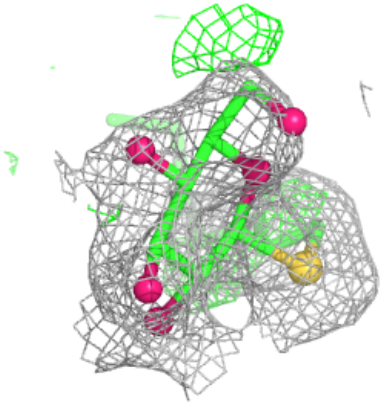


Electron density around HTG b 625:

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

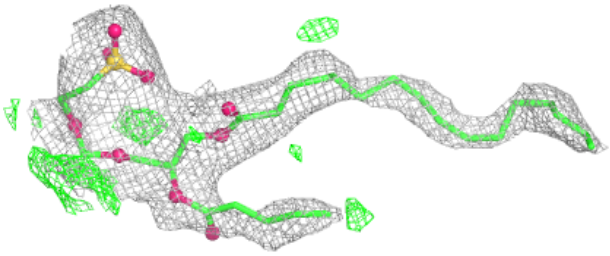


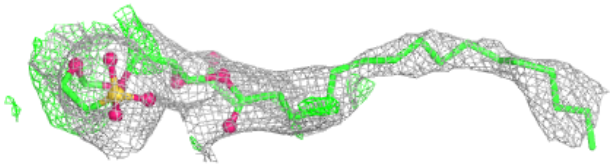


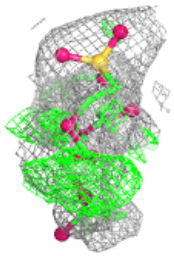


Electron density around SQD f 102:

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

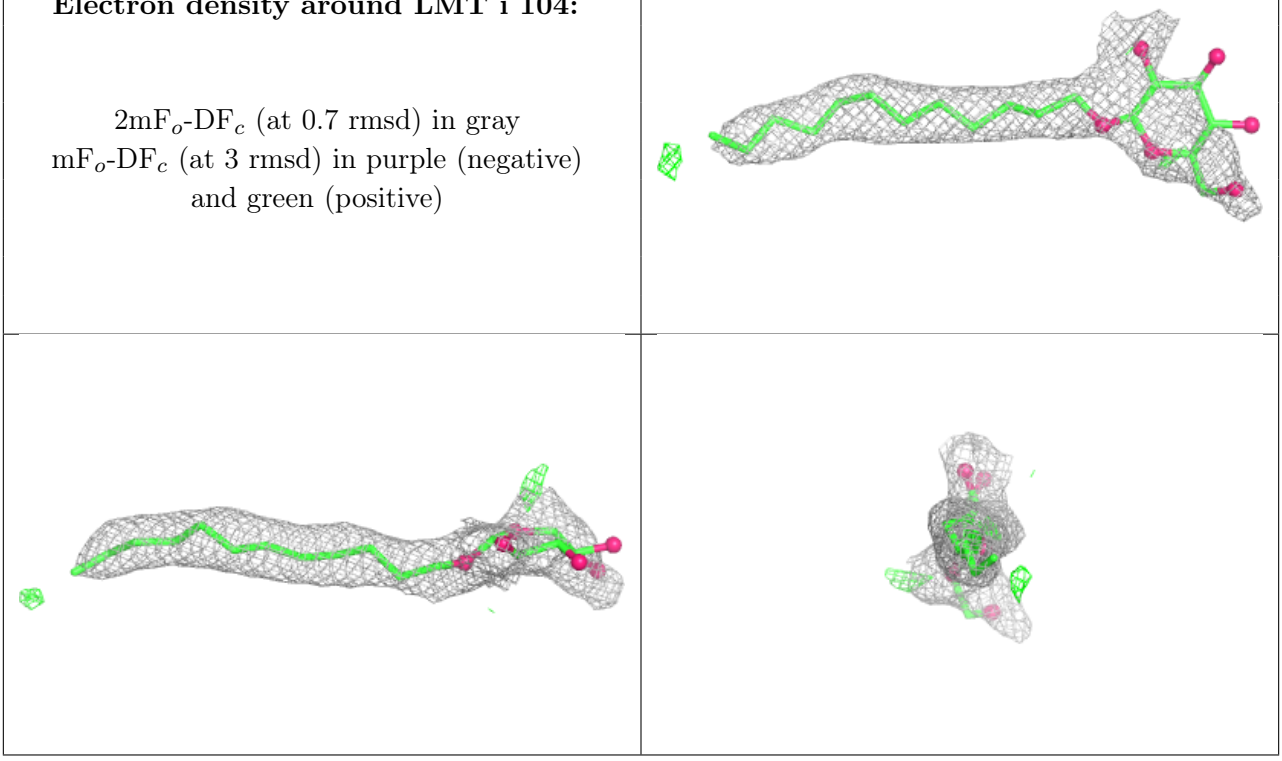






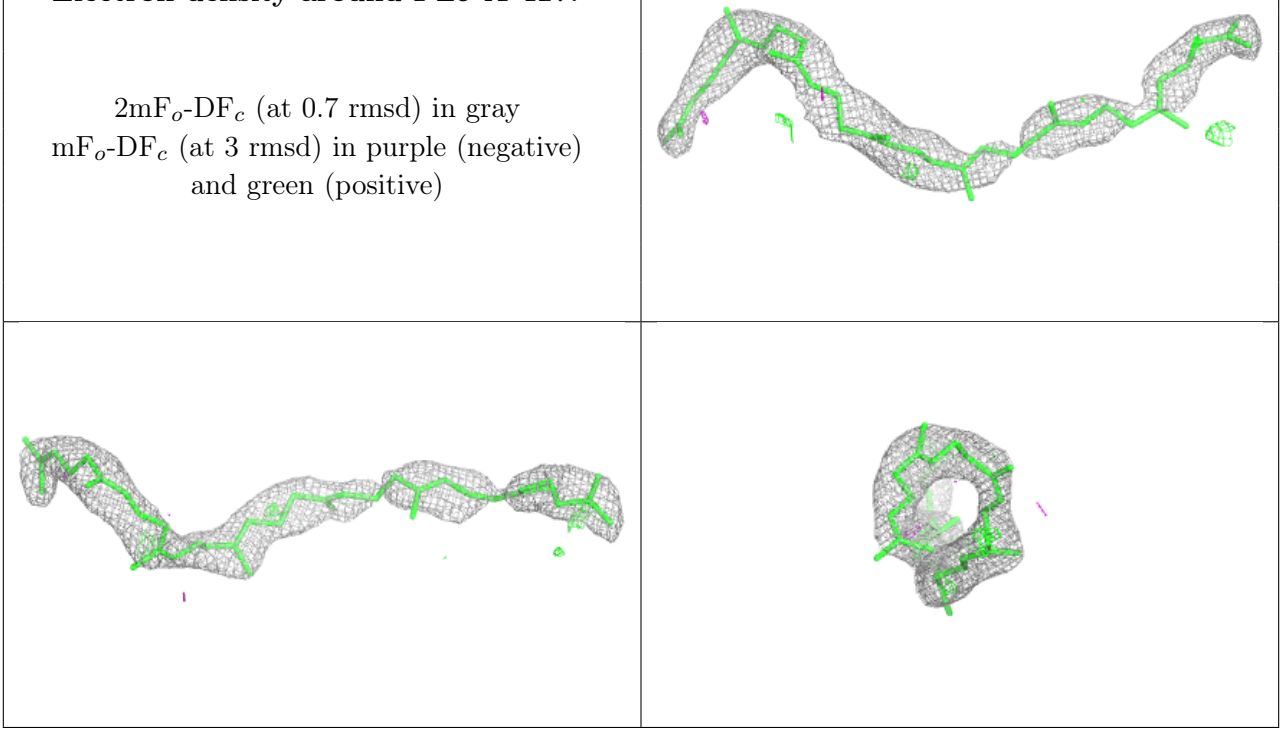
Electron density around LMT i 104:

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



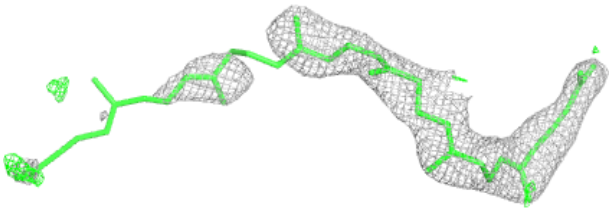
Electron density around PL9 A 417:

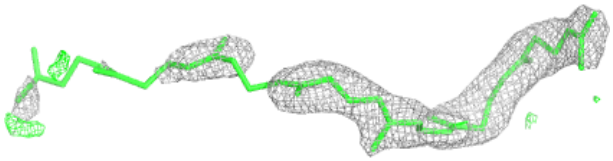
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

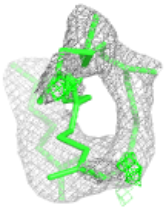


Electron density around PL9 x 801:

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

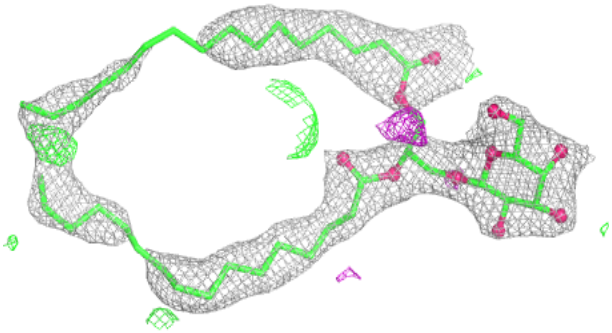


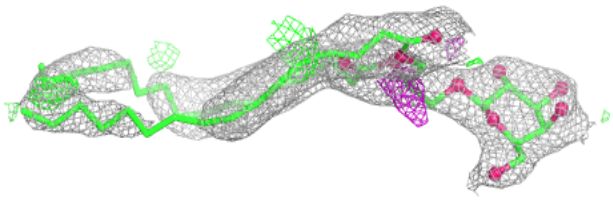


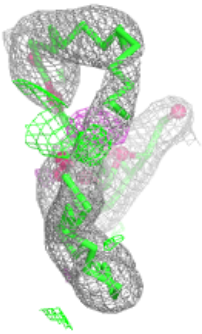


Electron density around LMG i 101:

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

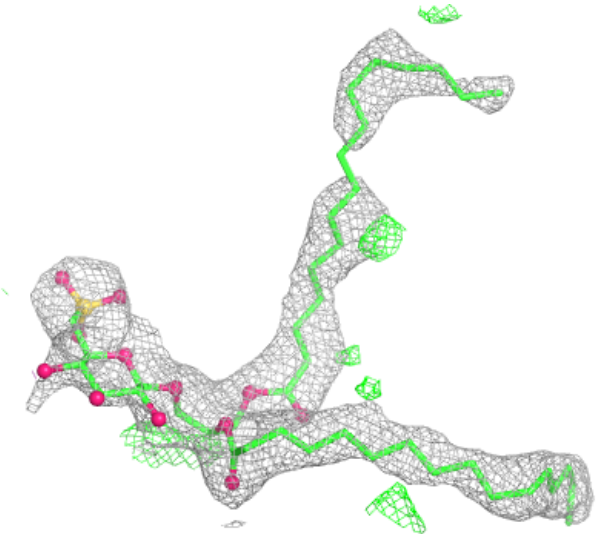


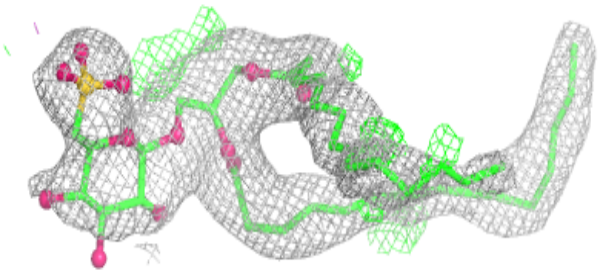


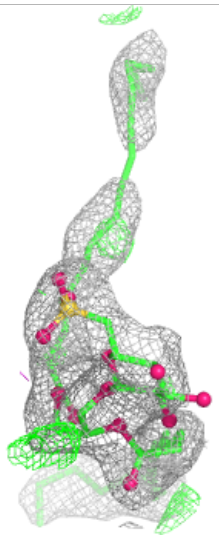


Electron density around SQD A 413:

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

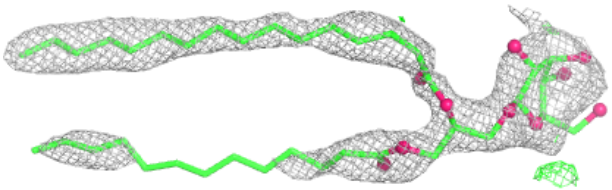


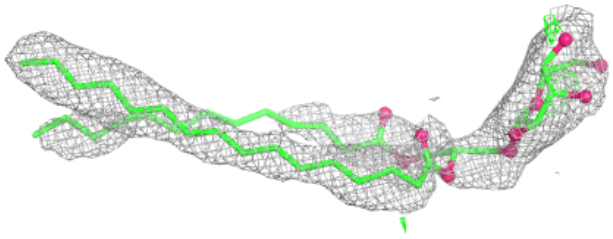


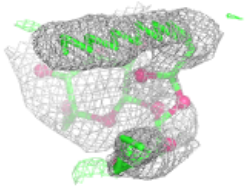


Electron density around LMG c 522:

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

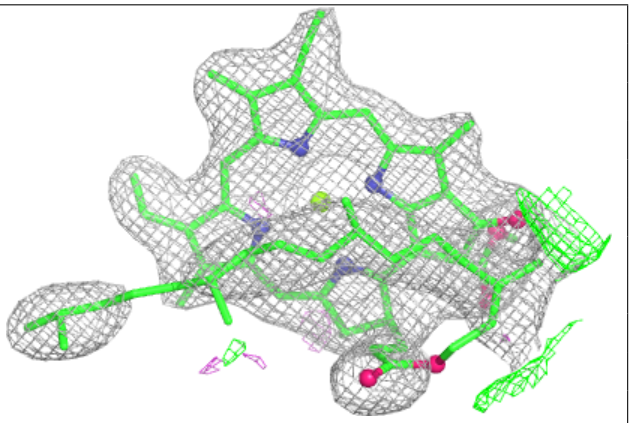


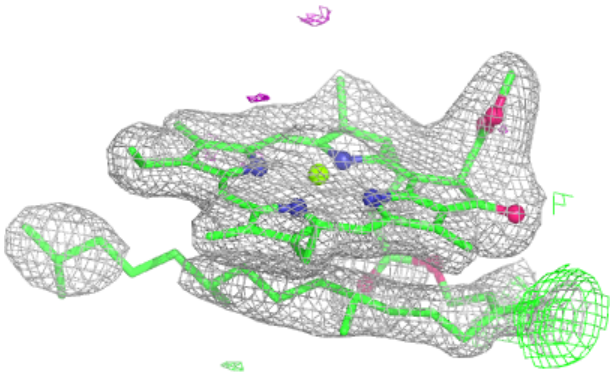


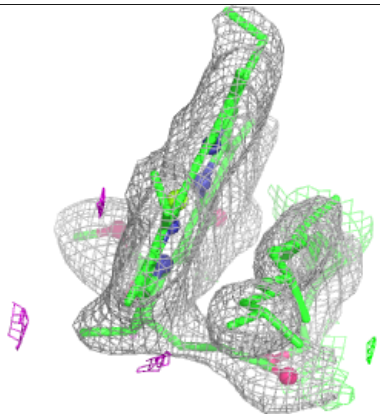


Electron density around CLA B 602:

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

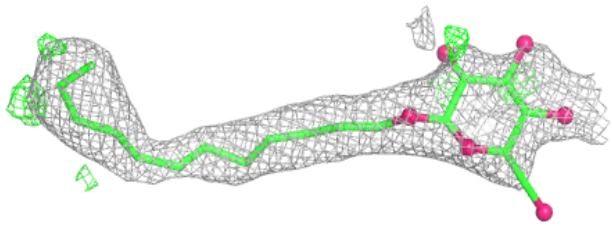


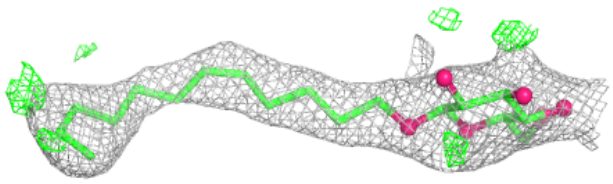


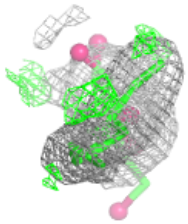


Electron density around LMT B 637:

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

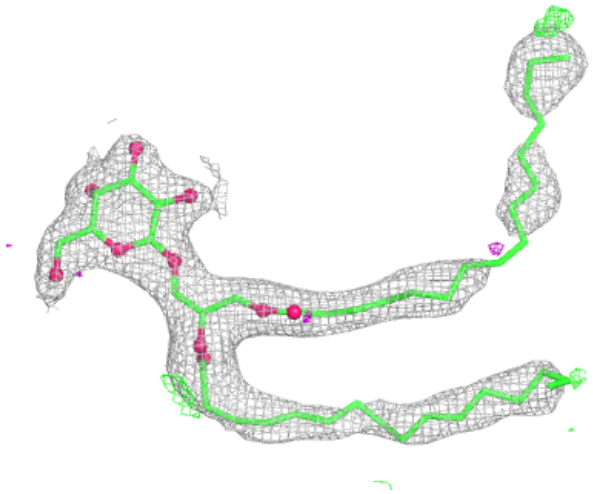


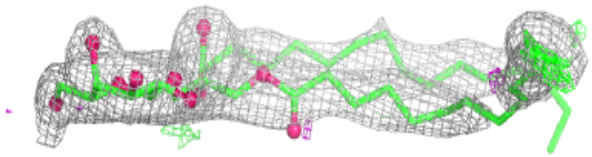


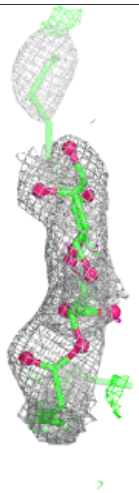


Electron density around LMG C 520:

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

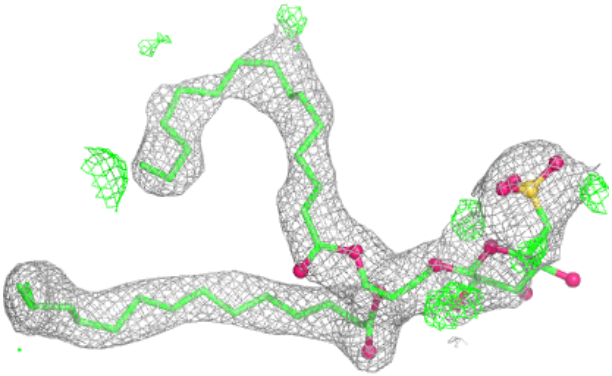


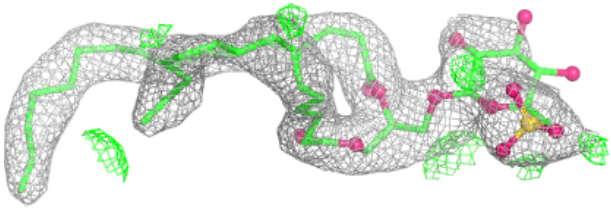


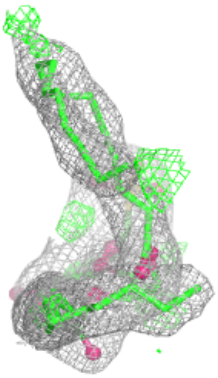


Electron density around SQD a 2102:

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

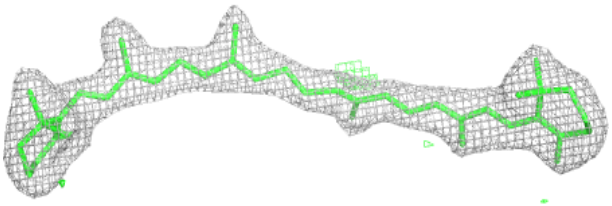


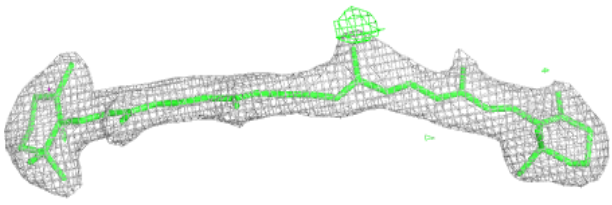


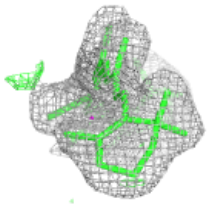


Electron density around BCR t 102:

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

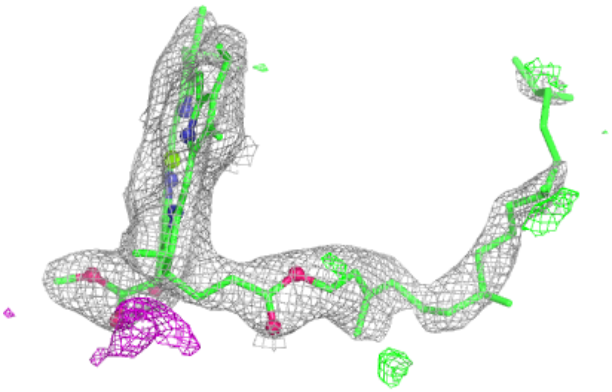


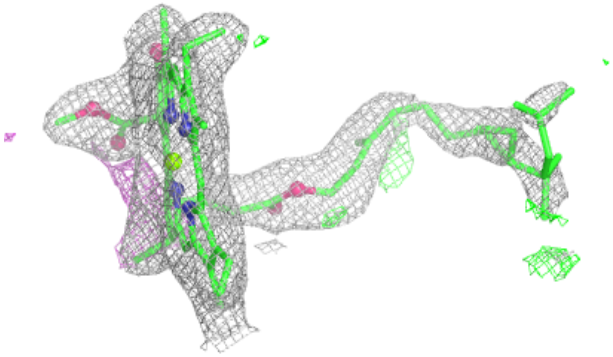


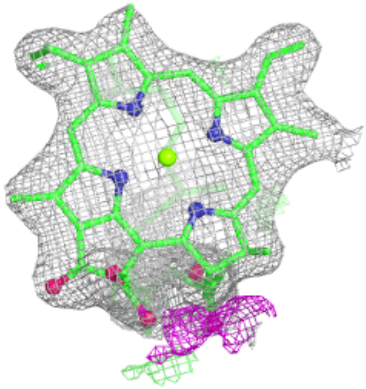


Electron density around CLA C 507:

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

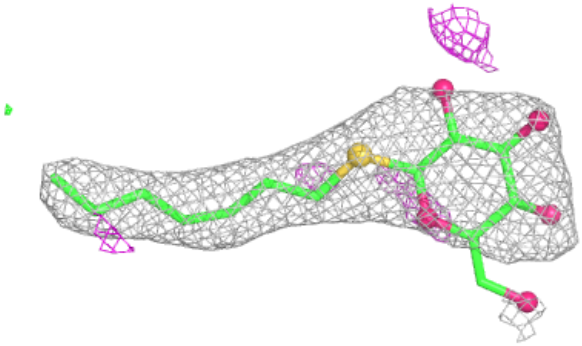


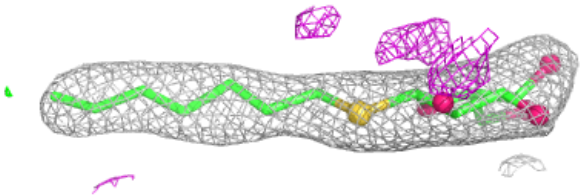


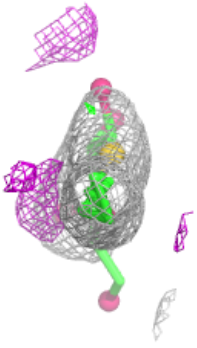


Electron density around HTG B 627:

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

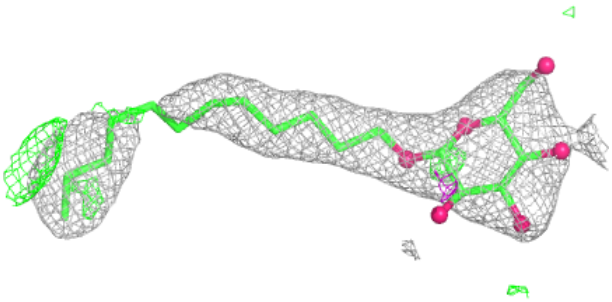


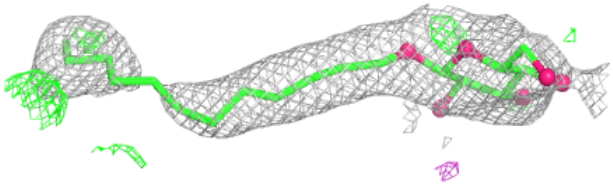


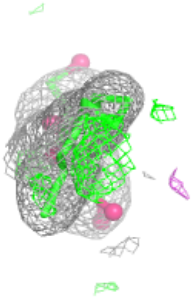


Electron density around LMT T 102:

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

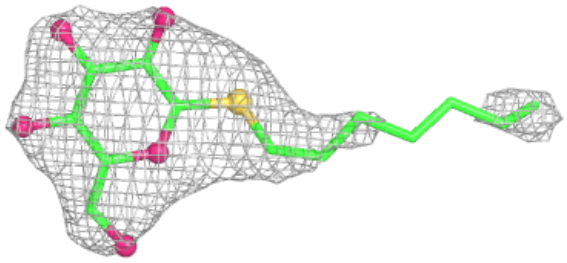


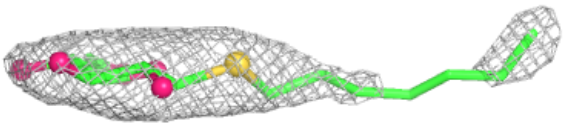


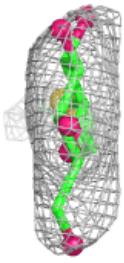


Electron density around HTG C 521:

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

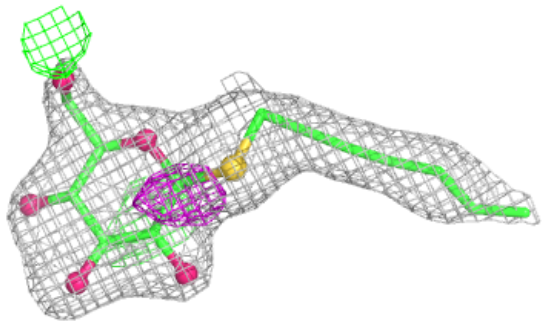


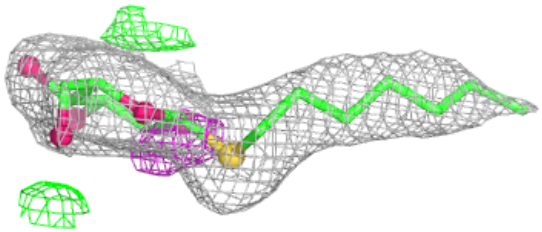


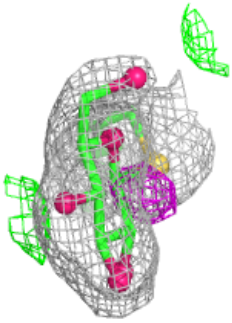


Electron density around HTG B 624:

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

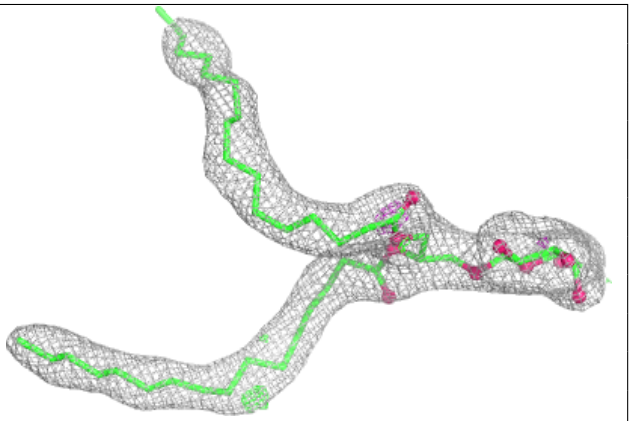


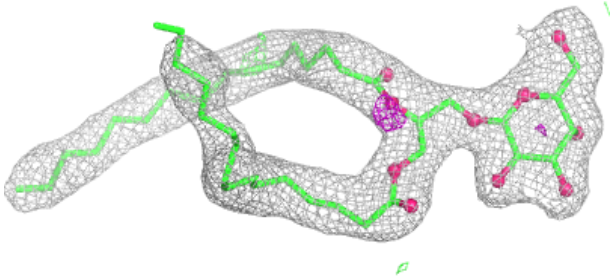


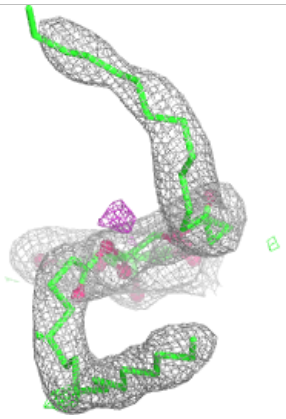


Electron density around LMG B 622:

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

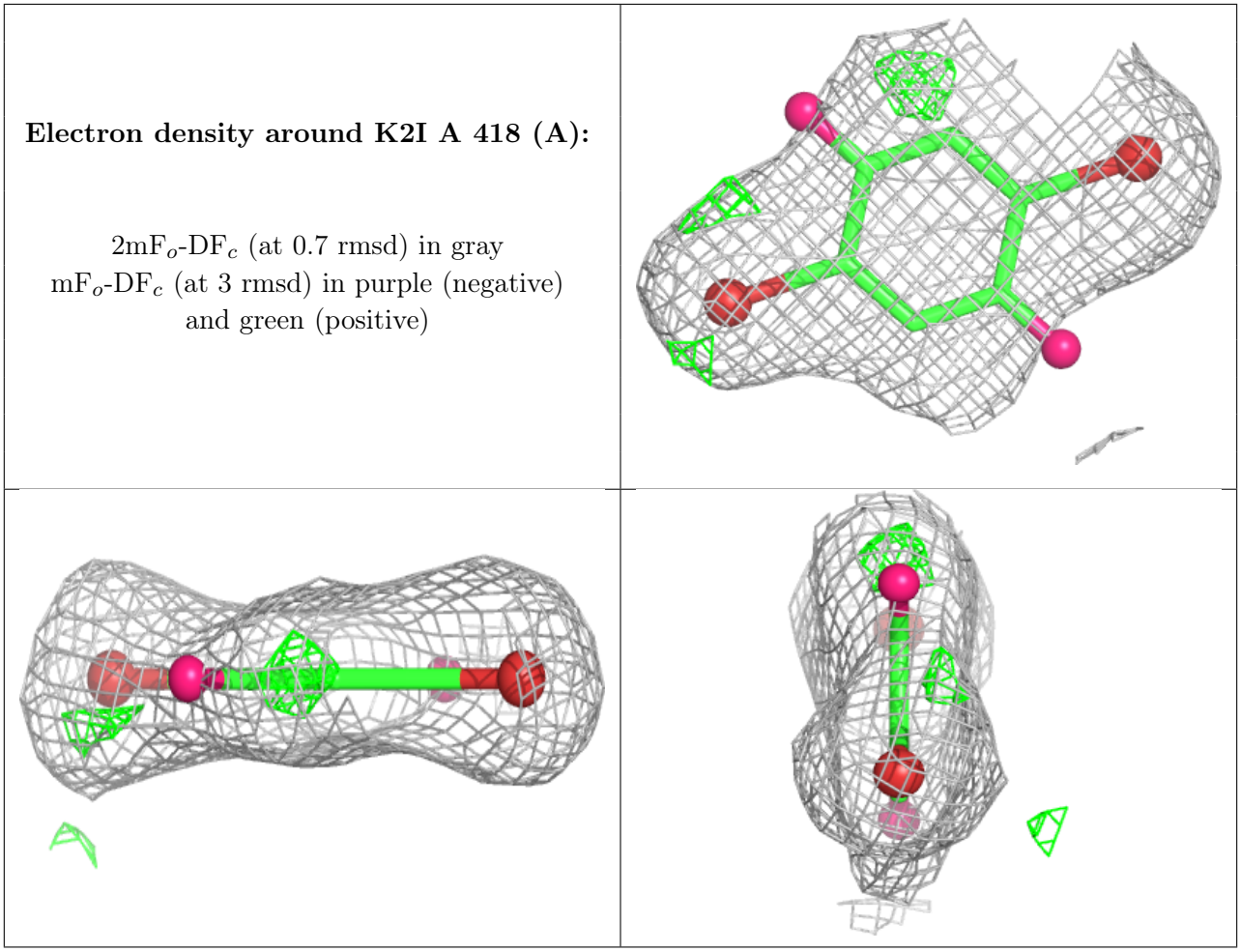






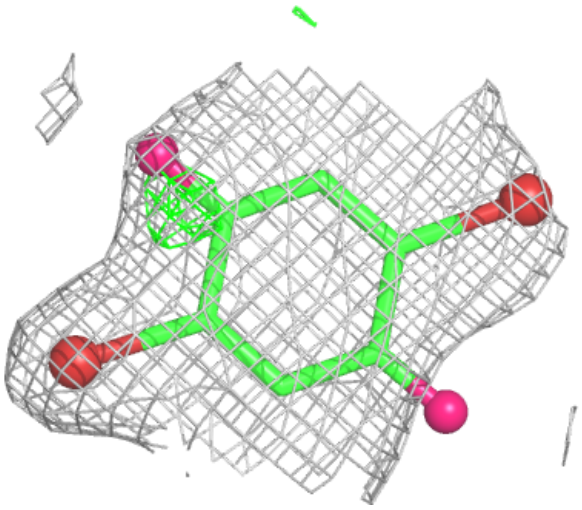
Electron density around K2I A 418 (A):

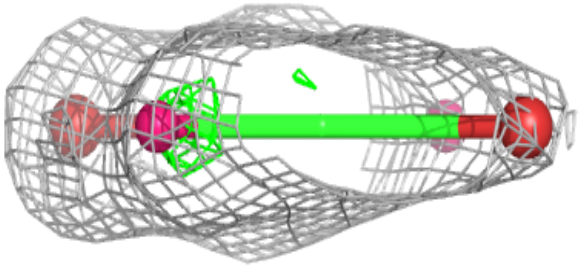
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

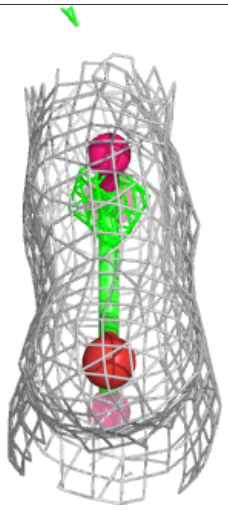


Electron density around K2I A 418 (B):

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



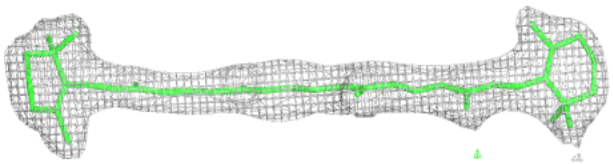




Electron density around BCR C 516:

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

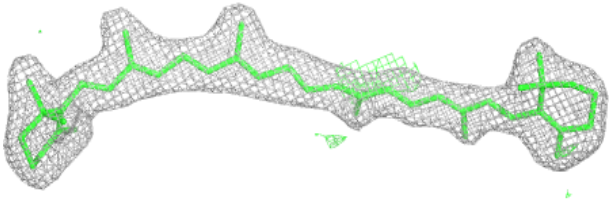


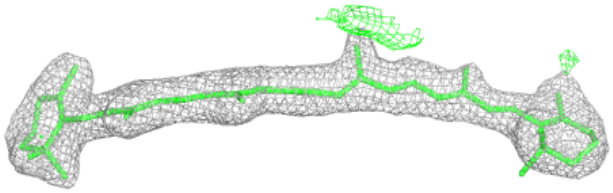


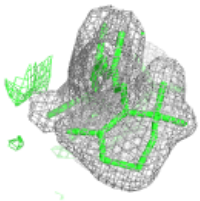


Electron density around BCR T 101:

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

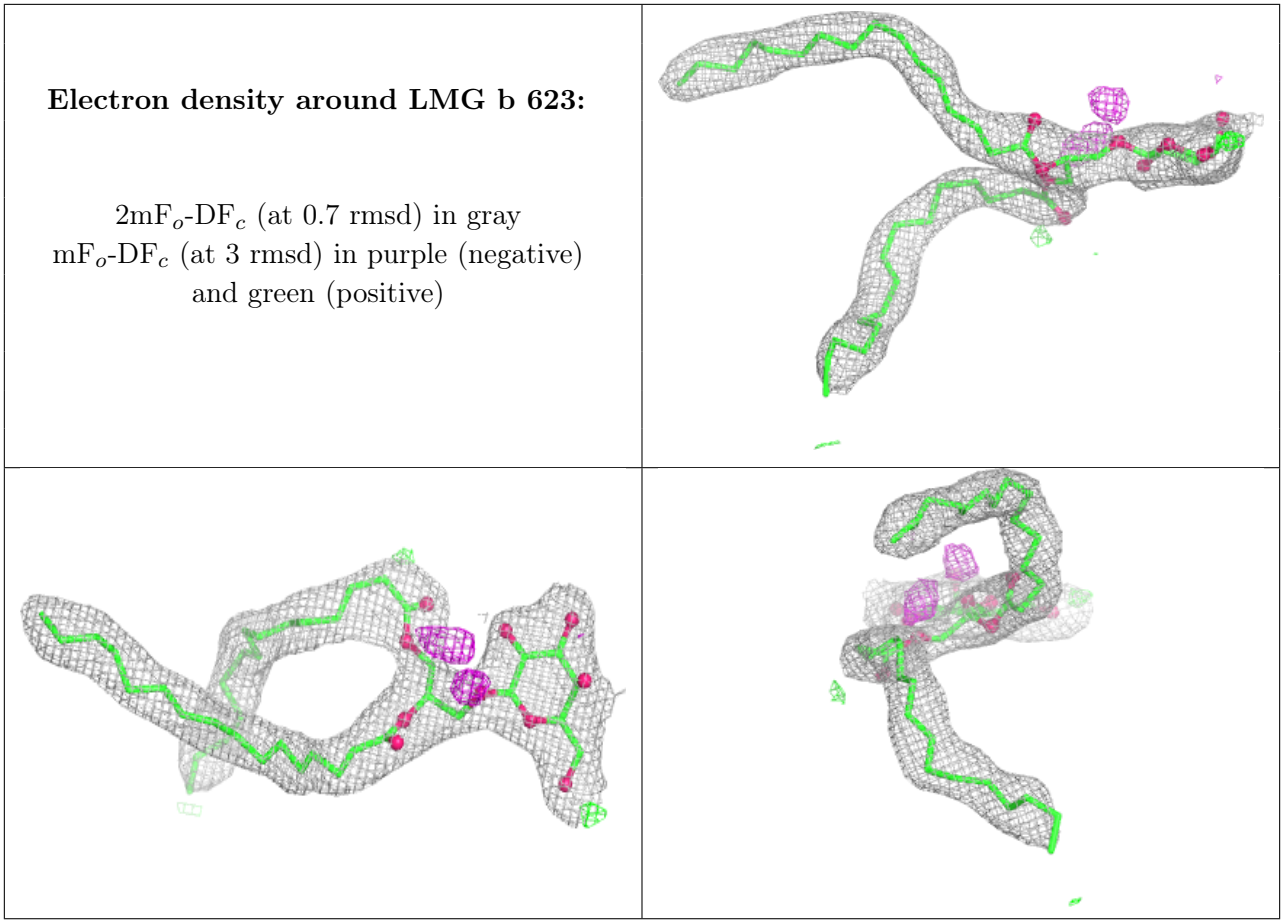






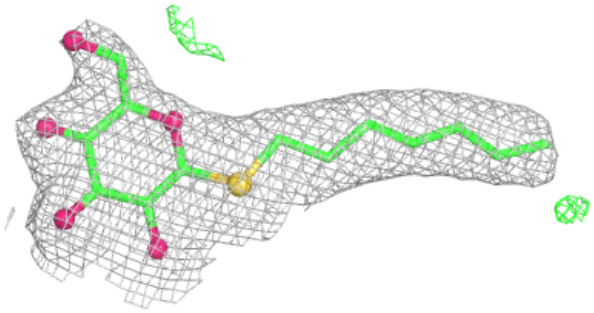
Electron density around LMG b 623:

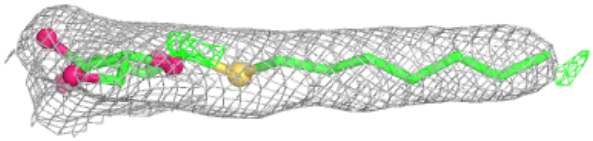
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

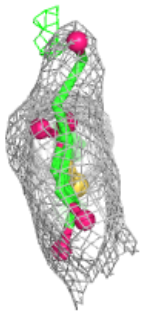


Electron density around HTG b 601:

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

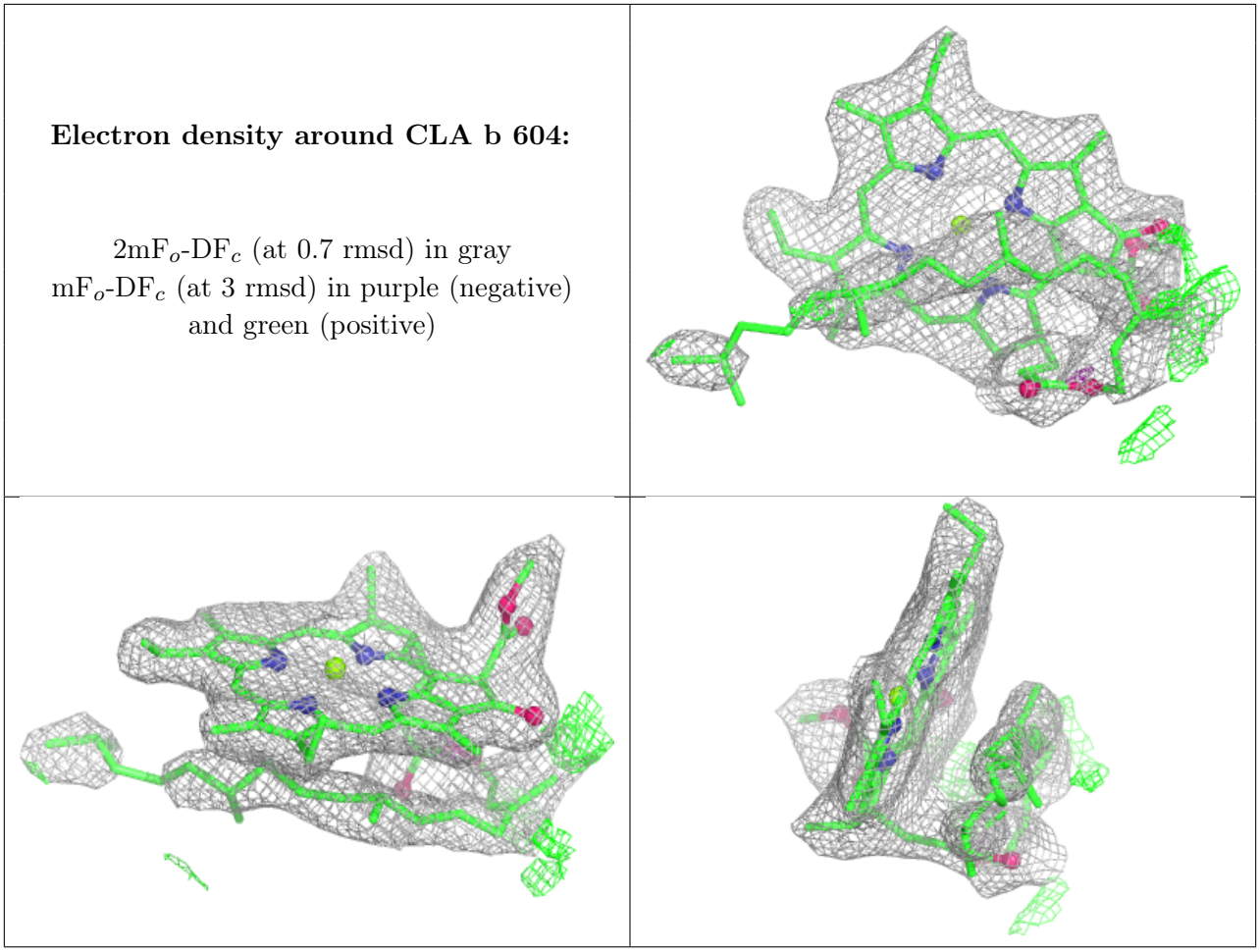






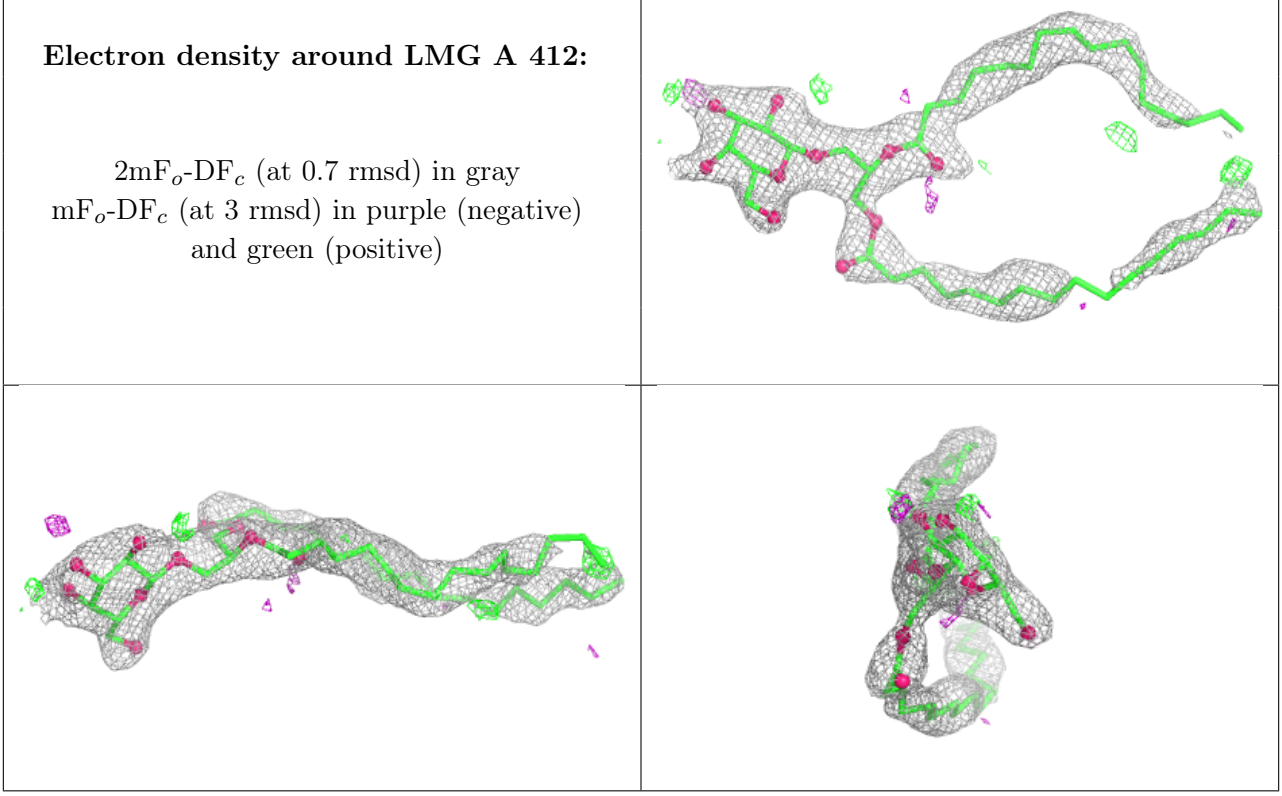
Electron density around CLA b 604:

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



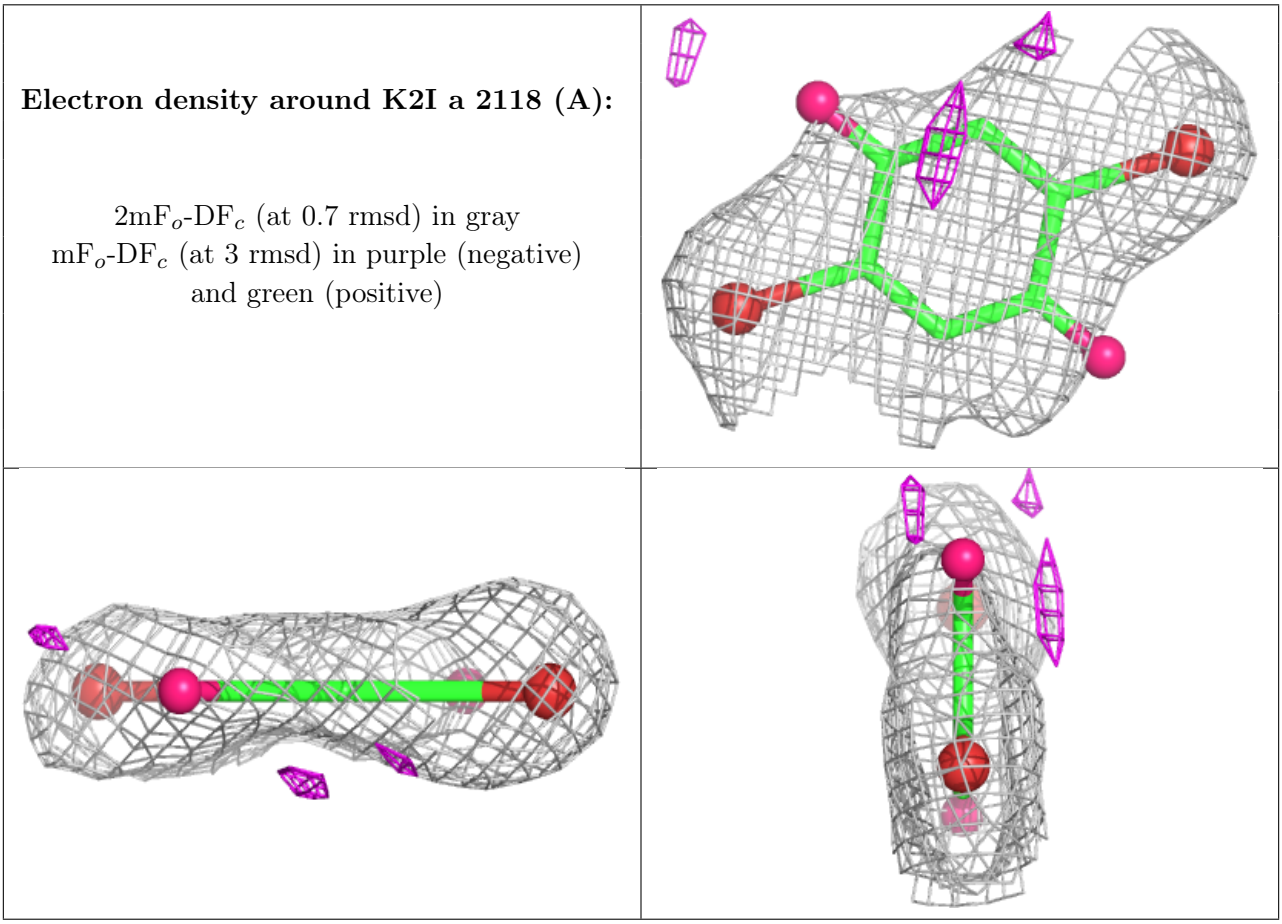
Electron density around LMG A 412:

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



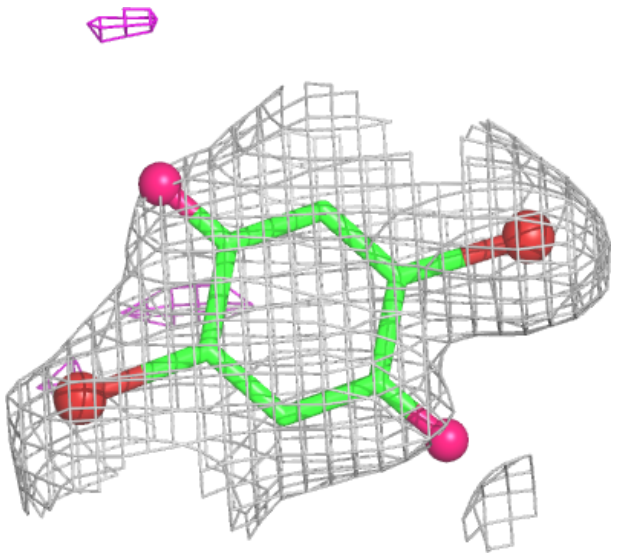
Electron density around K2I a 2118 (A):

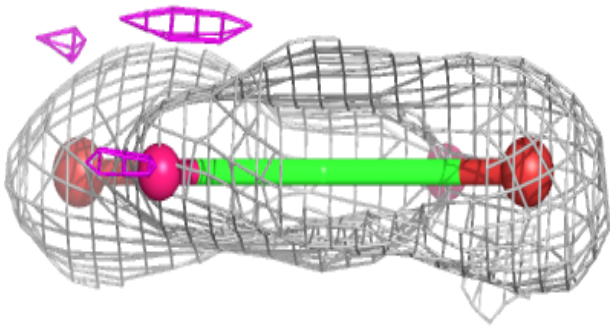
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

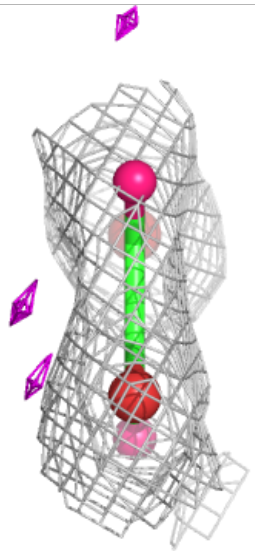


Electron density around K2I a 2118 (B):

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

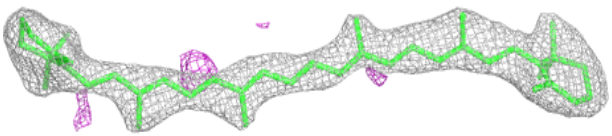


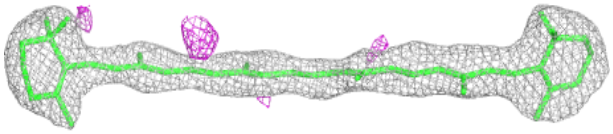


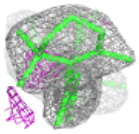


Electron density around BCR c 516:

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

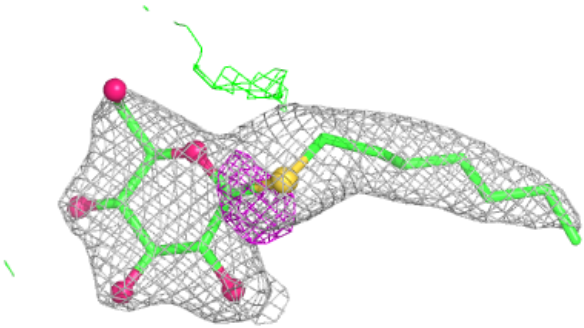


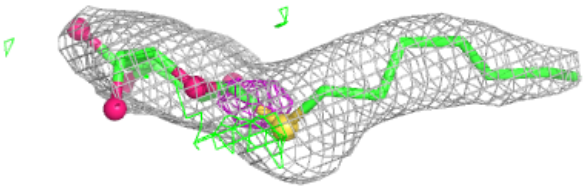


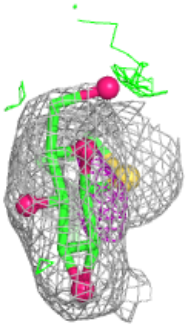


Electron density around HTG O 302:

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

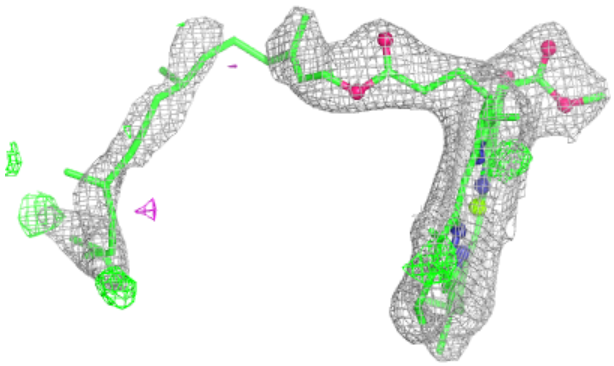


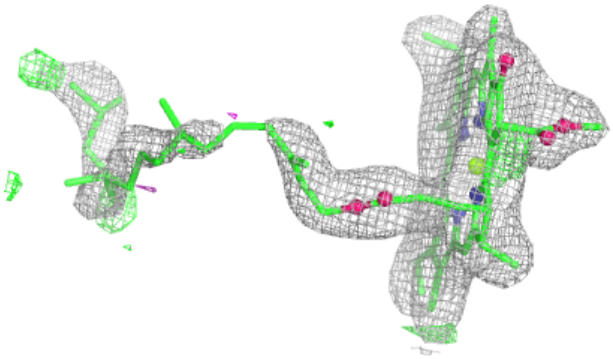


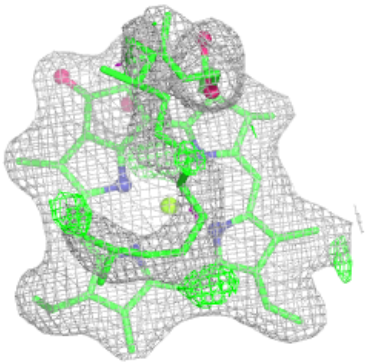


Electron density around CLA c 508:

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

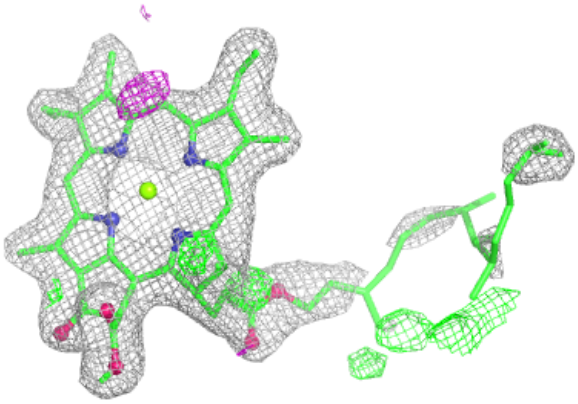


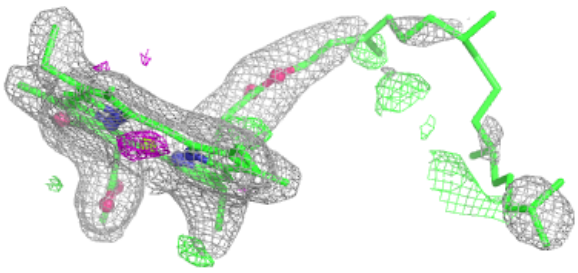




Electron density around CLA a 2113:

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

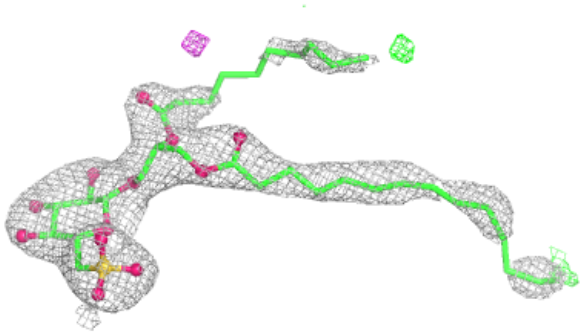


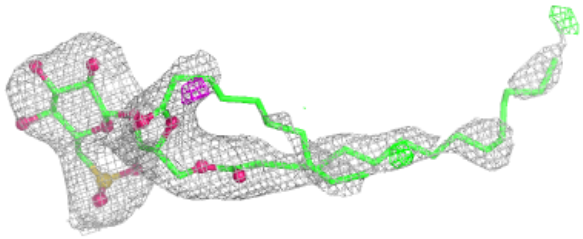


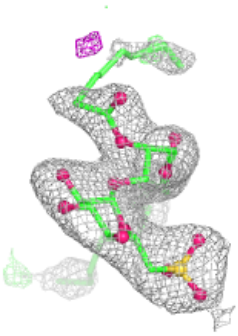


Electron density around SQD a 2115:

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

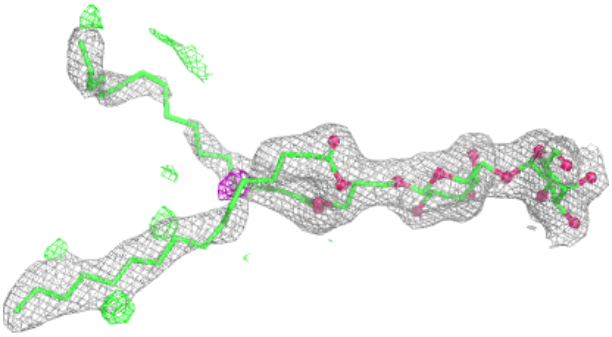


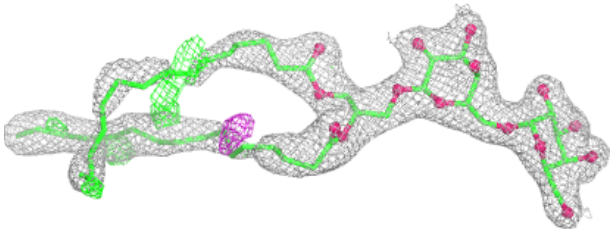


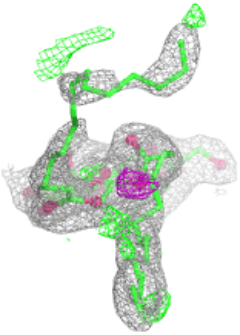


Electron density around DGD c 518:

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

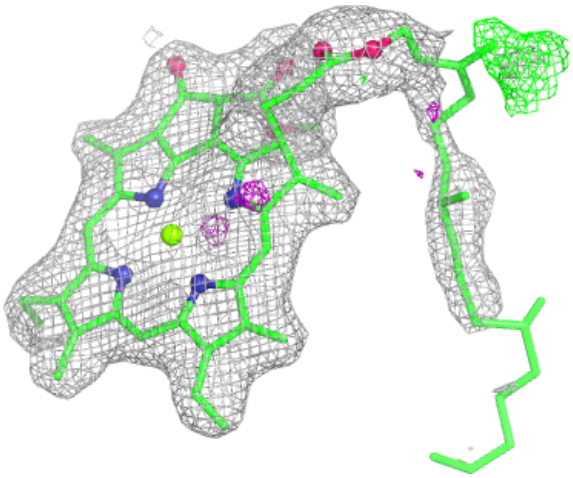


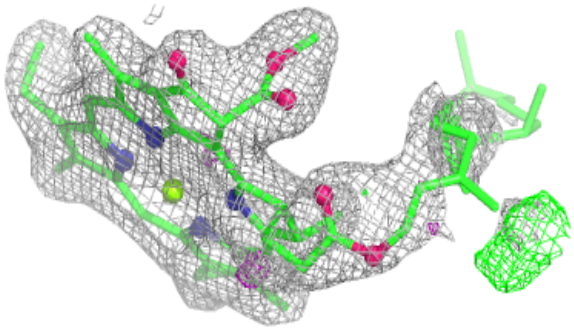


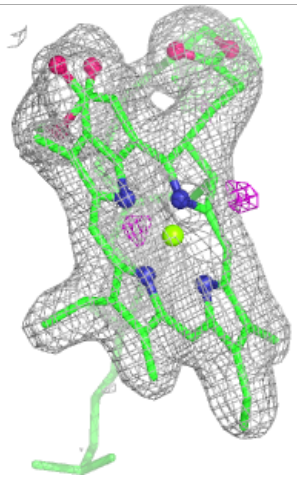


Electron density around CLA B 617:

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

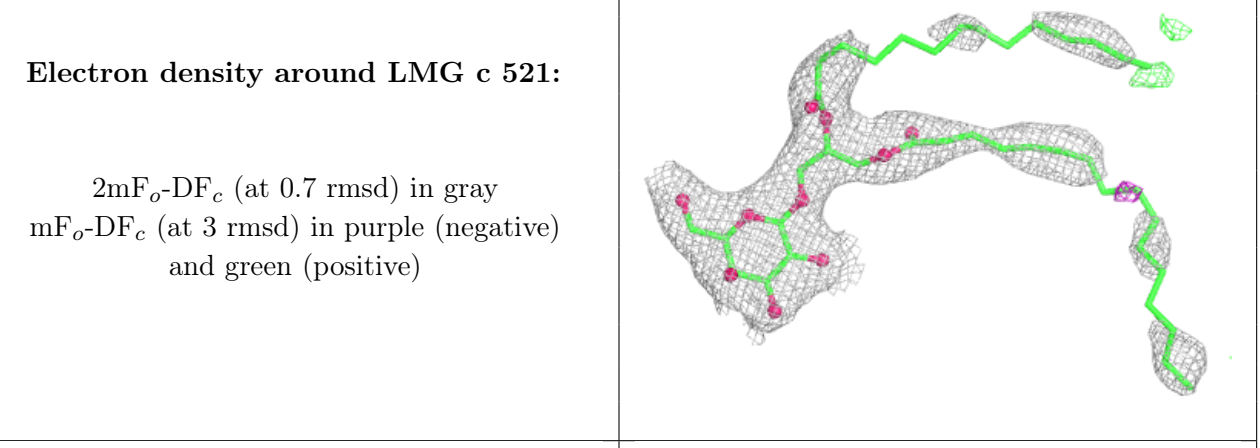






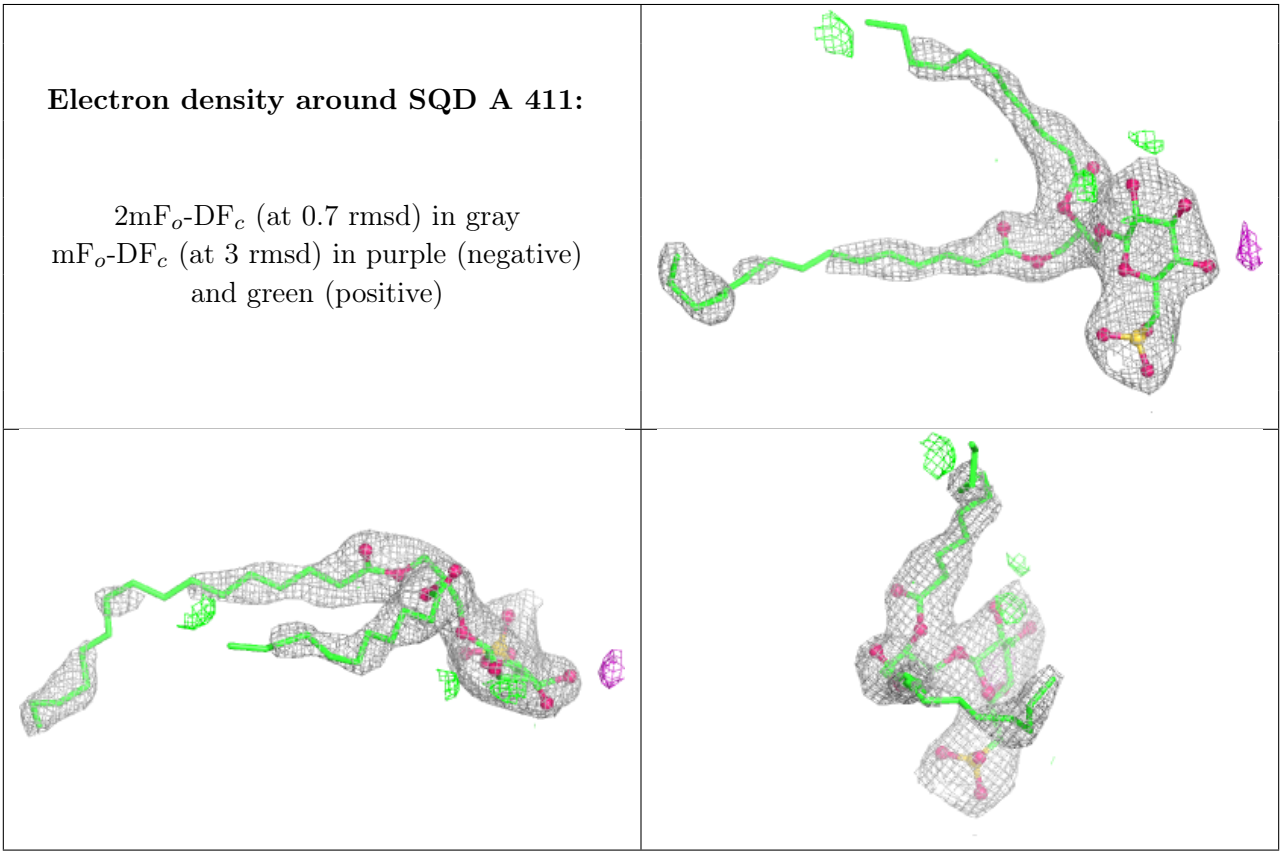
Electron density around LMG c 521:

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



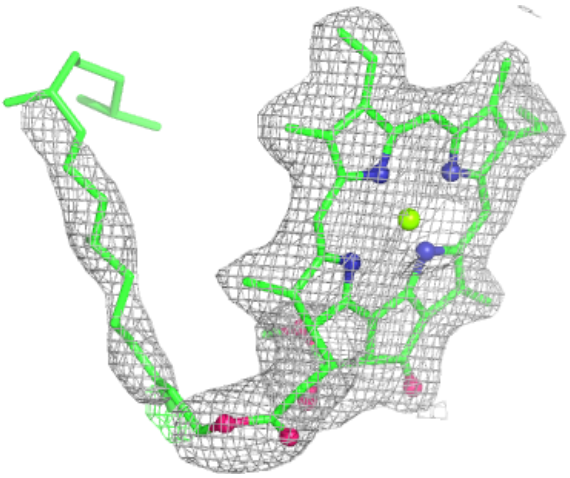
Electron density around SQD A 411:

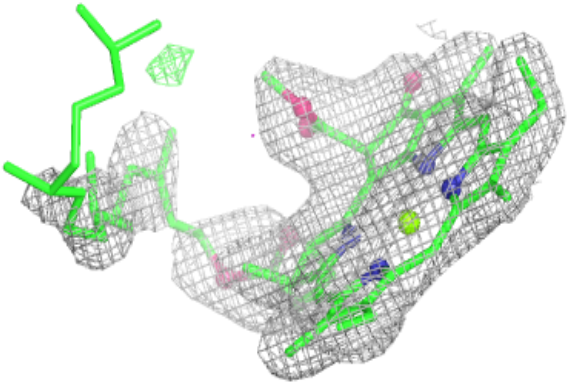
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

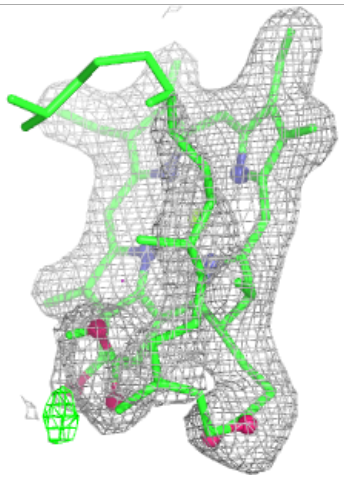


Electron density around CLA b 619:

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

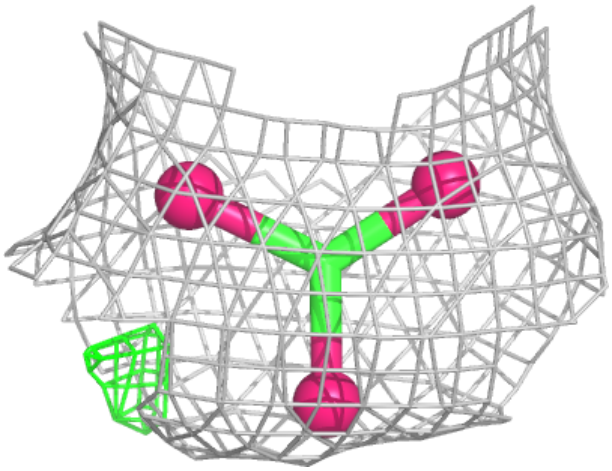


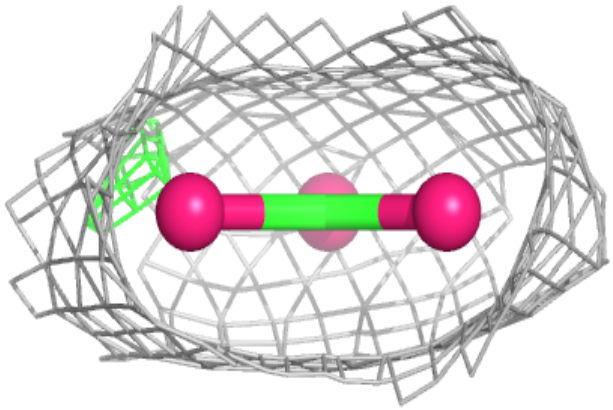


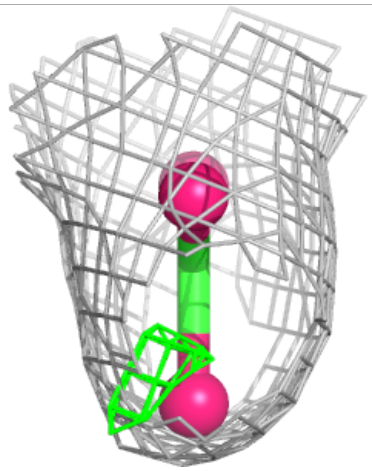


Electron density around BCT A 421:

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

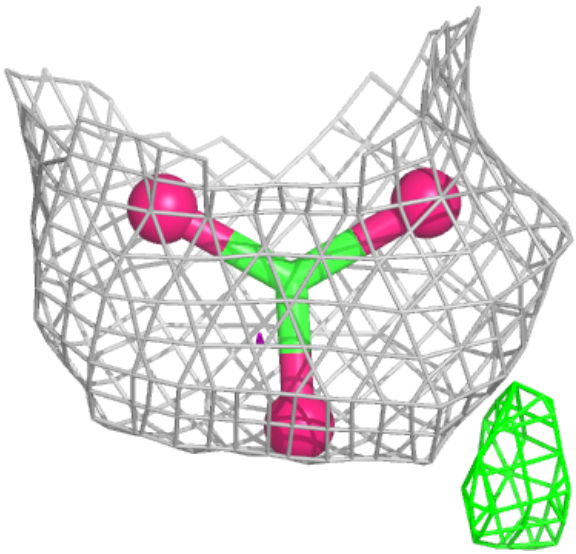


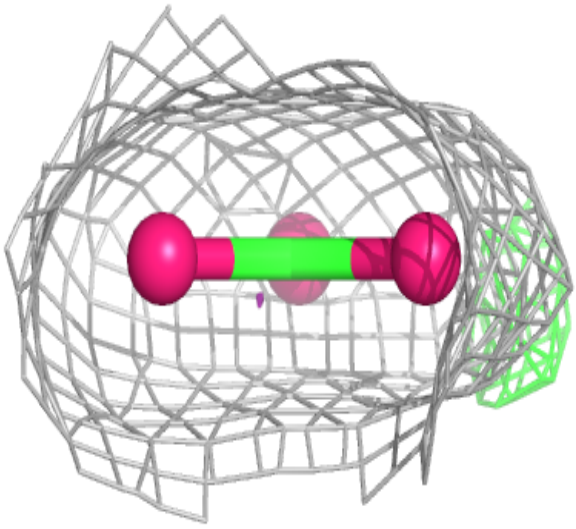


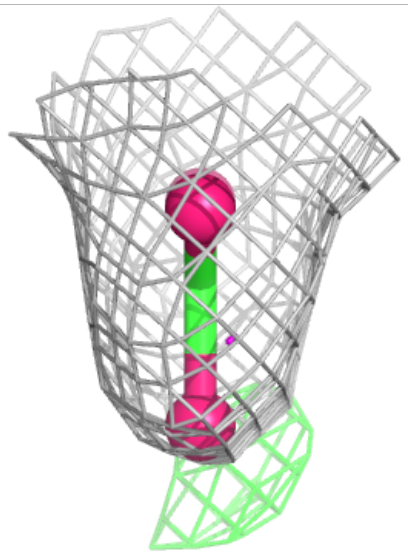


Electron density around BCT a 2108:

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

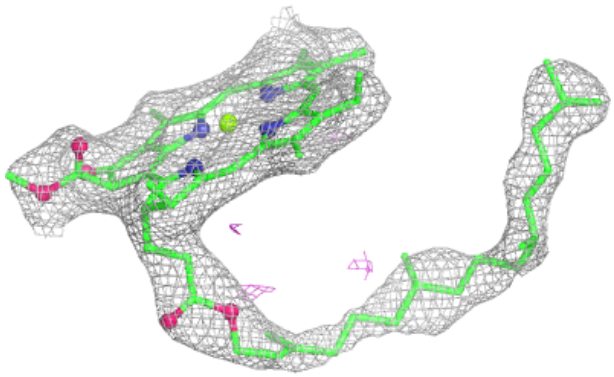


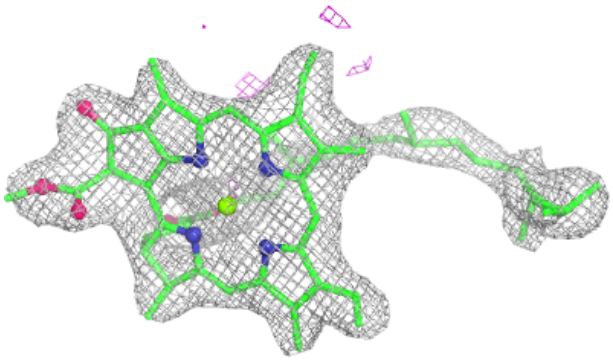


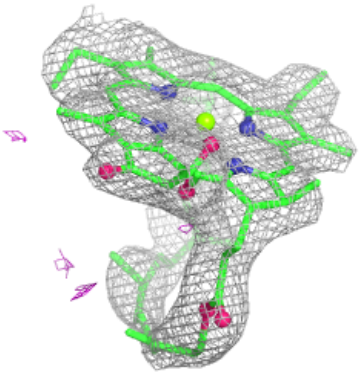


Electron density around CLA C 514:

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

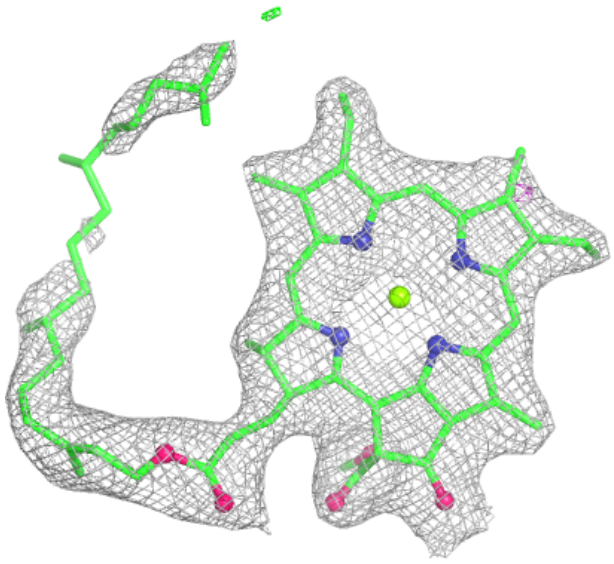


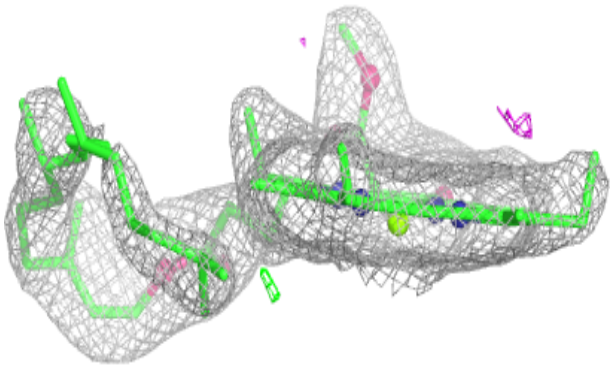


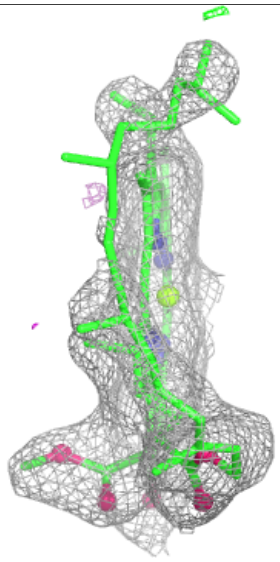


Electron density around CLA c 514:

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

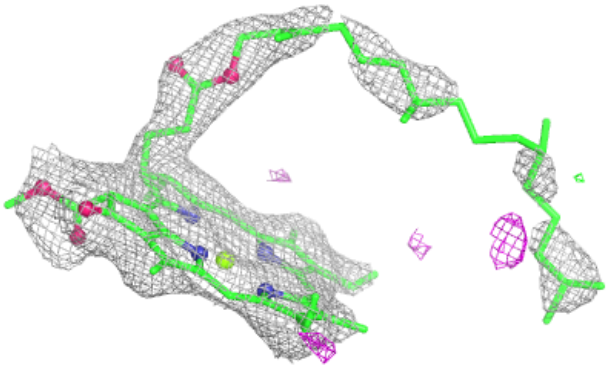


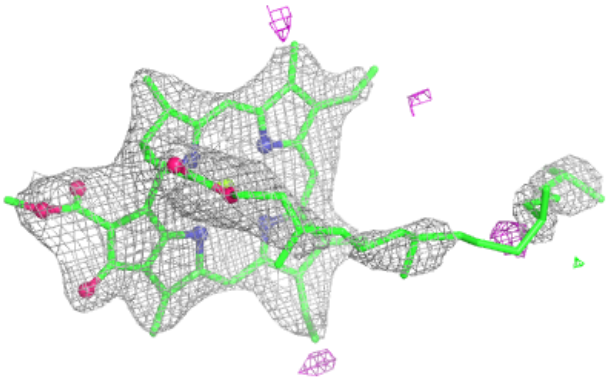


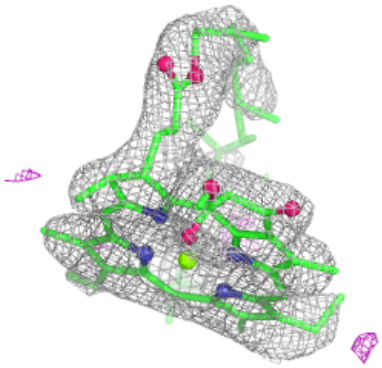


Electron density around CLA c 515:

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

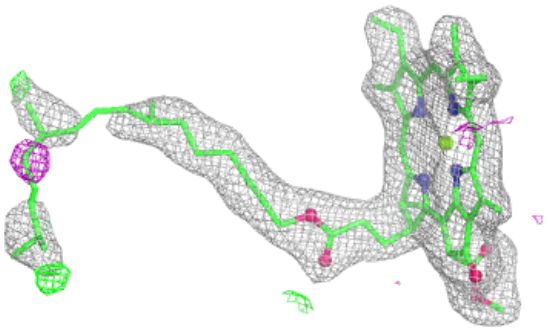


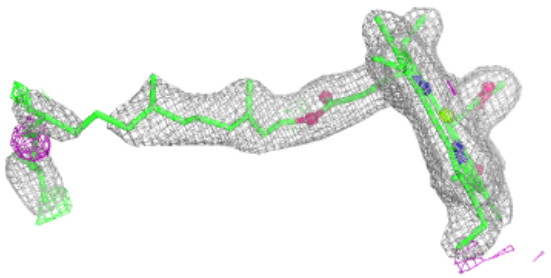


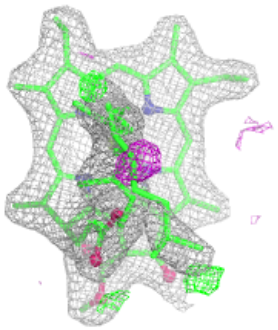


Electron density around CLA d 405:

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

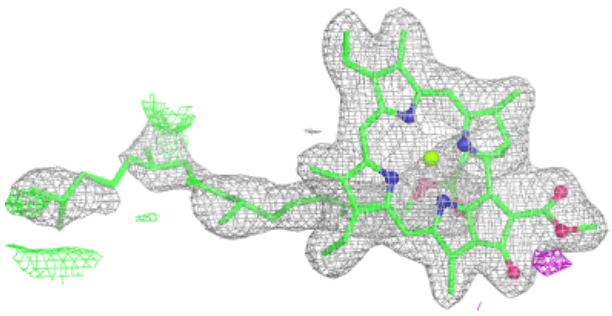


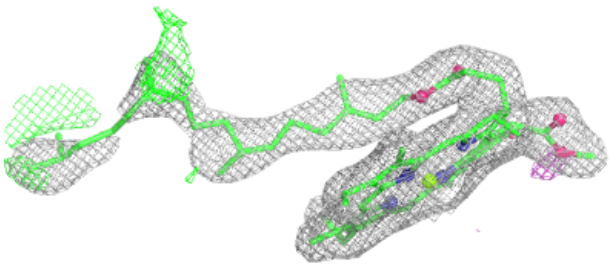


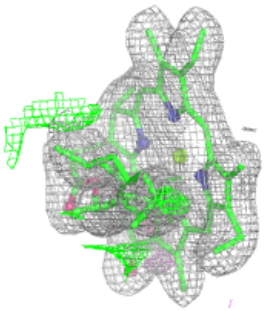


Electron density around CLA B 615:

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

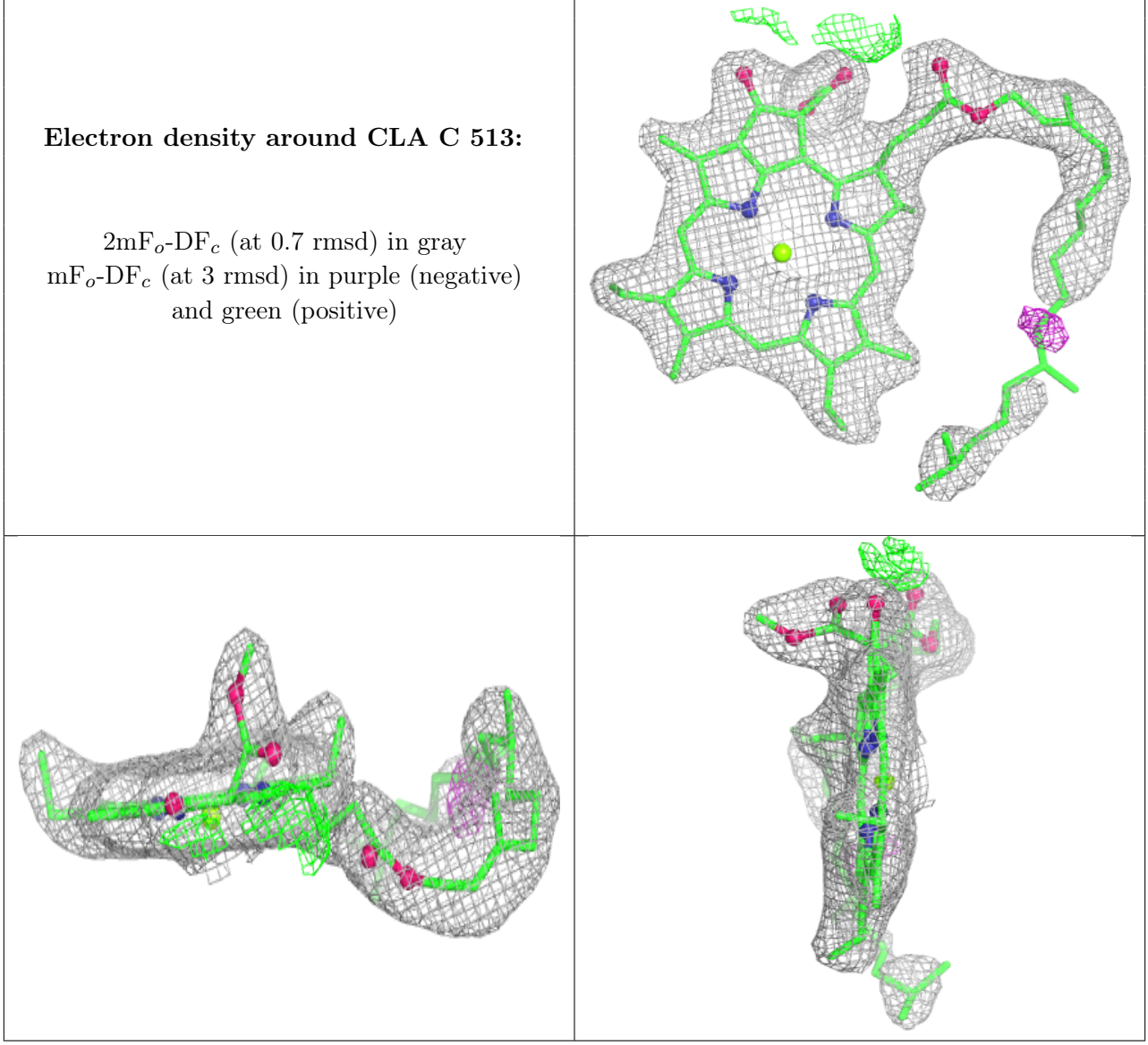






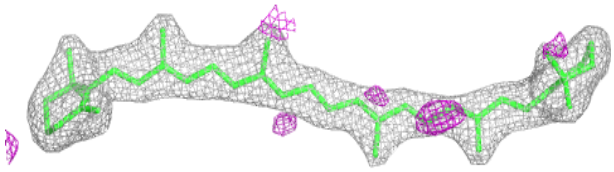
Electron density around CLA C 513:

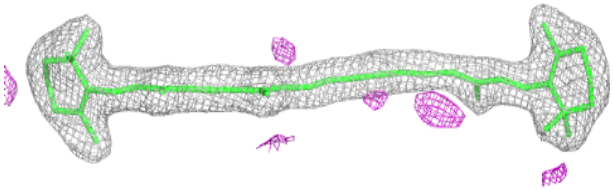
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

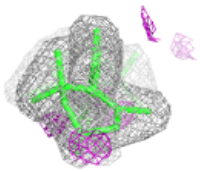


Electron density around BCR a 2114:

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

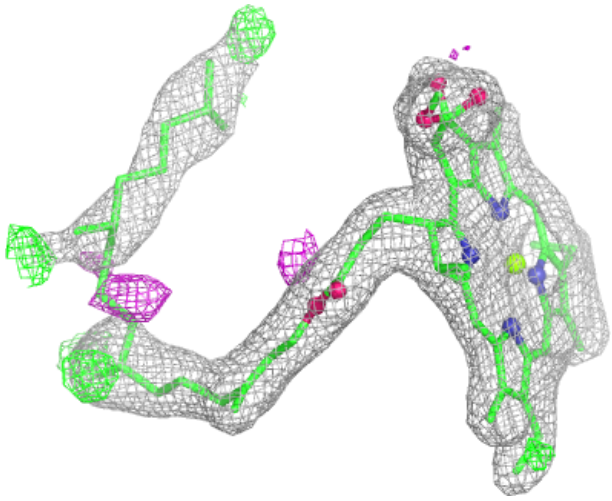


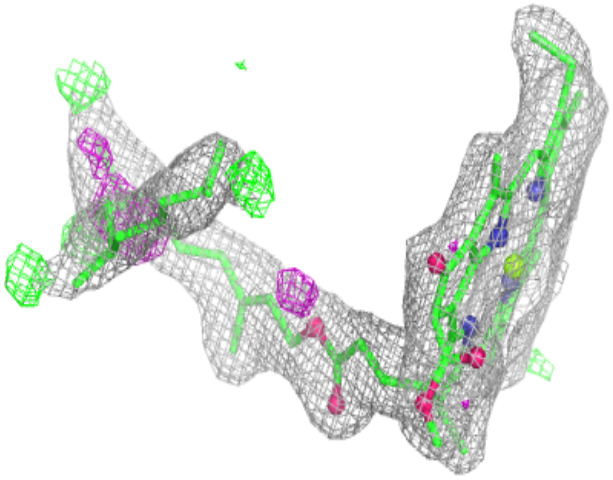


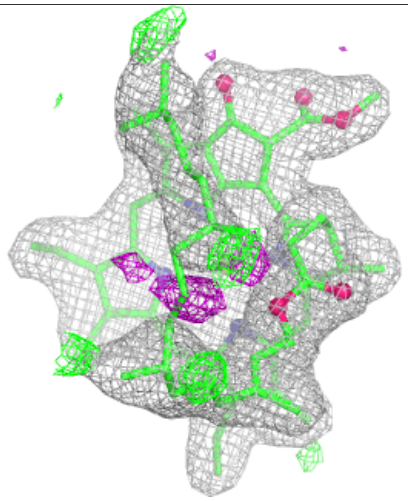


Electron density around CLA b 609:

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

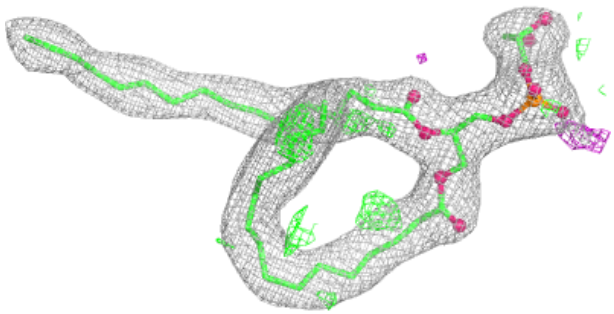


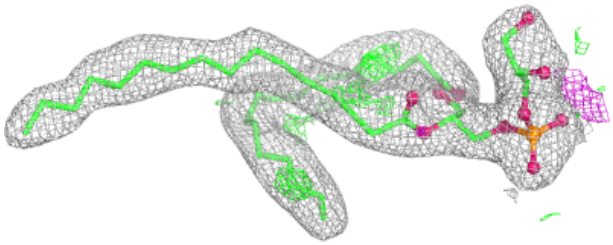


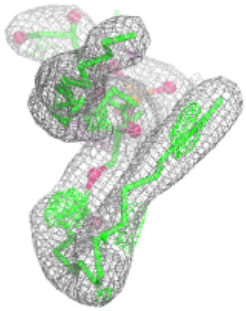


Electron density around LHG D 409:

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

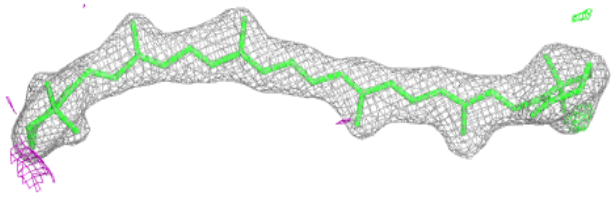


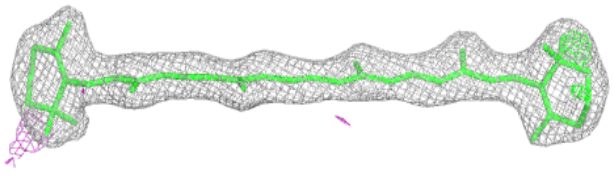


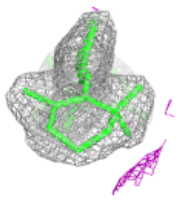


Electron density around BCR c 517:

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

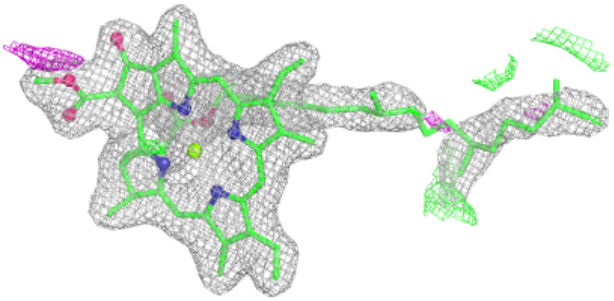


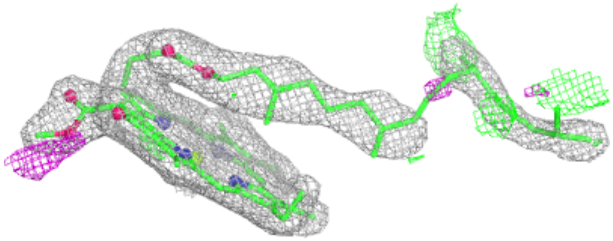


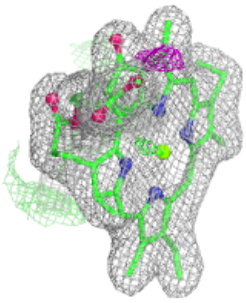


Electron density around CLA b 617:

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

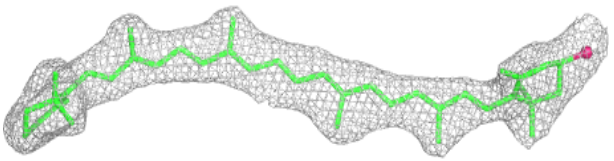


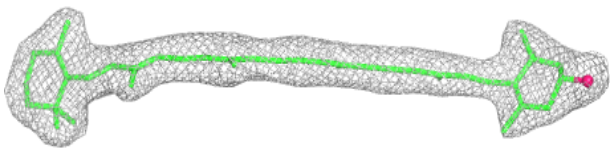


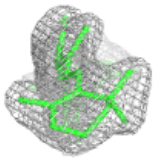


Electron density around RRX H 101:

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

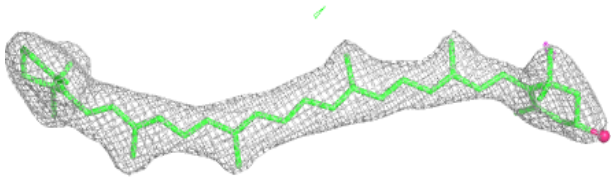


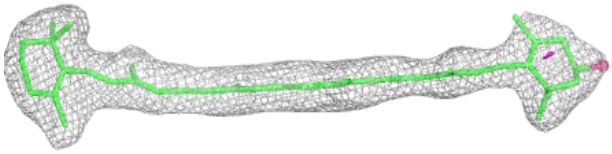


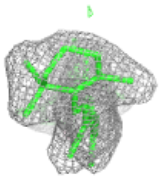


Electron density around RRX h 702:

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

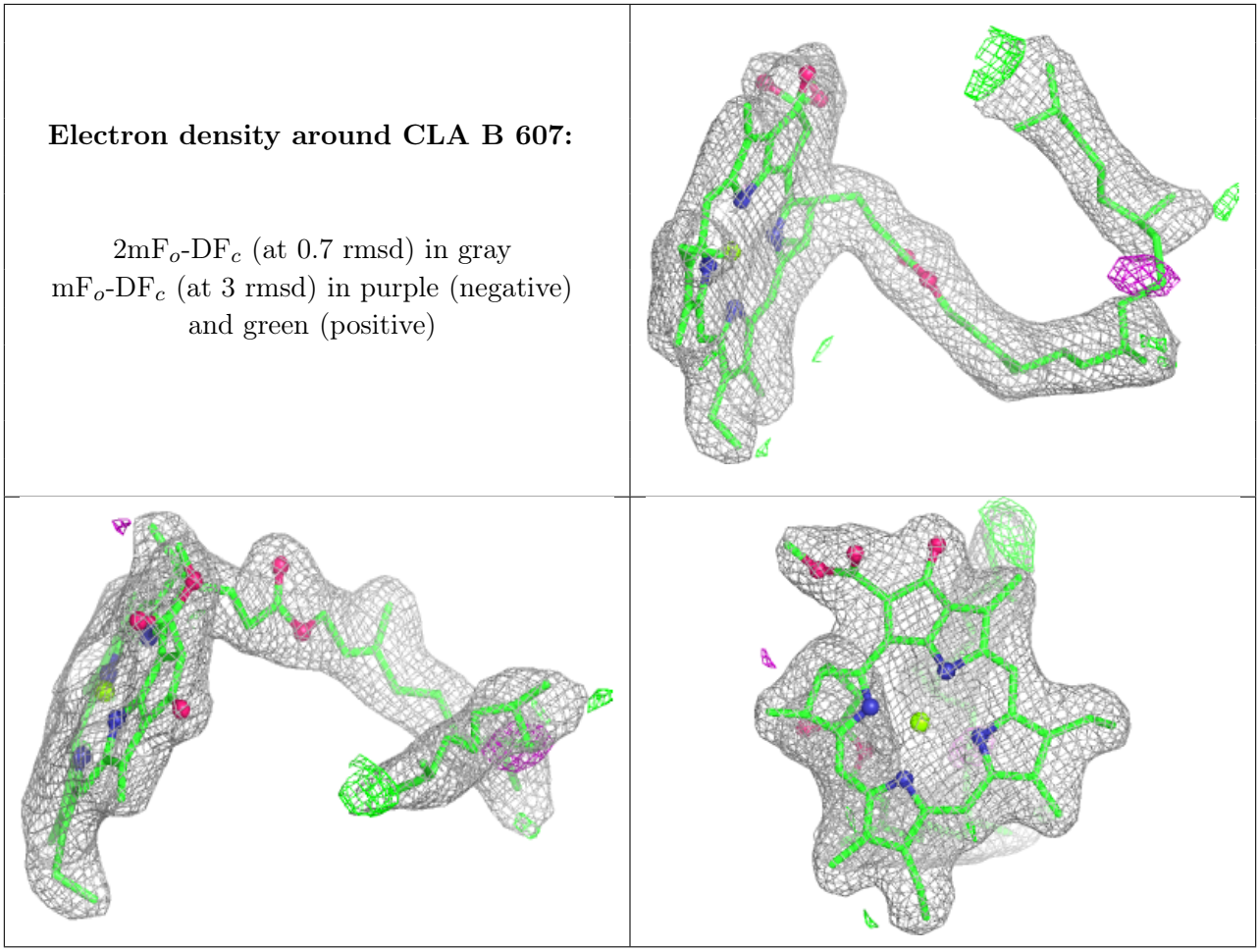






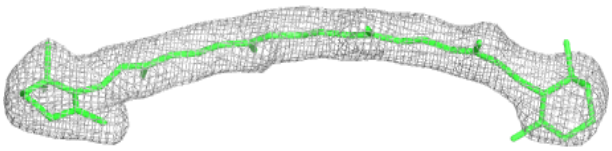
Electron density around CLA B 607:

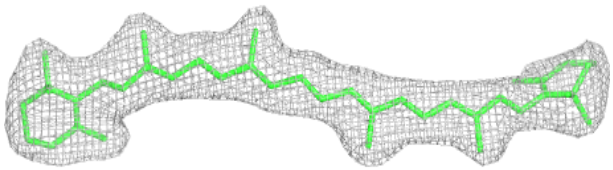
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

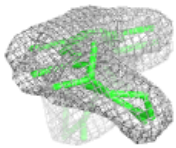


Electron density around BCR D 406:

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

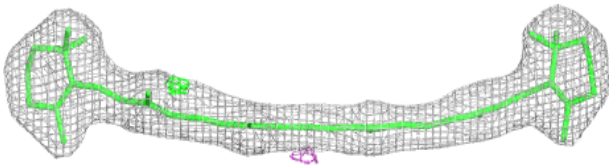


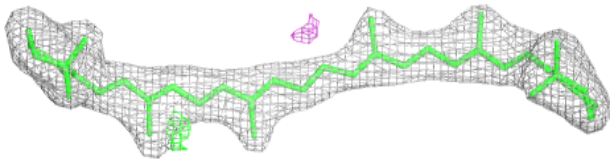


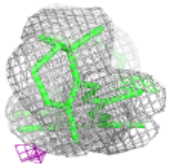


Electron density around BCR K 101:

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

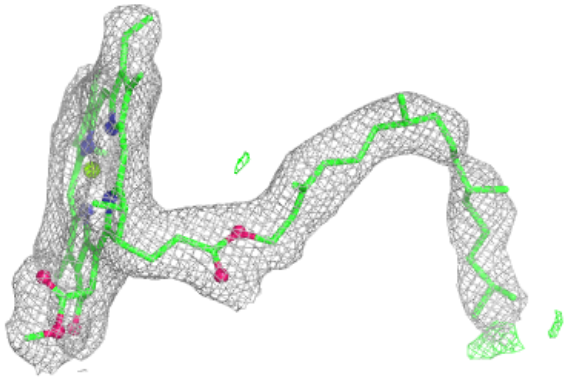


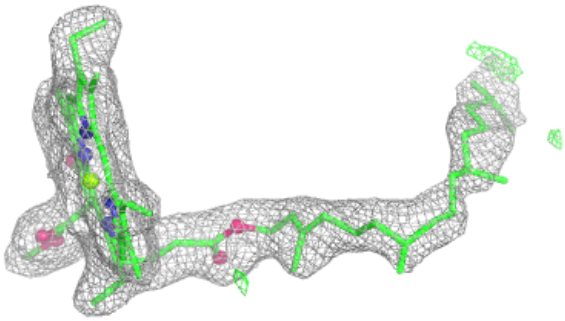


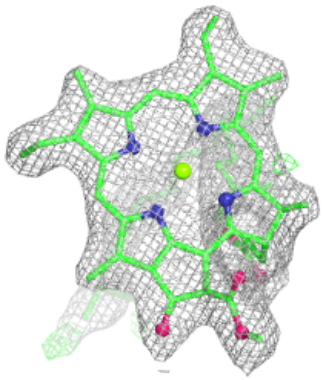


Electron density around CLA D 405:

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

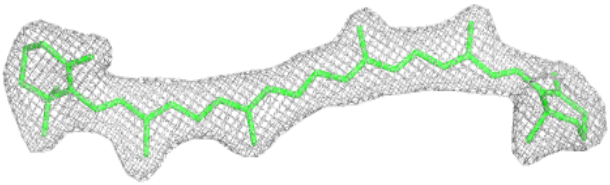


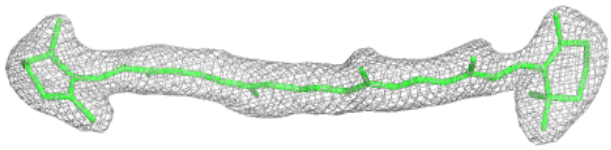


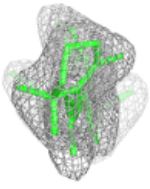


Electron density around BCR Y 302:

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

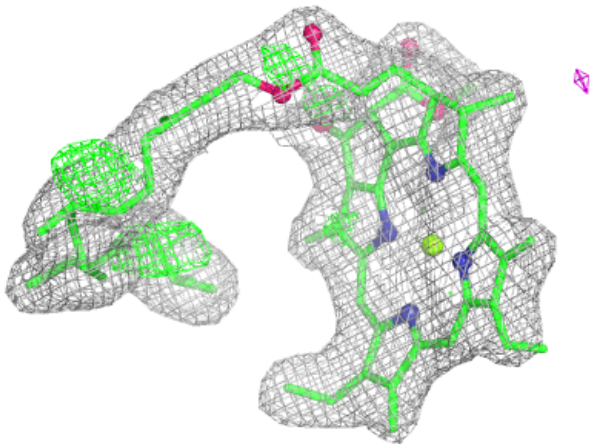


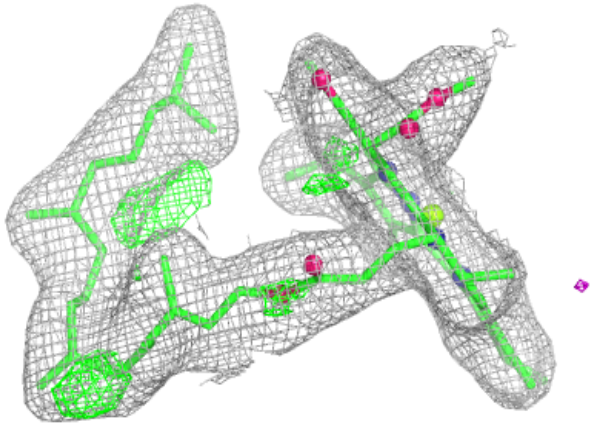


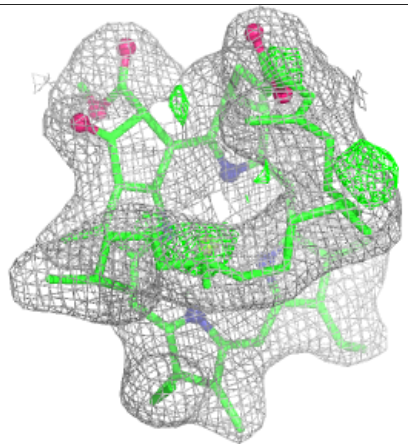


Electron density around CLA c 505:

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

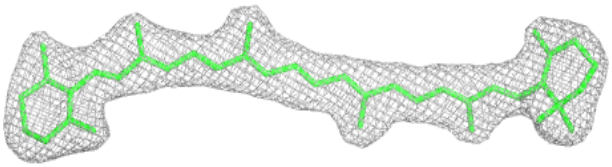


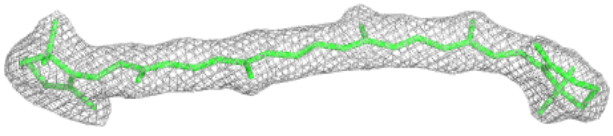


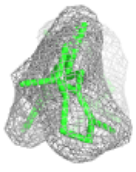


Electron density around BCR b 622:

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

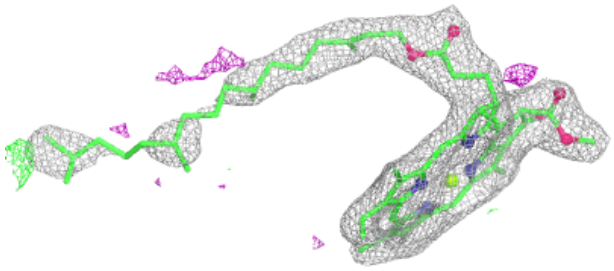


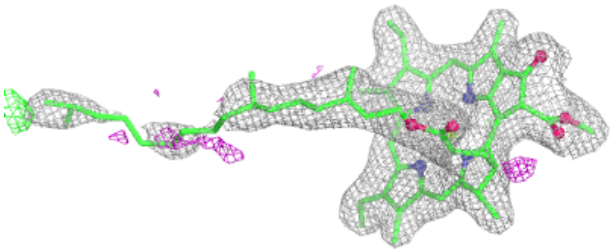


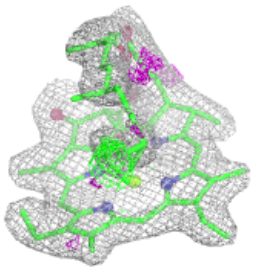


Electron density around CLA c 506:

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

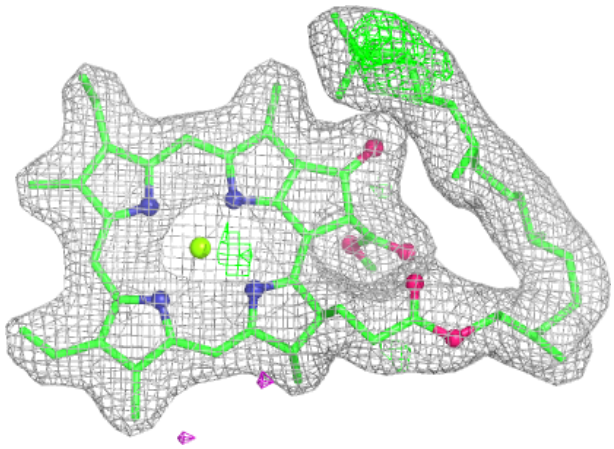


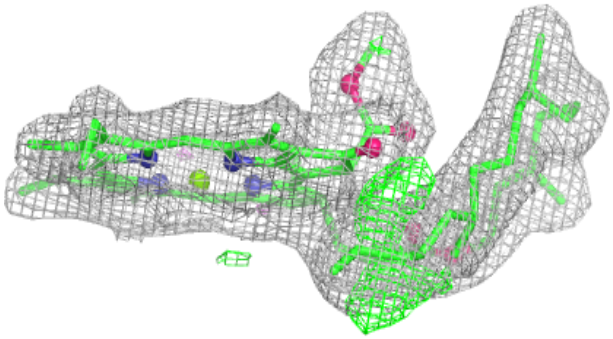


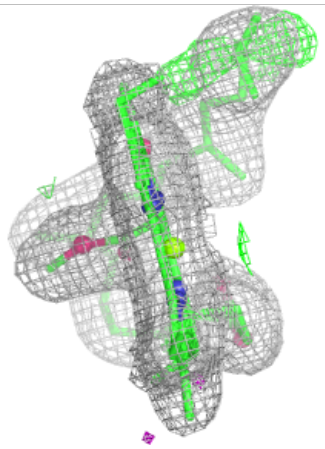


Electron density around CLA B 611:

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

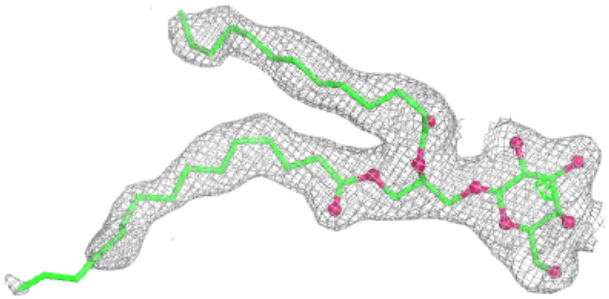


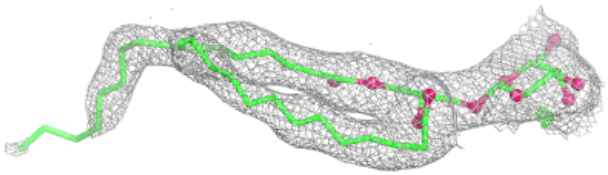


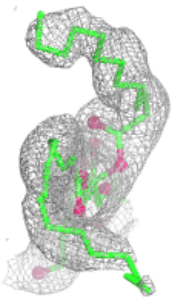


Electron density around LMG d 411:

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

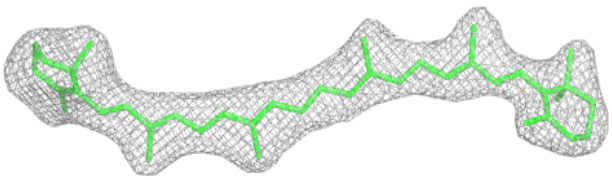


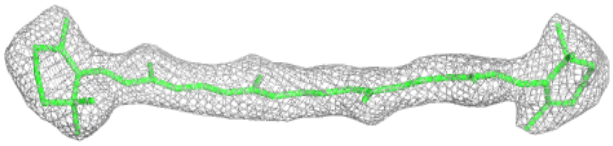


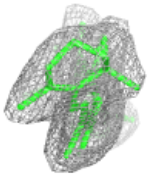


Electron density around BCR c 528:

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

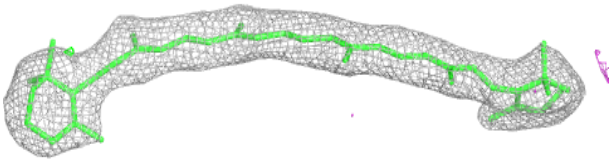


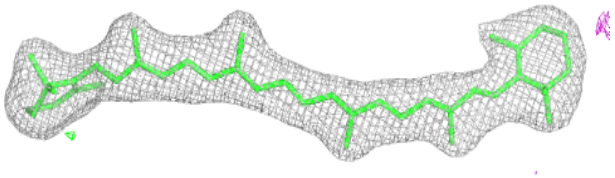


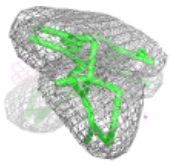


Electron density around BCR d 406:

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

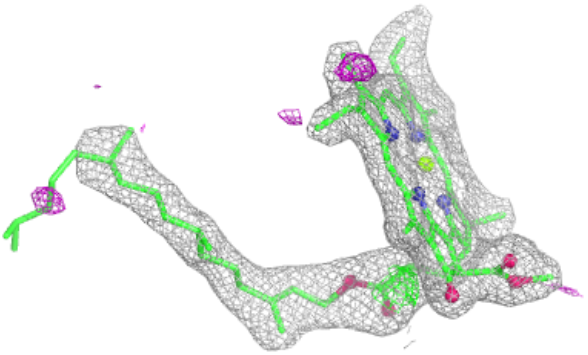


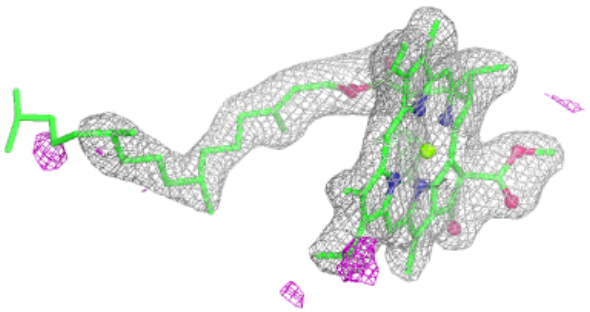


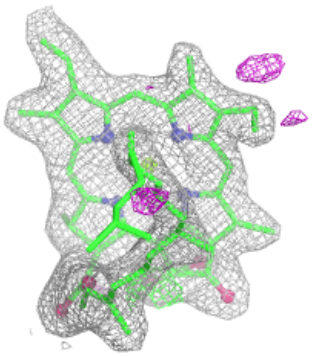


Electron density around CLA c 510:

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

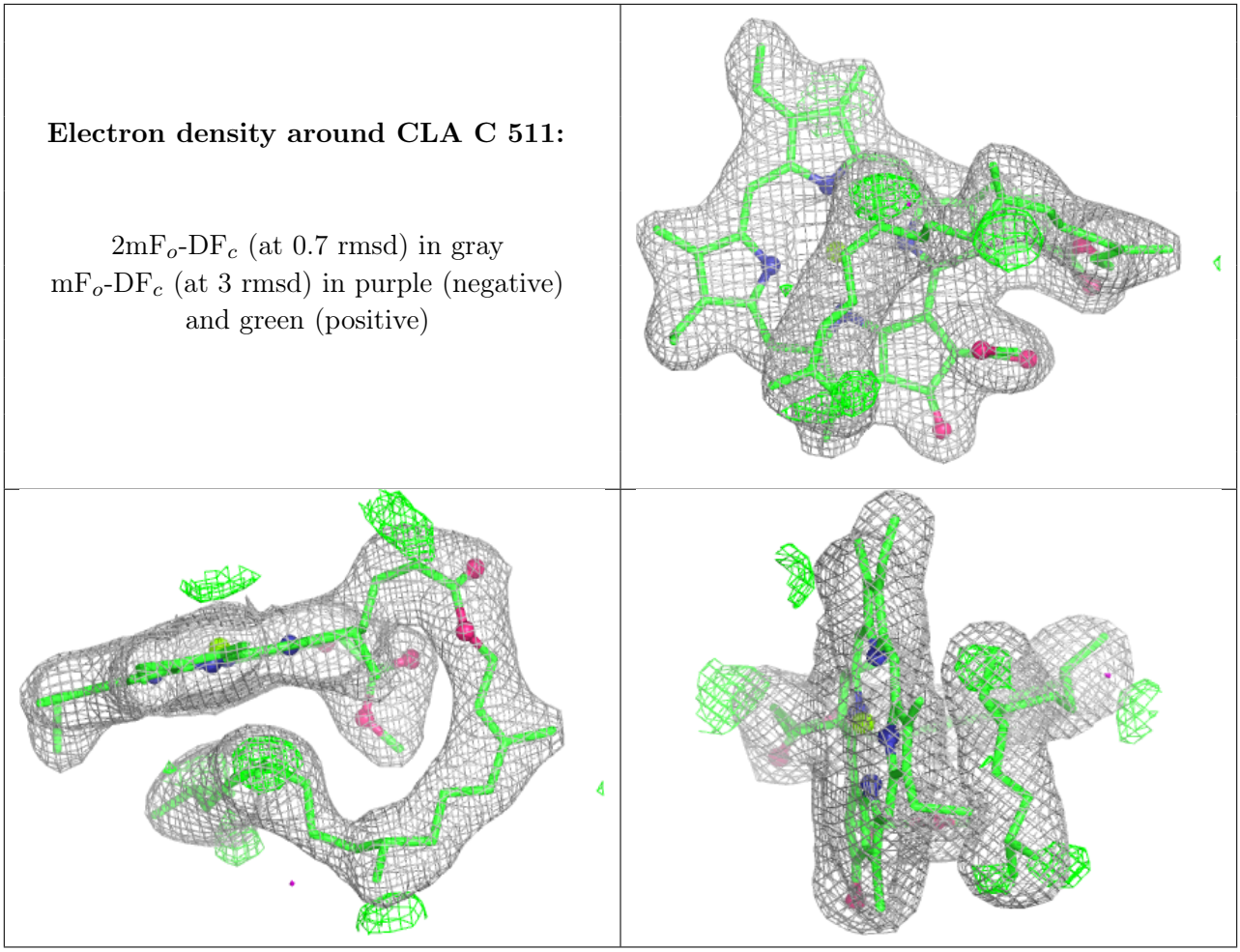






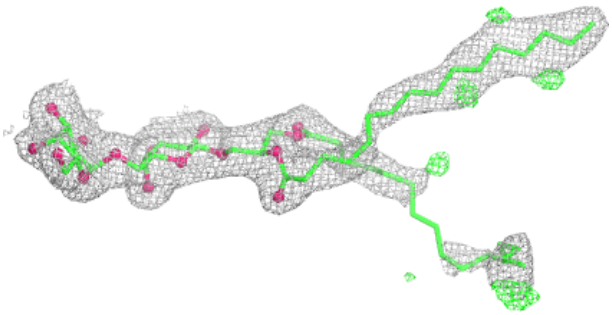
Electron density around CLA C 511:

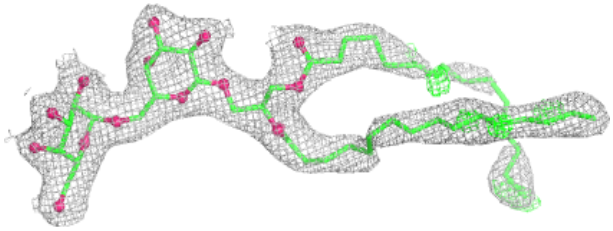
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

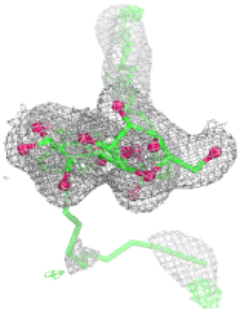


Electron density around DGD C 517:

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

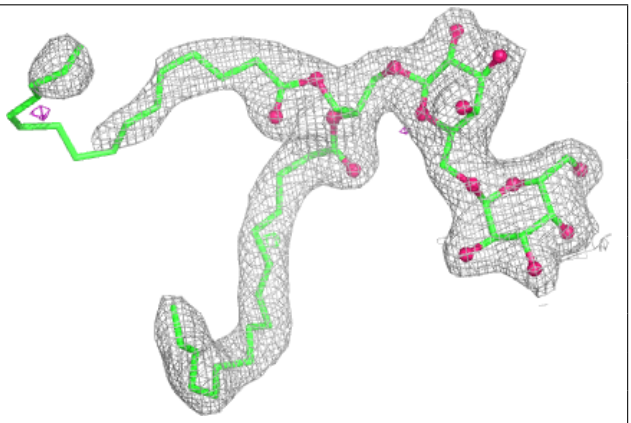


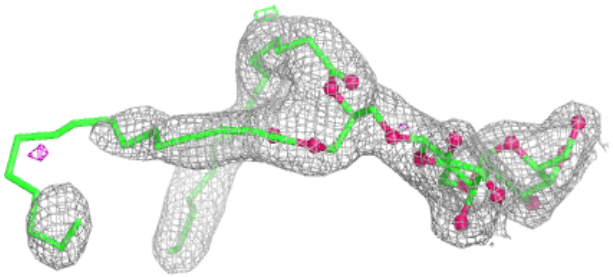


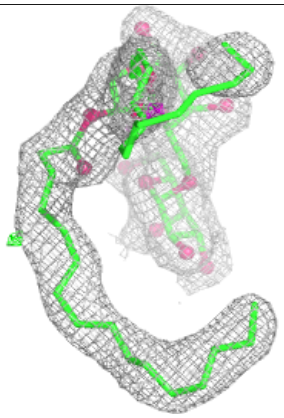


Electron density around DGD C 518:

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

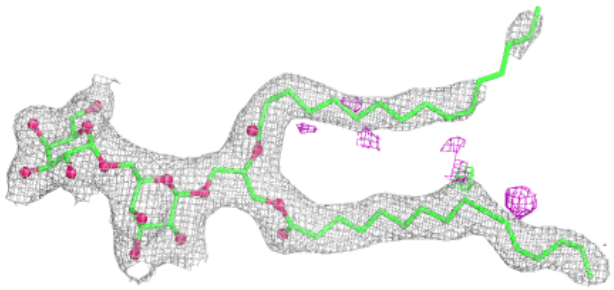


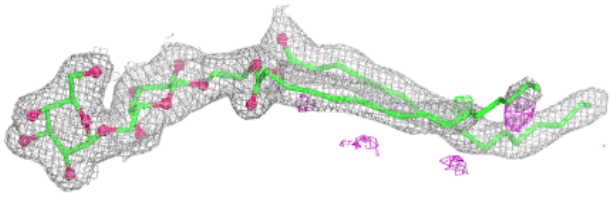


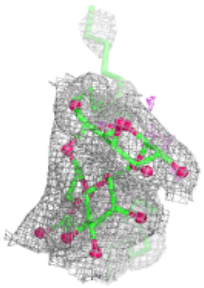


Electron density around DGD C 519:

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

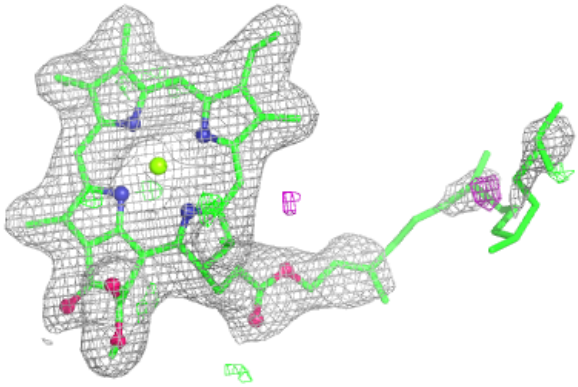


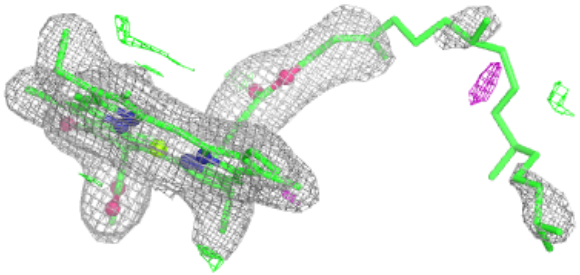


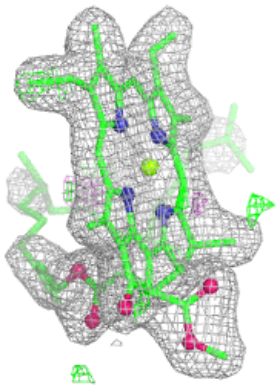


Electron density around CLA A 409:

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

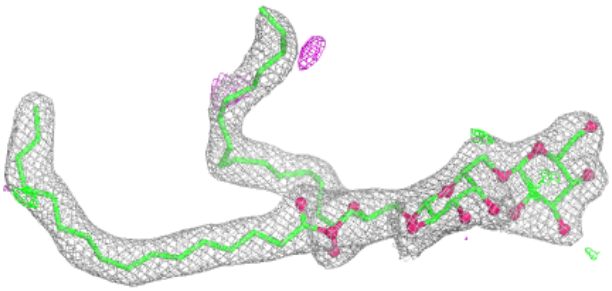


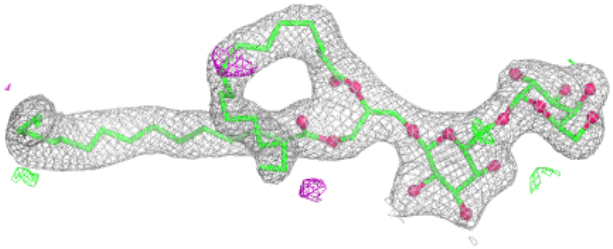


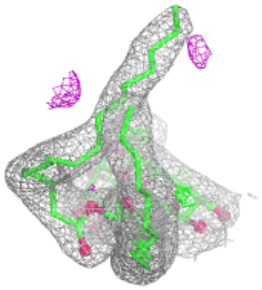


Electron density around DGD H 102:

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

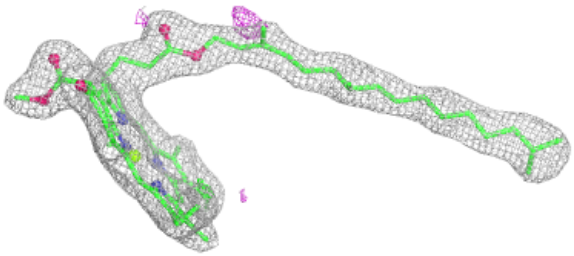


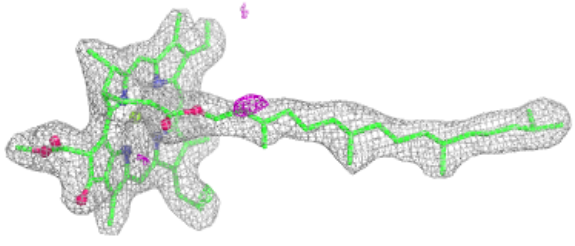


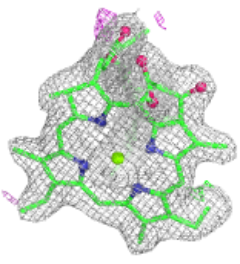


Electron density around CLA b 610:

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

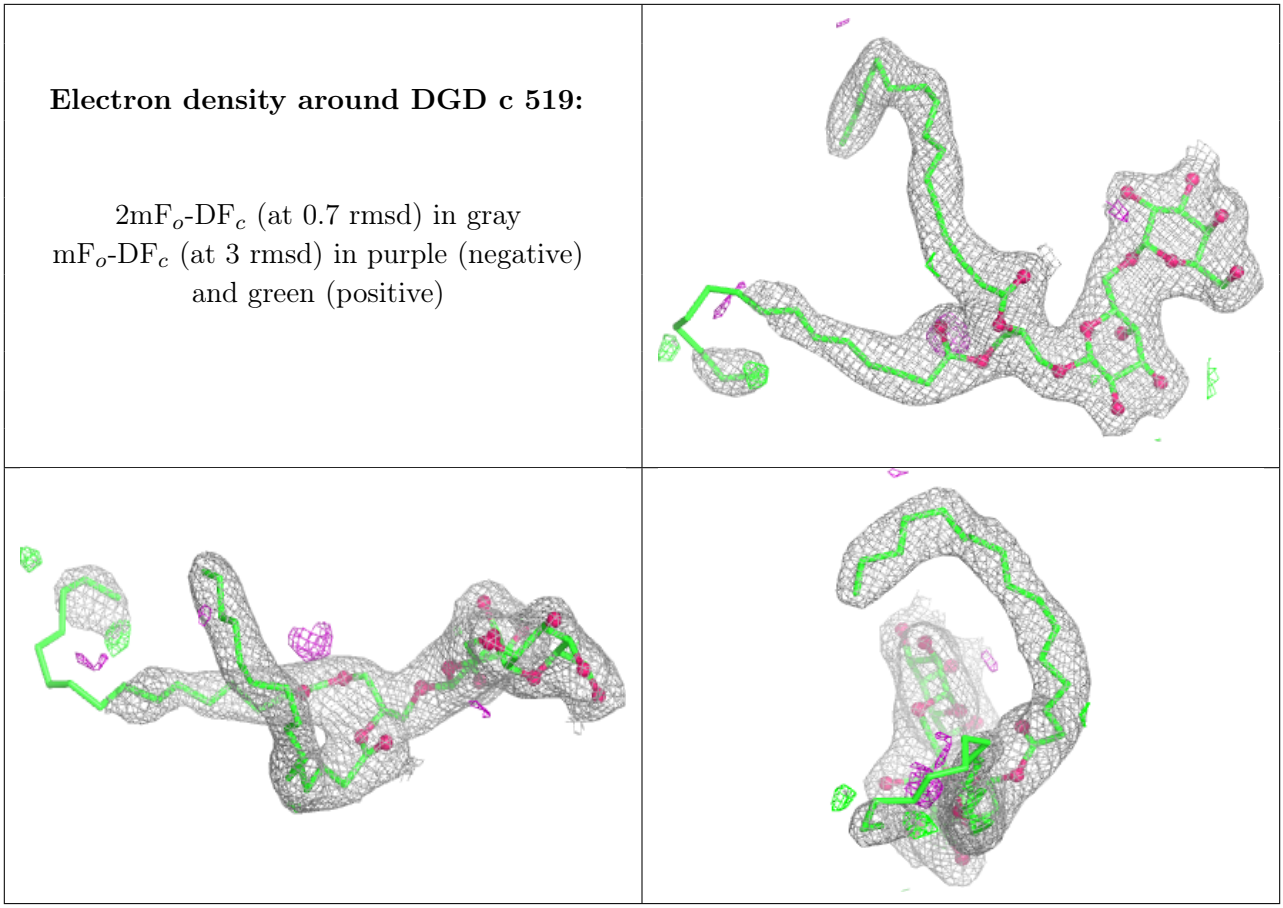






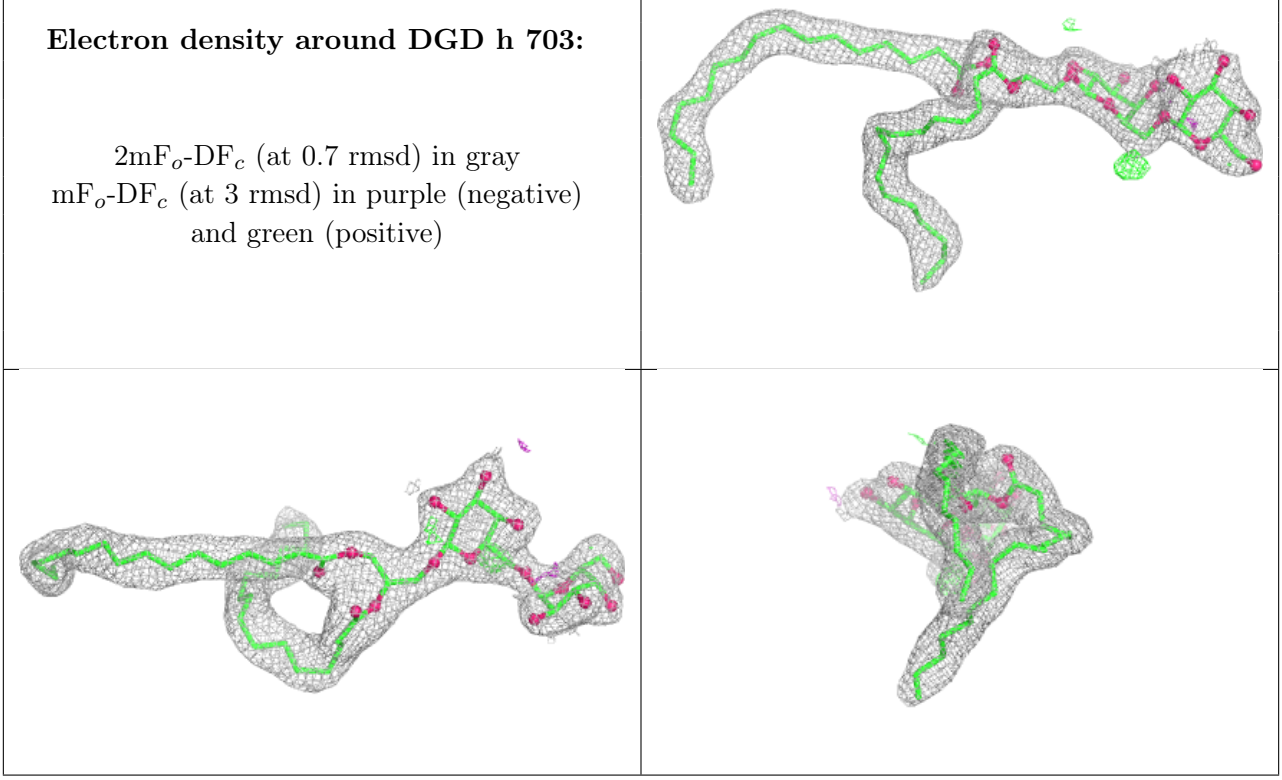
Electron density around DGD c 519:

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



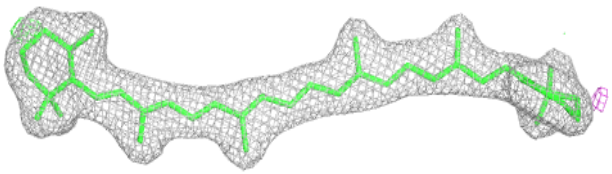
Electron density around DGD h 703:

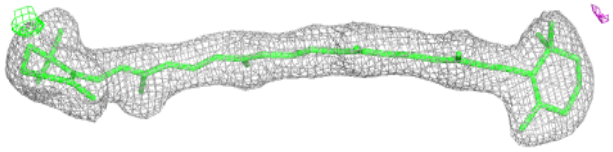
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

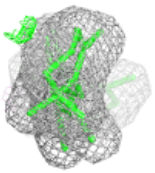


Electron density around BCR B 618:

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

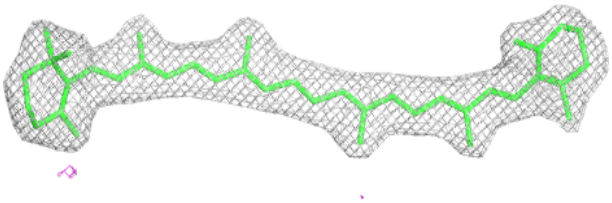


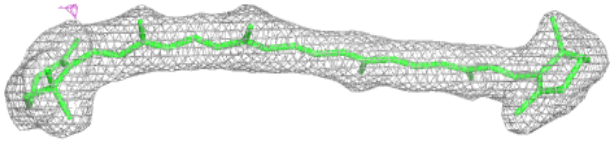


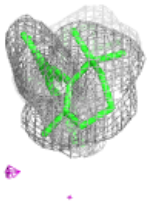


Electron density around BCR B 620:

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

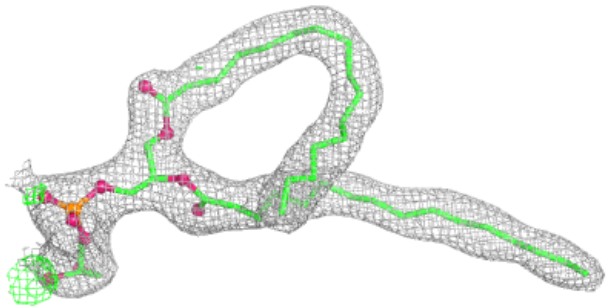


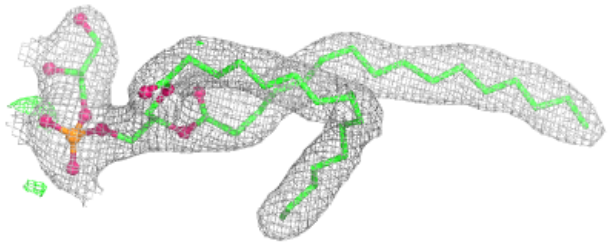


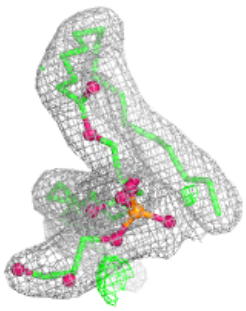


Electron density around LHG d 408:

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

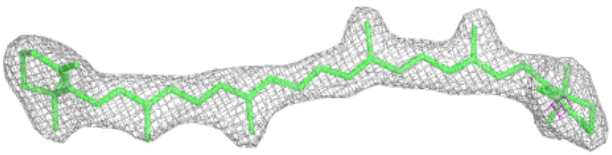


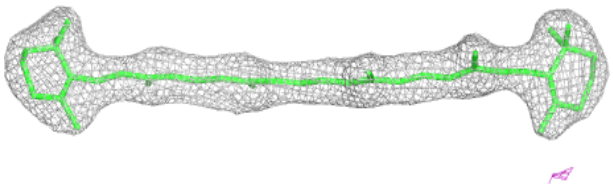


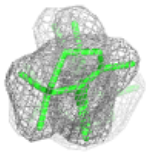


Electron density around BCR C 515:

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

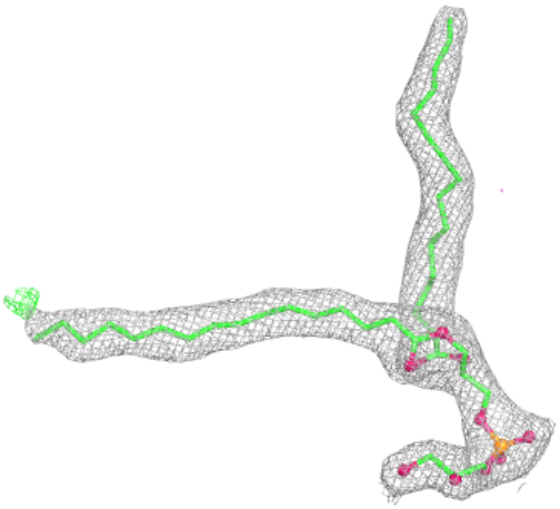


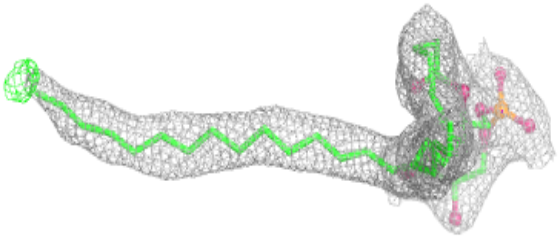


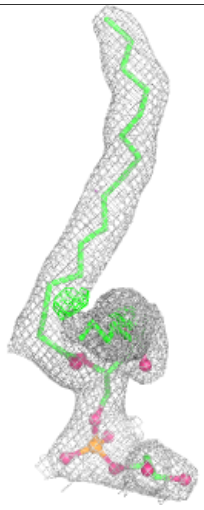


Electron density around LHG l 101:

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

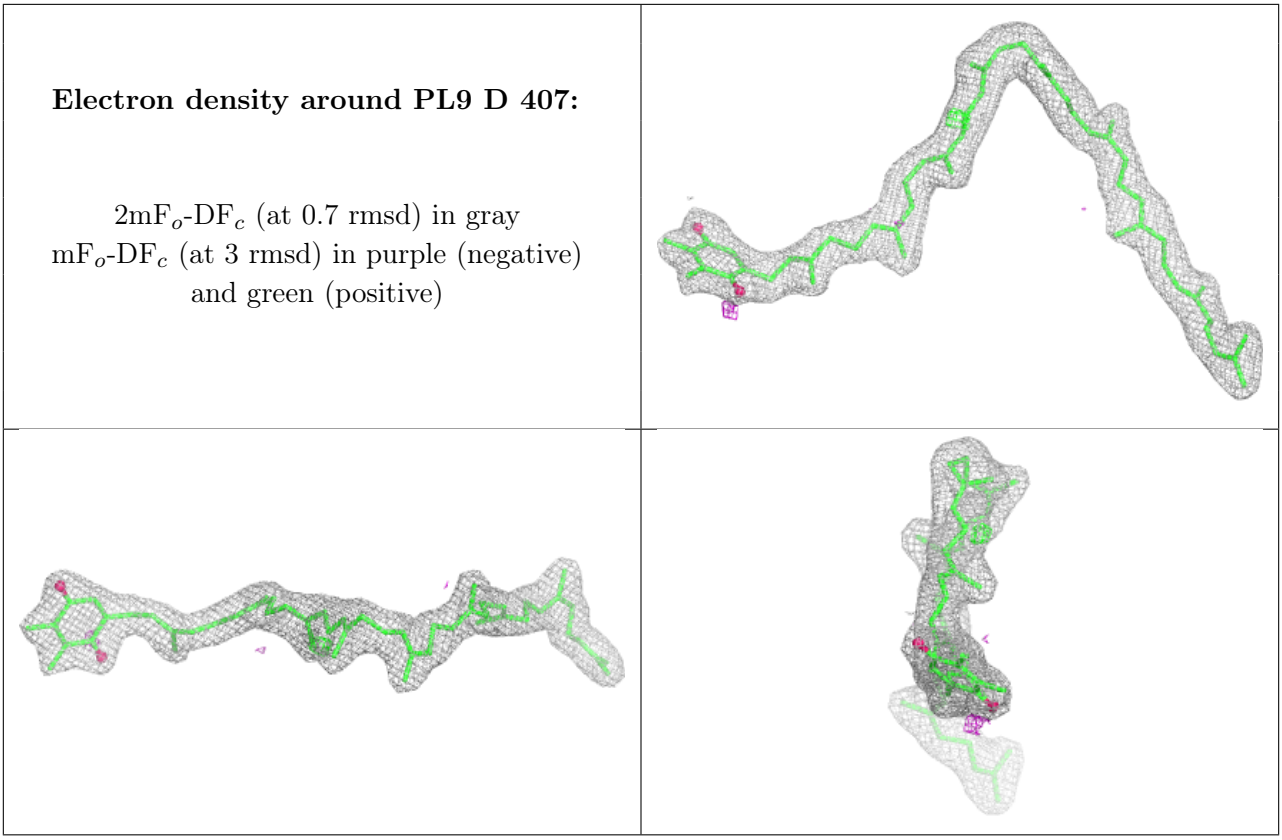






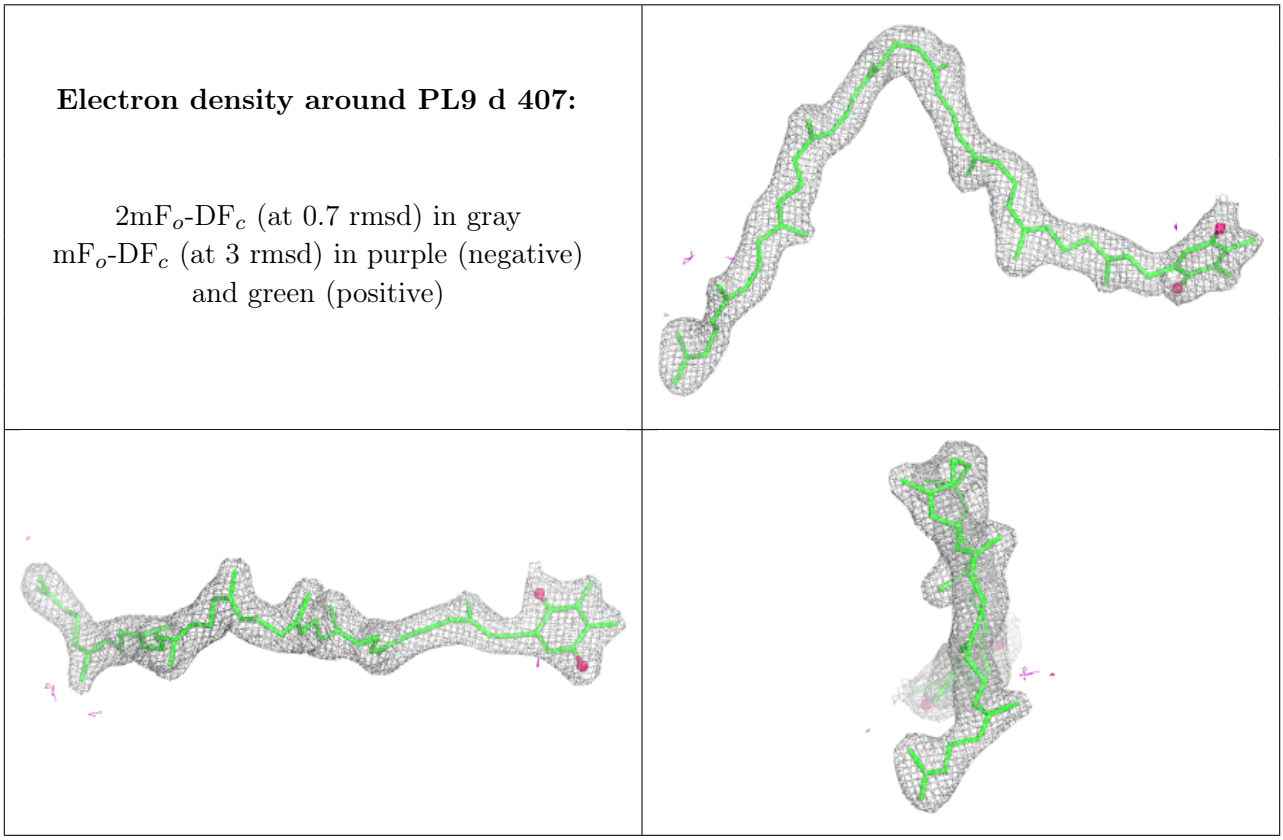
Electron density around PL9 D 407:

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



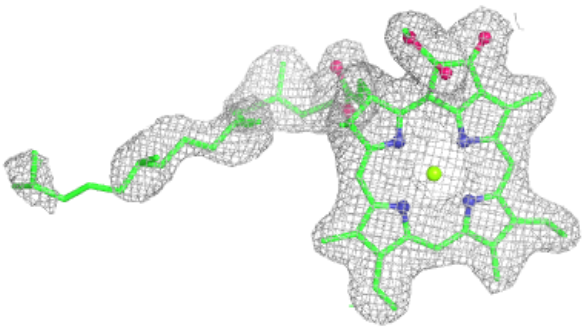
Electron density around PL9 d 407:

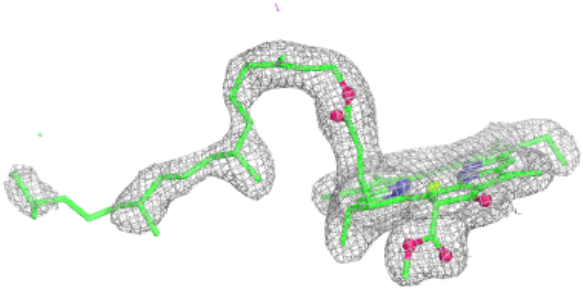
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

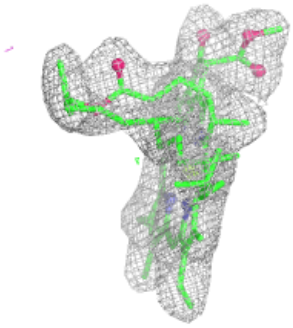


Electron density around CLA A 406:

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

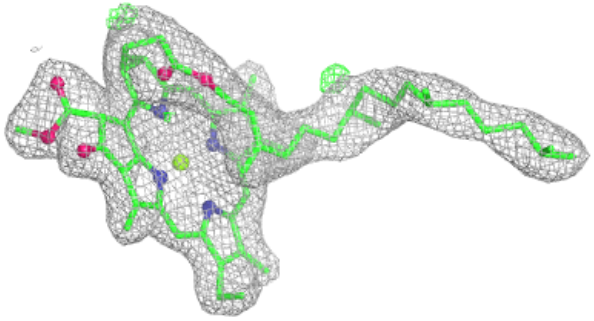


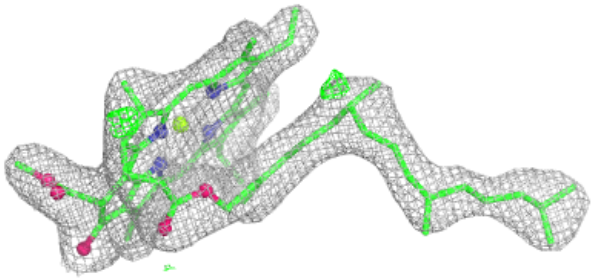


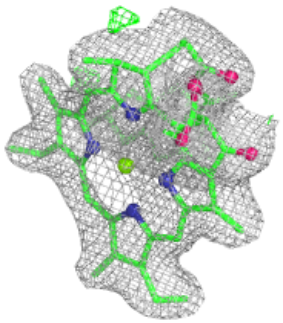


Electron density around CLA c 507:

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

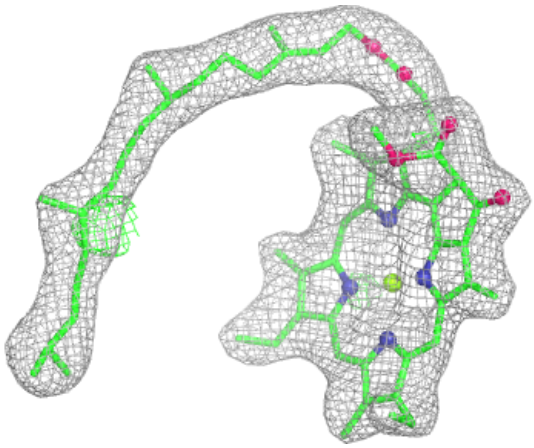


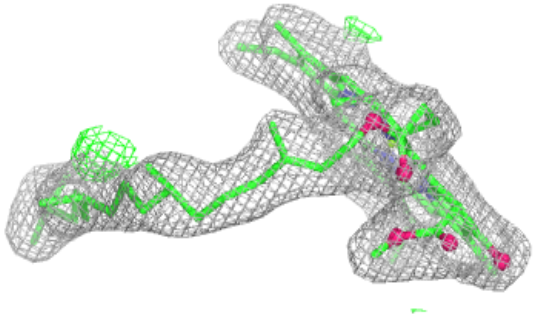


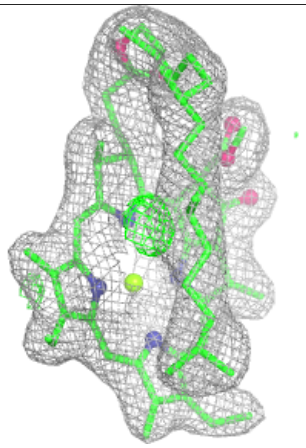


Electron density around CLA C 508:

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

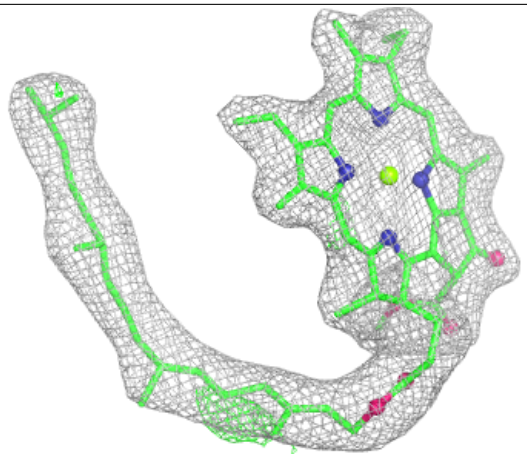


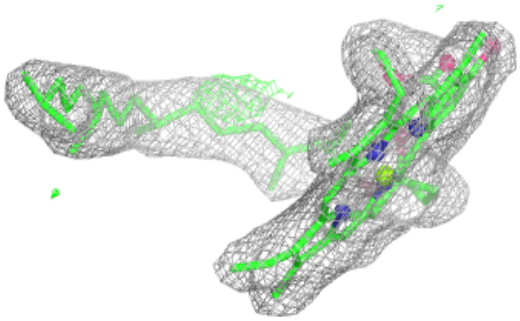




Electron density around CLA c 509:

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

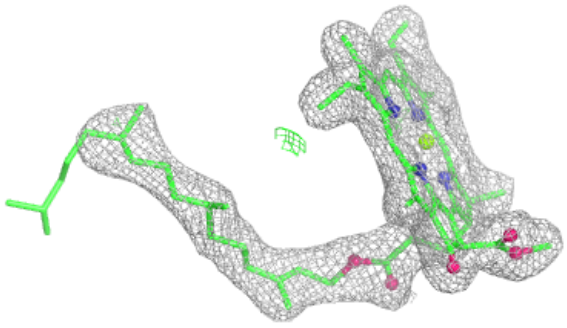


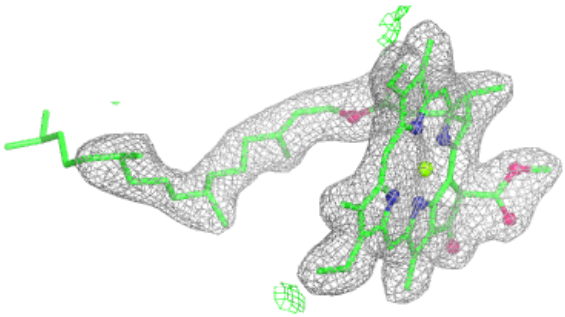


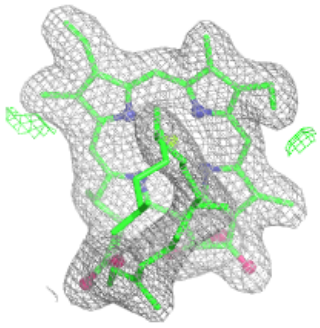


Electron density around CLA C 509:

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

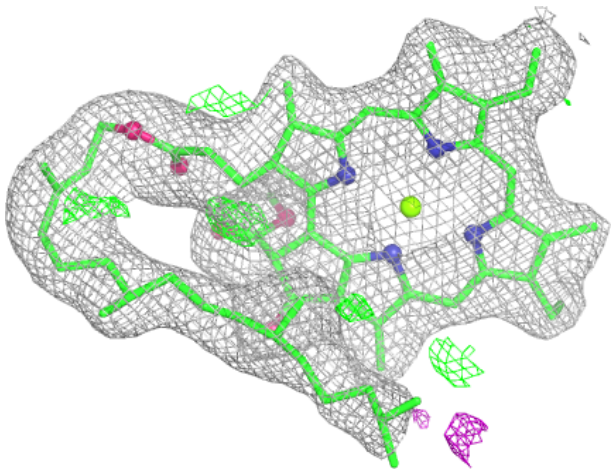


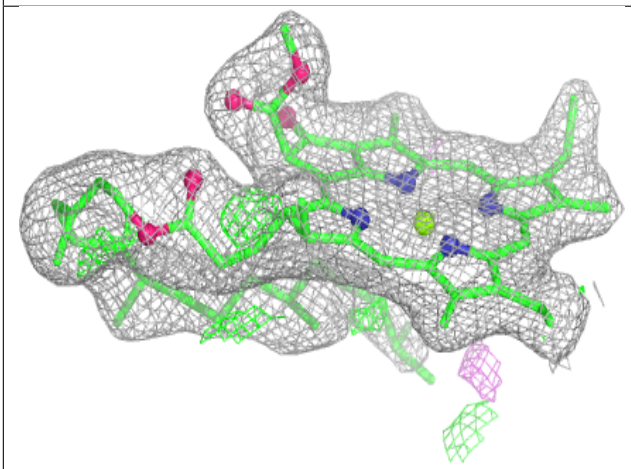


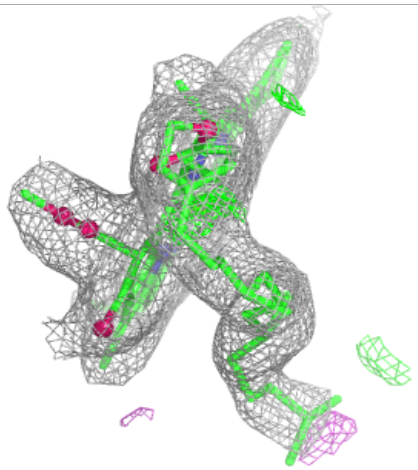


Electron density around CLA c 511:

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

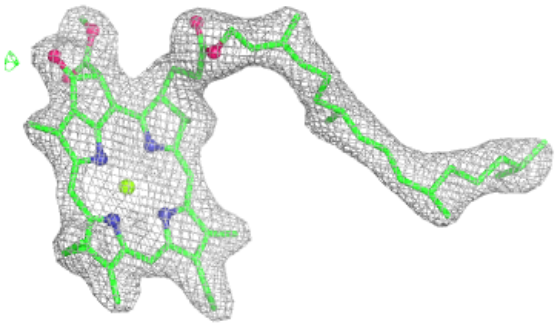


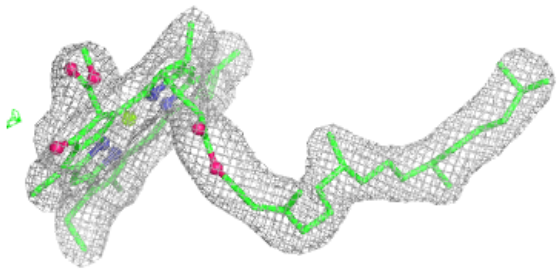


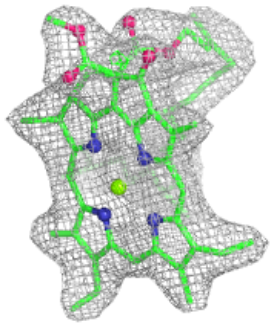


Electron density around CLA c 513:

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

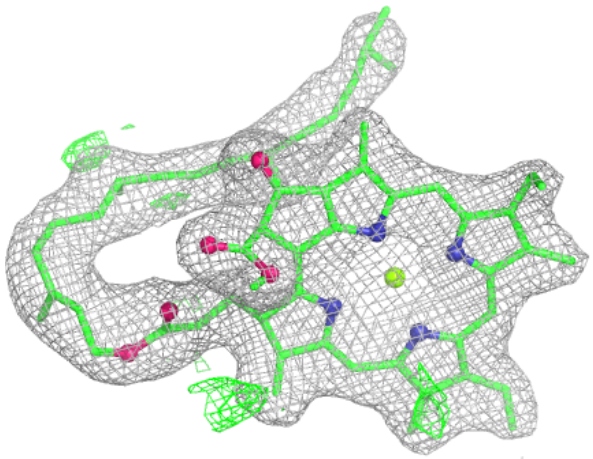


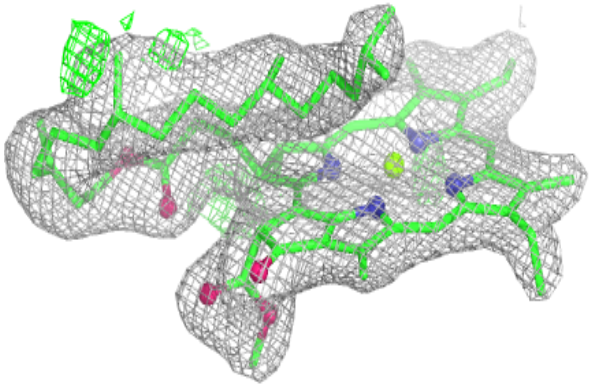


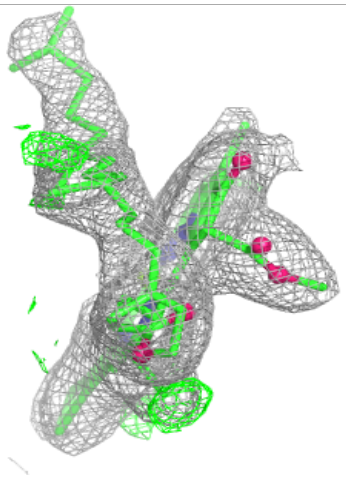


Electron density around CLA C 510:

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

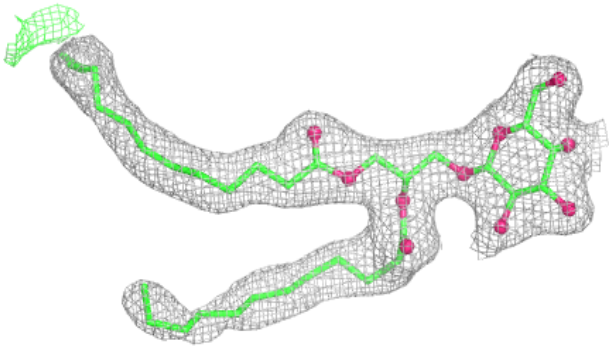


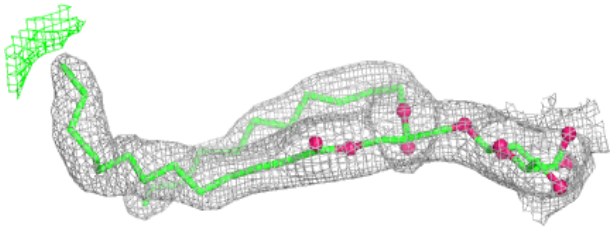


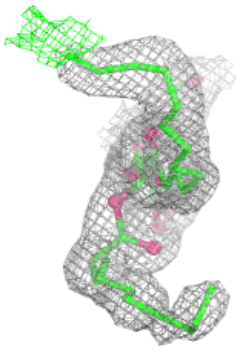


Electron density around LMG D 412:

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

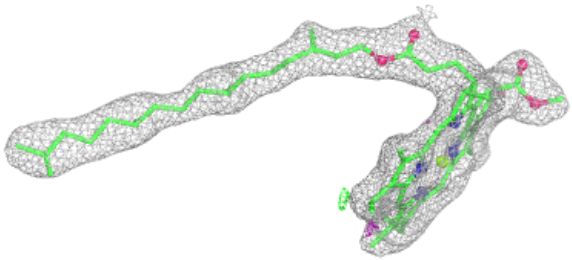


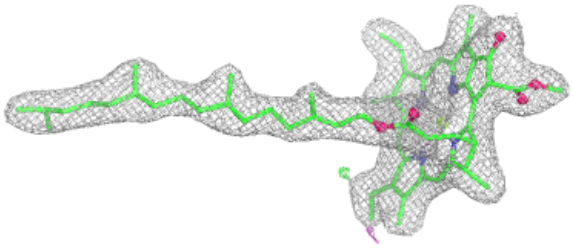


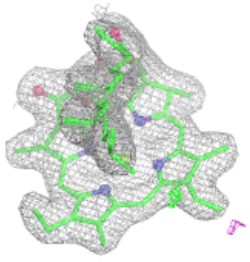


Electron density around CLA B 608:

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

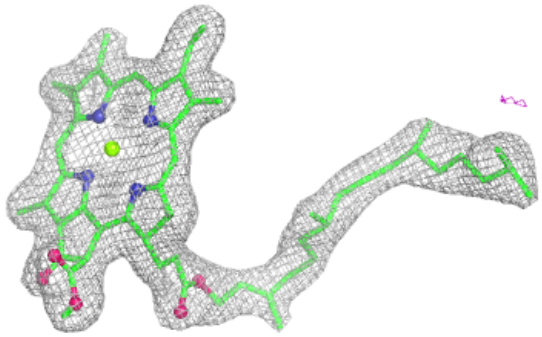


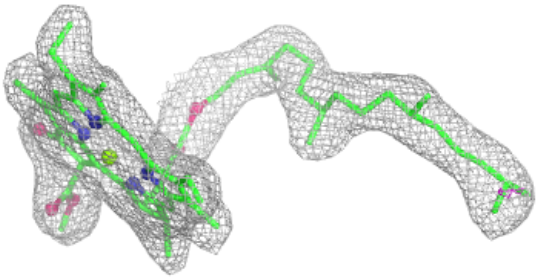


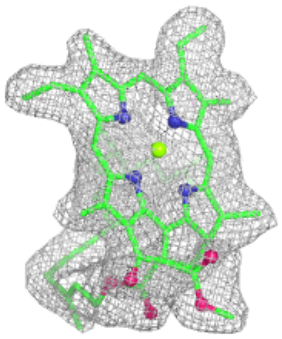


Electron density around CLA C 512:

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

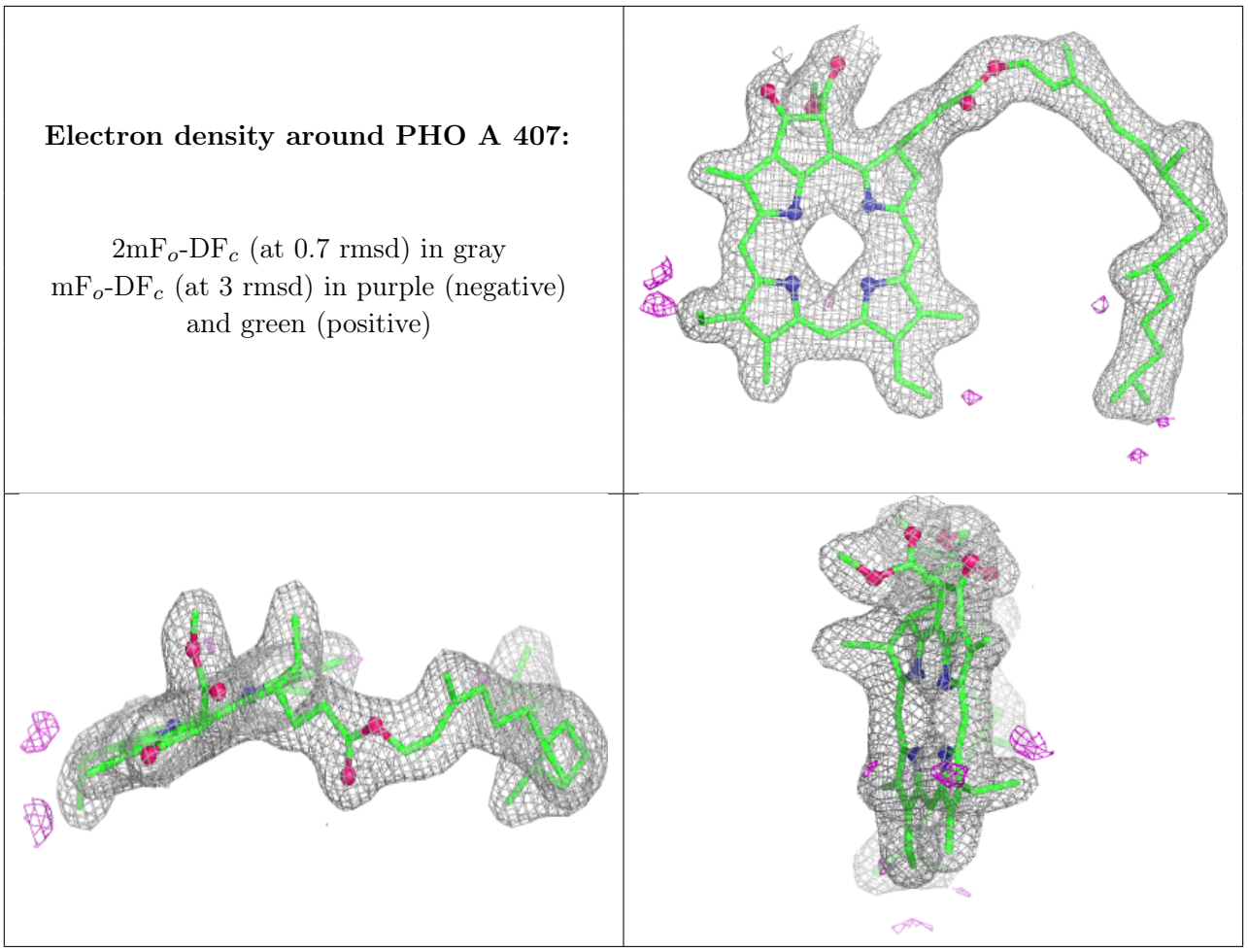






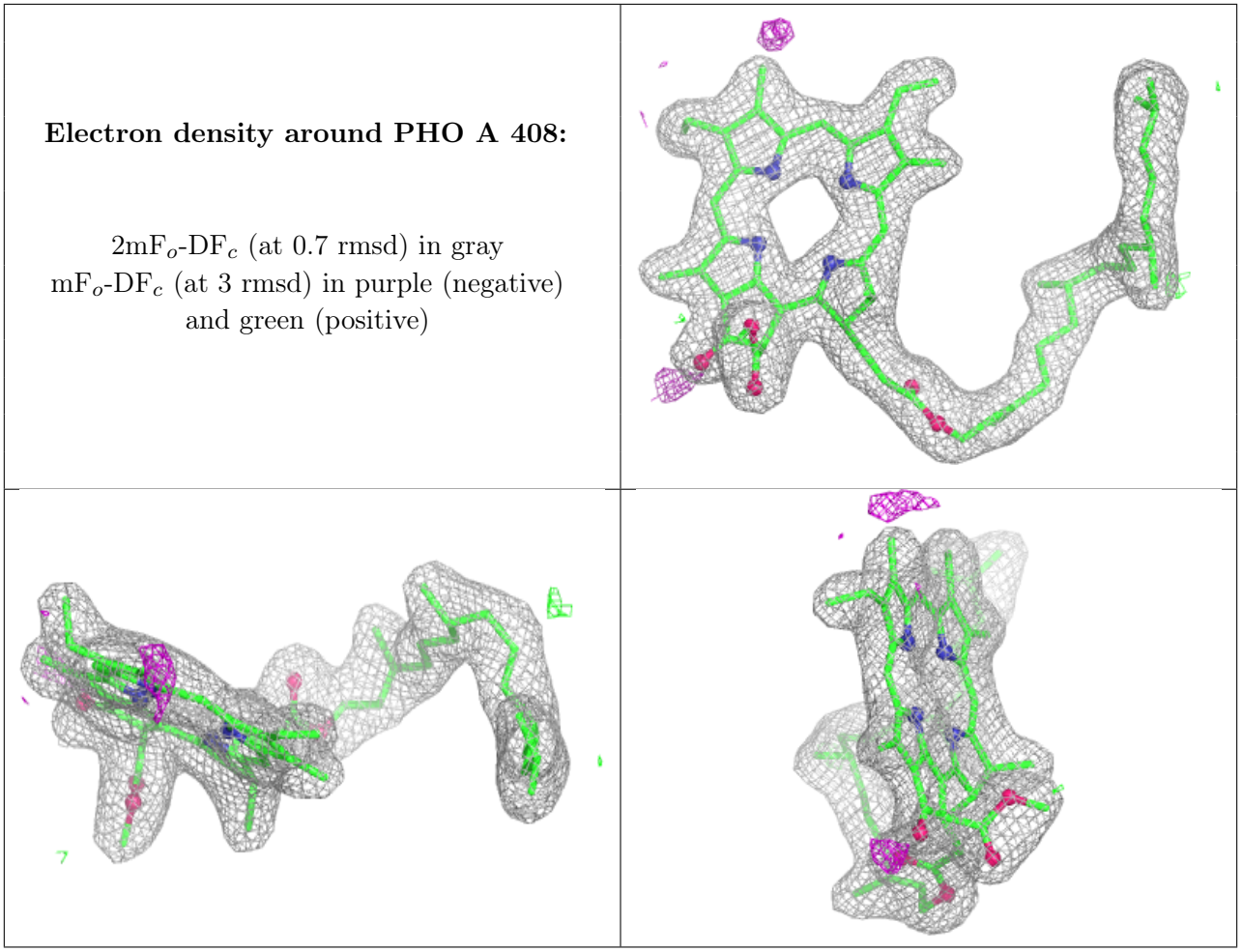
Electron density around PHO A 407:

$2mF_o$-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 408:

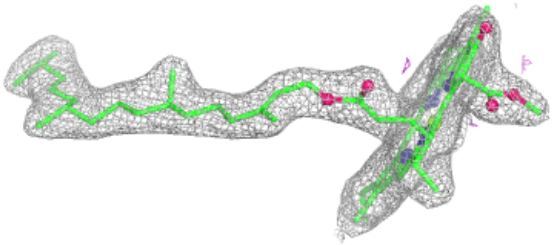
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

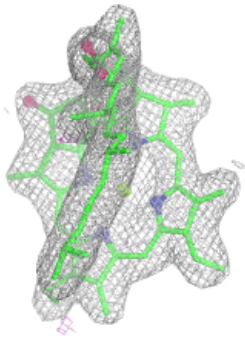


Electron density around CLA B 610:

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

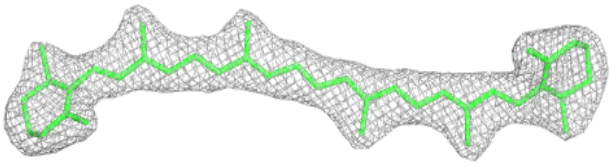


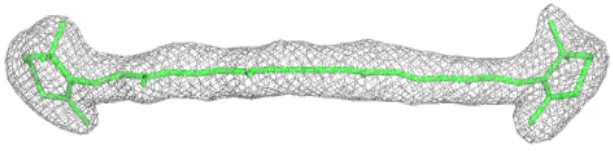


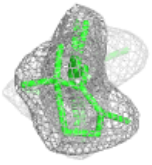


Electron density around BCR B 619:

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

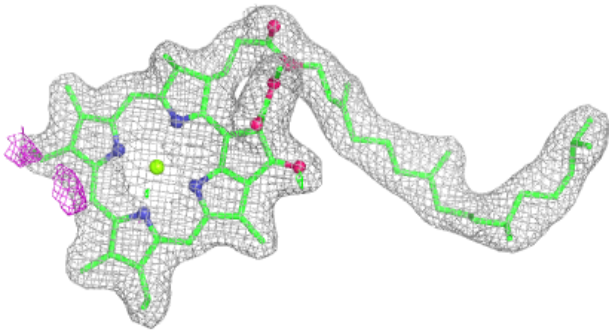


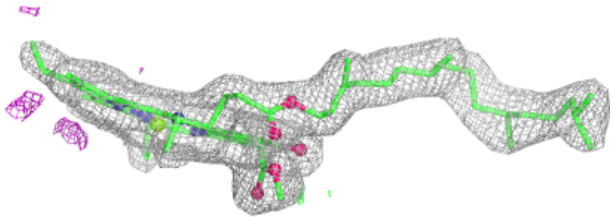


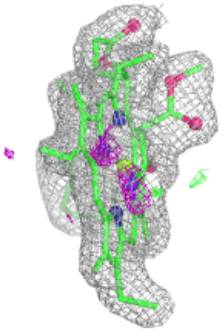


Electron density around CLA B 603:

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

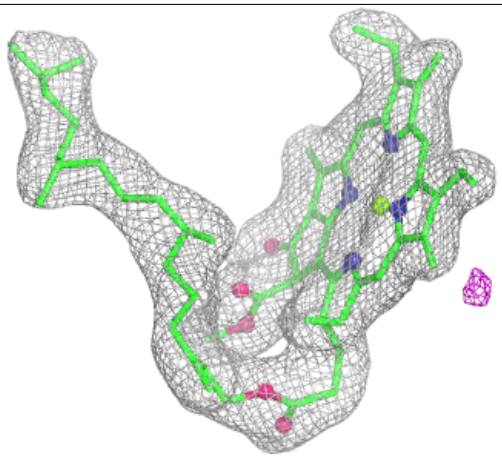


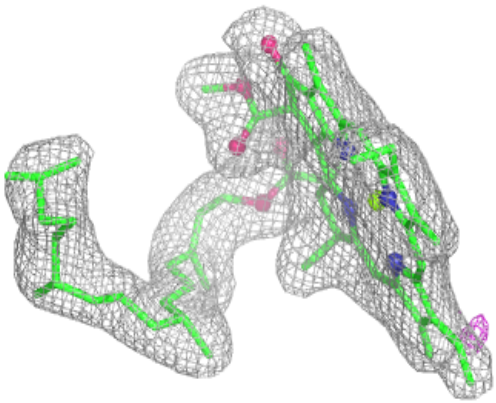


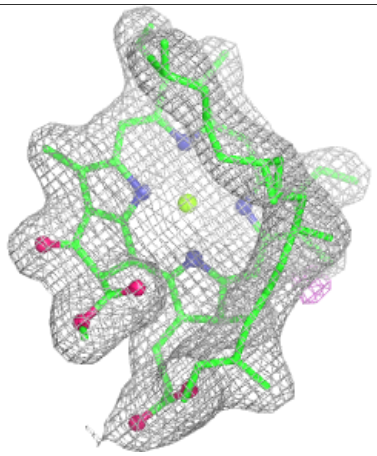


Electron density around CLA B 614:

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

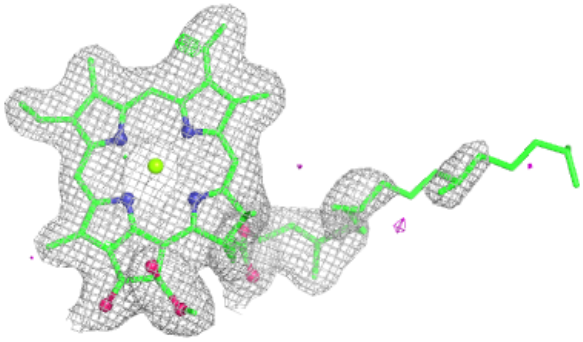


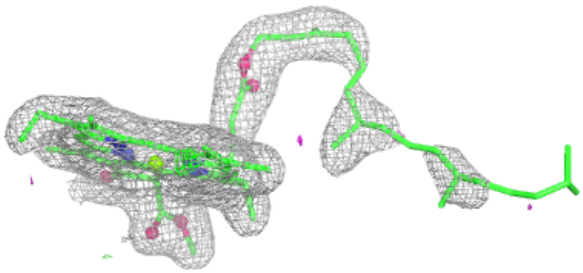


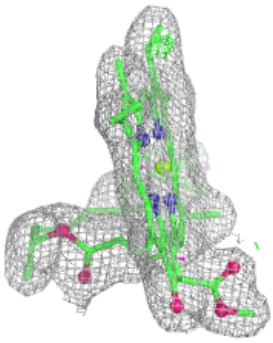


Electron density around CLA a 2110:

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

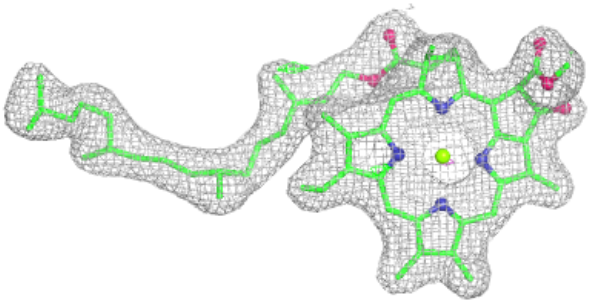


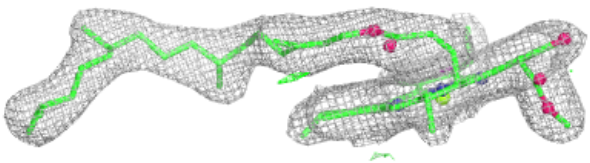


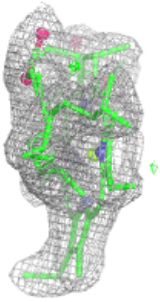


Electron density around CLA B 604:

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

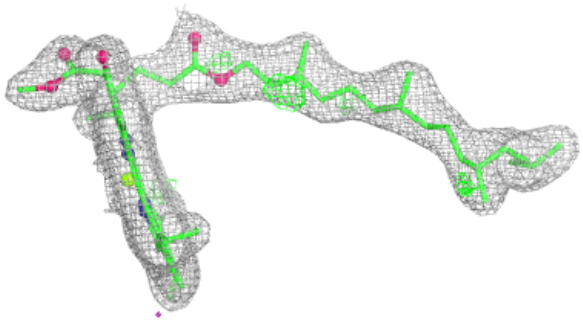


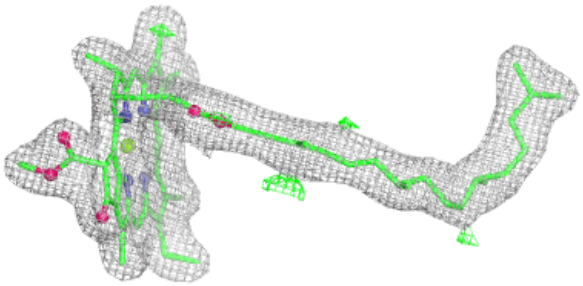


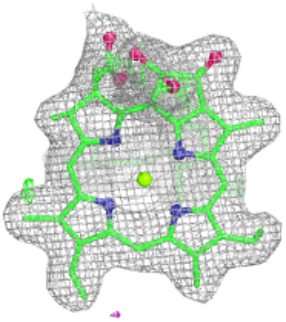


Electron density around CLA B 606:

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

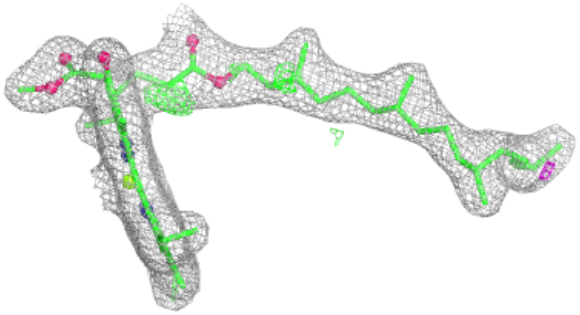


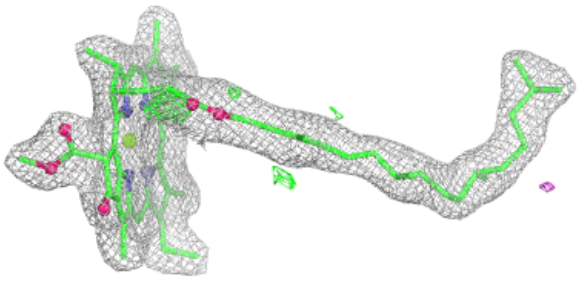


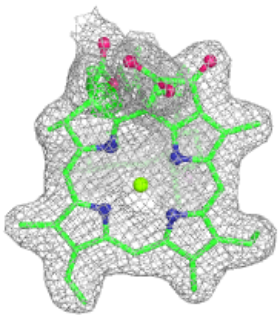


Electron density around CLA b 608:

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

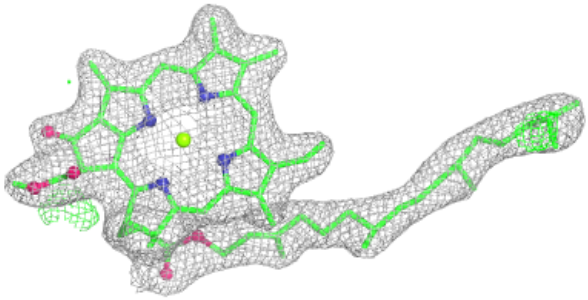


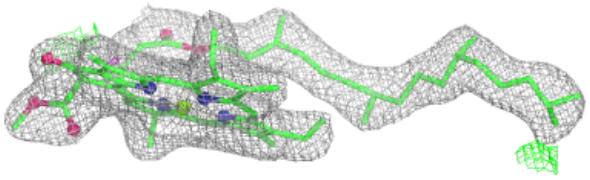


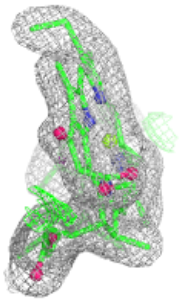


Electron density around CLA C 502:

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

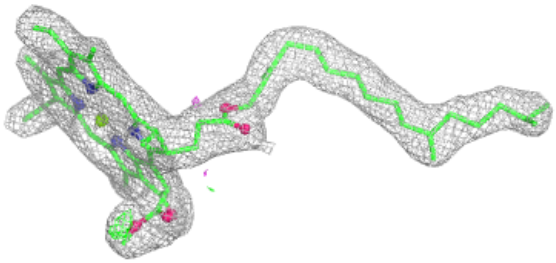


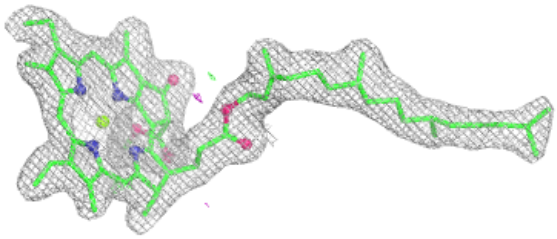


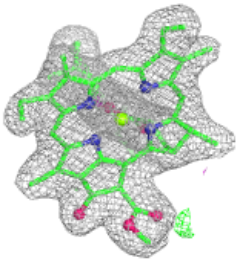


Electron density around CLA C 503:

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

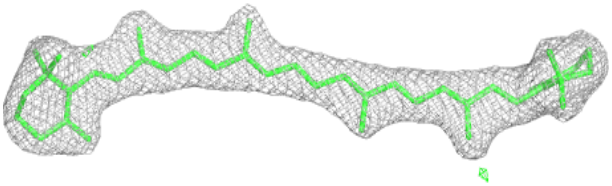


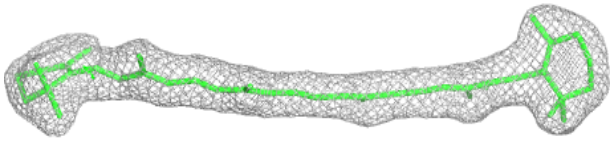


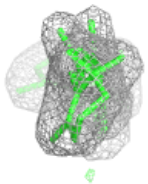


Electron density around BCR b 620:

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

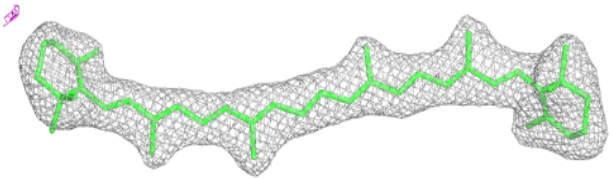


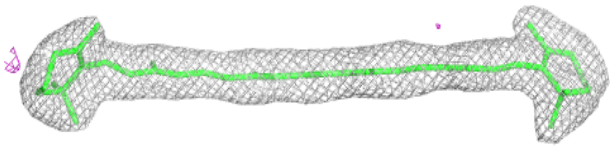


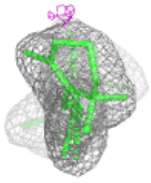


Electron density around BCR b 621:

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

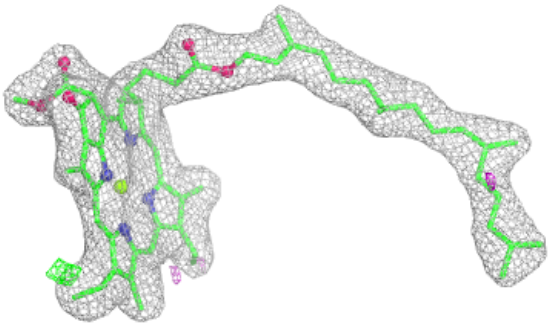


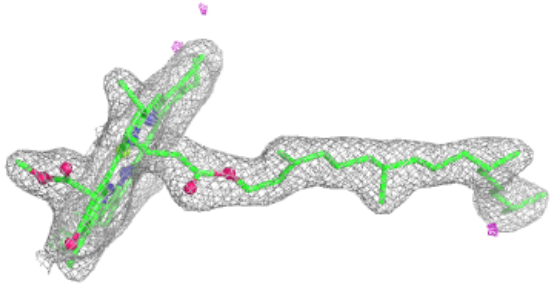


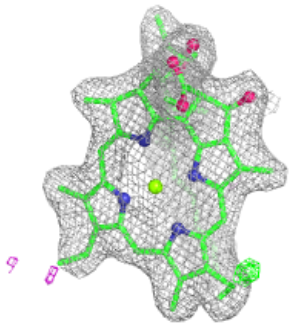


Electron density around CLA b 612:

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

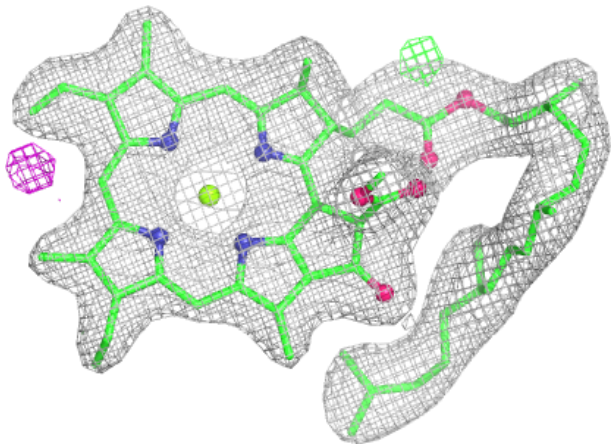


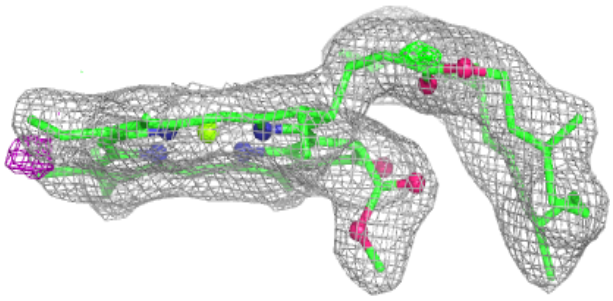


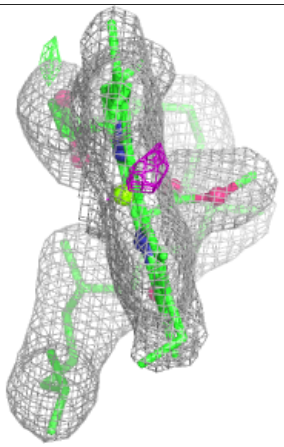


Electron density around CLA b 613:

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

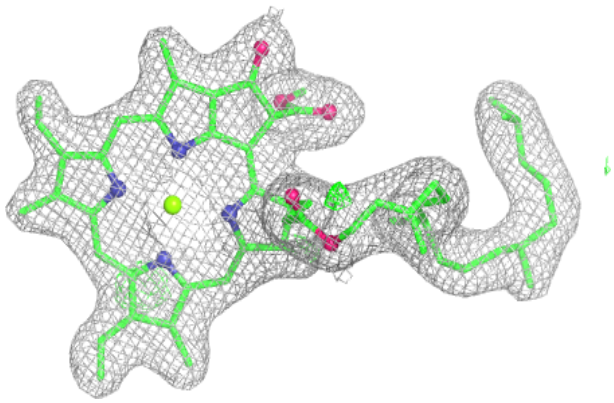


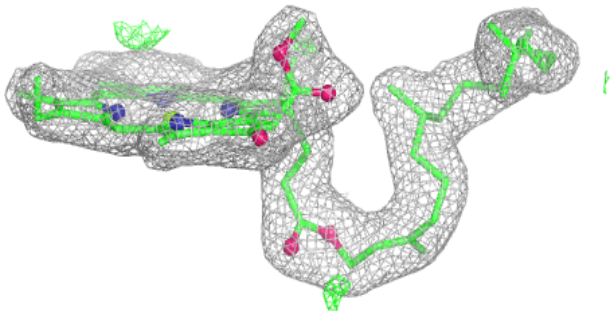


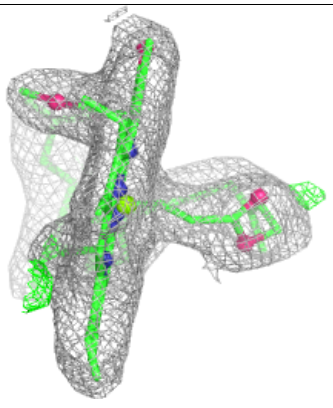


Electron density around CLA b 615:

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

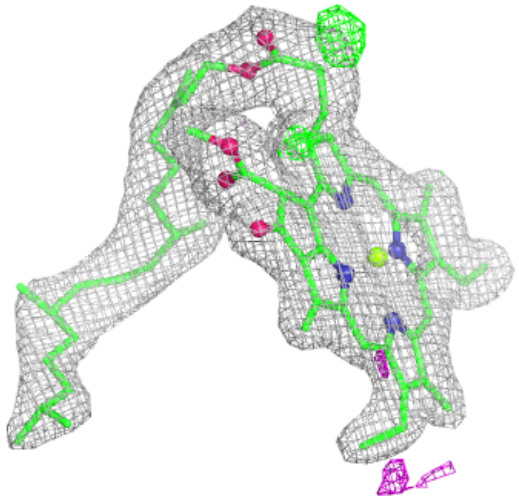


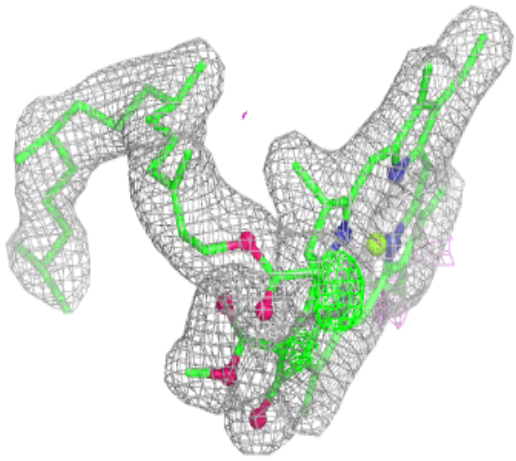


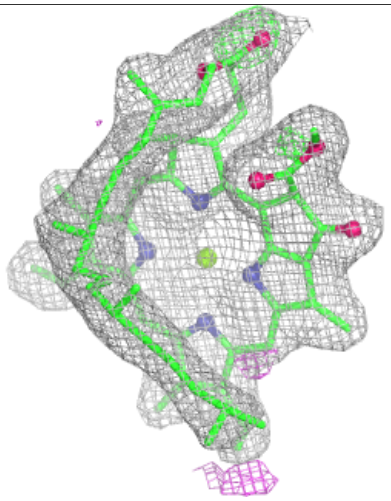


Electron density around CLA b 616:

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

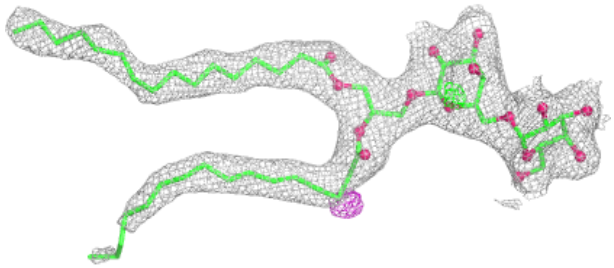


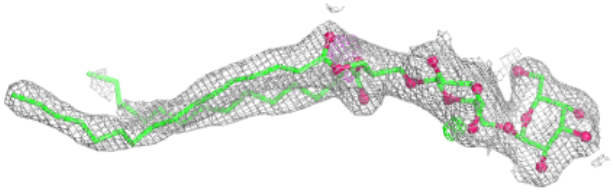


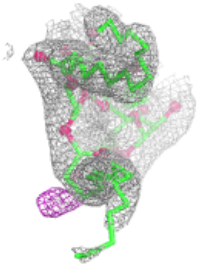


Electron density around DGD c 520:

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

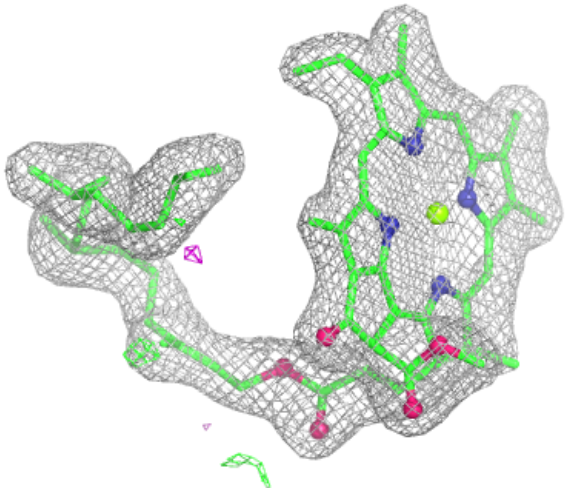


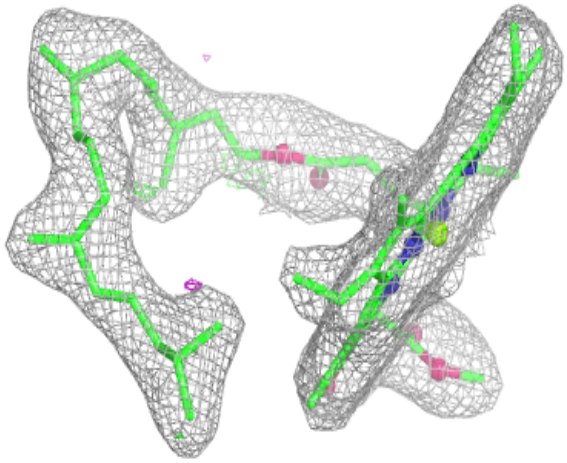


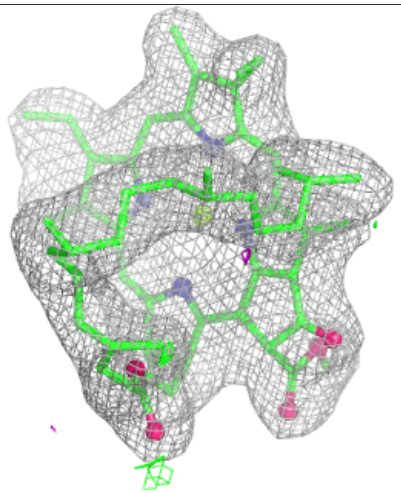


Electron density around CLA C 504:

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

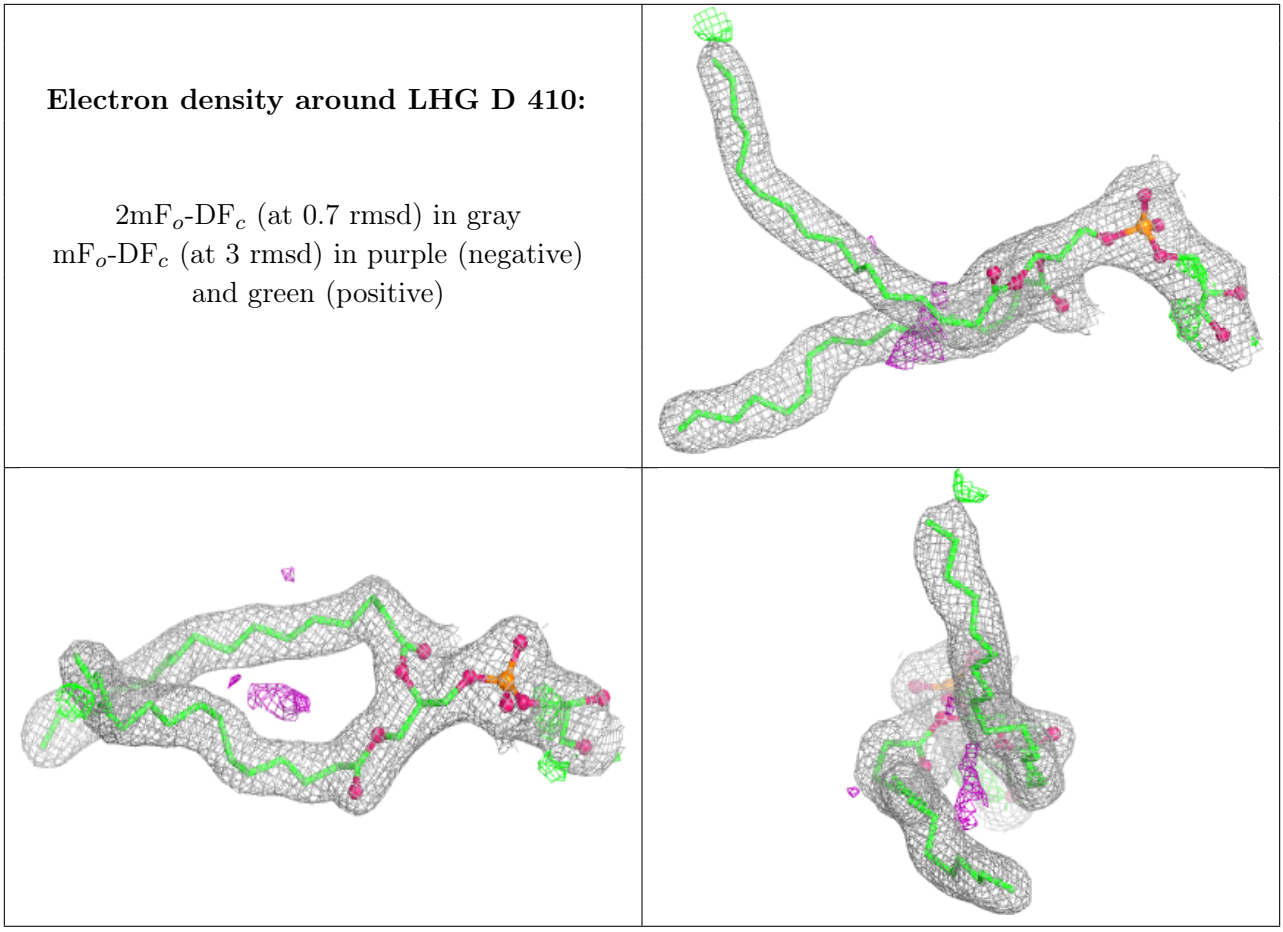






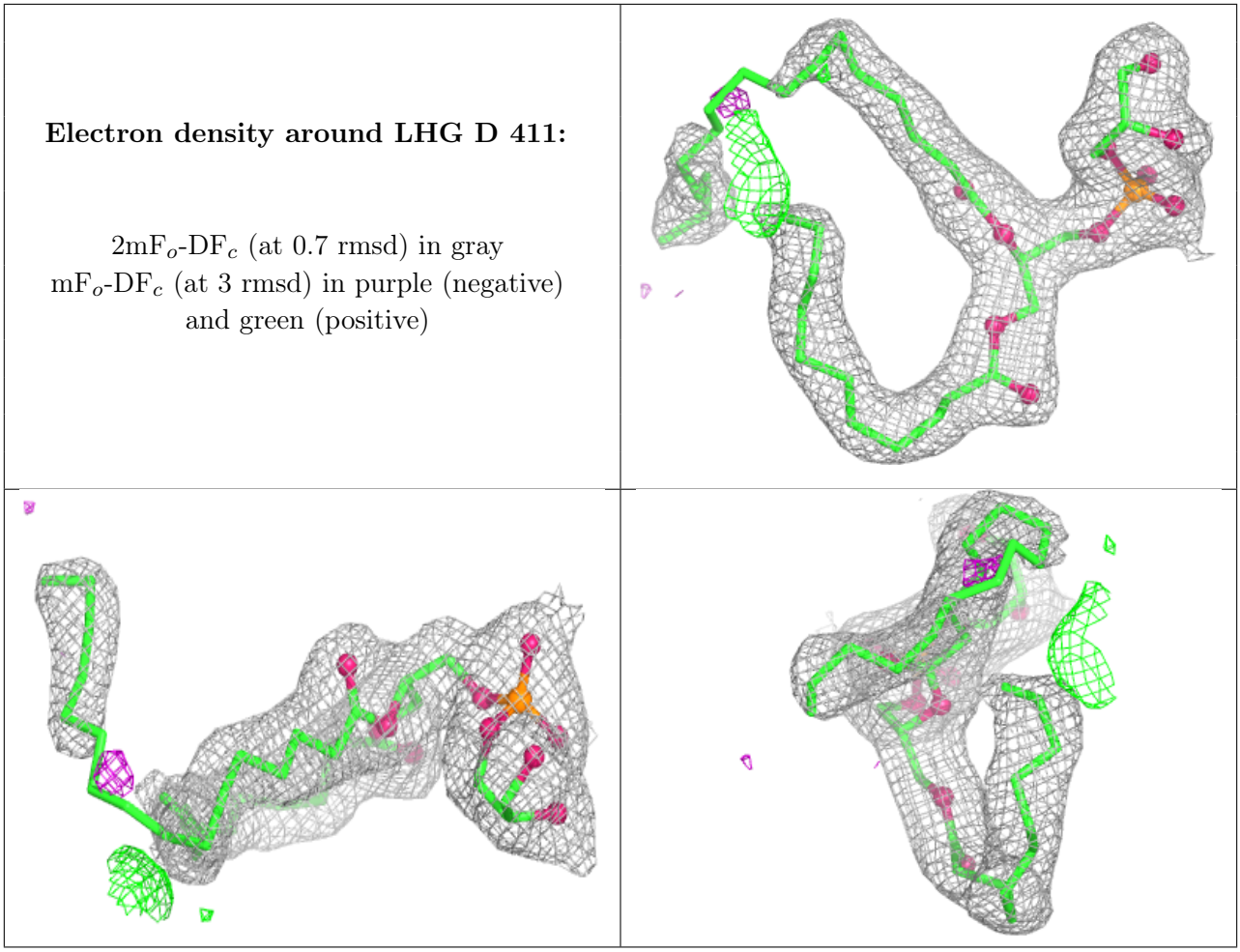
Electron density around LHG D 410:

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



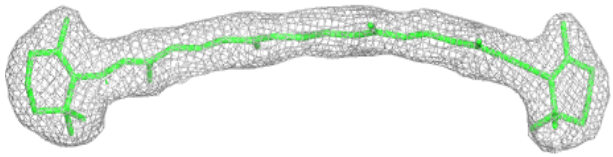
Electron density around LHG D 411:

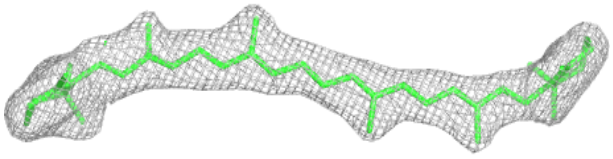
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

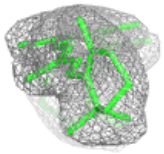


Electron density around BCR k 2003:

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

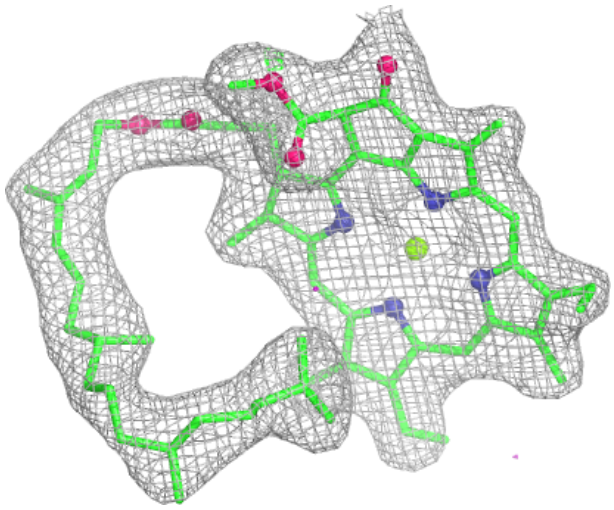


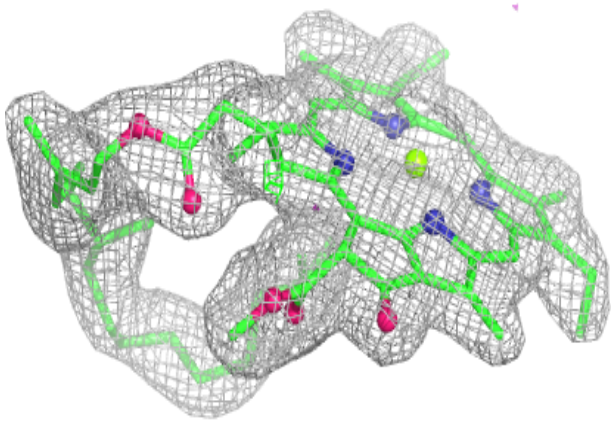




Electron density around CLA b 618:

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

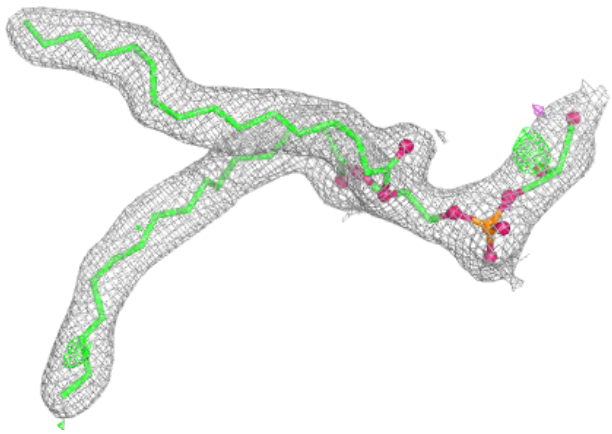


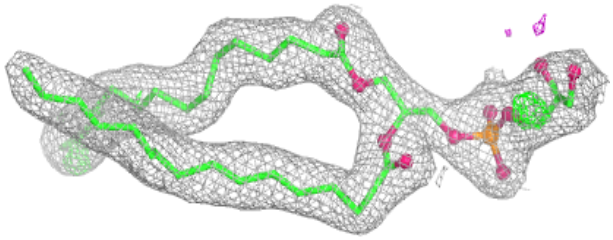


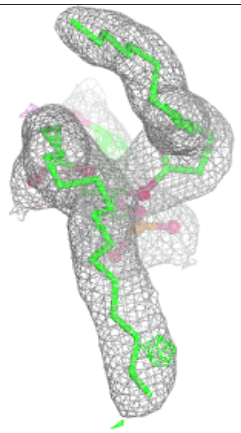


Electron density around LHG d 409:

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

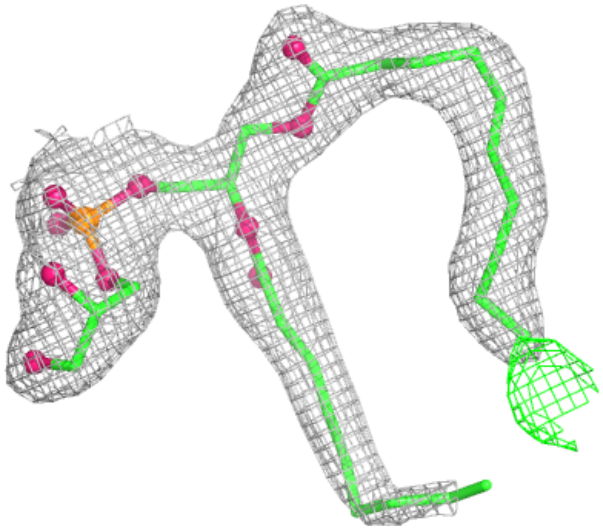


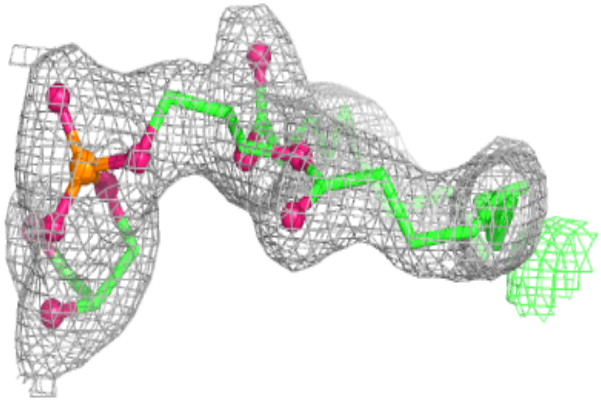




Electron density around LHG d 410:

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

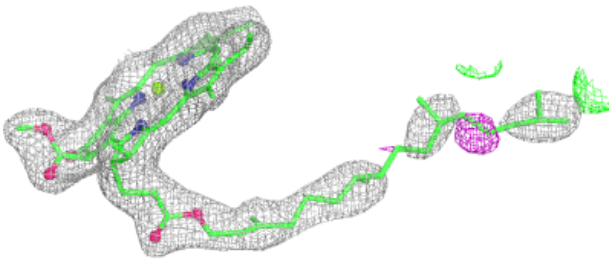


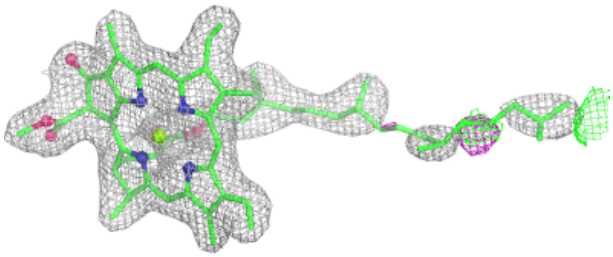


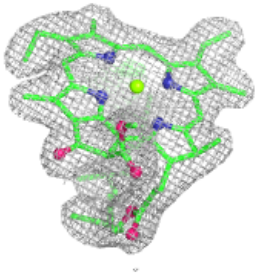


Electron density around CLA C 505:

