Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 03:53 PM JST

PDB ID	:	6JLJ / pdb_00006jlj
Title	:	XFEL structure of cyanobacterial photosystem II (dark state, dataset1)
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2019-03-06
Resolution	:	2.15 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:

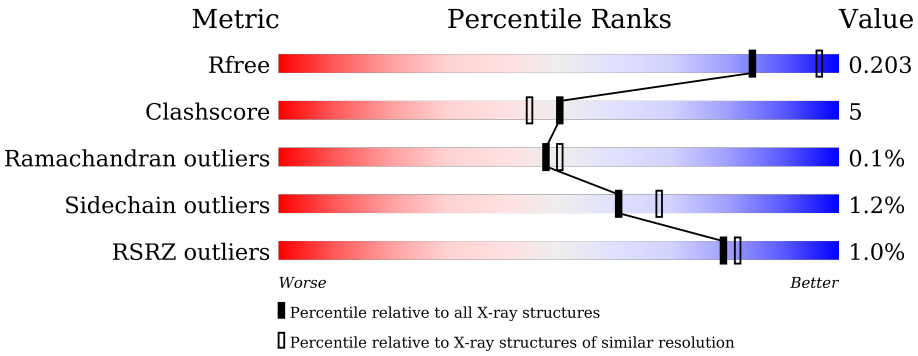
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.15 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.



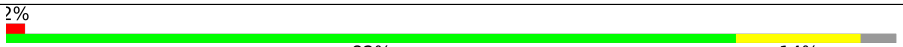
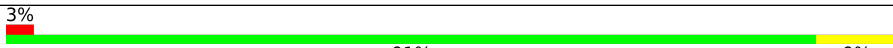
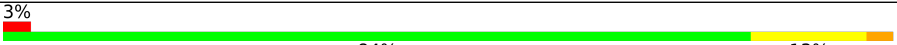
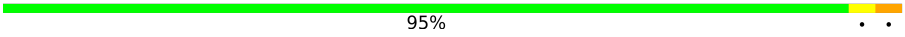
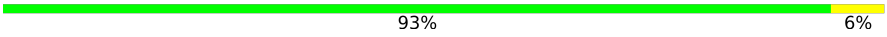
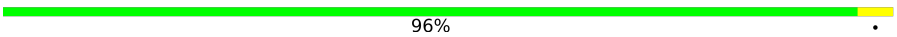
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	87% 10% .
2	B	505	90% 10%
2	b	505	% 90% 9%
3	C	455	91% 8% .
3	c	455	93% 7%

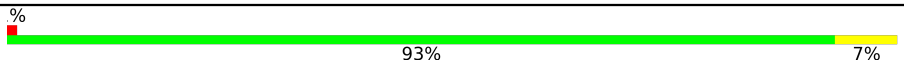
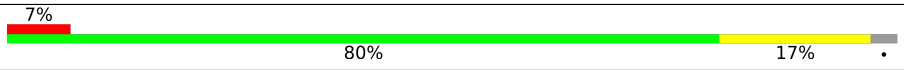
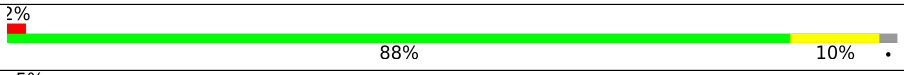
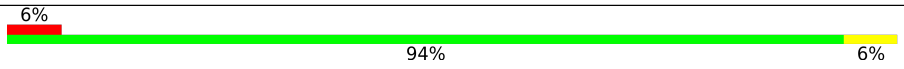
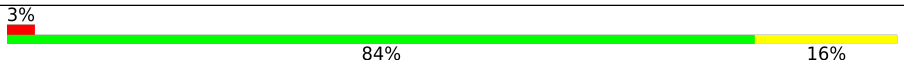
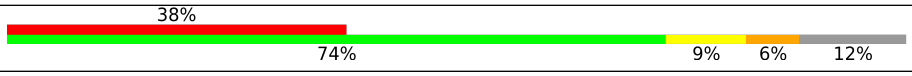
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	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	34	

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
40	HEC	V	205	X	-	-	-
40	HEC	v	205	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 54101 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
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	461	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

- 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	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			280	187	43	48	2			

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
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
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	0	0
			287	191	46	50			
18	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O	98	0	0
			239	163	41	35			

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

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

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

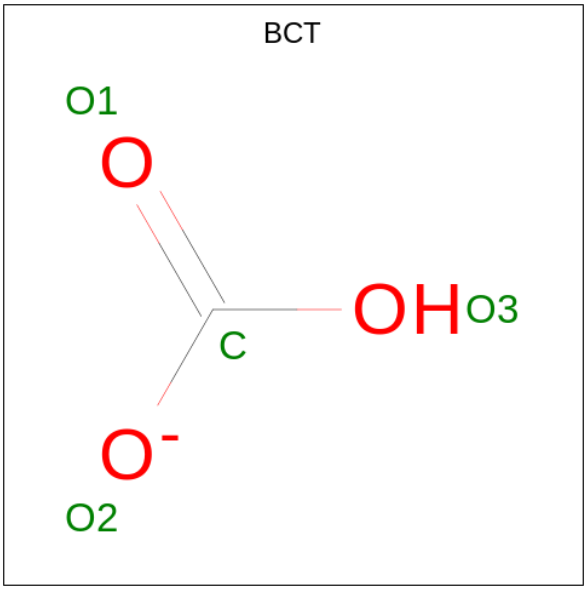
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

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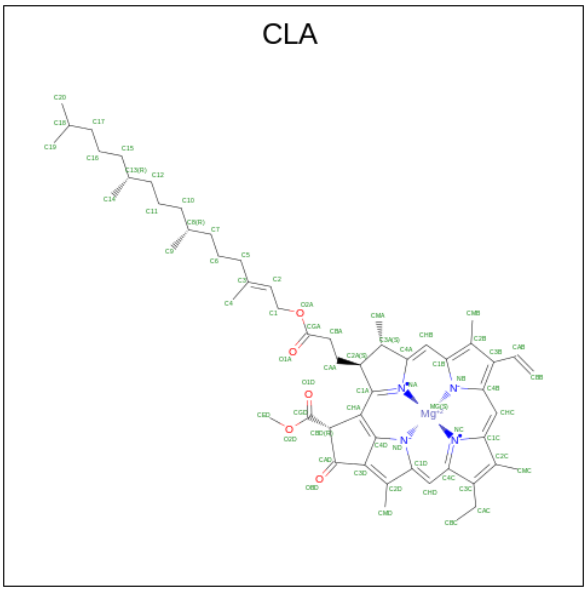
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 2 2	0	0
22	v	1	Total Cl 1 1	0	0

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



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

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



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

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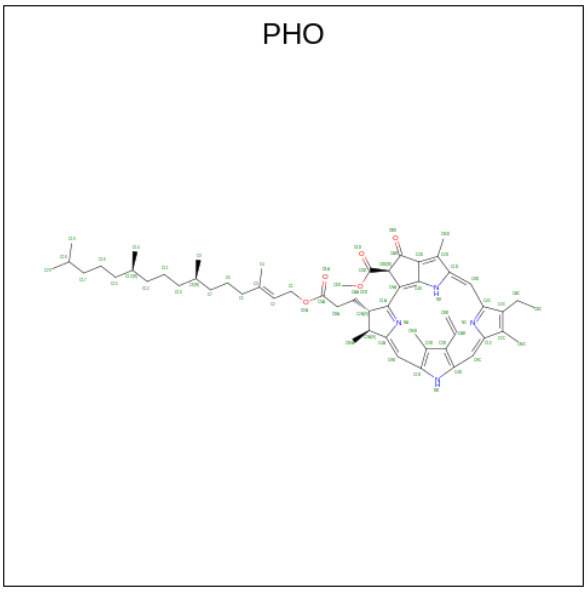
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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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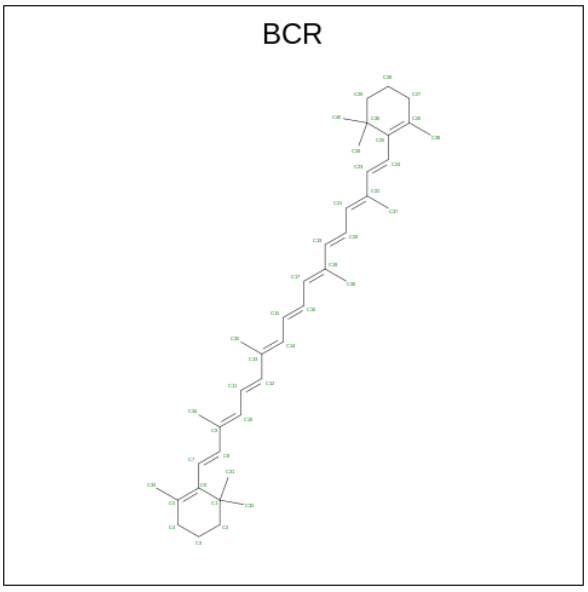
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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	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: $C_{55}H_{74}N_4O_5$).



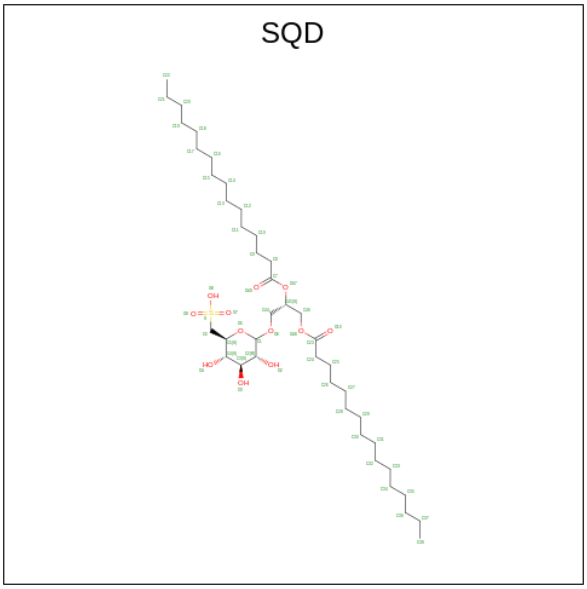
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



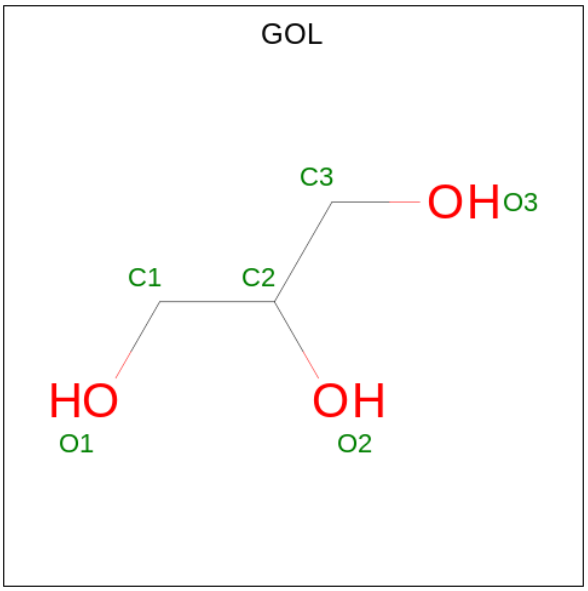
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total 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	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	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
			54	41	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
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



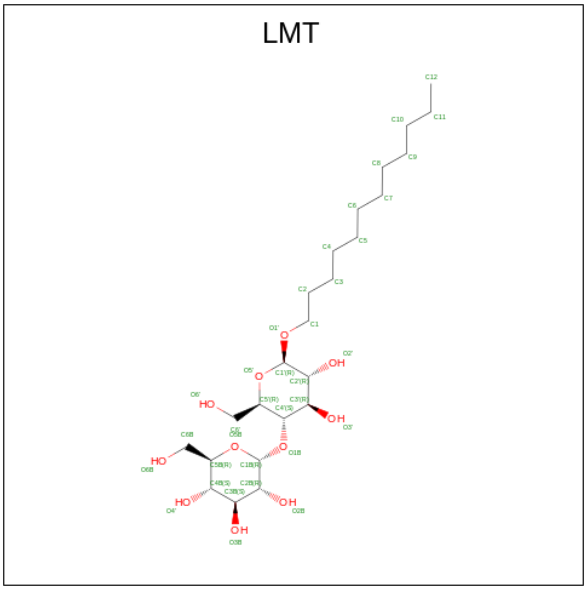
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	F	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	f	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

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



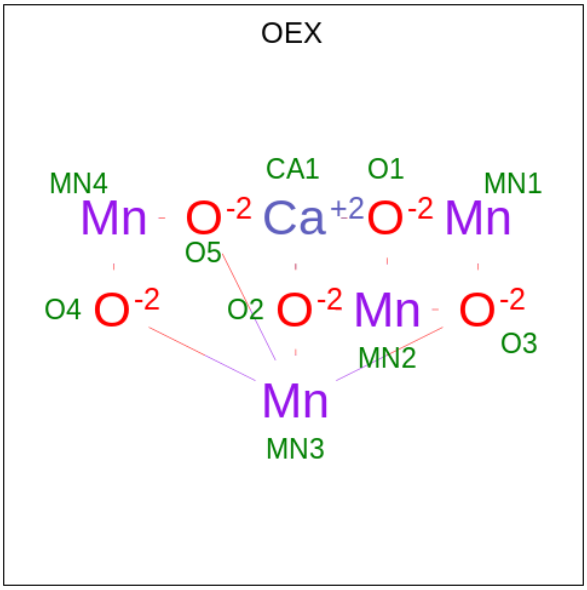
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 35 24 11	0	0
29	B	1	Total C O 35 24 11	0	0
29	B	1	Total C O 25 19 6	0	0
29	C	1	Total C O 35 24 11	0	0
29	F	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	T	1	Total C O 25 19 6	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
29	f	1	Total C O 35 24 11	0	0

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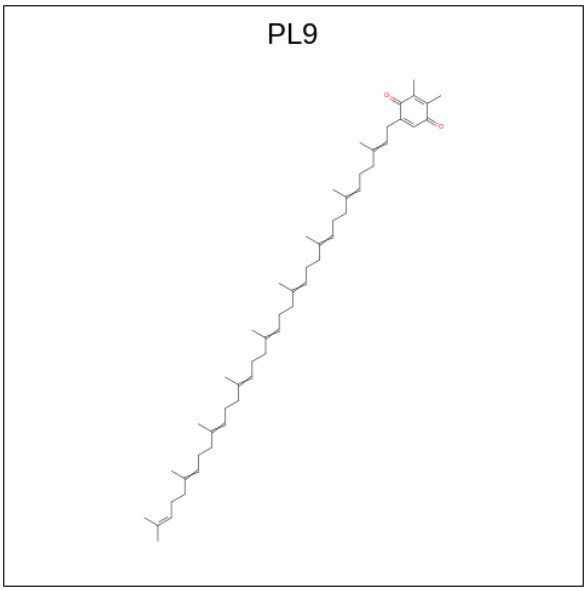
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	m	1	Total C O 35 24 11	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total Ca Mn O 10 1 4 5	0	0
30	a	1	Total Ca Mn O 10 1 4 5	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: $C_{53}H_{80}O_2$).



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

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	B	1	Total C O 33 28 5	0	0
32	C	1	Total C O 34 29 5	0	0
32	D	2	Total C O 57 51 6	0	0
32	I	1	Total C O 40 35 5	0	0
32	J	1	Total C 10 10	0	0
32	M	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0

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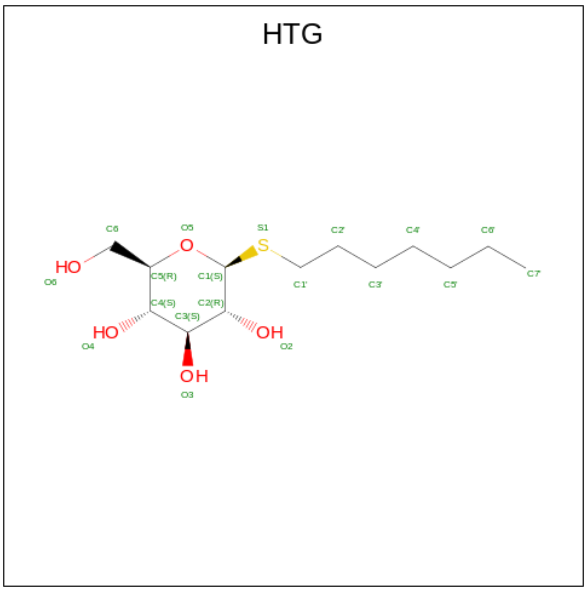
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	3	Total C O 71 63 8	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	C	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	c	2	Total Ca 2 2	0	0
33	f	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



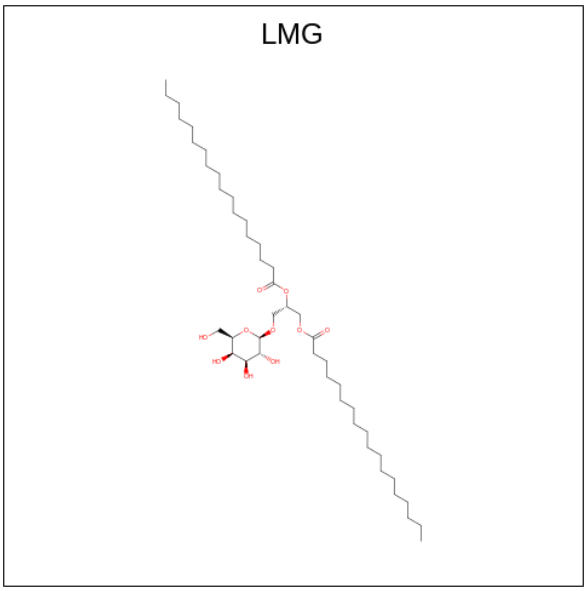
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16	10	5	1		
34	V	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	c	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0
34	d	1	Total C O S 16 10 5 1	0	0

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



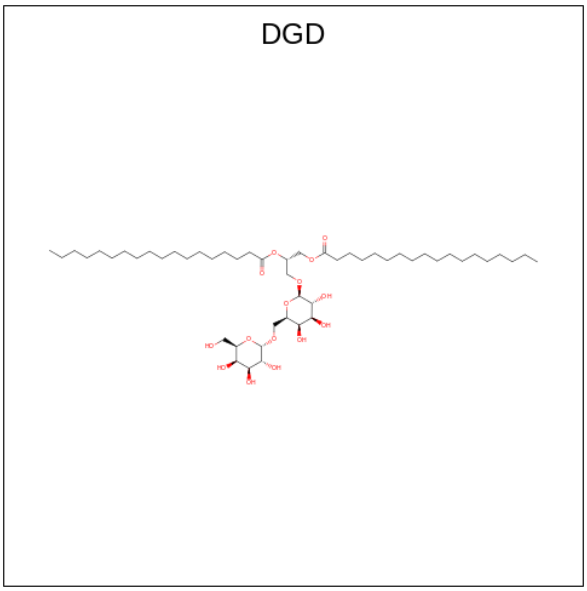
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 51 41 10	0	0
35	C	1	Total C O 51 41 10	0	0
35	C	1	Total C O 51 41 10	0	0
35	J	1	Total C O 51 41 10	0	0
35	M	1	Total C O 51 41 10	0	0
35	Z	1	Total C O 37 27 10	0	0
35	a	1	Total C O 51 41 10	0	0
35	b	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	c	1	Total C O 51 41 10	0	0
35	c	1	Total C O 51 41 10	0	0
35	j	1	Total C O 51 41 10	0	0
35	z	1	Total C O 39 29 10	0	0

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



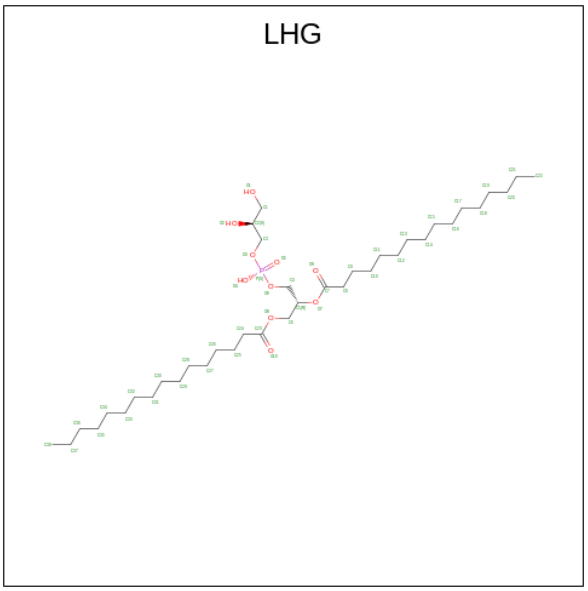
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	D	1	Total C O 52 42 10	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0

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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



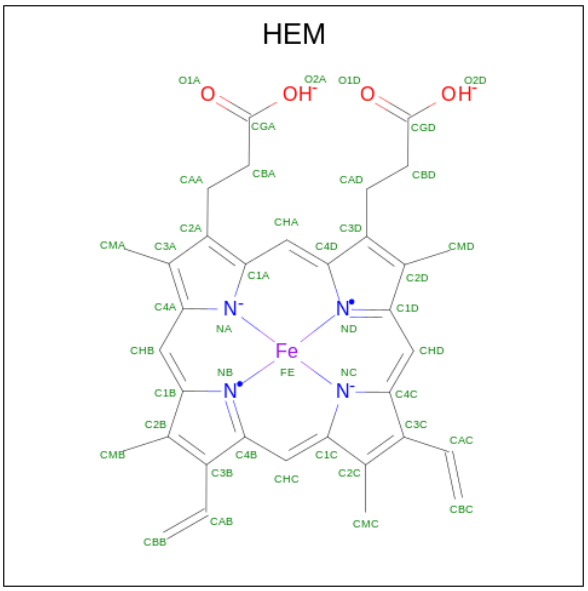
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	e	1	Total	C	O	P	0	0
			42	31	10	1		
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

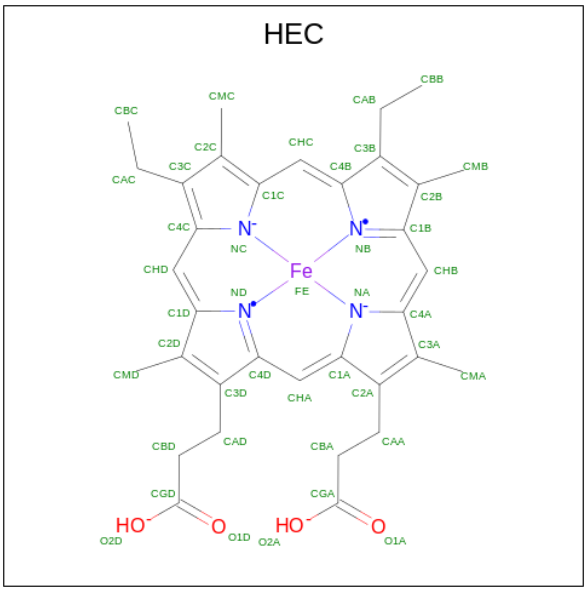


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	163	Total	O	0	3
			166	166		
41	B	291	Total	O	0	4
			295	295		
41	C	230	Total	O	0	2
			232	232		
41	D	139	Total	O	0	4
			143	143		
41	E	34	Total	O	0	0
			34	34		
41	F	8	Total	O	0	0
			8	8		
41	H	43	Total	O	0	1
			44	44		
41	I	4	Total	O	0	0
			4	4		
41	J	11	Total	O	0	0
			11	11		
41	K	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	16	Total O 17 17	0	1
41	M	24	Total O 24 24	0	0
41	O	177	Total O 179 179	0	2
41	T	16	Total O 17 17	0	1
41	U	85	Total O 85 85	0	0
41	V	115	Total O 117 117	0	2
41	Y	4	Total O 4 4	0	0
41	X	8	Total O 8 8	0	0
41	Z	1	Total O 1 1	0	0
41	a	158	Total O 159 159	0	1
41	b	258	Total O 261 261	0	3
41	c	201	Total O 204 204	0	3
41	d	128	Total O 131 131	0	3
41	e	20	Total O 20 20	0	0
41	f	8	Total O 8 8	0	0
41	h	42	Total O 42 42	0	0
41	i	6	Total O 6 6	0	0
41	j	6	Total O 6 6	0	0
41	k	7	Total O 7 7	0	0
41	l	8	Total O 8 8	0	0
41	m	14	Total O 14 14	0	0

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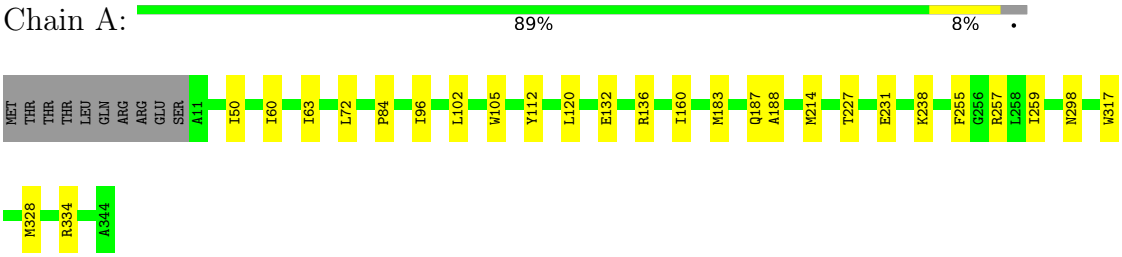
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	o	163	Total O 163 163	0	0
41	t	9	Total O 9 9	0	0
41	u	91	Total O 91 91	0	0
41	v	82	Total O 83 83	0	1
41	y	2	Total O 2 2	0	0
41	x	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

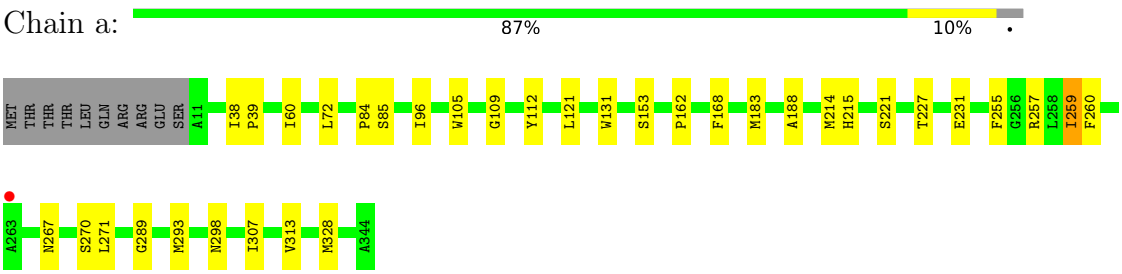
• Molecule 1: Photosystem II protein D1

Chain A:



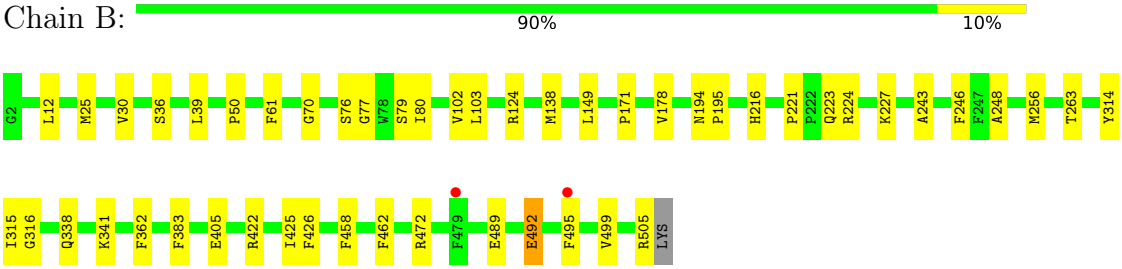
• Molecule 1: Photosystem II protein D1

Chain a:



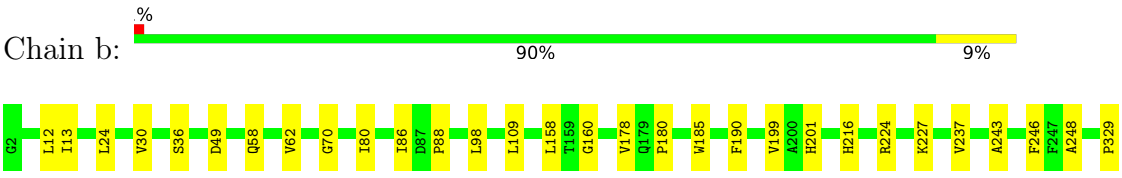
• Molecule 2: Photosystem II CP47 reaction center protein

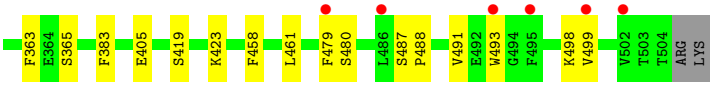
Chain B:



• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

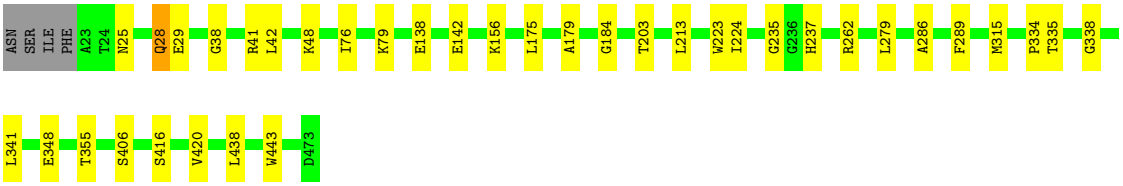




• Molecule 3: Photosystem II CP43 reaction center protein

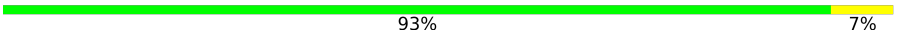
Chain C:

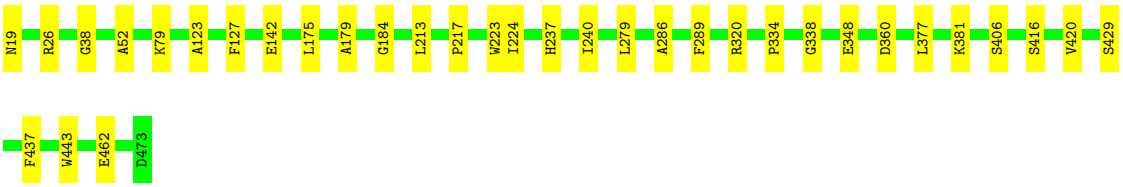




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

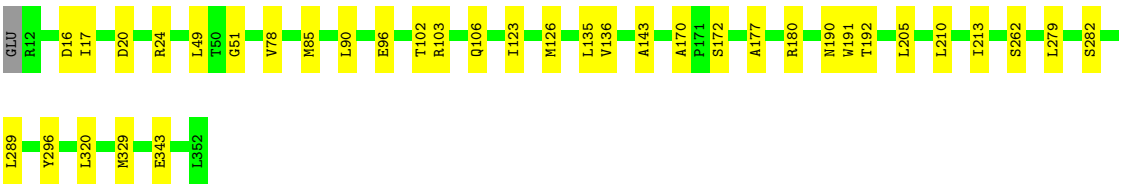




• Molecule 4: Photosystem II D2 protein

Chain D:

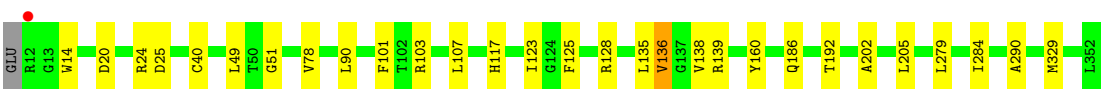




• Molecule 4: Photosystem II D2 protein

Chain d:

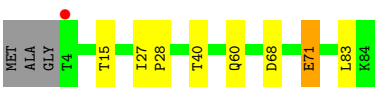




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

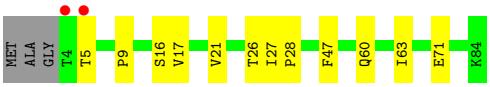




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

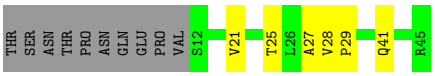




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

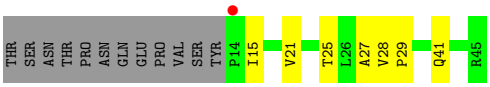




• Molecule 6: Cytochrome b559 subunit beta

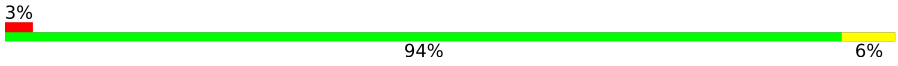
Chain f:





• Molecule 7: Photosystem II reaction center protein H

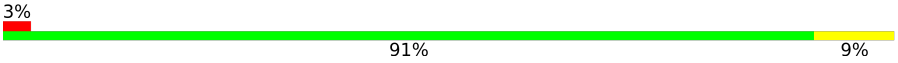
Chain H:

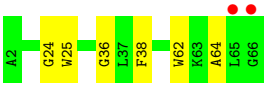




• Molecule 7: Photosystem II reaction center protein H

Chain h:





• Molecule 8: Photosystem II reaction center protein I

Chain I:





• Molecule 8: Photosystem II reaction center protein I

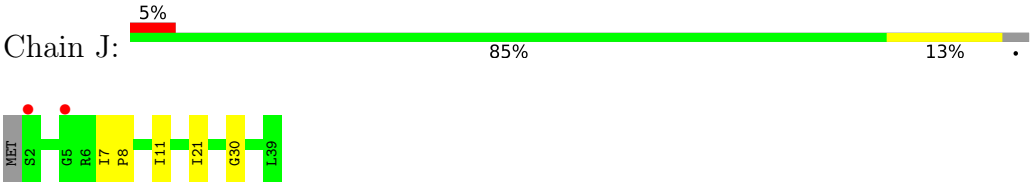
Chain i:





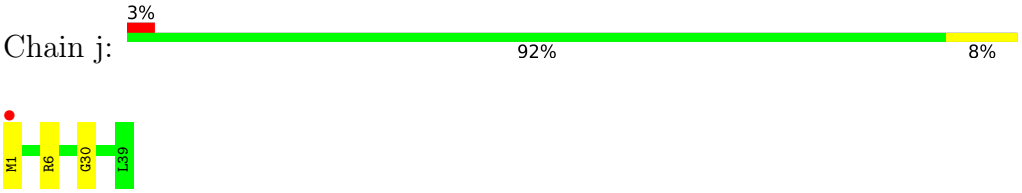
• Molecule 9: Photosystem II reaction center protein J

Chain J:



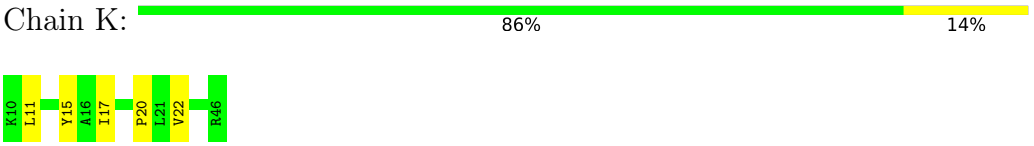
• Molecule 9: Photosystem II reaction center protein J

Chain j:



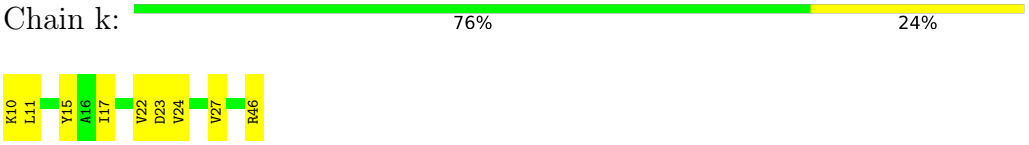
• Molecule 10: Photosystem II reaction center protein K

Chain K:



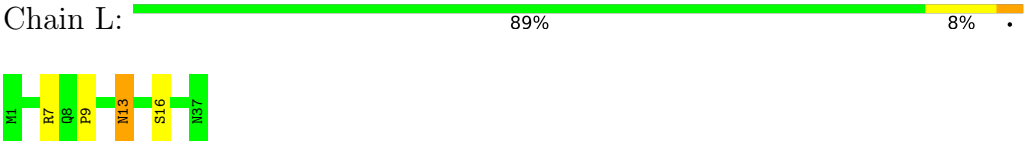
• Molecule 10: Photosystem II reaction center protein K

Chain k:



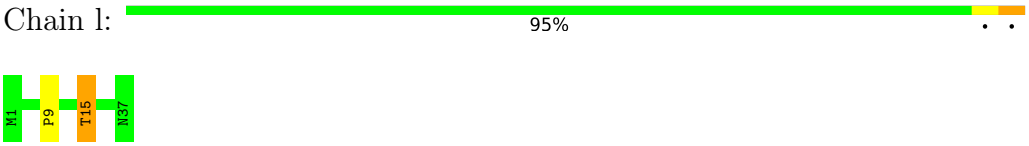
• Molecule 11: Photosystem II reaction center protein L

Chain L:



• Molecule 11: Photosystem II reaction center protein L

Chain l:



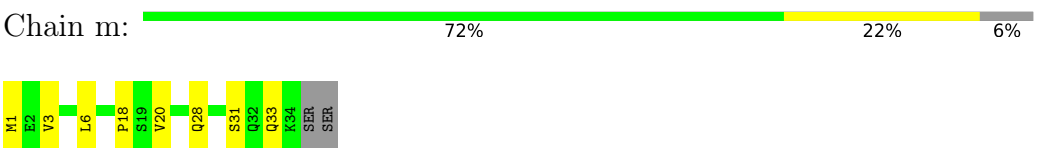
• Molecule 12: Photosystem II reaction center protein M

Chain M:



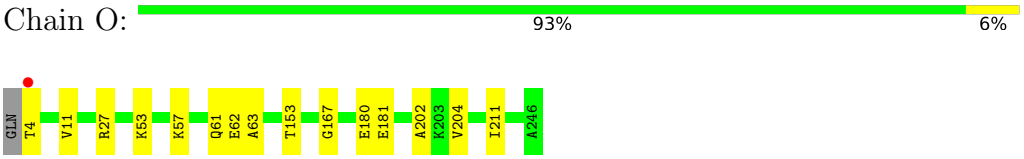
• Molecule 12: Photosystem II reaction center protein M

Chain m:



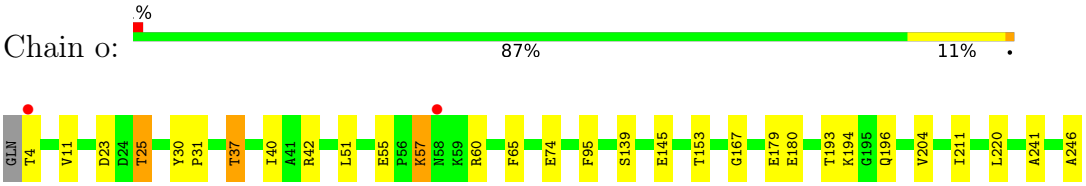
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



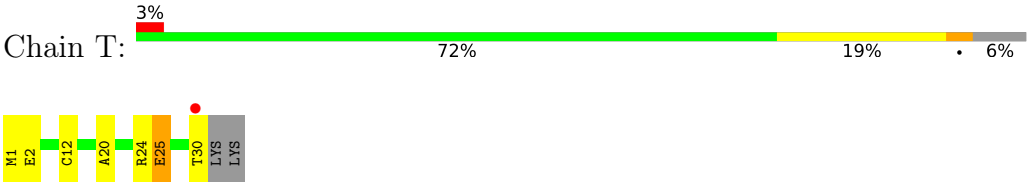
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



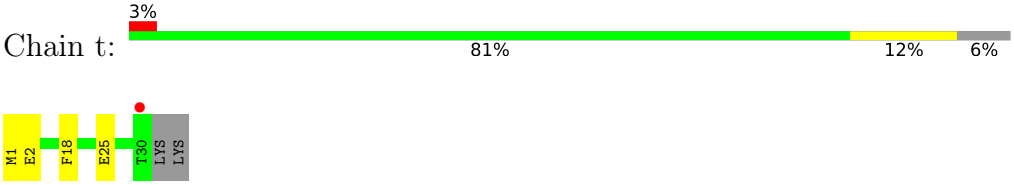
• Molecule 14: Photosystem II reaction center protein T

Chain T:



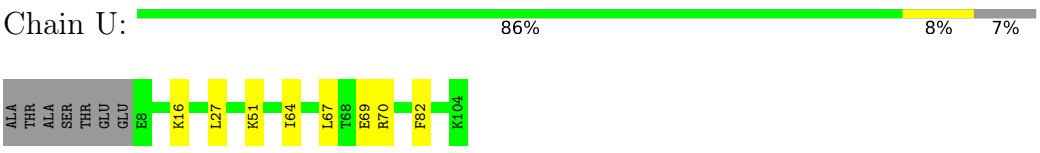
• Molecule 14: Photosystem II reaction center protein T

Chain t:



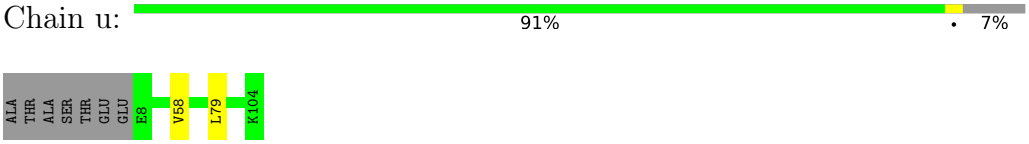
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



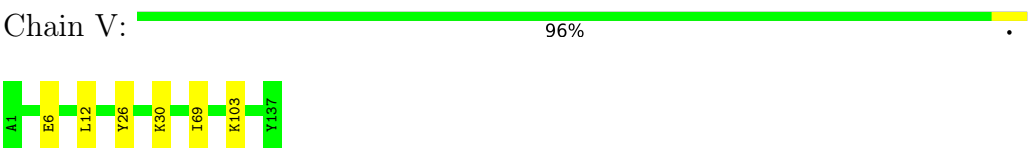
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



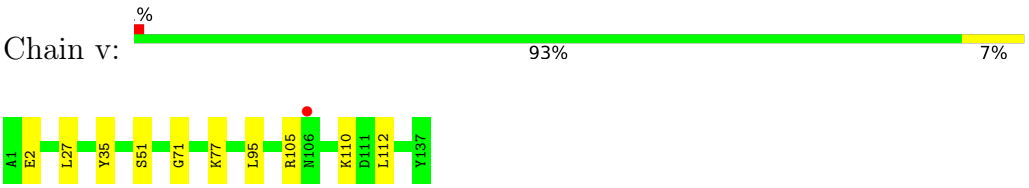
• Molecule 16: Cytochrome c-550

Chain V:



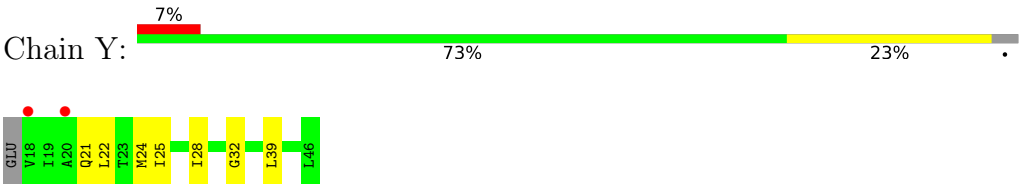
• Molecule 16: Cytochrome c-550

Chain v:



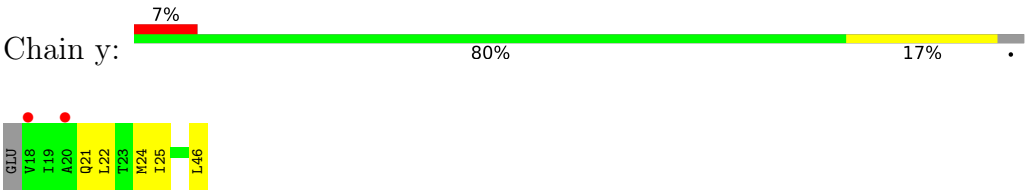
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



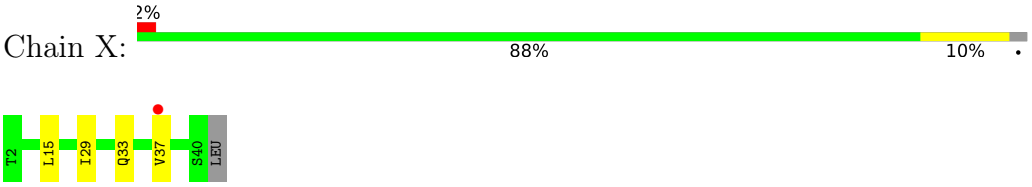
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



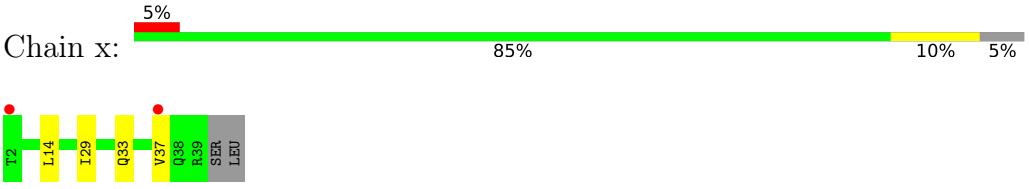
• Molecule 18: Photosystem II reaction center protein X

Chain X:



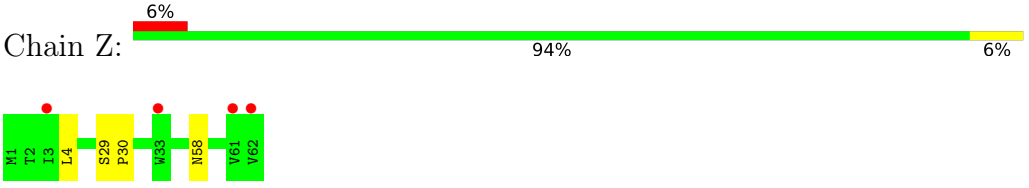
• Molecule 18: Photosystem II reaction center protein X

Chain x:



• Molecule 19: Photosystem II reaction center protein Z

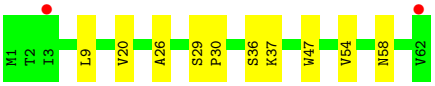
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:

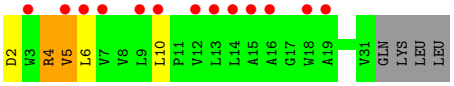




• Molecule 20: Photosystem II protein Y

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	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 19.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.15) 99.8 (19.99-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.152 , 0.198 0.159 , 0.203	Depositor DCC
R_{free} test set	26827 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	54101	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: BCR, DGD, LMG, FME, PHO, SQD, BCT, HTG, FE2, LMT, HEM, LHG, CL, CA, GOL, PL9, UNL, OEX, CLA, MG, HEC

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	0.60	0/2728	0.86	0/3719
1	a	0.61	0/2748	0.84	0/3746
2	B	0.54	0/4191	0.81	1/5709 (0.0%)
2	b	0.53	0/4198	0.80	1/5720 (0.0%)
3	C	0.49	0/3626	0.80	2/4936 (0.0%)
3	c	0.49	0/3676	0.79	0/5004
4	D	0.61	0/2818	0.83	3/3840 (0.1%)
4	d	0.57	0/2818	0.81	0/3840
5	E	0.45	0/693	0.80	1/944 (0.1%)
5	e	0.47	0/695	0.80	0/948
6	F	0.57	0/284	0.79	0/387
6	f	0.53	0/265	0.78	0/360
7	H	0.47	0/535	0.86	0/728
7	h	0.41	0/524	0.84	0/713
8	I	0.43	0/311	0.77	0/419
8	i	0.46	0/311	0.70	0/419
9	J	0.44	0/278	0.77	0/376
9	j	0.42	0/286	0.77	0/386
10	K	0.44	0/303	0.87	0/416
10	k	0.52	0/303	0.78	0/416
11	L	0.55	0/319	0.70	0/433
11	l	0.51	0/319	0.70	0/433
12	M	0.63	0/270	0.87	0/368
12	m	0.62	0/262	0.83	0/357
13	O	0.45	0/1958	0.77	0/2654
13	o	0.46	0/1937	0.81	2/2625 (0.1%)
14	T	0.60	0/266	0.72	0/362
14	t	0.60	0/266	0.71	0/362
15	U	0.48	0/785	0.75	0/1064
15	u	0.49	0/785	0.73	0/1064
16	V	0.51	0/1096	0.79	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
16	v	0.47	0/1085	0.79	1/1473 (0.1%)
17	Y	0.53	0/216	0.87	0/289
17	y	0.43	0/216	0.78	0/289
18	X	0.40	0/290	0.78	0/392
18	x	0.43	0/284	0.76	0/384
19	Z	0.41	0/490	0.77	0/669
19	z	0.38	0/490	0.83	0/669
20	R	0.36	0/245	0.67	0/338
All	All	0.52	0/43170	0.80	11/58738 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	170	ALA	CA-C-N	-6.04	113.72	119.76
4	D	170	ALA	C-N-CA	-6.04	113.72	119.76
4	D	262	SER	N-CA-C	-5.93	107.03	114.56
3	C	76	ILE	CA-C-N	5.81	125.67	119.28
3	C	76	ILE	C-N-CA	5.81	125.67	119.28
16	v	105	ARG	N-CA-C	5.71	117.50	111.28
2	b	13	ILE	N-CA-C	5.50	116.23	110.62
2	B	77	GLY	N-CA-C	5.31	121.06	114.37
13	o	55	GLU	CA-C-N	5.08	125.80	120.11
13	o	55	GLU	C-N-CA	5.08	125.80	120.11
5	E	83	LEU	N-CA-C	-5.04	107.63	112.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2634	0	2546	21	0
1	a	2645	0	2567	25	0
2	B	4021	0	3898	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	4022	0	3908	41	0
3	C	3501	0	3428	23	0
3	c	3544	0	3480	26	0
4	D	2720	0	2626	23	0
4	d	2720	0	2626	24	0
5	E	668	0	658	6	0
5	e	670	0	664	8	0
6	F	275	0	282	5	0
6	f	257	0	269	4	0
7	H	519	0	545	6	0
7	h	511	0	532	8	0
8	I	314	0	328	5	0
8	i	314	0	328	3	0
9	J	272	0	279	4	0
9	j	280	0	291	2	0
10	K	293	0	305	3	0
10	k	293	0	305	7	0
11	L	309	0	327	5	0
11	l	309	0	327	3	0
12	M	274	0	299	12	0
12	m	269	0	288	8	0
13	O	1903	0	1886	9	0
13	o	1891	0	1870	17	0
14	T	264	0	267	5	0
14	t	264	0	267	2	0
15	U	774	0	773	4	1
15	u	774	0	773	1	0
16	V	1072	0	1086	5	0
16	v	1064	0	1073	8	0
17	Y	215	0	246	5	0
17	y	215	0	246	4	0
18	X	287	0	317	3	0
18	x	281	0	312	3	0
19	Z	479	0	516	3	0
19	z	479	0	516	7	0
20	R	239	0	262	3	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	U	1	0	0	1	0
22	a	2	0	0	0	0
22	v	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	42	0
24	C	845	0	936	34	0
24	D	130	0	144	4	0
24	a	195	0	216	7	0
24	b	1040	0	1152	29	0
24	c	845	0	936	34	0
24	d	195	0	216	8	0
25	A	64	0	74	3	0
25	D	64	0	74	1	0
25	a	64	0	74	2	0
25	d	64	0	74	2	0
26	A	40	0	56	2	0
26	B	120	0	168	8	0
26	C	80	0	112	11	0
26	D	40	0	56	1	0
26	H	40	0	56	4	0
26	K	40	0	56	3	0
26	T	40	0	56	6	0
26	Y	40	0	56	3	0
26	a	40	0	56	1	0
26	b	120	0	168	8	0
26	c	80	0	112	5	0
26	d	40	0	56	3	0
26	h	40	0	56	4	0
26	k	40	0	56	1	0
26	t	40	0	56	6	0
26	y	40	0	56	2	0
27	A	108	0	156	7	0
27	B	54	0	78	1	0
27	F	43	0	53	1	0
27	L	54	0	78	2	0
27	a	108	0	156	4	0
27	f	43	0	53	2	1
28	A	18	0	24	1	0
28	B	42	0	56	1	0
28	C	12	0	16	0	0
28	F	6	0	8	0	0
28	O	6	0	8	0	0
28	T	12	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	V	24	0	32	0	0
28	a	12	0	16	1	0
28	b	30	0	40	1	0
28	c	12	0	16	2	0
28	f	6	0	7	1	0
28	o	6	0	8	0	0
28	t	6	0	8	0	0
28	v	18	0	24	1	0
29	A	35	0	46	2	0
29	B	60	0	81	1	0
29	C	35	0	46	2	0
29	F	35	0	46	0	0
29	M	105	0	138	4	0
29	T	25	0	35	0	0
29	a	70	0	92	4	0
29	b	25	0	35	3	0
29	f	35	0	46	1	0
29	m	35	0	46	2	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	55	0	80	5	0
31	D	55	0	80	2	0
31	a	55	0	80	6	0
31	d	55	0	80	1	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	C	34	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	2	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0
34	B	95	0	130	2	0
34	C	38	0	52	0	0
34	D	16	0	17	2	0
34	V	19	0	26	2	0
34	b	95	0	130	3	0
34	c	38	0	52	0	0
34	d	16	0	17	3	0
35	C	153	0	216	8	0
35	J	51	0	72	1	0
35	M	51	0	72	2	0
35	Z	37	0	44	1	0
35	a	51	0	72	1	0
35	b	51	0	72	3	0
35	c	102	0	144	4	0
35	j	51	0	72	2	0
35	z	39	0	48	4	0
36	C	186	0	246	5	0
36	D	52	0	71	2	0
36	H	62	0	82	0	0
36	c	186	0	246	4	0
36	e	62	0	82	9	0
36	h	62	0	82	0	0
37	D	147	0	222	9	0
37	E	42	0	57	2	0
37	L	49	0	74	2	0
37	d	147	0	222	9	0
37	e	42	0	57	4	0
37	l	49	0	74	2	0
38	E	43	0	30	3	0
38	e	43	0	30	2	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	166	0	0	1	0
41	B	295	0	0	2	0
41	C	232	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	D	143	0	0	1	0
41	E	34	0	0	0	0
41	F	8	0	0	0	0
41	H	44	0	0	0	0
41	I	4	0	0	1	0
41	J	11	0	0	0	0
41	K	7	0	0	0	0
41	L	17	0	0	0	0
41	M	24	0	0	0	0
41	O	179	0	0	0	0
41	T	17	0	0	1	0
41	U	85	0	0	2	0
41	V	117	0	0	3	0
41	X	8	0	0	0	0
41	Y	4	0	0	0	0
41	Z	1	0	0	1	0
41	a	159	0	0	2	0
41	b	261	0	0	2	0
41	c	204	0	0	2	0
41	d	131	0	0	1	0
41	e	20	0	0	0	0
41	f	8	0	0	0	0
41	h	42	0	0	0	0
41	i	6	0	0	0	0
41	j	6	0	0	0	0
41	k	7	0	0	1	0
41	l	8	0	0	0	0
41	m	14	0	0	0	0
41	o	163	0	0	2	0
41	t	9	0	0	0	0
41	u	91	0	0	0	0
41	v	83	0	0	1	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	54101	0	52739	547	1

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 5.

All (547) 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:214:MET:HG2	31:A:418:PL9:H102	1.47	0.95
24:B:616:CLA:H71	24:B:617:CLA:H192	1.52	0.88
24:c:517:CLA:HHC	24:c:517:CLA:HBB1	1.57	0.86
41:B:960:HOH:O	22:U:201:CL:CL	2.30	0.84
4:d:192:THR:HG23	24:d:403:CLA:HBC2	1.67	0.76
41:b:849:HOH:O	22:v:204:CL:CL	2.42	0.74
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.69	0.74
24:c:507:CLA:HBB1	24:c:507:CLA:HHC	1.70	0.73
1:a:298:ASN:ND2	41:a:502:HOH:O	2.21	0.72
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.71	0.72
31:A:418:PL9:H261	37:E:101:LHG:H223	1.71	0.72
1:a:214:MET:HG2	31:a:416:PL9:H102	1.69	0.72
24:a:410:CLA:H203	35:j:101:LMG:H412	1.72	0.72
15:U:51:LYS:NZ	41:U:301:HOH:O	2.23	0.71
31:a:416:PL9:H28	37:e:102:LHG:H222	1.72	0.70
16:v:71:GLY:HA2	28:v:201:GOL:H31	1.73	0.70
24:C:514:CLA:HBB1	26:C:515:BCR:H24C	1.72	0.70
24:B:615:CLA:H18	35:M:101:LMG:H421	1.74	0.69
24:C:504:CLA:HBB1	24:C:513:CLA:H41	1.72	0.69
27:a:414:SQD:H271	37:d:409:LHG:H141	1.73	0.69
26:T:103:BCR:H321	26:T:103:BCR:HC8	1.75	0.69
28:T:102:GOL:O1	41:T:201:HOH:O	2.10	0.68
24:C:506:CLA:CMD	24:C:508:CLA:HAB	2.24	0.68
35:c:522:LMG:H181	10:k:27:VAL:HG11	1.76	0.68
24:c:505:CLA:H202	24:c:511:CLA:HBB1	1.76	0.68
13:o:179[A]:GLU:OE2	41:o:401:HOH:O	2.12	0.68
1:A:298:ASN:ND2	41:A:501:HOH:O	2.28	0.67
24:C:514:CLA:H171	26:C:515:BCR:H373	1.76	0.66
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.77	0.66
24:b:624:CLA:H2	24:b:625:CLA:HBB2	1.77	0.66
37:D:409:LHG:H132	37:D:409:LHG:H372	1.78	0.66
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.78	0.65
4:D:192:THR:HG23	24:D:402:CLA:HBC2	1.78	0.65
24:D:403:CLA:H171	18:X:15:LEU:HD13	1.79	0.65
1:a:215:HIS:ND1	31:a:416:PL9:O1	2.27	0.64
13:o:74[B]:GLU:OE1	41:o:402:HOH:O	2.14	0.64
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.80	0.64
3:c:279:LEU:HD22	24:c:513:CLA:HED2	1.80	0.63
2:B:248:ALA:HA	24:B:604:CLA:H42	1.79	0.63
2:B:124:ARG:O	7:H:12[A]:ARG:NH1	2.29	0.63
8:I:37:LEU:O	41:I:201:HOH:O	2.15	0.62
12:m:6:LEU:HD11	29:m:102:LMT:H11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.81	0.62
3:C:286:ALA:HB2	24:C:503:CLA:HMD1	1.80	0.62
24:C:507:CLA:HMC2	24:C:508:CLA:H102	1.82	0.61
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.30	0.61
12:M:33:GLN:HB2	12:m:33:GLN:HB2	1.83	0.60
25:A:408:PHO:HBC3	4:D:279:LEU:HD22	1.83	0.60
24:c:517:CLA:H171	26:c:527:BCR:H373	1.83	0.60
1:a:271:LEU:HD11	31:a:416:PL9:HC8	1.84	0.60
37:D:409:LHG:H112	37:D:409:LHG:H382	1.84	0.60
24:B:607:CLA:H191	26:B:620:BCR:H363	1.85	0.59
15:U:16:LYS:NZ	41:U:302:HOH:O	2.35	0.59
3:c:213[A]:LEU:HG	24:c:510:CLA:H202	1.84	0.59
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.16	0.58
2:b:248:ALA:HA	24:b:612:CLA:H42	1.85	0.58
24:c:506:CLA:H61	24:c:516:CLA:H42	1.85	0.58
16:V:26:TYR:O	41:V:301:HOH:O	2.16	0.58
2:B:50:PRO:HB2	28:B:630:GOL:H12	1.85	0.58
36:e:101:DGD:HAW1	27:f:102:SQD:H382	1.86	0.58
24:c:512:CLA:HBC3	24:c:514:CLA:H71	1.85	0.57
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.86	0.57
3:c:79:LYS:HD2	16:v:35:TYR:HE1	1.68	0.57
36:e:101:DGD:HE3	36:e:101:DGD:HD4	1.87	0.57
24:C:503:CLA:H61	24:C:513:CLA:H42	1.86	0.57
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.86	0.57
24:C:506:CLA:HMD3	24:C:508:CLA:HAB	1.87	0.56
24:C:514:CLA:H202	35:C:521:LMG:H402	1.86	0.56
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.88	0.56
28:f:101:GOL:H11	16:v:27:LEU:HD21	1.86	0.56
4:d:139:ARG:NH2	41:d:502:HOH:O	2.39	0.56
1:a:72:LEU:HD11	29:a:404:LMT:H52	1.88	0.56
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.87	0.56
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.41	0.56
5:e:9:PRO:HA	37:e:102:LHG:HC31	1.87	0.56
2:b:98:LEU:HB2	34:b:601:HTG:H7'1	1.88	0.55
3:c:320:ARG:HB2	28:c:502:GOL:H32	1.88	0.55
29:f:103:LMT:O3'	29:f:103:LMT:O2B	2.23	0.55
1:A:238[A]:LYS:HG2	14:T:30:THR:HG21	1.89	0.55
4:D:102:THR:OG1	36:D:406:DGD:HG31	2.06	0.55
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.87	0.55
24:c:512:CLA:H201	35:c:522:LMG:H232	1.88	0.55
1:A:72:LEU:HD13	29:A:416:LMT:H11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:610:CLA:H193	26:h:101:BCR:H353	1.89	0.55
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.55
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.42	0.55
2:b:224:ARG:HH11	29:b:630:LMT:H1'	1.72	0.54
24:c:508:CLA:H201	37:d:409:LHG:H352	1.90	0.54
31:D:405:PL9:H201	37:L:101:LHG:H202	1.89	0.54
11:L:13:ASN:ND2	11:L:16:SER:H	2.05	0.54
24:c:516:CLA:O2D	24:c:517:CLA:HBB2	2.07	0.54
37:d:408:LHG:HC62	11:l:15:THR:HG23	1.88	0.54
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.07	0.54
2:B:338:GLN:HA	13:o:57:LYS:HE3	1.88	0.54
24:C:513:CLA:H101	24:C:514:CLA:H141	1.89	0.54
2:B:472:ARG:NH2	41:B:704:HOH:O	2.40	0.54
24:C:514:CLA:HBB1	26:C:515:BCR:H371	1.89	0.54
28:b:604:GOL:H11	16:v:51:SER:HA	1.90	0.54
31:a:416:PL9:HC2	31:a:416:PL9:H103	1.90	0.54
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.90	0.54
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.91	0.53
1:A:50:ILE:HG12	29:A:416:LMT:H102	1.89	0.53
13:O:27:ARG:NH1	13:O:202:ALA:O	2.40	0.53
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.44	0.53
3:c:286:ALA:HB2	24:c:506:CLA:HMD1	1.90	0.53
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.39	0.53
3:C:79:LYS:HG2	16:V:103:LYS:HD3	1.91	0.53
16:v:35:TYR:OH	41:v:301:HOH:O	2.14	0.53
2:b:216:HIS:HE1	24:b:618:CLA:C1A	2.21	0.53
24:c:512:CLA:H191	35:c:522:LMG:H232	1.90	0.53
10:k:24:VAL:HG13	17:y:25:ILE:HD13	1.91	0.53
13:o:37:THR:HG22	13:o:246:ALA:HB3	1.90	0.53
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.89	0.53
27:A:411:SQD:H251	37:D:409:LHG:H131	1.91	0.53
27:A:411:SQD:O7	3:C:28:GLN:NE2	2.42	0.53
27:A:411:SQD:H192	37:D:409:LHG:H201	1.90	0.53
29:M:102:LMT:H6'2	11:l:9:PRO:HB3	1.90	0.53
2:b:12:LEU:HB2	24:b:621:CLA:HMC2	1.90	0.53
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.44	0.53
1:a:183:MET:HA	24:a:409:CLA:HMD1	1.91	0.53
27:a:405:SQD:H141	26:t:101:BCR:HC41	1.91	0.53
3:c:26:ARG:NH2	17:y:46:LEU:OXT	2.37	0.53
3:c:217:PRO:HB2	36:c:519:DGD:HA21	1.90	0.53
24:b:622:CLA:HBB1	24:b:622:CLA:HMB1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:443:TRP:CZ2	24:C:509:CLA:HMD1	2.44	0.52
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.91	0.52
37:D:409:LHG:H352	37:D:409:LHG:H151	1.90	0.52
1:A:84:PRO:HA	1:A:112:TYR:CG	2.44	0.52
6:F:21:VAL:O	6:F:25:THR:HG23	2.09	0.52
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.45	0.52
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.52
24:c:509:CLA:CMD	24:c:511:CLA:HAB	2.40	0.52
37:d:409:LHG:H381	37:d:409:LHG:H122	1.91	0.52
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	1.92	0.52
29:C:522:LMT:O3B	41:C:601:HOH:O	2.19	0.52
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.92	0.51
4:d:14:TRP:CD1	34:d:412:HTG:H61	2.44	0.51
13:o:23:ASP:HB3	13:o:25:THR:HG23	1.92	0.51
1:a:121[A]:LEU:HD11	24:c:509:CLA:H152	1.92	0.51
37:d:409:LHG:H151	37:d:409:LHG:H342	1.92	0.51
19:z:47:TRP:CE2	35:z:101:LMG:H241	2.45	0.51
24:A:406:CLA:HED1	31:D:405:PL9:H362	1.91	0.51
35:C:501:LMG:H211	36:C:517:DGD:HA62	1.92	0.51
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.92	0.51
38:E:102:HEM:HAC	6:F:27:ALA:HB1	1.93	0.51
34:B:623:HTG:H7'3	29:a:404:LMT:H102	1.92	0.51
2:b:498:LYS:HD2	4:d:20:ASP:HA	1.92	0.51
25:A:408:PHO:HMA2	31:A:418:PL9:H221	1.93	0.51
29:a:419:LMT:O4'	41:a:501:HOH:O	2.19	0.51
1:a:227:THR:HB	1:a:231:GLU:HG3	1.93	0.51
24:a:410:CLA:HBB1	24:a:410:CLA:HHC	1.92	0.51
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.93	0.51
36:C:518:DGD:HB51	35:C:520:LMG:H392	1.93	0.51
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.46	0.51
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.41	0.50
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.93	0.50
24:c:509:CLA:HAA1	24:c:509:CLA:HBD	1.93	0.50
24:C:504:CLA:CBB	24:C:513:CLA:H41	2.41	0.50
3:c:334:PRO:HA	13:o:153:THR:OG1	2.10	0.50
24:B:612:CLA:HBC1	37:D:407:LHG:H322	1.93	0.50
3:C:223:TRP:CG	3:C:224:ILE:H	2.30	0.50
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.94	0.50
24:c:505:CLA:C4D	24:c:507:CLA:H2	2.41	0.50
34:d:412:HTG:H1	7:h:25:TRP:CD1	2.46	0.50
26:B:619:BCR:H363	26:t:101:BCR:H19C	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:443:TRP:CZ2	24:c:512:CLA:HMD1	2.46	0.50
24:A:409:CLA:H193	24:C:507:CLA:H93	1.93	0.50
27:A:415:SQD:H272	2:b:109:LEU:HD13	1.93	0.50
24:C:514:CLA:CBB	26:C:515:BCR:H24C	2.39	0.50
3:c:79:LYS:HD2	16:v:35:TYR:CE1	2.47	0.50
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.94	0.50
26:T:103:BCR:H19C	26:b:627:BCR:H363	1.93	0.50
3:c:213[B]:LEU:HD11	26:c:518:BCR:H373	1.93	0.50
24:c:517:CLA:HBB1	24:c:517:CLA:CHC	2.38	0.50
4:d:101:PHE:HB3	36:e:101:DGD:HG2	1.93	0.50
29:M:102:LMT:H6D	11:l:9:PRO:HA	1.94	0.50
2:B:499:VAL:HG12	4:D:135:LEU:HB3	1.94	0.49
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	1.93	0.49
4:D:205:LEU:HD13	25:D:401:PHO:HAB	1.94	0.49
8:I:2:GLU:O	8:I:6:ILE:HG12	2.11	0.49
2:B:76[B]:SER:HB2	34:B:623:HTG:HO6	1.77	0.49
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.46	0.49
12:M:27:VAL:HG12	12:m:28:GLN:HB3	1.93	0.49
3:c:38:GLY:HA3	24:c:515:CLA:HMD2	1.94	0.49
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.42	0.49
24:C:511:CLA:H43	37:D:409:LHG:H383	1.93	0.49
2:b:62:VAL:HB	24:b:614:CLA:HED3	1.93	0.49
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.47	0.49
24:b:624:CLA:H2	24:b:625:CLA:CBB	2.40	0.49
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.95	0.49
24:c:509:CLA:HHC	24:c:509:CLA:HBB1	1.94	0.49
24:c:517:CLA:H202	35:c:523:LMG:H402	1.94	0.49
2:B:405[B]:GLU:OE1	13:o:60:ARG:HD3	2.13	0.49
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.94	0.49
34:D:412:HTG:H1	7:H:25:TRP:CD1	2.47	0.49
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.48	0.49
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.95	0.49
31:A:418:PL9:H512	27:F:103:SQD:H301	1.95	0.48
3:C:279:LEU:HD22	24:C:510:CLA:HED2	1.95	0.48
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.94	0.48
2:B:149:LEU:HD22	24:B:605:CLA:H152	1.94	0.48
26:b:626:BCR:H12C	35:b:629:LMG:C43	2.43	0.48
2:b:224:ARG:NH1	29:b:630:LMT:H1'	2.29	0.48
24:B:607:CLA:H151	24:B:617:CLA:H122	1.95	0.48
10:k:15:TYR:OH	19:z:58:ASN:ND2	2.36	0.48
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:MET:HE3	24:B:616:CLA:CHD	2.44	0.48
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.49	0.48
29:B:622:LMT:O6'	4:D:16:ASP:OD2	2.32	0.48
13:O:53:LYS:HE2	13:O:63:ALA:HB3	1.95	0.48
4:d:136:VAL:HG12	4:d:138:VAL:HG13	1.95	0.48
24:B:616:CLA:H61	24:B:617:CLA:HBB1	1.96	0.48
3:C:25:ASN:O	3:C:41:ARG:HD3	2.14	0.48
3:C:156:LYS:HE3	41:C:740:HOH:O	2.13	0.48
36:e:101:DGD:HAF2	27:f:102:SQD:H372	1.96	0.48
11:L:13:ASN:C	11:L:13:ASN:HD22	2.20	0.48
2:B:39:LEU:HD22	29:a:404:LMT:H62	1.96	0.48
26:B:620:BCR:H331	26:B:620:BCR:C8	2.42	0.48
26:d:405:BCR:H313	36:e:101:DGD:HA91	1.95	0.48
28:A:413:GOL:H11	12:M:1:FME:HG2	1.96	0.47
1:A:257:ARG:NH2	2:B:492:GLU:O	2.47	0.47
24:B:602:CLA:H91	26:H:101:BCR:H21C	1.96	0.47
28:a:402:GOL:H2	5:e:63[A]:ILE:HD11	1.96	0.47
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.94	0.47
24:B:614:CLA:H162	24:B:614:CLA:H121	1.69	0.47
24:c:510:CLA:HMC2	24:c:511:CLA:H102	1.95	0.47
3:c:406:SER:HA	3:c:420:VAL:HG23	1.96	0.47
24:d:402:CLA:HMB1	24:d:402:CLA:HBB1	1.96	0.47
35:C:501:LMG:C25	24:C:506:CLA:HBB2	2.45	0.47
5:E:40:THR:HB	20:R:4:ARG:HG2	1.96	0.47
24:b:620:CLA:H71	37:l:101:LHG:H311	1.95	0.47
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.97	0.47
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.96	0.47
5:E:15:THR:HB	9:J:7:ILE:O	2.15	0.47
24:b:616:CLA:H122	35:b:629:LMG:H241	1.96	0.47
24:b:622:CLA:H18	37:d:407:LHG:H202	1.95	0.47
5:e:47:PHE:HZ	36:e:101:DGD:HBT2	1.79	0.47
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.45	0.47
26:d:405:BCR:H313	36:e:101:DGD:HAE1	1.97	0.47
3:C:334:PRO:HA	13:O:153:THR:OG1	2.15	0.47
20:R:6:LEU:O	20:R:10:LEU:HB2	2.15	0.47
36:c:520:DGD:HB32	36:c:520:DGD:HB61	1.63	0.47
7:h:38:PHE:HB2	26:h:101:BCR:C10	2.45	0.47
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.96	0.47
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.14	0.47
2:b:405:GLU:OE1	41:b:701:HOH:O	2.20	0.47
25:d:401:PHO:NC	25:d:401:PHO:ND	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:57:LYS:NZ	2:b:49:ASP:OD1	2.42	0.47
1:a:267:ASN:HB3	1:a:270[B]:SER:OG	2.15	0.47
24:b:617:CLA:HAB	4:d:123:ILE:HG12	1.97	0.47
24:A:409:CLA:H92	8:I:13:THR:HG23	1.97	0.46
37:L:101:LHG:H321	12:M:18:PRO:HB3	1.97	0.46
3:c:223:TRP:CG	3:c:224:ILE:H	2.33	0.46
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.83	0.46
3:C:338:GLY:HA3	3:C:341:LEU:O	2.15	0.46
34:D:412:HTG:H1'2	7:H:25:TRP:CD2	2.50	0.46
1:a:60:ILE:HD12	1:a:84:PRO:HD2	1.97	0.46
24:b:614:CLA:HHC	24:b:614:CLA:HBB1	1.97	0.46
3:c:360:ASP:OD1	41:c:601:HOH:O	2.20	0.46
26:T:103:BCR:H11C	26:T:103:BCR:H341	1.77	0.46
8:i:36:ASP:OD1	8:i:36:ASP:N	2.42	0.46
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.50	0.46
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.96	0.46
24:c:515:CLA:H171	19:z:20:VAL:HA	1.97	0.46
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.97	0.46
2:b:201:HIS:HB2	24:b:611:CLA:CHB	2.46	0.46
4:d:186:GLN:HB2	24:d:403:CLA:HBC1	1.96	0.46
2:B:256:MET:HA	2:B:263:THR:HG21	1.97	0.46
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.16	0.46
2:b:493:TRP:CD1	5:e:5:THR:HG22	2.50	0.46
24:b:623:CLA:H41	24:b:623:CLA:H62	1.67	0.46
35:b:629:LMG:H421	37:l:101:LHG:H371	1.98	0.46
3:c:437:PHE:CE1	24:c:514:CLA:HMB2	2.51	0.46
28:c:502:GOL:H2	41:c:731:HOH:O	2.15	0.46
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.98	0.46
24:c:509:CLA:H72	24:c:509:CLA:H112	1.80	0.46
26:H:101:BCR:H331	26:H:101:BCR:C8	2.46	0.45
13:O:180:GLU:CD	13:O:180:GLU:H	2.23	0.45
5:E:27:ILE:CD1	38:E:102:HEM:HBC2	2.47	0.45
24:b:610:CLA:H93	24:b:610:CLA:H111	1.75	0.45
24:b:613:CLA:H43	24:b:614:CLA:H2	1.98	0.45
10:k:10:LYS:HD2	10:k:10:LYS:N	2.31	0.45
2:B:458:PHE:HB3	24:B:605:CLA:HBC2	1.98	0.45
24:b:614:CLA:HAA1	24:b:614:CLA:HBD	1.97	0.45
1:A:227:THR:HB	1:A:231:GLU:HG3	1.98	0.45
24:A:406:CLA:HBA1	24:A:406:CLA:C4A	2.45	0.45
38:e:103:HEM:CAC	6:f:27:ALA:HB1	2.47	0.45
24:B:616:CLA:H152	24:B:616:CLA:H112	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:D:409:LHG:H242	37:D:409:LHG:H272	1.75	0.45
35:J:101:LMG:H152	35:J:101:LMG:H292	1.99	0.45
13:O:204:VAL:HG22	13:O:211:ILE:HG22	1.98	0.45
35:a:415:LMG:H242	24:c:509:CLA:H92	1.97	0.45
6:f:21:VAL:O	6:f:25:THR:HG23	2.17	0.45
13:o:145:GLU:HG2	13:o:196:GLN:HG3	1.98	0.45
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.99	0.45
1:a:153:SER:HB2	24:a:409:CLA:H43	1.99	0.45
2:b:36:SER:OG	26:b:627:BCR:H362	2.17	0.45
2:b:498:LYS:HA	4:d:24:ARG:HA	1.99	0.45
26:b:627:BCR:H15C	26:b:627:BCR:H351	1.83	0.45
24:A:406:CLA:H203	24:A:406:CLA:H162	1.74	0.45
24:C:514:CLA:CBB	26:C:515:BCR:H371	2.47	0.45
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.17	0.45
2:b:24:LEU:HG	24:b:624:CLA:HED2	1.99	0.45
2:b:227:LYS:NZ	29:b:630:LMT:O6'	2.50	0.45
3:c:52:ALA:HB2	24:c:515:CLA:HMA2	1.98	0.45
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.97	0.45
26:A:410:BCR:H24C	26:A:410:BCR:H371	1.74	0.45
4:D:343:GLU:O	41:D:534[B]:HOH:O	2.20	0.45
35:Z:101:LMG:HC8	35:Z:101:LMG:H111	1.63	0.45
25:a:411:PHO:HAB	4:d:205:LEU:HD13	1.99	0.45
2:b:30:VAL:HG12	24:b:614:CLA:HHD	1.97	0.45
24:d:402:CLA:H203	24:d:402:CLA:H162	1.69	0.45
4:D:49:LEU:HD13	26:D:404:BCR:C15	2.47	0.45
2:b:487:SER:HA	2:b:488:PRO:HD3	1.80	0.45
24:B:608:CLA:C4A	24:B:608:CLA:HBA2	2.48	0.44
29:C:522:LMT:H61	29:C:522:LMT:H32	1.77	0.44
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.99	0.44
4:d:40:CYS:HB3	4:d:117:HIS:O	2.17	0.44
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.44
35:C:501:LMG:H242	35:C:501:LMG:H212	1.78	0.44
16:V:6:GLU:OE2	41:V:302:HOH:O	2.20	0.44
17:Y:28:ILE:HG23	26:Y:101:BCR:H10C	2.00	0.44
2:B:223:GLN:NE2	2:B:227:LYS:HD3	2.31	0.44
24:b:624:CLA:HHC	24:b:624:CLA:HBB1	2.00	0.44
5:e:17:VAL:O	5:e:21:VAL:HG23	2.17	0.44
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.98	0.44
17:Y:32:GLY:HA3	26:Y:101:BCR:C15	2.48	0.44
2:b:458:PHE:HB3	24:b:613:CLA:HBC2	1.98	0.44
24:A:409:CLA:H162	24:A:409:CLA:H122	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:31:SER:OG	12:m:31:SER:OG	2.36	0.44
1:a:259:ILE:HG22	1:a:260:PHE:CD1	2.51	0.44
26:t:101:BCR:HC7	26:t:101:BCR:H331	1.60	0.44
19:z:37:LYS:NZ	35:z:101:LMG:HC4	2.32	0.44
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.73	0.44
36:D:406:DGD:O1B	36:D:406:DGD:O2D	2.28	0.44
31:a:416:PL9:H151	31:a:416:PL9:H171	1.70	0.44
31:A:418:PL9:H421	31:A:418:PL9:H401	1.79	0.44
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.73	0.44
4:d:103:ARG:O	4:d:107:LEU:HG	2.17	0.44
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.99	0.44
27:A:411:SQD:H122	27:A:411:SQD:H152	1.74	0.44
26:B:619:BCR:H24C	26:B:619:BCR:H371	1.77	0.44
9:j:6:ARG:HA	9:j:6:ARG:NH2	2.33	0.44
26:k:101:BCR:H371	26:k:101:BCR:H24C	1.63	0.44
35:C:501:LMG:H382	36:C:517:DGD:HB42	1.99	0.43
11:L:9:PRO:HA	29:M:105:LMT:H6D	1.99	0.43
16:V:30:LYS:NZ	41:V:304:HOH:O	2.39	0.43
2:b:86[A]:ILE:HD12	2:b:88:PRO:HD3	2.00	0.43
1:A:334:ARG:HD3	4:D:320:LEU:HD13	1.99	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.18	0.43
24:B:603:CLA:H111	24:B:603:CLA:H151	1.83	0.43
11:L:13:ASN:HD22	11:L:16:SER:H	1.64	0.43
14:T:20:ALA:O	14:T:24:ARG:HB3	2.18	0.43
3:c:429:SER:HA	36:c:520:DGD:HBW1	2.00	0.43
27:L:102:SQD:H1	27:L:102:SQD:H462	1.99	0.43
15:U:64:ILE:HB	15:U:67:LEU:HD11	2.00	0.43
34:V:206:HTG:H6'2	34:V:206:HTG:H3'2	1.81	0.43
18:X:29:ILE:O	18:X:33:GLN:HG2	2.19	0.43
36:e:101:DGD:HG2	36:e:101:DGD:HB21	1.85	0.43
12:M:4:ASN:ND2	35:M:101:LMG:O10	2.50	0.43
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.00	0.43
24:B:609:CLA:HAB	4:D:123:ILE:HG12	2.00	0.43
24:B:615:CLA:HAA1	24:B:615:CLA:HBD	2.00	0.43
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.98	0.43
37:d:409:LHG:H281	37:d:409:LHG:H251	1.80	0.43
37:d:409:LHG:H331	37:d:409:LHG:H361	1.68	0.43
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.54	0.43
27:A:411:SQD:H381	9:J:21:ILE:HD11	2.00	0.43
3:C:42:LEU:HD21	24:C:512:CLA:H2A	1.99	0.43
2:b:190:PHE:CZ	24:b:611:CLA:HBB1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:499:VAL:HG12	4:d:135:LEU:HB3	2.00	0.43
3:c:175:LEU:HD23	3:c:237:HIS:CG	2.53	0.43
4:d:279:LEU:HD22	25:d:401:PHO:HBC3	2.00	0.43
26:y:101:BCR:H15C	26:y:101:BCR:H351	1.86	0.43
1:A:132:GLU:O	1:A:136:ARG:HG2	2.19	0.43
3:C:213:LEU:HD21	26:C:516:BCR:C20	2.49	0.43
4:D:85:MET:CE	4:D:96:GLU:HG2	2.49	0.43
16:V:12:LEU:HD12	16:V:69:ILE:HB	2.00	0.43
34:V:206:HTG:H1'1	34:V:206:HTG:H4'1	1.73	0.43
8:i:2:GLU:O	8:i:6:ILE:HG12	2.18	0.43
27:A:411:SQD:H291	24:C:509:CLA:H71	2.01	0.43
26:C:516:BCR:H371	26:C:516:BCR:H24C	1.76	0.43
15:U:27:LEU:HD21	15:U:82:PHE:CG	2.54	0.43
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.01	0.43
2:b:224:ARG:HG3	7:h:24:GLY:O	2.19	0.43
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.48	0.43
3:C:48:LYS:HG3	3:C:138:GLU:HG3	2.00	0.43
3:C:262:ARG:HG2	8:I:38:GLU:HG2	2.00	0.43
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.99	0.43
26:K:101:BCR:H15C	26:K:101:BCR:H351	1.89	0.43
35:C:501:LMG:H221	36:C:517:DGD:HAE1	2.01	0.43
24:C:512:CLA:HMB1	26:K:101:BCR:H382	2.01	0.43
4:D:282:SER:OG	24:D:402:CLA:HED3	2.19	0.43
24:b:620:CLA:H112	24:b:620:CLA:H72	1.83	0.43
26:b:626:BCR:H15C	26:b:626:BCR:H351	1.89	0.43
5:e:26:THR:HB	38:e:103:HEM:HAB	2.00	0.43
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.42
13:o:193:THR:HG21	13:o:220:LEU:HD12	2.01	0.42
24:C:506:CLA:HAA1	24:C:506:CLA:HBD	2.00	0.42
26:T:103:BCR:H24C	26:T:103:BCR:H371	1.86	0.42
25:a:411:PHO:H61	25:a:411:PHO:H2	1.87	0.42
24:d:403:CLA:HAA2	24:d:403:CLA:HBD	2.02	0.42
36:e:101:DGD:HB71	36:e:101:DGD:HBW2	2.00	0.42
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.93	0.42
24:B:616:CLA:H2	24:B:617:CLA:CBB	2.49	0.42
9:J:8:PRO:HD2	9:J:11:ILE:HD12	2.00	0.42
26:T:103:BCR:H382	26:T:103:BCR:H23C	2.01	0.42
2:b:419:SER:HB3	34:b:631:HTG:H2'1	2.01	0.42
24:d:404:CLA:H2	18:x:14:LEU:HA	2.00	0.42
37:d:407:LHG:H212	12:m:18:PRO:HG3	2.00	0.42
37:e:102:LHG:H181	37:e:102:LHG:H151	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:615:CLA:H92	24:B:615:CLA:H61	1.74	0.42
26:C:516:BCR:H11C	26:C:516:BCR:H341	1.89	0.42
24:a:409:CLA:HAA2	24:a:409:CLA:HBD	2.01	0.42
24:a:410:CLA:H13	35:j:101:LMG:H242	2.01	0.42
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.42
5:e:27:ILE:HB	5:e:28:PRO:HD3	2.01	0.42
1:A:187:GLN:HB2	24:A:405:CLA:HAC2	2.02	0.42
24:A:409:CLA:H72	24:A:409:CLA:H112	1.71	0.42
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	2.01	0.42
24:C:506:CLA:HMD2	24:C:508:CLA:HAB	2.01	0.42
5:E:68:ASP:OD1	5:E:71:GLU:HB2	2.19	0.42
26:H:101:BCR:H15C	26:H:101:BCR:H351	1.90	0.42
2:b:190:PHE:HZ	24:b:611:CLA:HBB1	1.85	0.42
26:b:628:BCR:H20C	26:b:628:BCR:H361	1.92	0.42
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.01	0.42
26:C:516:BCR:H15C	26:C:516:BCR:H351	1.89	0.42
24:D:402:CLA:HAA2	24:D:402:CLA:HBD	2.02	0.42
1:a:131:TRP:CH2	24:c:509:CLA:HAA2	2.54	0.42
24:b:615:CLA:H122	24:b:615:CLA:H162	1.71	0.42
26:c:527:BCR:H15C	26:c:527:BCR:H351	1.87	0.42
1:A:160:ILE:HD11	36:C:517:DGD:HBT2	2.02	0.42
27:B:621:SQD:O8	11:L:7:ARG:HD3	2.18	0.42
26:T:103:BCR:H331	26:T:103:BCR:HC7	1.74	0.42
24:b:624:CLA:H92	24:b:624:CLA:H61	1.87	0.42
4:d:49:LEU:HD13	26:d:405:BCR:C15	2.50	0.42
24:d:404:CLA:H142	7:h:36:GLY:HA3	2.01	0.42
37:e:102:LHG:H201	37:e:102:LHG:H171	1.82	0.42
3:C:179:ALA:O	3:C:184:GLY:HA2	2.20	0.42
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.01	0.42
1:a:289:GLY:O	1:a:293:MET:HE3	2.19	0.42
13:o:180:GLU:H	13:o:180:GLU:CD	2.28	0.42
1:A:102:LEU:HD23	1:A:102:LEU:HA	1.93	0.42
24:C:514:CLA:HBA1	24:C:514:CLA:H3A	1.76	0.42
2:b:461:LEU:HD21	4:d:284:ILE:HD11	2.01	0.42
26:c:527:BCR:H11C	26:c:527:BCR:H341	1.81	0.42
26:h:101:BCR:H24C	26:h:101:BCR:H371	1.75	0.42
1:A:63:ILE:HB	3:C:335:THR:HG21	2.01	0.42
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.54	0.42
24:C:513:CLA:O2D	24:C:514:CLA:HBB2	2.19	0.42
24:c:517:CLA:H61	26:c:527:BCR:H281	2.02	0.42
26:t:101:BCR:H11C	26:t:101:BCR:H341	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:510:CLA:H141	24:C:510:CLA:H161	1.83	0.41
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.01	0.41
18:x:29:ILE:O	18:x:33:GLN:HG2	2.19	0.41
2:B:102:VAL:HA	26:B:619:BCR:C40	2.49	0.41
24:B:611:CLA:H152	24:B:611:CLA:OBD	2.19	0.41
24:B:616:CLA:H172	24:B:616:CLA:H13	1.95	0.41
3:C:438:LEU:HD11	24:C:506:CLA:HBB1	2.01	0.41
3:c:348:GLU:OE1	13:o:11:VAL:HA	2.20	0.41
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.55	0.41
24:C:513:CLA:H202	24:C:513:CLA:HMB2	2.01	0.41
12:M:25:LEU:HD23	12:M:25:LEU:HA	1.87	0.41
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.55	0.41
14:t:18:PHE:CD1	26:t:101:BCR:H343	2.55	0.41
25:A:408:PHO:NC	25:A:408:PHO:ND	2.67	0.41
4:D:126:MET:HE3	4:D:143:ALA:O	2.20	0.41
24:c:507:CLA:HBB1	24:c:507:CLA:CHC	2.46	0.41
13:o:30:TYR:HA	13:o:31:PRO:HD3	1.89	0.41
4:D:17:ILE:O	4:D:20:ASP:HB2	2.21	0.41
38:E:102:HEM:CAC	6:F:27:ALA:HB1	2.51	0.41
24:a:409:CLA:CBD	24:d:402:CLA:HAC2	2.51	0.41
12:M:34:LYS:HG2	29:M:102:LMT:O3B	2.20	0.41
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.02	0.41
27:a:405:SQD:H192	27:a:405:SQD:H161	1.88	0.41
2:b:160:GLY:HA3	2:b:180:PRO:HB3	2.02	0.41
2:b:237:VAL:HG11	24:b:619:CLA:H201	2.02	0.41
24:c:511:CLA:H92	24:c:511:CLA:H61	1.81	0.41
3:C:223:TRP:CD1	35:C:501:LMG:H321	2.56	0.41
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.88	0.41
3:c:179:ALA:O	3:c:184:GLY:HA2	2.21	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.87	0.41
4:d:24:ARG:HD3	18:x:37:VAL:HG22	2.01	0.41
2:B:221:PRO:HA	24:B:610:CLA:HED3	2.03	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.41
2:B:462:PHE:CE1	24:B:614:CLA:HMB3	2.55	0.41
24:B:615:CLA:H62	24:B:615:CLA:H41	1.82	0.41
3:C:348:GLU:OE1	13:O:11:VAL:HA	2.20	0.41
24:C:506:CLA:H43	26:C:516:BCR:HC7	2.02	0.41
12:M:6:LEU:HA	12:M:6:LEU:HD23	1.84	0.41
28:T:102:GOL:H12	29:m:102:LMT:H12	2.02	0.41
24:b:614:CLA:H41	24:b:614:CLA:H62	1.83	0.41
26:B:620:BCR:H15C	26:B:620:BCR:H351	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:GLY:HA3	24:C:512:CLA:HMD2	2.03	0.41
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.41
24:C:512:CLA:H41	17:Y:39:LEU:HD13	2.03	0.41
37:D:409:LHG:H112	37:D:409:LHG:C38	2.48	0.41
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.71	0.41
2:b:363:PHE:HB3	2:b:365:SER:O	2.21	0.41
2:B:61:PHE:CZ	24:B:608:CLA:HBB1	2.56	0.41
24:B:606:CLA:HAA1	24:B:606:CLA:HBD	2.02	0.41
19:Z:30:PRO:HD2	41:Z:201:HOH:O	2.20	0.41
4:d:202:ALA:HB2	31:d:406:PL9:H353	2.03	0.41
34:d:412:HTG:H1	7:h:25:TRP:CG	2.56	0.41
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.02	0.40
24:B:605:CLA:H161	24:B:605:CLA:H141	1.87	0.40
24:B:612:CLA:H192	24:B:612:CLA:H161	1.81	0.40
24:B:612:CLA:H203	24:B:614:CLA:NB	2.36	0.40
24:B:617:CLA:H92	24:B:617:CLA:H61	1.88	0.40
3:C:406:SER:HA	3:C:420:VAL:HG23	2.03	0.40
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.79	0.40
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.56	0.40
27:L:102:SQD:H342	14:T:12:CYS:HB3	2.02	0.40
2:B:25:MET:HG2	26:B:618:BCR:H23C	2.03	0.40
24:B:609:CLA:H3A	24:B:609:CLA:HBA2	1.89	0.40
2:b:185:TRP:CZ2	34:b:632:HTG:H2'1	2.56	0.40
3:c:127:PHE:CE1	35:z:101:LMG:H152	2.56	0.40
24:c:512:CLA:H203	24:c:512:CLA:H161	1.78	0.40
36:c:519:DGD:HA21	36:c:519:DGD:HA52	1.98	0.40
4:d:125:PHE:O	4:d:128:ARG:HB3	2.22	0.40
8:i:33:LYS:HB3	8:i:34:ARG:H	1.60	0.40
19:z:29:SER:HA	19:z:30:PRO:HD3	1.88	0.40
2:B:315:ILE:HG22	2:B:426:PHE:HB3	2.02	0.40
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.57	0.40
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.03	0.40
1:a:257:ARG:NH2	4:d:25:ASP:OD1	2.45	0.40
26:b:628:BCR:C8	26:b:628:BCR:H331	2.52	0.40
7:h:62:TRP:C	7:h:64:ALA:H	2.30	0.40
24:A:407:CLA:H192	37:E:101:LHG:H172	2.03	0.40
2:B:194:ASN:HA	2:B:195:PRO:HD2	1.91	0.40
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.03	0.40
1:a:121[B]:LEU:HD23	1:a:121[B]:LEU:HA	1.97	0.40
27:a:414:SQD:H321	24:c:512:CLA:H71	2.02	0.40
3:c:123:ALA:HB1	35:z:101:LMG:H242	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:h:101:BCR:H331	26:h:101:BCR:C8	2.51	0.40
10:k:46:ARG:NH2	41:k:201:HOH:O	2.47	0.40
26:A:410:BCR:H11C	26:A:410:BCR:H341	1.95	0.40
24:B:617:CLA:H112	24:B:617:CLA:H91	1.84	0.40
8:I:33:LYS:HB3	8:I:34:ARG:H	1.52	0.40
13:O:61:GLN:HG2	13:O:62:GLU:N	2.36	0.40
1:a:85:SER:HA	1:a:109:GLY:HA3	2.04	0.40
26:a:413:BCR:H24C	26:a:413:BCR:H371	1.88	0.40
26:b:628:BCR:H24C	26:b:628:BCR:H371	1.90	0.40
16:v:77:LYS:HG2	16:v:95:LEU:HD12	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:69:GLU:OE1	27:f:102:SQD:O3[2_554]	2.16	0.04

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%)	327 (98%)	7 (2%)	1 (0%)	36	34
1	a	338/344 (98%)	332 (98%)	5 (2%)	1 (0%)	36	34
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	502 (98%)	11 (2%)	0	100	100
3	C	453/455 (100%)	444 (98%)	7 (2%)	2 (0%)	30	26
3	c	459/455 (101%)	449 (98%)	8 (2%)	2 (0%)	30	26
4	D	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	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	64/65 (98%)	60 (94%)	4 (6%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (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	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	36 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5282/5384 (98%)	5166 (98%)	110 (2%)	6 (0%)	48 50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	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	272/279 (98%)	272 (100%)	0	100 100
1	a	275/279 (99%)	275 (100%)	0	100 100
2	B	412/403 (102%)	407 (99%)	5 (1%)	63 70
2	b	413/403 (102%)	410 (99%)	3 (1%)	76 82
3	C	356/356 (100%)	350 (98%)	6 (2%)	53 60
3	c	362/356 (102%)	357 (99%)	5 (1%)	59 66
4	D	277/277 (100%)	274 (99%)	3 (1%)	65 72
4	d	277/277 (100%)	274 (99%)	3 (1%)	65 72
5	E	74/73 (101%)	73 (99%)	1 (1%)	59 66
5	e	74/73 (101%)	72 (97%)	2 (3%)	39 41
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	25 (96%)	1 (4%)	29 29
7	H	55/54 (102%)	54 (98%)	1 (2%)	51 58
7	h	54/54 (100%)	54 (100%)	0	100 100
8	I	34/34 (100%)	34 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 39
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30 30
10	K	30/30 (100%)	29 (97%)	1 (3%)	33 34
10	k	30/30 (100%)	29 (97%)	1 (3%)	33 34
11	L	36/35 (103%)	35 (97%)	1 (3%)	38 40
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 40
12	M	31/32 (97%)	30 (97%)	1 (3%)	34 36
12	m	30/32 (94%)	30 (100%)	0	100 100
13	O	214/207 (103%)	211 (99%)	3 (1%)	59 66
13	o	211/207 (102%)	205 (97%)	6 (3%)	38 40
14	T	27/28 (96%)	25 (93%)	2 (7%)	13 8
14	t	27/28 (96%)	25 (93%)	2 (7%)	13 8
15	U	84/89 (94%)	83 (99%)	1 (1%)	63 70
15	u	84/89 (94%)	84 (100%)	0	100 100
16	V	118/117 (101%)	118 (100%)	0	100 100
16	v	117/117 (100%)	115 (98%)	2 (2%)	53 60
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24 22
17	y	22/23 (96%)	21 (96%)	1 (4%)	24 22
18	X	32/33 (97%)	32 (100%)	0	100 100
18	x	31/33 (94%)	31 (100%)	0	100 100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50 56
19	z	52/52 (100%)	52 (100%)	0	100 100
20	R	25/29 (86%)	23 (92%)	2 (8%)	11 7
All	All	4387/4403 (100%)	4329 (99%)	58 (1%)	61 68

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	79	SER
2	B	80	ILE
2	B	362	PHE
2	B	492	GLU
2	B	505	ARG

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Mol	Chain	Res	Type
3	C	28	GLN
3	C	29	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	90	LEU
4	D	136	VAL
4	D	329	MET
5	E	71	GLU
7	H	65	LEU
10	K	17	ILE
11	L	13	ASN
12	M	5	GLN
13	O	4	THR
13	O	181[A]	GLU
13	O	181[B]	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	70	ARG
17	Y	24	MET
19	Z	4	LEU
20	R	4	ARG
20	R	5	VAL
2	b	80	ILE
2	b	479	PHE
2	b	480	SER
3	c	19	ASN
3	c	142	GLU
3	c	289	PHE
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	136	VAL
4	d	329	MET
5	e	16	SER
5	e	71	GLU
6	f	15	ILE
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
11	l	15	THR

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Mol	Chain	Res	Type
13	o	4	THR
13	o	25	THR
13	o	37	THR
13	o	57	LYS
13	o	139	SER
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
16	v	2	GLU
16	v	110	LYS
17	y	24	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	296	ASN
2	B	53	ASN
2	B	490	GLN
3	C	44	ASN
3	C	418	ASN
4	D	61	HIS
4	D	83	ASN
4	D	186	GLN
4	D	332	GLN
5	E	74	GLN
11	L	13	ASN
13	O	61	GLN
13	O	124	ASN
13	O	147	ASN
19	Z	58	ASN
1	a	12	ASN
1	a	165	GLN
1	a	315	ASN
2	b	53	ASN
2	b	281	GLN
2	b	331	ASN
2	b	490	GLN
3	c	28	GLN
3	c	373	ASN
3	c	418	ASN
4	d	83	ASN