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

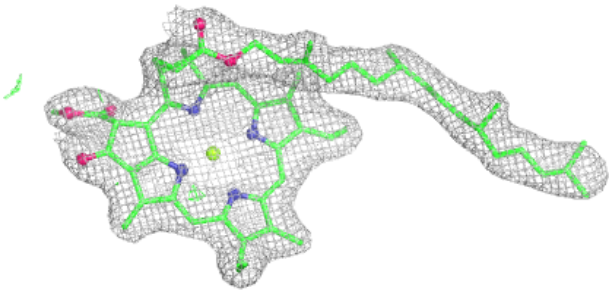


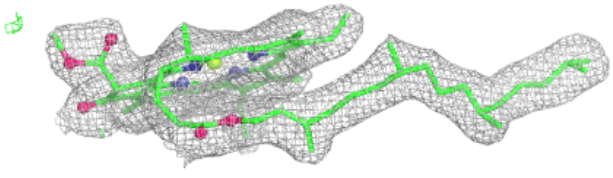




Electron density around CLA c 503:

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

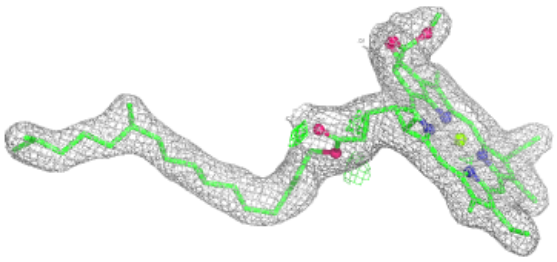


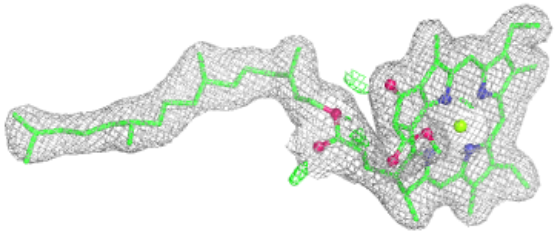


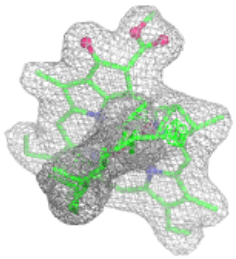


Electron density around CLA c 504:

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

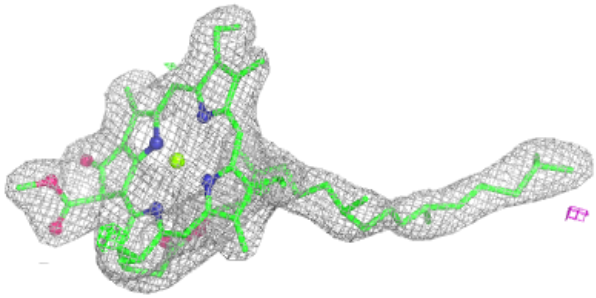


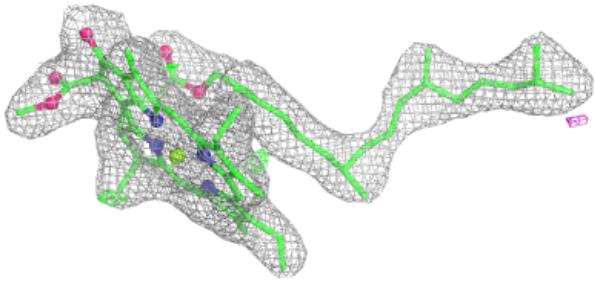


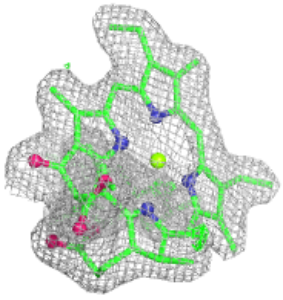


Electron density around CLA C 506:

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

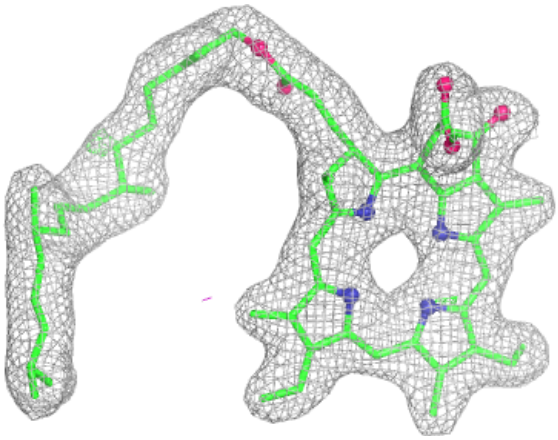


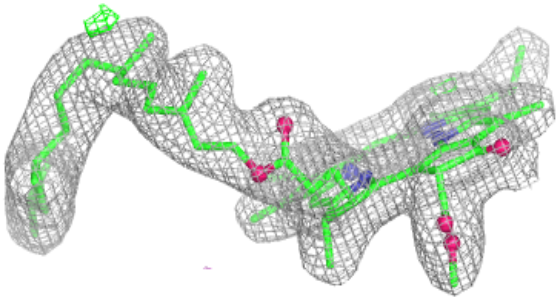


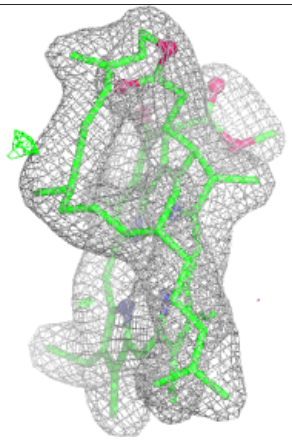


Electron density around PHO a 2112:

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

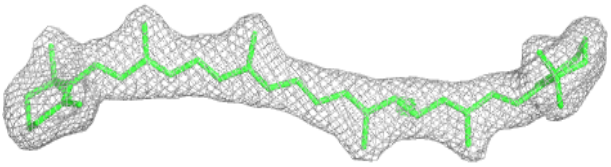


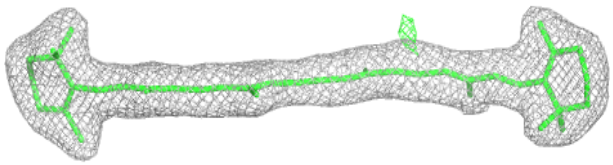


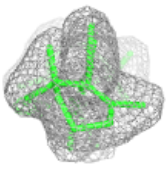


Electron density around BCR A 410:

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

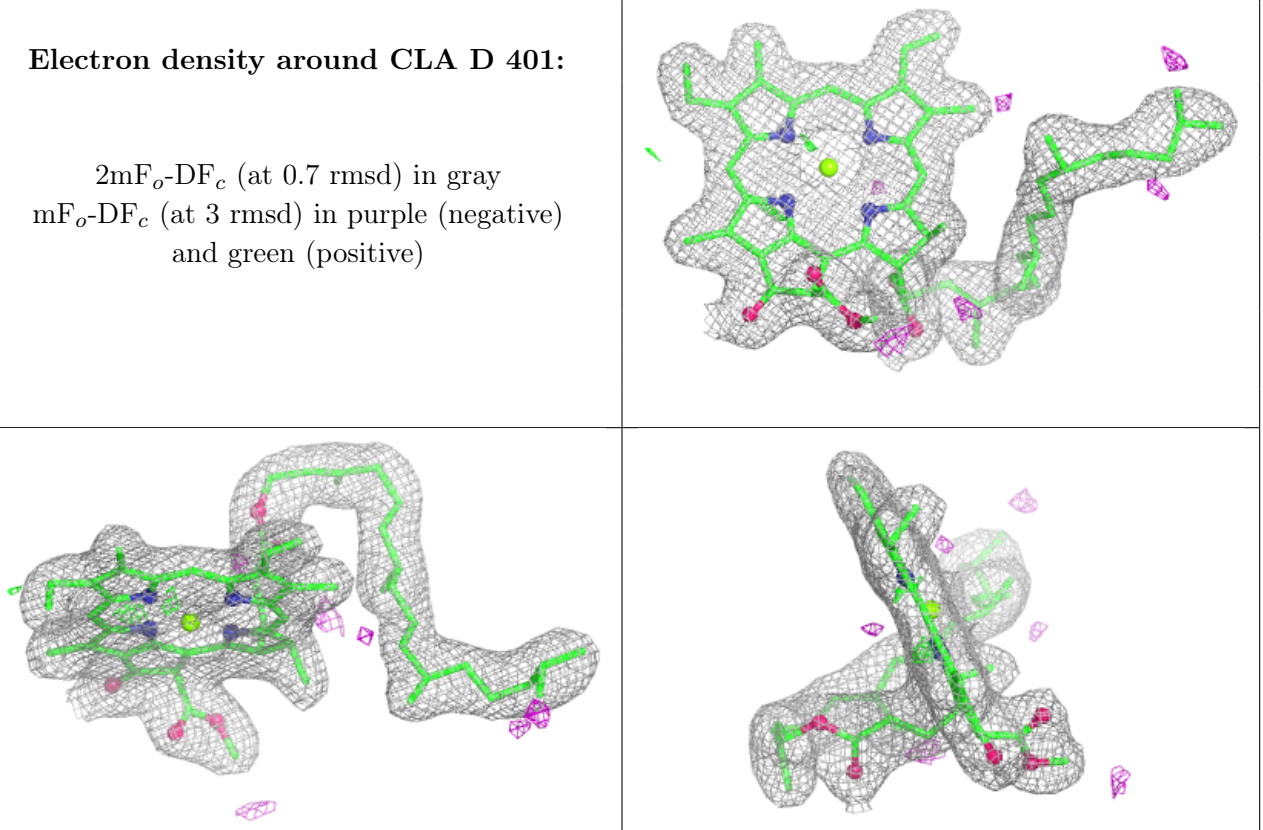






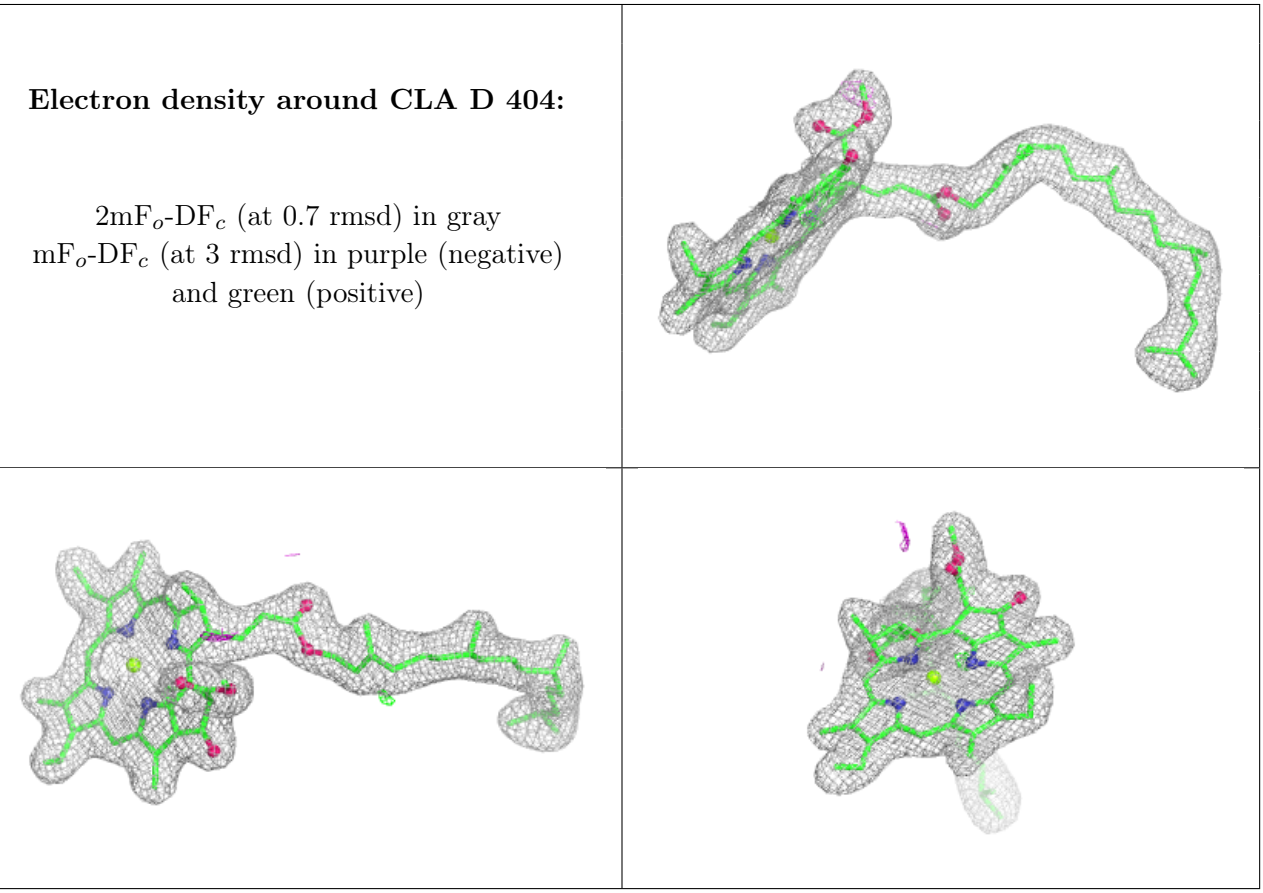
Electron density around CLA D 401:

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



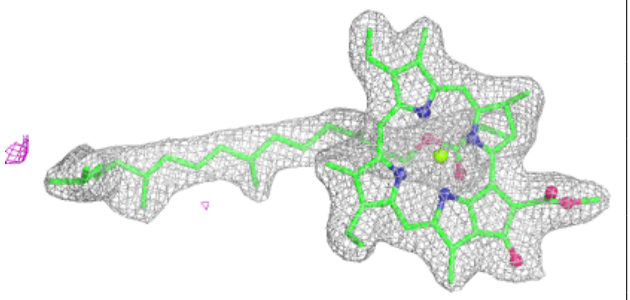
Electron density around CLA D 404:

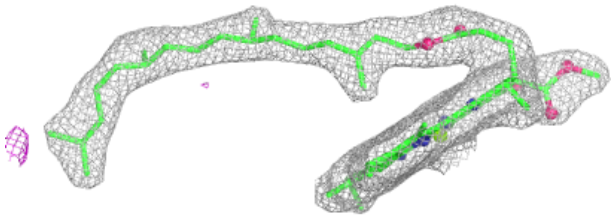
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

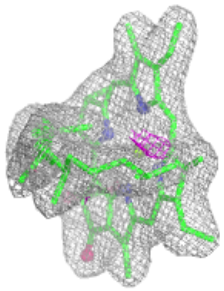


Electron density around CLA b 611:

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

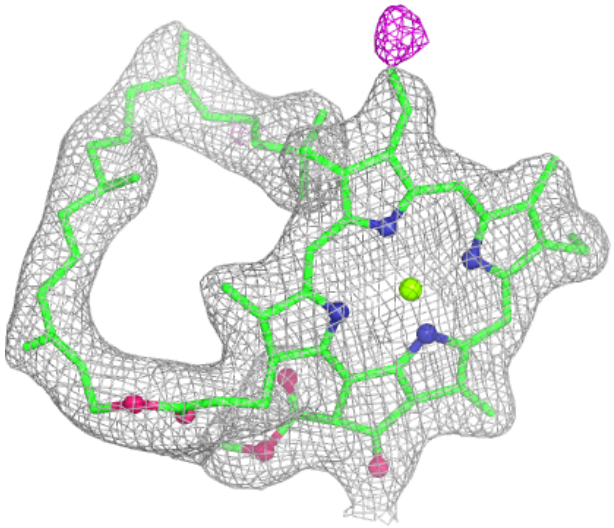


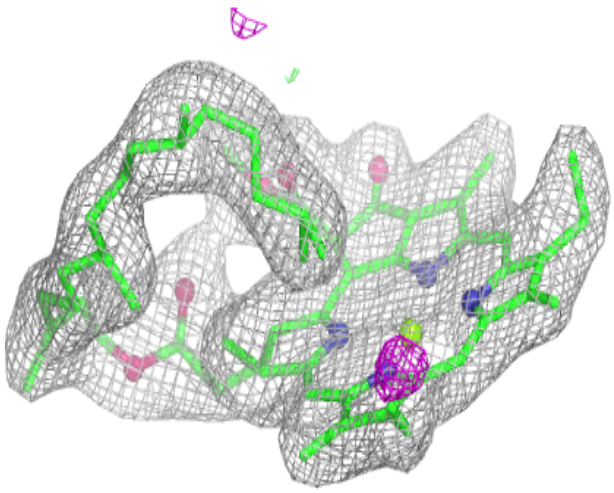


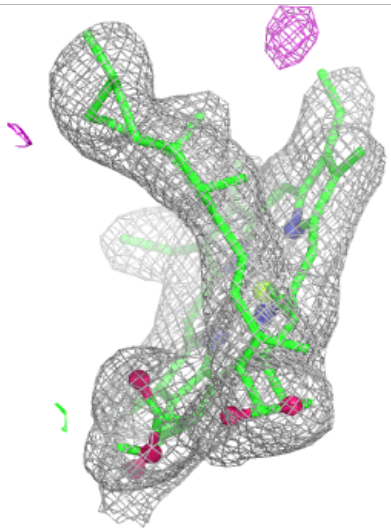


Electron density around CLA B 616:

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

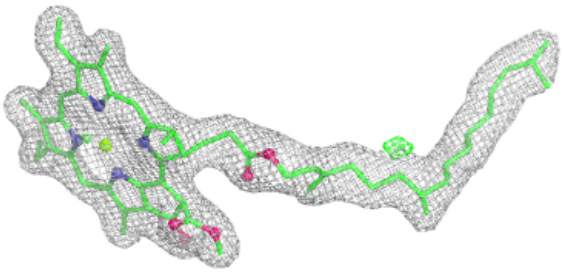


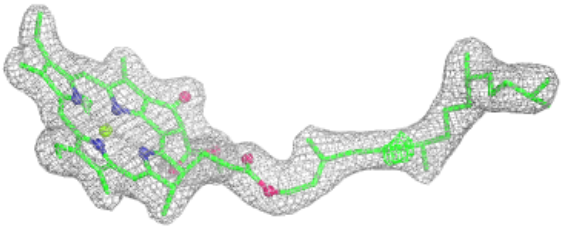


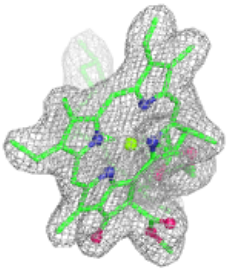


Electron density around CLA a 2109:

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

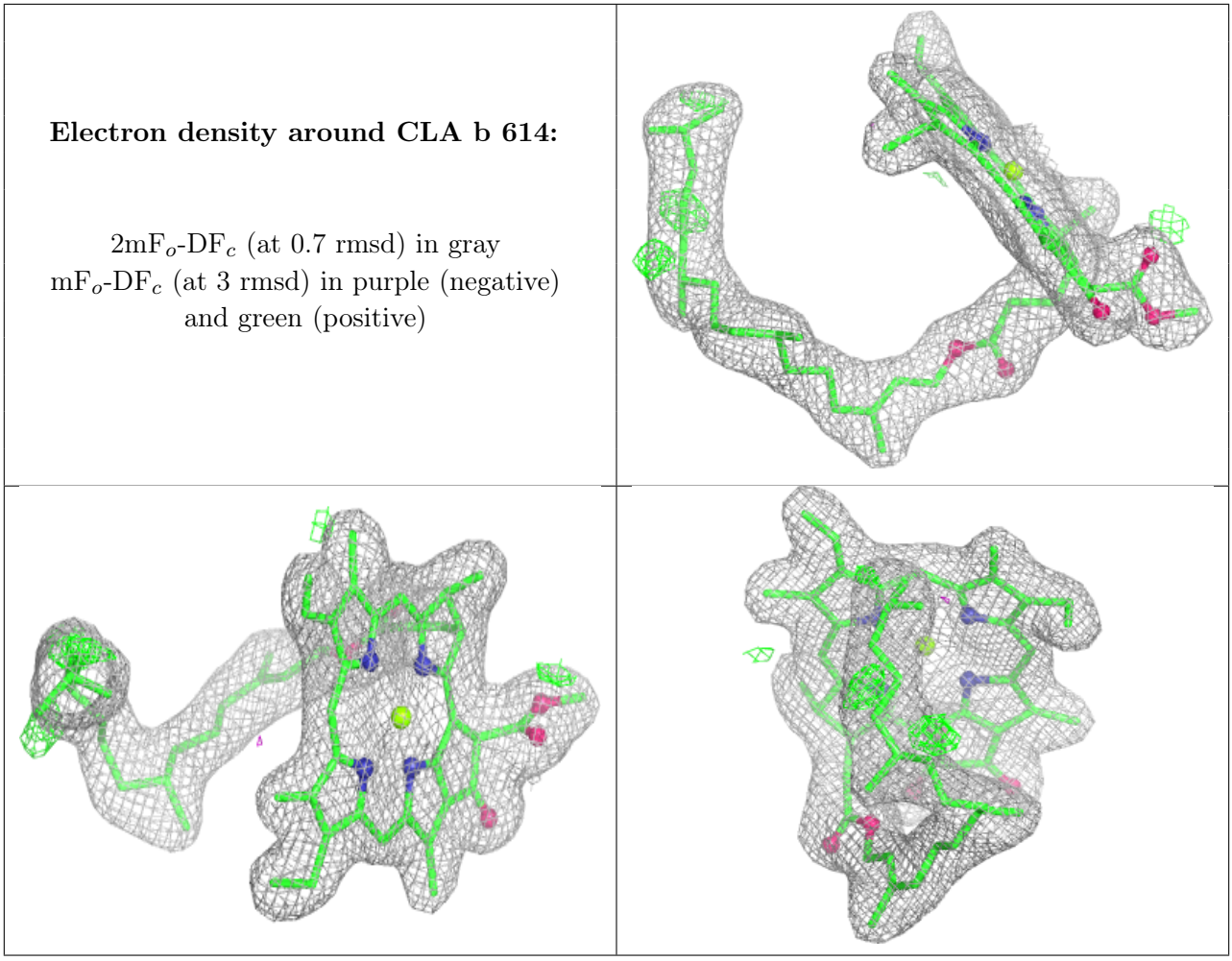






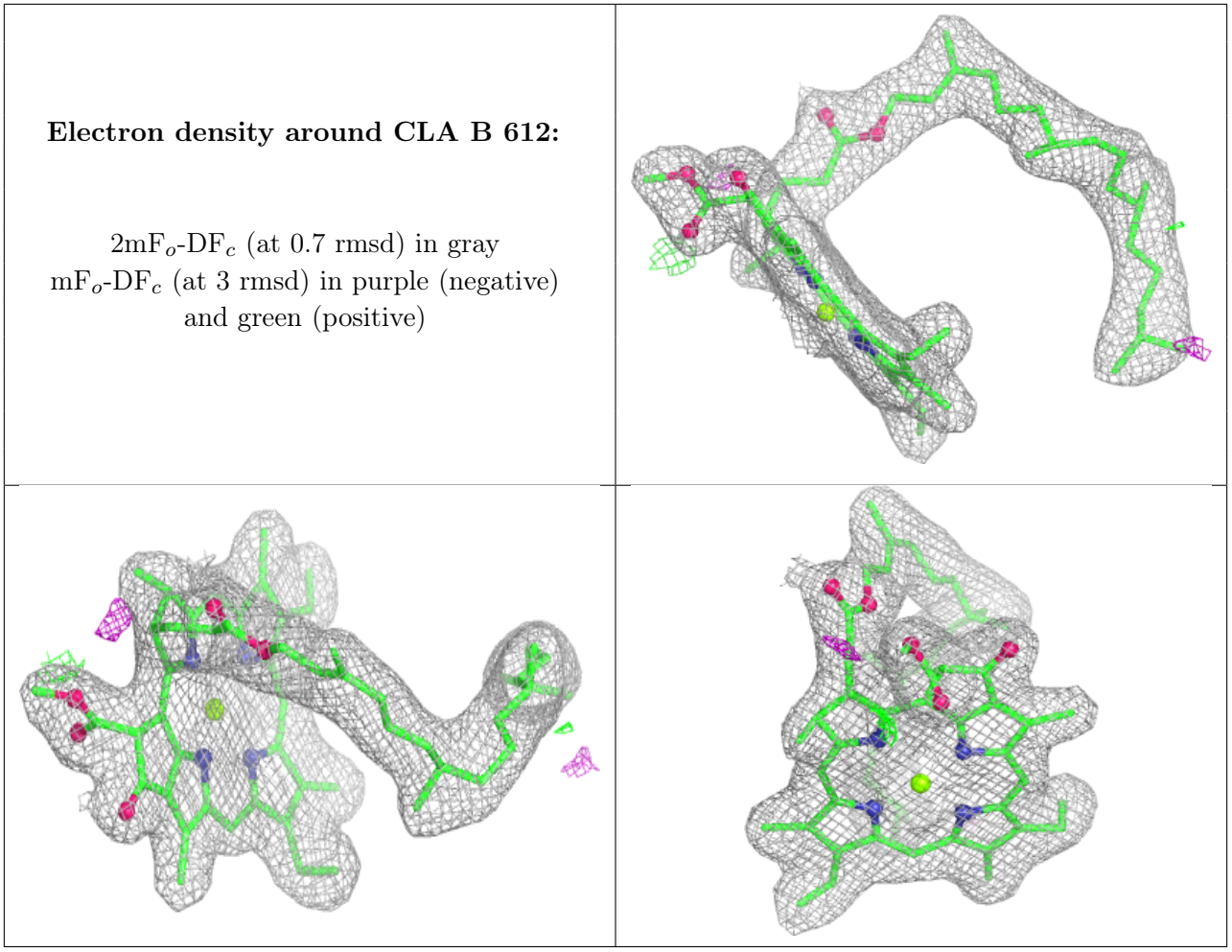
Electron density around CLA b 614:

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



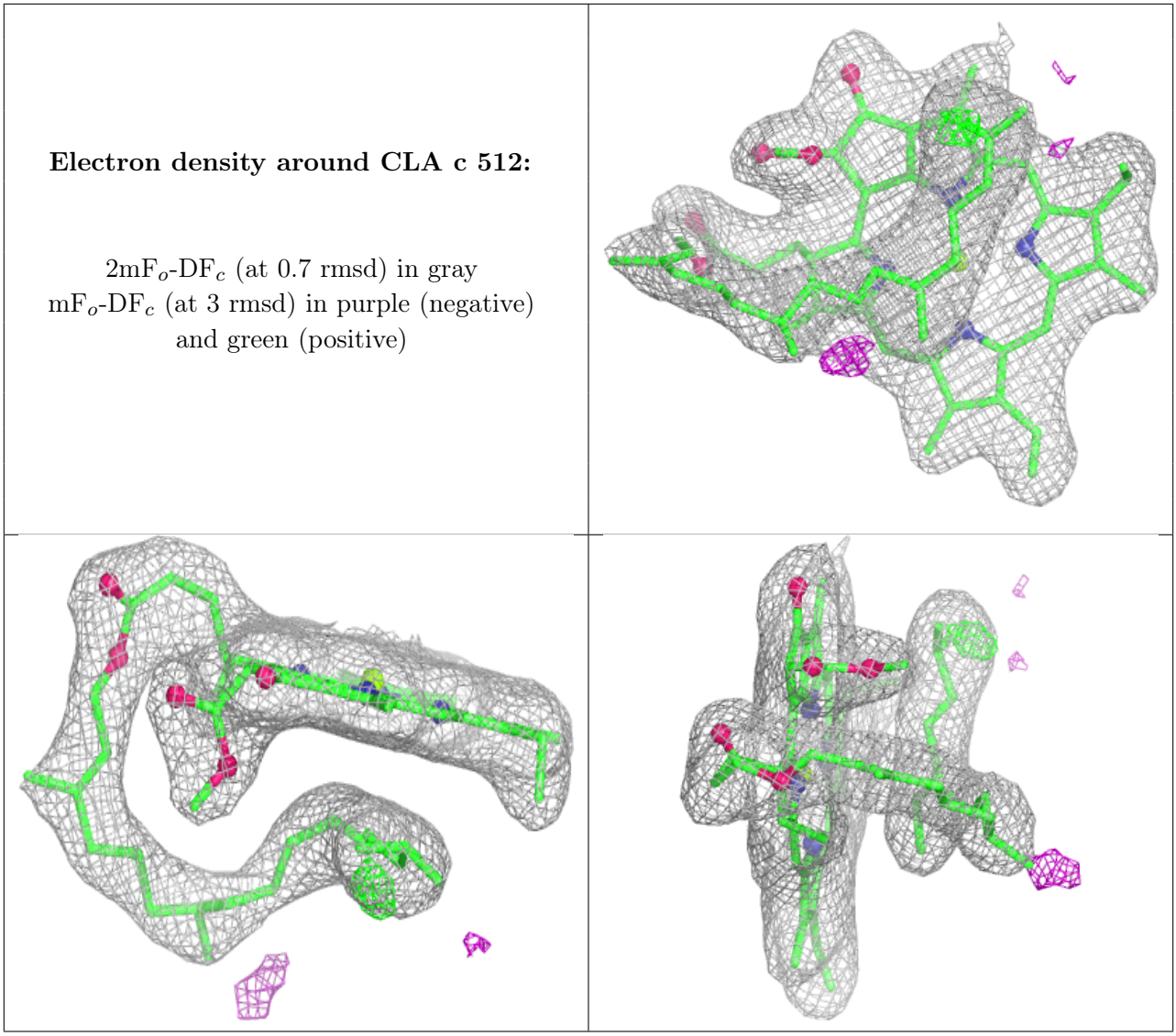
Electron density around CLA B 612:

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



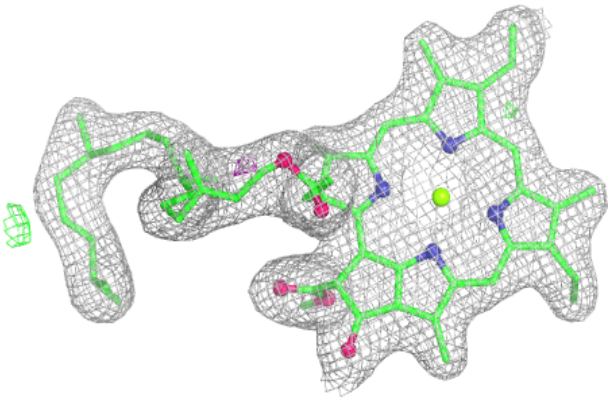
Electron density around CLA c 512:

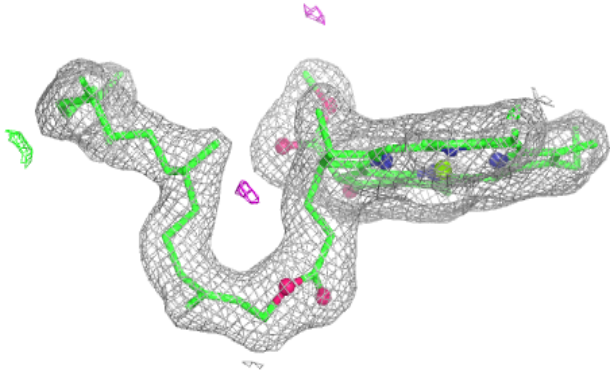
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

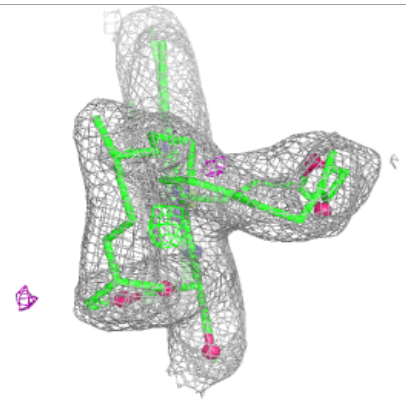


Electron density around CLA B 613:

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

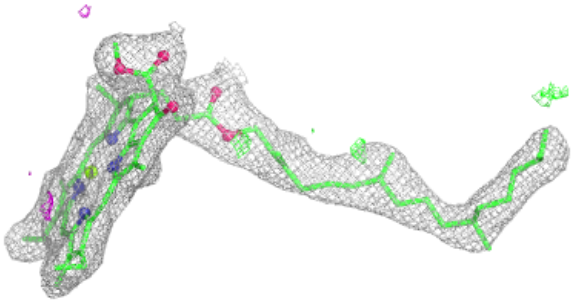


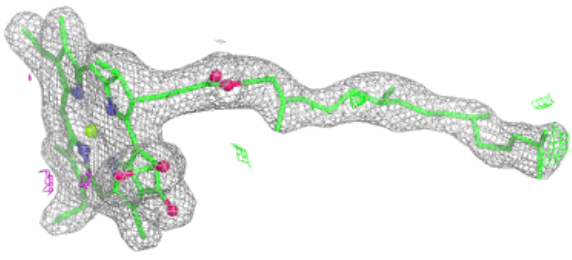


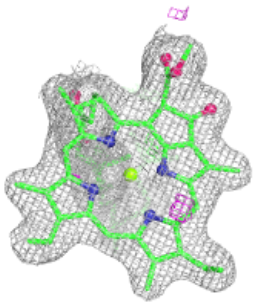


Electron density around CLA B 605:

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



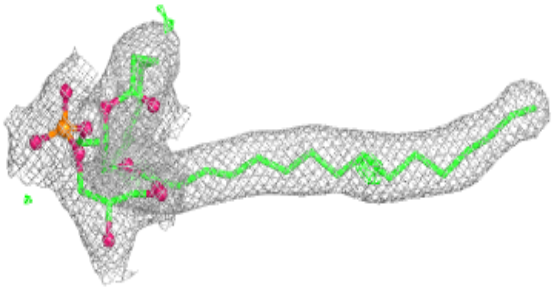


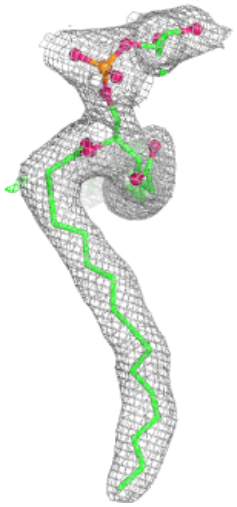


Electron density around LHG L 101:

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

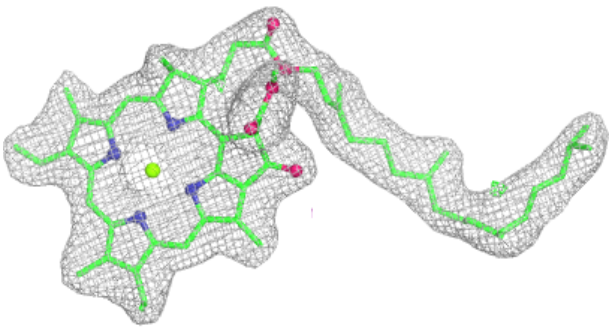


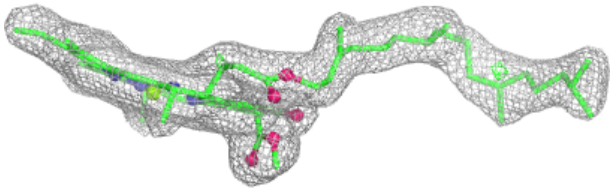




Electron density around CLA b 605:

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

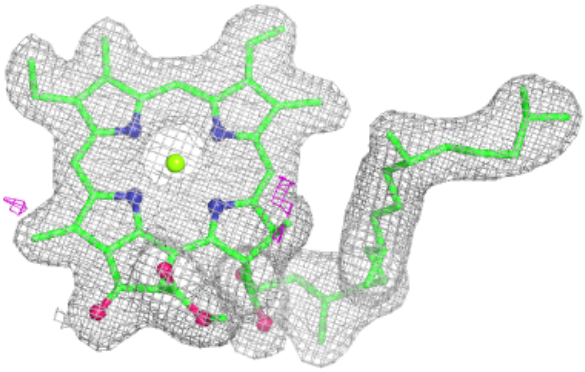


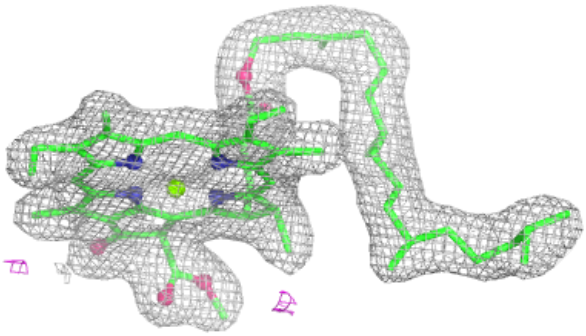


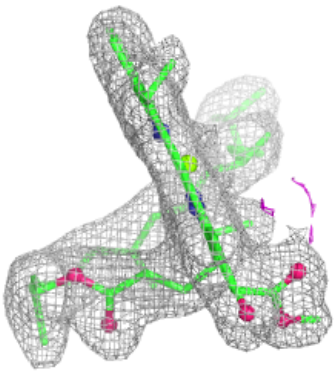


Electron density around CLA d 401:

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

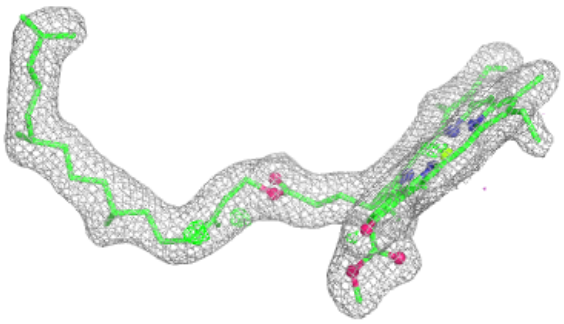


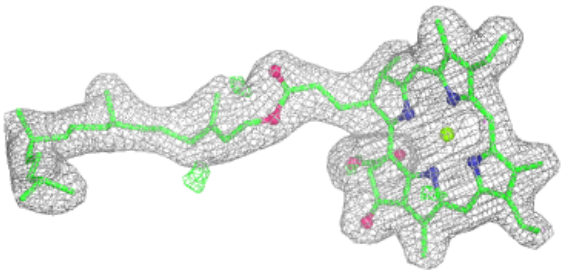


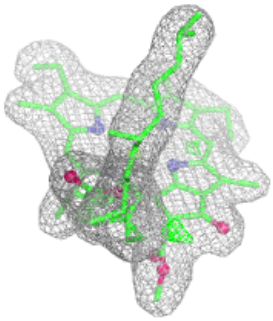


Electron density around CLA d 404:

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

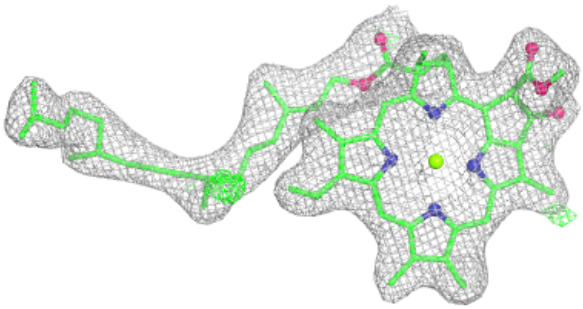


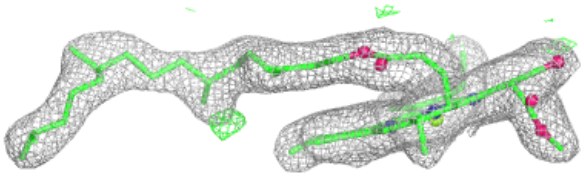


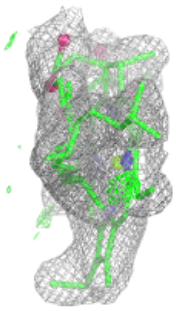


Electron density around CLA b 606:

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

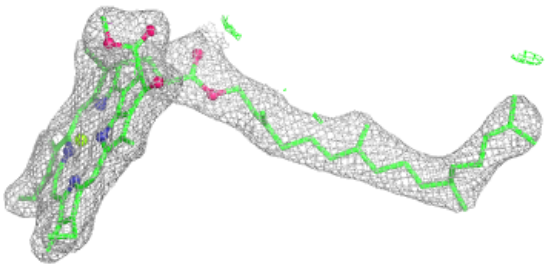


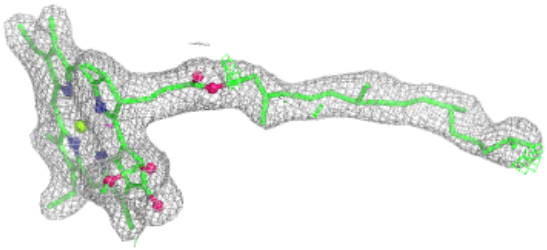


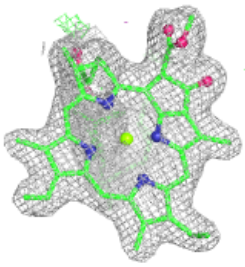


Electron density around CLA b 607:

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

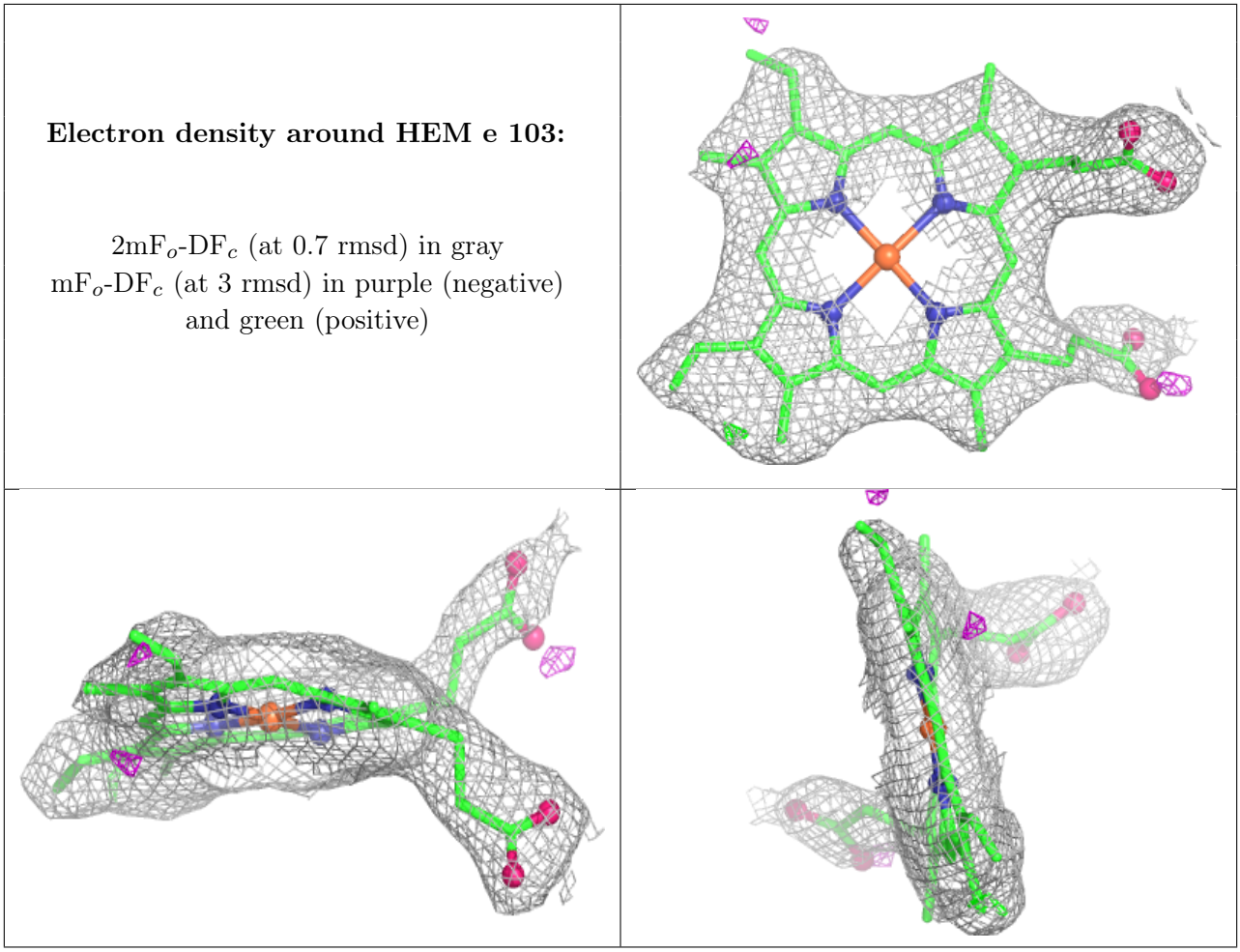






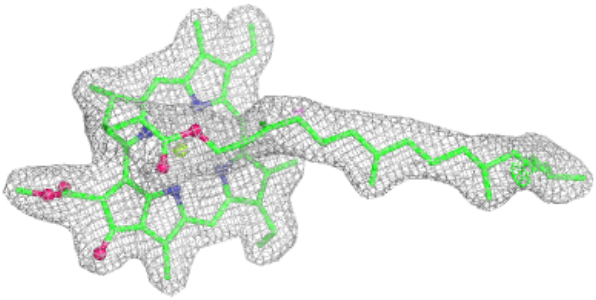
Electron density around HEM e 103:

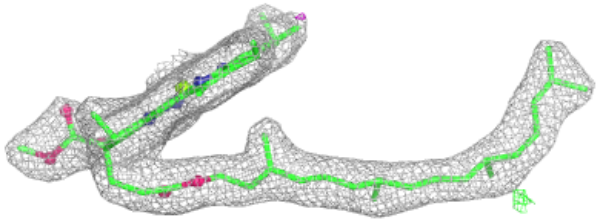
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 609:

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

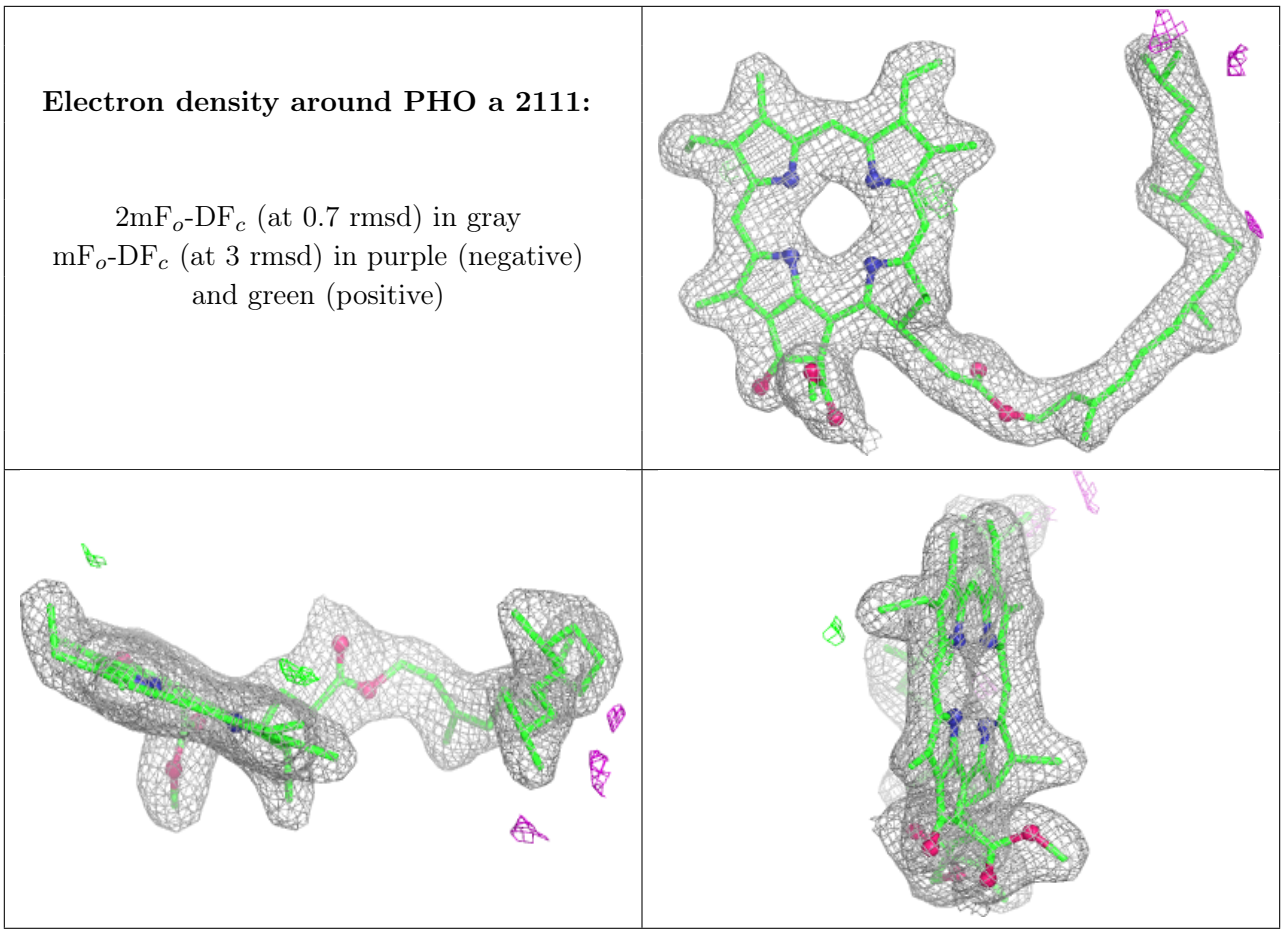






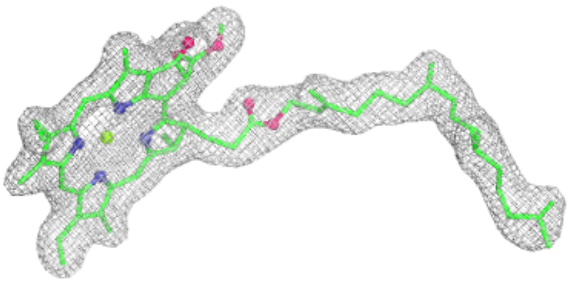
Electron density around PHO a 2111:

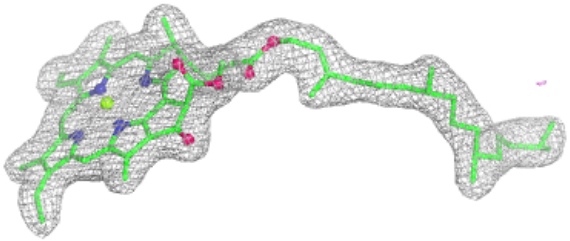
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

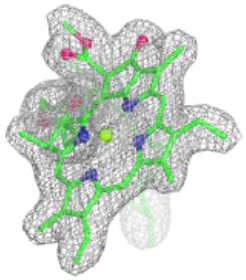


Electron density around CLA A 405:

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

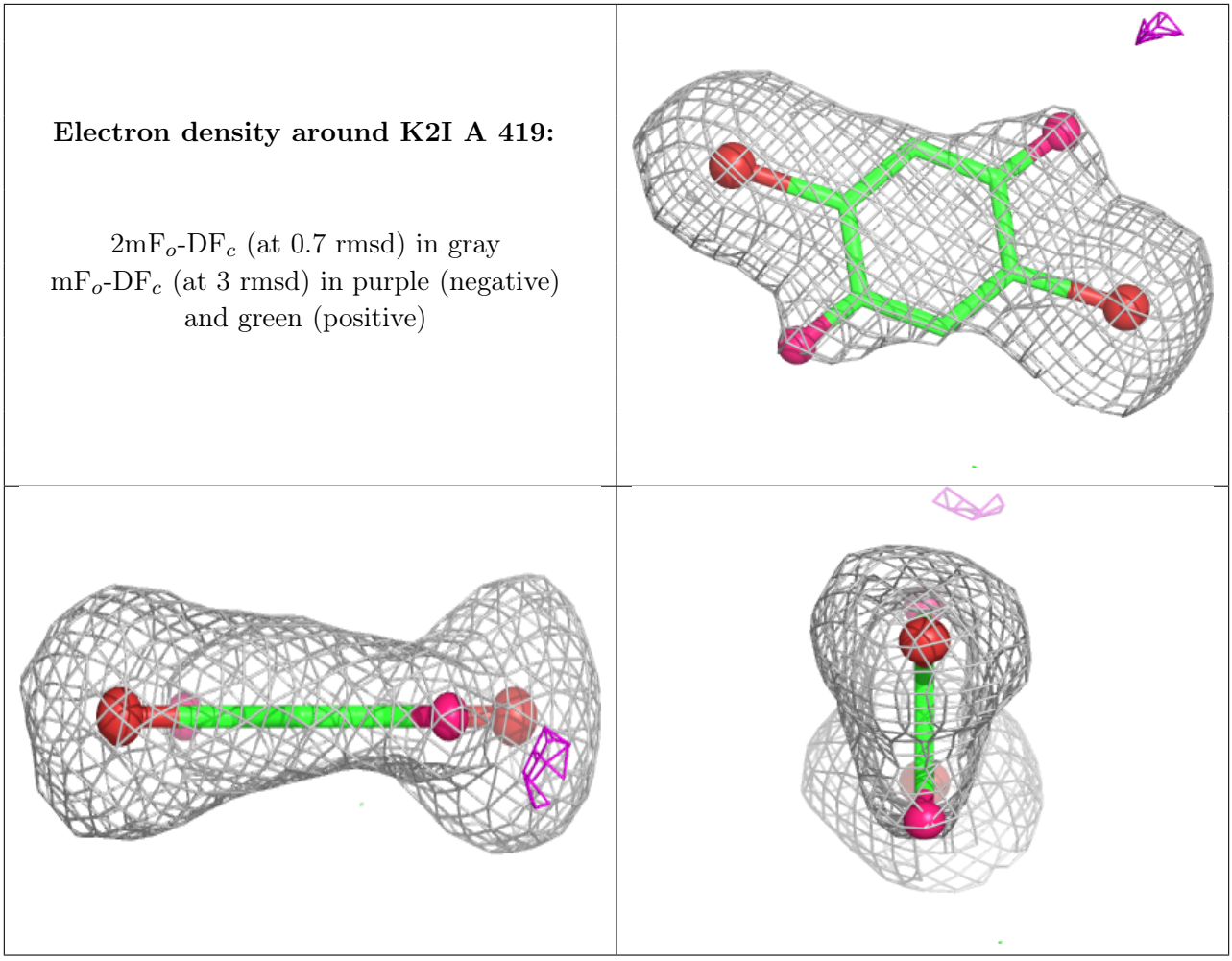






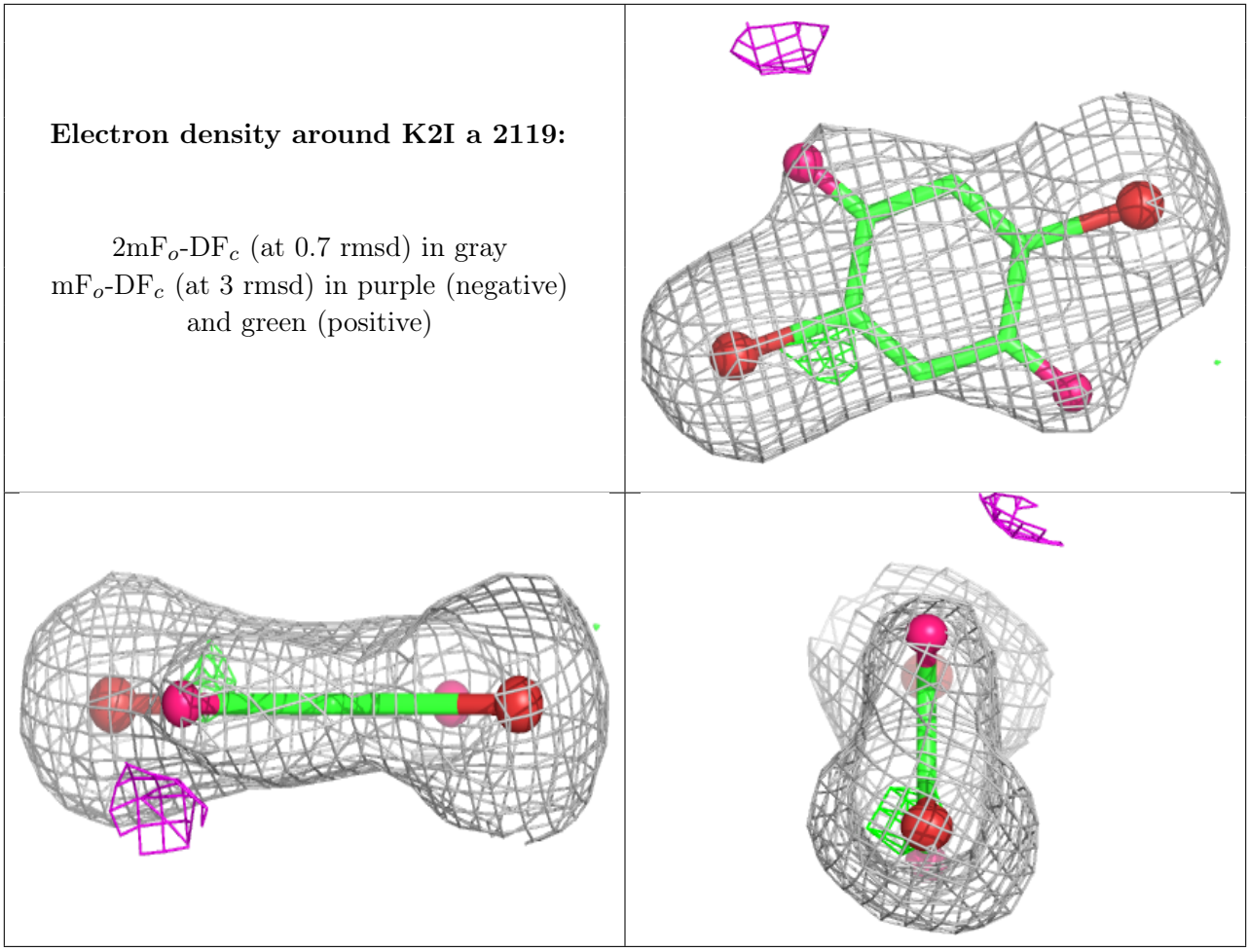
Electron density around K2I A 419:

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



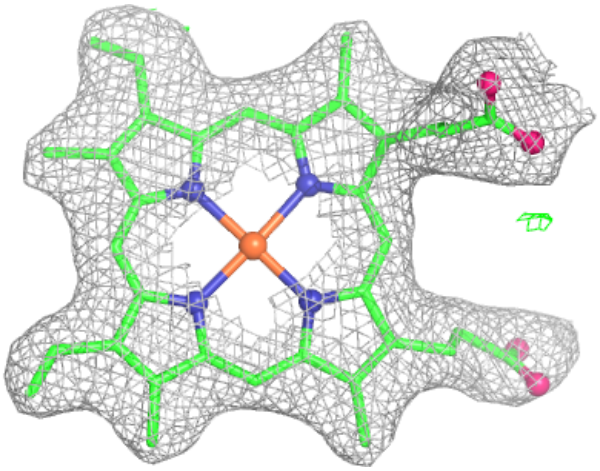
Electron density around K2I a 2119:

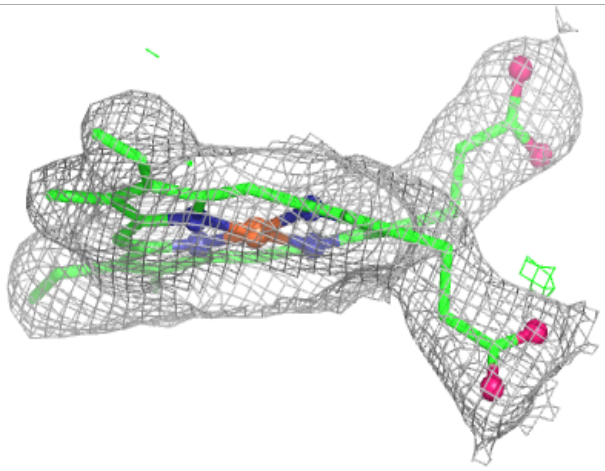
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

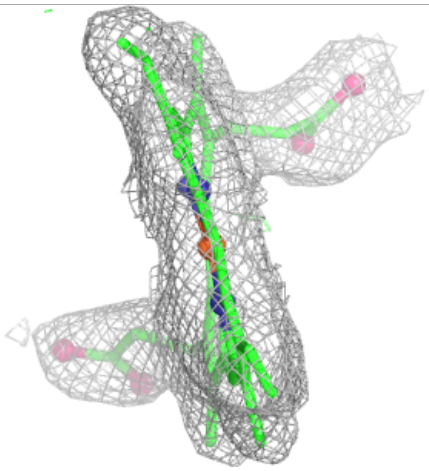


Electron density around HEM F 102:

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

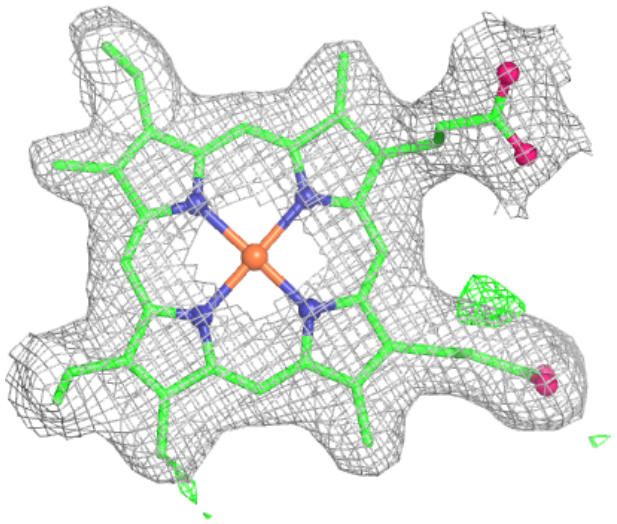


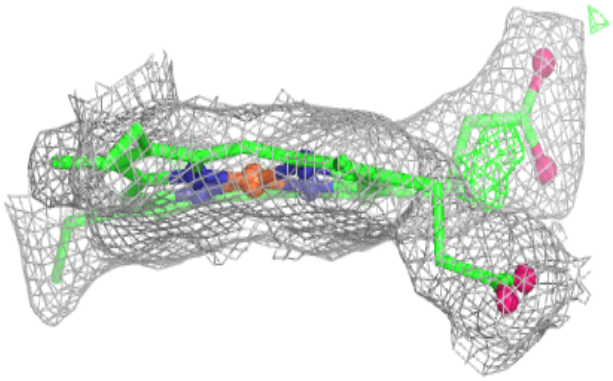


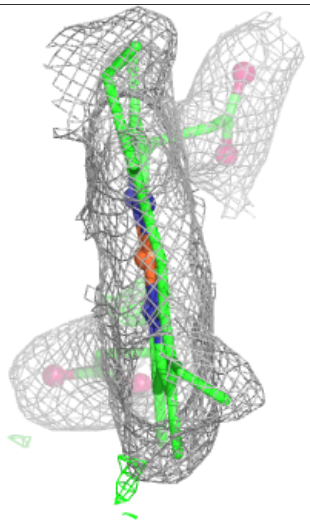


Electron density around HEC V 201:

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

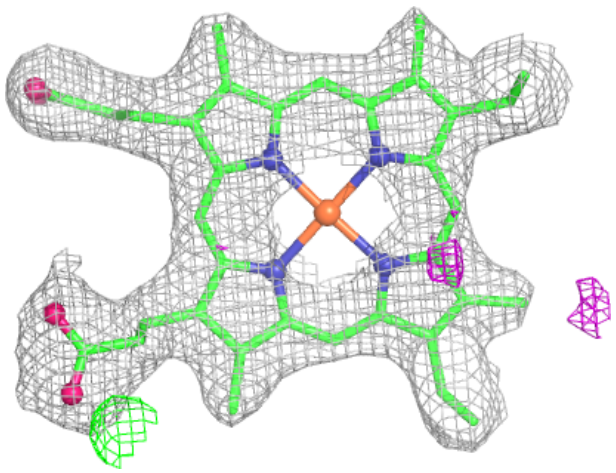


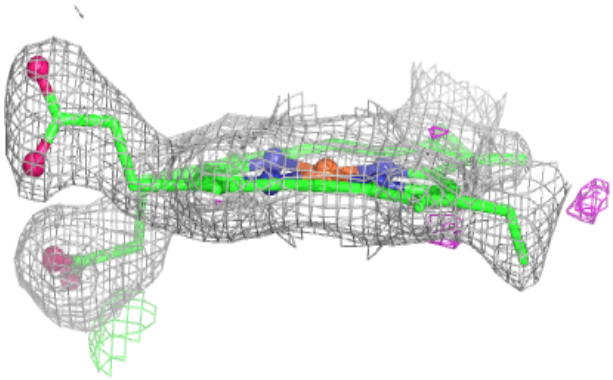




Electron density around HEC v 201:

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

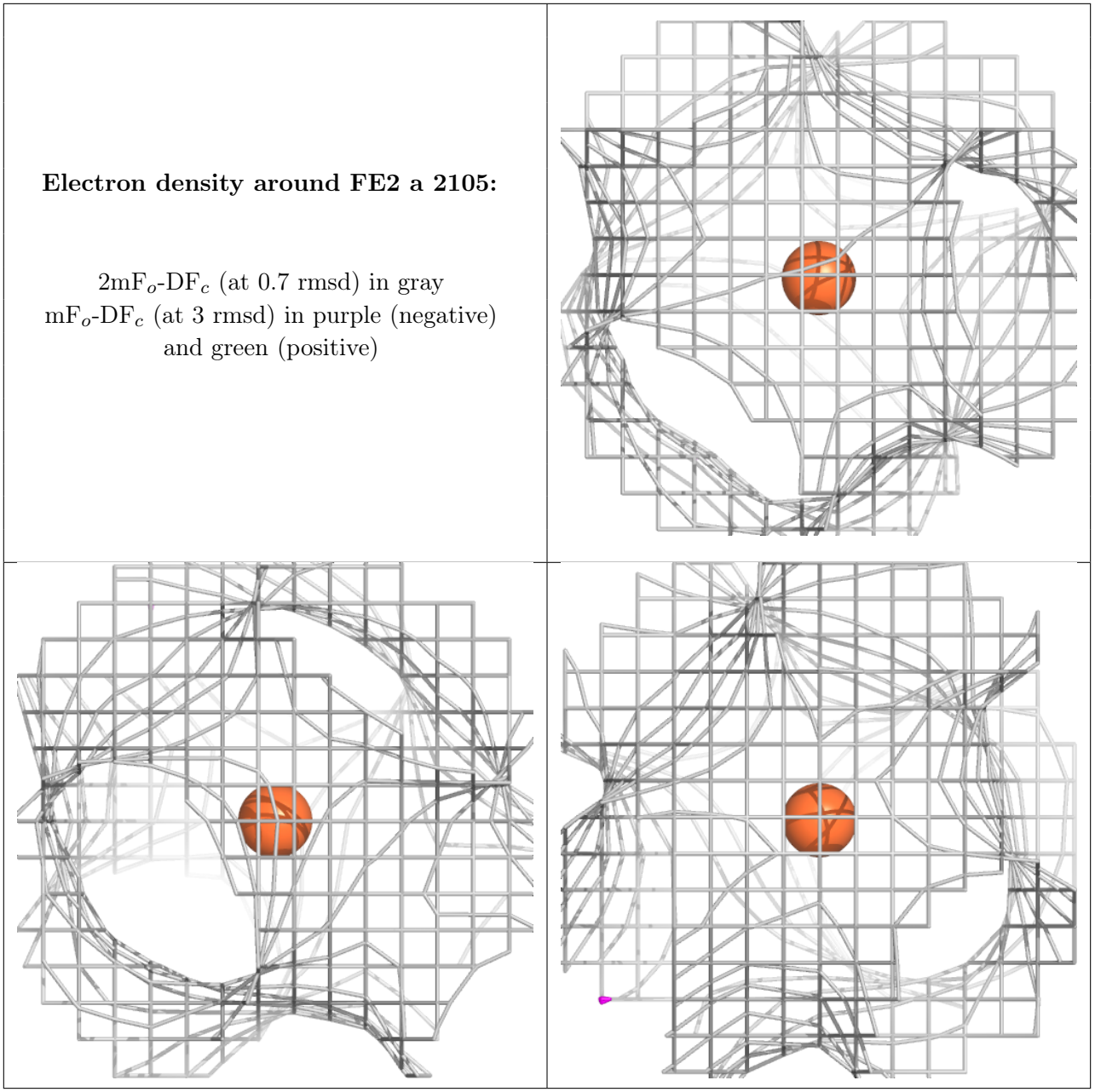






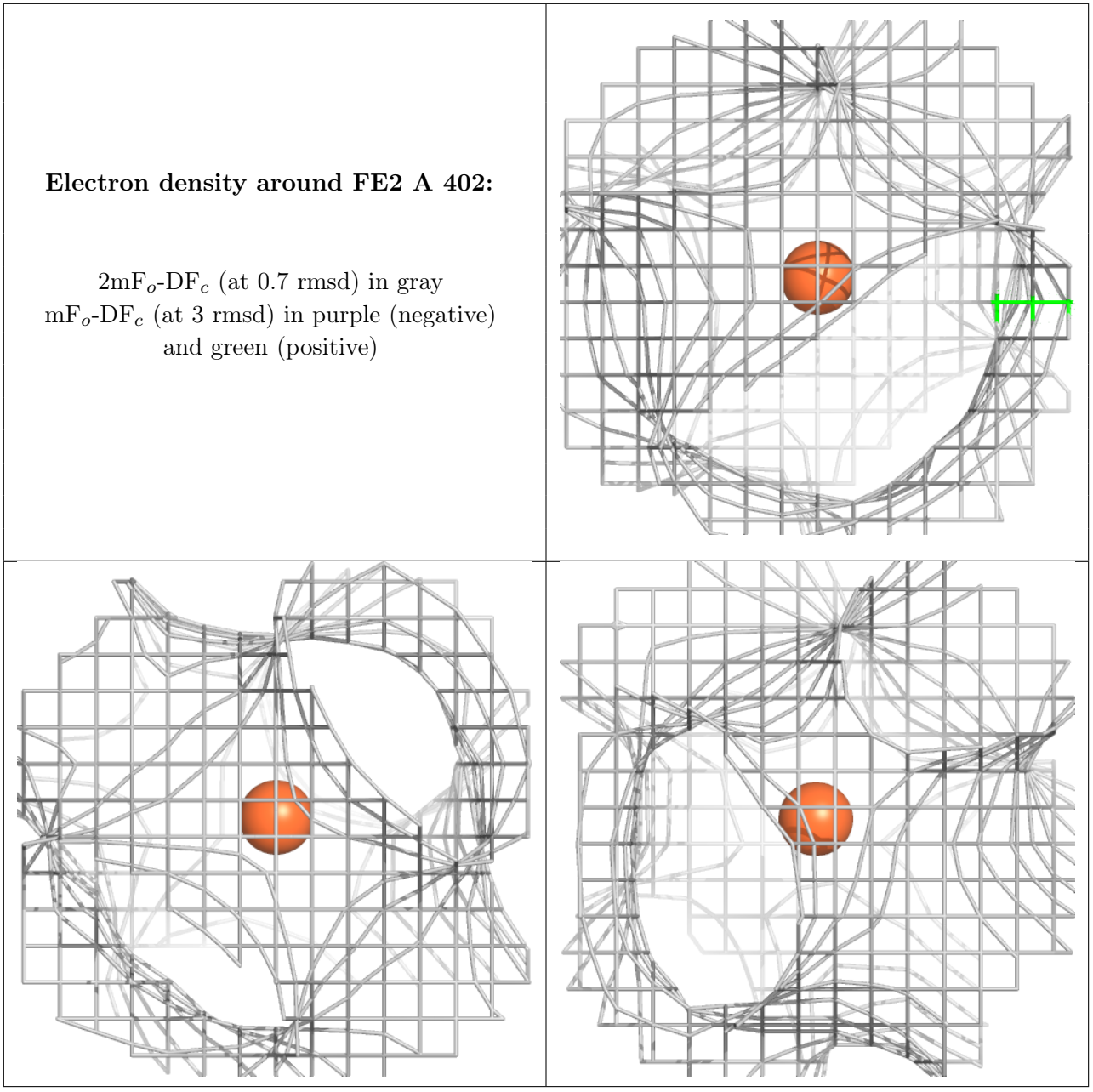
Electron density around FE2 a 2105:

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



Electron density around FE2 A 402:

$2mF_o$-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.