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Mol	Chain	Res	Type
4	d	186	GLN
4	d	301	GLN
4	d	332	GLN
5	e	74	GLN
12	m	5	GLN
13	o	124	ASN
13	o	147	ASN
13	o	155	ASN
15	u	81	HIS
19	z	6	GLN
19	z	31	GLN
19	z	58	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	2.25	4 (57%)
8	FME	I	1	8	8,9,10	0.66	0	7,9,11	1.17	1 (14%)
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.37	2 (28%)
12	FME	m	1	12	8,9,10	0.68	0	7,9,11	1.53	2 (28%)
14	FME	T	1	14	8,9,10	0.71	0	7,9,11	1.36	1 (14%)
12	FME	M	1	12	8,9,10	0.63	0	7,9,11	1.36	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
14	FME	t	1	14	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-3.38	117.62	122.82
14	t	1	FME	C-CA-N	2.62	114.47	109.73
12	m	1	FME	CA-N-CN	-2.46	119.03	122.82
8	i	1	FME	CA-N-CN	-2.45	119.05	122.82
14	t	1	FME	O1-CN-N	-2.43	118.87	125.27
14	T	1	FME	O-C-CA	-2.30	118.76	124.78
14	t	1	FME	O-C-CA	-2.28	118.80	124.78
8	I	1	FME	O-C-CA	-2.19	119.04	124.78
12	m	1	FME	O1-CN-N	-2.16	119.58	125.27
8	i	1	FME	O-C-CA	-2.08	119.33	124.78
12	M	1	FME	O-C-CA	-2.07	119.35	124.78
12	M	1	FME	CA-N-CN	-2.03	119.69	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	O1-CN-N-CA
12	m	1	FME	CA-CB-CG-SD
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 251 ligands modelled in this entry, 19 are monoatomic and 18 are unknown - leaving 214 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	GOL	A	412	-	5,5,5	0.32	0	5,5,5	0.36	0
37	LHG	d	409	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	2 (3%)
24	CLA	B	607	2	69,73,73	2.02	20 (28%)	83,113,113	2.91	30 (36%)
24	CLA	b	614	2	69,73,73	2.04	19 (27%)	83,113,113	2.96	29 (34%)
29	LMT	M	105	-	36,36,36	0.47	0	47,47,47	0.85	0
28	GOL	V	203	-	5,5,5	0.40	0	5,5,5	0.28	0
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.57	9 (16%)
29	LMT	f	103	-	36,36,36	0.48	0	47,47,47	0.94	2 (4%)
30	OEX	A	417	1,41,3	0,14,14	-	-	-		
40	HEC	v	205	16	50,50,50	1.67	10 (20%)	68,82,82	1.80	18 (26%)
24	CLA	C	503	3	69,73,73	2.07	20 (28%)	83,113,113	2.74	29 (34%)
37	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.11	5 (9%)
27	SQD	a	405	-	53,54,54	1.06	3 (5%)	62,65,65	1.24	6 (9%)
37	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.10	3 (6%)
24	CLA	c	515	3	69,73,73	2.02	19 (27%)	83,113,113	2.75	31 (37%)
25	PHO	d	401	-	58,69,69	2.76	14 (24%)	56,99,99	2.93	14 (25%)
24	CLA	d	403	4	69,73,73	2.02	19 (27%)	83,113,113	2.77	29 (34%)
26	BCR	A	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.23	7 (12%)
26	BCR	a	413	-	41,41,41	1.07	1 (2%)	56,56,56	1.14	4 (7%)
27	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.53	9 (14%)
27	SQD	A	415	-	53,54,54	1.05	3 (5%)	62,65,65	1.15	4 (6%)
35	LMG	c	523	-	51,51,55	0.96	2 (3%)	59,59,63	1.22	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	609	2	69,73,73	2.02	20 (28%)	83,113,113	2.76	32 (38%)
24	CLA	b	611	2	69,73,73	2.07	21 (30%)	83,113,113	2.88	30 (36%)
28	GOL	B	628	-	5,5,5	0.36	0	5,5,5	0.52	0
28	GOL	B	631	-	5,5,5	0.37	0	5,5,5	0.38	0
26	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.57	7 (12%)
24	CLA	C	508	41	69,73,73	2.03	20 (28%)	83,113,113	2.72	28 (33%)
24	CLA	b	624	2	69,73,73	2.02	19 (27%)	83,113,113	2.84	27 (32%)
35	LMG	J	101	39	51,51,55	0.86	2 (3%)	59,59,63	0.99	4 (6%)
24	CLA	C	506	3	69,73,73	1.99	20 (28%)	83,113,113	2.69	28 (33%)
29	LMT	F	102	-	36,36,36	0.46	0	47,47,47	1.01	2 (4%)
35	LMG	b	629	-	51,51,55	0.90	2 (3%)	59,59,63	1.01	3 (5%)
24	CLA	D	402	4	69,73,73	1.96	20 (28%)	83,113,113	2.89	30 (36%)
26	BCR	B	619	-	41,41,41	1.10	1 (2%)	56,56,56	1.38	6 (10%)
24	CLA	C	507	3	69,73,73	2.05	20 (28%)	83,113,113	2.71	29 (34%)
26	BCR	Y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.53	9 (16%)
28	GOL	B	626	-	5,5,5	0.43	0	5,5,5	0.30	0
24	CLA	a	410	41	69,73,73	2.00	20 (28%)	83,113,113	2.83	30 (36%)
29	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.90	1 (2%)
37	LHG	e	102	-	41,41,48	1.03	2 (4%)	44,47,54	0.93	2 (4%)
24	CLA	C	510	3	69,73,73	2.11	20 (28%)	83,113,113	2.77	28 (33%)
24	CLA	A	407	41	69,73,73	2.03	19 (27%)	83,113,113	2.89	32 (38%)
24	CLA	A	406	41	69,73,73	2.03	20 (28%)	83,113,113	2.91	32 (38%)
37	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.98	3 (5%)
24	CLA	a	409	1	69,73,73	2.05	20 (28%)	83,113,113	2.82	31 (37%)
24	CLA	c	513	3	69,73,73	2.09	20 (28%)	83,113,113	2.77	29 (34%)
24	CLA	B	604	2	69,73,73	2.08	20 (28%)	83,113,113	2.76	30 (36%)
24	CLA	c	506	3	69,73,73	2.03	21 (30%)	83,113,113	2.75	29 (34%)
36	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.88	2 (2%)
36	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	1.12	7 (9%)
36	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.12	7 (9%)
29	LMT	T	104	-	25,25,36	0.52	0	30,30,47	0.92	1 (3%)
28	GOL	b	603	-	5,5,5	0.33	0	5,5,5	0.20	0
26	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	9 (16%)
28	GOL	o	301	-	5,5,5	0.38	0	5,5,5	0.26	0
24	CLA	B	612	2	69,73,73	2.02	20 (28%)	83,113,113	2.78	27 (32%)
28	GOL	C	525	-	5,5,5	0.38	0	5,5,5	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	625	2	69,73,73	2.02	20 (28%)	83,113,113	2.79	30 (36%)
24	CLA	c	512	3	69,73,73	2.07	20 (28%)	83,113,113	2.75	29 (34%)
35	LMG	c	522	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)
24	CLA	B	611	41	69,73,73	2.08	18 (26%)	83,113,113	2.84	34 (40%)
29	LMT	b	630	-	25,25,36	0.52	0	30,30,47	0.64	0
34	HTG	c	525	-	19,19,19	1.03	2 (10%)	23,24,24	1.49	3 (13%)
35	LMG	j	101	39	51,51,55	0.92	2 (3%)	59,59,63	1.04	3 (5%)
24	CLA	C	514	3	69,73,73	2.05	19 (27%)	83,113,113	2.81	31 (37%)
28	GOL	a	401	-	5,5,5	0.42	0	5,5,5	0.46	0
24	CLA	B	610	2	69,73,73	2.02	18 (26%)	83,113,113	2.76	29 (34%)
37	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
28	GOL	B	630	-	5,5,5	0.40	0	5,5,5	0.36	0
34	HTG	b	631	-	19,19,19	0.79	1 (5%)	23,24,24	1.26	2 (8%)
35	LMG	C	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.18	5 (8%)
28	GOL	B	629	-	5,5,5	0.37	0	5,5,5	0.28	0
35	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.10	4 (6%)
24	CLA	C	511	3	69,73,73	2.07	20 (28%)	83,113,113	2.70	32 (38%)
34	HTG	b	608	-	19,19,19	1.07	2 (10%)	23,24,24	1.27	3 (13%)
35	LMG	a	415	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	5 (8%)
24	CLA	b	619	41	69,73,73	2.05	21 (30%)	83,113,113	2.84	31 (37%)
37	LHG	d	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.00	4 (7%)
28	GOL	A	413	-	5,5,5	0.46	0	5,5,5	0.46	0
29	LMT	B	622	-	36,36,36	0.43	0	47,47,47	1.06	2 (4%)
26	BCR	B	620	-	41,41,41	1.05	1 (2%)	56,56,56	1.50	10 (17%)
31	PL9	A	418	-	55,55,55	0.66	2 (3%)	68,69,69	1.77	20 (29%)
34	HTG	C	523	-	19,19,19	0.99	2 (10%)	23,24,24	1.58	2 (8%)
26	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	13 (23%)
24	CLA	c	508	41	69,73,73	2.04	20 (28%)	83,113,113	2.84	31 (37%)
24	CLA	B	614	2	69,73,73	2.04	19 (27%)	83,113,113	2.76	32 (38%)
24	CLA	C	513	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	30 (36%)
24	CLA	b	622	2	69,73,73	2.04	20 (28%)	83,113,113	2.70	31 (37%)
38	HEM	e	103	6,5	50,50,50	1.52	7 (14%)	66,82,82	1.72	15 (22%)
36	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.21	7 (9%)
24	CLA	C	502	3	69,73,73	2.03	18 (26%)	83,113,113	2.81	30 (36%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.30	0
24	CLA	c	509	3	69,73,73	1.99	20 (28%)	83,113,113	2.69	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	a	412	1	69,73,73	2.05	19 (27%)	83,113,113	2.84	32 (38%)
35	LMG	M	101	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
24	CLA	b	623	2	69,73,73	1.99	19 (27%)	83,113,113	2.92	32 (38%)
24	CLA	c	505	3	69,73,73	2.01	20 (28%)	83,113,113	2.79	29 (34%)
28	GOL	v	203	-	5,5,5	0.41	0	5,5,5	0.27	0
24	CLA	C	509	3	69,73,73	2.06	20 (28%)	83,113,113	2.85	29 (34%)
28	GOL	t	102	-	5,5,5	0.45	0	5,5,5	0.12	0
37	LHG	D	409	-	48,48,48	0.96	2 (4%)	51,54,54	1.04	3 (5%)
24	CLA	B	613	2	69,73,73	2.00	19 (27%)	83,113,113	2.90	29 (34%)
26	BCR	k	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.47	11 (19%)
24	CLA	B	603	2	69,73,73	2.06	21 (30%)	83,113,113	2.89	28 (33%)
24	CLA	C	512	3	69,73,73	2.06	20 (28%)	83,113,113	2.80	32 (38%)
34	HTG	b	632	-	19,19,19	1.14	2 (10%)	23,24,24	1.75	3 (13%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	11 (19%)
28	GOL	V	202	-	5,5,5	0.38	0	5,5,5	0.32	0
24	CLA	b	610	41	69,73,73	2.07	20 (28%)	83,113,113	2.81	26 (31%)
26	BCR	d	405	-	41,41,41	1.06	1 (2%)	56,56,56	1.65	13 (23%)
34	HTG	c	524	-	19,19,19	1.04	2 (10%)	23,24,24	1.49	1 (4%)
24	CLA	A	409	1	69,73,73	2.07	20 (28%)	83,113,113	2.79	31 (37%)
28	GOL	f	101	33	5,5,5	0.32	0	5,5,5	0.49	0
29	LMT	a	404	-	36,36,36	0.48	1 (2%)	47,47,47	1.10	2 (4%)
36	DGD	c	521	-	63,63,67	0.89	2 (3%)	77,77,81	1.01	4 (5%)
34	HTG	B	623	-	19,19,19	1.07	1 (5%)	23,24,24	1.09	1 (4%)
24	CLA	c	507	3	69,73,73	2.06	19 (27%)	83,113,113	2.77	27 (32%)
34	HTG	D	412	-	16,16,19	1.10	2 (12%)	20,21,24	1.49	1 (5%)
34	HTG	C	524	-	19,19,19	1.01	2 (10%)	23,24,24	1.78	4 (17%)
28	GOL	b	604	-	5,5,5	0.37	0	5,5,5	0.24	0
29	LMT	m	102	-	36,36,36	0.49	0	47,47,47	0.98	2 (4%)
36	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	0.98	4 (5%)
25	PHO	A	408	-	58,69,69	2.78	15 (25%)	56,99,99	2.81	13 (23%)
24	CLA	c	510	3	69,73,73	2.02	20 (28%)	83,113,113	2.75	30 (36%)
28	GOL	T	101	-	5,5,5	0.43	0	5,5,5	0.17	0
24	CLA	B	602	41	69,73,73	2.07	20 (28%)	83,113,113	2.85	29 (34%)
34	HTG	d	412	-	16,16,19	1.22	2 (12%)	20,21,24	1.80	3 (15%)
29	LMT	M	104	-	36,36,36	0.54	1 (2%)	47,47,47	1.04	4 (8%)
24	CLA	B	616	2	69,73,73	2.01	18 (26%)	83,113,113	2.88	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	606	2	69,73,73	2.03	18 (26%)	83,113,113	2.92	30 (36%)
24	CLA	c	511	41	69,73,73	2.00	20 (28%)	83,113,113	2.76	27 (32%)
26	BCR	c	527	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	8 (14%)
27	SQD	A	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.52	11 (17%)
38	HEM	E	102	6,5	50,50,50	1.55	6 (12%)	66,82,82	1.84	14 (21%)
36	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.02	5 (6%)
24	CLA	b	620	2	69,73,73	2.00	19 (27%)	83,113,113	2.79	29 (34%)
34	HTG	B	624	-	19,19,19	0.78	1 (5%)	23,24,24	1.56	3 (13%)
36	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	6 (7%)
31	PL9	d	406	-	55,55,55	0.71	2 (3%)	68,69,69	1.54	16 (23%)
28	GOL	A	414	-	5,5,5	0.39	0	5,5,5	0.17	0
28	GOL	C	526	-	5,5,5	0.34	0	5,5,5	0.52	0
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.27	0
24	CLA	b	621	2	69,73,73	2.03	21 (30%)	83,113,113	2.79	33 (39%)
24	CLA	c	517	3	69,73,73	2.08	20 (28%)	83,113,113	2.84	32 (38%)
24	CLA	d	404	4	69,73,73	2.03	21 (30%)	83,113,113	2.86	32 (38%)
27	SQD	a	414	-	53,54,54	0.97	3 (5%)	62,65,65	1.59	13 (20%)
28	GOL	V	201	-	5,5,5	0.37	0	5,5,5	0.32	0
34	HTG	b	601	-	19,19,19	0.96	1 (5%)	23,24,24	1.04	1 (4%)
35	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)
24	CLA	d	402	41	69,73,73	2.04	20 (28%)	83,113,113	2.79	32 (38%)
24	CLA	c	516	3	69,73,73	2.04	19 (27%)	83,113,113	2.95	32 (38%)
24	CLA	b	616	41	69,73,73	2.03	19 (27%)	83,113,113	2.80	30 (36%)
34	HTG	B	632	-	19,19,19	1.02	2 (10%)	23,24,24	1.39	3 (13%)
24	CLA	C	505	41	69,73,73	2.05	20 (28%)	83,113,113	2.84	30 (36%)
23	BCT	a	418	21	2,3,3	0.64	0	2,3,3	0.73	0
26	BCR	K	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.43	11 (19%)
34	HTG	V	206	-	19,19,19	1.04	2 (10%)	23,24,24	1.30	3 (13%)
26	BCR	B	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.38	7 (12%)
25	PHO	D	401	-	58,69,69	2.77	12 (20%)	56,99,99	2.67	14 (25%)
34	HTG	B	633	-	19,19,19	1.03	2 (10%)	23,24,24	1.41	1 (4%)
24	CLA	b	615	2	69,73,73	2.01	20 (28%)	83,113,113	2.88	29 (34%)
23	BCT	A	404	21	2,3,3	0.59	0	2,3,3	1.30	0
29	LMT	a	419	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
29	LMT	B	635	-	25,25,36	0.55	1 (4%)	30,30,47	0.80	1 (3%)
24	CLA	A	405	1	69,73,73	2.05	20 (28%)	83,113,113	2.73	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	b	628	-	41,41,41	1.07	1 (2%)	56,56,56	1.25	7 (12%)
28	GOL	b	602	-	5,5,5	0.41	0	5,5,5	0.44	0
37	LHG	d	407	-	48,48,48	0.88	3 (6%)	51,54,54	1.04	5 (9%)
26	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.38	7 (12%)
28	GOL	c	501	-	5,5,5	0.37	0	5,5,5	0.29	0
36	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.92	4 (5%)
28	GOL	b	606	-	5,5,5	0.37	0	5,5,5	0.28	0
28	GOL	B	627	-	5,5,5	0.30	0	5,5,5	0.45	0
30	OEX	a	417	1,41,3	0,14,14	-	-	-		
24	CLA	B	605	2	69,73,73	1.97	21 (30%)	83,113,113	2.77	32 (38%)
31	PL9	D	405	-	55,55,55	0.65	1 (1%)	68,69,69	1.71	18 (26%)
24	CLA	B	608	41	69,73,73	2.01	20 (28%)	83,113,113	2.71	31 (37%)
40	HEC	V	205	16	50,50,50	1.71	9 (18%)	68,82,82	1.73	20 (29%)
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.21	0
24	CLA	D	403	4	69,73,73	2.05	21 (30%)	83,113,113	2.80	30 (36%)
24	CLA	b	618	2	69,73,73	2.00	18 (26%)	83,113,113	2.78	30 (36%)
26	BCR	D	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.73	14 (25%)
35	LMG	Z	101	-	37,37,55	0.96	2 (5%)	45,45,63	1.38	6 (13%)
37	LHG	D	408	-	48,48,48	0.89	2 (4%)	51,54,54	0.89	4 (7%)
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.83	4 (17%)
29	LMT	C	522	-	36,36,36	0.50	0	47,47,47	1.22	3 (6%)
28	GOL	c	502	-	5,5,5	0.40	0	5,5,5	0.48	0
26	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	16 (28%)
29	LMT	A	416	-	36,36,36	0.56	1 (2%)	47,47,47	1.28	3 (6%)
31	PL9	a	416	-	55,55,55	0.64	2 (3%)	68,69,69	1.91	18 (26%)
26	BCR	T	103	-	41,41,41	1.08	1 (2%)	56,56,56	1.62	13 (23%)
34	HTG	b	607	-	19,19,19	1.08	2 (10%)	23,24,24	1.32	1 (4%)
27	SQD	L	102	-	53,54,54	1.02	3 (5%)	62,65,65	1.58	10 (16%)
27	SQD	F	103	-	42,43,54	1.15	3 (7%)	51,54,65	1.59	11 (21%)
24	CLA	b	613	2	69,73,73	2.01	20 (28%)	83,113,113	2.72	31 (37%)
26	BCR	b	626	-	41,41,41	1.02	1 (2%)	56,56,56	1.45	8 (14%)
28	GOL	V	204	-	5,5,5	0.35	0	5,5,5	0.29	0
27	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.47	8 (15%)
28	GOL	F	101	33	5,5,5	0.37	0	5,5,5	0.22	0
24	CLA	B	615	2	69,73,73	2.03	20 (28%)	83,113,113	2.86	29 (34%)
28	GOL	O	301	-	5,5,5	0.35	0	5,5,5	0.40	0
36	DGD	D	406	-	52,52,67	1.02	3 (5%)	60,60,81	1.21	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	617	2	69,73,73	2.10	20 (28%)	83,113,113	2.70	31 (37%)
24	CLA	c	514	3	69,73,73	2.05	20 (28%)	83,113,113	2.81	33 (39%)
26	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	8 (14%)
25	PHO	a	411	-	58,69,69	2.77	14 (24%)	56,99,99	2.70	16 (28%)
35	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.11	3 (6%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	B	617	2	69,73,73	2.03	20 (28%)	83,113,113	2.77	29 (34%)
28	GOL	b	605	-	5,5,5	0.37	0	5,5,5	0.30	0
24	CLA	b	612	2	69,73,73	2.03	20 (28%)	83,113,113	2.86	32 (38%)
28	GOL	v	202	-	5,5,5	0.34	0	5,5,5	0.28	0
24	CLA	C	504	3	69,73,73	2.08	19 (27%)	83,113,113	2.77	27 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	A	412	-	-	0/4/4/4	-
37	LHG	d	409	-	-	13/53/53/53	-
24	CLA	B	607	2	-	5/39/115/115	-
24	CLA	b	614	2	-	3/39/115/115	-
29	LMT	M	105	-	-	7/21/61/61	0/2/2/2
28	GOL	V	203	-	-	1/4/4/4	-
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
29	LMT	f	103	-	-	10/21/61/61	0/2/2/2
40	HEC	v	205	16	1/1/3/7	5/14/54/54	-
24	CLA	C	503	3	-	5/39/115/115	-
37	LHG	D	407	-	-	13/53/53/53	-
27	SQD	a	405	-	-	16/49/69/69	0/1/1/1
37	LHG	E	101	-	-	22/46/46/53	-
24	CLA	c	515	3	-	5/39/115/115	-
25	PHO	d	401	-	-	1/37/103/103	0/5/6/6
24	CLA	d	403	4	-	4/39/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	415	-	-	14/49/69/69	0/1/1/1
35	LMG	c	523	-	-	3/46/66/70	0/1/1/1
24	CLA	B	609	2	-	1/39/115/115	-
24	CLA	b	611	2	-	7/39/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-
28	GOL	B	631	-	-	0/4/4/4	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	C	508	41	-	7/39/115/115	-
24	CLA	b	624	2	-	4/39/115/115	-
35	LMG	J	101	39	-	9/46/66/70	0/1/1/1
24	CLA	C	506	3	-	6/39/115/115	-
29	LMT	F	102	-	-	3/21/61/61	0/2/2/2
35	LMG	b	629	-	-	10/46/66/70	0/1/1/1
24	CLA	D	402	4	-	0/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	C	507	3	-	9/39/115/115	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	a	410	41	-	10/39/115/115	-
29	LMT	M	102	-	-	5/21/61/61	0/2/2/2
37	LHG	e	102	-	-	20/46/46/53	-
24	CLA	C	510	3	-	11/39/115/115	-
24	CLA	A	407	41	-	4/39/115/115	-
24	CLA	A	406	41	-	4/39/115/115	-
37	LHG	l	101	-	-	14/53/53/53	-
24	CLA	a	409	1	-	6/39/115/115	-
24	CLA	c	513	3	-	11/39/115/115	-
24	CLA	B	604	2	-	8/39/115/115	-
24	CLA	c	506	3	-	7/39/115/115	-
36	DGD	C	519	-	-	8/51/91/95	0/2/2/2
36	DGD	C	517	-	-	16/51/91/95	0/2/2/2
36	DGD	c	519	-	-	15/51/91/95	0/2/2/2
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
28	GOL	b	603	-	-	0/4/4/4	-
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	o	301	-	-	3/4/4/4	-
24	CLA	B	612	2	-	6/39/115/115	-
28	GOL	C	525	-	-	2/4/4/4	-
24	CLA	b	625	2	-	8/39/115/115	-
24	CLA	c	512	3	-	4/39/115/115	-
35	LMG	c	522	-	-	13/46/66/70	0/1/1/1
24	CLA	B	611	41	-	6/39/115/115	-
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
34	HTG	c	525	-	-	0/10/30/30	0/1/1/1
35	LMG	j	101	39	-	12/46/66/70	0/1/1/1
24	CLA	C	514	3	-	6/39/115/115	-
28	GOL	a	401	-	-	2/4/4/4	-
24	CLA	B	610	2	-	5/39/115/115	-
37	LHG	L	101	-	-	15/53/53/53	-
28	GOL	B	630	-	-	4/4/4/4	-
34	HTG	b	631	-	-	3/10/30/30	0/1/1/1
35	LMG	C	521	-	-	9/46/66/70	0/1/1/1
28	GOL	B	629	-	-	3/4/4/4	-
35	LMG	C	501	-	-	18/46/66/70	0/1/1/1
24	CLA	C	511	3	-	8/39/115/115	-
34	HTG	b	608	-	-	1/10/30/30	0/1/1/1
35	LMG	a	415	-	-	18/46/66/70	0/1/1/1
24	CLA	b	619	41	-	6/39/115/115	-
37	LHG	d	408	-	-	9/53/53/53	-
28	GOL	A	413	-	-	2/4/4/4	-
29	LMT	B	622	-	-	10/21/61/61	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
31	PL9	A	418	-	-	13/53/73/73	0/1/1/1
34	HTG	C	523	-	-	0/10/30/30	0/1/1/1
26	BCR	C	516	-	-	4/29/63/63	0/2/2/2
24	CLA	c	508	41	-	8/39/115/115	-
24	CLA	B	614	2	-	7/39/115/115	-
24	CLA	C	513	3	-	12/39/115/115	-
24	CLA	b	622	2	-	4/39/115/115	-
38	HEM	e	103	6,5	-	10/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	e	101	-	-	26/51/91/95	0/2/2/2
24	CLA	C	502	3	-	5/39/115/115	-
28	GOL	T	102	-	-	2/4/4/4	-
24	CLA	c	509	3	-	4/39/115/115	-
24	CLA	a	412	1	-	9/39/115/115	-
35	LMG	M	101	-	-	7/46/66/70	0/1/1/1
24	CLA	b	623	2	-	20/39/115/115	-
24	CLA	c	505	3	-	5/39/115/115	-
28	GOL	v	203	-	-	2/4/4/4	-
24	CLA	C	509	3	-	5/39/115/115	-
28	GOL	t	102	-	-	0/4/4/4	-
37	LHG	D	409	-	-	14/53/53/53	-
24	CLA	B	613	2	-	1/39/115/115	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
24	CLA	B	603	2	-	7/39/115/115	-
24	CLA	C	512	3	-	3/39/115/115	-
34	HTG	b	632	-	-	5/10/30/30	0/1/1/1
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-
24	CLA	b	610	41	-	16/39/115/115	-
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
34	HTG	c	524	-	-	3/10/30/30	0/1/1/1
24	CLA	A	409	1	-	10/39/115/115	-
28	GOL	f	101	33	-	3/4/4/4	-
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
36	DGD	c	521	-	-	16/51/91/95	0/2/2/2
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	c	507	3	-	2/39/115/115	-
34	HTG	D	412	-	-	1/7/27/30	0/1/1/1
34	HTG	C	524	-	-	3/10/30/30	0/1/1/1
28	GOL	b	604	-	-	2/4/4/4	-
29	LMT	m	102	-	-	5/21/61/61	0/2/2/2
36	DGD	c	520	-	-	16/51/91/95	0/2/2/2
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
24	CLA	c	510	3	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	B	602	41	-	12/39/115/115	-
34	HTG	d	412	-	-	0/7/27/30	0/1/1/1
29	LMT	M	104	-	-	10/21/61/61	0/2/2/2
24	CLA	B	616	2	-	11/39/115/115	-
24	CLA	B	606	2	-	6/39/115/115	-
24	CLA	c	511	41	-	7/39/115/115	-
26	BCR	c	527	-	-	0/29/63/63	0/2/2/2
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
38	HEM	E	102	6,5	-	9/14/54/54	-
36	DGD	C	518	-	-	18/51/91/95	0/2/2/2
24	CLA	b	620	2	-	3/39/115/115	-
34	HTG	B	624	-	-	5/10/30/30	0/1/1/1
36	DGD	H	102	-	-	13/51/91/95	0/2/2/2
31	PL9	d	406	-	-	3/53/73/73	0/1/1/1
28	GOL	A	414	-	-	2/4/4/4	-
28	GOL	C	526	-	-	0/4/4/4	-
28	GOL	a	402	-	-	2/4/4/4	-
24	CLA	b	621	2	-	2/39/115/115	-
24	CLA	c	517	3	-	5/39/115/115	-
24	CLA	d	404	4	-	3/39/115/115	-
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
28	GOL	V	201	-	-	2/4/4/4	-
34	HTG	b	601	-	-	3/10/30/30	0/1/1/1
35	LMG	C	520	-	-	11/46/66/70	0/1/1/1
24	CLA	d	402	41	-	8/39/115/115	-
24	CLA	c	516	3	-	11/39/115/115	-
24	CLA	b	616	41	-	4/39/115/115	-
34	HTG	B	632	-	-	3/10/30/30	0/1/1/1
24	CLA	C	505	41	-	8/39/115/115	-
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
34	HTG	V	206	-	-	4/10/30/30	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
25	PHO	D	401	-	-	5/37/103/103	0/5/6/6
34	HTG	B	633	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	615	2	-	11/39/115/115	-
29	LMT	a	419	-	-	5/21/61/61	0/2/2/2
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
24	CLA	A	405	1	-	4/39/115/115	-
26	BCR	b	628	-	-	2/29/63/63	0/2/2/2
28	GOL	b	602	-	-	4/4/4/4	-
37	LHG	d	407	-	-	12/53/53/53	-
26	BCR	b	627	-	-	2/29/63/63	0/2/2/2
28	GOL	c	501	-	-	0/4/4/4	-
36	DGD	h	102	-	-	10/51/91/95	0/2/2/2
28	GOL	b	606	-	-	3/4/4/4	-
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	B	605	2	-	6/39/115/115	-
31	PL9	D	405	-	-	8/53/73/73	0/1/1/1
40	HEC	V	205	16	1/1/3/7	4/14/54/54	-
24	CLA	B	608	41	-	4/39/115/115	-
28	GOL	v	201	-	-	2/4/4/4	-
24	CLA	D	403	4	-	5/39/115/115	-
24	CLA	b	618	2	-	8/39/115/115	-
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
35	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
37	LHG	D	408	-	-	11/53/53/53	-
34	HTG	B	625	-	-	5/10/30/30	0/1/1/1
29	LMT	C	522	-	-	10/21/61/61	0/2/2/2
28	GOL	c	502	-	-	0/4/4/4	-
26	BCR	t	101	-	-	3/29/63/63	0/2/2/2
29	LMT	A	416	-	-	5/21/61/61	0/2/2/2
31	PL9	a	416	-	-	15/53/73/73	0/1/1/1
26	BCR	T	103	-	-	2/29/63/63	0/2/2/2
34	HTG	b	607	-	-	2/10/30/30	0/1/1/1
27	SQD	L	102	-	-	20/49/69/69	0/1/1/1
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1
24	CLA	b	613	2	-	3/39/115/115	-
26	BCR	b	626	-	-	2/29/63/63	0/2/2/2
28	GOL	V	204	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
28	GOL	F	101	33	-	2/4/4/4	-
24	CLA	B	615	2	-	14/39/115/115	-
28	GOL	O	301	-	-	2/4/4/4	-
36	DGD	D	406	-	-	21/47/67/95	0/1/1/2
24	CLA	b	617	2	-	3/39/115/115	-
24	CLA	c	514	3	-	9/39/115/115	-
26	BCR	c	518	-	-	2/29/63/63	0/2/2/2
25	PHO	a	411	-	-	5/37/103/103	0/5/6/6
35	LMG	z	101	-	-	13/34/54/70	0/1/1/1
28	GOL	B	636	-	-	0/4/4/4	-
24	CLA	B	617	2	-	6/39/115/115	-
28	GOL	b	605	-	-	2/4/4/4	-
24	CLA	b	612	2	-	5/39/115/115	-
28	GOL	v	202	-	-	3/4/4/4	-
24	CLA	C	504	3	-	1/39/115/115	-

All (1622) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	C1B-C2B	9.25	1.49	1.39
25	D	401	PHO	C1D-C2D	9.21	1.49	1.39
25	d	401	PHO	C1B-C2B	9.14	1.49	1.39
25	a	411	PHO	C1D-C2D	8.92	1.49	1.39
25	A	408	PHO	C1D-C2D	8.78	1.49	1.39
25	d	401	PHO	C1D-C2D	8.53	1.49	1.39
25	a	411	PHO	C1B-C2B	8.36	1.48	1.39
25	A	408	PHO	C1B-C2B	8.22	1.48	1.39
25	d	401	PHO	C3B-C4B	7.00	1.49	1.41
25	A	408	PHO	C3B-C4B	6.99	1.49	1.41
25	a	411	PHO	C3B-C4B	6.98	1.49	1.41
25	A	408	PHO	C4D-CHA	6.77	1.50	1.39
25	a	411	PHO	C4D-CHA	6.49	1.49	1.39
25	D	401	PHO	C4D-CHA	6.40	1.49	1.39
25	A	408	PHO	C3B-C2B	6.36	1.49	1.40
25	d	401	PHO	C4D-CHA	6.25	1.49	1.39
25	D	401	PHO	C3B-C2B	6.11	1.48	1.40
25	D	401	PHO	C3B-C4B	6.10	1.48	1.41
25	a	411	PHO	C3B-C2B	6.08	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	401	PHO	C3C-C2C	6.07	1.49	1.36
25	A	408	PHO	C3D-C2D	5.84	1.49	1.39
25	d	401	PHO	C3B-C2B	5.79	1.48	1.40
25	a	411	PHO	C3C-C2C	5.77	1.49	1.36
24	B	614	CLA	C1D-ND	5.77	1.44	1.37
24	C	503	CLA	C1D-ND	5.74	1.44	1.37
25	D	401	PHO	C3C-C2C	5.69	1.48	1.36
24	C	504	CLA	C3C-C2C	5.66	1.48	1.36
24	B	603	CLA	C3C-C2C	5.65	1.48	1.36
24	C	509	CLA	C3C-C2C	5.61	1.48	1.36
24	B	604	CLA	C3C-C2C	5.56	1.48	1.36
25	a	411	PHO	C3D-C2D	5.55	1.49	1.39
24	b	610	CLA	C3C-C2C	5.54	1.48	1.36
24	d	402	CLA	C1D-ND	5.51	1.44	1.37
25	A	408	PHO	C3C-C2C	5.49	1.48	1.36
24	A	407	CLA	C3C-C2C	5.48	1.48	1.36
24	c	517	CLA	C3C-C2C	5.46	1.48	1.36
24	B	605	CLA	C1D-ND	5.46	1.44	1.37
24	B	611	CLA	C3C-C2C	5.46	1.48	1.36
25	d	401	PHO	C3D-C2D	5.45	1.49	1.39
25	D	401	PHO	C3D-C2D	5.45	1.49	1.39
24	b	619	CLA	C3C-C2C	5.45	1.48	1.36
24	b	617	CLA	C3C-C2C	5.44	1.48	1.36
24	b	614	CLA	C3C-C2C	5.43	1.48	1.36
24	A	406	CLA	C1D-ND	5.43	1.44	1.37
24	D	402	CLA	C3C-C2C	5.42	1.48	1.36
24	b	622	CLA	C3C-C2C	5.41	1.48	1.36
26	k	101	BCR	C23-C22	-5.39	1.34	1.45
24	c	512	CLA	C3C-C2C	5.39	1.48	1.36
24	c	513	CLA	C1D-ND	5.38	1.44	1.37
24	D	403	CLA	C1D-ND	5.38	1.44	1.37
24	a	409	CLA	C1D-ND	5.38	1.44	1.37
24	a	409	CLA	C3C-C2C	5.37	1.48	1.36
24	C	510	CLA	C3C-C2C	5.37	1.48	1.36
24	C	514	CLA	C3C-C2C	5.37	1.48	1.36
24	c	514	CLA	C3C-C2C	5.36	1.48	1.36
24	b	610	CLA	C1D-ND	5.35	1.44	1.37
24	D	403	CLA	C3C-C2C	5.35	1.48	1.36
24	A	406	CLA	C3C-C2C	5.34	1.48	1.36
24	C	510	CLA	C1D-ND	5.34	1.44	1.37
24	B	602	CLA	C1D-ND	5.33	1.44	1.37
24	C	513	CLA	C3C-C2C	5.33	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C3C-C2C	5.33	1.48	1.36
24	C	511	CLA	C3C-C2C	5.32	1.48	1.36
26	b	628	BCR	C23-C22	-5.32	1.34	1.45
24	a	412	CLA	C3C-C2C	5.31	1.48	1.36
24	B	606	CLA	O2D-CGD	5.31	1.46	1.33
24	C	511	CLA	C1D-ND	5.31	1.44	1.37
24	B	606	CLA	C1D-ND	5.31	1.44	1.37
24	b	611	CLA	C3C-C2C	5.30	1.48	1.36
24	C	504	CLA	C1D-ND	5.30	1.44	1.37
24	b	624	CLA	C1D-ND	5.29	1.44	1.37
24	b	616	CLA	C3C-C2C	5.29	1.48	1.36
24	d	402	CLA	C3C-C2C	5.28	1.48	1.36
24	c	514	CLA	C1D-ND	5.28	1.44	1.37
24	C	507	CLA	C1D-ND	5.28	1.44	1.37
24	b	621	CLA	O2D-CGD	5.27	1.46	1.33
38	e	103	HEM	FE-NB	5.27	2.11	1.94
24	c	510	CLA	C3C-C2C	5.26	1.47	1.36
24	C	503	CLA	C3C-C2C	5.26	1.47	1.36
24	c	508	CLA	C3C-C2C	5.26	1.47	1.36
24	B	602	CLA	C3C-C2C	5.26	1.47	1.36
24	b	622	CLA	O2D-CGD	5.25	1.46	1.33
24	b	622	CLA	C1D-ND	5.25	1.44	1.37
24	B	615	CLA	C1D-ND	5.25	1.44	1.37
24	c	512	CLA	C1D-ND	5.25	1.44	1.37
24	B	608	CLA	C3C-C2C	5.24	1.47	1.36
24	A	409	CLA	C1D-ND	5.23	1.44	1.37
24	b	617	CLA	C1D-ND	5.23	1.44	1.37
24	c	513	CLA	C3C-C2C	5.23	1.47	1.36
24	c	516	CLA	C3C-C2C	5.22	1.47	1.36
24	C	512	CLA	C1D-ND	5.21	1.44	1.37
24	C	502	CLA	C1D-ND	5.21	1.44	1.37
40	V	205	HEC	FE-NB	5.21	2.11	1.94
24	c	509	CLA	C3C-C2C	5.21	1.47	1.36
24	d	404	CLA	C3C-C2C	5.20	1.47	1.36
24	B	616	CLA	O2D-CGD	5.20	1.45	1.33
24	d	404	CLA	O2D-CGD	5.19	1.45	1.33
24	c	506	CLA	C3C-C2C	5.19	1.47	1.36
24	C	509	CLA	O2D-CGD	5.19	1.45	1.33
24	a	412	CLA	C1D-ND	5.19	1.44	1.37
24	c	507	CLA	C3C-C2C	5.19	1.47	1.36
24	b	623	CLA	C3C-C2C	5.19	1.47	1.36
24	C	512	CLA	C3C-C2C	5.18	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	C3C-C2C	5.18	1.47	1.36
24	b	625	CLA	C1D-ND	5.17	1.44	1.37
24	b	624	CLA	C3C-C2C	5.17	1.47	1.36
24	b	620	CLA	O2D-CGD	5.17	1.45	1.33
24	C	508	CLA	C3C-C2C	5.17	1.47	1.36
24	B	611	CLA	C1D-ND	5.17	1.44	1.37
24	B	615	CLA	C3C-C2C	5.17	1.47	1.36
24	C	503	CLA	CHC-C1C	5.16	1.49	1.38
24	B	612	CLA	C3C-C2C	5.15	1.47	1.36
24	C	505	CLA	C3C-C2C	5.15	1.47	1.36
24	B	617	CLA	C1D-ND	5.14	1.44	1.37
24	b	623	CLA	O2D-CGD	5.14	1.45	1.33
24	c	510	CLA	C1D-ND	5.13	1.44	1.37
24	c	513	CLA	O2D-CGD	5.13	1.45	1.33
24	C	505	CLA	C1D-ND	5.13	1.44	1.37
24	c	516	CLA	O2D-CGD	5.12	1.45	1.33
24	C	507	CLA	C3C-C2C	5.12	1.47	1.36
24	c	517	CLA	C1D-ND	5.12	1.44	1.37
24	C	513	CLA	C1D-ND	5.11	1.44	1.37
24	C	506	CLA	C3C-C2C	5.11	1.47	1.36
24	c	511	CLA	C3C-C2C	5.11	1.47	1.36
24	b	613	CLA	C1D-ND	5.10	1.44	1.37
25	a	411	PHO	O2D-CGD	5.10	1.45	1.33
24	c	505	CLA	C3C-C2C	5.10	1.47	1.36
26	C	515	BCR	C23-C22	-5.09	1.35	1.45
24	B	606	CLA	C3C-C2C	5.09	1.47	1.36
24	b	621	CLA	C3C-C2C	5.09	1.47	1.36
24	B	610	CLA	CHC-C1C	5.08	1.48	1.38
24	B	614	CLA	C3C-C2C	5.08	1.47	1.36
26	Y	101	BCR	C23-C22	-5.08	1.35	1.45
24	B	617	CLA	O2D-CGD	5.08	1.45	1.33
24	C	511	CLA	O2D-CGD	5.07	1.45	1.33
24	d	403	CLA	C3C-C2C	5.07	1.47	1.36
24	A	409	CLA	C3C-C2C	5.07	1.47	1.36
24	B	610	CLA	C3C-C2C	5.06	1.47	1.36
24	b	618	CLA	C3C-C2C	5.05	1.47	1.36
38	E	102	HEM	FE-NB	5.05	2.10	1.94
24	A	409	CLA	O2D-CGD	5.05	1.45	1.33
24	b	618	CLA	O2D-CGD	5.05	1.45	1.33
24	A	405	CLA	C1D-ND	5.04	1.44	1.37
24	b	616	CLA	O2D-CGD	5.04	1.45	1.33
24	a	412	CLA	O2D-CGD	5.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	516	CLA	CHC-C1C	5.04	1.48	1.38
24	B	605	CLA	C3C-C2C	5.04	1.47	1.36
24	A	405	CLA	C3C-C2C	5.04	1.47	1.36
24	B	609	CLA	C3C-C2C	5.04	1.47	1.36
24	b	625	CLA	O2D-CGD	5.03	1.45	1.33
24	c	508	CLA	O2D-CGD	5.03	1.45	1.33
40	v	205	HEC	FE-NB	5.03	2.10	1.94
24	B	603	CLA	O2D-CGD	5.03	1.45	1.33
24	A	405	CLA	CHC-C1C	5.03	1.48	1.38
24	B	607	CLA	C3C-C2C	5.03	1.47	1.36
24	d	402	CLA	O2D-CGD	5.02	1.45	1.33
24	b	619	CLA	C1D-ND	5.02	1.44	1.37
24	B	613	CLA	C3C-C2C	5.02	1.47	1.36
24	b	615	CLA	C1D-ND	5.01	1.43	1.37
24	C	504	CLA	CHC-C1C	5.01	1.48	1.38
26	B	620	BCR	C23-C22	-5.00	1.35	1.45
24	B	617	CLA	C3C-C2C	5.00	1.47	1.36
24	c	508	CLA	C1D-ND	5.00	1.43	1.37
24	d	404	CLA	C1D-ND	5.00	1.43	1.37
24	b	614	CLA	O2D-CGD	5.00	1.45	1.33
24	c	515	CLA	C1D-ND	5.00	1.43	1.37
24	c	510	CLA	O2D-CGD	5.00	1.45	1.33
24	C	507	CLA	O2D-CGD	4.99	1.45	1.33
24	B	608	CLA	O2D-CGD	4.99	1.45	1.33
24	B	614	CLA	O2D-CGD	4.99	1.45	1.33
24	b	612	CLA	C3C-C2C	4.99	1.47	1.36
25	A	408	PHO	O2D-CGD	4.98	1.45	1.33
24	c	505	CLA	C1D-ND	4.98	1.43	1.37
26	H	101	BCR	C23-C22	-4.98	1.35	1.45
24	c	507	CLA	C1D-ND	4.98	1.43	1.37
24	b	623	CLA	C1D-ND	4.98	1.43	1.37
24	c	517	CLA	O2D-CGD	4.97	1.45	1.33
24	c	515	CLA	C3C-C2C	4.97	1.47	1.36
24	B	616	CLA	C1D-ND	4.96	1.43	1.37
24	a	410	CLA	C3C-C2C	4.96	1.47	1.36
24	C	510	CLA	O2D-CGD	4.96	1.45	1.33
24	b	611	CLA	C1D-ND	4.96	1.43	1.37
24	C	512	CLA	O2D-CGD	4.95	1.45	1.33
24	C	514	CLA	O2D-CGD	4.95	1.45	1.33
24	c	506	CLA	O2D-CGD	4.95	1.45	1.33
24	c	507	CLA	CHC-C1C	4.94	1.48	1.38
26	T	103	BCR	C23-C22	-4.94	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	O2D-CGD	4.93	1.45	1.33
24	B	603	CLA	C1D-ND	4.93	1.43	1.37
24	A	405	CLA	O2D-CGD	4.93	1.45	1.33
24	B	602	CLA	O2D-CGD	4.93	1.45	1.33
24	b	620	CLA	C3C-C2C	4.92	1.47	1.36
24	C	502	CLA	CHC-C1C	4.92	1.48	1.38
24	B	607	CLA	O2D-CGD	4.92	1.45	1.33
24	D	403	CLA	O2D-CGD	4.91	1.45	1.33
24	b	610	CLA	O2D-CGD	4.91	1.45	1.33
24	C	508	CLA	CHC-C1C	4.90	1.48	1.38
24	b	624	CLA	O2D-CGD	4.89	1.45	1.33
24	c	512	CLA	O2D-CGD	4.89	1.45	1.33
24	c	514	CLA	O2D-CGD	4.88	1.45	1.33
24	B	609	CLA	C1D-ND	4.88	1.43	1.37
24	A	407	CLA	O2D-CGD	4.88	1.45	1.33
24	B	610	CLA	O2D-CGD	4.88	1.45	1.33
24	c	505	CLA	O2D-CGD	4.87	1.45	1.33
24	b	612	CLA	O2D-CGD	4.87	1.45	1.33
24	c	516	CLA	C1D-ND	4.87	1.43	1.37
25	a	411	PHO	OBD-CAD	4.87	1.29	1.22
24	B	616	CLA	C3C-C2C	4.87	1.47	1.36
24	b	612	CLA	C1D-ND	4.86	1.43	1.37
24	D	402	CLA	C1D-ND	4.86	1.43	1.37
24	B	603	CLA	CHC-C1C	4.86	1.48	1.38
24	B	612	CLA	O2D-CGD	4.85	1.45	1.33
24	b	618	CLA	C1D-ND	4.85	1.43	1.37
24	b	621	CLA	C1D-ND	4.85	1.43	1.37
24	b	620	CLA	C1D-ND	4.84	1.43	1.37
24	c	506	CLA	C1D-ND	4.84	1.43	1.37
24	a	409	CLA	O2D-CGD	4.84	1.45	1.33
24	b	613	CLA	O2D-CGD	4.83	1.45	1.33
24	C	502	CLA	C3C-C2C	4.83	1.47	1.36
24	C	505	CLA	CHC-C1C	4.83	1.48	1.38
24	A	407	CLA	CHC-C1C	4.82	1.48	1.38
24	c	517	CLA	CHC-C1C	4.82	1.48	1.38
24	C	506	CLA	O2D-CGD	4.81	1.44	1.33
24	b	617	CLA	O2D-CGD	4.81	1.44	1.33
24	b	619	CLA	O2D-CGD	4.81	1.44	1.33
24	B	606	CLA	CHC-C1C	4.81	1.48	1.38
24	C	502	CLA	O2D-CGD	4.80	1.44	1.33
24	A	409	CLA	CHC-C1C	4.80	1.48	1.38
24	c	509	CLA	O2D-CGD	4.80	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	C1D-ND	4.80	1.43	1.37
24	A	406	CLA	O2D-CGD	4.79	1.44	1.33
24	B	617	CLA	CHC-C1C	4.79	1.48	1.38
24	C	509	CLA	C1D-ND	4.78	1.43	1.37
26	t	101	BCR	C23-C22	-4.78	1.35	1.45
24	a	410	CLA	CHC-C1C	4.78	1.48	1.38
24	C	503	CLA	O2D-CGD	4.77	1.44	1.33
24	D	402	CLA	O2D-CGD	4.77	1.44	1.33
24	b	610	CLA	CHC-C1C	4.77	1.48	1.38
24	C	513	CLA	CHC-C1C	4.76	1.48	1.38
24	a	410	CLA	O2D-CGD	4.76	1.44	1.33
24	b	614	CLA	C1D-ND	4.75	1.43	1.37
26	y	101	BCR	C23-C22	-4.75	1.35	1.45
26	C	516	BCR	C23-C22	-4.75	1.35	1.45
24	B	607	CLA	C1D-ND	4.75	1.43	1.37
26	c	527	BCR	C23-C22	-4.74	1.35	1.45
24	B	604	CLA	CHC-C1C	4.74	1.48	1.38
24	B	616	CLA	CHC-C1C	4.73	1.48	1.38
24	a	409	CLA	CHC-C1C	4.73	1.48	1.38
24	B	612	CLA	C1D-ND	4.73	1.43	1.37
24	b	614	CLA	CHC-C1C	4.73	1.48	1.38
24	C	508	CLA	O2D-CGD	4.73	1.44	1.33
24	c	511	CLA	C1D-ND	4.72	1.43	1.37
26	K	101	BCR	C23-C22	-4.71	1.35	1.45
24	B	615	CLA	O2D-CGD	4.71	1.44	1.33
26	d	405	BCR	C23-C22	-4.71	1.35	1.45
24	C	506	CLA	CHC-C1C	4.71	1.48	1.38
25	D	401	PHO	O2D-CGD	4.71	1.44	1.33
25	D	401	PHO	OBD-CAD	4.71	1.28	1.22
26	h	101	BCR	C23-C22	-4.70	1.35	1.45
24	B	602	CLA	O2A-CGA	4.70	1.47	1.33
24	b	611	CLA	O2D-CGD	4.69	1.44	1.33
25	d	401	PHO	O2D-CGD	4.69	1.44	1.33
24	B	609	CLA	O2D-CGD	4.69	1.44	1.33
24	b	617	CLA	CHC-C1C	4.69	1.48	1.38
24	a	412	CLA	CHC-C1C	4.68	1.48	1.38
24	B	613	CLA	CHC-C1C	4.68	1.48	1.38
24	B	611	CLA	O2D-CGD	4.68	1.44	1.33
24	c	507	CLA	O2D-CGD	4.66	1.44	1.33
24	c	511	CLA	O2D-CGD	4.66	1.44	1.33
24	c	515	CLA	O2D-CGD	4.66	1.44	1.33
24	c	513	CLA	CHC-C1C	4.65	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	C1D-ND	4.65	1.43	1.37
24	b	617	CLA	CHD-C1D	4.64	1.47	1.38
26	D	404	BCR	C23-C22	-4.64	1.36	1.45
24	B	602	CLA	CHC-C1C	4.63	1.47	1.38
24	c	509	CLA	CHC-C1C	4.63	1.47	1.38
24	d	403	CLA	CHC-C1C	4.63	1.47	1.38
24	C	510	CLA	CHC-C1C	4.62	1.47	1.38
24	B	613	CLA	O2D-CGD	4.62	1.44	1.33
27	A	415	SQD	O48-C23	4.61	1.46	1.33
24	C	514	CLA	CHC-C1C	4.61	1.47	1.38
24	B	607	CLA	CHC-C1C	4.60	1.47	1.38
24	c	508	CLA	CHC-C1C	4.60	1.47	1.38
24	C	508	CLA	C1D-ND	4.59	1.43	1.37
24	B	604	CLA	O2D-CGD	4.59	1.44	1.33
24	b	625	CLA	C3C-C2C	4.59	1.46	1.36
24	b	611	CLA	CHC-C1C	4.58	1.47	1.38
27	a	405	SQD	O48-C23	4.57	1.46	1.33
24	d	403	CLA	O2D-CGD	4.56	1.44	1.33
26	a	413	BCR	C23-C22	-4.56	1.36	1.45
24	C	511	CLA	CHC-C1C	4.56	1.47	1.38
24	c	507	CLA	CHD-C1D	4.55	1.47	1.38
24	B	611	CLA	CHD-C1D	4.55	1.47	1.38
24	C	504	CLA	O2D-CGD	4.54	1.44	1.33
24	C	510	CLA	O2A-CGA	4.54	1.46	1.33
27	f	102	SQD	O47-C7	4.53	1.47	1.34
36	D	406	DGD	O1G-C1A	4.53	1.46	1.33
24	C	505	CLA	O2D-CGD	4.52	1.44	1.33
24	b	611	CLA	CHD-C1D	4.52	1.47	1.38
24	B	604	CLA	C1D-ND	4.51	1.43	1.37
24	d	404	CLA	CHC-C1C	4.51	1.47	1.38
24	B	605	CLA	O2D-CGD	4.51	1.44	1.33
24	a	410	CLA	C1D-ND	4.51	1.43	1.37
24	B	612	CLA	CHD-C1D	4.51	1.47	1.38
26	c	518	BCR	C23-C22	-4.51	1.36	1.45
24	b	615	CLA	CHD-C1D	4.50	1.47	1.38
24	b	619	CLA	CHC-C1C	4.50	1.47	1.38
24	b	623	CLA	CHC-C1C	4.49	1.47	1.38
24	b	616	CLA	CHC-C1C	4.49	1.47	1.38
24	c	512	CLA	CHD-C1D	4.49	1.47	1.38
24	C	509	CLA	CHC-C1C	4.48	1.47	1.38
24	c	514	CLA	CHC-C1C	4.48	1.47	1.38
24	b	612	CLA	CHC-C1C	4.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	CHC-C1C	4.47	1.47	1.38
24	b	620	CLA	CHC-C1C	4.47	1.47	1.38
24	b	615	CLA	O2D-CGD	4.46	1.44	1.33
24	c	512	CLA	CHC-C1C	4.46	1.47	1.38
24	B	615	CLA	CHC-C1C	4.46	1.47	1.38
24	b	616	CLA	C1D-ND	4.46	1.43	1.37
24	c	512	CLA	O2A-CGA	4.45	1.46	1.33
26	B	618	BCR	C23-C22	-4.45	1.36	1.45
24	C	509	CLA	CHD-C1D	4.45	1.47	1.38
24	b	624	CLA	CHC-C1C	4.45	1.47	1.38
24	b	618	CLA	CHD-C1D	4.45	1.47	1.38
24	A	409	CLA	CHD-C1D	4.45	1.47	1.38
35	z	101	LMG	O8-C28	4.45	1.46	1.33
24	b	622	CLA	CHC-C1C	4.45	1.47	1.38
24	C	502	CLA	CHD-C1D	4.44	1.47	1.38
24	b	610	CLA	CHD-C1D	4.44	1.47	1.38
26	b	626	BCR	C23-C22	-4.44	1.36	1.45
24	C	507	CLA	CHD-C1D	4.44	1.47	1.38
24	b	624	CLA	O2A-CGA	4.43	1.46	1.33
24	C	511	CLA	CHD-C1D	4.43	1.47	1.38
24	B	608	CLA	C1D-ND	4.43	1.43	1.37
24	b	618	CLA	CHC-C1C	4.43	1.47	1.38
24	C	509	CLA	O2A-CGA	4.43	1.46	1.33
24	c	506	CLA	CHC-C1C	4.42	1.47	1.38
24	A	407	CLA	CHD-C1D	4.42	1.47	1.38
24	c	515	CLA	CHD-C1D	4.42	1.47	1.38
24	B	609	CLA	CHD-C1D	4.42	1.47	1.38
24	B	607	CLA	CHD-C1D	4.41	1.47	1.38
24	B	608	CLA	CHC-C1C	4.41	1.47	1.38
24	c	515	CLA	O2A-CGA	4.41	1.46	1.33
26	B	619	BCR	C23-C22	-4.41	1.36	1.45
24	c	511	CLA	CHC-C1C	4.40	1.47	1.38
24	B	608	CLA	CHD-C1D	4.40	1.46	1.38
24	B	610	CLA	C1D-ND	4.40	1.43	1.37
27	F	103	SQD	O47-C7	4.40	1.46	1.34
24	B	605	CLA	CHC-C1C	4.40	1.47	1.38
36	e	101	DGD	O2G-C1B	4.39	1.46	1.34
24	c	510	CLA	CHC-C1C	4.39	1.47	1.38
24	c	513	CLA	O2A-CGA	4.39	1.46	1.33
24	C	508	CLA	O2A-CGA	4.39	1.46	1.33
24	B	602	CLA	CHD-C1D	4.39	1.46	1.38
26	A	410	BCR	C23-C22	-4.38	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	CHD-C1D	4.38	1.46	1.38
36	D	406	DGD	O2G-C1B	4.38	1.46	1.34
24	c	513	CLA	CHD-C1D	4.38	1.46	1.38
24	C	506	CLA	C1D-ND	4.37	1.43	1.37
37	E	101	LHG	O8-C23	4.37	1.46	1.33
24	b	610	CLA	O2A-CGA	4.37	1.46	1.33
24	c	511	CLA	O2A-CGA	4.37	1.46	1.33
24	a	409	CLA	CHD-C1D	4.37	1.46	1.38
24	C	513	CLA	O2A-CGA	4.36	1.46	1.33
24	B	612	CLA	CHC-C1C	4.36	1.47	1.38
35	C	520	LMG	O8-C28	4.36	1.46	1.33
24	b	615	CLA	CHC-C1C	4.35	1.47	1.38
24	B	610	CLA	O2A-CGA	4.35	1.46	1.33
24	C	512	CLA	CHC-C1C	4.34	1.47	1.38
24	C	510	CLA	CHD-C1D	4.34	1.46	1.38
27	B	621	SQD	O47-C7	4.34	1.46	1.34
24	b	621	CLA	CHC-C1C	4.34	1.47	1.38
24	D	403	CLA	CHC-C1C	4.33	1.47	1.38
24	c	505	CLA	CHC-C1C	4.33	1.47	1.38
24	b	616	CLA	CHD-C1D	4.33	1.46	1.38
27	a	405	SQD	O47-C7	4.32	1.46	1.34
24	B	611	CLA	CHC-C1C	4.32	1.47	1.38
24	B	609	CLA	O2A-CGA	4.32	1.46	1.33
24	c	515	CLA	CHC-C1C	4.32	1.47	1.38
35	C	501	LMG	O7-C10	4.32	1.46	1.34
24	C	512	CLA	O2A-CGA	4.32	1.46	1.33
24	C	514	CLA	CHD-C1D	4.32	1.46	1.38
24	D	403	CLA	CHD-C1D	4.31	1.46	1.38
24	b	613	CLA	CHC-C1C	4.31	1.47	1.38
24	a	409	CLA	CHD-C4C	4.31	1.49	1.39
35	C	521	LMG	O7-C10	4.31	1.46	1.34
24	c	506	CLA	CHD-C1D	4.30	1.46	1.38
24	d	403	CLA	CHD-C1D	4.30	1.46	1.38
24	B	617	CLA	CHD-C1D	4.30	1.46	1.38
24	C	512	CLA	CHD-C1D	4.30	1.46	1.38
37	l	101	LHG	O8-C23	4.30	1.45	1.33
36	e	101	DGD	O1G-C1A	4.29	1.45	1.33
24	b	625	CLA	CHD-C1D	4.29	1.46	1.38
24	d	402	CLA	O2A-CGA	4.28	1.45	1.33
24	B	613	CLA	C1B-NB	-4.28	1.32	1.37
37	D	409	LHG	O7-C7	4.27	1.46	1.34
24	d	402	CLA	CHD-C1D	4.27	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	e	102	LHG	O8-C23	4.27	1.45	1.33
24	C	504	CLA	CHD-C1D	4.26	1.46	1.38
24	C	506	CLA	CHD-C1D	4.26	1.46	1.38
24	d	404	CLA	O2A-CGA	4.26	1.45	1.33
24	B	606	CLA	O2A-CGA	4.26	1.45	1.33
37	d	409	LHG	O8-C23	4.26	1.45	1.33
35	c	523	LMG	O7-C10	4.25	1.46	1.34
24	b	621	CLA	CHB-C1B	4.24	1.48	1.39
24	b	617	CLA	O2A-CGA	4.24	1.45	1.33
24	B	604	CLA	CHD-C1D	4.24	1.46	1.38
36	C	518	DGD	O1G-C1A	4.24	1.45	1.33
24	C	507	CLA	O2A-CGA	4.24	1.45	1.33
27	f	102	SQD	O48-C23	4.24	1.45	1.33
35	C	501	LMG	O8-C28	4.24	1.45	1.33
24	c	509	CLA	C1D-ND	4.24	1.43	1.37
24	B	617	CLA	O2A-CGA	4.24	1.45	1.33
24	A	407	CLA	C1D-ND	4.23	1.43	1.37
24	b	615	CLA	O2A-CGA	4.23	1.45	1.33
24	c	517	CLA	O2A-CGA	4.23	1.45	1.33
24	B	605	CLA	CHD-C1D	4.23	1.46	1.38
24	c	516	CLA	O2A-CGA	4.23	1.45	1.33
24	C	511	CLA	CHB-C1B	4.23	1.48	1.39
24	A	406	CLA	O2A-CGA	4.23	1.45	1.33
24	c	517	CLA	CHD-C1D	4.22	1.46	1.38
24	b	622	CLA	CHD-C1D	4.22	1.46	1.38
35	c	523	LMG	O8-C28	4.22	1.45	1.33
26	b	627	BCR	C23-C22	-4.21	1.36	1.45
24	C	504	CLA	CHD-C4C	4.21	1.48	1.39
24	B	613	CLA	O2A-CGA	4.21	1.45	1.33
24	b	625	CLA	CHB-C1B	4.21	1.48	1.39
24	C	514	CLA	O2A-CGA	4.21	1.45	1.33
35	M	101	LMG	O8-C28	4.20	1.45	1.33
24	b	621	CLA	CHD-C1D	4.20	1.46	1.38
27	a	414	SQD	O48-C23	4.20	1.45	1.33
24	b	619	CLA	CHD-C1D	4.20	1.46	1.38
24	B	609	CLA	CHC-C1C	4.19	1.47	1.38
24	b	625	CLA	O2A-CGA	4.19	1.45	1.33
24	c	506	CLA	C3D-C2D	4.19	1.50	1.39
24	a	412	CLA	CHD-C4C	4.18	1.48	1.39
24	B	613	CLA	C1D-ND	4.18	1.42	1.37
24	B	610	CLA	CHD-C1D	4.18	1.46	1.38
24	A	409	CLA	O2A-CGA	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	410	CLA	O2A-CGA	4.18	1.45	1.33
35	a	415	LMG	O8-C28	4.18	1.45	1.33
24	C	508	CLA	CHC-C4B	4.17	1.48	1.39
36	c	521	DGD	O1G-C1A	4.17	1.45	1.33
24	C	513	CLA	CHD-C1D	4.17	1.46	1.38
24	D	402	CLA	O2A-CGA	4.17	1.45	1.33
35	c	522	LMG	O8-C28	4.17	1.45	1.33
24	B	603	CLA	CHD-C1D	4.17	1.46	1.38
24	B	614	CLA	CHB-C1B	4.16	1.48	1.39
27	L	102	SQD	O47-C7	4.16	1.46	1.34
36	C	517	DGD	O1G-C1A	4.16	1.45	1.33
24	b	623	CLA	O2A-CGA	4.16	1.45	1.33
24	C	502	CLA	O2A-CGA	4.16	1.45	1.33
34	B	623	HTG	C1'-S1	-4.16	1.76	1.81
24	D	402	CLA	CHC-C1C	4.16	1.47	1.38
24	c	510	CLA	CHD-C1D	4.16	1.46	1.38
35	C	521	LMG	O8-C28	4.15	1.45	1.33
24	b	614	CLA	CHD-C1D	4.15	1.46	1.38
36	h	102	DGD	O1G-C1A	4.15	1.45	1.33
37	e	102	LHG	O7-C7	4.15	1.46	1.34
36	H	102	DGD	O1G-C1A	4.15	1.45	1.33
24	B	616	CLA	O2A-CGA	4.15	1.45	1.33
24	C	508	CLA	CHD-C1D	4.14	1.46	1.38
38	e	103	HEM	FE-NC	4.14	2.09	1.95
24	b	612	CLA	CHD-C1D	4.14	1.46	1.38
24	C	507	CLA	CHD-C4C	4.14	1.48	1.39
37	L	101	LHG	O8-C23	4.14	1.45	1.33
36	h	102	DGD	O2G-C1B	4.13	1.46	1.34
24	B	615	CLA	O2A-CGA	4.13	1.45	1.33
24	d	402	CLA	CHC-C1C	4.13	1.46	1.38
24	C	505	CLA	O2A-CGA	4.13	1.45	1.33
27	A	415	SQD	O47-C7	4.13	1.45	1.34
38	E	102	HEM	FE-NC	4.13	2.09	1.95
24	b	620	CLA	O2A-CGA	4.12	1.45	1.33
24	d	403	CLA	CHD-C4C	4.12	1.48	1.39
24	b	617	CLA	CHD-C4C	4.12	1.48	1.39
36	C	519	DGD	O1G-C1A	4.12	1.45	1.33
25	d	401	PHO	O2A-CGA	4.12	1.45	1.33
24	C	504	CLA	O2A-CGA	4.12	1.45	1.33
24	b	625	CLA	C3D-C2D	4.11	1.50	1.39
24	B	616	CLA	CHC-C4B	4.11	1.48	1.39
35	b	629	LMG	O8-C28	4.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	Z	101	LMG	O7-C10	4.11	1.45	1.34
27	L	102	SQD	O48-C23	4.10	1.45	1.33
24	b	611	CLA	O2A-CGA	4.10	1.45	1.33
24	d	404	CLA	CHD-C1D	4.10	1.46	1.38
24	B	607	CLA	O2A-CGA	4.09	1.45	1.33
24	b	612	CLA	O2A-CGA	4.09	1.45	1.33
24	C	503	CLA	C3D-C2D	4.09	1.50	1.39
24	b	625	CLA	CHC-C1C	4.09	1.46	1.38
36	c	520	DGD	O1G-C1A	4.09	1.45	1.33
27	F	103	SQD	O48-C23	4.08	1.45	1.33
35	M	101	LMG	O7-C10	4.08	1.45	1.34
37	d	409	LHG	O7-C7	4.08	1.45	1.34
24	C	512	CLA	CHB-C1B	4.08	1.48	1.39
35	j	101	LMG	O8-C28	4.08	1.45	1.33
24	A	409	CLA	CHC-C4B	4.08	1.48	1.39
24	C	511	CLA	O2A-CGA	4.08	1.45	1.33
24	B	612	CLA	CHB-C1B	4.07	1.48	1.39
24	a	412	CLA	CHD-C1D	4.07	1.46	1.38
24	b	623	CLA	CHD-C4C	4.07	1.48	1.39
24	B	610	CLA	C3D-C2D	4.07	1.50	1.39
24	c	511	CLA	CHD-C1D	4.06	1.46	1.38
24	b	618	CLA	O2A-CGA	4.06	1.45	1.33
24	B	611	CLA	C3D-C2D	4.05	1.50	1.39
24	c	512	CLA	CHD-C4C	4.05	1.48	1.39
25	A	408	PHO	OBD-CAD	4.05	1.28	1.22
35	z	101	LMG	O7-C10	4.05	1.45	1.34
24	A	406	CLA	C3D-C2D	4.05	1.50	1.39
24	B	609	CLA	C3D-C2D	4.05	1.50	1.39
24	c	517	CLA	CHD-C4C	4.05	1.48	1.39
24	B	614	CLA	CHC-C1C	4.05	1.46	1.38
24	C	504	CLA	CHC-C4B	4.05	1.48	1.39
24	B	604	CLA	CHC-C4B	4.04	1.48	1.39
24	c	505	CLA	O2A-CGA	4.04	1.45	1.33
24	B	604	CLA	O2A-CGA	4.04	1.45	1.33
24	b	611	CLA	CHD-C4C	4.04	1.48	1.39
24	b	610	CLA	CHD-C4C	4.04	1.48	1.39
24	b	616	CLA	C1B-NB	-4.04	1.32	1.37
34	b	632	HTG	C1'-S1	-4.04	1.76	1.81
40	V	205	HEC	CBC-CAC	-4.04	1.33	1.51
24	b	613	CLA	CHD-C1D	4.03	1.46	1.38
24	c	505	CLA	CHD-C1D	4.03	1.46	1.38
37	D	408	LHG	O7-C7	4.03	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	412	CLA	O2A-CGA	4.03	1.45	1.33
24	c	516	CLA	CHD-C1D	4.03	1.46	1.38
24	B	604	CLA	C3D-C2D	4.03	1.50	1.39
24	c	507	CLA	CHD-C4C	4.03	1.48	1.39
24	B	608	CLA	O2A-CGA	4.02	1.45	1.33
24	c	506	CLA	CHD-C4C	4.02	1.48	1.39
24	b	613	CLA	O2A-CGA	4.02	1.45	1.33
24	C	505	CLA	CHB-C1B	4.02	1.48	1.39
24	c	509	CLA	CHD-C1D	4.02	1.46	1.38
24	A	406	CLA	CHD-C1D	4.02	1.46	1.38
24	A	407	CLA	OBD-CAD	4.02	1.29	1.22
24	c	507	CLA	O2A-CGA	4.02	1.45	1.33
24	b	620	CLA	CHD-C1D	4.02	1.46	1.38
24	c	512	CLA	CHB-C1B	4.01	1.48	1.39
24	c	513	CLA	CHB-C1B	4.01	1.48	1.39
24	C	512	CLA	CHD-C4C	4.01	1.48	1.39
24	c	515	CLA	C3D-C2D	4.01	1.50	1.39
24	C	507	CLA	C3D-C2D	4.01	1.50	1.39
24	B	612	CLA	C3D-C2D	4.01	1.50	1.39
24	B	607	CLA	CHD-C4C	4.01	1.48	1.39
40	v	205	HEC	CBC-CAC	-4.01	1.33	1.51
24	A	405	CLA	CHD-C4C	4.00	1.48	1.39
24	c	513	CLA	CHD-C4C	4.00	1.48	1.39
37	E	101	LHG	O7-C7	4.00	1.45	1.34
24	d	403	CLA	O2A-CGA	3.99	1.45	1.33
24	b	617	CLA	CHC-C4B	3.99	1.48	1.39
24	C	512	CLA	C3D-C2D	3.99	1.50	1.39
35	j	101	LMG	O7-C10	3.99	1.45	1.34
24	B	603	CLA	O2A-CGA	3.99	1.45	1.33
27	B	621	SQD	O48-C23	3.99	1.45	1.33
24	c	514	CLA	CHD-C4C	3.99	1.48	1.39
24	C	513	CLA	C3D-C2D	3.99	1.50	1.39
24	C	505	CLA	CHD-C4C	3.99	1.48	1.39
25	D	401	PHO	O2A-CGA	3.99	1.45	1.33
36	c	521	DGD	O2G-C1B	3.98	1.45	1.34
24	b	614	CLA	O2A-CGA	3.98	1.45	1.33
24	C	510	CLA	CHD-C4C	3.98	1.48	1.39
24	B	614	CLA	O2A-CGA	3.98	1.45	1.33
35	C	520	LMG	O7-C10	3.98	1.45	1.34
24	b	615	CLA	CHD-C4C	3.98	1.48	1.39
24	c	508	CLA	CHD-C1D	3.97	1.46	1.38
24	c	517	CLA	CHC-C4B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	C3D-C2D	3.97	1.50	1.39
24	C	505	CLA	CHD-C1D	3.97	1.46	1.38
24	a	410	CLA	CHD-C1D	3.97	1.46	1.38
24	c	508	CLA	O2A-CGA	3.97	1.44	1.33
24	c	512	CLA	C3D-C2D	3.97	1.50	1.39
24	c	506	CLA	O2A-CGA	3.97	1.44	1.33
24	C	503	CLA	CHD-C1D	3.97	1.46	1.38
24	C	505	CLA	C3D-C2D	3.97	1.49	1.39
24	b	616	CLA	CHB-C1B	3.97	1.48	1.39
25	A	408	PHO	O2A-CGA	3.96	1.44	1.33
24	b	610	CLA	C3D-C2D	3.96	1.49	1.39
24	A	405	CLA	CHD-C1D	3.96	1.46	1.38
24	A	407	CLA	O2A-CGA	3.95	1.44	1.33
36	C	519	DGD	O2G-C1B	3.95	1.45	1.34
37	D	409	LHG	O8-C23	3.95	1.44	1.33
24	C	502	CLA	CHC-C4B	3.95	1.48	1.39
24	B	602	CLA	CHD-C4C	3.95	1.48	1.39
24	C	504	CLA	C3D-C2D	3.95	1.49	1.39
35	c	522	LMG	O7-C10	3.95	1.45	1.34
24	b	623	CLA	C3D-C2D	3.94	1.49	1.39
24	c	512	CLA	OBD-CAD	3.94	1.29	1.22
24	b	619	CLA	O2A-CGA	3.94	1.44	1.33
24	B	615	CLA	CHD-C4C	3.94	1.48	1.39
24	c	515	CLA	CHD-C4C	3.94	1.48	1.39
24	c	509	CLA	CHB-C1B	3.94	1.48	1.39
24	b	616	CLA	O2A-CGA	3.93	1.44	1.33
40	v	205	HEC	FE-NC	3.93	2.08	1.95
24	B	603	CLA	OBD-CAD	3.93	1.29	1.22
24	A	406	CLA	CHD-C4C	3.93	1.48	1.39
34	d	412	HTG	C1'-S1	-3.93	1.76	1.81
24	C	514	CLA	CHD-C4C	3.93	1.48	1.39
24	c	516	CLA	CHD-C4C	3.93	1.48	1.39
24	C	506	CLA	O2A-CGA	3.93	1.44	1.33
24	b	623	CLA	CHD-C1D	3.92	1.46	1.38
24	c	507	CLA	CHC-C4B	3.92	1.48	1.39
24	c	510	CLA	CHD-C4C	3.92	1.48	1.39
24	D	403	CLA	CHD-C4C	3.92	1.48	1.39
24	C	502	CLA	CHD-C4C	3.92	1.48	1.39
24	b	622	CLA	CHB-C1B	3.92	1.48	1.39
24	b	613	CLA	CHB-C1B	3.92	1.48	1.39
36	c	520	DGD	O2G-C1B	3.92	1.45	1.34
24	a	410	CLA	CHB-C1B	3.91	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	CHD-C4C	3.91	1.48	1.39
24	c	514	CLA	OBD-CAD	3.91	1.29	1.22
24	B	608	CLA	CHC-C4B	3.91	1.48	1.39
24	B	606	CLA	C3D-C2D	3.91	1.49	1.39
36	C	517	DGD	O2G-C1B	3.91	1.45	1.34
24	C	510	CLA	C3D-C2D	3.91	1.49	1.39
24	D	403	CLA	O2A-CGA	3.90	1.44	1.33
36	H	102	DGD	O2G-C1B	3.90	1.45	1.34
35	a	415	LMG	O7-C10	3.90	1.45	1.34
24	B	608	CLA	CHD-C4C	3.90	1.48	1.39
24	C	503	CLA	CHC-C4B	3.90	1.48	1.39
24	B	610	CLA	CHB-C1B	3.90	1.48	1.39
24	d	402	CLA	C3D-C2D	3.89	1.49	1.39
24	b	624	CLA	C3D-C2D	3.89	1.49	1.39
24	c	510	CLA	O2A-CGA	3.89	1.44	1.33
27	a	414	SQD	O47-C7	3.89	1.45	1.34
24	B	611	CLA	O2A-CGA	3.89	1.44	1.33
24	b	625	CLA	CHD-C4C	3.89	1.48	1.39
24	b	621	CLA	O2A-CGA	3.88	1.44	1.33
24	B	604	CLA	CHD-C4C	3.88	1.48	1.39
24	c	516	CLA	CHC-C4B	3.88	1.48	1.39
24	C	503	CLA	O2A-CGA	3.88	1.44	1.33
34	b	607	HTG	C1'-S1	-3.88	1.76	1.81
24	D	403	CLA	C3D-C2D	3.88	1.49	1.39
24	b	618	CLA	CHD-C4C	3.88	1.48	1.39
24	B	615	CLA	CHB-C1B	3.87	1.48	1.39
24	C	506	CLA	CHB-C1B	3.87	1.48	1.39
24	b	616	CLA	CHC-C4B	3.87	1.48	1.39
24	b	620	CLA	CHB-C1B	3.87	1.48	1.39
24	d	403	CLA	CHB-C1B	3.87	1.48	1.39
24	B	604	CLA	OBD-CAD	3.87	1.29	1.22
40	V	205	HEC	FE-NC	3.87	2.08	1.95
24	b	622	CLA	O2A-CGA	3.87	1.44	1.33
24	B	603	CLA	CHD-C4C	3.87	1.48	1.39
24	b	622	CLA	C3D-C2D	3.87	1.49	1.39
24	B	614	CLA	CHD-C4C	3.87	1.48	1.39
24	c	508	CLA	CHB-C1B	3.87	1.48	1.39
24	A	406	CLA	CHC-C1C	3.87	1.46	1.38
24	B	609	CLA	CHB-C1B	3.87	1.48	1.39
24	B	613	CLA	CHC-C4B	3.86	1.48	1.39
24	B	606	CLA	CHC-C4B	3.86	1.48	1.39
24	a	412	CLA	CHB-C1B	3.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	411	SQD	O48-C23	3.86	1.44	1.33
24	B	604	CLA	C1B-NB	-3.86	1.33	1.37
24	B	612	CLA	CHC-C4B	3.86	1.48	1.39
24	A	405	CLA	C3D-C2D	3.86	1.49	1.39
24	c	514	CLA	O2A-CGA	3.86	1.44	1.33
24	B	616	CLA	CHD-C1D	3.86	1.45	1.38
24	B	614	CLA	C3D-C2D	3.85	1.49	1.39
36	C	518	DGD	O2G-C1B	3.85	1.45	1.34
24	d	402	CLA	CHB-C1B	3.85	1.48	1.39
24	C	513	CLA	CHD-C4C	3.85	1.48	1.39
24	d	402	CLA	CHD-C4C	3.85	1.48	1.39
24	b	611	CLA	OBD-CAD	3.85	1.29	1.22
40	v	205	HEC	CBB-CAB	-3.85	1.34	1.51
27	A	411	SQD	O47-C7	3.85	1.45	1.34
24	b	621	CLA	C3D-C2D	3.84	1.49	1.39
24	C	514	CLA	CHC-C4B	3.84	1.48	1.39
24	c	516	CLA	C3D-C2D	3.84	1.49	1.39
24	b	617	CLA	CHB-C1B	3.84	1.48	1.39
24	b	618	CLA	OBD-CAD	3.84	1.29	1.22
24	A	407	CLA	CHC-C4B	3.84	1.48	1.39
24	a	409	CLA	CHC-C4B	3.84	1.48	1.39
35	b	629	LMG	O7-C10	3.83	1.45	1.34
24	B	612	CLA	CHD-C4C	3.83	1.48	1.39
24	b	619	CLA	OBD-CAD	3.83	1.29	1.22
37	D	407	LHG	O8-C23	3.83	1.44	1.33
24	B	611	CLA	CHD-C4C	3.83	1.48	1.39
24	C	503	CLA	CHD-C4C	3.82	1.48	1.39
24	b	612	CLA	CHB-C1B	3.82	1.48	1.39
24	c	511	CLA	C3D-C2D	3.82	1.49	1.39
24	c	510	CLA	CHB-C1B	3.82	1.48	1.39
24	B	613	CLA	CHD-C1D	3.82	1.45	1.38
36	c	519	DGD	O1G-C1A	3.82	1.44	1.33
24	A	405	CLA	CHB-C1B	3.82	1.48	1.39
24	b	618	CLA	C3D-C2D	3.82	1.49	1.39
24	C	511	CLA	CHD-C4C	3.82	1.48	1.39
37	d	408	LHG	O7-C7	3.82	1.45	1.34
24	A	409	CLA	CHD-C4C	3.82	1.47	1.39
24	c	505	CLA	C3D-C2D	3.82	1.49	1.39
24	B	602	CLA	CHB-C1B	3.82	1.48	1.39
24	B	613	CLA	CHB-C1B	3.82	1.48	1.39
36	c	519	DGD	O2G-C1B	3.82	1.45	1.34
24	C	509	CLA	CHD-C4C	3.82	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	C3D-C2D	3.82	1.49	1.39
24	c	514	CLA	CHB-C1B	3.82	1.48	1.39
25	d	401	PHO	OBD-CAD	3.81	1.27	1.22
24	c	509	CLA	CHC-C4B	3.81	1.48	1.39
37	l	101	LHG	O7-C7	3.81	1.45	1.34
24	c	505	CLA	CHD-C4C	3.81	1.47	1.39
24	b	611	CLA	C3D-C2D	3.81	1.49	1.39
24	A	407	CLA	CHD-C4C	3.81	1.47	1.39
24	C	503	CLA	CHB-C1B	3.81	1.48	1.39
24	A	409	CLA	CHB-C1B	3.81	1.47	1.39
24	b	622	CLA	CHD-C4C	3.81	1.47	1.39
24	b	624	CLA	CHD-C1D	3.80	1.45	1.38
24	B	610	CLA	CHC-C4B	3.80	1.47	1.39
35	J	101	LMG	O8-C28	3.80	1.44	1.33
24	C	510	CLA	OBD-CAD	3.79	1.29	1.22
24	c	514	CLA	C3D-C2D	3.79	1.49	1.39
24	B	615	CLA	OBD-CAD	3.79	1.29	1.22
24	b	619	CLA	CHC-C4B	3.79	1.47	1.39
24	A	405	CLA	O2A-CGA	3.79	1.44	1.33
40	V	205	HEC	CBB-CAB	-3.79	1.34	1.51
37	d	407	LHG	O8-C23	3.79	1.44	1.33
24	B	611	CLA	OBD-CAD	3.79	1.29	1.22
24	C	508	CLA	C3D-C2D	3.79	1.49	1.39
37	d	408	LHG	O8-C23	3.79	1.44	1.33
24	b	618	CLA	CHB-C1B	3.79	1.47	1.39
24	d	403	CLA	OBD-CAD	3.78	1.29	1.22
24	B	614	CLA	CHD-C1D	3.78	1.45	1.38
24	D	403	CLA	OBD-CAD	3.78	1.29	1.22
24	b	614	CLA	CHD-C4C	3.78	1.47	1.39
24	b	613	CLA	C3D-C2D	3.78	1.49	1.39
24	c	515	CLA	CHB-C1B	3.78	1.47	1.39
24	c	511	CLA	CHD-C4C	3.78	1.47	1.39
24	b	617	CLA	C3D-C2D	3.78	1.49	1.39
24	b	614	CLA	CHB-C1B	3.78	1.47	1.39
38	E	102	HEM	C4D-ND	-3.78	1.33	1.40
24	b	624	CLA	CHB-C1B	3.77	1.47	1.39
24	b	621	CLA	OBD-CAD	3.77	1.29	1.22
24	C	514	CLA	C3D-C2D	3.77	1.49	1.39
24	c	510	CLA	C3D-C2D	3.77	1.49	1.39
24	B	605	CLA	CHD-C4C	3.77	1.47	1.39
24	c	513	CLA	C3D-C2D	3.77	1.49	1.39
24	B	602	CLA	C3D-C2D	3.76	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	CHC-C4B	3.76	1.47	1.39
24	A	407	CLA	C3D-C2D	3.76	1.49	1.39
24	B	606	CLA	OBD-CAD	3.76	1.29	1.22
24	b	616	CLA	CHD-C4C	3.76	1.47	1.39
24	c	516	CLA	OBD-CAD	3.76	1.29	1.22
24	b	620	CLA	CHD-C4C	3.76	1.47	1.39
24	B	606	CLA	CHD-C1D	3.76	1.45	1.38
24	b	615	CLA	CHB-C1B	3.76	1.47	1.39
24	B	615	CLA	CHC-C4B	3.76	1.47	1.39
24	c	513	CLA	OBD-CAD	3.76	1.29	1.22
24	b	619	CLA	CHD-C4C	3.76	1.47	1.39
24	b	619	CLA	CHB-C1B	3.76	1.47	1.39
37	D	408	LHG	O8-C23	3.76	1.44	1.33
24	b	617	CLA	OBD-CAD	3.76	1.29	1.22
24	b	610	CLA	CHC-C4B	3.75	1.47	1.39
24	D	402	CLA	C3D-C2D	3.75	1.49	1.39
24	B	617	CLA	C3D-C2D	3.75	1.49	1.39
24	b	612	CLA	CHC-C4B	3.75	1.47	1.39
24	B	606	CLA	CHD-C4C	3.75	1.47	1.39
24	B	617	CLA	CHC-C4B	3.75	1.47	1.39
24	a	410	CLA	OBD-CAD	3.75	1.28	1.22
24	d	404	CLA	CHD-C4C	3.75	1.47	1.39
24	B	605	CLA	CHB-C1B	3.75	1.47	1.39
24	B	609	CLA	CHD-C4C	3.75	1.47	1.39
24	c	508	CLA	C3D-C2D	3.74	1.49	1.39
24	d	404	CLA	CHC-C4B	3.74	1.47	1.39
24	d	403	CLA	C1B-NB	-3.74	1.33	1.37
24	c	508	CLA	CHC-C4B	3.74	1.47	1.39
24	a	412	CLA	C3D-C2D	3.74	1.49	1.39
34	V	206	HTG	C1'-S1	-3.74	1.76	1.81
24	a	412	CLA	OBD-CAD	3.74	1.28	1.22
24	B	615	CLA	C3D-C2D	3.73	1.49	1.39
24	B	617	CLA	CHB-C1B	3.73	1.47	1.39
24	B	616	CLA	CHD-C4C	3.73	1.47	1.39
24	c	505	CLA	CHB-C1B	3.73	1.47	1.39
24	B	617	CLA	CHD-C4C	3.73	1.47	1.39
24	C	505	CLA	OBD-CAD	3.72	1.28	1.22
24	c	509	CLA	CHD-C4C	3.72	1.47	1.39
24	b	620	CLA	C3D-C2D	3.72	1.49	1.39
24	B	614	CLA	OBD-CAD	3.72	1.28	1.22
24	B	602	CLA	OBD-CAD	3.72	1.28	1.22
24	C	507	CLA	CHB-C1B	3.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3D-C2D	3.72	1.49	1.39
37	L	101	LHG	O7-C7	3.71	1.44	1.34
24	A	405	CLA	C4B-NB	-3.71	1.33	1.37
24	B	613	CLA	C3D-C2D	3.71	1.49	1.39
24	d	403	CLA	C3D-C2D	3.71	1.49	1.39
24	b	624	CLA	OBD-CAD	3.71	1.28	1.22
24	c	507	CLA	OBD-CAD	3.71	1.28	1.22
24	b	625	CLA	OBD-CAD	3.71	1.28	1.22
24	B	602	CLA	CHC-C4B	3.70	1.47	1.39
24	d	404	CLA	C3D-C2D	3.70	1.49	1.39
24	c	507	CLA	C3D-C2D	3.70	1.49	1.39
24	c	509	CLA	O2A-CGA	3.70	1.44	1.33
24	B	605	CLA	O2A-CGA	3.70	1.44	1.33
24	B	615	CLA	CHD-C1D	3.70	1.45	1.38
24	C	511	CLA	CHC-C4B	3.69	1.47	1.39
24	c	517	CLA	C3D-C2D	3.69	1.49	1.39
24	b	620	CLA	CHC-C4B	3.69	1.47	1.39
24	C	513	CLA	CHC-C4B	3.69	1.47	1.39
24	C	510	CLA	CHB-C1B	3.68	1.47	1.39
24	d	403	CLA	CHC-C4B	3.68	1.47	1.39
24	C	513	CLA	CHB-C1B	3.68	1.47	1.39
24	B	611	CLA	C4B-NB	-3.68	1.33	1.37
24	D	403	CLA	CHB-C1B	3.67	1.47	1.39
24	C	511	CLA	OBD-CAD	3.67	1.28	1.22
24	d	402	CLA	CHC-C4B	3.67	1.47	1.39
24	B	604	CLA	CHB-C1B	3.67	1.47	1.39
24	C	506	CLA	CHD-C4C	3.67	1.47	1.39
24	b	621	CLA	CHC-C4B	3.67	1.47	1.39
24	A	409	CLA	OBD-CAD	3.67	1.28	1.22
24	B	608	CLA	C1B-NB	-3.67	1.33	1.37
24	c	510	CLA	C1B-NB	-3.66	1.33	1.37
24	b	612	CLA	C3D-C2D	3.66	1.49	1.39
24	b	614	CLA	CHC-C4B	3.66	1.47	1.39
35	J	101	LMG	O7-C10	3.66	1.44	1.34
24	c	508	CLA	C1B-NB	-3.65	1.33	1.37
24	C	509	CLA	C3D-C2D	3.65	1.49	1.39
24	B	610	CLA	OBD-CAD	3.65	1.28	1.22
34	b	608	HTG	C1'-S1	-3.65	1.76	1.81
24	c	511	CLA	OBD-CAD	3.64	1.28	1.22
24	d	402	CLA	OBD-CAD	3.64	1.28	1.22
24	b	624	CLA	CHD-C4C	3.64	1.47	1.39
24	A	406	CLA	OBD-CAD	3.64	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	412	CLA	CHC-C4B	3.64	1.47	1.39
24	c	506	CLA	CHB-C1B	3.64	1.47	1.39
24	B	612	CLA	O2A-CGA	3.64	1.44	1.33
24	B	611	CLA	CHC-C4B	3.64	1.47	1.39
24	c	509	CLA	C3D-C2D	3.64	1.49	1.39
24	C	510	CLA	CHC-C4B	3.63	1.47	1.39
24	d	404	CLA	C1B-NB	-3.63	1.33	1.37
24	a	410	CLA	CHD-C4C	3.63	1.47	1.39
24	C	512	CLA	OBD-CAD	3.63	1.28	1.22
24	B	603	CLA	CHC-C4B	3.63	1.47	1.39
24	d	404	CLA	CHB-C1B	3.63	1.47	1.39
24	b	619	CLA	C3D-C2D	3.62	1.49	1.39
24	D	402	CLA	CHD-C1D	3.62	1.45	1.38
24	B	617	CLA	OBD-CAD	3.62	1.28	1.22
24	c	511	CLA	CHB-C1B	3.62	1.47	1.39
24	B	606	CLA	CHB-C1B	3.62	1.47	1.39
24	B	607	CLA	CHB-C1B	3.62	1.47	1.39
24	D	402	CLA	CHB-C1B	3.61	1.47	1.39
24	B	603	CLA	C3D-C2D	3.61	1.49	1.39
34	B	633	HTG	C1'-S1	-3.61	1.76	1.81
24	B	611	CLA	CHB-C1B	3.61	1.47	1.39
24	b	624	CLA	CHC-C4B	3.61	1.47	1.39
24	C	509	CLA	CHC-C4B	3.61	1.47	1.39
24	C	508	CLA	CHB-C1B	3.60	1.47	1.39
34	B	625	HTG	C1'-S1	-3.60	1.76	1.81
24	b	614	CLA	OBD-CAD	3.60	1.28	1.22
24	b	612	CLA	OBD-CAD	3.60	1.28	1.22
24	a	409	CLA	OBD-CAD	3.60	1.28	1.22
24	c	513	CLA	CHC-C4B	3.59	1.47	1.39
24	B	603	CLA	C1B-NB	-3.59	1.33	1.37
24	B	616	CLA	CHB-C1B	3.59	1.47	1.39
24	c	508	CLA	OBD-CAD	3.59	1.28	1.22
24	B	607	CLA	CHC-C4B	3.59	1.47	1.39
24	b	616	CLA	C3D-C2D	3.59	1.48	1.39
24	C	513	CLA	OBD-CAD	3.58	1.28	1.22
24	B	610	CLA	CHD-C4C	3.58	1.47	1.39
34	B	632	HTG	C1'-S1	-3.58	1.76	1.81
24	a	410	CLA	C1B-NB	-3.58	1.33	1.37
24	c	505	CLA	OBD-CAD	3.58	1.28	1.22
24	b	620	CLA	OBD-CAD	3.58	1.28	1.22
24	D	402	CLA	CHD-C4C	3.58	1.47	1.39
24	C	508	CLA	CHD-C4C	3.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	CHC-C4B	3.57	1.47	1.39
24	B	609	CLA	OBD-CAD	3.57	1.28	1.22
24	b	612	CLA	CHD-C4C	3.57	1.47	1.39
24	a	410	CLA	C3D-C2D	3.56	1.48	1.39
24	B	607	CLA	OBD-CAD	3.56	1.28	1.22
24	B	612	CLA	OBD-CAD	3.56	1.28	1.22
34	c	525	HTG	C1'-S1	-3.55	1.76	1.81
24	b	621	CLA	CHD-C4C	3.55	1.47	1.39
24	b	615	CLA	C3D-C2D	3.55	1.48	1.39
34	c	524	HTG	C1'-S1	-3.55	1.76	1.81
24	b	619	CLA	C1B-NB	-3.55	1.33	1.37
24	c	511	CLA	CHC-C4B	3.55	1.47	1.39
24	A	405	CLA	CHC-C4B	3.55	1.47	1.39
25	a	411	PHO	O2A-CGA	3.54	1.43	1.33
24	D	403	CLA	CHC-C4B	3.54	1.47	1.39
24	C	505	CLA	CHC-C4B	3.53	1.47	1.39
24	C	502	CLA	CHB-C1B	3.53	1.47	1.39
24	B	613	CLA	OBD-CAD	3.52	1.28	1.22
24	B	605	CLA	C3D-C2D	3.52	1.48	1.39
37	D	407	LHG	O7-C7	3.52	1.44	1.34
24	a	409	CLA	O2A-CGA	3.52	1.43	1.33
24	a	409	CLA	C3D-C2D	3.52	1.48	1.39
24	C	514	CLA	CHB-C1B	3.52	1.47	1.39
24	b	615	CLA	C1B-NB	-3.51	1.33	1.37
34	D	412	HTG	C1'-S1	-3.51	1.76	1.81
24	c	515	CLA	OBD-CAD	3.51	1.28	1.22
34	C	524	HTG	C1'-S1	-3.51	1.76	1.81
24	C	505	CLA	C1B-NB	-3.51	1.33	1.37
24	b	614	CLA	C3D-C2D	3.50	1.48	1.39
24	B	616	CLA	OBD-CAD	3.50	1.28	1.22
24	A	407	CLA	C3B-C4B	3.50	1.50	1.42
24	C	502	CLA	OBD-CAD	3.49	1.28	1.22
24	B	616	CLA	C3D-C2D	3.49	1.48	1.39
24	c	517	CLA	OBD-CAD	3.49	1.28	1.22
24	b	611	CLA	CHB-C1B	3.49	1.47	1.39
24	C	509	CLA	OBD-CAD	3.49	1.28	1.22
24	c	514	CLA	CHC-C4B	3.49	1.47	1.39
24	B	603	CLA	CHB-C1B	3.48	1.47	1.39
24	c	517	CLA	CHB-C1B	3.48	1.47	1.39
24	b	616	CLA	OBD-CAD	3.47	1.28	1.22
24	b	610	CLA	OBD-CAD	3.47	1.28	1.22
24	B	614	CLA	C4B-NB	-3.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C4B-NB	-3.46	1.33	1.37
24	c	505	CLA	C4B-NB	-3.46	1.33	1.37
37	d	407	LHG	O7-C7	3.46	1.44	1.34
24	C	504	CLA	OBD-CAD	3.46	1.28	1.22
24	A	406	CLA	C1B-NB	-3.45	1.33	1.37
24	C	504	CLA	CHB-C1B	3.45	1.47	1.39
24	C	507	CLA	CHC-C4B	3.45	1.47	1.39
24	B	608	CLA	C3D-C2D	3.45	1.48	1.39
24	b	623	CLA	CHC-C4B	3.45	1.47	1.39
24	C	510	CLA	C1B-NB	-3.44	1.33	1.37
24	C	507	CLA	C1B-NB	-3.44	1.33	1.37
24	c	506	CLA	C4B-NB	-3.44	1.33	1.37
24	b	622	CLA	OBD-CAD	3.44	1.28	1.22
24	a	409	CLA	CHB-C1B	3.44	1.47	1.39
24	C	514	CLA	OBD-CAD	3.44	1.28	1.22
24	A	406	CLA	CHB-C1B	3.43	1.47	1.39
24	b	618	CLA	CHC-C4B	3.43	1.47	1.39
24	b	623	CLA	CHB-C1B	3.43	1.47	1.39
24	b	611	CLA	C1B-NB	-3.43	1.33	1.37
24	A	405	CLA	OBD-CAD	3.42	1.28	1.22
40	v	205	HEC	C1D-ND	-3.42	1.34	1.40
24	b	615	CLA	CHC-C4B	3.42	1.47	1.39
24	B	607	CLA	C3D-C2D	3.41	1.48	1.39
38	e	103	HEM	C4D-ND	-3.41	1.34	1.40
24	B	608	CLA	CHB-C1B	3.41	1.47	1.39
24	c	510	CLA	CHC-C4B	3.41	1.47	1.39
24	A	406	CLA	C4B-NB	-3.40	1.33	1.37
24	c	510	CLA	OBD-CAD	3.39	1.28	1.22
24	b	610	CLA	CHB-C1B	3.39	1.47	1.39
24	B	616	CLA	C1B-NB	-3.39	1.33	1.37
24	b	623	CLA	OBD-CAD	3.37	1.28	1.22
24	B	614	CLA	CHC-C4B	3.37	1.47	1.39
24	a	410	CLA	CHC-C4B	3.37	1.47	1.39
24	c	509	CLA	OBD-CAD	3.37	1.28	1.22
24	b	613	CLA	CHD-C4C	3.36	1.46	1.39
24	c	512	CLA	CHC-C4B	3.36	1.47	1.39
34	b	601	HTG	C1'-S1	-3.36	1.77	1.81
24	A	406	CLA	CHC-C4B	3.36	1.46	1.39
24	b	618	CLA	C1B-NB	-3.36	1.33	1.37
24	C	509	CLA	CHB-C1B	3.35	1.46	1.39
24	b	614	CLA	C1B-NB	-3.35	1.33	1.37
24	c	515	CLA	CHC-C4B	3.35	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C1B-C2B	3.34	1.51	1.43
24	c	507	CLA	CHB-C1B	3.34	1.46	1.39
24	C	503	CLA	OBD-CAD	3.34	1.28	1.22
34	C	523	HTG	C1'-S1	-3.34	1.77	1.81
24	C	506	CLA	C1B-NB	-3.33	1.33	1.37
24	B	609	CLA	CHC-C4B	3.33	1.46	1.39
24	b	625	CLA	CHC-C4B	3.33	1.46	1.39
24	c	506	CLA	CHC-C4B	3.32	1.46	1.39
24	B	607	CLA	C1B-NB	-3.32	1.33	1.37
24	b	611	CLA	C4B-NB	-3.32	1.33	1.37
24	C	506	CLA	C3D-C2D	3.32	1.48	1.39
24	b	623	CLA	C1B-NB	-3.32	1.33	1.37
24	b	613	CLA	CHC-C4B	3.32	1.46	1.39
24	c	506	CLA	OBD-CAD	3.31	1.28	1.22
24	A	407	CLA	CHB-C1B	3.30	1.46	1.39
38	E	102	HEM	C1B-NB	-3.30	1.34	1.40
24	b	613	CLA	OBD-CAD	3.30	1.28	1.22
24	D	402	CLA	CHC-C4B	3.30	1.46	1.39
24	c	516	CLA	CHB-C1B	3.30	1.46	1.39
24	c	505	CLA	C1B-NB	-3.29	1.33	1.37
24	B	610	CLA	C1B-NB	-3.29	1.33	1.37
24	C	510	CLA	C4B-NB	-3.29	1.33	1.37
24	B	615	CLA	C1B-NB	-3.28	1.33	1.37
38	e	103	HEM	C1B-NB	-3.28	1.34	1.40
24	C	507	CLA	OBD-CAD	3.28	1.28	1.22
24	D	403	CLA	C4B-NB	-3.28	1.33	1.37
40	V	205	HEC	C1D-ND	-3.28	1.34	1.40
24	b	610	CLA	C1B-NB	-3.28	1.33	1.37
24	a	412	CLA	C4B-NB	-3.28	1.33	1.37
24	c	513	CLA	C4B-NB	-3.27	1.33	1.37
24	d	404	CLA	OBD-CAD	3.27	1.28	1.22
24	B	608	CLA	OBD-CAD	3.27	1.28	1.22
24	B	611	CLA	C1B-NB	-3.27	1.33	1.37
24	b	620	CLA	C1B-NB	-3.25	1.33	1.37
24	c	505	CLA	CHC-C4B	3.25	1.46	1.39
24	B	605	CLA	CHC-C4B	3.25	1.46	1.39
24	C	511	CLA	C1B-NB	-3.25	1.33	1.37
24	b	610	CLA	C3B-C4B	3.24	1.50	1.42
24	B	604	CLA	C4B-NB	-3.24	1.33	1.37
24	C	504	CLA	C3B-C4B	3.24	1.50	1.42
24	C	506	CLA	OBD-CAD	3.23	1.28	1.22
24	b	615	CLA	OBD-CAD	3.23	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C1C-C2C	3.23	1.50	1.44
24	C	502	CLA	C1B-NB	-3.22	1.33	1.37
24	C	508	CLA	OBD-CAD	3.22	1.28	1.22
24	c	517	CLA	C3B-C4B	3.22	1.50	1.42
24	c	507	CLA	C3B-C4B	3.21	1.50	1.42
24	b	612	CLA	C1B-NB	-3.20	1.33	1.37
24	D	402	CLA	C1B-NB	-3.19	1.33	1.37
24	b	612	CLA	C4B-NB	-3.18	1.33	1.37
24	C	514	CLA	C3B-C4B	3.18	1.50	1.42
40	V	205	HEC	C4B-NB	-3.17	1.34	1.40
24	b	622	CLA	CHC-C4B	3.17	1.46	1.39
24	B	609	CLA	C4B-NB	-3.15	1.33	1.37
24	b	613	CLA	C1B-NB	-3.15	1.33	1.37
24	b	613	CLA	C4D-CHA	3.14	1.49	1.38
24	C	514	CLA	C1B-NB	-3.13	1.33	1.37
24	C	508	CLA	C1B-NB	-3.13	1.33	1.37
24	C	508	CLA	C1C-C2C	3.12	1.50	1.44
24	c	516	CLA	C1B-NB	-3.11	1.34	1.37
24	c	514	CLA	C4B-NB	-3.11	1.34	1.37
24	B	613	CLA	CHD-C4C	3.11	1.46	1.39
24	B	607	CLA	C4B-NB	-3.10	1.34	1.37
24	c	516	CLA	C3B-C4B	3.10	1.50	1.42
24	c	515	CLA	C4B-NB	-3.09	1.34	1.37
24	b	617	CLA	C3B-C4B	3.09	1.50	1.42
24	c	517	CLA	C1B-NB	-3.08	1.34	1.37
24	C	512	CLA	CHC-C4B	3.07	1.46	1.39
24	b	614	CLA	C3B-C4B	3.06	1.49	1.42
24	b	621	CLA	C1B-C2B	3.06	1.50	1.43
24	C	507	CLA	C4B-NB	-3.06	1.34	1.37
24	C	505	CLA	C4B-NB	-3.06	1.34	1.37
24	C	506	CLA	C4B-NB	-3.05	1.34	1.37
24	c	516	CLA	C4B-NB	-3.05	1.34	1.37
24	c	511	CLA	C4B-NB	-3.05	1.34	1.37
24	b	622	CLA	C4C-C3C	3.05	1.50	1.45
24	b	625	CLA	C4B-NB	-3.04	1.34	1.37
24	b	624	CLA	C1B-NB	-3.04	1.34	1.37
24	b	615	CLA	C4B-NB	-3.03	1.34	1.37
24	B	611	CLA	C3B-C4B	3.03	1.49	1.42
24	D	402	CLA	C4B-NB	-3.03	1.34	1.37
24	b	625	CLA	C1B-C2B	3.03	1.50	1.43
24	b	619	CLA	C4B-NB	-3.03	1.34	1.37
24	B	605	CLA	C1B-C2B	3.03	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C3B-C4B	3.03	1.49	1.42
24	B	602	CLA	C3B-C4B	3.02	1.49	1.42
27	f	102	SQD	C6-S	-3.02	1.66	1.77
24	b	617	CLA	C1B-NB	-3.01	1.34	1.37
24	C	508	CLA	C3B-C4B	3.01	1.49	1.42
24	b	611	CLA	C3B-C4B	3.01	1.49	1.42
24	B	612	CLA	C1B-NB	-3.01	1.34	1.37
24	c	507	CLA	C1B-NB	-3.00	1.34	1.37
24	C	513	CLA	C1B-C2B	3.00	1.50	1.43
24	C	502	CLA	C3B-C4B	3.00	1.49	1.42
24	c	509	CLA	C3B-C4B	2.99	1.49	1.42
24	C	509	CLA	C4B-NB	-2.99	1.34	1.37
24	B	610	CLA	C1B-C2B	2.99	1.50	1.43
40	v	205	HEC	C4B-NB	-2.99	1.35	1.40
24	c	513	CLA	C1B-NB	-2.99	1.34	1.37
24	b	616	CLA	C1B-C2B	2.98	1.50	1.43
24	c	514	CLA	C1B-NB	-2.98	1.34	1.37
24	C	503	CLA	C1B-NB	-2.98	1.34	1.37
24	B	608	CLA	C4C-C3C	2.97	1.50	1.45
24	C	509	CLA	C4C-C3C	2.97	1.50	1.45
24	C	512	CLA	C4B-NB	-2.97	1.34	1.37
24	B	605	CLA	OBD-CAD	2.97	1.27	1.22
24	c	507	CLA	C1C-C2C	2.96	1.50	1.44
24	c	517	CLA	C4B-NB	-2.96	1.34	1.37
24	C	503	CLA	C3B-C4B	2.96	1.49	1.42
24	b	613	CLA	C1B-C2B	2.96	1.50	1.43
24	b	625	CLA	C1B-NB	-2.96	1.34	1.37
27	A	415	SQD	C6-S	-2.96	1.66	1.77
24	C	509	CLA	C3B-C4B	2.95	1.49	1.42
24	b	624	CLA	C3B-C4B	2.94	1.49	1.42
24	d	402	CLA	C1B-C2B	2.94	1.50	1.43
24	C	513	CLA	C1B-NB	-2.94	1.34	1.37
24	B	606	CLA	C1C-C2C	2.94	1.50	1.44
24	a	412	CLA	C3B-C4B	2.94	1.49	1.42
24	A	409	CLA	C1B-NB	-2.94	1.34	1.37
24	D	402	CLA	OBD-CAD	2.94	1.27	1.22
24	B	617	CLA	C1B-NB	-2.93	1.34	1.37
24	c	511	CLA	C1B-NB	-2.92	1.34	1.37
24	c	512	CLA	C1B-NB	-2.91	1.34	1.37
24	C	510	CLA	C3B-C4B	2.91	1.49	1.42
24	C	514	CLA	C4B-NB	-2.91	1.34	1.37
24	C	513	CLA	C3B-C4B	2.91	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	C1B-C2B	2.91	1.50	1.43
24	B	616	CLA	C3B-C4B	2.91	1.49	1.42
24	a	410	CLA	C3B-C4B	2.91	1.49	1.42
24	A	407	CLA	C1B-NB	-2.90	1.34	1.37
24	C	506	CLA	C1B-C2B	2.90	1.50	1.43
24	A	409	CLA	C3B-C4B	2.90	1.49	1.42
24	C	504	CLA	C1B-NB	-2.90	1.34	1.37
24	B	605	CLA	C4D-CHA	2.90	1.48	1.38
24	c	511	CLA	C4D-CHA	2.90	1.48	1.38
24	B	610	CLA	C3B-C4B	2.89	1.49	1.42
24	B	613	CLA	C4B-NB	-2.89	1.34	1.37
24	b	614	CLA	C4B-NB	-2.89	1.34	1.37
24	B	605	CLA	C1B-NB	-2.88	1.34	1.37
24	b	612	CLA	C1C-C2C	2.88	1.50	1.44
24	B	609	CLA	C1B-NB	-2.87	1.34	1.37
24	c	515	CLA	C1B-C2B	2.87	1.50	1.43
24	B	606	CLA	C3B-C4B	2.87	1.49	1.42
24	B	611	CLA	C4D-CHA	2.87	1.48	1.38
24	d	402	CLA	C4B-NB	-2.87	1.34	1.37
24	d	403	CLA	C4B-NB	-2.87	1.34	1.37
24	c	510	CLA	C4B-NB	-2.86	1.34	1.37
24	b	614	CLA	C1C-C2C	2.86	1.50	1.44
24	b	621	CLA	C4B-NB	-2.86	1.34	1.37
24	c	506	CLA	C4D-CHA	2.86	1.48	1.38
24	b	622	CLA	C1B-C2B	2.86	1.50	1.43
24	c	509	CLA	C1B-C2B	2.85	1.50	1.43
24	c	515	CLA	C1B-NB	-2.85	1.34	1.37
24	B	614	CLA	C4C-C3C	2.84	1.49	1.45
24	B	608	CLA	C1B-C2B	2.84	1.49	1.43
24	B	602	CLA	C4B-NB	-2.84	1.34	1.37
24	D	403	CLA	C4C-C3C	2.83	1.49	1.45
34	b	631	HTG	C1'-S1	-2.83	1.77	1.81
24	C	509	CLA	C1B-NB	-2.83	1.34	1.37
24	C	511	CLA	C1B-C2B	2.83	1.49	1.43
25	d	401	PHO	C3A-C2A	-2.83	1.52	1.54
24	c	506	CLA	C1B-C2B	2.83	1.49	1.43
24	A	409	CLA	C4B-NB	-2.82	1.34	1.37
24	B	602	CLA	C1B-NB	-2.82	1.34	1.37
24	C	503	CLA	C1B-C2B	2.82	1.49	1.43
24	B	615	CLA	C1B-C2B	2.82	1.49	1.43
24	b	612	CLA	C3B-C4B	2.82	1.49	1.42
24	C	509	CLA	C1C-C2C	2.82	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	C4B-NB	-2.82	1.34	1.37
24	c	517	CLA	C1C-C2C	2.81	1.50	1.44
24	C	512	CLA	C4D-CHA	2.81	1.48	1.38
24	d	404	CLA	C4B-NB	-2.81	1.34	1.37
24	a	409	CLA	C4B-NB	-2.81	1.34	1.37
24	c	506	CLA	C3B-C4B	2.81	1.49	1.42
38	E	102	HEM	C1C-C2C	-2.80	1.39	1.45
24	A	405	CLA	C4C-C3C	2.80	1.49	1.45
24	b	624	CLA	C1B-C2B	2.80	1.49	1.43
24	C	505	CLA	C1B-C2B	2.79	1.49	1.43
24	c	509	CLA	C4C-C3C	2.79	1.49	1.45
24	c	514	CLA	C1B-C2B	2.79	1.49	1.43
24	c	512	CLA	C1B-C2B	2.79	1.49	1.43
27	a	405	SQD	C6-S	-2.78	1.67	1.77
24	B	609	CLA	C3B-C4B	2.78	1.49	1.42
24	b	622	CLA	C1B-NB	-2.78	1.34	1.37
24	b	621	CLA	C4D-CHA	2.78	1.48	1.38
34	B	624	HTG	C1'-S1	-2.78	1.77	1.81
24	B	609	CLA	C1B-C2B	2.78	1.49	1.43
24	B	604	CLA	C1C-C2C	2.78	1.49	1.44
25	A	408	PHO	CHA-CBD	-2.78	1.48	1.51
24	B	614	CLA	C1B-NB	-2.78	1.34	1.37
24	B	617	CLA	C1B-C2B	2.77	1.49	1.43
24	C	510	CLA	C1B-C2B	2.77	1.49	1.43
24	D	403	CLA	C1B-NB	-2.77	1.34	1.37
24	C	510	CLA	C4C-C3C	2.77	1.49	1.45
24	c	509	CLA	C1C-C2C	2.77	1.49	1.44
24	C	508	CLA	C4D-CHA	2.77	1.48	1.38
24	C	511	CLA	C4D-CHA	2.77	1.48	1.38
24	B	603	CLA	C3B-C4B	2.76	1.49	1.42
24	B	613	CLA	C1B-C2B	2.76	1.49	1.43
24	B	612	CLA	C4B-NB	-2.76	1.34	1.37
24	C	504	CLA	C1C-C2C	2.76	1.49	1.44
24	B	616	CLA	C4B-NB	-2.76	1.34	1.37
24	C	512	CLA	C4C-C3C	2.76	1.49	1.45
24	B	616	CLA	C1B-C2B	2.76	1.49	1.43
24	a	409	CLA	C4C-C3C	2.75	1.49	1.45
24	d	402	CLA	C1B-NB	-2.75	1.34	1.37
24	b	623	CLA	C4B-NB	-2.75	1.34	1.37
24	A	406	CLA	C4D-CHA	2.74	1.48	1.38
27	F	103	SQD	C6-S	-2.74	1.67	1.77
24	b	622	CLA	C4D-CHA	2.73	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C4D-CHA	2.73	1.48	1.38
24	B	612	CLA	C1B-C2B	2.73	1.49	1.43
24	A	405	CLA	C4D-CHA	2.72	1.48	1.38
24	c	511	CLA	C1C-C2C	2.72	1.49	1.44
24	c	509	CLA	C1B-NB	-2.72	1.34	1.37
24	b	624	CLA	C4D-CHA	2.72	1.48	1.38
24	B	611	CLA	C4C-C3C	2.72	1.49	1.45
24	B	614	CLA	C4D-CHA	2.71	1.48	1.38
24	d	404	CLA	C1B-C2B	2.71	1.49	1.43
27	A	411	SQD	C6-S	-2.71	1.67	1.77
24	b	620	CLA	C4D-CHA	2.71	1.48	1.38
24	D	402	CLA	C1B-C2B	2.71	1.49	1.43
24	a	412	CLA	C1B-C2B	2.71	1.49	1.43
24	A	406	CLA	C1B-C2B	2.71	1.49	1.43
24	b	616	CLA	C4D-CHA	2.71	1.48	1.38
24	B	602	CLA	C1B-C2B	2.70	1.49	1.43
24	c	512	CLA	C4B-NB	-2.70	1.34	1.37
24	C	502	CLA	C4B-NB	-2.69	1.34	1.37
24	B	612	CLA	C1C-C2C	2.69	1.49	1.44
24	A	409	CLA	C4D-CHA	2.69	1.48	1.38
24	b	620	CLA	C1B-C2B	2.69	1.49	1.43
24	b	617	CLA	C1B-C2B	2.69	1.49	1.43
24	B	617	CLA	C4D-CHA	2.69	1.48	1.38
24	a	409	CLA	C1B-NB	-2.69	1.34	1.37
24	C	505	CLA	C4D-CHA	2.68	1.47	1.38
24	B	614	CLA	C1B-C2B	2.68	1.49	1.43
24	a	412	CLA	C1B-NB	-2.68	1.34	1.37
24	b	615	CLA	C4D-CHA	2.68	1.47	1.38
24	C	506	CLA	C3B-C4B	2.68	1.49	1.42
24	B	607	CLA	C1C-C2C	2.68	1.49	1.44
24	b	622	CLA	C4B-NB	-2.67	1.34	1.37
24	C	510	CLA	C4D-CHA	2.67	1.47	1.38
24	c	513	CLA	C4D-CHA	2.67	1.47	1.38
24	c	505	CLA	C1B-C2B	2.67	1.49	1.43
24	b	618	CLA	C4B-NB	-2.66	1.34	1.37
24	c	511	CLA	C1B-C2B	2.66	1.49	1.43
24	b	615	CLA	C3B-C4B	2.66	1.49	1.42
24	C	503	CLA	C4D-CHA	2.66	1.47	1.38
24	c	507	CLA	C4B-NB	-2.66	1.34	1.37
24	c	515	CLA	C3B-C4B	2.66	1.49	1.42
24	b	617	CLA	C4B-NB	-2.66	1.34	1.37
24	c	512	CLA	C3B-C4B	2.66	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C3B-C4B	2.65	1.49	1.42
24	D	403	CLA	C1B-C2B	2.65	1.49	1.43
24	B	607	CLA	C4D-CHA	2.65	1.47	1.38
24	B	608	CLA	C4D-CHA	2.65	1.47	1.38
24	B	609	CLA	C4C-C3C	2.65	1.49	1.45
24	b	621	CLA	C3B-C4B	2.65	1.49	1.42
24	c	505	CLA	C4D-CHA	2.65	1.47	1.38
24	D	402	CLA	C1C-C2C	2.65	1.49	1.44
24	B	606	CLA	C4B-NB	-2.64	1.34	1.37
24	b	612	CLA	C1B-C2B	2.64	1.49	1.43
24	A	405	CLA	C1B-NB	-2.64	1.34	1.37
24	C	504	CLA	C4B-NB	-2.64	1.34	1.37
24	B	615	CLA	C1C-C2C	2.64	1.49	1.44
24	a	410	CLA	C1C-C2C	2.64	1.49	1.44
24	C	503	CLA	C1C-C2C	2.63	1.49	1.44
40	V	205	HEC	C4B-C3B	2.63	1.49	1.45
24	C	506	CLA	C3D-C4D	-2.63	1.38	1.44
24	B	607	CLA	C3B-C4B	2.63	1.48	1.42
24	C	514	CLA	C4D-CHA	2.63	1.47	1.38
24	a	409	CLA	C1C-C2C	2.63	1.49	1.44
24	B	604	CLA	C4D-CHA	2.63	1.47	1.38
24	C	509	CLA	C4D-CHA	2.63	1.47	1.38
24	d	403	CLA	C4C-C3C	2.62	1.49	1.45
24	b	612	CLA	C4D-CHA	2.62	1.47	1.38
24	c	510	CLA	C1B-C2B	2.62	1.49	1.43
27	B	621	SQD	C6-S	-2.62	1.67	1.77
24	B	609	CLA	C4D-CHA	2.62	1.47	1.38
24	c	505	CLA	C4C-C3C	2.62	1.49	1.45
24	C	505	CLA	C1C-C2C	2.61	1.49	1.44
24	b	614	CLA	C3D-C4D	-2.61	1.38	1.44
24	C	513	CLA	C4D-CHA	2.61	1.47	1.38
24	b	618	CLA	C1B-C2B	2.61	1.49	1.43
24	b	625	CLA	C4D-CHA	2.61	1.47	1.38
24	c	508	CLA	C4D-CHA	2.60	1.47	1.38
24	B	607	CLA	C4C-C3C	2.60	1.49	1.45
24	b	615	CLA	C1C-C2C	2.60	1.49	1.44
35	Z	101	LMG	O8-C28	2.60	1.46	1.33
24	c	516	CLA	C1C-C2C	2.60	1.49	1.44
24	b	619	CLA	C3B-C4B	2.60	1.48	1.42
24	A	407	CLA	C1C-C2C	2.60	1.49	1.44
24	B	610	CLA	C4D-CHA	2.60	1.47	1.38
24	A	409	CLA	C1C-C2C	2.59	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C1B-C2B	2.59	1.49	1.43
24	c	513	CLA	C1C-C2C	2.59	1.49	1.44
31	a	416	PL9	C6-C5	2.59	1.48	1.35
24	B	614	CLA	C1C-C2C	2.59	1.49	1.44
24	A	409	CLA	C1B-C2B	2.59	1.49	1.43
24	c	506	CLA	C1B-NB	-2.59	1.34	1.37
24	B	602	CLA	C4D-CHA	2.59	1.47	1.38
24	D	403	CLA	C3B-C4B	2.59	1.48	1.42
27	a	414	SQD	C6-S	-2.59	1.67	1.77
27	L	102	SQD	C6-S	-2.58	1.67	1.77
24	c	515	CLA	C4D-CHA	2.58	1.47	1.38
24	C	507	CLA	C4D-CHA	2.58	1.47	1.38
24	B	607	CLA	C1B-C2B	2.58	1.49	1.43
24	C	514	CLA	C1C-C2C	2.58	1.49	1.44
24	B	610	CLA	C3D-C4D	-2.58	1.38	1.44
24	b	622	CLA	C1C-C2C	2.58	1.49	1.44
24	c	514	CLA	C4D-CHA	2.58	1.47	1.38
24	b	623	CLA	C1B-C2B	2.57	1.49	1.43
24	b	611	CLA	C4D-CHA	2.57	1.47	1.38
24	C	508	CLA	C1B-C2B	2.57	1.49	1.43
24	b	611	CLA	C4C-C3C	2.57	1.49	1.45
24	B	603	CLA	C4D-CHA	2.57	1.47	1.38
24	C	512	CLA	C3B-C4B	2.57	1.48	1.42
24	C	502	CLA	C4D-CHA	2.57	1.47	1.38
24	B	612	CLA	C4D-CHA	2.57	1.47	1.38
24	b	621	CLA	C1B-NB	-2.56	1.34	1.37
31	A	418	PL9	C6-C5	2.56	1.48	1.35
24	C	514	CLA	C1B-C2B	2.56	1.49	1.43
24	b	610	CLA	C4D-CHA	2.56	1.47	1.38
24	b	615	CLA	C1B-C2B	2.56	1.49	1.43
24	C	502	CLA	C1C-C2C	2.56	1.49	1.44
24	B	611	CLA	C1B-C2B	2.56	1.49	1.43
24	C	512	CLA	C1B-NB	-2.56	1.34	1.37
24	B	617	CLA	C3B-C4B	2.56	1.48	1.42
24	b	616	CLA	C3D-C4D	-2.55	1.38	1.44
24	B	615	CLA	C4D-CHA	2.55	1.47	1.38
24	d	404	CLA	C3B-C4B	2.55	1.48	1.42
24	B	615	CLA	C4C-C3C	2.55	1.49	1.45
24	a	409	CLA	C4D-CHA	2.54	1.47	1.38
24	b	614	CLA	C4D-CHA	2.54	1.47	1.38
24	b	613	CLA	C3B-C4B	2.54	1.48	1.42
24	C	510	CLA	C1C-C2C	2.54	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C4D-CHA	2.53	1.47	1.38
24	C	513	CLA	C1C-C2C	2.53	1.49	1.44
24	D	402	CLA	C4D-CHA	2.53	1.47	1.38
24	b	613	CLA	C4C-C3C	2.53	1.49	1.45
24	b	620	CLA	C3B-C4B	2.53	1.48	1.42
24	b	610	CLA	C4B-NB	-2.53	1.34	1.37
24	C	506	CLA	C1C-C2C	2.53	1.49	1.44
24	C	507	CLA	C3B-C4B	2.53	1.48	1.42
24	C	511	CLA	C3B-C4B	2.52	1.48	1.42
24	B	603	CLA	C1B-C2B	2.52	1.49	1.43
24	b	619	CLA	C4C-C3C	2.52	1.49	1.45
24	b	611	CLA	C1B-C2B	2.52	1.49	1.43
31	d	406	PL9	C6-C5	2.52	1.48	1.35
24	A	407	CLA	C1B-C2B	2.52	1.49	1.43
24	b	620	CLA	C4B-NB	-2.52	1.34	1.37
24	B	616	CLA	C1C-C2C	2.51	1.49	1.44
24	B	603	CLA	C4B-NB	-2.51	1.34	1.37
24	B	615	CLA	C3B-C4B	2.50	1.48	1.42
24	b	617	CLA	C1C-C2C	2.50	1.49	1.44
24	B	613	CLA	C3B-C4B	2.50	1.48	1.42
24	c	517	CLA	C4C-C3C	2.50	1.49	1.45
24	d	404	CLA	C1C-C2C	2.50	1.49	1.44
24	B	615	CLA	C4B-NB	-2.50	1.34	1.37
25	d	401	PHO	C4B-NB	-2.50	1.33	1.38
24	C	511	CLA	C4B-NB	-2.50	1.34	1.37
24	c	510	CLA	C3B-C4B	2.50	1.48	1.42
34	d	412	HTG	C1-S1	-2.50	1.76	1.80
24	a	412	CLA	C4D-CHA	2.49	1.47	1.38
24	B	603	CLA	C1C-C2C	2.49	1.49	1.44
24	c	507	CLA	C3D-C4D	-2.49	1.38	1.44
24	C	511	CLA	C1C-C2C	2.49	1.49	1.44
24	C	504	CLA	C4D-CHA	2.49	1.47	1.38
24	C	508	CLA	C4B-NB	-2.49	1.34	1.37
25	A	408	PHO	C1B-NB	-2.49	1.34	1.38
24	b	613	CLA	C4B-NB	-2.48	1.34	1.37
24	c	516	CLA	C4D-CHA	2.48	1.47	1.38
24	C	514	CLA	C4C-C3C	2.48	1.49	1.45
24	c	509	CLA	C4D-CHA	2.48	1.47	1.38
24	B	606	CLA	C1B-NB	-2.48	1.34	1.37
24	a	409	CLA	C3B-C4B	2.48	1.48	1.42
24	c	512	CLA	C4D-CHA	2.48	1.47	1.38
24	D	403	CLA	C4D-CHA	2.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C4D-CHA	2.47	1.47	1.38
34	b	607	HTG	C1-S1	-2.47	1.76	1.80
24	c	508	CLA	C1C-C2C	2.47	1.49	1.44
24	A	405	CLA	C3B-C4B	2.46	1.48	1.42
24	b	619	CLA	C1B-C2B	2.46	1.49	1.43
25	A	408	PHO	C4B-NB	-2.46	1.34	1.38
24	b	616	CLA	C1C-C2C	2.46	1.49	1.44
24	B	608	CLA	C3B-C4B	2.46	1.48	1.42
25	d	401	PHO	CHA-CBD	-2.46	1.48	1.51
24	c	513	CLA	C3B-C4B	2.45	1.48	1.42
24	c	507	CLA	C4C-C3C	2.45	1.49	1.45
24	C	511	CLA	C4C-C3C	2.45	1.49	1.45
24	c	514	CLA	C3B-C4B	2.44	1.48	1.42
24	d	404	CLA	C4D-CHA	2.44	1.47	1.38
31	D	405	PL9	C6-C5	2.44	1.48	1.35
24	A	407	CLA	C3D-C4D	-2.44	1.38	1.44
25	D	401	PHO	C3A-C2A	-2.44	1.52	1.54
24	c	517	CLA	C4D-CHA	2.44	1.47	1.38
24	a	410	CLA	C4D-CHA	2.44	1.47	1.38
24	b	615	CLA	C3D-C4D	-2.44	1.38	1.44
24	c	507	CLA	C1B-C2B	2.44	1.49	1.43
24	C	510	CLA	C3B-C2B	2.44	1.49	1.41
24	b	613	CLA	C1C-C2C	2.43	1.49	1.44
29	A	416	LMT	O1'-C1'	2.43	1.44	1.40
24	a	410	CLA	C4B-NB	-2.43	1.34	1.37
24	c	507	CLA	C4D-CHA	2.43	1.47	1.38
34	c	524	HTG	C1-S1	-2.43	1.77	1.80
24	c	510	CLA	C4D-CHA	2.43	1.47	1.38
24	B	613	CLA	C4C-C3C	2.42	1.49	1.45
24	A	407	CLA	C4B-NB	-2.42	1.34	1.37
24	C	509	CLA	C3D-C4D	-2.42	1.38	1.44
25	a	411	PHO	CHA-CBD	-2.42	1.48	1.51
24	C	512	CLA	C1C-C2C	2.42	1.49	1.44
24	b	623	CLA	C3D-C4D	-2.42	1.38	1.44
24	d	404	CLA	C4C-C3C	2.42	1.49	1.45
24	c	514	CLA	C4C-C3C	2.42	1.49	1.45
24	B	609	CLA	C1C-C2C	2.42	1.49	1.44
24	d	403	CLA	C1B-C2B	2.42	1.48	1.43
24	b	618	CLA	C3B-C4B	2.42	1.48	1.42
24	C	509	CLA	C1B-C2B	2.42	1.48	1.43
24	c	506	CLA	C3D-C4D	-2.42	1.38	1.44
24	B	605	CLA	C3B-C4B	2.42	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C3B-C4B	2.41	1.48	1.42
24	C	505	CLA	C3B-C2B	2.41	1.49	1.41
24	B	610	CLA	C1C-C2C	2.41	1.49	1.44
24	b	617	CLA	C3D-C4D	-2.41	1.38	1.44
24	B	616	CLA	C4D-CHA	2.41	1.47	1.38
24	B	604	CLA	C4C-C3C	2.40	1.49	1.45
38	e	103	HEM	C1C-C2C	-2.40	1.40	1.45
24	B	605	CLA	C3B-C2B	2.40	1.49	1.41
24	b	610	CLA	C1B-C2B	2.40	1.48	1.43
24	B	604	CLA	C1B-C2B	2.40	1.48	1.43
24	b	612	CLA	C3D-C4D	-2.40	1.38	1.44
24	c	513	CLA	C3B-C2B	2.40	1.49	1.41
24	c	514	CLA	C1C-C2C	2.40	1.49	1.44
24	C	505	CLA	C3D-C4D	-2.40	1.38	1.44
24	C	505	CLA	C3B-C4B	2.39	1.48	1.42
24	C	506	CLA	C4C-C3C	2.39	1.49	1.45
24	c	513	CLA	C4C-C3C	2.39	1.49	1.45
24	c	510	CLA	C3D-C4D	-2.39	1.38	1.44
24	b	617	CLA	C4C-C3C	2.39	1.49	1.45
24	d	403	CLA	C4D-CHA	2.38	1.46	1.38
34	b	632	HTG	C1-S1	-2.38	1.77	1.80
24	B	604	CLA	C3D-C4D	-2.38	1.38	1.44
24	B	605	CLA	C4B-NB	-2.38	1.34	1.37
34	c	525	HTG	C1-S1	-2.38	1.77	1.80
24	C	502	CLA	C1B-C2B	2.38	1.48	1.43
24	A	405	CLA	C1B-C2B	2.37	1.48	1.43
34	D	412	HTG	C1-S1	-2.37	1.77	1.80
24	B	613	CLA	C3B-C2B	2.37	1.49	1.41
24	b	625	CLA	C1C-NC	-2.37	1.34	1.37
24	A	406	CLA	C3D-C4D	-2.37	1.38	1.44
24	B	613	CLA	C4D-CHA	2.37	1.46	1.38
24	A	405	CLA	C3D-C4D	-2.37	1.38	1.44
24	c	509	CLA	C3D-C4D	-2.37	1.38	1.44
24	A	407	CLA	C4D-CHA	2.36	1.46	1.38
24	b	619	CLA	C4D-CHA	2.36	1.46	1.38
24	C	503	CLA	C4B-NB	-2.36	1.34	1.37
24	C	509	CLA	C3B-C2B	2.36	1.49	1.41
24	C	514	CLA	C3D-C4D	-2.36	1.38	1.44
24	b	621	CLA	C1C-C2C	2.35	1.49	1.44
24	c	517	CLA	C3D-C4D	-2.35	1.38	1.44
24	a	410	CLA	C1B-C2B	2.35	1.48	1.43
40	V	205	HEC	C4D-ND	-2.35	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	C3D-C4D	-2.35	1.38	1.44
24	B	603	CLA	C4C-C3C	2.35	1.49	1.45
36	D	406	DGD	O3G-C1D	2.35	1.44	1.40
34	C	523	HTG	C1-S1	-2.35	1.77	1.80
24	d	402	CLA	C3B-C2B	2.34	1.49	1.41
24	C	504	CLA	C1B-C2B	2.34	1.48	1.43
24	b	614	CLA	C1B-C2B	2.34	1.48	1.43
24	c	508	CLA	C1B-C2B	2.34	1.48	1.43
24	b	613	CLA	C3B-C2B	2.34	1.49	1.41
34	b	608	HTG	C1-S1	-2.34	1.77	1.80
24	a	409	CLA	C3B-C2B	2.33	1.49	1.41
24	C	507	CLA	C3D-C4D	-2.33	1.38	1.44
24	A	407	CLA	C4C-C3C	2.33	1.49	1.45
24	C	511	CLA	C3D-C4D	-2.33	1.38	1.44
24	d	402	CLA	C4D-CHA	2.33	1.46	1.38
24	d	403	CLA	C3D-C4D	-2.33	1.38	1.44
24	C	507	CLA	C1B-C2B	2.32	1.48	1.43
24	b	620	CLA	C3B-C2B	2.32	1.49	1.41
24	c	508	CLA	C4C-C3C	2.32	1.49	1.45
24	A	405	CLA	C1C-C2C	2.32	1.49	1.44
24	b	621	CLA	C3B-C2B	2.32	1.49	1.41
24	c	511	CLA	C4C-C3C	2.32	1.49	1.45
24	c	505	CLA	C3B-C4B	2.32	1.48	1.42
24	C	508	CLA	C4C-C3C	2.31	1.49	1.45
34	B	632	HTG	C1-S1	-2.31	1.77	1.80
24	B	617	CLA	C3B-C2B	2.31	1.49	1.41
24	C	512	CLA	C3B-C2B	2.31	1.49	1.41
24	C	507	CLA	C4C-C3C	2.31	1.49	1.45
24	B	602	CLA	C1C-C2C	2.31	1.49	1.44
24	b	622	CLA	C3B-C2B	2.31	1.49	1.41
24	D	402	CLA	C3B-C2B	2.31	1.49	1.41
24	b	620	CLA	C4C-C3C	2.31	1.49	1.45
24	D	403	CLA	C3D-C4D	-2.30	1.39	1.44
24	c	513	CLA	C3D-C4D	-2.30	1.39	1.44
24	B	603	CLA	C3D-C4D	-2.30	1.39	1.44
24	c	510	CLA	C3B-C2B	2.30	1.49	1.41
34	V	206	HTG	C1-S1	-2.30	1.77	1.80
24	C	510	CLA	C3D-C4D	-2.30	1.39	1.44
24	B	611	CLA	C3D-C4D	-2.30	1.39	1.44
24	D	402	CLA	C3D-C4D	-2.30	1.39	1.44
24	c	506	CLA	C1C-C2C	2.30	1.49	1.44
24	C	507	CLA	C1C-C2C	2.30	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	C3B-C4B	2.29	1.48	1.42
24	c	505	CLA	C3B-C2B	2.29	1.48	1.41
24	B	612	CLA	C4C-C3C	2.29	1.49	1.45
24	b	620	CLA	C3D-C4D	-2.29	1.39	1.44
24	d	402	CLA	C1C-C2C	2.29	1.49	1.44
24	c	512	CLA	C3B-C2B	2.29	1.48	1.41
24	c	508	CLA	C3B-C4B	2.28	1.48	1.42
40	v	205	HEC	C1B-NB	-2.28	1.34	1.38
24	b	624	CLA	C4B-NB	-2.28	1.35	1.37
24	D	403	CLA	C1C-C2C	2.28	1.49	1.44
24	a	412	CLA	C1C-C2C	2.28	1.49	1.44
24	b	625	CLA	C3B-C4B	2.28	1.48	1.42
24	c	509	CLA	C4B-NB	-2.28	1.35	1.37
24	a	410	CLA	C3D-C4D	-2.28	1.39	1.44
24	c	515	CLA	C4C-C3C	2.28	1.49	1.45
24	b	623	CLA	C3B-C4B	2.28	1.48	1.42
24	a	409	CLA	C3D-C4D	-2.27	1.39	1.44
24	b	625	CLA	C3B-C2B	2.27	1.48	1.41
24	A	406	CLA	C3B-C4B	2.27	1.48	1.42
24	B	605	CLA	C3D-C4D	-2.27	1.39	1.44
38	e	103	HEM	C3C-C4C	-2.27	1.42	1.46
24	c	517	CLA	C1B-C2B	2.27	1.48	1.43
24	B	605	CLA	C1C-C2C	2.27	1.48	1.44
24	b	623	CLA	C4D-CHA	2.26	1.46	1.38
24	d	404	CLA	C3B-C2B	2.26	1.48	1.41
24	c	511	CLA	C3B-C2B	2.26	1.48	1.41
24	a	412	CLA	C3D-C4D	-2.25	1.39	1.44
24	A	406	CLA	C3B-C2B	2.25	1.48	1.41
24	B	607	CLA	C3D-C4D	-2.25	1.39	1.44
24	C	503	CLA	C4C-C3C	2.25	1.48	1.45
24	A	409	CLA	C4C-C3C	2.25	1.48	1.45
24	A	409	CLA	C3D-C4D	-2.25	1.39	1.44
24	c	515	CLA	C3B-C2B	2.25	1.48	1.41
24	B	603	CLA	C3B-C2B	2.25	1.48	1.41
24	c	508	CLA	C3D-C4D	-2.24	1.39	1.44
24	a	409	CLA	C1B-C2B	2.24	1.48	1.43
24	b	624	CLA	C1C-C2C	2.23	1.48	1.44
24	B	608	CLA	C4B-NB	-2.23	1.35	1.37
25	D	401	PHO	C4B-NB	-2.23	1.34	1.38
24	C	508	CLA	C3D-C4D	-2.23	1.39	1.44
38	E	102	HEM	C1D-ND	-2.23	1.34	1.38
24	b	611	CLA	C1C-C2C	2.23	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3B-C2B	2.23	1.48	1.41
24	A	406	CLA	C1C-C2C	2.22	1.48	1.44
24	c	514	CLA	C3B-C2B	2.22	1.48	1.41
24	C	511	CLA	C3B-C2B	2.22	1.48	1.41
24	c	510	CLA	C1C-C2C	2.22	1.48	1.44
25	A	408	PHO	C1D-ND	-2.22	1.34	1.38
24	B	615	CLA	C3D-C4D	-2.22	1.39	1.44
24	B	606	CLA	C4D-CHA	2.21	1.46	1.38
24	b	610	CLA	C3D-C4D	-2.21	1.39	1.44
24	B	609	CLA	C3D-C4D	-2.21	1.39	1.44
24	b	622	CLA	C3B-C4B	2.21	1.47	1.42
24	c	516	CLA	C1B-C2B	2.21	1.48	1.43
24	b	622	CLA	C3D-C4D	-2.21	1.39	1.44
25	a	411	PHO	C4B-NB	-2.21	1.34	1.38
24	b	619	CLA	C3B-C2B	2.21	1.48	1.41
24	c	508	CLA	C3B-C2B	2.20	1.48	1.41
40	V	205	HEC	C1B-NB	-2.20	1.34	1.38
24	b	610	CLA	C1C-C2C	2.20	1.48	1.44
24	b	612	CLA	C3B-C2B	2.20	1.48	1.41
24	C	503	CLA	C3B-C2B	2.20	1.48	1.41
24	c	515	CLA	C1C-C2C	2.20	1.48	1.44
24	b	621	CLA	C1C-NC	-2.20	1.34	1.37
24	b	623	CLA	C3B-C2B	2.20	1.48	1.41
24	b	614	CLA	C4C-C3C	2.19	1.48	1.45
24	C	513	CLA	C4C-C3C	2.19	1.48	1.45
24	C	512	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	615	CLA	C3B-C2B	2.19	1.48	1.41
24	b	611	CLA	C1D-C2D	2.19	1.49	1.45
34	B	633	HTG	C1-S1	-2.19	1.77	1.80
24	b	618	CLA	C3D-C4D	-2.18	1.39	1.44
24	A	405	CLA	C3B-C2B	2.18	1.48	1.41
24	b	610	CLA	C3B-C2B	2.18	1.48	1.41
24	D	402	CLA	C4C-C3C	2.18	1.48	1.45
24	c	512	CLA	C3D-C4D	-2.18	1.39	1.44
24	d	404	CLA	C1D-C2D	2.18	1.49	1.45
24	c	506	CLA	C1C-NC	-2.18	1.34	1.37
24	B	608	CLA	C1C-C2C	2.18	1.48	1.44
24	B	610	CLA	C4C-C3C	2.17	1.48	1.45
24	b	617	CLA	C3B-C2B	2.17	1.48	1.41
24	D	402	CLA	C3B-C4B	2.17	1.47	1.42
24	C	513	CLA	C4B-NB	-2.17	1.35	1.37
40	v	205	HEC	C4A-C3A	-2.17	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C4C-C3C	2.17	1.48	1.45
24	d	403	CLA	C3B-C2B	2.16	1.48	1.41
24	B	609	CLA	C3B-C2B	2.16	1.48	1.41
24	b	619	CLA	C1C-C2C	2.16	1.48	1.44
24	B	617	CLA	C1C-C2C	2.16	1.48	1.44
24	B	612	CLA	C3B-C2B	2.16	1.48	1.41
24	C	502	CLA	C3D-C4D	-2.16	1.39	1.44
25	A	408	PHO	C3A-C2A	-2.15	1.52	1.54
31	d	406	PL9	C2-C3	2.15	1.40	1.34
24	A	409	CLA	C3B-C2B	2.15	1.48	1.41
24	C	504	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	605	CLA	C4C-C3C	2.15	1.48	1.45
36	h	102	DGD	O5D-C1E	2.15	1.43	1.40
24	B	605	CLA	C1A-CHA	2.15	1.52	1.43
24	b	611	CLA	C3D-C4D	-2.14	1.39	1.44
24	b	623	CLA	C1C-C2C	2.14	1.48	1.44
24	C	506	CLA	C3B-C2B	2.14	1.48	1.41
24	C	508	CLA	C3B-C2B	2.14	1.48	1.41
24	b	615	CLA	C3B-C2B	2.14	1.48	1.41
24	d	404	CLA	C3D-C4D	-2.14	1.39	1.44
24	D	403	CLA	C1C-NC	-2.14	1.34	1.37
24	d	402	CLA	C3B-C4B	2.13	1.47	1.42
31	a	416	PL9	C2-C3	2.13	1.40	1.34
24	D	403	CLA	C3B-C2B	2.13	1.48	1.41
24	b	616	CLA	C4B-NB	-2.13	1.35	1.37
24	a	410	CLA	C4C-C3C	2.12	1.48	1.45
29	B	635	LMT	O1'-C1'	2.12	1.43	1.40
24	B	607	CLA	C3B-C2B	2.12	1.48	1.41
24	b	618	CLA	C1C-C2C	2.12	1.48	1.44
24	b	612	CLA	C4C-C3C	2.12	1.48	1.45
24	c	510	CLA	C4C-C3C	2.12	1.48	1.45
24	b	619	CLA	C3D-C4D	-2.12	1.39	1.44
24	B	616	CLA	C3D-C4D	-2.12	1.39	1.44
24	c	506	CLA	C4C-C3C	2.11	1.48	1.45
24	c	505	CLA	C3D-C4D	-2.11	1.39	1.44
24	c	509	CLA	C3B-C2B	2.11	1.48	1.41
24	c	516	CLA	C3B-C2B	2.11	1.48	1.41
25	a	411	PHO	CBD-CGD	-2.11	1.49	1.52
24	B	612	CLA	C3D-C4D	-2.11	1.39	1.44
24	b	621	CLA	C1A-CHA	2.11	1.51	1.43
24	B	608	CLA	C3D-C4D	-2.10	1.39	1.44
25	d	401	PHO	C1B-NB	-2.10	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C3B-C2B	2.10	1.48	1.41
29	M	104	LMT	O1'-C1'	2.10	1.43	1.40
24	C	505	CLA	C4C-C3C	2.09	1.48	1.45
24	c	511	CLA	C3D-C4D	-2.09	1.39	1.44
24	A	406	CLA	C4C-C3C	2.09	1.48	1.45
24	B	602	CLA	C3B-C2B	2.09	1.48	1.41
29	a	404	LMT	O1'-C1'	2.09	1.43	1.40
24	C	513	CLA	C3D-C4D	-2.09	1.39	1.44
24	c	506	CLA	C3B-C2B	2.09	1.48	1.41
31	A	418	PL9	C2-C3	2.08	1.40	1.34
24	c	514	CLA	C3D-C4D	-2.08	1.39	1.44
24	B	608	CLA	C3B-C2B	2.08	1.48	1.41
24	c	512	CLA	C4C-C3C	2.08	1.48	1.45
40	v	205	HEC	C4D-ND	-2.07	1.34	1.38
24	c	505	CLA	C1C-C2C	2.06	1.48	1.44
24	B	602	CLA	C1D-C2D	2.06	1.49	1.45
24	B	617	CLA	C4C-C3C	2.05	1.48	1.45
40	v	205	HEC	C4B-C3B	2.05	1.48	1.45
24	b	610	CLA	C4C-C3C	2.05	1.48	1.45
24	c	511	CLA	C3B-C4B	2.05	1.47	1.42
24	d	402	CLA	C3D-C4D	-2.05	1.39	1.44
34	B	625	HTG	C1-S1	-2.04	1.77	1.80
24	b	615	CLA	C4C-C3C	2.04	1.48	1.45
24	b	611	CLA	C3B-C2B	2.04	1.48	1.41
37	d	407	LHG	O7-C5	-2.04	1.41	1.46
24	b	625	CLA	C3D-C4D	-2.04	1.39	1.44
24	b	625	CLA	C4C-C3C	2.04	1.48	1.45
25	a	411	PHO	C3A-C2A	-2.04	1.52	1.54
24	d	402	CLA	C1C-NC	-2.03	1.34	1.37
24	B	606	CLA	C3D-C4D	-2.03	1.39	1.44
24	b	624	CLA	C3B-C2B	2.03	1.48	1.41
24	C	503	CLA	C3D-C4D	-2.03	1.39	1.44
24	b	624	CLA	C4C-C3C	2.03	1.48	1.45
24	b	621	CLA	C4C-C3C	2.03	1.48	1.45
24	b	619	CLA	C1D-C2D	2.03	1.49	1.45
24	B	602	CLA	C4C-C3C	2.03	1.48	1.45
24	a	410	CLA	C3B-C2B	2.03	1.48	1.41
24	c	512	CLA	C1C-C2C	2.02	1.48	1.44
24	a	412	CLA	C4C-C3C	2.02	1.48	1.45
24	c	516	CLA	C3D-C4D	-2.02	1.39	1.44
38	e	103	HEM	C1D-ND	-2.02	1.34	1.38
24	c	517	CLA	C3B-C2B	2.01	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C4C-C3C	2.01	1.48	1.45
24	B	614	CLA	C3B-C4B	2.01	1.47	1.42
34	C	524	HTG	C1-S1	-2.01	1.77	1.80
24	B	603	CLA	C1D-C2D	2.01	1.49	1.45
24	C	507	CLA	C3B-C2B	2.00	1.48	1.41
24	b	613	CLA	C3D-C4D	-2.00	1.39	1.44
24	B	604	CLA	C3B-C2B	2.00	1.48	1.41

All (2777) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	PHO	C2D-C1D-ND	11.95	117.78	109.53
25	d	401	PHO	C2D-C1D-ND	11.26	117.30	109.53
25	a	411	PHO	C2D-C1D-ND	10.82	117.00	109.53
24	a	410	CLA	C1D-ND-C4D	-10.50	98.87	106.33
24	B	606	CLA	C1D-ND-C4D	-10.46	98.90	106.33
25	D	401	PHO	C2D-C1D-ND	10.37	116.69	109.53
24	b	614	CLA	C1D-ND-C4D	-10.09	99.17	106.33
24	B	613	CLA	C1D-ND-C4D	-10.05	99.20	106.33
24	B	616	CLA	C1D-ND-C4D	-10.01	99.23	106.33
24	A	407	CLA	C1D-ND-C4D	-9.89	99.31	106.33
24	b	624	CLA	C1D-ND-C4D	-9.88	99.31	106.33
24	B	602	CLA	C1D-ND-C4D	-9.85	99.34	106.33
24	C	502	CLA	C1D-ND-C4D	-9.59	99.52	106.33
24	C	504	CLA	C1D-ND-C4D	-9.58	99.53	106.33
24	c	515	CLA	C1D-ND-C4D	-9.57	99.54	106.33
24	d	404	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	c	517	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	D	402	CLA	C1D-ND-C4D	-9.48	99.60	106.33
24	b	618	CLA	C1D-ND-C4D	-9.43	99.63	106.33
24	c	516	CLA	C1D-ND-C4D	-9.42	99.64	106.33
24	A	409	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	B	607	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	b	620	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	B	603	CLA	C1D-ND-C4D	-9.35	99.69	106.33
24	b	619	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	C	512	CLA	C1D-ND-C4D	-9.30	99.73	106.33
24	C	514	CLA	C1D-ND-C4D	-9.28	99.74	106.33
24	B	613	CLA	C2D-C1D-ND	9.28	116.94	110.10
24	a	409	CLA	C1D-ND-C4D	-9.26	99.76	106.33
24	a	412	CLA	C1D-ND-C4D	-9.25	99.77	106.33
24	C	513	CLA	C1D-ND-C4D	-9.23	99.78	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	623	CLA	C1D-ND-C4D	-9.21	99.80	106.33
24	c	507	CLA	C1D-ND-C4D	-9.18	99.81	106.33
24	c	508	CLA	C1D-ND-C4D	-9.18	99.81	106.33
24	B	615	CLA	C1D-ND-C4D	-9.16	99.83	106.33
24	B	606	CLA	C2D-C1D-ND	9.15	116.84	110.10
24	D	403	CLA	C1D-ND-C4D	-9.14	99.84	106.33
24	C	509	CLA	C1D-ND-C4D	-9.14	99.84	106.33
24	b	621	CLA	C1D-ND-C4D	-9.11	99.86	106.33
24	d	403	CLA	C1D-ND-C4D	-9.11	99.86	106.33
24	c	510	CLA	C1D-ND-C4D	-9.06	99.90	106.33
24	C	503	CLA	C1D-ND-C4D	-9.03	99.92	106.33
24	a	410	CLA	C2D-C1D-ND	9.02	116.75	110.10
24	B	612	CLA	C1D-ND-C4D	-9.00	99.94	106.33
24	A	406	CLA	C1D-ND-C4D	-8.94	99.98	106.33
24	b	624	CLA	C2D-C1D-ND	8.93	116.69	110.10
24	c	505	CLA	C1D-ND-C4D	-8.93	99.99	106.33
24	b	610	CLA	C1D-ND-C4D	-8.93	99.99	106.33
24	c	512	CLA	C1D-ND-C4D	-8.93	99.99	106.33
24	b	612	CLA	C1D-ND-C4D	-8.85	100.05	106.33
24	d	402	CLA	C1D-ND-C4D	-8.83	100.06	106.33
24	c	514	CLA	C1D-ND-C4D	-8.82	100.07	106.33
24	B	617	CLA	C1D-ND-C4D	-8.80	100.09	106.33
24	B	610	CLA	C1D-ND-C4D	-8.79	100.09	106.33
24	D	402	CLA	C2D-C1D-ND	8.79	116.58	110.10
24	B	614	CLA	C2D-C1D-ND	8.78	116.57	110.10
24	C	505	CLA	C1D-ND-C4D	-8.78	100.10	106.33
24	B	608	CLA	C1D-ND-C4D	-8.77	100.11	106.33
24	b	625	CLA	C1D-ND-C4D	-8.74	100.13	106.33
24	b	611	CLA	C1D-ND-C4D	-8.73	100.13	106.33
24	C	508	CLA	C1D-ND-C4D	-8.72	100.14	106.33
24	b	616	CLA	C1D-ND-C4D	-8.69	100.16	106.33
24	B	609	CLA	C1D-ND-C4D	-8.69	100.16	106.33
24	B	614	CLA	C1D-ND-C4D	-8.68	100.17	106.33
24	c	513	CLA	C1D-ND-C4D	-8.67	100.18	106.33
24	B	611	CLA	C1D-ND-C4D	-8.66	100.18	106.33
24	C	510	CLA	C1D-ND-C4D	-8.61	100.22	106.33
24	b	621	CLA	C2D-C1D-ND	8.60	116.44	110.10
24	c	516	CLA	C2D-C1D-ND	8.52	116.38	110.10
24	c	516	CLA	C2B-C1B-NB	8.51	115.94	110.23
24	C	511	CLA	C1D-ND-C4D	-8.48	100.31	106.33
24	b	615	CLA	C1D-ND-C4D	-8.48	100.31	106.33
24	d	404	CLA	C2D-C1D-ND	8.47	116.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	623	CLA	C2D-C1D-ND	8.47	116.35	110.10
24	c	506	CLA	C1D-ND-C4D	-8.47	100.32	106.33
24	C	513	CLA	C2D-C1D-ND	8.45	116.33	110.10
24	c	509	CLA	C1D-ND-C4D	-8.44	100.34	106.33
24	C	507	CLA	C1D-ND-C4D	-8.43	100.35	106.33
24	C	506	CLA	C1D-ND-C4D	-8.42	100.35	106.33
24	B	604	CLA	C1D-ND-C4D	-8.42	100.35	106.33
24	B	611	CLA	C2B-C1B-NB	8.39	115.86	110.23
24	c	511	CLA	C1D-ND-C4D	-8.35	100.40	106.33
24	B	616	CLA	C2D-C1D-ND	8.30	116.22	110.10
24	C	509	CLA	C2B-C1B-NB	8.28	115.78	110.23
24	A	406	CLA	C2D-C1D-ND	8.27	116.20	110.10
24	C	508	CLA	C2D-C1D-ND	8.24	116.17	110.10
24	b	614	CLA	C2D-C1D-ND	8.23	116.17	110.10
24	C	503	CLA	C2D-C1D-ND	8.22	116.16	110.10
24	c	505	CLA	C2D-C1D-ND	8.22	116.16	110.10
24	C	505	CLA	C2D-C1D-ND	8.22	116.16	110.10
24	b	617	CLA	C1D-ND-C4D	-8.21	100.50	106.33
24	C	504	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	A	409	CLA	C2D-C1D-ND	8.14	116.10	110.10
24	b	625	CLA	C2D-C1D-ND	8.14	116.10	110.10
24	b	622	CLA	C1D-ND-C4D	-8.14	100.56	106.33
24	c	508	CLA	C2D-C1D-ND	8.13	116.09	110.10
24	C	502	CLA	C2D-C1D-ND	8.11	116.08	110.10
24	C	514	CLA	C2B-C1B-NB	8.09	115.66	110.23
24	B	607	CLA	C2D-C1D-ND	8.07	116.05	110.10
24	b	618	CLA	C2D-C1D-ND	8.06	116.04	110.10
24	C	512	CLA	C2D-C1D-ND	8.05	116.04	110.10
24	b	620	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	C	504	CLA	C2B-C1B-NB	8.03	115.62	110.23
24	a	412	CLA	C2D-C1D-ND	8.02	116.01	110.10
24	B	602	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	c	515	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	C	509	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	A	407	CLA	C2D-C1D-ND	7.99	115.99	110.10
24	A	405	CLA	C1D-ND-C4D	-7.97	100.67	106.33
24	b	622	CLA	C2D-C1D-ND	7.95	115.96	110.10
24	b	610	CLA	C2B-C1B-NB	7.94	115.55	110.23
24	B	615	CLA	C2D-C1D-ND	7.92	115.94	110.10
24	b	619	CLA	C2D-C1D-ND	7.91	115.94	110.10
24	A	407	CLA	C2B-C1B-NB	7.91	115.54	110.23
24	b	611	CLA	C2B-C1B-NB	7.88	115.51	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	402	CLA	C2D-C1D-ND	7.88	115.91	110.10
24	c	510	CLA	C2D-C1D-ND	7.87	115.90	110.10
24	B	617	CLA	C2D-C1D-ND	7.86	115.89	110.10
24	c	517	CLA	C2B-C1B-NB	7.82	115.48	110.23
24	c	506	CLA	C2D-C1D-ND	7.82	115.87	110.10
24	B	610	CLA	C2D-C1D-ND	7.79	115.85	110.10
24	C	514	CLA	C2D-C1D-ND	7.78	115.84	110.10
24	c	511	CLA	C2D-C1D-ND	7.76	115.83	110.10
25	d	401	PHO	O2D-CGD-CBD	7.76	120.82	111.00
24	B	608	CLA	C2D-C1D-ND	7.74	115.81	110.10
24	B	603	CLA	C2D-C1D-ND	7.73	115.80	110.10
24	B	609	CLA	C2D-C1D-ND	7.72	115.79	110.10
24	c	507	CLA	C2B-C1B-NB	7.71	115.40	110.23
24	b	615	CLA	C2B-C1B-NB	7.69	115.39	110.23
24	b	610	CLA	C2D-C1D-ND	7.68	115.76	110.10
24	c	517	CLA	C2D-C1D-ND	7.67	115.76	110.10
24	B	612	CLA	C2D-C1D-ND	7.66	115.75	110.10
24	b	616	CLA	C2D-C1D-ND	7.63	115.73	110.10
24	D	403	CLA	C2D-C1D-ND	7.62	115.72	110.10
24	c	512	CLA	C2D-C1D-ND	7.61	115.71	110.10
24	B	605	CLA	CMD-C2D-C1D	7.60	138.11	124.71
24	b	617	CLA	C2B-C1B-NB	7.60	115.33	110.23
24	B	611	CLA	C2D-C1D-ND	7.59	115.70	110.10
24	c	507	CLA	C2D-C1D-ND	7.58	115.69	110.10
24	b	615	CLA	C2D-C1D-ND	7.57	115.69	110.10
24	B	605	CLA	C1D-ND-C4D	-7.52	100.99	106.33
24	A	409	CLA	C2B-C1B-NB	7.52	115.27	110.23
24	c	506	CLA	C2B-C1B-NB	7.49	115.25	110.23
24	B	605	CLA	C2D-C1D-ND	7.48	115.61	110.10
24	a	409	CLA	C2D-C1D-ND	7.47	115.61	110.10
24	b	613	CLA	C2D-C1D-ND	7.47	115.61	110.10
24	c	513	CLA	C2D-C1D-ND	7.47	115.61	110.10
24	C	513	CLA	C2B-C1B-NB	7.45	115.23	110.23
24	B	607	CLA	C2B-C1B-NB	7.45	115.22	110.23
24	C	510	CLA	C2B-C1B-NB	7.44	115.22	110.23
24	b	612	CLA	C2D-C1D-ND	7.44	115.58	110.10
24	A	406	CLA	C2B-C1B-NB	7.42	115.21	110.23
24	b	611	CLA	C4A-NA-C1A	-7.42	103.37	106.71
24	c	514	CLA	C2D-C1D-ND	7.39	115.55	110.10
25	D	401	PHO	C1C-C2C-C3C	-7.38	102.47	108.61
24	a	409	CLA	C2B-C1B-NB	7.34	115.15	110.23
24	c	515	CLA	C2B-C1B-NB	7.32	115.14	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	412	CLA	C2B-C1B-NB	7.32	115.14	110.23
24	B	603	CLA	C2B-C1B-NB	7.31	115.13	110.23
24	C	507	CLA	C2D-C1D-ND	7.29	115.47	110.10
24	B	602	CLA	C2B-C1B-NB	7.28	115.11	110.23
24	B	616	CLA	C2B-C1B-NB	7.26	115.10	110.23
24	b	614	CLA	CMD-C2D-C1D	7.24	137.47	124.71
24	b	615	CLA	C4A-NA-C1A	-7.24	103.45	106.71
24	d	403	CLA	C2D-C1D-ND	7.22	115.43	110.10
24	b	623	CLA	C2B-C1B-NB	7.22	115.07	110.23
24	C	510	CLA	C2D-C1D-ND	7.22	115.42	110.10
24	B	609	CLA	C2B-C1B-NB	7.20	115.06	110.23
24	b	613	CLA	C1D-ND-C4D	-7.15	101.26	106.33
24	b	616	CLA	CMD-C2D-C1D	7.14	137.30	124.71
24	D	403	CLA	C2B-C1B-NB	7.13	115.01	110.23
24	c	514	CLA	C2B-C1B-NB	7.12	115.01	110.23
24	b	611	CLA	C2D-C1D-ND	7.10	115.33	110.10
24	d	403	CLA	C4A-NA-C1A	-7.05	103.54	106.71
24	B	604	CLA	C2D-C1D-ND	7.02	115.28	110.10
24	A	405	CLA	C2B-C1B-NB	7.02	114.94	110.23
24	b	614	CLA	C2B-C1B-NB	7.02	114.94	110.23
24	B	606	CLA	C2B-C1B-NB	7.02	114.94	110.23
25	d	401	PHO	C4D-ND-C1D	-7.01	101.70	108.83
24	C	511	CLA	C2D-C1D-ND	7.01	115.27	110.10
24	b	619	CLA	CMD-C2D-C1D	7.00	137.04	124.71
25	a	411	PHO	C2B-C1B-NB	6.99	114.35	109.53
24	B	606	CLA	CHD-C4C-C3C	-6.99	114.56	124.84
25	a	411	PHO	O2D-CGD-CBD	6.96	119.81	111.00
24	c	509	CLA	C4A-NA-C1A	-6.95	103.58	106.71
24	C	512	CLA	C2B-C1B-NB	6.94	114.88	110.23
24	C	505	CLA	CMD-C2D-C1D	6.91	136.90	124.71
24	c	505	CLA	C2B-C1B-NB	6.89	114.85	110.23
24	c	513	CLA	C2B-C1B-NB	6.86	114.83	110.23
24	b	612	CLA	C2B-C1B-NB	6.86	114.83	110.23
24	b	614	CLA	CHD-C4C-C3C	-6.84	114.78	124.84
24	B	603	CLA	CMD-C2D-C1D	6.84	136.78	124.71
24	d	404	CLA	CMD-C2D-C1D	6.83	136.75	124.71
24	c	512	CLA	C2B-C1B-NB	6.83	114.81	110.23
24	d	404	CLA	C2B-C1B-NB	6.82	114.80	110.23
24	B	613	CLA	C2B-C1B-NB	6.80	114.79	110.23
24	B	604	CLA	C2B-C1B-NB	6.79	114.79	110.23
24	A	405	CLA	C2D-C1D-ND	6.75	115.08	110.10
25	d	401	PHO	C2B-C1B-NB	6.74	114.18	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	C2D-C1D-ND	6.73	115.07	110.10
24	A	405	CLA	C4A-NA-C1A	-6.73	103.68	106.71
24	a	409	CLA	CMD-C2D-C1D	6.71	136.54	124.71
24	b	613	CLA	C2C-C1C-NC	6.70	116.25	109.97
24	b	619	CLA	C2B-C1B-NB	6.70	114.72	110.23
24	C	508	CLA	C2B-C1B-NB	6.69	114.72	110.23
24	B	612	CLA	C2B-C1B-NB	6.67	114.71	110.23
24	b	614	CLA	CHD-C1D-ND	-6.66	118.33	124.45
24	C	506	CLA	C2D-C1D-ND	6.65	115.00	110.10
24	B	616	CLA	CMD-C2D-C1D	6.64	136.41	124.71
24	B	614	CLA	CMD-C2D-C1D	6.64	136.41	124.71
24	d	403	CLA	CMD-C2D-C1D	6.64	136.41	124.71
24	b	620	CLA	C2B-C1B-NB	6.63	114.68	110.23
24	b	611	CLA	CMD-C2D-C1D	6.63	136.40	124.71
24	b	617	CLA	C4A-NA-C1A	-6.62	103.73	106.71
24	c	508	CLA	CMD-C2D-C1D	6.61	136.37	124.71
24	C	505	CLA	C2B-C1B-NB	6.60	114.66	110.23
24	B	617	CLA	C2B-C1B-NB	6.59	114.65	110.23
24	b	624	CLA	C2B-C1B-NB	6.59	114.65	110.23
24	c	516	CLA	C4A-NA-C1A	-6.59	103.75	106.71
24	c	508	CLA	C2B-C1B-NB	6.58	114.64	110.23
24	b	616	CLA	C2B-C1B-NB	6.58	114.64	110.23
24	C	503	CLA	C2B-C1B-NB	6.57	114.64	110.23
24	B	615	CLA	C2B-C1B-NB	6.57	114.64	110.23
24	A	407	CLA	CHD-C1D-ND	-6.56	118.42	124.45
24	c	511	CLA	O2D-CGD-CBD	6.56	122.93	111.27
24	b	622	CLA	C2B-C1B-NB	6.56	114.63	110.23
24	B	603	CLA	CHD-C1D-ND	-6.55	118.44	124.45
24	b	614	CLA	C4A-NA-C1A	-6.53	103.77	106.71
24	C	502	CLA	C2B-C1B-NB	6.52	114.60	110.23
24	b	621	CLA	CHD-C4C-C3C	-6.51	115.26	124.84
24	B	616	CLA	CHD-C1D-ND	-6.51	118.47	124.45
24	c	509	CLA	C2D-C1D-ND	6.51	114.90	110.10
24	d	404	CLA	CHD-C1D-ND	-6.51	118.47	124.45
25	A	408	PHO	C2B-C1B-NB	6.50	114.02	109.53
24	C	506	CLA	C2B-C1B-NB	6.48	114.58	110.23
24	b	624	CLA	CMD-C2D-C1D	6.48	136.12	124.71
24	B	607	CLA	CMD-C2D-C1D	6.47	136.12	124.71
24	C	511	CLA	CMD-C2D-C1D	6.47	136.11	124.71
24	b	623	CLA	O2D-CGD-CBD	6.46	122.75	111.27
24	c	514	CLA	CMD-C2D-C1D	6.45	136.07	124.71
24	B	615	CLA	CMD-C2D-C1D	6.45	136.07	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	624	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
25	A	408	PHO	C4D-ND-C1D	-6.43	102.28	108.83
24	c	517	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	b	613	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	C	508	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
24	b	611	CLA	CHD-C1D-ND	-6.42	118.55	124.45
24	B	616	CLA	CHD-C4C-C3C	-6.42	115.41	124.84
24	a	410	CLA	C2B-C1B-NB	6.41	114.53	110.23
24	B	613	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	B	602	CLA	CMD-C2D-C1D	6.40	135.99	124.71
34	d	412	HTG	C1'-S1-C1	6.39	112.05	100.09
24	a	410	CLA	CHD-C4C-C3C	-6.39	115.44	124.84
24	d	403	CLA	CHD-C1D-ND	-6.39	118.58	124.45
24	c	517	CLA	C4A-NA-C1A	-6.37	103.84	106.71
24	B	614	CLA	C2C-C1C-NC	6.37	115.94	109.97
24	C	514	CLA	CHD-C1D-ND	-6.37	118.60	124.45
24	B	612	CLA	C4A-NA-C1A	-6.36	103.85	106.71
24	b	620	CLA	CMD-C2D-C1D	6.36	135.92	124.71
24	c	507	CLA	CMD-C2D-C1D	6.36	135.92	124.71
24	C	507	CLA	C2B-C1B-NB	6.36	114.49	110.23
24	B	603	CLA	C4A-NA-C1A	-6.35	103.85	106.71
24	c	509	CLA	C2C-C1C-NC	6.34	115.92	109.97
24	d	403	CLA	C2C-C1C-NC	6.34	115.91	109.97
24	B	616	CLA	C4A-NA-C1A	-6.34	103.86	106.71
24	C	514	CLA	CMD-C2D-C1D	6.33	135.86	124.71
24	b	615	CLA	CMD-C2D-C1D	6.32	135.85	124.71
24	D	402	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
24	c	510	CLA	C2B-C1B-NB	6.32	114.47	110.23
24	b	610	CLA	CMD-C2D-C1D	6.32	135.85	124.71
25	D	401	PHO	C4D-ND-C1D	-6.32	102.40	108.83
24	b	612	CLA	CMD-C2D-C1D	6.31	135.84	124.71
24	C	506	CLA	C4A-NA-C1A	-6.31	103.87	106.71
34	C	523	HTG	C1'-S1-C1	6.30	111.88	100.09
24	C	504	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
24	c	510	CLA	CMD-C2D-C1D	6.29	135.80	124.71
24	C	513	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
24	B	608	CLA	CMD-C2D-C1D	6.29	135.79	124.71
24	D	403	CLA	CMD-C2D-C1D	6.29	135.79	124.71
24	D	402	CLA	C2B-C1B-NB	6.28	114.44	110.23
24	B	607	CLA	C4A-NA-C1A	-6.26	103.89	106.71
24	B	605	CLA	C2C-C1C-NC	6.26	115.83	109.97
24	b	612	CLA	CHD-C4C-C3C	-6.25	115.65	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	CMD-C2D-C1D	6.25	135.72	124.71
24	B	602	CLA	CHD-C1D-ND	-6.24	118.72	124.45
24	b	610	CLA	O2D-CGD-CBD	6.24	122.36	111.27
24	c	511	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
24	C	502	CLA	O2D-CGD-CBD	6.23	122.35	111.27
24	B	612	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
24	b	621	CLA	C2B-C1B-NB	6.23	114.41	110.23
24	B	607	CLA	CHD-C1D-ND	-6.22	118.74	124.45
24	C	505	CLA	CHD-C1D-ND	-6.21	118.75	124.45
24	B	610	CLA	C2B-C1B-NB	6.20	114.39	110.23
24	b	616	CLA	CHD-C1D-ND	-6.20	118.76	124.45
25	a	411	PHO	C4D-ND-C1D	-6.19	102.53	108.83
24	c	517	CLA	CHD-C1D-ND	-6.18	118.77	124.45
24	c	505	CLA	CMD-C2D-C1D	6.18	135.60	124.71
24	b	619	CLA	C4A-NA-C1A	-6.18	103.93	106.71
24	c	516	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
24	C	507	CLA	CMD-C2D-C1D	6.17	135.59	124.71
24	B	610	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
24	c	508	CLA	CHD-C1D-ND	-6.16	118.79	124.45
24	C	503	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
24	B	602	CLA	O2D-CGD-CBD	6.15	122.20	111.27
24	B	617	CLA	O2D-CGD-CBD	6.14	122.18	111.27
24	D	402	CLA	CMD-C2D-C1D	6.14	135.53	124.71
24	c	505	CLA	C2C-C1C-NC	6.14	115.72	109.97
24	b	615	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
24	C	510	CLA	CMD-C2D-C1D	6.14	135.53	124.71
24	d	402	CLA	C2C-C1C-NC	6.13	115.71	109.97
25	A	408	PHO	O2D-CGD-CBD	6.12	118.75	111.00
24	b	622	CLA	C2C-C1C-NC	6.12	115.70	109.97
24	b	613	CLA	O2D-CGD-CBD	6.11	122.13	111.27
24	B	617	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
24	a	412	CLA	CMD-C2D-C1D	6.10	135.47	124.71
24	c	513	CLA	CMD-C2D-C1D	6.10	135.47	124.71
24	b	616	CLA	C2C-C1C-NC	6.10	115.68	109.97
24	B	611	CLA	CMD-C2D-C1D	6.09	135.45	124.71
24	C	509	CLA	CMD-C2D-C1D	6.09	135.44	124.71
24	d	402	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
24	B	603	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
24	C	512	CLA	C2C-C1C-NC	6.06	115.65	109.97
24	B	610	CLA	CMD-C2D-C1D	6.06	135.40	124.71
24	C	509	CLA	CHD-C1D-ND	-6.06	118.89	124.45
24	A	406	CLA	C2C-C1C-NC	6.06	115.65	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	512	CLA	CMD-C2D-C1D	6.05	135.37	124.71
24	b	610	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
24	b	618	CLA	CMD-C2D-C1D	6.04	135.35	124.71
24	b	616	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
24	C	508	CLA	CMD-C2D-C1D	6.04	135.35	124.71
24	D	402	CLA	CHD-C1D-ND	-6.03	118.91	124.45
24	b	623	CLA	CHD-C1D-ND	-6.03	118.91	124.45
24	b	612	CLA	C4A-NA-C1A	-6.02	104.00	106.71
24	B	606	CLA	CMD-C2D-C1D	6.01	135.31	124.71
24	c	513	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
24	C	511	CLA	C2B-C1B-NB	6.00	114.26	110.23
24	A	406	CLA	CMD-C2D-C1D	6.00	135.29	124.71
24	B	605	CLA	C2B-C1B-NB	6.00	114.25	110.23
24	B	609	CLA	C2C-C1C-NC	6.00	115.59	109.97
24	b	624	CLA	CHD-C1D-ND	-6.00	118.94	124.45
24	C	502	CLA	CMD-C2D-C1D	5.99	135.27	124.71
24	A	407	CLA	CMD-C2D-C1D	5.99	135.27	124.71
24	a	409	CLA	CHD-C1D-ND	-5.98	118.95	124.45
24	b	625	CLA	O2D-CGD-CBD	5.98	121.89	111.27
25	A	408	PHO	C1C-C2C-C3C	-5.97	103.64	108.61
24	c	507	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
24	b	610	CLA	CHD-C1D-ND	-5.96	118.97	124.45
24	b	613	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
24	B	602	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
24	C	511	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
24	a	412	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
24	A	409	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
24	b	617	CLA	CMD-C2D-C1D	5.93	135.17	124.71
24	d	402	CLA	C2B-C1B-NB	5.93	114.21	110.23
24	B	608	CLA	CHD-C1D-ND	-5.93	119.01	124.45
24	b	618	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
24	d	404	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
24	C	506	CLA	CMD-C2D-C1D	5.92	135.16	124.71
24	b	618	CLA	CHD-C1D-ND	-5.92	119.02	124.45
24	c	507	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	B	611	CLA	CHD-C1D-ND	-5.91	119.02	124.45
24	B	610	CLA	CHD-C1D-ND	-5.91	119.03	124.45
25	a	411	PHO	C1C-C2C-C3C	-5.90	103.70	108.61
24	b	618	CLA	C2B-C1B-NB	5.90	114.19	110.23
25	D	401	PHO	C2B-C1B-NB	5.90	113.60	109.53
24	c	516	CLA	CHD-C1D-ND	-5.90	119.03	124.45
24	c	510	CLA	CHD-C1D-ND	-5.90	119.03	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	c	511	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	C	504	CLA	CHD-C1D-ND	-5.90	119.04	124.45
24	b	623	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	b	619	CLA	CHD-C1D-ND	-5.88	119.05	124.45
24	C	513	CLA	O2D-CGD-CBD	5.87	121.70	111.27
24	C	507	CLA	CHD-C1D-ND	-5.87	119.06	124.45
24	c	509	CLA	C2B-C1B-NB	5.87	114.16	110.23
24	d	402	CLA	CMD-C2D-C1D	5.86	135.05	124.71
24	c	505	CLA	CHD-C1D-ND	-5.86	119.07	124.45
24	B	604	CLA	O2D-CGD-CBD	5.86	121.68	111.27
24	D	402	CLA	C2C-C1C-NC	5.86	115.46	109.97
24	C	504	CLA	CMD-C2D-C1D	5.85	135.03	124.71
24	B	604	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
24	B	617	CLA	CMD-C2D-C1D	5.85	135.02	124.71
24	c	510	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
24	b	623	CLA	CHD-C4C-C3C	-5.83	116.26	124.84
24	c	510	CLA	C2C-C1C-NC	5.83	115.43	109.97
24	c	511	CLA	CMD-C2D-C1D	5.83	134.98	124.71
24	A	406	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	B	614	CLA	CHD-C4C-C3C	-5.81	116.29	124.84
24	B	617	CLA	C4A-NA-C1A	-5.81	104.09	106.71
24	c	516	CLA	O2D-CGD-CBD	5.81	121.58	111.27
24	b	625	CLA	CMD-C2D-C1D	5.80	134.94	124.71
24	B	605	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
24	A	407	CLA	C4A-NA-C1A	-5.80	104.10	106.71
24	c	516	CLA	CMD-C2D-C1D	5.80	134.93	124.71
24	c	515	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
24	C	506	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
24	B	611	CLA	C2C-C1C-NC	5.78	115.39	109.97
24	B	615	CLA	CHD-C1D-ND	-5.78	119.14	124.45
34	D	412	HTG	C1'-S1-C1	5.77	110.89	100.09
24	a	412	CLA	CHD-C1D-ND	-5.77	119.15	124.45
24	B	615	CLA	CHD-C4C-C3C	-5.77	116.37	124.84
24	D	403	CLA	CHD-C1D-ND	-5.76	119.16	124.45
24	c	509	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
24	c	512	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	c	511	CLA	C2B-C1B-NB	5.75	114.08	110.23
24	a	409	CLA	C4A-NA-C1A	-5.74	104.12	106.71
24	C	512	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
24	B	609	CLA	CMD-C2D-C1D	5.74	134.82	124.71
24	c	514	CLA	C2C-C1C-NC	5.73	115.34	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C2C-C1C-NC	5.72	115.33	109.97
25	D	401	PHO	O2D-CGD-CBD	5.72	118.24	111.00
24	b	620	CLA	C2C-C1C-NC	5.72	115.33	109.97
24	b	622	CLA	CMD-C2D-C1D	5.70	134.76	124.71
24	c	517	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
24	b	625	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
24	C	502	CLA	CHD-C1D-ND	-5.69	119.22	124.45
24	c	509	CLA	O2D-CGD-CBD	5.69	121.38	111.27
24	b	620	CLA	CHD-C1D-ND	-5.68	119.23	124.45
34	c	524	HTG	C1'-S1-C1	5.68	110.72	100.09
24	b	613	CLA	C2B-C1B-NB	5.68	114.04	110.23
24	B	614	CLA	C2B-C1B-NB	5.68	114.04	110.23
24	B	607	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
24	c	512	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
24	B	615	CLA	O2D-CGD-CBD	5.66	121.33	111.27
24	C	502	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
24	d	403	CLA	C2B-C1B-NB	5.66	114.03	110.23
24	C	506	CLA	C2C-C1C-NC	5.65	115.27	109.97
24	c	508	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
24	A	407	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
24	c	514	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
24	B	613	CLA	CHD-C1D-ND	-5.65	119.27	124.45
24	b	617	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
24	b	625	CLA	CHD-C1D-ND	-5.64	119.27	124.45
24	B	607	CLA	C2C-C1C-NC	5.64	115.25	109.97
24	b	619	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
24	b	618	CLA	C2C-C1C-NC	5.62	115.24	109.97
24	b	621	CLA	C2C-C1C-NC	5.61	115.23	109.97
24	c	515	CLA	CHD-C1D-ND	-5.61	119.30	124.45
34	B	633	HTG	C1'-S1-C1	5.61	110.59	100.09
24	B	613	CLA	O2D-CGD-CBD	5.61	121.23	111.27
24	C	503	CLA	CMD-C2D-C1D	5.60	134.59	124.71
24	c	506	CLA	C4A-NA-C1A	-5.60	104.19	106.71
24	a	410	CLA	CMD-C2D-C1D	5.60	134.58	124.71
24	C	512	CLA	CHD-C1D-ND	-5.60	119.31	124.45
24	a	409	CLA	C2C-C1C-NC	5.60	115.21	109.97
24	B	604	CLA	C4A-NA-C1A	-5.59	104.19	106.71
24	c	506	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
24	B	609	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
24	b	612	CLA	O2D-CGD-CBD	5.58	121.19	111.27
24	B	608	CLA	C2B-C1B-NB	5.58	113.97	110.23
24	c	514	CLA	CHD-C1D-ND	-5.58	119.33	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
24	a	410	CLA	CHD-C1D-ND	-5.56	119.34	124.45
24	b	615	CLA	C2C-C1C-NC	5.56	115.19	109.97
24	a	412	CLA	C2C-C1C-NC	5.56	115.18	109.97
24	A	406	CLA	CHD-C1D-ND	-5.56	119.34	124.45
24	c	506	CLA	CHD-C1D-ND	-5.56	119.34	124.45
38	E	102	HEM	CHC-C4B-NB	5.56	130.46	124.42
24	D	403	CLA	C2C-C1C-NC	5.56	115.18	109.97
24	C	507	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
24	C	514	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
24	b	620	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
24	B	606	CLA	CHD-C1D-ND	-5.52	119.38	124.45
24	b	615	CLA	CHD-C1D-ND	-5.52	119.38	124.45
24	c	513	CLA	C2C-C1C-NC	5.52	115.14	109.97
24	C	505	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
27	f	102	SQD	O47-C7-C8	5.51	123.37	111.50
24	c	509	CLA	CMD-C2D-C1D	5.50	134.40	124.71
24	D	402	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	A	405	CLA	C2C-C1C-NC	5.50	115.12	109.97
24	A	409	CLA	CMD-C2D-C1D	5.50	134.40	124.71
24	C	509	CLA	O2D-CGD-CBD	5.50	121.03	111.27
24	C	513	CLA	CMD-C2D-C1D	5.49	134.38	124.71
24	c	508	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	C	510	CLA	C2C-C1C-NC	5.48	115.10	109.97
24	C	504	CLA	C4A-NA-C1A	-5.47	104.25	106.71
24	A	407	CLA	O2D-CGD-CBD	5.46	120.98	111.27
24	B	615	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	C	510	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
24	B	604	CLA	C2C-C1C-NC	5.45	115.08	109.97
24	C	507	CLA	C2C-C1C-NC	5.45	115.08	109.97
24	B	609	CLA	CHD-C1D-ND	-5.45	119.45	124.45
24	c	512	CLA	CHD-C1D-ND	-5.44	119.46	124.45
24	b	610	CLA	C4A-NA-C1A	-5.43	104.27	106.71
24	C	508	CLA	CHD-C1D-ND	-5.42	119.47	124.45
24	B	615	CLA	C2C-C1C-NC	5.42	115.05	109.97
24	c	505	CLA	O2D-CGD-CBD	5.41	120.88	111.27
24	c	512	CLA	CMD-C2D-C1D	5.41	134.25	124.71
25	d	401	PHO	C1C-C2C-C3C	-5.40	104.12	108.61
24	C	509	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	d	404	CLA	C4A-NA-C1A	-5.40	104.28	106.71
24	b	625	CLA	C2B-C1B-NB	5.40	113.85	110.23
24	C	513	CLA	CHD-C1D-ND	-5.39	119.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	CHD-C1D-ND	-5.39	119.50	124.45
34	B	625	HTG	C1'-S1-C1	5.38	110.16	100.09
25	D	401	PHO	C3D-C4D-ND	5.37	115.04	107.72
27	L	102	SQD	O6-C1-C2	5.37	116.69	108.30
24	b	612	CLA	C2C-C1C-NC	5.36	115.00	109.97
24	c	511	CLA	CHD-C1D-ND	-5.35	119.54	124.45
24	C	511	CLA	C2C-C1C-NC	5.35	114.98	109.97
24	a	409	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
24	B	610	CLA	C4A-NA-C1A	-5.33	104.31	106.71
24	d	402	CLA	CHD-C1D-ND	-5.33	119.55	124.45
24	b	624	CLA	C2C-C1C-NC	5.33	114.97	109.97
24	C	508	CLA	O2D-CGD-CBD	5.32	120.72	111.27
24	b	625	CLA	C2C-C1C-NC	5.31	114.95	109.97
24	D	403	CLA	C4A-NA-C1A	-5.30	104.32	106.71
24	B	604	CLA	CMD-C2D-C1D	5.30	134.05	124.71
24	C	507	CLA	C4A-NA-C1A	-5.29	104.33	106.71
24	c	515	CLA	C2C-C1C-NC	5.29	114.92	109.97
34	c	525	HTG	C1'-S1-C1	5.28	109.97	100.09
24	C	509	CLA	C4A-NA-C1A	-5.28	104.33	106.71
24	C	510	CLA	CHD-C1D-ND	-5.28	119.60	124.45
24	B	611	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
24	B	603	CLA	C2C-C1C-NC	5.26	114.90	109.97
24	B	612	CLA	CHD-C1D-ND	-5.26	119.62	124.45
27	B	621	SQD	O6-C1-C2	5.26	116.51	108.30
24	b	615	CLA	O2D-CGD-CBD	5.26	120.61	111.27
24	B	613	CLA	CMD-C2D-C1D	5.25	133.97	124.71
24	c	506	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	B	607	CLA	O2D-CGD-CBD	5.25	120.60	111.27
24	B	614	CLA	C3D-C2D-C1D	-5.24	98.67	105.83
24	B	605	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	b	617	CLA	C2C-C1C-NC	5.23	114.88	109.97
24	b	614	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	b	612	CLA	CHD-C1D-ND	-5.23	119.65	124.45
24	C	511	CLA	CHD-C1D-ND	-5.22	119.65	124.45
24	D	403	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
27	a	414	SQD	O6-C1-C2	5.21	116.44	108.30
24	b	620	CLA	C4A-NA-C1A	-5.21	104.36	106.71
24	c	505	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
24	B	608	CLA	C4A-NA-C1A	-5.20	104.37	106.71
34	C	524	HTG	C1'-S1-C1	5.20	109.82	100.09
24	b	611	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
24	b	623	CLA	C2C-C1C-NC	5.19	114.83	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CMD-C2D-C1D	5.18	133.85	124.71
24	c	508	CLA	O2D-CGD-CBD	5.18	120.47	111.27
24	B	611	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
24	C	505	CLA	C2C-C1C-NC	5.17	114.82	109.97
24	B	614	CLA	CHD-C1D-ND	-5.17	119.70	124.45
24	C	506	CLA	O2D-CGD-CBD	5.17	120.45	111.27
24	a	410	CLA	C2C-C1C-NC	5.16	114.80	109.97
24	C	514	CLA	C2C-C1C-NC	5.15	114.80	109.97
24	b	625	CLA	C4A-NA-C1A	-5.14	104.39	106.71
24	A	406	CLA	O2D-CGD-CBD	5.13	120.39	111.27
24	c	515	CLA	CMD-C2D-C1D	5.13	133.75	124.71
24	C	505	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
24	C	502	CLA	C2C-C1C-NC	5.12	114.77	109.97
26	Y	101	BCR	C33-C5-C6	-5.12	118.78	124.53
24	C	503	CLA	CHD-C1D-ND	-5.12	119.75	124.45
24	b	622	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
24	A	409	CLA	C2C-C1C-NC	5.12	114.76	109.97
24	A	406	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
24	b	611	CLA	C2C-C1C-NC	5.10	114.75	109.97
24	d	404	CLA	C2C-C1C-NC	5.10	114.75	109.97
24	b	611	CLA	O2D-CGD-CBD	5.09	120.32	111.27
24	A	409	CLA	CHD-C1D-ND	-5.08	119.78	124.45
24	d	404	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
24	c	512	CLA	C4A-NA-C1A	-5.08	104.42	106.71
24	C	513	CLA	C2C-C1C-NC	5.07	114.72	109.97
24	B	610	CLA	C2C-C1C-NC	5.06	114.71	109.97
24	c	506	CLA	C3B-C2B-C1B	-5.06	101.06	107.16
24	c	516	CLA	C3B-C2B-C1B	-5.06	101.06	107.16
34	B	625	HTG	O5-C1-C2	5.05	116.67	110.31
25	A	408	PHO	C1-C2-C3	-5.05	117.31	126.04
24	B	602	CLA	C2C-C1C-NC	5.04	114.70	109.97
25	d	401	PHO	C1-C2-C3	-5.04	117.32	126.04
24	B	608	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
24	C	511	CLA	O2D-CGD-CBD	5.01	120.18	111.27
24	c	512	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	b	621	CLA	C3C-C4C-NC	5.01	116.19	110.57
24	c	508	CLA	C4A-NA-C1A	-5.01	104.45	106.71
27	F	103	SQD	O47-C7-C8	5.01	122.29	111.50
24	A	407	CLA	C3D-C4D-ND	5.00	118.33	110.24
24	C	514	CLA	C4A-NA-C1A	-5.00	104.46	106.71
34	b	632	HTG	C1'-S1-C1	5.00	109.44	100.09
24	C	505	CLA	O2D-CGD-CBD	4.99	120.14	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	509	CLA	C3C-C4C-NC	4.99	116.17	110.57
24	B	605	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
24	c	513	CLA	O2D-CGD-CBD	4.98	120.11	111.27
24	c	506	CLA	CMD-C2D-C1D	4.98	133.49	124.71
25	d	401	PHO	C3D-C4D-ND	4.98	114.50	107.72
24	b	623	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
27	A	411	SQD	O47-C7-C8	4.97	122.21	111.50
26	t	101	BCR	C33-C5-C6	-4.96	118.96	124.53
38	E	102	HEM	CAD-CBD-CGD	4.96	124.28	113.60
24	b	622	CLA	C4A-NA-C1A	-4.96	104.48	106.71
24	B	605	CLA	CHD-C1D-ND	-4.95	119.90	124.45
24	b	622	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
24	C	513	CLA	C4A-NA-C1A	-4.95	104.48	106.71
24	c	513	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
24	A	405	CLA	CHD-C4C-C3C	-4.95	117.57	124.84
24	B	609	CLA	O2D-CGD-CBD	4.95	120.06	111.27
24	B	613	CLA	C3C-C4C-NC	4.94	116.11	110.57
24	b	617	CLA	CHD-C1D-ND	-4.94	119.92	124.45
24	b	624	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
24	c	513	CLA	C4A-NA-C1A	-4.93	104.49	106.71
24	D	402	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
24	B	616	CLA	C2C-C1C-NC	4.93	114.59	109.97
34	B	624	HTG	C1'-S1-C1	4.93	109.31	100.09
24	C	509	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
24	c	511	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
24	b	623	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
24	C	504	CLA	C2C-C1C-NC	4.92	114.58	109.97
24	b	619	CLA	C2C-C1C-NC	4.92	114.58	109.97
24	C	503	CLA	C4A-NA-C1A	-4.92	104.50	106.71
24	b	616	CLA	O2D-CGD-CBD	4.92	120.00	111.27
24	A	406	CLA	C4A-NA-C1A	-4.92	104.50	106.71
24	C	510	CLA	C4A-NA-C1A	-4.92	104.50	106.71
24	c	513	CLA	CHD-C1D-ND	-4.91	119.94	124.45
24	C	514	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
24	C	510	CLA	C1-C2-C3	-4.90	117.57	126.04
24	b	611	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
24	C	510	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
24	B	603	CLA	O2D-CGD-CBD	4.87	119.93	111.27
24	a	409	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
24	A	409	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
24	A	406	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
24	A	405	CLA	CHD-C1D-ND	-4.87	119.98	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
24	c	511	CLA	C3C-C4C-NC	4.86	116.02	110.57
24	D	403	CLA	O2D-CGD-CBD	4.86	119.90	111.27
24	b	613	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
24	b	622	CLA	CHD-C1D-ND	-4.84	120.00	124.45
24	C	508	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
24	c	505	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	B	606	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	b	624	CLA	C4A-NA-C1A	-4.83	104.53	106.71
24	B	613	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
24	A	409	CLA	C4A-NA-C1A	-4.83	104.53	106.71
24	c	517	CLA	C2C-C1C-NC	4.83	114.50	109.97
34	C	524	HTG	C1-O5-C5	4.82	121.48	112.58
24	B	617	CLA	C2C-C1C-NC	4.82	114.49	109.97
24	C	512	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
24	B	606	CLA	O2D-CGD-CBD	4.82	119.83	111.27
24	b	621	CLA	O2D-CGD-CBD	4.81	119.82	111.27
24	B	604	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
24	c	508	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
24	A	405	CLA	C3B-C2B-C1B	-4.80	101.37	107.16
24	a	410	CLA	O2D-CGD-CBD	4.80	119.79	111.27
27	B	621	SQD	O47-C7-C8	4.79	121.83	111.50
24	c	517	CLA	C3B-C2B-C1B	-4.79	101.37	107.16
24	c	514	CLA	O2D-CGD-CBD	4.79	119.78	111.27
24	B	607	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
24	B	613	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	C	503	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	b	610	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	C	506	CLA	C3C-C4C-NC	4.78	115.94	110.57
24	C	502	CLA	C4A-NA-C1A	-4.78	104.56	106.71
24	c	507	CLA	C2C-C1C-NC	4.78	114.45	109.97
24	B	604	CLA	CHD-C1D-ND	-4.78	120.06	124.45
24	C	513	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	b	615	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	B	614	CLA	C3C-C4C-NC	4.77	115.92	110.57
24	c	510	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
24	b	614	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
24	b	625	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
24	d	402	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
24	c	505	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
24	C	508	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
24	C	504	CLA	C3B-C2B-C1B	-4.75	101.42	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	410	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	C	509	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	b	616	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	B	615	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	A	407	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
26	B	618	BCR	C33-C5-C6	-4.74	119.20	124.53
24	c	509	CLA	CHD-C1D-ND	-4.74	120.10	124.45
24	a	412	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
24	B	604	CLA	O2D-CGD-O1D	-4.73	114.59	123.84
24	a	410	CLA	C3D-C4D-ND	4.73	117.89	110.24
24	b	617	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
26	b	626	BCR	C33-C5-C6	-4.72	119.23	124.53
24	d	403	CLA	C3D-C4D-ND	4.72	117.87	110.24
24	b	615	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
36	C	517	DGD	O2G-C1B-C2B	4.72	121.67	111.50
24	b	614	CLA	O2D-CGD-CBD	4.72	119.65	111.27
24	B	606	CLA	C3D-C4D-ND	4.71	117.86	110.24
24	D	403	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
24	c	514	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
29	A	416	LMT	C1'-O5'-C5'	4.71	122.93	113.69
26	y	101	BCR	C33-C5-C6	-4.71	119.24	124.53
24	C	503	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	A	407	CLA	C2C-C1C-NC	4.70	114.37	109.97
24	b	619	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	C	503	CLA	O2D-CGD-CBD	4.69	119.61	111.27
24	B	617	CLA	CHD-C1D-ND	-4.69	120.14	124.45
24	b	619	CLA	O2D-CGD-CBD	4.69	119.60	111.27
24	d	402	CLA	O2D-CGD-CBD	4.68	119.59	111.27
24	C	506	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
24	B	609	CLA	C3B-C2B-C1B	-4.68	101.52	107.16
24	A	406	CLA	C1C-C2C-C3C	-4.68	102.04	106.96
24	c	507	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
26	D	404	BCR	C7-C8-C9	-4.67	119.18	126.23
24	b	613	CLA	C4A-NA-C1A	-4.66	104.61	106.71
24	c	515	CLA	C3D-C4D-ND	4.66	117.77	110.24
24	b	614	CLA	C3D-C4D-ND	4.65	117.76	110.24
24	B	602	CLA	C3D-C4D-ND	4.65	117.75	110.24
25	A	408	PHO	C3D-C4D-ND	4.64	114.05	107.72
34	b	632	HTG	O5-C1-C2	4.64	116.15	110.31
24	C	513	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
24	B	607	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	b	618	CLA	C4A-NA-C1A	-4.64	104.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	516	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	616	CLA	C1C-C2C-C3C	-4.63	102.09	106.96
24	b	618	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	610	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
24	b	614	CLA	C3C-C4C-NC	4.62	115.76	110.57
24	b	612	CLA	C3C-C4C-NC	4.62	115.75	110.57
27	L	102	SQD	O47-C7-C8	4.62	121.46	111.50
24	d	403	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
24	b	623	CLA	C4A-NA-C1A	-4.62	104.63	106.71
24	B	606	CLA	C3C-C4C-NC	4.62	115.75	110.57
24	B	615	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
24	b	613	CLA	CHD-C1D-ND	-4.61	120.22	124.45
24	B	611	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	a	412	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	b	619	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
25	a	411	PHO	C3D-C4D-ND	4.59	113.98	107.72
24	C	505	CLA	C4A-NA-C1A	-4.59	104.64	106.71
24	D	402	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
24	B	617	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
24	C	507	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
24	B	616	CLA	C3D-C4D-ND	4.59	117.66	110.24
24	c	507	CLA	C3C-C4C-NC	4.59	115.71	110.57
24	C	502	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
36	e	101	DGD	O2G-C1B-C2B	4.58	121.38	111.50
24	B	613	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
24	d	402	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
24	D	402	CLA	C3C-C4C-NC	4.58	115.70	110.57
24	B	616	CLA	C3B-C2B-C1B	-4.58	101.64	107.16
24	B	614	CLA	C4A-NA-C1A	-4.58	104.65	106.71
24	B	610	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	c	506	CLA	O2D-CGD-CBD	4.57	119.39	111.27
24	b	618	CLA	C3D-C4D-ND	4.57	117.63	110.24
24	B	617	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
26	B	620	BCR	C15-C14-C13	-4.56	120.80	127.31
24	b	613	CLA	C3C-C4C-NC	4.56	115.69	110.57
24	B	606	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
24	c	511	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	B	616	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	D	403	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
24	B	608	CLA	O2D-CGD-CBD	4.55	119.35	111.27
24	C	510	CLA	O2D-CGD-CBD	4.55	119.35	111.27
24	b	612	CLA	C3B-C2B-C1B	-4.55	101.67	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
24	c	517	CLA	C3D-C4D-ND	4.54	117.59	110.24
35	C	521	LMG	O7-C10-C11	4.54	121.29	111.50
24	B	603	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
24	A	409	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	A	409	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
24	c	508	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
24	C	504	CLA	C3C-C4C-NC	4.53	115.66	110.57
24	b	621	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
24	B	606	CLA	CMB-C2B-C1B	4.53	132.27	125.37
24	b	613	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
24	c	511	CLA	C4A-NA-C1A	-4.53	104.67	106.71
24	b	621	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	611	CLA	O2D-CGD-CBD	4.53	119.32	111.27
35	C	501	LMG	O7-C10-C11	4.53	121.26	111.50
24	B	602	CLA	C3B-C2B-C1B	-4.53	101.70	107.16
24	a	412	CLA	O2D-CGD-CBD	4.52	119.31	111.27
24	C	508	CLA	C4A-NA-C1A	-4.52	104.67	106.71
24	c	506	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
40	V	205	HEC	C4B-NB-C1B	4.52	109.74	105.07
24	C	504	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
24	b	621	CLA	CMD-C2D-C1D	4.51	132.65	124.71
24	C	508	CLA	C3C-C4C-NC	4.50	115.62	110.57
24	d	404	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
24	C	512	CLA	C3B-C4B-NB	4.50	114.69	110.52
24	d	402	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
35	a	415	LMG	O7-C10-C11	4.50	121.19	111.50
24	B	612	CLA	C3C-C4C-NC	4.49	115.61	110.57
24	B	613	CLA	C3D-C4D-ND	4.49	117.51	110.24
24	B	603	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
38	e	103	HEM	CHC-C4B-NB	4.49	129.30	124.42
24	c	507	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
35	c	523	LMG	O7-C10-C11	4.48	121.16	111.50
24	C	508	CLA	C2C-C1C-NC	4.48	114.17	109.97
24	C	511	CLA	C1-C2-C3	-4.48	118.30	126.04
24	b	620	CLA	O2D-CGD-CBD	4.48	119.22	111.27
24	C	504	CLA	C3D-C4D-ND	4.47	117.47	110.24
24	c	516	CLA	C2C-C1C-NC	4.47	114.16	109.97
34	b	631	HTG	C1'-S1-C1	4.47	108.44	100.09
24	c	513	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
24	d	404	CLA	O2D-CGD-CBD	4.45	119.18	111.27
24	C	511	CLA	C4A-NA-C1A	-4.45	104.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	412	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
24	C	514	CLA	C3D-C4D-ND	4.45	117.44	110.24
24	b	619	CLA	C3D-C4D-ND	4.44	117.43	110.24
24	b	615	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	C	514	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	B	606	CLA	C2C-C1C-NC	4.44	114.13	109.97
24	c	512	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
24	b	610	CLA	C3B-C2B-C1B	-4.44	101.81	107.16
24	B	612	CLA	C3D-C4D-ND	4.44	117.41	110.24
24	a	410	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	C	505	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
24	b	611	CLA	C3D-C4D-ND	4.43	117.41	110.24
24	C	502	CLA	C3D-C4D-ND	4.43	117.41	110.24
24	b	622	CLA	C3B-C4B-NB	4.43	114.62	110.52
34	B	632	HTG	C1'-S1-C1	4.43	108.37	100.09
24	b	612	CLA	CAA-C2A-C3A	-4.42	100.66	112.78
24	B	612	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
24	C	512	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
24	B	611	CLA	C4A-NA-C1A	-4.42	104.72	106.71
24	b	623	CLA	C1-C2-C3	-4.42	118.40	126.04
24	A	409	CLA	C3D-C4D-ND	4.42	117.38	110.24
24	B	615	CLA	C3C-C4C-NC	4.41	115.52	110.57
24	B	603	CLA	C3D-C4D-ND	4.41	117.37	110.24
24	b	620	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
24	C	507	CLA	O2D-CGD-CBD	4.41	119.10	111.27
24	b	616	CLA	C3C-C4C-NC	4.40	115.51	110.57
24	a	412	CLA	C4A-NA-C1A	-4.40	104.73	106.71
24	B	605	CLA	C3C-C4C-NC	4.40	115.50	110.57
24	c	517	CLA	C3D-C2D-C1D	-4.39	99.83	105.83
24	D	403	CLA	C3D-C4D-ND	4.39	117.34	110.24
24	B	614	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
24	b	622	CLA	C3B-C2B-C1B	-4.39	101.87	107.16
24	c	505	CLA	C4A-NA-C1A	-4.38	104.73	106.71
24	b	612	CLA	C1D-CHD-C4C	-4.38	116.60	126.06
24	c	507	CLA	C3D-C4D-ND	4.38	117.33	110.24
34	b	607	HTG	C1'-S1-C1	4.38	108.28	100.09
24	b	620	CLA	C3D-C4D-ND	4.38	117.32	110.24
24	B	602	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
24	c	512	CLA	C3D-C4D-ND	4.37	117.31	110.24
24	C	513	CLA	C3C-C4C-NC	4.36	115.47	110.57
24	c	509	CLA	C3D-C4D-ND	4.36	117.30	110.24
24	C	506	CLA	CHD-C1D-ND	-4.36	120.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	C	503	CLA	C3C-C4C-NC	4.36	115.46	110.57
24	a	409	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	d	404	CLA	C3D-C4D-ND	4.35	117.28	110.24
24	b	621	CLA	C1D-CHD-C4C	-4.35	116.68	126.06
24	b	620	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
24	b	615	CLA	C1D-CHD-C4C	-4.34	116.69	126.06
24	b	624	CLA	C3C-C4C-NC	4.34	115.44	110.57
24	B	609	CLA	C4A-NA-C1A	-4.34	104.76	106.71
36	e	101	DGD	O6E-C5E-C4E	4.33	117.56	109.69
24	c	509	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
24	D	402	CLA	O2D-CGD-CBD	4.33	118.96	111.27
24	b	625	CLA	C3B-C4B-NB	4.32	114.52	110.52
24	c	512	CLA	C3B-C2B-C1B	-4.31	101.95	107.16
24	B	604	CLA	C3C-C4C-NC	4.31	115.41	110.57
24	B	610	CLA	C3D-C4D-ND	4.31	117.21	110.24
24	b	612	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
24	b	624	CLA	C3D-C4D-ND	4.31	117.20	110.24
24	B	609	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
24	B	610	CLA	O2D-CGD-CBD	4.30	118.91	111.27
24	B	606	CLA	C4A-NA-C1A	-4.30	104.77	106.71
24	b	610	CLA	C3D-C4D-ND	4.29	117.18	110.24
27	A	411	SQD	O6-C1-C2	4.29	115.00	108.30
24	C	503	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
24	b	625	CLA	CAC-C3C-C4C	4.29	130.37	124.81
24	c	516	CLA	C3D-C4D-ND	4.28	117.17	110.24
27	L	102	SQD	C3-C4-C5	4.28	117.88	110.24
24	A	407	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
38	E	102	HEM	C1B-NB-C4B	4.28	109.50	105.07
24	B	604	CLA	C3D-C4D-ND	4.28	117.16	110.24
24	b	618	CLA	O2D-CGD-CBD	4.28	118.87	111.27
24	c	514	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	B	612	CLA	O2D-CGD-CBD	4.27	118.86	111.27
24	A	406	CLA	C3B-C4B-NB	4.27	114.48	110.52
24	B	616	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	B	610	CLA	C3C-C4C-NC	4.26	115.35	110.57
26	H	101	BCR	C16-C17-C18	-4.26	121.23	127.31
24	b	611	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	B	605	CLA	C4A-NA-C1A	-4.25	104.80	106.71
24	B	617	CLA	C1D-CHD-C4C	-4.25	116.90	126.06
24	b	623	CLA	O2D-CGD-O1D	-4.25	115.54	123.84
24	B	609	CLA	C3D-C4D-ND	4.25	117.11	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
24	c	514	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
24	c	508	CLA	C3D-C4D-ND	4.24	117.10	110.24
40	v	205	HEC	C4B-NB-C1B	4.24	109.45	105.07
24	b	621	CLA	CHD-C1D-ND	-4.24	120.56	124.45
24	C	510	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
24	a	409	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	C	512	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	B	607	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	B	612	CLA	CMC-C2C-C1C	4.23	131.47	125.04
24	b	614	CLA	C3B-C2B-C1B	-4.22	102.06	107.16
24	c	510	CLA	O2D-CGD-CBD	4.22	118.77	111.27
24	c	510	CLA	C3D-C4D-ND	4.22	117.07	110.24
24	b	616	CLA	C3D-C4D-ND	4.22	117.06	110.24
24	B	610	CLA	CMB-C2B-C1B	4.22	131.79	125.37
24	C	509	CLA	C3D-C4D-ND	4.21	117.05	110.24
24	c	514	CLA	C3D-C4D-ND	4.21	117.04	110.24
24	a	412	CLA	C3D-C4D-ND	4.21	117.04	110.24
24	c	510	CLA	C4A-NA-C1A	-4.21	104.81	106.71
24	B	605	CLA	C3B-C4B-NB	4.21	114.42	110.52
24	c	513	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
24	C	513	CLA	C3D-C4D-ND	4.19	117.02	110.24
24	b	623	CLA	C3D-C4D-ND	4.19	117.02	110.24
24	C	505	CLA	CBC-CAC-C3C	-4.19	100.88	112.43
24	B	607	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
24	A	405	CLA	CAC-C3C-C4C	4.19	130.24	124.81
24	B	606	CLA	C1D-CHD-C4C	-4.19	117.03	126.06
24	c	515	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
24	B	604	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
24	A	406	CLA	CBC-CAC-C3C	-4.18	100.91	112.43
27	a	414	SQD	O47-C7-C8	4.18	120.51	111.50
24	B	617	CLA	C3C-C4C-NC	4.18	115.26	110.57
24	A	405	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
24	C	504	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
24	D	402	CLA	C3D-C4D-ND	4.17	116.99	110.24
24	c	513	CLA	C3C-C4C-NC	4.17	115.25	110.57
24	c	512	CLA	C3C-C4C-NC	4.17	115.25	110.57
24	C	503	CLA	C1-C2-C3	-4.17	118.83	126.04
24	c	510	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
24	B	611	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	d	403	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
36	D	406	DGD	O2G-C1B-C2B	4.17	120.48	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	406	CLA	C3D-C4D-ND	4.15	116.95	110.24
24	B	612	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
24	c	507	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
24	c	505	CLA	C3C-C4C-NC	4.14	115.22	110.57
24	d	402	CLA	C3D-C4D-ND	4.14	116.94	110.24
40	v	205	HEC	C4C-NC-C1C	4.13	109.39	105.35
24	C	505	CLA	C3B-C4B-NB	4.13	114.35	110.52
26	b	626	BCR	C7-C8-C9	-4.13	119.99	126.23
37	D	409	LHG	O7-C7-C8	4.13	120.40	111.50
24	C	507	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
24	C	511	CLA	C3D-C4D-ND	4.13	116.92	110.24
24	C	511	CLA	C3C-C4C-NC	4.13	115.20	110.57
25	d	401	PHO	O2D-CGD-O1D	-4.13	115.77	123.84
24	C	509	CLA	C3C-C4C-NC	4.12	115.20	110.57
24	C	507	CLA	C3D-C4D-ND	4.12	116.91	110.24
24	B	605	CLA	C3B-C2B-C1B	-4.12	102.18	107.16
24	d	402	CLA	C1D-CHD-C4C	-4.12	117.16	126.06
24	C	506	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
24	B	615	CLA	C3D-C4D-ND	4.12	116.90	110.24
24	C	514	CLA	C3C-C4C-NC	4.12	115.19	110.57
24	b	617	CLA	O2D-CGD-CBD	4.11	118.58	111.27
26	d	405	BCR	C24-C23-C22	-4.11	120.03	126.23
24	c	515	CLA	C1D-CHD-C4C	-4.10	117.20	126.06
24	D	403	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	C	512	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
24	b	612	CLA	C3D-C4D-ND	4.10	116.87	110.24
24	b	625	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
24	b	618	CLA	CMB-C2B-C1B	4.10	131.61	125.37
24	A	405	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
27	B	621	SQD	O7-S-C6	4.10	111.81	106.94
24	b	619	CLA	C1-C2-C3	-4.09	118.96	126.04
40	v	205	HEC	CHB-C1B-NB	4.09	128.87	124.42
24	B	605	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
24	b	610	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
24	D	402	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
24	b	624	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
24	c	515	CLA	C4A-NA-C1A	-4.09	104.87	106.71
24	d	403	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
24	C	502	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
24	b	613	CLA	C3B-C4B-NB	4.09	114.31	110.52
29	A	416	LMT	O5'-C5'-C4'	4.08	118.36	109.75
26	T	103	BCR	C11-C10-C9	-4.08	121.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C3D-C4D-ND	4.08	116.83	110.24
36	c	521	DGD	O2G-C1B-C2B	4.08	120.29	111.50
24	b	617	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
24	d	402	CLA	C4A-NA-C1A	-4.06	104.88	106.71
36	c	520	DGD	O2G-C1B-C2B	4.06	120.25	111.50
24	c	510	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
24	c	514	CLA	C3B-C4B-NB	4.06	114.28	110.52
24	c	505	CLA	C3D-C4D-ND	4.05	116.80	110.24
24	C	510	CLA	C3D-C4D-ND	4.05	116.80	110.24
38	e	103	HEM	CHD-C1D-ND	4.05	128.82	124.42
24	c	512	CLA	C3B-C4B-NB	4.05	114.27	110.52
24	b	616	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
24	a	410	CLA	C4A-NA-C1A	-4.04	104.89	106.71
31	a	416	PL9	C7-C3-C4	4.04	120.16	116.88
24	C	505	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	b	625	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
24	b	619	CLA	C3C-C4C-NC	4.04	115.10	110.57
24	c	514	CLA	C4-C3-C5	4.03	122.06	115.27
24	B	614	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	C	503	CLA	C3D-C4D-ND	4.03	116.76	110.24
24	a	409	CLA	C1-C2-C3	-4.03	119.07	126.04
24	b	625	CLA	C3D-C4D-ND	4.03	116.75	110.24
24	b	617	CLA	C3C-C4C-NC	4.03	115.08	110.57
24	C	506	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	B	612	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	c	506	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	B	615	CLA	O2D-CGD-O1D	-4.02	115.99	123.84
24	a	409	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
24	c	508	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
29	C	522	LMT	O1B-C4'-C3'	4.01	117.94	107.28
24	B	603	CLA	C3C-C4C-NC	4.01	115.06	110.57
24	C	510	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	d	402	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	B	603	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	b	622	CLA	C3C-C4C-NC	4.00	115.06	110.57
29	B	622	LMT	O1B-C4'-C3'	4.00	117.92	107.28
35	Z	101	LMG	O7-C10-C11	4.00	120.12	111.50
24	B	617	CLA	C3D-C4D-ND	4.00	116.71	110.24
24	A	406	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
24	c	509	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
40	V	205	HEC	C4C-NC-C1C	4.00	109.26	105.35
27	a	405	SQD	O47-C7-C8	4.00	120.11	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	620	CLA	CAC-C3C-C4C	3.99	129.99	124.81
24	b	624	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
31	a	416	PL9	C22-C23-C24	-3.99	118.06	127.66
24	B	613	CLA	C4A-NA-C1A	-3.99	104.91	106.71
24	A	405	CLA	C3D-C4D-ND	3.98	116.68	110.24
24	B	616	CLA	C1D-CHD-C4C	-3.98	117.46	126.06
24	c	508	CLA	C3C-C4C-NC	3.98	115.04	110.57
24	C	508	CLA	CMC-C2C-C1C	3.98	131.11	125.04
24	b	618	CLA	C3C-C4C-NC	3.98	115.04	110.57
24	B	604	CLA	CAA-C2A-C3A	-3.98	101.87	112.78
24	c	517	CLA	O2D-CGD-CBD	3.98	118.34	111.27
24	C	502	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
24	C	506	CLA	CMB-C2B-C1B	3.97	131.42	125.37
24	b	617	CLA	C3D-C4D-ND	3.97	116.67	110.24
24	B	602	CLA	C4A-NA-C1A	-3.97	104.92	106.71
24	c	514	CLA	C1-C2-C3	-3.97	119.18	126.04
24	c	511	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	B	612	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
24	b	621	CLA	C4A-NA-C1A	-3.96	104.92	106.71
24	C	511	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
24	a	410	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
24	c	510	CLA	C3C-C4C-NC	3.96	115.01	110.57
24	b	614	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
24	B	615	CLA	CAC-C3C-C4C	3.96	129.94	124.81
26	D	404	BCR	C33-C5-C6	-3.96	120.08	124.53
24	B	605	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
24	B	614	CLA	C3B-C4B-NB	3.95	114.18	110.52
24	C	505	CLA	C3D-C4D-ND	3.95	116.63	110.24
24	C	512	CLA	C4A-NA-C1A	-3.95	104.93	106.71
24	c	513	CLA	C3D-C4D-ND	3.95	116.63	110.24
31	a	416	PL9	C32-C33-C34	-3.95	118.15	127.66
27	A	415	SQD	O48-C23-C24	3.94	124.29	111.91
24	d	402	CLA	C3B-C4B-NB	3.94	114.17	110.52
24	c	509	CLA	CMB-C2B-C1B	3.94	131.37	125.37
40	v	205	HEC	CHC-C4B-NB	3.94	129.23	124.37
24	C	512	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	b	611	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
24	c	514	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
24	b	623	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
37	D	407	LHG	O7-C7-C8	3.93	119.98	111.50
24	C	502	CLA	C1D-CHD-C4C	-3.93	117.57	126.06
24	b	618	CLA	C1C-C2C-C3C	-3.93	102.82	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	622	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
24	B	613	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
36	D	406	DGD	C1D-C2D-C3D	3.93	118.18	110.00
24	c	516	CLA	C3C-C4C-NC	3.93	114.98	110.57
24	b	616	CLA	C4A-NA-C1A	-3.93	104.94	106.71
24	b	611	CLA	C3C-C4C-NC	3.93	114.97	110.57
24	c	514	CLA	C3C-C4C-NC	3.93	114.97	110.57
24	a	410	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
27	a	414	SQD	C44-O6-C1	-3.91	106.10	113.74
40	v	205	HEC	CHA-C4D-ND	3.91	128.67	124.42
24	c	510	CLA	C3B-C4B-NB	3.91	114.14	110.52
24	c	517	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
24	c	506	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
38	e	103	HEM	C4C-NC-C1C	3.91	109.17	105.35
24	D	403	CLA	CAC-C3C-C4C	3.91	129.88	124.81
26	C	515	BCR	C15-C14-C13	-3.90	121.74	127.31
24	B	607	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
24	b	621	CLA	C3D-C4D-ND	3.90	116.54	110.24
24	B	607	CLA	C3C-C4C-NC	3.90	114.94	110.57
24	b	620	CLA	C3C-C4C-NC	3.89	114.94	110.57
26	C	515	BCR	C16-C17-C18	-3.89	121.76	127.31
24	B	604	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
24	c	508	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
26	H	101	BCR	C38-C26-C25	-3.88	120.17	124.53
24	a	409	CLA	C3C-C4C-NC	3.88	114.92	110.57
24	b	618	CLA	C3B-C2B-C1B	-3.88	102.48	107.16
24	b	613	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
24	c	512	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
24	C	513	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
24	C	511	CLA	C3B-C4B-NB	3.87	114.10	110.52
24	b	613	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
27	A	411	SQD	C45-O47-C7	-3.86	108.28	117.79
24	c	505	CLA	C3B-C4B-NB	3.86	114.10	110.52
26	k	101	BCR	C24-C23-C22	-3.86	120.40	126.23
26	d	405	BCR	C38-C26-C25	-3.86	120.19	124.53
37	E	101	LHG	O7-C7-C8	3.86	119.82	111.50
24	c	507	CLA	O2D-CGD-CBD	3.86	118.12	111.27
26	D	404	BCR	C24-C23-C22	-3.86	120.41	126.23
24	C	512	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
24	C	514	CLA	O2D-CGD-CBD	3.86	118.12	111.27
24	C	512	CLA	O2D-CGD-CBD	3.85	118.12	111.27
24	B	608	CLA	C1C-C2C-C3C	-3.85	102.90	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	B	611	CLA	C3C-C4C-NC	3.85	114.89	110.57
38	E	102	HEM	CHD-C4C-NC	3.85	128.60	124.44
24	c	505	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	B	602	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
24	b	611	CLA	CAC-C3C-C4C	3.85	129.80	124.81
24	B	613	CLA	CMC-C2C-C1C	3.84	130.89	125.04
24	C	504	CLA	O2D-CGD-CBD	3.84	118.09	111.27
24	c	511	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
24	b	624	CLA	CMB-C2B-C1B	3.83	131.21	125.37
24	B	615	CLA	O2A-CGA-O1A	-3.83	113.92	123.59
24	B	611	CLA	CAA-C2A-C3A	-3.83	102.29	112.78
24	B	608	CLA	C3B-C2B-C1B	-3.83	102.54	107.16
24	c	511	CLA	C3D-C4D-ND	3.83	116.43	110.24
24	C	508	CLA	C3D-C4D-ND	3.82	116.42	110.24
24	b	614	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
24	A	405	CLA	C3C-C4C-NC	3.82	114.85	110.57
24	C	503	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
36	e	101	DGD	C3E-C4E-C5E	3.81	117.04	110.24
37	L	101	LHG	O7-C7-C8	3.81	119.71	111.50
24	C	507	CLA	C3C-C4C-NC	3.81	114.84	110.57
24	B	609	CLA	C3C-C4C-NC	3.81	114.84	110.57
24	B	608	CLA	C3C-C4C-NC	3.81	114.84	110.57
36	c	519	DGD	O2G-C1B-C2B	3.81	119.70	111.50
25	a	411	PHO	O1D-CGD-CBD	-3.81	118.40	124.74
24	d	404	CLA	C3C-C4C-NC	3.80	114.83	110.57
27	A	415	SQD	O47-C7-C8	3.80	119.69	111.50
24	C	502	CLA	CMC-C2C-C1C	3.80	130.83	125.04
24	C	511	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
24	b	615	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
24	C	502	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
26	T	103	BCR	C15-C16-C17	-3.79	115.70	123.47
26	C	515	BCR	C7-C8-C9	-3.79	120.50	126.23
24	c	513	CLA	C1-C2-C3	-3.79	119.48	126.04
24	c	517	CLA	C3C-C4C-NC	3.79	114.82	110.57
26	k	101	BCR	C11-C10-C9	-3.79	121.91	127.31
24	b	610	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
24	c	515	CLA	C3B-C4B-NB	3.78	114.03	110.52
24	c	516	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
24	b	625	CLA	C3C-C4C-NC	3.78	114.81	110.57
25	d	401	PHO	C4D-CHA-CBD	3.77	110.22	108.52
24	b	623	CLA	C3C-C4C-NC	3.77	114.80	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	512	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	C	507	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	C	506	CLA	C3D-C2D-C1D	-3.76	100.70	105.83
24	C	505	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
24	A	407	CLA	C3C-C4C-NC	3.76	114.78	110.57
38	e	103	HEM	C1B-NB-C4B	3.75	108.95	105.07
24	B	602	CLA	C3C-C4C-NC	3.75	114.78	110.57
24	b	610	CLA	C3C-C4C-NC	3.75	114.78	110.57
24	A	405	CLA	O2D-CGD-CBD	3.75	117.93	111.27
24	c	505	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
24	a	412	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
24	B	604	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
24	B	602	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
24	C	508	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
24	C	505	CLA	C3C-C4C-NC	3.73	114.75	110.57
24	c	515	CLA	C3C-C4C-NC	3.73	114.75	110.57
24	c	510	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
24	C	514	CLA	C1D-CHD-C4C	-3.72	118.02	126.06
24	d	403	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
24	b	611	CLA	CAA-C2A-C3A	-3.72	102.58	112.78
24	d	403	CLA	C3B-C4B-NB	3.72	113.97	110.52
24	A	409	CLA	O2D-CGD-CBD	3.72	117.88	111.27
31	d	406	PL9	C42-C43-C44	-3.72	118.71	127.66
24	B	608	CLA	CAA-C2A-C3A	-3.72	102.60	112.78
24	B	610	CLA	C3B-C2B-C1B	-3.71	102.68	107.16
26	c	518	BCR	C7-C8-C9	-3.71	120.63	126.23
24	B	605	CLA	C1-C2-C3	-3.71	119.63	126.04
24	d	404	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
27	a	405	SQD	O8-S-C6	3.70	111.64	105.74
24	b	620	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	b	612	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	c	506	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	D	403	CLA	C3B-C4B-NB	3.69	113.94	110.52
31	a	416	PL9	C15-C14-C16	3.69	121.48	115.27
24	a	412	CLA	C3C-C4C-NC	3.69	114.71	110.57
24	A	407	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	c	506	CLA	C3C-C4C-NC	3.69	114.70	110.57
24	a	410	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
24	D	402	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
24	C	502	CLA	C3C-C4C-NC	3.68	114.70	110.57
24	a	412	CLA	CMB-C2B-C1B	3.68	130.97	125.37
24	c	509	CLA	C1D-CHD-C4C	-3.68	118.12	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	C3B-C4B-NB	3.68	113.93	110.52
24	b	615	CLA	C3D-C4D-ND	3.67	116.18	110.24
24	b	617	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
24	d	403	CLA	O2D-CGD-CBD	3.67	117.79	111.27
24	c	513	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
24	c	514	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
24	b	623	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
27	a	414	SQD	C1-C2-C3	-3.67	102.36	110.00
25	D	401	PHO	C1A-C2A-C3A	-3.66	99.35	102.84
24	B	609	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
24	C	513	CLA	CMB-C2B-C1B	3.66	130.95	125.37
24	A	409	CLA	C1D-CHD-C4C	-3.65	118.17	126.06
24	B	611	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
24	B	603	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
24	C	503	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
24	c	513	CLA	C3B-C4B-NB	3.65	113.90	110.52
24	A	405	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	D	403	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
24	b	622	CLA	C3D-C4D-ND	3.64	116.13	110.24
24	b	615	CLA	C3B-C4B-NB	3.64	113.89	110.52
24	b	622	CLA	C1-C2-C3	-3.64	119.75	126.04
24	C	502	CLA	CBC-CAC-C3C	-3.64	102.41	112.43
26	y	101	BCR	C15-C14-C13	-3.63	122.13	127.31
24	C	509	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
24	C	509	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
24	C	510	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
24	D	403	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
24	c	507	CLA	CMB-C2B-C1B	3.62	130.88	125.37
38	e	103	HEM	CHD-C4C-NC	3.61	128.35	124.44
24	B	602	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	612	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
24	b	621	CLA	C3B-C4B-NB	3.61	113.86	110.52
24	C	507	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
24	d	404	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
24	b	611	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
24	b	621	CLA	C4C-C3C-C2C	-3.59	101.67	106.90
24	b	617	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
24	c	517	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
38	E	102	HEM	C4C-NC-C1C	3.58	108.85	105.35
26	D	404	BCR	C38-C26-C25	-3.58	120.51	124.53
34	V	206	HTG	C1'-S1-C1	3.58	106.78	100.09
24	B	607	CLA	CMC-C2C-C1C	3.58	130.48	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	615	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
35	c	522	LMG	O7-C10-C11	3.57	119.20	111.50
24	C	513	CLA	C1-C2-C3	-3.57	119.86	126.04
24	a	412	CLA	C1-C2-C3	-3.57	119.86	126.04
24	C	512	CLA	CAC-C3C-C4C	3.57	129.44	124.81
24	A	405	CLA	C3B-C4B-NB	3.57	113.83	110.52
24	b	619	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
35	z	101	LMG	O7-C10-C11	3.57	119.19	111.50
24	C	510	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
24	D	402	CLA	C3B-C4B-NB	3.57	113.82	110.52
24	C	507	CLA	CBC-CAC-C3C	-3.57	102.60	112.43
36	C	518	DGD	O2G-C1B-C2B	3.56	119.18	111.50
24	b	618	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
24	b	619	CLA	CAC-C3C-C4C	3.56	129.43	124.81
29	C	522	LMT	C1'-O5'-C5'	3.56	120.68	113.69
26	b	627	BCR	C29-C30-C25	3.56	115.96	110.48
24	c	505	CLA	CAC-C3C-C4C	3.56	129.43	124.81
24	b	620	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
27	a	405	SQD	O48-C23-C24	3.55	123.05	111.91
24	d	403	CLA	C3C-C4C-NC	3.55	114.55	110.57
35	c	523	LMG	C3-C4-C5	3.55	116.57	110.24
31	a	416	PL9	C20-C19-C21	3.55	121.24	115.27
24	b	612	CLA	CMC-C2C-C1C	3.54	130.43	125.04
24	b	620	CLA	C3B-C4B-NB	3.54	113.80	110.52
35	C	520	LMG	O7-C10-C11	3.54	119.13	111.50
24	b	614	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
24	c	511	CLA	CMC-C2C-C1C	3.54	130.43	125.04
24	B	610	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
24	B	616	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
26	t	101	BCR	C15-C14-C13	3.53	132.34	127.31
24	A	407	CLA	C4-C3-C5	3.52	121.19	115.27
25	D	401	PHO	CBC-CAC-C3C	-3.52	107.73	112.88
24	B	616	CLA	CMB-C2B-C1B	3.52	130.72	125.37
25	d	401	PHO	C4-C3-C5	3.51	121.17	115.27
24	A	406	CLA	C3C-C4C-NC	3.51	114.50	110.57
26	C	516	BCR	C33-C5-C6	-3.51	120.59	124.53
24	B	616	CLA	CMC-C2C-C1C	3.51	130.38	125.04
24	c	516	CLA	C1-C2-C3	-3.51	119.98	126.04
40	v	205	HEC	C1D-ND-C4D	3.50	108.69	105.07
24	C	514	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
24	B	614	CLA	C3D-C4D-ND	3.50	115.91	110.24
24	B	608	CLA	C1D-CHD-C4C	-3.50	118.50	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	414	SQD	O8-S-C6	3.50	111.32	105.74
24	C	504	CLA	CMB-C2B-C1B	3.50	130.70	125.37
24	d	403	CLA	CAC-C3C-C4C	3.50	129.35	124.81
35	c	523	LMG	O6-C5-C4	3.49	116.04	109.69
24	B	605	CLA	CMB-C2B-C1B	3.49	130.69	125.37
24	b	624	CLA	O2D-CGD-CBD	3.49	117.47	111.27
24	c	508	CLA	C4-C3-C5	3.49	121.14	115.27
24	B	612	CLA	CAC-C3C-C4C	3.49	129.34	124.81
34	B	624	HTG	C1-O5-C5	3.49	119.01	112.58
29	a	404	LMT	O5'-C5'-C4'	3.48	117.09	109.75
24	B	606	CLA	CHD-C4C-NC	3.48	129.69	124.20
24	b	622	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	b	615	CLA	CMC-C2C-C1C	3.47	130.33	125.04
24	c	506	CLA	CMB-C2B-C1B	3.47	130.66	125.37
24	b	616	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
38	E	102	HEM	C4A-NA-C1A	3.47	108.75	105.35
24	d	404	CLA	C3B-C4B-NB	3.47	113.73	110.52
24	c	511	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
24	C	506	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
26	c	527	BCR	C11-C10-C9	-3.46	122.37	127.31
26	K	101	BCR	C7-C8-C9	-3.46	121.01	126.23
24	c	516	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
27	f	102	SQD	C1-O5-C5	3.46	120.48	113.69
24	c	507	CLA	CAC-C3C-C4C	3.46	129.29	124.81
24	b	619	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
24	C	509	CLA	C3B-C4B-NB	3.45	113.72	110.52
36	h	102	DGD	O2G-C1B-C2B	3.45	118.94	111.50
24	B	615	CLA	CMC-C2C-C1C	3.45	130.30	125.04
34	B	623	HTG	C1'-S1-C1	3.45	106.54	100.09
26	c	527	BCR	C16-C17-C18	-3.45	122.39	127.31
34	b	608	HTG	C1'-S1-C1	3.45	106.54	100.09
24	b	614	CLA	C4-C3-C5	3.45	121.07	115.27
31	D	405	PL9	C40-C39-C41	3.45	121.07	115.27
31	a	416	PL9	C7-C8-C9	-3.44	121.06	126.79
24	B	606	CLA	CMC-C2C-C1C	3.44	130.28	125.04
25	d	401	PHO	C1A-C2A-C3A	-3.44	99.56	102.84
24	d	403	CLA	C1-C2-C3	-3.44	120.09	126.04
24	c	515	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
24	A	407	CLA	CMB-C2B-C1B	3.44	130.60	125.37
37	d	409	LHG	O7-C7-C8	3.44	118.91	111.50
31	A	418	PL9	C20-C19-C21	3.44	121.05	115.27
24	D	402	CLA	C1-C2-C3	-3.44	120.10	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C3B-C4B-NB	3.44	113.70	110.52
26	b	627	BCR	C38-C26-C25	-3.43	120.67	124.53
24	C	505	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
26	t	101	BCR	C15-C16-C17	-3.43	116.45	123.47
35	b	629	LMG	O7-C10-C11	3.43	118.89	111.50
24	C	511	CLA	C4-C3-C5	3.43	121.04	115.27
26	C	516	BCR	C7-C8-C9	-3.43	121.06	126.23
31	A	418	PL9	C37-C38-C39	-3.42	119.42	127.66
24	c	509	CLA	C3D-C2D-C1D	-3.42	101.16	105.83
24	B	610	CLA	CAC-C3C-C4C	3.42	129.25	124.81
24	C	513	CLA	C3B-C4B-NB	3.42	113.69	110.52
24	c	507	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
24	c	506	CLA	C3B-C4B-NB	3.41	113.68	110.52
29	a	404	LMT	C1'-O5'-C5'	3.41	120.39	113.69
26	B	619	BCR	C28-C27-C26	-3.41	107.98	114.08
24	C	511	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
24	c	515	CLA	O2D-CGD-CBD	3.41	117.33	111.27
26	T	103	BCR	C33-C5-C6	-3.41	120.70	124.53
24	b	618	CLA	C3B-C4B-NB	3.41	113.68	110.52
24	b	624	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
24	b	615	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
24	D	402	CLA	CMC-C2C-C1C	3.41	130.23	125.04
24	B	612	CLA	C3B-C4B-NB	3.41	113.68	110.52
34	b	601	HTG	C1'-S1-C1	3.41	106.46	100.09
27	F	103	SQD	O6-C1-C2	3.40	113.61	108.30
24	D	403	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
24	B	604	CLA	CMC-C2C-C1C	3.40	130.22	125.04
31	D	405	PL9	C42-C43-C44	-3.40	119.47	127.66
24	C	513	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
24	C	510	CLA	C3B-C4B-NB	3.39	113.66	110.52
31	a	416	PL9	C17-C18-C19	-3.39	119.49	127.66
31	D	405	PL9	C7-C8-C9	-3.39	121.15	126.79
24	B	611	CLA	CAC-C3C-C4C	3.39	129.21	124.81
31	D	405	PL9	C10-C9-C11	3.39	120.97	115.27
24	c	515	CLA	CAC-C3C-C4C	3.39	129.21	124.81
24	d	403	CLA	CHC-C1C-C2C	-3.39	117.33	126.73
24	a	409	CLA	CAA-C2A-C3A	-3.38	103.51	112.78
24	B	611	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
24	B	613	CLA	CAC-C3C-C4C	3.38	129.20	124.81
24	B	614	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
31	A	418	PL9	C32-C33-C34	-3.38	119.53	127.66
24	C	510	CLA	CAC-C3C-C4C	3.38	129.19	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
24	B	615	CLA	O2A-CGA-CBA	3.38	122.50	111.91
40	V	205	HEC	CHB-C1B-NB	3.37	128.08	124.42
24	A	409	CLA	CAC-C3C-C4C	3.37	129.18	124.81
24	C	502	CLA	CMB-C2B-C1B	3.37	130.50	125.37
24	B	617	CLA	C3B-C4B-NB	3.37	113.64	110.52
40	V	205	HEC	CHA-C4D-ND	3.36	128.07	124.42
24	B	607	CLA	C3B-C4B-NB	3.36	113.63	110.52
24	B	607	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
40	V	205	HEC	CHC-C4B-NB	3.36	128.51	124.37
35	c	522	LMG	O8-C28-C29	3.36	122.44	111.91
24	B	613	CLA	C3B-C4B-NB	3.36	113.63	110.52
37	d	408	LHG	O7-C7-C8	3.35	118.72	111.50
24	B	611	CLA	O2A-CGA-CBA	3.34	122.40	111.91
24	c	510	CLA	C1-C2-C3	-3.34	120.26	126.04
24	B	613	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	B	613	CLA	C4-C3-C5	3.33	120.88	115.27
24	c	511	CLA	CMB-C2B-C1B	3.33	130.45	125.37
24	c	505	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
24	b	614	CLA	CHD-C4C-NC	3.33	129.46	124.20
24	D	402	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
24	c	508	CLA	CBC-CAC-C3C	-3.33	103.25	112.43
24	B	615	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
24	C	510	CLA	C1-O2A-CGA	3.33	125.18	116.44
24	A	406	CLA	CHC-C1C-C2C	-3.33	117.49	126.73
24	C	506	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	b	613	CLA	CMC-C2C-C1C	3.33	130.10	125.04
24	D	403	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
24	B	604	CLA	O2A-CGA-O1A	-3.32	115.21	123.59
24	b	625	CLA	CHC-C1C-C2C	-3.32	117.51	126.73
25	A	408	PHO	C4-C3-C5	3.32	120.85	115.27
24	b	614	CLA	C2A-C1A-CHA	-3.31	118.06	123.86
24	b	611	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
24	A	407	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
24	b	622	CLA	CHC-C1C-C2C	-3.31	117.53	126.73
26	b	627	BCR	C15-C14-C13	-3.31	122.58	127.31
24	c	508	CLA	C3B-C4B-NB	3.31	113.59	110.52
24	C	508	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
24	B	602	CLA	C3B-C4B-NB	3.31	113.58	110.52
26	B	618	BCR	C7-C8-C9	-3.31	121.24	126.23
24	C	504	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
24	b	622	CLA	C1D-CHD-C4C	-3.31	118.93	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	618	BCR	C24-C23-C22	-3.30	121.24	126.23
35	J	101	LMG	O7-C10-C11	3.30	118.62	111.50
24	A	405	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
24	d	402	CLA	CBC-CAC-C3C	-3.30	103.33	112.43
35	a	415	LMG	C8-O7-C10	-3.30	109.67	117.79
25	A	408	PHO	CMB-C2B-C3B	3.30	130.84	124.68
26	C	515	BCR	C33-C5-C6	-3.29	120.83	124.53
24	B	614	CLA	O2D-CGD-CBD	3.29	117.12	111.27
24	B	613	CLA	C1-C2-C3	-3.29	120.35	126.04
31	d	406	PL9	C10-C9-C11	3.29	120.81	115.27
24	B	610	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
24	B	613	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
24	C	504	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
24	A	409	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
24	b	625	CLA	CBC-CAC-C3C	-3.28	103.38	112.43
24	C	505	CLA	CMC-C2C-C1C	3.28	130.04	125.04
24	B	602	CLA	CMB-C2B-C1B	3.28	130.37	125.37
24	c	510	CLA	CBC-CAC-C3C	-3.28	103.39	112.43
24	b	624	CLA	C3B-C4B-NB	3.28	113.56	110.52
24	b	612	CLA	C3B-C4B-NB	3.27	113.55	110.52
31	d	406	PL9	C40-C39-C41	3.27	120.77	115.27
24	B	614	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
24	a	412	CLA	C3B-C4B-NB	3.27	113.54	110.52
24	b	617	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
24	A	406	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
24	B	613	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
35	M	101	LMG	O7-C10-C11	3.26	118.53	111.50
24	B	617	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
24	C	514	CLA	C1-C2-C3	-3.26	120.41	126.04
27	F	103	SQD	O7-S-C6	3.25	110.81	106.94
37	l	101	LHG	O7-C7-C8	3.25	118.51	111.50
24	C	506	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
31	A	418	PL9	C7-C3-C4	3.25	119.52	116.88
25	a	411	PHO	CBC-CAC-C3C	-3.25	108.12	112.88
24	B	605	CLA	CAC-C3C-C4C	3.25	129.03	124.81
26	d	405	BCR	C7-C8-C9	-3.25	121.33	126.23
24	c	509	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
24	b	615	CLA	CAC-C3C-C4C	3.24	129.01	124.81
24	b	621	CLA	CMB-C2B-C1B	3.24	130.30	125.37
24	C	503	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
24	c	509	CLA	CAC-C3C-C4C	3.23	129.01	124.81
24	B	606	CLA	C4C-C3C-C2C	-3.23	102.19	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	619	BCR	C29-C30-C25	3.23	115.46	110.48
27	f	102	SQD	O5-C5-C4	3.23	115.56	109.69
26	y	101	BCR	C16-C17-C18	-3.23	122.70	127.31
24	B	611	CLA	C3B-C4B-NB	3.23	113.51	110.52
24	c	509	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
24	b	620	CLA	CHC-C1C-C2C	-3.23	117.77	126.73
24	b	621	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
24	b	610	CLA	CHD-C4C-NC	3.22	129.27	124.20
24	b	621	CLA	O2A-CGA-CBA	3.21	122.00	111.91
24	B	611	CLA	CHC-C1C-C2C	-3.21	117.81	126.73
24	B	610	CLA	C3B-C4B-NB	3.21	113.50	110.52
24	c	516	CLA	CHD-C4C-NC	3.21	129.26	124.20
24	b	621	CLA	C1-C2-C3	-3.21	120.50	126.04
24	C	508	CLA	CMB-C2B-C1B	3.21	130.25	125.37
24	C	513	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
24	B	611	CLA	CMA-C3A-C4A	-3.20	103.17	111.77
24	B	605	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
24	A	409	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
24	b	616	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
24	c	507	CLA	C1-C2-C3	-3.20	120.51	126.04
24	C	512	CLA	CHC-C1C-C2C	-3.20	117.85	126.73
24	b	621	CLA	C4-C3-C5	3.20	120.65	115.27
26	k	101	BCR	C20-C21-C22	-3.20	122.75	127.31
24	A	409	CLA	C1-C2-C3	-3.19	120.52	126.04
24	c	506	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
24	B	616	CLA	CHD-C4C-NC	3.19	129.23	124.20
26	b	628	BCR	C38-C26-C25	-3.19	120.95	124.53
38	e	103	HEM	C4D-ND-C1D	3.18	108.36	105.07
26	b	626	BCR	C15-C14-C13	-3.18	122.77	127.31
26	d	405	BCR	C33-C5-C6	-3.18	120.95	124.53
26	B	619	BCR	C2-C1-C6	3.18	115.38	110.48
37	D	408	LHG	O7-C7-C8	3.18	118.35	111.50
24	b	616	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
24	A	406	CLA	CHD-C4C-NC	3.18	129.21	124.20
24	A	407	CLA	CBC-CAC-C3C	-3.18	103.68	112.43
24	B	617	CLA	CBC-CAC-C3C	-3.18	103.68	112.43
24	A	405	CLA	O2A-CGA-CBA	3.17	121.85	111.91
31	a	416	PL9	C10-C9-C11	3.17	120.60	115.27
24	b	624	CLA	CHD-C4C-NC	3.17	129.19	124.20
24	b	624	CLA	C4-C3-C5	3.17	120.60	115.27
24	a	412	CLA	CHD-C4C-NC	3.17	129.19	124.20
31	A	418	PL9	C53-C6-C1	3.16	121.45	114.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	403	CLA	CMB-C2B-C1B	3.16	130.18	125.37
27	A	411	SQD	O8-S-C6	3.15	110.76	105.74
24	B	611	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	c	516	CLA	CMC-C2C-C1C	3.15	129.84	125.04
24	c	505	CLA	CHC-C1C-C2C	-3.15	117.98	126.73
24	C	503	CLA	O2A-CGA-O1A	-3.15	115.65	123.59
24	C	507	CLA	C3B-C4B-NB	3.15	113.44	110.52
24	C	507	CLA	CAC-C3C-C4C	3.15	128.89	124.81
24	b	624	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	d	402	CLA	C2A-C1A-CHA	-3.14	118.36	123.86
24	b	625	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
31	a	416	PL9	C42-C43-C44	-3.14	120.09	127.66
37	l	101	LHG	O8-C23-C24	3.14	121.77	111.91
24	b	623	CLA	C3B-C4B-NB	3.14	113.43	110.52
24	b	625	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
24	B	602	CLA	O2A-CGA-CBA	3.13	121.74	111.91
24	b	613	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
31	a	416	PL9	C27-C28-C29	-3.13	120.11	127.66
34	C	524	HTG	O5-C5-C4	3.13	115.38	109.69
31	A	418	PL9	C45-C44-C46	3.13	120.53	115.27
24	C	510	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
24	b	618	CLA	CBC-CAC-C3C	-3.12	103.82	112.43
24	B	616	CLA	O2D-CGD-CBD	3.12	116.82	111.27
24	B	602	CLA	CHD-C4C-NC	3.12	129.12	124.20
24	B	615	CLA	C4-C3-C5	3.12	120.52	115.27
24	B	608	CLA	C1-C2-C3	-3.12	120.65	126.04
24	D	403	CLA	C4-C3-C5	3.12	120.52	115.27
24	d	403	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
24	b	610	CLA	C4-C3-C5	3.12	120.51	115.27
24	A	407	CLA	C1D-CHD-C4C	-3.11	119.34	126.06
24	B	609	CLA	CMB-C2B-C1B	3.11	130.11	125.37
24	B	603	CLA	C3B-C4B-NB	3.11	113.40	110.52
24	D	403	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
24	C	513	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	b	614	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
26	D	404	BCR	C29-C30-C25	3.11	115.27	110.48
24	C	514	CLA	CAC-C3C-C4C	3.11	128.84	124.81
24	a	412	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
24	d	403	CLA	C2A-C1A-CHA	-3.11	118.43	123.86
35	Z	101	LMG	O6-C5-C4	3.11	115.33	109.69
26	h	101	BCR	C16-C17-C18	-3.11	122.88	127.31
24	b	616	CLA	C3B-C4B-NB	3.11	113.40	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	409	CLA	C4-C3-C5	3.10	120.49	115.27
26	c	518	BCR	C33-C5-C6	-3.10	121.05	124.53
24	B	615	CLA	C2A-C1A-CHA	-3.10	118.44	123.86
37	D	407	LHG	O8-C23-C24	3.10	121.63	111.91
24	a	410	CLA	CMC-C2C-C1C	3.09	129.75	125.04
26	T	103	BCR	C34-C9-C10	-3.09	118.59	122.92
24	B	604	CLA	O2A-CGA-CBA	3.09	121.61	111.91
24	B	606	CLA	C4-C3-C5	3.09	120.47	115.27
24	b	625	CLA	O2A-CGA-CBA	3.09	121.61	111.91
26	h	101	BCR	C38-C26-C25	-3.09	121.06	124.53
24	b	613	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
24	C	514	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
24	A	407	CLA	C2A-C1A-CHA	-3.09	118.46	123.86
24	B	606	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
24	C	511	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
31	A	418	PL9	C8-C7-C3	3.09	120.70	111.98
24	C	503	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
24	b	620	CLA	CBC-CAC-C3C	-3.08	103.94	112.43
24	d	402	CLA	CMB-C2B-C1B	3.08	130.06	125.37
24	d	404	CLA	CAC-C3C-C4C	3.08	128.81	124.81
24	c	511	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
24	d	403	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
26	B	620	BCR	C32-C1-C6	-3.08	105.31	110.30
24	c	506	CLA	CAC-C3C-C4C	3.08	128.80	124.81
27	F	103	SQD	C3-C4-C5	3.08	115.73	110.24
24	b	618	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
24	c	514	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
40	v	205	HEC	CBC-CAC-C3C	3.07	120.91	112.43
24	d	402	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	d	402	CLA	CHD-C4C-NC	3.07	129.04	124.20
24	B	609	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
24	C	509	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
24	c	505	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
24	b	621	CLA	O2A-CGA-O1A	-3.06	115.86	123.59
24	B	615	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
24	B	616	CLA	C3B-C4B-NB	3.06	113.36	110.52
36	H	102	DGD	O2G-C1B-C2B	3.06	118.10	111.50
29	T	104	LMT	C1'-O5'-C5'	3.06	119.70	113.69
24	c	510	CLA	CHC-C1C-C2C	-3.06	118.22	126.73
24	b	610	CLA	C3B-C4B-NB	3.06	113.35	110.52
24	B	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	B	603	CLA	CHD-C4C-NC	3.06	129.02	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	404	CLA	CHD-C4C-NC	3.06	129.02	124.20
24	B	603	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	d	402	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
24	C	507	CLA	C4-C3-C5	3.06	120.41	115.27
24	b	615	CLA	C4-C3-C5	3.06	120.41	115.27
24	C	507	CLA	C1-C2-C3	-3.06	120.76	126.04
24	b	611	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
35	j	101	LMG	O7-C10-C11	3.05	118.08	111.50
27	L	102	SQD	O8-S-C6	3.05	110.60	105.74
31	D	405	PL9	C36-C37-C38	-3.05	101.87	111.88
24	a	410	CLA	CHD-C4C-NC	3.05	129.00	124.20
24	A	409	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
31	D	405	PL9	C53-C6-C1	3.04	121.21	114.99
24	B	614	CLA	CMB-C2B-C1B	3.04	130.00	125.37
24	B	613	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
24	a	409	CLA	O2D-CGD-CBD	3.04	116.67	111.27
25	a	411	PHO	C1A-C2A-C3A	-3.04	99.95	102.84
24	a	412	CLA	CBC-CAC-C3C	-3.04	104.05	112.43
24	c	517	CLA	CMC-C2C-C1C	3.04	129.66	125.04
26	K	101	BCR	C33-C5-C6	-3.04	121.12	124.53
24	B	609	CLA	CMC-C2C-C1C	3.03	129.66	125.04
24	b	614	CLA	CMB-C2B-C1B	3.03	129.99	125.37
24	a	409	CLA	C2A-C1A-CHA	-3.03	118.56	123.86
40	V	205	HEC	CBC-CAC-C3C	3.03	120.79	112.43
26	c	527	BCR	C33-C5-C6	-3.03	121.12	124.53
24	c	514	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
24	C	508	CLA	CHD-C4C-NC	3.03	128.98	124.20
24	c	515	CLA	C4-C3-C5	3.03	120.37	115.27
24	B	610	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
26	Y	101	BCR	C15-C14-C13	-3.03	122.99	127.31
24	b	621	CLA	CAC-C3C-C4C	3.03	128.74	124.81
24	b	616	CLA	CMB-C2B-C1B	3.02	129.97	125.37
38	E	102	HEM	CBD-CAD-C3D	-3.02	104.23	112.63
24	A	409	CLA	CMB-C2B-C1B	3.02	129.97	125.37
24	C	514	CLA	CMB-C2B-C1B	3.02	129.97	125.37
24	B	606	CLA	C2A-C1A-CHA	-3.02	118.58	123.86
24	c	511	CLA	C4-C3-C5	3.02	120.35	115.27
24	C	503	CLA	C3B-C4B-NB	3.02	113.32	110.52
31	A	418	PL9	C22-C23-C24	-3.02	120.39	127.66
36	D	406	DGD	O1G-C1A-C2A	3.02	121.37	111.91
37	d	407	LHG	O8-C23-O10	-3.01	115.98	123.59
24	B	610	CLA	CHC-C1C-C2C	-3.01	118.36	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	622	CLA	CED-O2D-CGD	3.01	122.75	115.94
24	b	624	CLA	CAC-C3C-C4C	3.01	128.72	124.81
24	B	616	CLA	CBC-CAC-C3C	-3.01	104.14	112.43
24	C	510	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
24	C	513	CLA	CHD-C4C-NC	3.01	128.94	124.20
34	b	608	HTG	C1-O5-C5	3.01	118.13	112.58
24	b	623	CLA	CHD-C4C-NC	3.01	128.94	124.20
24	c	512	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
35	C	520	LMG	O8-C28-C29	3.00	121.33	111.91
24	c	515	CLA	CMC-C2C-C1C	3.00	129.61	125.04
24	C	508	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
24	B	615	CLA	C3B-C4B-NB	3.00	113.30	110.52
24	D	402	CLA	O2A-CGA-CBA	3.00	121.32	111.91
24	b	623	CLA	CBC-CAC-C3C	-3.00	104.17	112.43
24	c	515	CLA	CHD-C4C-NC	3.00	128.92	124.20
27	F	103	SQD	O5-C5-C4	2.99	115.13	109.69
24	c	507	CLA	CMC-C2C-C1C	2.99	129.59	125.04
24	c	512	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
24	a	410	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	b	613	CLA	C3D-C4D-ND	2.98	115.07	110.24
26	D	404	BCR	C28-C27-C26	-2.98	108.75	114.08
24	b	611	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
24	B	608	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
24	C	507	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
24	b	611	CLA	C3B-C4B-NB	2.98	113.28	110.52
24	b	625	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
24	b	619	CLA	C4-C3-C5	2.98	120.28	115.27
24	b	622	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
24	B	607	CLA	C1-C2-C3	-2.98	120.90	126.04
24	C	509	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
24	B	603	CLA	CHC-C1C-C2C	-2.98	118.47	126.73
24	C	504	CLA	O2A-CGA-CBA	2.97	121.23	111.91
36	C	519	DGD	O2G-C1B-C2B	2.97	117.90	111.50
24	C	505	CLA	CAC-C3C-C4C	2.97	128.66	124.81
24	b	613	CLA	C1-C2-C3	-2.97	120.91	126.04
26	B	619	BCR	C37-C22-C21	-2.97	118.77	122.92
24	C	506	CLA	C3B-C4B-NB	2.97	113.27	110.52
24	B	617	CLA	CHD-C4C-NC	2.96	128.88	124.20
24	B	610	CLA	CHD-C4C-NC	2.96	128.87	124.20
24	a	412	CLA	C4-C3-C5	2.96	120.25	115.27
31	a	416	PL9	C35-C34-C36	2.96	120.25	115.27
24	B	610	CLA	O2D-CGD-O1D	-2.96	118.06	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	612	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
24	B	617	CLA	CAC-C3C-C4C	2.95	128.64	124.81
24	A	405	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
24	c	513	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
37	E	101	LHG	O8-C23-C24	2.95	121.17	111.91
26	B	620	BCR	C38-C26-C25	-2.95	121.22	124.53
24	c	515	CLA	C1-C2-C3	-2.95	120.94	126.04
26	C	516	BCR	C24-C23-C22	-2.95	121.78	126.23
24	b	617	CLA	C3B-C4B-NB	2.95	113.25	110.52
24	c	517	CLA	C1-C2-C3	-2.95	120.95	126.04
27	a	414	SQD	O9-S-C6	2.95	110.44	106.94
24	d	403	CLA	O2A-CGA-CBA	2.94	121.15	111.91
37	D	409	LHG	O8-C23-C24	2.94	121.15	111.91
24	B	605	CLA	C3D-C4D-ND	2.94	115.00	110.24
24	C	511	CLA	CAC-C3C-C4C	2.94	128.63	124.81
24	b	617	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	b	610	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
24	d	402	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
25	D	401	PHO	C4-C3-C5	2.94	120.21	115.27
24	b	610	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
24	b	618	CLA	CHD-C4C-NC	2.94	128.83	124.20
24	c	515	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
24	c	512	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
24	A	405	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
24	c	506	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
27	F	103	SQD	O48-C23-C24	2.93	121.11	111.91
31	a	416	PL9	C37-C38-C39	-2.93	120.60	127.66
35	j	101	LMG	O6-C5-C4	2.93	115.01	109.69
24	C	503	CLA	O2A-CGA-CBA	2.93	121.09	111.91
24	b	619	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
24	a	410	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
24	D	402	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	A	405	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
27	A	415	SQD	O48-C23-O10	-2.92	116.22	123.59
24	b	622	CLA	CMB-C2B-C1B	2.92	129.81	125.37
24	A	406	CLA	C4-C3-C5	2.92	120.18	115.27
37	L	101	LHG	C5-O7-C7	-2.92	110.61	117.79
24	B	605	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
36	H	102	DGD	C3G-O3G-C1D	-2.92	108.04	113.74
24	d	404	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
24	c	512	CLA	C1-C2-C3	-2.91	121.00	126.04
24	B	605	CLA	CMC-C2C-C1C	2.91	129.48	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	603	CLA	C1-C2-C3	-2.91	121.01	126.04
31	A	418	PL9	C27-C28-C29	-2.91	120.65	127.66
24	c	512	CLA	CAC-C3C-C4C	2.91	128.59	124.81
24	b	624	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
24	b	625	CLA	CMB-C2B-C1B	2.91	129.80	125.37
24	B	607	CLA	CAC-C3C-C4C	2.91	128.58	124.81
24	C	502	CLA	CHD-C4C-NC	2.91	128.78	124.20
24	C	503	CLA	CAC-C3C-C4C	2.90	128.58	124.81
24	c	507	CLA	C4-C3-C5	2.90	120.16	115.27
24	C	511	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
24	c	509	CLA	CMC-C2C-C1C	2.90	129.46	125.04
24	a	409	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
24	c	514	CLA	O2A-CGA-CBA	2.90	121.00	111.91
36	C	518	DGD	O1G-C1A-C2A	2.89	120.99	111.91
24	d	402	CLA	CHB-C1B-NB	-2.89	121.19	124.26
24	B	610	CLA	CBC-CAC-C3C	-2.89	104.45	112.43
35	c	522	LMG	C8-O7-C10	-2.89	110.67	117.79
38	E	102	HEM	CHD-C1D-ND	2.89	127.56	124.42
24	C	505	CLA	C4-C3-C5	2.89	120.13	115.27
24	b	611	CLA	C4-C3-C5	2.88	120.12	115.27
24	d	404	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
24	b	612	CLA	CAC-C3C-C4C	2.88	128.55	124.81
24	b	623	CLA	C2A-C1A-CHA	-2.88	118.82	123.86
24	C	503	CLA	CHD-C4C-NC	2.88	128.75	124.20
24	C	504	CLA	CHD-C4C-NC	2.88	128.75	124.20
24	c	512	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
24	B	607	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
24	b	622	CLA	O2D-CGD-CBD	2.88	116.38	111.27
24	c	513	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	B	617	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
24	c	508	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
24	c	510	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	b	623	CLA	O2A-CGA-CBA	2.88	120.93	111.91
40	V	205	HEC	C1D-ND-C4D	2.88	108.04	105.07
24	b	612	CLA	CMA-C3A-C2A	-2.88	102.23	113.83
24	a	409	CLA	CAA-C2A-C1A	-2.87	102.56	111.97
24	c	513	CLA	CMB-C2B-C1B	2.87	129.75	125.37
31	D	405	PL9	C32-C33-C34	-2.87	120.74	127.66
24	b	623	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	b	616	CLA	CBC-CAC-C3C	-2.87	104.52	112.43
24	c	517	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	a	412	CLA	CHC-C1C-C2C	-2.87	118.76	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	B	604	CLA	CMB-C2B-C1B	2.87	129.74	125.37
24	D	402	CLA	CHD-C4C-NC	2.87	128.72	124.20
24	b	615	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
24	b	625	CLA	CHD-C4C-NC	2.87	128.72	124.20
24	C	513	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
36	h	102	DGD	O1G-C1A-C2A	2.86	120.89	111.91
24	B	610	CLA	CMC-C2C-C1C	2.86	129.40	125.04
24	A	409	CLA	CED-O2D-CGD	2.86	122.41	115.94
24	c	510	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
24	c	516	CLA	C4-C3-C5	2.86	120.08	115.27
24	B	612	CLA	CHD-C4C-NC	2.86	128.71	124.20
24	c	517	CLA	CHD-C4C-NC	2.86	128.71	124.20
26	y	101	BCR	C24-C23-C22	-2.86	121.92	126.23
24	B	616	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
24	B	602	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
24	C	503	CLA	CMB-C2B-C1B	2.86	129.72	125.37
24	C	512	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
24	C	511	CLA	CHD-C4C-NC	2.85	128.70	124.20
24	c	506	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
24	a	409	CLA	CAC-C3C-C4C	2.85	128.51	124.81
24	B	617	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
26	h	101	BCR	C11-C10-C9	-2.85	123.24	127.31
24	B	617	CLA	CMB-C2B-C1B	2.85	129.71	125.37
31	D	405	PL9	C15-C14-C16	2.85	120.06	115.27
31	A	418	PL9	C7-C8-C9	-2.85	122.05	126.79
24	b	621	CLA	CED-O2D-CGD	2.85	122.38	115.94
24	B	617	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	B	612	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
31	a	416	PL9	C53-C6-C1	2.85	120.81	114.99
27	F	103	SQD	C44-O6-C1	-2.85	108.18	113.74
24	C	506	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
24	b	619	CLA	CAA-C2A-C3A	-2.84	104.99	112.78
24	B	605	CLA	C4-C3-C5	2.84	120.05	115.27
24	c	513	CLA	CHB-C1B-NB	-2.84	121.25	124.26
25	D	401	PHO	CMA-C3A-C4A	-2.84	108.15	114.38
34	b	608	HTG	O5-C1-C2	2.84	113.89	110.31
24	A	407	CLA	CHD-C4C-NC	2.84	128.68	124.20
24	B	612	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	C	506	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	c	527	BCR	C15-C14-C13	-2.84	123.26	127.31
26	d	405	BCR	C28-C27-C26	-2.84	109.00	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	513	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
24	a	410	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
24	C	510	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
24	c	513	CLA	O2A-CGA-CBA	2.84	120.81	111.91
24	a	409	CLA	C3B-C4B-NB	2.84	113.15	110.52
24	C	502	CLA	CAC-C3C-C4C	2.84	128.49	124.81
24	c	505	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
24	c	506	CLA	CHD-C4C-NC	2.83	128.67	124.20
24	b	621	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
24	B	607	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
24	b	617	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
24	a	410	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
24	B	614	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
24	B	602	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
24	b	613	CLA	CAC-C3C-C4C	2.83	128.48	124.81
24	c	513	CLA	CMC-C2C-C1C	2.83	129.34	125.04
26	T	103	BCR	C35-C13-C12	2.82	122.53	118.08
29	M	104	LMT	O5'-C5'-C4'	2.82	115.70	109.75
24	b	613	CLA	O2A-CGA-CBA	2.82	120.77	111.91
24	D	403	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
31	A	418	PL9	C12-C13-C14	-2.82	120.87	127.66
37	D	407	LHG	C5-O7-C7	-2.82	110.85	117.79
37	d	407	LHG	O8-C23-C24	2.82	120.75	111.91
25	A	408	PHO	C1A-C2A-C3A	-2.82	100.16	102.84
24	C	502	CLA	C1-O2A-CGA	2.82	123.83	116.44
24	c	506	CLA	O2A-CGA-CBA	2.82	120.75	111.91
24	d	404	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
24	B	605	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
24	c	514	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
24	C	512	CLA	CMB-C2B-C1B	2.81	129.65	125.37
24	d	403	CLA	C4-C3-C5	2.81	120.00	115.27
31	D	405	PL9	C12-C13-C14	-2.81	120.89	127.66
24	B	608	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
24	B	615	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
38	e	103	HEM	CHA-C4D-ND	2.81	127.84	124.37
24	b	623	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
36	H	102	DGD	O1G-C1A-C2A	2.81	120.72	111.91
24	c	507	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
24	C	505	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
36	c	519	DGD	O6D-C5D-C6D	2.81	112.33	106.67
24	C	509	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	b	615	CLA	CHD-C4C-NC	2.80	128.62	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	629	LMG	O8-C28-C29	2.80	120.71	111.91
35	M	101	LMG	O8-C28-C29	2.80	120.71	111.91
24	b	613	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	b	618	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
31	D	405	PL9	C7-C3-C4	2.80	119.15	116.88
24	B	603	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	c	517	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
26	c	518	BCR	C15-C14-C13	-2.80	123.32	127.31
24	c	517	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
24	c	506	CLA	C1-C2-C3	-2.80	121.20	126.04
38	e	103	HEM	C4A-NA-C1A	2.80	108.09	105.35
24	C	507	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	A	405	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
24	b	616	CLA	CMC-C2C-C1C	2.79	129.29	125.04
24	A	407	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	C	512	CLA	CHD-C4C-NC	2.79	128.60	124.20
24	c	515	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	c	516	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	b	615	CLA	O2A-CGA-CBA	2.79	120.67	111.91
24	C	512	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
24	c	516	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
35	z	101	LMG	O8-C28-C29	2.79	120.66	111.91
26	d	405	BCR	C29-C30-C25	2.79	114.77	110.48
24	b	612	CLA	O2A-CGA-CBA	2.79	120.65	111.91
29	f	103	LMT	C1B-O5B-C5B	2.79	119.16	113.69
24	c	514	CLA	CMB-C2B-C1B	2.79	129.61	125.37
24	b	612	CLA	CHD-C4C-NC	2.78	128.59	124.20
24	b	618	CLA	C4-C3-C5	2.78	119.95	115.27
26	c	518	BCR	C3-C4-C5	-2.78	109.11	114.08
38	e	103	HEM	CHB-C1B-NB	2.78	127.80	124.37
24	B	604	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
24	c	508	CLA	C1-C2-C3	-2.78	121.24	126.04
26	b	628	BCR	C24-C23-C22	-2.77	122.05	126.23
26	b	627	BCR	C33-C5-C6	-2.77	121.42	124.53
24	B	607	CLA	CHD-C4C-NC	2.77	128.56	124.20
40	V	205	HEC	CHA-C1A-NA	2.77	127.43	124.44
24	C	512	CLA	CMC-C2C-C1C	2.77	129.25	125.04
24	b	620	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
24	B	603	CLA	CAA-C2A-C3A	-2.77	105.21	112.78
26	A	410	BCR	C38-C26-C25	-2.76	121.42	124.53
24	c	511	CLA	C1-C2-C3	-2.76	121.26	126.04
24	B	609	CLA	CBC-CAC-C3C	-2.76	104.81	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	C1-O2A-CGA	2.76	123.69	116.44
24	b	617	CLA	O2A-CGA-CBA	2.76	120.57	111.91
31	d	406	PL9	C20-C19-C21	2.76	119.92	115.27
24	b	611	CLA	CMB-C2B-C1B	2.76	129.57	125.37
24	C	509	CLA	CAC-C3C-C4C	2.76	128.39	124.81
24	a	409	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
37	D	407	LHG	O8-C23-O10	-2.76	116.63	123.59
24	C	512	CLA	CHB-C1B-NB	-2.76	121.34	124.26
24	c	509	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
24	c	510	CLA	C4-C3-C5	2.76	119.91	115.27
26	k	101	BCR	C7-C8-C9	-2.76	122.07	126.23
24	b	614	CLA	C3B-C4B-NB	2.75	113.07	110.52
36	C	519	DGD	O1G-C1A-C2A	2.75	120.55	111.91
24	D	402	CLA	CHC-C1C-C2C	-2.75	119.08	126.73
24	A	409	CLA	C3B-C4B-NB	2.75	113.07	110.52
24	C	510	CLA	O2A-CGA-CBA	2.75	120.54	111.91
24	b	621	CLA	CHD-C4C-NC	2.75	128.54	124.20
26	h	101	BCR	C10-C11-C12	-2.75	114.64	123.22
26	y	101	BCR	C38-C26-C25	-2.75	121.44	124.53
37	L	101	LHG	O8-C23-C24	2.75	120.53	111.91
24	c	513	CLA	CAC-C3C-C4C	2.75	128.37	124.81
26	d	405	BCR	C3-C4-C5	-2.74	109.18	114.08
34	b	632	HTG	C1-O5-C5	2.74	117.64	112.58
24	B	609	CLA	CHD-C4C-NC	2.74	128.52	124.20
31	a	416	PL9	C40-C39-C41	2.74	119.88	115.27
24	b	616	CLA	CHD-C4C-NC	2.74	128.52	124.20
24	C	506	CLA	C4-C3-C5	2.74	119.88	115.27
24	B	603	CLA	CMA-C3A-C4A	-2.74	104.42	111.77
36	h	102	DGD	O1G-C1A-O1A	-2.74	116.68	123.59
37	d	407	LHG	O7-C7-C8	2.74	117.40	111.50
27	A	411	SQD	O9-S-C6	2.74	110.19	106.94
26	K	101	BCR	C24-C23-C22	-2.74	122.10	126.23
24	C	514	CLA	C3B-C4B-NB	2.74	113.05	110.52
27	L	102	SQD	O48-C23-C24	2.73	120.48	111.91
24	b	618	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
24	C	505	CLA	CHD-C4C-NC	2.73	128.50	124.20
24	C	514	CLA	CHC-C1C-C2C	-2.73	119.15	126.73
24	B	605	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
24	c	512	CLA	CMC-C2C-C1C	2.73	129.19	125.04
38	e	103	HEM	CAD-CBD-CGD	2.72	119.47	113.60
24	c	508	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	c	517	CLA	C4-C3-C5	2.72	119.85	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	517	CLA	O2A-CGA-CBA	2.72	120.45	111.91
24	d	403	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	a	409	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
24	A	407	CLA	CMC-C2C-C1C	2.72	129.18	125.04
24	c	514	CLA	CHD-C4C-NC	2.72	128.49	124.20
24	B	614	CLA	CHB-C1B-NB	-2.72	121.38	124.26
24	C	508	CLA	O2A-CGA-CBA	2.72	120.44	111.91
24	B	609	CLA	O2A-CGA-CBA	2.72	120.43	111.91
24	b	619	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
31	a	416	PL9	C25-C24-C26	2.71	119.84	115.27
26	Y	101	BCR	C37-C22-C23	2.71	122.35	118.08
24	d	404	CLA	CMC-C2C-C1C	2.71	129.17	125.04
26	B	620	BCR	C10-C11-C12	-2.71	114.75	123.22
24	C	507	CLA	CHD-C4C-NC	2.71	128.47	124.20
24	B	613	CLA	O2A-CGA-CBA	2.71	120.41	111.91
24	a	409	CLA	O2A-CGA-CBA	2.71	120.41	111.91
24	C	502	CLA	C4-C3-C5	2.71	119.83	115.27
24	b	619	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	B	604	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
24	A	407	CLA	C1-C2-C3	-2.71	121.36	126.04
37	e	102	LHG	O7-C7-C8	2.70	117.33	111.50
27	A	415	SQD	O8-S-C6	2.70	110.05	105.74
24	b	616	CLA	CED-O2D-CGD	2.70	122.05	115.94
24	B	606	CLA	O2A-CGA-CBA	2.70	120.38	111.91
24	c	510	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
24	B	613	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	C	510	CLA	C4-C3-C5	2.70	119.81	115.27
24	b	612	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
31	a	416	PL9	C7-C3-C2	-2.70	119.75	123.30
24	C	509	CLA	C4-C3-C5	2.69	119.80	115.27
25	d	401	PHO	CMB-C2B-C3B	2.69	129.72	124.68
24	B	612	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
40	v	205	HEC	CHA-C1A-NA	2.69	127.35	124.44
24	B	607	CLA	O2A-CGA-O1A	-2.69	116.80	123.59
27	L	102	SQD	C44-O6-C1	-2.69	108.48	113.74
26	B	619	BCR	C33-C5-C6	-2.69	121.51	124.53
24	c	516	CLA	O2A-CGA-CBA	2.69	120.34	111.91
27	B	621	SQD	O48-C23-C24	2.69	120.34	111.91
24	C	503	CLA	CHC-C1C-C2C	-2.69	119.27	126.73
37	D	409	LHG	O8-C23-O10	-2.68	116.82	123.59
24	D	402	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
24	c	515	CLA	O2A-CGA-CBA	2.68	120.32	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	619	CLA	C3B-C4B-NB	2.68	113.00	110.52
24	c	508	CLA	CHD-C4C-NC	2.68	128.43	124.20
24	c	515	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
34	V	206	HTG	C1-C2-C3	-2.68	105.30	110.59
24	A	409	CLA	CMC-C2C-C1C	2.68	129.12	125.04
31	D	405	PL9	C22-C23-C24	-2.68	121.21	127.66
26	c	518	BCR	C38-C26-C25	-2.68	121.52	124.53
25	d	401	PHO	C4A-C3A-C2A	-2.68	100.29	102.84
24	C	512	CLA	C4-C3-C5	2.67	119.77	115.27
24	B	614	CLA	C1-C2-C3	-2.67	121.42	126.04
24	D	403	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
24	c	508	CLA	CMC-C2C-C1C	2.67	129.10	125.04
27	A	411	SQD	O48-C23-C24	2.67	120.28	111.91
25	A	408	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
27	a	405	SQD	C3-C4-C5	2.67	115.00	110.24
24	b	612	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
37	e	102	LHG	O8-C23-C24	2.66	120.25	111.91
29	m	102	LMT	O5'-C5'-C4'	2.66	115.36	109.75
24	C	510	CLA	CMC-C2C-C1C	2.66	129.09	125.04
24	b	620	CLA	CMC-C2C-C1C	2.66	129.09	125.04
24	C	511	CLA	O2A-CGA-CBA	2.66	120.24	111.91
24	C	507	CLA	CMB-C2B-C1B	2.66	129.41	125.37
24	B	606	CLA	C3B-C4B-NB	2.65	112.98	110.52
24	C	507	CLA	CMC-C2C-C1C	2.65	129.08	125.04
26	H	101	BCR	C15-C14-C13	-2.65	123.52	127.31
24	D	402	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
27	B	621	SQD	C3-C4-C5	2.65	114.97	110.24
24	C	514	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	B	603	CLA	C4-C3-C5	2.65	119.73	115.27
24	b	622	CLA	C4-C3-C5	2.65	119.73	115.27
31	d	406	PL9	C53-C6-C1	2.65	120.40	114.99
24	b	617	CLA	CHD-C4C-NC	2.65	128.37	124.20
24	B	616	CLA	CAC-C3C-C4C	2.65	128.24	124.81
31	A	418	PL9	C25-C24-C26	2.65	119.72	115.27
36	e	101	DGD	O5D-C1E-C2E	2.65	112.43	108.30
26	T	103	BCR	C12-C13-C14	-2.64	114.88	118.94
24	A	409	CLA	CMA-C3A-C4A	-2.64	104.67	111.77
24	a	410	CLA	CHC-C1C-C2C	-2.64	119.39	126.73
24	b	614	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
24	c	513	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
24	b	618	CLA	O2A-CGA-CBA	2.64	120.19	111.91
36	H	102	DGD	O1G-C1A-O1A	-2.64	116.93	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
24	b	625	CLA	C1-C2-C3	-2.64	121.48	126.04
26	A	410	BCR	C37-C22-C21	-2.64	119.23	122.92
24	B	608	CLA	C4-C3-C5	2.63	119.70	115.27
24	C	507	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
24	b	619	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	C	508	CLA	CAC-C3C-C4C	2.63	128.22	124.81
24	B	604	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	a	410	CLA	C3B-C4B-NB	2.63	112.95	110.52
26	b	627	BCR	C37-C22-C21	-2.63	119.24	122.92
37	d	409	LHG	O8-C23-C24	2.63	120.16	111.91
24	B	611	CLA	CAA-CBA-CGA	-2.63	105.58	113.25
24	B	606	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	y	101	BCR	C21-C20-C19	-2.63	115.02	123.22
24	C	506	CLA	CMC-C2C-C1C	2.62	129.04	125.04
24	b	615	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
24	c	515	CLA	C1-O2A-CGA	2.62	123.32	116.44
26	t	101	BCR	C1-C6-C7	2.62	123.19	115.78
24	b	620	CLA	CHD-C4C-NC	2.62	128.33	124.20
34	V	206	HTG	O5-C1-C2	-2.62	107.02	110.31
36	C	517	DGD	C2G-O2G-C1B	-2.62	111.34	117.79
24	b	615	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
24	b	624	CLA	CMC-C2C-C1C	2.62	129.03	125.04
24	b	622	CLA	O2A-CGA-CBA	2.62	120.12	111.91
26	y	101	BCR	C10-C11-C12	-2.61	115.06	123.22
24	C	512	CLA	C1-C2-C3	-2.61	121.52	126.04
24	b	623	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
40	v	205	HEC	C3C-C4C-NC	-2.61	107.23	110.15
24	B	605	CLA	O2A-CGA-CBA	2.61	120.10	111.91
24	a	412	CLA	CMA-C3A-C2A	-2.61	103.29	113.83
24	d	404	CLA	CMB-C2B-C1B	2.61	129.34	125.37
35	C	521	LMG	O8-C28-C29	2.61	120.10	111.91
24	a	412	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
24	C	512	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
24	B	607	CLA	C4-C3-C5	2.61	119.66	115.27
27	f	102	SQD	O47-C7-O49	-2.61	117.40	123.70
24	c	508	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
24	b	612	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
38	E	102	HEM	CHA-C1A-NA	2.60	128.64	123.85
24	d	404	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
24	C	514	CLA	C4-C3-C5	2.60	119.64	115.27
27	a	414	SQD	C45-O47-C7	-2.60	111.39	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	517	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	d	404	CLA	C4-C3-C5	2.59	119.64	115.27
31	D	405	PL9	C25-C24-C26	2.59	119.63	115.27
24	c	511	CLA	CHD-C4C-NC	2.59	128.29	124.20
27	L	102	SQD	O7-S-C6	2.59	110.02	106.94
24	B	608	CLA	CAC-C3C-C4C	2.59	128.17	124.81
38	E	102	HEM	CHB-C1B-NB	2.59	127.57	124.37
24	B	604	CLA	CHC-C1C-C2C	-2.59	119.54	126.73
24	b	623	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
26	c	527	BCR	C28-C27-C26	-2.59	109.45	114.08
24	b	614	CLA	CHC-C1C-C2C	-2.59	119.54	126.73
24	c	512	CLA	C4-C3-C5	2.59	119.62	115.27
24	D	402	CLA	CMB-C2B-C1B	2.58	129.30	125.37
24	a	410	CLA	C4-C3-C5	2.58	119.62	115.27
24	C	504	CLA	CHC-C1C-C2C	-2.58	119.55	126.73
24	C	514	CLA	CMC-C2C-C1C	2.58	128.97	125.04
26	C	516	BCR	C28-C27-C26	-2.58	109.47	114.08
27	L	102	SQD	O47-C7-O49	-2.58	117.47	123.70
24	B	609	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
24	b	618	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
24	b	621	CLA	CHB-C1B-NB	-2.58	121.53	124.26
24	C	511	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	C	508	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	A	405	CLA	CAA-C2A-C1A	-2.58	103.53	111.97
31	a	416	PL9	C51-C49-C50	2.58	120.30	114.60
26	K	101	BCR	C15-C14-C13	-2.58	123.64	127.31
24	c	511	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
26	Y	101	BCR	C10-C11-C12	-2.57	115.19	123.22
24	C	505	CLA	CHB-C1B-NB	-2.57	121.53	124.26
31	d	406	PL9	C27-C28-C29	-2.57	121.47	127.66
31	d	406	PL9	C37-C38-C39	-2.57	121.47	127.66
24	b	623	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
27	F	103	SQD	O9-S-C6	2.57	109.99	106.94
35	a	415	LMG	O8-C28-C29	2.57	119.97	111.91
24	c	517	CLA	CMB-C2B-C1B	2.57	129.28	125.37
24	B	611	CLA	CMB-C2B-C1B	2.57	129.28	125.37
24	C	502	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
24	c	512	CLA	CHD-C4C-NC	2.56	128.24	124.20
24	C	507	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
26	C	516	BCR	C11-C10-C9	-2.56	123.65	127.31
24	c	516	CLA	C3B-C4B-NB	2.56	112.89	110.52
24	C	511	CLA	CBC-CAC-C3C	-2.56	105.37	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	620	CLA	CMB-C2B-C1B	2.56	129.27	125.37
24	b	618	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
24	B	605	CLA	OBD-CAD-C3D	-2.56	122.36	128.52
24	b	617	CLA	C1-C2-C3	-2.56	121.62	126.04
24	B	602	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
24	B	614	CLA	OBD-CAD-C3D	-2.56	122.37	128.52
24	B	609	CLA	CAC-C3C-C4C	2.56	128.13	124.81
24	b	613	CLA	CHD-C4C-NC	2.55	128.23	124.20
27	A	411	SQD	O48-C23-O10	-2.55	117.14	123.59
24	A	409	CLA	CHD-C4C-NC	2.55	128.23	124.20
24	A	405	CLA	CMC-C2C-C1C	2.55	128.93	125.04
24	C	512	CLA	O2A-CGA-CBA	2.55	119.92	111.91
24	A	409	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
24	b	617	CLA	OBD-CAD-C3D	-2.55	122.38	128.52
24	b	613	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
35	C	521	LMG	C3-C4-C5	2.55	114.79	110.24
27	a	414	SQD	O48-C23-C24	2.55	119.91	111.91
26	h	101	BCR	C7-C8-C9	-2.55	122.38	126.23
24	c	511	CLA	CAC-C3C-C4C	2.55	128.12	124.81
24	c	507	CLA	O2A-CGA-CBA	2.55	119.91	111.91
34	B	625	HTG	C1-O5-C5	2.55	117.28	112.58
24	C	505	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
27	f	102	SQD	O48-C23-C24	2.54	119.89	111.91
24	d	403	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
24	c	507	CLA	CHD-C4C-NC	2.54	128.21	124.20
24	d	404	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	A	418	PL9	C15-C14-C16	2.54	119.55	115.27
24	B	603	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
36	e	101	DGD	C1E-O6E-C5E	2.54	118.67	113.69
35	J	101	LMG	C9-C8-C7	-2.54	105.78	111.79
27	A	411	SQD	O47-C7-O49	-2.54	117.57	123.70
36	c	521	DGD	O1G-C1A-C2A	2.54	119.87	111.91
24	B	602	CLA	CBC-CAC-C3C	-2.54	105.44	112.43
24	b	611	CLA	C1-C2-C3	-2.54	121.66	126.04
24	B	612	CLA	CBC-CAC-C3C	-2.53	105.44	112.43
24	b	612	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
24	A	409	CLA	CHB-C4A-NA	2.53	128.02	124.51
34	c	525	HTG	C1-O5-C5	2.53	117.25	112.58
26	k	101	BCR	C10-C11-C12	-2.53	115.31	123.22
24	a	409	CLA	CMC-C2C-C1C	2.53	128.90	125.04
24	b	614	CLA	CMC-C2C-C1C	2.53	128.89	125.04
24	d	402	CLA	C4C-C3C-C2C	-2.53	103.21	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	PHO	C4A-C3A-C2A	-2.53	100.43	102.84
24	B	605	CLA	CHD-C4C-NC	2.53	128.19	124.20
24	c	516	CLA	CBA-CAA-C2A	-2.53	106.40	113.86
26	d	405	BCR	C2-C1-C6	2.53	114.37	110.48
24	c	516	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
34	C	524	HTG	O5-C1-C2	2.52	113.49	110.31
24	B	617	CLA	O2A-CGA-CBA	2.52	119.83	111.91
24	C	503	CLA	CMC-C2C-C1C	2.52	128.88	125.04
24	B	602	CLA	CMC-C2C-C1C	2.52	128.88	125.04
24	D	402	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
24	c	515	CLA	CMB-C2B-C1B	2.52	129.21	125.37
24	B	607	CLA	O2A-CGA-CBA	2.52	119.82	111.91
24	c	508	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
31	A	418	PL9	C30-C29-C31	2.52	119.51	115.27
24	C	506	CLA	C1-O2A-CGA	2.52	123.05	116.44
26	d	405	BCR	C15-C14-C13	-2.52	123.72	127.31
24	A	409	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
26	c	527	BCR	C29-C30-C25	2.52	114.36	110.48
24	C	513	CLA	C4-C3-C5	2.52	119.50	115.27
36	e	101	DGD	O1G-C1A-C2A	2.51	119.80	111.91
24	b	619	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
24	B	607	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
24	B	602	CLA	CAC-C3C-C4C	2.51	128.07	124.81
24	b	621	CLA	CMC-C2C-C1C	2.51	128.86	125.04
24	b	622	CLA	CHB-C1B-NB	-2.51	121.60	124.26
35	a	415	LMG	C7-O1-C1	-2.51	108.83	113.74
34	B	625	HTG	C1-C2-C3	2.51	115.54	110.59
29	M	104	LMT	O5B-C5B-C4B	2.51	114.25	109.69
24	C	509	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	B	612	CLA	C1-C2-C3	-2.51	121.70	126.04
26	a	413	BCR	C3-C4-C5	-2.51	109.60	114.08
26	c	527	BCR	C7-C8-C9	-2.51	122.45	126.23
26	k	101	BCR	C39-C30-C25	-2.51	106.23	110.30
35	Z	101	LMG	C1-O6-C5	2.50	118.60	113.69
35	c	523	LMG	O8-C28-C29	2.50	119.77	111.91
24	B	616	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
24	a	412	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
24	b	617	CLA	CMB-C2B-C1B	2.50	129.18	125.37
24	c	508	CLA	CAC-C3C-C4C	2.50	128.05	124.81
24	A	406	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
24	B	612	CLA	C2A-C1A-CHA	-2.50	119.50	123.86
40	V	205	HEC	C3B-C4B-NB	-2.49	107.39	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	101	BCR	C29-C30-C25	2.49	114.32	110.48
38	E	102	HEM	C4D-ND-C1D	2.49	107.65	105.07
24	a	410	CLA	O2A-CGA-CBA	2.49	119.73	111.91
24	c	505	CLA	O2A-CGA-CBA	2.49	119.73	111.91
24	D	403	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
24	b	620	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
24	C	513	CLA	C1-O2A-CGA	2.49	122.97	116.44
24	B	611	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	H	101	BCR	C24-C23-C22	-2.49	122.48	126.23
24	c	517	CLA	CHC-C1C-C2C	-2.48	119.83	126.73
26	C	515	BCR	C20-C21-C22	-2.48	123.77	127.31
36	c	519	DGD	C2G-O2G-C1B	-2.48	111.68	117.79
26	B	620	BCR	C3-C4-C5	-2.48	109.64	114.08
24	B	608	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
25	a	411	PHO	CMA-C3A-C4A	-2.48	108.94	114.38
24	C	510	CLA	CHD-C4C-NC	2.48	128.12	124.20
36	D	406	DGD	C4D-C3D-C2D	2.48	115.16	110.82
24	a	410	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
24	C	514	CLA	CHD-C4C-NC	2.48	128.11	124.20
26	h	101	BCR	C16-C15-C14	-2.48	118.40	123.47
34	d	412	HTG	C1-O5-C5	2.48	117.15	112.58
24	B	615	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	d	402	CLA	C1-C2-C3	-2.48	121.76	126.04
24	A	407	CLA	CHC-C1C-C2C	-2.48	119.85	126.73
24	B	616	CLA	CED-O2D-CGD	2.47	121.53	115.94
24	B	616	CLA	C2A-C1A-CHA	-2.47	119.53	123.86
24	C	509	CLA	C1-C2-C3	-2.47	121.77	126.04
31	A	418	PL9	C10-C9-C11	2.47	119.43	115.27
24	C	511	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
24	C	502	CLA	C3B-C4B-NB	2.47	112.81	110.52
24	C	504	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
27	A	411	SQD	C1-C2-C3	-2.47	104.85	110.00
24	c	516	CLA	CHC-C1C-C2C	-2.47	119.88	126.73
24	B	606	CLA	CAC-C3C-C4C	2.47	128.01	124.81
24	a	410	CLA	CMB-C2B-C1B	2.47	129.13	125.37
24	C	505	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
24	B	613	CLA	CHB-C1B-NB	-2.47	121.65	124.26
24	B	614	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	b	620	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	C	513	CLA	CHB-C1B-NB	-2.46	121.65	124.26
24	B	606	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
24	a	409	CLA	CHD-C4C-NC	2.46	128.08	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	C4-C3-C5	2.46	119.41	115.27
24	B	608	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	B	616	CLA	CHC-C1C-C2C	-2.46	119.91	126.73
26	t	101	BCR	C7-C6-C5	-2.45	115.52	121.46
31	D	405	PL9	C27-C28-C29	-2.45	121.75	127.66
24	A	406	CLA	CHB-C1B-NB	-2.45	121.66	124.26
24	C	512	CLA	C1-O2A-CGA	2.45	122.87	116.44
24	b	616	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
24	a	409	CLA	C4-C3-C5	2.45	119.39	115.27
24	b	617	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
37	d	408	LHG	O8-C23-C24	2.45	119.59	111.91
24	C	509	CLA	O2A-CGA-CBA	2.45	119.58	111.91
24	B	617	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
24	c	510	CLA	CMC-C2C-C1C	2.44	128.76	125.04
26	t	101	BCR	C21-C20-C19	-2.44	115.59	123.22
24	b	625	CLA	C4-C3-C5	2.44	119.38	115.27
26	C	516	BCR	C21-C20-C19	-2.44	115.60	123.22
26	C	516	BCR	C15-C14-C13	-2.44	123.83	127.31
24	c	512	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
24	C	502	CLA	C1-C2-C3	-2.44	121.82	126.04
31	a	416	PL9	C30-C29-C31	2.44	119.37	115.27
26	a	413	BCR	C33-C5-C6	-2.44	121.79	124.53
24	d	403	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
24	B	607	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
24	B	607	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
26	t	101	BCR	C2-C1-C6	2.43	114.23	110.48
24	B	608	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
24	B	606	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
24	c	507	CLA	CHC-C1C-C2C	-2.43	119.98	126.73
26	K	101	BCR	C16-C17-C18	-2.43	123.84	127.31
24	B	610	CLA	C1-C2-C3	-2.43	121.85	126.04
24	b	624	CLA	C11-C10-C8	-2.42	108.08	115.92
24	B	608	CLA	CMB-C2B-C1B	2.42	129.06	125.37
24	a	412	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	b	615	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
24	c	516	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
37	d	408	LHG	O8-C23-O10	-2.42	117.48	123.59
35	C	521	LMG	C8-O7-C10	-2.42	111.83	117.79
24	c	516	CLA	CMB-C2B-C1B	2.42	129.05	125.37
24	B	612	CLA	CMB-C2B-C1B	2.42	129.05	125.37
24	b	617	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
24	C	506	CLA	CHB-C1B-NB	-2.41	121.70	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	CHD-C4C-NC	2.41	128.01	124.20
24	B	617	CLA	O1D-CGD-CBD	-2.41	119.54	124.48
24	d	402	CLA	C1-O2A-CGA	2.41	122.78	116.44
26	B	619	BCR	C31-C1-C6	-2.41	106.39	110.30
40	v	205	HEC	CHD-C1D-ND	2.41	127.35	124.37
24	B	615	CLA	CMB-C2B-C1B	2.41	129.04	125.37
24	c	507	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
31	A	418	PL9	C42-C43-C44	-2.41	121.86	127.66
24	a	412	CLA	CMC-C2C-C1C	2.41	128.71	125.04
40	v	205	HEC	CHB-C1B-C2B	-2.41	121.22	124.98
24	c	506	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
24	b	619	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
26	C	515	BCR	C37-C22-C23	2.41	121.87	118.08
24	B	614	CLA	CAC-C3C-C4C	2.41	127.93	124.81
24	b	614	CLA	CAC-C3C-C2C	2.41	131.64	127.53
26	b	626	BCR	C16-C17-C18	-2.40	123.88	127.31
38	e	103	HEM	CHA-C1A-NA	2.40	128.27	123.85
24	B	604	CLA	C3B-C4B-NB	2.40	112.74	110.52
24	B	610	CLA	C1-O2A-CGA	2.40	122.74	116.44
27	F	103	SQD	O47-C7-O49	-2.40	117.90	123.70
24	B	605	CLA	C11-C10-C8	-2.40	108.16	115.92
36	c	520	DGD	O1G-C1A-C2A	2.40	119.44	111.91
26	A	410	BCR	C33-C5-C6	-2.40	121.83	124.53
26	t	101	BCR	C12-C13-C14	-2.40	115.26	118.94
24	b	620	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
24	b	616	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
24	c	514	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
24	D	402	CLA	C4-C3-C5	2.40	119.30	115.27
24	C	509	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
24	b	623	CLA	CMB-C2B-C1B	2.40	129.02	125.37
24	A	406	CLA	CAA-CBA-CGA	2.40	120.25	113.25
24	a	412	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
35	Z	101	LMG	C1-C2-C3	2.39	114.98	110.00
24	b	611	CLA	O2A-CGA-CBA	2.39	119.42	111.91
35	c	522	LMG	O8-C28-O10	-2.39	117.56	123.59
24	B	604	CLA	CMA-C3A-C2A	-2.39	104.19	113.83
24	a	412	CLA	O2A-CGA-CBA	2.39	119.41	111.91
24	d	403	CLA	CMA-C3A-C2A	-2.39	104.19	113.83
37	L	101	LHG	O7-C7-O9	-2.39	117.93	123.70
24	c	515	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
27	B	621	SQD	O47-C7-O49	-2.39	117.94	123.70
24	c	510	CLA	O2A-CGA-CBA	2.39	119.39	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	CMC-C2C-C1C	2.38	128.67	125.04
27	B	621	SQD	C44-O6-C1	-2.38	109.08	113.74
24	C	513	CLA	CMC-C2C-C1C	2.38	128.67	125.04
40	V	205	HEC	O2D-CGD-CBD	2.38	121.68	114.03
24	b	616	CLA	C4-C3-C5	2.38	119.28	115.27
29	M	104	LMT	O1B-C1B-C2B	2.38	114.27	108.10
24	B	611	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
24	d	404	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	C	502	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
24	A	409	CLA	O2A-CGA-CBA	2.38	119.36	111.91
24	B	606	CLA	C1-C2-C3	-2.38	121.93	126.04
24	a	410	CLA	CAC-C3C-C4C	2.38	127.89	124.81
29	A	416	LMT	C4B-C3B-C2B	-2.37	106.68	110.82
24	C	513	CLA	O2A-CGA-CBA	2.37	119.35	111.91
24	d	402	CLA	CMA-C3A-C2A	-2.37	104.27	113.83
24	C	510	CLA	CHB-C1B-NB	-2.37	121.75	124.26
24	c	509	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	c	511	CLA	C3B-C4B-NB	2.36	112.71	110.52
24	C	514	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
27	a	405	SQD	O48-C23-O10	-2.36	117.63	123.59
24	b	613	CLA	CMB-C2B-C1B	2.36	128.97	125.37
24	C	503	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
26	H	101	BCR	C10-C11-C12	-2.36	115.85	123.22
26	C	515	BCR	C38-C26-C25	-2.36	121.88	124.53
24	d	404	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
24	b	623	CLA	CHB-C4A-NA	2.36	127.77	124.51
29	C	522	LMT	O5'-C5'-C4'	2.36	114.72	109.75
24	C	508	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
26	T	103	BCR	C16-C15-C14	2.36	128.30	123.47
35	c	523	LMG	C8-O7-C10	-2.36	111.99	117.79
26	K	101	BCR	C3-C4-C5	-2.35	109.88	114.08
24	c	517	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	b	619	CLA	CMB-C2B-C1B	2.35	128.95	125.37
31	A	418	PL9	C17-C18-C19	-2.35	122.00	127.66
24	c	505	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
24	c	506	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
26	A	410	BCR	C24-C23-C22	-2.35	122.68	126.23
24	b	625	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
36	C	517	DGD	O1G-C1A-O1A	-2.35	117.66	123.59
24	B	604	CLA	CAC-C3C-C4C	2.35	127.86	124.81
31	d	406	PL9	O1-C4-C3	-2.35	118.13	120.72
26	c	518	BCR	C21-C20-C19	-2.35	115.88	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
38	e	103	HEM	C2A-C1A-NA	-2.35	107.52	110.15
24	c	510	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
36	D	406	DGD	O6D-C5D-C6D	2.35	111.40	106.67
34	B	632	HTG	C3-C4-C5	2.35	114.42	110.24
26	Y	101	BCR	C28-C27-C26	-2.35	109.89	114.08
26	t	101	BCR	C20-C21-C22	-2.35	123.96	127.31
36	C	518	DGD	O1G-C1A-O1A	-2.34	117.68	123.59
24	c	513	CLA	C4-C3-C5	2.34	119.21	115.27
24	A	407	CLA	CAC-C3C-C4C	2.34	127.85	124.81
24	b	625	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
24	B	608	CLA	CED-O2D-CGD	2.34	121.23	115.94
24	C	514	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
24	b	614	CLA	O2A-CGA-CBA	2.34	119.24	111.91
24	b	610	CLA	C2A-C1A-CHA	-2.34	119.78	123.86
34	B	624	HTG	O5-C1-C2	2.33	113.25	110.31
24	B	604	CLA	C1-O2A-CGA	2.33	122.57	116.44
24	A	406	CLA	C4C-C3C-C2C	-2.33	103.50	106.90
29	M	102	LMT	O6'-C6'-C5'	-2.33	103.29	111.29
24	B	609	CLA	CHB-C4A-NA	2.33	127.74	124.51
29	F	102	LMT	C1B-O5B-C5B	2.33	118.26	113.69
35	Z	101	LMG	C9-O8-C28	2.33	122.95	117.10
40	V	205	HEC	CHD-C4C-NC	2.33	128.13	123.85
24	C	508	CLA	CHC-C1C-C2C	-2.33	120.26	126.73
24	B	613	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
24	C	511	CLA	CMB-C2B-C1B	2.33	128.91	125.37
24	c	511	CLA	O2A-CGA-CBA	2.33	119.21	111.91
26	B	620	BCR	C28-C27-C26	-2.33	109.92	114.08
24	C	504	CLA	C3B-C4B-NB	2.33	112.67	110.52
24	B	609	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
24	d	404	CLA	CHB-C1B-NB	-2.32	121.80	124.26
31	d	406	PL9	C36-C37-C38	-2.32	104.25	111.88
31	D	405	PL9	C37-C38-C39	-2.32	122.07	127.66
36	c	520	DGD	C3B-C2B-C1B	-2.32	105.18	113.62
24	a	410	CLA	C1-C2-C3	-2.32	122.03	126.04
24	a	412	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
27	L	102	SQD	C1-C2-C3	-2.32	105.17	110.00
24	b	621	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
24	b	611	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
24	c	510	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
24	c	509	CLA	C4-C3-C5	2.32	119.17	115.27
29	m	102	LMT	C1'-O5'-C5'	2.31	118.23	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	c	519	DGD	O2G-C1B-O1B	-2.31	118.11	123.70
26	t	101	BCR	C7-C8-C9	-2.31	122.74	126.23
24	c	510	CLA	CAC-C3C-C4C	2.31	127.81	124.81
40	v	205	HEC	C3B-C4B-NB	-2.31	107.60	110.17
24	c	512	CLA	O2A-CGA-CBA	2.31	119.15	111.91
24	A	406	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
35	j	101	LMG	C1-O6-C5	2.31	118.22	113.69
24	C	508	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
27	a	405	SQD	O5-C5-C4	2.30	113.88	109.69
24	c	508	CLA	C11-C10-C8	-2.30	108.47	115.92
24	b	613	CLA	CHA-C1A-NA	-2.30	121.12	126.40
24	c	506	CLA	CMC-C2C-C1C	2.30	128.54	125.04
24	A	406	CLA	CMA-C3A-C2A	-2.30	104.55	113.83
31	D	405	PL9	C51-C49-C50	2.30	119.68	114.60
24	b	611	CLA	CHD-C4C-NC	2.30	127.83	124.20
24	b	618	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
24	C	513	CLA	CAC-C3C-C4C	2.30	127.79	124.81
26	b	626	BCR	C33-C5-C4	2.29	118.02	113.62
24	B	610	CLA	O2A-CGA-CBA	2.29	119.10	111.91
24	c	507	CLA	C3B-C4B-NB	2.29	112.64	110.52
24	c	508	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
24	B	603	CLA	CMC-C2C-C1C	2.29	128.53	125.04
24	C	504	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
27	B	621	SQD	C1-C2-C3	-2.29	105.23	110.00
31	d	406	PL9	C25-C24-C26	2.29	119.12	115.27
40	V	205	HEC	CAB-C3B-C4B	2.29	127.78	124.81
24	B	609	CLA	C1-C2-C3	-2.29	122.09	126.04
24	A	406	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
26	T	103	BCR	C21-C20-C19	-2.28	116.09	123.22
24	C	511	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
26	Y	101	BCR	C40-C30-C25	-2.28	106.60	110.30
26	k	101	BCR	C15-C14-C13	-2.28	124.06	127.31
24	C	505	CLA	CMB-C2B-C1B	2.28	128.84	125.37
36	h	102	DGD	C2G-O2G-C1B	-2.28	112.19	117.79
24	A	407	CLA	CAA-CBA-CGA	2.28	119.91	113.25
24	b	620	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
36	C	517	DGD	C3G-C2G-C1G	-2.28	106.41	111.79
24	b	610	CLA	CMB-C2B-C1B	2.27	128.83	125.37
24	c	514	CLA	CAC-C3C-C4C	2.27	127.76	124.81
24	B	614	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
24	B	614	CLA	CHD-C4C-NC	2.27	127.78	124.20
24	B	611	CLA	O2A-CGA-O1A	-2.27	117.86	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	CHC-C1C-C2C	-2.27	120.42	126.73
26	T	103	BCR	C36-C18-C19	2.27	121.65	118.08
31	d	406	PL9	C15-C14-C16	2.27	119.09	115.27
24	B	611	CLA	CHB-C1B-NB	-2.27	121.86	124.26
35	Z	101	LMG	C8-O7-C10	-2.27	112.21	117.79
24	C	505	CLA	C1-O2A-CGA	2.27	122.39	116.44
26	b	628	BCR	C2-C1-C6	2.27	113.97	110.48
27	B	621	SQD	O9-S-C6	2.26	109.63	106.94
24	b	623	CLA	C4-C3-C5	2.26	119.08	115.27
26	D	404	BCR	C21-C20-C19	-2.26	116.16	123.22
24	c	516	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
24	B	616	CLA	C4-C3-C5	2.26	119.08	115.27
26	b	628	BCR	C8-C7-C6	-2.26	120.85	127.20
40	v	205	HEC	C2A-C1A-NA	-2.26	108.12	110.32
24	d	402	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
24	B	602	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	C	502	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
27	L	102	SQD	O5-C5-C4	2.26	113.80	109.69
24	b	622	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	D	403	CLA	O2A-CGA-CBA	2.26	118.99	111.91
24	C	507	CLA	C2A-C1A-CHA	-2.26	119.92	123.86
24	b	610	CLA	CAC-C3C-C4C	2.26	127.74	124.81
24	c	514	CLA	CHB-C1B-NB	-2.25	121.87	124.26
24	a	409	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	D	401	PHO	C1-C2-C3	-2.25	122.15	126.04
37	d	408	LHG	C6-C5-C4	-2.25	106.46	111.79
26	B	620	BCR	C36-C18-C19	2.25	121.62	118.08
24	b	620	CLA	C1-C2-C3	-2.25	122.15	126.04
24	c	505	CLA	CMB-C2B-C1B	2.25	128.80	125.37
40	V	205	HEC	CHD-C1D-ND	2.25	127.15	124.37
35	z	101	LMG	C8-O7-C10	-2.25	112.25	117.79
24	B	610	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
26	B	618	BCR	C16-C17-C18	-2.25	124.10	127.31
37	D	407	LHG	O7-C7-O9	-2.25	118.27	123.70
37	L	101	LHG	O8-C23-O10	-2.25	117.92	123.59
24	B	614	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
24	b	625	CLA	CHB-C1B-NB	-2.25	121.88	124.26
24	c	517	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
24	A	405	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
24	C	514	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
24	B	602	CLA	C1-C2-C3	-2.24	122.17	126.04
31	d	406	PL9	C12-C13-C14	-2.24	122.27	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	CHB-C1B-NB	-2.24	121.89	124.26
35	C	501	LMG	O8-C28-C29	2.24	118.93	111.91
24	b	613	CLA	C6-C5-C3	-2.24	107.59	113.45
26	H	101	BCR	C29-C30-C25	2.23	113.92	110.48
24	b	624	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
40	V	205	HEC	CMD-C2D-C1D	2.23	128.44	125.04
27	a	414	SQD	O47-C7-O49	-2.23	118.31	123.70
24	b	614	CLA	C1-C2-C3	-2.23	122.18	126.04
24	c	515	CLA	CHB-C1B-NB	-2.23	121.89	124.26
24	C	506	CLA	CHD-C4C-NC	2.23	127.72	124.20
24	B	614	CLA	CMC-C2C-C1C	2.23	128.44	125.04
27	A	411	SQD	C1-O5-C5	-2.23	109.31	113.69
24	C	506	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
24	C	503	CLA	C4-C3-C5	2.23	119.02	115.27
24	a	409	CLA	CHB-C1B-C2B	-2.22	120.96	127.24
37	D	408	LHG	O8-C23-O10	-2.22	117.98	123.59
24	d	402	CLA	O2A-CGA-CBA	2.22	118.87	111.91
40	v	205	HEC	O2A-CGA-CBA	2.22	121.16	114.03
24	B	608	CLA	CHD-C4C-NC	2.22	127.70	124.20
24	B	613	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
40	v	205	HEC	CBB-CAB-C3B	2.22	118.54	112.43
24	c	506	CLA	C4-C3-C5	2.22	119.00	115.27
26	T	103	BCR	C10-C11-C12	-2.22	116.30	123.22
24	b	617	CLA	C4-C3-C5	2.21	119.00	115.27
24	b	613	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
24	B	609	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
26	t	101	BCR	C35-C13-C12	2.21	121.56	118.08
24	B	614	CLA	C4-C3-C5	2.21	118.99	115.27
26	B	618	BCR	C15-C14-C13	-2.21	124.15	127.31
24	B	607	CLA	CMB-C2B-C1B	2.21	128.74	125.37
26	D	404	BCR	C1-C6-C7	2.21	122.03	115.78
26	A	410	BCR	C3-C4-C5	-2.21	110.13	114.08
36	c	521	DGD	C2G-O2G-C1B	-2.21	112.35	117.79
29	B	635	LMT	C1'-O5'-C5'	2.21	118.02	113.69
24	B	616	CLA	O2A-CGA-CBA	2.21	118.83	111.91
24	A	406	CLA	O2A-CGA-CBA	2.21	118.83	111.91
26	b	626	BCR	C10-C11-C12	-2.21	116.33	123.22
24	c	511	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
24	c	515	CLA	CED-O2D-CGD	2.20	120.92	115.94
25	D	401	PHO	CBA-CAA-C2A	-2.20	107.38	113.81
24	A	407	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
24	A	409	CLA	O2A-CGA-O1A	-2.20	118.04	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	O2A-CGA-CBA	2.20	118.82	111.91
24	b	625	CLA	CHC-C1C-NC	2.20	127.54	124.20
24	C	513	CLA	CHB-C4A-NA	2.20	127.56	124.51
26	D	404	BCR	C3-C4-C5	-2.20	110.15	114.08
24	b	615	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
24	b	619	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
29	B	622	LMT	C1-O1'-C1'	-2.20	110.19	113.84
24	b	619	CLA	CMC-C2C-C1C	2.20	128.39	125.04
24	D	402	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
24	c	508	CLA	O2A-CGA-CBA	2.20	118.80	111.91
26	t	101	BCR	C11-C10-C9	-2.19	124.18	127.31
24	C	502	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
25	a	411	PHO	C1-O2A-CGA	2.19	122.20	116.44
40	V	205	HEC	C4A-NA-C1A	2.19	107.50	105.35
24	b	621	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
24	b	623	CLA	CED-O2D-CGD	2.19	120.90	115.94
24	B	604	CLA	C4-C3-C5	2.19	118.96	115.27
24	b	611	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
34	b	631	HTG	C1-C2-C3	2.19	114.92	110.59
24	D	403	CLA	CHD-C4C-NC	2.19	127.66	124.20
24	A	405	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
26	k	101	BCR	C29-C30-C25	2.19	113.85	110.48
24	B	611	CLA	C1-C2-C3	-2.19	122.26	126.04
24	A	407	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
25	a	411	PHO	C4-C3-C5	2.19	118.95	115.27
35	c	523	LMG	O8-C28-O10	-2.19	118.07	123.59
24	d	404	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
26	t	101	BCR	C29-C28-C27	-2.19	106.49	111.38
38	e	103	HEM	CHD-C1D-C2D	-2.18	121.57	124.98
24	c	513	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	c	508	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
24	C	502	CLA	O2A-CGA-CBA	2.18	118.76	111.91
26	D	404	BCR	C39-C30-C25	-2.18	106.76	110.30
35	b	629	LMG	O8-C28-O10	-2.18	118.10	123.59
24	B	615	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
26	K	101	BCR	C2-C1-C6	2.18	113.83	110.48
24	c	506	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	C	511	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
27	F	103	SQD	C1-C2-C3	-2.18	105.47	110.00
24	B	616	CLA	C1-C2-C3	-2.18	122.28	126.04
24	b	619	CLA	CMA-C3A-C4A	-2.17	105.93	111.77
24	c	517	CLA	CHB-C1B-C2B	-2.17	121.10	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
40	v	205	HEC	O2D-CGD-CBD	2.17	121.00	114.03
24	B	617	CLA	C4-C3-C5	2.17	118.92	115.27
24	c	516	CLA	CAC-C3C-C4C	2.17	127.63	124.81
24	C	511	CLA	C6-C7-C8	-2.17	108.90	115.92
24	b	618	CLA	CED-O2D-CGD	2.17	120.84	115.94
24	b	622	CLA	CHD-C4C-NC	2.17	127.62	124.20
24	b	616	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
26	h	101	BCR	C24-C23-C22	-2.17	122.96	126.23
24	b	610	CLA	O2A-CGA-CBA	2.17	118.71	111.91
26	b	626	BCR	C3-C4-C5	-2.17	110.21	114.08
24	b	616	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
24	c	514	CLA	C4-C3-C2	-2.17	118.12	123.68
38	E	102	HEM	O2A-CGA-CBA	2.17	120.99	114.03
24	c	510	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
24	D	403	CLA	CHB-C1B-NB	-2.16	121.97	124.26
26	b	626	BCR	C29-C30-C25	2.16	113.81	110.48
27	a	414	SQD	C1-O5-C5	-2.16	109.44	113.69
26	T	103	BCR	C16-C17-C18	-2.16	124.23	127.31
26	B	618	BCR	C34-C9-C10	-2.16	119.90	122.92
26	c	518	BCR	C16-C17-C18	-2.16	124.23	127.31
24	c	505	CLA	OBD-CAD-C3D	-2.16	123.33	128.52
26	t	101	BCR	C23-C24-C25	-2.16	121.14	127.20
24	b	617	CLA	CMC-C2C-C1C	2.16	128.32	125.04
25	a	411	PHO	CMB-C2B-C3B	2.16	128.71	124.68
26	K	101	BCR	C10-C11-C12	-2.16	116.49	123.22
24	b	624	CLA	O2A-CGA-CBA	2.16	118.67	111.91
24	b	618	CLA	CMC-C2C-C1C	2.16	128.32	125.04
36	e	101	DGD	O2G-C1B-O1B	-2.15	118.50	123.70
24	B	612	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
36	H	102	DGD	C3E-C4E-C5E	-2.15	106.40	110.24
26	d	405	BCR	C29-C28-C27	-2.15	106.57	111.38
24	B	617	CLA	CHB-C1B-NB	-2.15	121.98	124.26
24	c	505	CLA	CHD-C4C-NC	2.15	127.59	124.20
26	B	620	BCR	C2-C1-C6	2.15	113.79	110.48
40	v	205	HEC	CMD-C2D-C1D	2.15	128.31	125.04
24	C	511	CLA	C4-C3-C2	-2.15	118.17	123.68
24	C	504	CLA	CMC-C2C-C1C	2.15	128.31	125.04
24	C	509	CLA	CHB-C4A-NA	2.14	127.48	124.51
26	a	413	BCR	C8-C7-C6	-2.14	121.18	127.20
38	e	103	HEM	CBD-CAD-C3D	-2.14	106.67	112.63
24	C	512	CLA	CED-O2D-CGD	2.14	120.78	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	517	CLA	C3B-C4B-NB	2.14	112.50	110.52
24	B	603	CLA	CMB-C2B-C1B	2.14	128.63	125.37
26	h	101	BCR	C36-C18-C17	-2.14	119.92	122.92
36	C	517	DGD	O1G-C1A-C2A	2.14	118.62	111.91
24	c	514	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
24	c	514	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
26	b	627	BCR	C32-C1-C6	-2.14	106.84	110.30
26	k	101	BCR	C34-C9-C10	-2.13	119.93	122.92
24	c	514	CLA	CHB-C4A-NA	2.13	127.46	124.51
24	C	504	CLA	C4-C3-C5	2.13	118.86	115.27
40	V	205	HEC	C3C-C4C-NC	-2.13	107.76	110.15
31	A	418	PL9	C7-C3-C2	-2.13	120.50	123.30
24	C	514	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
24	A	406	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
24	A	405	CLA	CHD-C4C-NC	2.13	127.56	124.20
31	D	405	PL9	C42-C41-C39	-2.13	105.98	112.98
26	C	516	BCR	C3-C4-C5	-2.13	110.28	114.08
24	B	606	CLA	CED-O2D-CGD	2.13	120.75	115.94
24	B	614	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
24	C	514	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
24	C	510	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
36	c	521	DGD	C1D-O6D-C5D	2.12	117.86	113.69
26	Y	101	BCR	C24-C23-C22	-2.12	123.03	126.23
24	c	507	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	c	508	CLA	CMB-C2B-C1B	2.12	128.60	125.37
24	B	611	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
24	d	404	CLA	CGD-CBD-CAD	-2.12	103.87	110.73
26	H	101	BCR	C36-C18-C17	-2.12	119.95	122.92
24	b	614	CLA	OBD-CAD-C3D	-2.12	123.42	128.52
25	D	401	PHO	O1D-CGD-CBD	-2.12	121.21	124.74
26	b	628	BCR	C21-C20-C19	-2.12	116.61	123.22
27	f	102	SQD	O48-C23-O10	-2.12	118.25	123.59
26	d	405	BCR	C10-C11-C12	-2.12	116.61	123.22
24	b	623	CLA	C4-C3-C2	-2.12	118.25	123.68
24	b	612	CLA	C4-C3-C5	2.11	118.83	115.27
26	t	101	BCR	C37-C22-C23	2.11	121.41	118.08
35	C	501	LMG	C8-O7-C10	-2.11	112.59	117.79
26	d	405	BCR	C38-C26-C27	2.11	117.68	113.62
26	A	410	BCR	C8-C7-C6	-2.11	121.27	127.20
26	T	103	BCR	C2-C1-C6	2.11	113.73	110.48
24	a	410	CLA	CAA-CBA-CGA	2.11	119.42	113.25
35	C	521	LMG	O6-C5-C4	2.11	113.52	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	CMA-C3A-C4A	-2.11	106.11	111.77
24	b	617	CLA	CAC-C3C-C4C	2.11	127.55	124.81
36	C	517	DGD	O2G-C1B-O1B	-2.11	118.61	123.70
24	d	404	CLA	C6-C7-C8	-2.11	109.11	115.92
37	d	407	LHG	O7-C7-O9	-2.11	118.61	123.70
24	C	508	CLA	CED-O2D-CGD	2.11	120.70	115.94
24	c	505	CLA	C4-C3-C5	2.10	118.81	115.27
40	V	205	HEC	CAD-CBD-CGD	2.10	118.13	113.60
26	y	101	BCR	C40-C30-C25	-2.10	106.89	110.30
34	C	523	HTG	C1-O5-C5	2.10	116.46	112.58
26	H	101	BCR	C39-C30-C25	-2.10	106.89	110.30
24	B	611	CLA	CGD-CBD-CAD	-2.10	103.93	110.73
24	b	619	CLA	CMA-C3A-C2A	-2.10	105.35	113.83
24	B	614	CLA	CHB-C4A-NA	2.10	127.42	124.51
40	V	205	HEC	C2A-C1A-NA	-2.10	108.28	110.32
31	d	406	PL9	C40-C39-C38	-2.10	118.29	123.68
24	c	514	CLA	CMA-C3A-C4A	-2.10	106.13	111.77
24	C	512	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
24	B	606	CLA	CHB-C1B-NB	-2.10	122.03	124.26
24	B	610	CLA	C7-C6-C5	-2.10	107.66	113.36
25	a	411	PHO	CBA-CAA-C2A	-2.10	107.68	113.81
24	C	509	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
27	f	102	SQD	O9-S-C6	2.10	109.43	106.94
24	C	508	CLA	C1-C2-C3	-2.10	122.42	126.04
25	d	401	PHO	CMA-C3A-C4A	-2.10	109.78	114.38
24	B	609	CLA	CMA-C3A-C2A	-2.09	105.38	113.83
26	B	618	BCR	C21-C20-C19	-2.09	116.69	123.22
24	D	403	CLA	CHB-C4A-NA	2.09	127.41	124.51
26	h	101	BCR	C29-C30-C25	2.09	113.70	110.48
31	D	405	PL9	C45-C44-C46	2.09	118.79	115.27
24	B	614	CLA	CMA-C3A-C2A	-2.09	105.40	113.83
26	D	404	BCR	C15-C14-C13	-2.09	124.33	127.31
26	B	620	BCR	C23-C24-C25	-2.09	121.33	127.20
24	b	612	CLA	C7-C6-C5	-2.09	107.69	113.36
35	a	415	LMG	O7-C10-O9	-2.09	118.66	123.70
24	b	618	CLA	CAC-C3C-C4C	2.09	127.52	124.81
29	F	102	LMT	C2'-C3'-C4'	2.09	114.45	109.68
24	D	403	CLA	C1-C2-C3	-2.09	122.44	126.04
26	d	405	BCR	C21-C20-C19	-2.08	116.72	123.22
24	B	609	CLA	CMA-C3A-C4A	-2.08	106.18	111.77
24	C	506	CLA	CHA-C1A-NA	-2.08	121.63	126.40
36	c	519	DGD	O1G-C1A-C2A	2.08	118.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	M	104	LMT	C1B-O5B-C5B	2.08	117.77	113.69
24	C	509	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
25	A	408	PHO	O2A-CGA-CBA	2.08	118.42	111.91
40	V	205	HEC	CHB-C1B-C2B	-2.08	121.73	124.98
36	c	520	DGD	O1G-C1A-O1A	-2.08	118.35	123.59
25	a	411	PHO	CAA-CBA-CGA	-2.08	107.19	113.25
24	C	508	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
24	C	509	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
31	A	418	PL9	C40-C39-C41	2.08	118.76	115.27
27	f	102	SQD	O7-S-C6	2.07	109.41	106.94
24	C	511	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
27	a	414	SQD	O6-C44-C45	-2.07	105.89	110.90
24	B	605	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
24	c	510	CLA	CGD-CBD-CAD	-2.07	104.02	110.73
31	A	418	PL9	C51-C49-C50	2.07	119.18	114.60
38	E	102	HEM	C2A-C1A-NA	-2.07	107.83	110.15
36	C	517	DGD	O3G-C3G-C2G	-2.07	105.90	110.90
24	c	509	CLA	CED-O2D-CGD	2.07	120.62	115.94
26	h	101	BCR	C20-C21-C22	-2.07	124.36	127.31
37	D	408	LHG	O8-C23-C24	2.07	118.40	111.91
26	k	101	BCR	C34-C9-C8	2.07	121.34	118.08
24	c	512	CLA	CMB-C2B-C1B	2.07	128.52	125.37
24	b	624	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
26	D	404	BCR	C38-C26-C27	2.07	117.59	113.62
24	b	622	CLA	CMC-C2C-C1C	2.07	128.19	125.04
35	C	501	LMG	C7-O1-C1	-2.07	109.70	113.74
26	Y	101	BCR	C16-C17-C18	-2.07	124.36	127.31
24	C	503	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
27	a	414	SQD	O48-C23-O10	-2.07	118.38	123.59
27	A	411	SQD	C44-O6-C1	-2.06	109.70	113.74
24	A	406	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
24	b	621	CLA	OBD-CAD-C3D	-2.06	123.55	128.52
26	A	410	BCR	C20-C21-C22	-2.06	124.37	127.31
24	c	509	CLA	CHD-C4C-NC	2.06	127.45	124.20
36	c	519	DGD	O5D-C6D-C5D	-2.06	105.23	109.05
29	a	419	LMT	C1B-O1B-C4'	-2.06	112.87	117.96
24	b	615	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
27	a	414	SQD	O9-S-O7	-2.06	106.82	113.95
24	b	622	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
35	J	101	LMG	O8-C28-O10	-2.06	118.40	123.59
26	T	103	BCR	C29-C28-C27	-2.05	106.79	111.38
29	f	103	LMT	C4B-C3B-C2B	-2.05	107.24	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	F	103	SQD	O48-C23-O10	-2.05	118.41	123.59
24	b	622	CLA	CHA-C1A-NA	-2.05	121.69	126.40
26	k	101	BCR	C2-C1-C6	2.05	113.64	110.48
26	c	518	BCR	C37-C22-C21	-2.05	120.05	122.92
34	c	525	HTG	O5-C5-C4	2.05	113.42	109.69
40	v	205	HEC	CHD-C4C-NC	2.05	127.62	123.85
24	C	505	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
24	b	611	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
36	C	518	DGD	O2G-C1B-O1B	-2.05	118.75	123.70
24	C	504	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
24	c	514	CLA	CED-O2D-CGD	2.05	120.57	115.94
37	E	101	LHG	O8-C23-O10	-2.05	118.42	123.59
24	C	507	CLA	CED-O2D-CGD	2.05	120.57	115.94
26	B	620	BCR	C36-C18-C17	-2.05	120.05	122.92
31	D	405	PL9	C40-C39-C38	-2.05	118.42	123.68
24	d	403	CLA	CMB-C2B-C1B	2.05	128.49	125.37
24	b	612	CLA	CMB-C2B-C1B	2.05	128.49	125.37
24	c	517	CLA	CED-O2D-CGD	2.05	120.57	115.94
36	H	102	DGD	C2G-O2G-C1B	-2.05	112.75	117.79
24	A	405	CLA	C11-C10-C8	-2.04	109.31	115.92
24	C	505	CLA	C11-C10-C8	-2.04	109.31	115.92
24	b	616	CLA	CAA-CBA-CGA	2.04	119.22	113.25
24	B	603	CLA	C1-O2A-CGA	2.04	121.80	116.44
37	D	408	LHG	O7-C7-O9	-2.04	118.77	123.70
24	c	513	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
24	A	407	CLA	CHB-C1B-C2B	-2.04	121.47	127.24
24	B	615	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
26	K	101	BCR	C36-C18-C17	-2.04	120.06	122.92
24	c	509	CLA	C3B-C4B-NB	2.04	112.41	110.52
26	D	404	BCR	C16-C17-C18	-2.04	124.40	127.31
26	b	628	BCR	C16-C17-C18	-2.04	124.40	127.31
24	C	512	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
31	d	406	PL9	C45-C44-C46	2.04	118.70	115.27
26	Y	101	BCR	C21-C20-C19	-2.04	116.86	123.22
24	B	605	CLA	CHA-C1A-NA	-2.04	121.73	126.40
35	C	520	LMG	O8-C28-O10	-2.04	118.45	123.59
26	a	413	BCR	C37-C22-C21	-2.04	120.07	122.92
24	C	514	CLA	CHB-C1B-NB	-2.03	122.10	124.26
24	A	407	CLA	CMA-C3A-C2A	-2.03	105.62	113.83
24	c	512	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	c	516	CLA	C1-O2A-CGA	2.03	121.78	116.44
26	b	627	BCR	C8-C7-C6	-2.03	121.49	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	CLA	C3B-C4B-NB	2.03	112.40	110.52
24	c	517	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
24	b	613	CLA	C6-C7-C8	-2.03	109.35	115.92
25	a	411	PHO	O2A-CGA-CBA	2.03	118.28	111.91
24	b	611	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	b	610	CLA	CHB-C1B-C2B	-2.03	121.51	127.24
24	B	602	CLA	C4-C3-C5	2.03	118.68	115.27
24	B	608	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
26	c	527	BCR	C11-C12-C13	-2.03	120.72	126.42
34	d	412	HTG	C4-C3-C2	-2.03	107.29	110.82
26	b	628	BCR	C15-C14-C13	-2.02	124.42	127.31
24	b	622	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
26	K	101	BCR	C32-C1-C6	-2.02	107.02	110.30
24	A	405	CLA	CMA-C3A-C2A	-2.02	105.67	113.83
38	e	103	HEM	C4C-CHD-C1D	-2.02	121.70	126.06
24	d	403	CLA	CHD-C4C-NC	2.02	127.39	124.20
26	H	101	BCR	C7-C8-C9	-2.02	123.18	126.23
24	a	412	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
24	b	620	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
40	V	205	HEC	O2A-CGA-CBA	2.02	120.51	114.03
26	D	404	BCR	C7-C6-C5	-2.02	116.58	121.46
36	C	518	DGD	C3G-O3G-C1D	-2.02	109.80	113.74
24	D	402	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
24	b	621	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
24	c	516	CLA	CMA-C3A-C4A	-2.02	106.36	111.77
34	B	632	HTG	C6-C5-C4	-2.01	108.28	113.00
24	B	616	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
26	C	516	BCR	C15-C16-C17	-2.01	119.35	123.47
26	C	516	BCR	C29-C28-C27	-2.01	106.88	111.38
24	C	513	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
31	d	406	PL9	C11-C9-C8	-2.01	117.04	121.12
26	h	101	BCR	C37-C22-C21	-2.01	120.10	122.92
35	M	101	LMG	C9-C8-C7	-2.01	107.03	111.79
24	d	402	CLA	CAA-CBA-CGA	2.01	119.13	113.25
24	b	613	CLA	C4-C3-C5	2.01	118.65	115.27
24	A	406	CLA	CMB-C2B-C1B	2.01	128.43	125.37
35	c	523	LMG	O7-C10-O9	-2.01	118.84	123.70
38	E	102	HEM	CHA-C4D-ND	2.01	126.85	124.37
24	b	616	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
24	b	617	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
26	C	516	BCR	C36-C18-C19	2.01	121.24	118.08
24	d	402	CLA	CED-O2D-CGD	2.01	120.48	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	504	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
31	d	406	PL9	C30-C29-C31	2.01	118.64	115.27
24	b	612	CLA	C1-O2A-CGA	2.01	121.71	116.44
26	C	516	BCR	C37-C22-C23	2.00	121.24	118.08
26	C	516	BCR	C40-C30-C25	-2.00	107.05	110.30
26	t	101	BCR	C33-C5-C4	2.00	117.47	113.62
24	B	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
24	b	621	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	c	505	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
26	y	101	BCR	C11-C10-C9	-2.00	124.45	127.31
37	l	101	LHG	O8-C23-O10	-2.00	118.53	123.59
35	J	101	LMG	C7-O1-C1	-2.00	109.83	113.74
36	c	519	DGD	C4D-C3D-C2D	-2.00	107.33	110.82
25	D	401	PHO	O2A-CGA-CBA	2.00	118.19	111.91
24	c	515	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
37	d	407	LHG	O4-P-O5	2.00	122.13	112.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	205	HEC	NA
40	v	205	HEC	NA

All (1342) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	C2-C3-C5-C6
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	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	C4B-C3B-CAB-CBB
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	C2-C1-O2A-CGA
24	b	614	CLA	C2-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	b	615	CLA	CHA-CBD-CGD-O1D
24	b	615	CLA	CHA-CBD-CGD-O2D
24	b	623	CLA	CHA-CBD-CGD-O1D
24	b	623	CLA	CHA-CBD-CGD-O2D
24	b	623	CLA	CAD-CBD-CGD-O1D
24	b	623	CLA	CAD-CBD-CGD-O2D
24	b	623	CLA	C2-C3-C5-C6
24	b	623	CLA	C4-C3-C5-C6
24	c	512	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O2D
24	c	516	CLA	C2B-C3B-CAB-CBB
24	c	516	CLA	C4B-C3B-CAB-CBB
26	B	618	BCR	C1-C6-C7-C8
26	D	404	BCR	C7-C8-C9-C10
26	D	404	BCR	C7-C8-C9-C34
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C37-C22-C23-C24
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	d	405	BCR	C21-C22-C23-C24
26	d	405	BCR	C37-C22-C23-C24
26	d	405	BCR	C23-C24-C25-C30
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
26	y	101	BCR	C37-C22-C23-C24
27	A	415	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	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O8
27	B	621	SQD	C5-C6-S-O9
27	F	103	SQD	O49-C7-O47-C45
27	F	103	SQD	C8-C7-O47-C45
27	F	103	SQD	C5-C6-S-O7
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
27	a	405	SQD	O6-C44-C45-O47
27	a	405	SQD	O5-C5-C6-S
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	C5-C6-S-O9
28	A	413	GOL	C1-C2-C3-O3
28	A	414	GOL	C1-C2-C3-O3
28	B	627	GOL	O1-C1-C2-C3
28	B	628	GOL	O1-C1-C2-C3
28	B	630	GOL	O1-C1-C2-C3
28	B	630	GOL	C1-C2-C3-O3
28	C	525	GOL	O1-C1-C2-C3
28	F	101	GOL	O1-C1-C2-C3
28	O	301	GOL	O1-C1-C2-C3
28	T	102	GOL	O1-C1-C2-C3
28	V	201	GOL	C1-C2-C3-O3
28	a	401	GOL	C1-C2-C3-O3
28	a	402	GOL	O1-C1-C2-C3
28	b	606	GOL	O1-C1-C2-C3
28	f	101	GOL	O1-C1-C2-C3
29	A	416	LMT	C2'-C1'-O1'-C1
29	A	416	LMT	O5'-C1'-O1'-C1
29	B	635	LMT	C2'-C1'-O1'-C1
29	B	635	LMT	O5'-C1'-O1'-C1
29	C	522	LMT	C2'-C1'-O1'-C1
29	C	522	LMT	O5'-C1'-O1'-C1
29	F	102	LMT	C2'-C1'-O1'-C1
29	F	102	LMT	O5'-C1'-O1'-C1
29	M	104	LMT	O5'-C1'-O1'-C1
29	T	104	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
29	a	404	LMT	C2'-C1'-O1'-C1
29	a	404	LMT	O5'-C1'-O1'-C1
29	a	419	LMT	C2'-C1'-O1'-C1
29	a	419	LMT	O5'-C1'-O1'-C1
29	b	630	LMT	C2'-C1'-O1'-C1
29	b	630	LMT	O5'-C1'-O1'-C1
29	f	103	LMT	C2'-C1'-O1'-C1
29	f	103	LMT	O5'-C1'-O1'-C1
31	a	416	PL9	C9-C11-C12-C13
31	a	416	PL9	C20-C19-C21-C22
34	B	624	HTG	C2'-C1'-S1-C1
34	B	625	HTG	O5-C1-S1-C1'
34	b	632	HTG	O5-C1-S1-C1'
34	b	632	HTG	C2'-C1'-S1-C1
34	c	524	HTG	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
35	C	521	LMG	C11-C10-O7-C8
35	Z	101	LMG	O6-C1-O1-C7
35	Z	101	LMG	O9-C10-O7-C8
35	Z	101	LMG	C11-C10-O7-C8
35	z	101	LMG	O6-C1-O1-C7
35	z	101	LMG	O9-C10-O7-C8
36	D	406	DGD	C2B-C1B-O2G-C2G
36	D	406	DGD	C2D-C1D-O3G-C3G
36	D	406	DGD	O6D-C1D-O3G-C3G
36	e	101	DGD	C2B-C1B-O2G-C2G
36	e	101	DGD	O1B-C1B-O2G-C2G
36	e	101	DGD	O6E-C1E-O5D-C6D
37	D	408	LHG	C4-O6-P-O4
37	E	101	LHG	C3-O3-P-O4
37	E	101	LHG	C3-O3-P-O5
37	E	101	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O5
37	L	101	LHG	C4-O6-P-O4
37	d	408	LHG	O2-C2-C3-O3
37	d	408	LHG	C3-O3-P-O4
37	e	102	LHG	C3-O3-P-O5
37	e	102	LHG	C3-O3-P-O6
37	l	101	LHG	C4-O6-P-O4
37	l	101	LHG	C4-O6-P-O5
38	E	102	HEM	C2B-C3B-CAB-CBB
38	E	102	HEM	C2C-C3C-CAC-CBC
29	C	522	LMT	C3'-C4'-O1B-C1B
37	e	102	LHG	O10-C23-O8-C6
29	B	622	LMT	C3'-C4'-O1B-C1B
37	e	102	LHG	C24-C23-O8-C6
37	E	101	LHG	O10-C23-O8-C6
35	C	521	LMG	O9-C10-O7-C8
36	D	406	DGD	O1B-C1B-O2G-C2G
24	A	409	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
24	b	623	CLA	C3-C5-C6-C7
37	E	101	LHG	C24-C23-O8-C6
27	B	621	SQD	C8-C7-O47-C45
27	L	102	SQD	C8-C7-O47-C45
35	z	101	LMG	C11-C10-O7-C8
24	c	511	CLA	C4-C3-C5-C6
31	a	416	PL9	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
24	c	511	CLA	C2-C3-C5-C6
31	a	416	PL9	C18-C19-C21-C22
24	B	607	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C3-C5-C6-C7
24	c	510	CLA	C3-C5-C6-C7
35	z	101	LMG	O6-C5-C6-O5
34	b	632	HTG	S1-C1'-C2'-C3'
26	T	103	BCR	C13-C14-C15-C16
29	M	104	LMT	O5'-C5'-C6'-O6'
37	E	101	LHG	O2-C2-C3-O3
24	B	602	CLA	C3-C5-C6-C7
24	c	509	CLA	CBD-CGD-O2D-CED
29	M	102	LMT	O5B-C5B-C6B-O6B
36	C	518	DGD	CBB-CCB-CDB-CEB
29	f	103	LMT	C4'-C5'-C6'-O6'
29	M	104	LMT	O5B-C5B-C6B-O6B
29	M	104	LMT	C4'-C5'-C6'-O6'
38	e	103	HEM	C3D-CAD-CBD-CGD
35	C	521	LMG	O6-C5-C6-O5
24	B	615	CLA	C4-C3-C5-C6
31	A	418	PL9	C25-C24-C26-C27
31	a	416	PL9	C15-C14-C16-C17
31	a	416	PL9	C25-C24-C26-C27
31	A	418	PL9	C23-C24-C26-C27
31	a	416	PL9	C13-C14-C16-C17
31	a	416	PL9	C23-C24-C26-C27
24	b	615	CLA	C2A-CAA-CBA-CGA
35	z	101	LMG	C4-C5-C6-O5
31	D	405	PL9	C39-C41-C42-C43
31	d	406	PL9	C39-C41-C42-C43
24	C	510	CLA	CBA-CGA-O2A-C1
29	f	103	LMT	O5'-C5'-C6'-O6'
37	l	101	LHG	C7-C8-C9-C10
34	B	625	HTG	O5-C5-C6-O6
35	M	101	LMG	C15-C16-C17-C18
36	C	517	DGD	C2A-C3A-C4A-C5A
24	A	409	CLA	C13-C15-C16-C17
24	b	624	CLA	C10-C11-C12-C13
36	e	101	DGD	C2E-C1E-O5D-C6D
24	B	602	CLA	C11-C10-C8-C9
24	B	603	CLA	C14-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	502	CLA	C11-C12-C13-C14
24	c	510	CLA	C6-C7-C8-C9
24	c	513	CLA	C11-C10-C8-C9
34	B	632	HTG	C4-C5-C6-O6
35	Z	101	LMG	C10-C11-C12-C13
24	B	615	CLA	C10-C11-C12-C13
24	C	509	CLA	C5-C6-C7-C8
24	B	617	CLA	C10-C11-C12-C13
24	C	502	CLA	C15-C16-C17-C18
24	b	615	CLA	C13-C15-C16-C17
24	c	512	CLA	C15-C16-C17-C18
29	B	622	LMT	O5B-C5B-C6B-O6B
35	C	521	LMG	C28-C29-C30-C31
35	c	522	LMG	C10-C11-C12-C13
37	L	101	LHG	C7-C8-C9-C10
34	b	601	HTG	C1'-C2'-C3'-C4'
29	m	102	LMT	O5'-C5'-C6'-O6'
24	B	602	CLA	C10-C11-C12-C13
24	B	615	CLA	C5-C6-C7-C8
24	B	615	CLA	C8-C10-C11-C12
24	B	616	CLA	C8-C10-C11-C12
36	C	517	DGD	C4A-C5A-C6A-C7A
28	A	413	GOL	O2-C2-C3-O3
28	B	627	GOL	O1-C1-C2-O2
28	B	628	GOL	O1-C1-C2-O2
28	T	102	GOL	O1-C1-C2-O2
28	b	605	GOL	O1-C1-C2-O2
28	f	101	GOL	O1-C1-C2-O2
24	C	510	CLA	O1A-CGA-O2A-C1
27	A	415	SQD	C23-C24-C25-C26
36	C	518	DGD	C1B-C2B-C3B-C4B
37	D	407	LHG	C23-C24-C25-C26
35	j	101	LMG	O6-C5-C6-O5
24	C	505	CLA	C15-C16-C17-C18
24	C	507	CLA	C13-C15-C16-C17
24	a	412	CLA	C8-C10-C11-C12
24	C	510	CLA	C3-C5-C6-C7
24	c	513	CLA	C3-C5-C6-C7
35	a	415	LMG	C17-C18-C19-C20
29	A	416	LMT	O5B-C5B-C6B-O6B
24	b	610	CLA	C2-C1-O2A-CGA
36	c	521	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
29	C	522	LMT	O5B-C5B-C6B-O6B
24	b	615	CLA	C12-C13-C15-C16
24	b	625	CLA	C11-C12-C13-C15
35	a	415	LMG	C10-C11-C12-C13
29	T	104	LMT	O1'-C1-C2-C3
29	M	102	LMT	C4B-C5B-C6B-O6B
36	e	101	DGD	O6D-C1D-O3G-C3G
24	b	623	CLA	C5-C6-C7-C8
34	V	206	HTG	S1-C1'-C2'-C3'
24	a	412	CLA	C10-C11-C12-C13
24	c	513	CLA	C13-C15-C16-C17
35	C	521	LMG	C4-C5-C6-O5
35	C	501	LMG	C11-C10-O7-C8
37	e	102	LHG	C11-C12-C13-C14
24	C	507	CLA	C5-C6-C7-C8
24	C	509	CLA	C10-C11-C12-C13
24	c	511	CLA	C5-C6-C7-C8
37	L	101	LHG	C4-O6-P-O3
37	d	408	LHG	C3-O3-P-O6
37	l	101	LHG	C4-O6-P-O3
27	B	621	SQD	C7-C8-C9-C10
34	b	632	HTG	C1'-C2'-C3'-C4'
24	B	605	CLA	CBD-CGD-O2D-CED
37	E	101	LHG	C1-C2-C3-O3
35	C	501	LMG	O9-C10-O7-C8
24	B	615	CLA	C2-C3-C5-C6
24	b	623	CLA	C13-C15-C16-C17
24	b	622	CLA	CBD-CGD-O2D-CED
27	F	103	SQD	C26-C27-C28-C29
29	M	104	LMT	C4B-C5B-C6B-O6B
36	C	519	DGD	C8A-C9A-CAA-CBA
24	B	614	CLA	C13-C15-C16-C17
26	t	101	BCR	C13-C14-C15-C16
35	C	501	LMG	C11-C12-C13-C14
34	c	524	HTG	C1'-C2'-C3'-C4'
27	B	621	SQD	C31-C32-C33-C34
29	T	104	LMT	C4-C5-C6-C7
36	C	517	DGD	C4B-C5B-C6B-C7B
36	c	519	DGD	C5A-C6A-C7A-C8A
36	c	521	DGD	C6A-C7A-C8A-C9A
24	a	412	CLA	C16-C17-C18-C19
34	c	524	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
27	A	411	SQD	C9-C10-C11-C12
36	C	518	DGD	C9A-CAA-CBA-CCA
37	e	102	LHG	C24-C25-C26-C27
29	T	104	LMT	C11-C10-C9-C8
34	B	624	HTG	C2'-C3'-C4'-C5'
35	j	101	LMG	C19-C20-C21-C22
36	D	406	DGD	C6A-C7A-C8A-C9A
36	c	520	DGD	C9A-CAA-CBA-CCA
37	L	101	LHG	C14-C15-C16-C17
27	A	415	SQD	C30-C31-C32-C33
36	e	101	DGD	CCA-CDA-CEA-CFA
36	e	101	DGD	C8B-C9B-CAB-CBB
37	D	408	LHG	O2-C2-C3-O3
29	M	104	LMT	C2-C3-C4-C5
36	H	102	DGD	CBB-CCB-CDB-CEB
27	A	415	SQD	C2-C1-O6-C44
29	B	622	LMT	C2'-C1'-O1'-C1
36	C	518	DGD	C2E-C1E-O5D-C6D
36	c	520	DGD	C2E-C1E-O5D-C6D
36	e	101	DGD	C2D-C1D-O3G-C3G
27	L	102	SQD	C12-C13-C14-C15
29	B	635	LMT	C3-C4-C5-C6
35	c	522	LMG	C34-C35-C36-C37
37	D	407	LHG	C24-C25-C26-C27
31	a	416	PL9	C12-C11-C9-C8
24	B	604	CLA	C6-C7-C8-C9
24	a	410	CLA	C11-C12-C13-C14
36	c	519	DGD	O6D-C5D-C6D-O5D
35	C	501	LMG	C14-C15-C16-C17
35	C	501	LMG	C30-C31-C32-C33
35	b	629	LMG	C32-C33-C34-C35
24	c	514	CLA	C8-C10-C11-C12
34	B	632	HTG	O5-C5-C6-O6
35	M	101	LMG	C36-C37-C38-C39
36	c	521	DGD	C7A-C8A-C9A-CAA
28	B	626	GOL	C1-C2-C3-O3
28	B	629	GOL	O1-C1-C2-C3
28	V	202	GOL	O1-C1-C2-C3
28	b	602	GOL	O1-C1-C2-C3
28	b	602	GOL	C1-C2-C3-O3
28	b	604	GOL	O1-C1-C2-C3
28	b	605	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	o	301	GOL	C1-C2-C3-O3
28	v	201	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
37	d	409	LHG	O1-C1-C2-C3
35	c	522	LMG	C11-C10-O7-C8
29	T	104	LMT	C7-C8-C9-C10
35	M	101	LMG	C29-C30-C31-C32
36	C	519	DGD	CAA-CBA-CCA-CDA
37	D	409	LHG	C29-C30-C31-C32
37	d	407	LHG	C32-C33-C34-C35
27	L	102	SQD	C27-C28-C29-C30
35	a	415	LMG	C21-C22-C23-C24
35	b	629	LMG	C38-C39-C40-C41
35	z	101	LMG	C12-C13-C14-C15
36	D	406	DGD	C2A-C3A-C4A-C5A
34	b	632	HTG	O5-C5-C6-O6
24	B	604	CLA	C4B-C3B-CAB-CBB
24	B	608	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
24	C	513	CLA	C4B-C3B-CAB-CBB
24	b	611	CLA	C4B-C3B-CAB-CBB
24	b	616	CLA	C4B-C3B-CAB-CBB
24	b	618	CLA	C4B-C3B-CAB-CBB
24	c	506	CLA	C4B-C3B-CAB-CBB
24	c	511	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C4B-C3B-CAB-CBB
24	a	412	CLA	C16-C17-C18-C20
24	b	620	CLA	C16-C17-C18-C19
36	C	518	DGD	O6E-C1E-O5D-C6D
27	a	405	SQD	C31-C32-C33-C34
27	a	414	SQD	C11-C12-C13-C14
36	h	102	DGD	CAA-CBA-CCA-CDA
24	c	515	CLA	CBD-CGD-O2D-CED
35	C	520	LMG	C11-C12-C13-C14
35	J	101	LMG	C19-C20-C21-C22
27	L	102	SQD	C24-C23-O48-C46
27	a	414	SQD	C29-C30-C31-C32
29	M	104	LMT	C2-C1-O1'-C1'
27	a	405	SQD	C25-C26-C27-C28
35	M	101	LMG	C31-C32-C33-C34
36	C	517	DGD	C5B-C6B-C7B-C8B
37	l	101	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
36	c	521	DGD	C7B-C8B-C9B-CAB
37	D	407	LHG	C34-C35-C36-C37
29	a	404	LMT	C4B-C5B-C6B-O6B
27	B	621	SQD	C30-C31-C32-C33
35	j	101	LMG	C14-C15-C16-C17
36	C	517	DGD	C3B-C4B-C5B-C6B
36	C	517	DGD	O6D-C5D-C6D-O5D
36	e	101	DGD	O6D-C5D-C6D-O5D
34	C	524	HTG	O5-C5-C6-O6
27	A	415	SQD	C26-C27-C28-C29
36	c	520	DGD	C4A-C5A-C6A-C7A
24	C	511	CLA	C4-C3-C5-C6
31	D	405	PL9	C15-C14-C16-C17
24	c	516	CLA	CBA-CGA-O2A-C1
36	e	101	DGD	C2A-C1A-O1G-C1G
24	C	511	CLA	C2-C3-C5-C6
24	c	514	CLA	C2-C3-C5-C6
31	D	405	PL9	C13-C14-C16-C17
29	a	404	LMT	C2-C3-C4-C5
36	c	521	DGD	C6B-C7B-C8B-C9B
28	B	630	GOL	O1-C1-C2-O2
28	C	525	GOL	O1-C1-C2-O2
28	O	301	GOL	O1-C1-C2-O2
28	a	401	GOL	O2-C2-C3-O3
28	a	402	GOL	O1-C1-C2-O2
28	v	201	GOL	O1-C1-C2-O2
35	Z	101	LMG	C19-C20-C21-C22
36	c	519	DGD	C9A-CAA-CBA-CCA
36	c	519	DGD	C8B-C9B-CAB-CBB
29	C	522	LMT	O5'-C5'-C6'-O6'
27	A	411	SQD	C14-C15-C16-C17
29	T	104	LMT	C1-C2-C3-C4
24	B	608	CLA	C2B-C3B-CAB-CBB
24	C	503	CLA	C2B-C3B-CAB-CBB
24	C	506	CLA	C2B-C3B-CAB-CBB
24	C	508	CLA	C2B-C3B-CAB-CBB
24	C	513	CLA	C2B-C3B-CAB-CBB
24	b	611	CLA	C2B-C3B-CAB-CBB
24	b	616	CLA	C2B-C3B-CAB-CBB
24	b	618	CLA	C2B-C3B-CAB-CBB
24	c	506	CLA	C2B-C3B-CAB-CBB
24	c	511	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	d	403	CLA	C2B-C3B-CAB-CBB
29	B	635	LMT	C11-C10-C9-C8
36	C	518	DGD	C1A-C2A-C3A-C4A
37	d	408	LHG	C1-C2-C3-O3
35	a	415	LMG	C29-C30-C31-C32
35	b	629	LMG	C16-C17-C18-C19
24	B	617	CLA	C2-C1-O2A-CGA
24	c	513	CLA	C2-C1-O2A-CGA
24	c	517	CLA	C10-C11-C12-C13
27	A	411	SQD	C13-C14-C15-C16
36	e	101	DGD	C2A-C3A-C4A-C5A
26	B	618	BCR	C5-C6-C7-C8
26	b	626	BCR	C1-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
34	B	625	HTG	C3'-C4'-C5'-C6'
27	L	102	SQD	C35-C36-C37-C38
24	c	516	CLA	O1A-CGA-O2A-C1
24	B	602	CLA	C8-C10-C11-C12
24	c	514	CLA	C4-C3-C5-C6
24	B	604	CLA	C6-C7-C8-C10
24	B	615	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	C	507	CLA	C6-C7-C8-C10
24	a	410	CLA	C11-C12-C13-C15
24	b	612	CLA	C6-C7-C8-C10
25	D	401	PHO	C2-C3-C5-C6
27	L	102	SQD	O10-C23-O48-C46
36	e	101	DGD	O1A-C1A-O1G-C1G
35	c	522	LMG	O9-C10-O7-C8
24	C	513	CLA	CBA-CGA-O2A-C1
35	a	415	LMG	C12-C13-C14-C15
29	a	419	LMT	C6-C7-C8-C9
35	a	415	LMG	C14-C15-C16-C17
37	d	409	LHG	C31-C32-C33-C34
27	L	102	SQD	C30-C31-C32-C33
35	z	101	LMG	C15-C16-C17-C18
36	e	101	DGD	C2B-C3B-C4B-C5B
35	j	101	LMG	C38-C39-C40-C41
36	c	519	DGD	C4D-C5D-C6D-O5D
24	b	623	CLA	C16-C17-C18-C19
27	A	415	SQD	O5-C1-O6-C44
36	c	520	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
29	A	416	LMT	C6-C7-C8-C9
34	b	631	HTG	C2'-C3'-C4'-C5'
35	z	101	LMG	C13-C14-C15-C16
36	H	102	DGD	C3B-C4B-C5B-C6B
36	C	517	DGD	C1B-C2B-C3B-C4B
37	e	102	LHG	C23-C24-C25-C26
36	c	519	DGD	C7B-C8B-C9B-CAB
37	E	101	LHG	C24-C25-C26-C27
38	E	102	HEM	C4B-C3B-CAB-CBB
38	E	102	HEM	C4C-C3C-CAC-CBC
27	F	103	SQD	C31-C32-C33-C34
37	d	409	LHG	C29-C30-C31-C32
27	F	103	SQD	C2-C1-O6-C44
35	Z	101	LMG	O6-C5-C6-O5
37	D	409	LHG	C24-C23-O8-C6
27	L	102	SQD	C29-C30-C31-C32
37	D	407	LHG	C25-C26-C27-C28
37	l	101	LHG	C33-C34-C35-C36
34	b	601	HTG	C2'-C3'-C4'-C5'
35	b	629	LMG	C33-C34-C35-C36
36	c	519	DGD	O6E-C5E-C6E-O5E
24	b	610	CLA	C8-C10-C11-C12
24	c	508	CLA	C4-C3-C5-C6
25	D	401	PHO	C4-C3-C5-C6
35	C	501	LMG	C10-C11-C12-C13
34	B	625	HTG	C4-C5-C6-O6
24	c	508	CLA	C2-C3-C5-C6
31	A	418	PL9	C4-C3-C7-C8
31	a	416	PL9	C4-C3-C7-C8
27	L	102	SQD	C28-C29-C30-C31
24	B	615	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	C	507	CLA	C6-C7-C8-C9
24	b	612	CLA	C6-C7-C8-C9
24	b	619	CLA	C11-C12-C13-C14
24	b	623	CLA	C11-C12-C13-C14
24	b	625	CLA	C11-C12-C13-C14
24	c	513	CLA	C6-C7-C8-C9
34	b	631	HTG	C3'-C4'-C5'-C6'
36	D	406	DGD	C8B-C9B-CAB-CBB
36	h	102	DGD	C5B-C6B-C7B-C8B
24	c	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	b	620	CLA	C16-C17-C18-C20
24	b	623	CLA	C16-C17-C18-C20
37	d	408	LHG	C34-C35-C36-C37
24	a	409	CLA	C2C-C3C-CAC-CBC
36	C	518	DGD	C8A-C9A-CAA-CBA
36	e	101	DGD	C5A-C6A-C7A-C8A
35	c	523	LMG	C10-C11-C12-C13
35	C	501	LMG	C32-C33-C34-C35
36	c	519	DGD	CAB-CBB-CCB-CDB
38	e	103	HEM	C2A-CAA-CBA-CGA
24	B	616	CLA	C13-C15-C16-C17
35	C	501	LMG	C12-C13-C14-C15
34	C	524	HTG	S1-C1'-C2'-C3'
36	c	520	DGD	C3B-C4B-C5B-C6B
24	C	512	CLA	CBA-CGA-O2A-C1
27	B	621	SQD	C24-C23-O48-C46
37	d	408	LHG	C24-C23-O8-C6
35	j	101	LMG	C17-C18-C19-C20
29	f	103	LMT	C5-C6-C7-C8
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	510	CLA	C16-C17-C18-C19
36	C	517	DGD	C4D-C5D-C6D-O5D
27	A	415	SQD	O6-C44-C45-C46
27	B	621	SQD	C44-C45-C46-O48
27	B	621	SQD	C35-C36-C37-C38
27	F	103	SQD	C44-C45-C46-O48
27	a	405	SQD	O6-C44-C45-C46
27	a	414	SQD	O6-C44-C45-C46
35	Z	101	LMG	C7-C8-C9-O8
35	a	415	LMG	C7-C8-C9-O8
35	c	522	LMG	C7-C8-C9-O8
36	D	406	DGD	O1G-C1G-C2G-C3G
36	e	101	DGD	O1G-C1G-C2G-C3G
37	E	101	LHG	C4-C5-C6-O8
24	C	512	CLA	O1A-CGA-O2A-C1
37	d	408	LHG	O10-C23-O8-C6
35	C	521	LMG	C8-C7-O1-C1
36	C	518	DGD	C2G-C3G-O3G-C1D
36	c	520	DGD	C2G-C3G-O3G-C1D
36	c	520	DGD	C5D-C6D-O5D-C1E
29	C	522	LMT	C9-C10-C11-C12
36	H	102	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
35	b	629	LMG	C40-C41-C42-C43
36	D	406	DGD	C7A-C8A-C9A-CAA
36	C	517	DGD	O6E-C5E-C6E-O5E
37	E	101	LHG	C19-C20-C21-C22
29	B	622	LMT	O5'-C1'-O1'-C1
28	A	414	GOL	O2-C2-C3-O3
28	V	201	GOL	O2-C2-C3-O3
28	V	202	GOL	O1-C1-C2-O2
27	F	103	SQD	C30-C31-C32-C33
27	a	405	SQD	C28-C29-C30-C31
36	C	519	DGD	CDA-CEA-CFA-CGA
37	d	407	LHG	C29-C30-C31-C32
24	b	623	CLA	C10-C11-C12-C13
35	c	522	LMG	C20-C21-C22-C23
27	a	414	SQD	C9-C10-C11-C12
36	C	518	DGD	CAB-CBB-CCB-CDB
24	B	604	CLA	C5-C6-C7-C8
27	L	102	SQD	C24-C25-C26-C27
29	a	404	LMT	C7-C8-C9-C10
24	c	506	CLA	C16-C17-C18-C19
36	C	519	DGD	C2A-C1A-O1G-C1G
35	j	101	LMG	C36-C37-C38-C39
24	a	412	CLA	C15-C16-C17-C18
36	H	102	DGD	CDA-CEA-CFA-CGA
35	J	101	LMG	O6-C5-C6-O5
24	c	510	CLA	C15-C16-C17-C18
24	C	513	CLA	CBD-CGD-O2D-CED
24	D	403	CLA	C3-C5-C6-C7
36	H	102	DGD	C7B-C8B-C9B-CAB
24	c	509	CLA	O1D-CGD-O2D-CED
24	C	510	CLA	C5-C6-C7-C8
27	A	415	SQD	C24-C23-O48-C46
35	M	101	LMG	C16-C17-C18-C19
35	a	415	LMG	C33-C34-C35-C36
37	D	409	LHG	O10-C23-O8-C6
29	f	103	LMT	C4-C5-C6-C7
37	l	101	LHG	C12-C13-C14-C15
27	A	411	SQD	C7-C8-C9-C10
27	a	405	SQD	C23-C24-C25-C26
24	a	410	CLA	C10-C11-C12-C13
24	c	508	CLA	C15-C16-C17-C18
35	Z	101	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	O6-C44-C45-O47
35	c	522	LMG	O1-C7-C8-O7
37	L	101	LHG	C13-C14-C15-C16
27	a	414	SQD	C34-C35-C36-C37
36	e	101	DGD	C4D-C5D-C6D-O5D
24	B	602	CLA	C11-C10-C8-C7
24	B	603	CLA	C12-C13-C15-C16
24	B	616	CLA	C11-C12-C13-C15
24	B	616	CLA	C12-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C7
24	b	610	CLA	C6-C7-C8-C10
24	b	623	CLA	C11-C12-C13-C15
24	c	513	CLA	C6-C7-C8-C10
24	c	513	CLA	C12-C13-C15-C16
35	j	101	LMG	C35-C36-C37-C38
24	B	616	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C9
24	a	410	CLA	C6-C7-C8-C9
24	a	410	CLA	C14-C13-C15-C16
24	b	610	CLA	C6-C7-C8-C9
24	b	610	CLA	C11-C10-C8-C9
24	b	615	CLA	C14-C13-C15-C16
24	c	510	CLA	C11-C10-C8-C9
24	c	513	CLA	C14-C13-C15-C16
35	j	101	LMG	C13-C14-C15-C16
36	c	521	DGD	C5B-C6B-C7B-C8B
37	e	102	LHG	C14-C15-C16-C17
24	b	613	CLA	C13-C15-C16-C17
27	A	415	SQD	C11-C12-C13-C14
29	B	635	LMT	C4-C5-C6-C7
24	c	515	CLA	O1D-CGD-O2D-CED
24	B	611	CLA	C16-C17-C18-C20
27	L	102	SQD	C11-C12-C13-C14
34	B	624	HTG	C1'-C2'-C3'-C4'
26	y	101	BCR	C21-C22-C23-C24
29	m	102	LMT	C2-C3-C4-C5
29	b	630	LMT	C3'-C4'-O1B-C1B
24	B	602	CLA	CBA-CGA-O2A-C1
24	b	610	CLA	CBA-CGA-O2A-C1
35	C	501	LMG	C13-C14-C15-C16
36	H	102	DGD	C4E-C5E-C6E-O5E
35	a	415	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
24	C	508	CLA	C4B-C3B-CAB-CBB
24	c	516	CLA	C15-C16-C17-C18
37	l	101	LHG	O6-C4-C5-C6
31	a	416	PL9	C14-C16-C17-C18
29	a	404	LMT	O5B-C5B-C6B-O6B
24	C	511	CLA	CBA-CGA-O2A-C1
24	c	514	CLA	CBA-CGA-O2A-C1
29	M	105	LMT	O5'-C5'-C6'-O6'
35	c	523	LMG	O6-C5-C6-O5
27	B	621	SQD	C11-C10-C9-C8
27	a	414	SQD	C17-C18-C19-C20
36	H	102	DGD	C7A-C8A-C9A-CAA
31	A	418	PL9	C15-C14-C16-C17
31	a	416	PL9	C45-C44-C46-C47
27	B	621	SQD	O10-C23-O48-C46
34	B	632	HTG	C2'-C3'-C4'-C5'
24	B	611	CLA	C16-C17-C18-C19
37	L	101	LHG	C30-C31-C32-C33
36	c	521	DGD	C2A-C1A-O1G-C1G
24	C	514	CLA	C3A-C2A-CAA-CBA
24	b	617	CLA	C13-C15-C16-C17
27	L	102	SQD	C32-C33-C34-C35
29	B	635	LMT	C2-C3-C4-C5
36	D	406	DGD	C4B-C5B-C6B-C7B
27	F	103	SQD	C32-C33-C34-C35
35	C	520	LMG	C14-C15-C16-C17
35	c	522	LMG	C40-C41-C42-C43
24	c	515	CLA	CBA-CGA-O2A-C1
27	L	102	SQD	C44-C45-C46-O48
35	C	501	LMG	C7-C8-C9-O8
37	e	102	LHG	C4-C5-C6-O8
36	D	406	DGD	C1B-C2B-C3B-C4B
37	D	409	LHG	C12-C13-C14-C15
27	a	414	SQD	C15-C16-C17-C18
27	a	414	SQD	C19-C20-C21-C22
36	C	518	DGD	C6B-C7B-C8B-C9B
36	c	519	DGD	C2A-C3A-C4A-C5A
24	b	610	CLA	C16-C17-C18-C20
31	a	416	PL9	C43-C44-C46-C47
35	J	101	LMG	C13-C14-C15-C16
36	h	102	DGD	C9B-CAB-CBB-CCB
36	C	518	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
24	b	622	CLA	O1D-CGD-O2D-CED
28	B	630	GOL	O2-C2-C3-O3
28	F	101	GOL	O1-C1-C2-O2
28	b	602	GOL	O2-C2-C3-O3
28	b	604	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2
27	f	102	SQD	C24-C25-C26-C27
36	C	519	DGD	O1A-C1A-O1G-C1G
24	B	604	CLA	C2B-C3B-CAB-CBB
35	j	101	LMG	C16-C17-C18-C19
36	c	520	DGD	C2A-C3A-C4A-C5A
36	c	521	DGD	CBA-CCA-CDA-CEA
29	B	622	LMT	O5B-C1B-O1B-C4'
27	a	414	SQD	O6-C44-C45-O47
35	Z	101	LMG	O1-C7-C8-O7
35	Z	101	LMG	O7-C8-C9-O8
36	D	406	DGD	O2G-C2G-C3G-O3G
29	a	404	LMT	C6-C7-C8-C9
29	M	105	LMT	O5'-C1'-O1'-C1
24	b	615	CLA	C10-C11-C12-C13
24	b	625	CLA	C10-C11-C12-C13
31	A	418	PL9	C13-C14-C16-C17
24	D	403	CLA	C11-C10-C8-C9
24	b	615	CLA	C11-C10-C8-C9
24	b	623	CLA	C11-C10-C8-C9
24	c	516	CLA	C11-C10-C8-C9
27	a	405	SQD	C19-C20-C21-C22
31	A	418	PL9	C2-C3-C7-C8
36	c	519	DGD	C3A-C4A-C5A-C6A
27	a	405	SQD	C27-C28-C29-C30
26	C	516	BCR	C1-C6-C7-C8
26	C	516	BCR	C5-C6-C7-C8
26	D	404	BCR	C1-C6-C7-C8
26	D	404	BCR	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C30
26	b	627	BCR	C23-C24-C25-C26
26	b	627	BCR	C23-C24-C25-C30
24	b	610	CLA	C10-C11-C12-C13
26	Y	101	BCR	C37-C22-C23-C24
27	B	621	SQD	C17-C18-C19-C20
26	Y	101	BCR	C21-C22-C23-C24
29	m	102	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
35	a	415	LMG	O9-C10-O7-C8
37	E	101	LHG	C8-C7-O7-C5
27	a	414	SQD	C35-C36-C37-C38
24	c	506	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C20
37	L	101	LHG	C16-C17-C18-C19
24	C	511	CLA	O1A-CGA-O2A-C1
24	b	610	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	O1A-CGA-O2A-C1
27	A	415	SQD	O10-C23-O48-C46
36	c	521	DGD	C4A-C5A-C6A-C7A
37	e	102	LHG	O6-C4-C5-C6
36	h	102	DGD	O2G-C1B-C2B-C3B
35	C	520	LMG	C30-C31-C32-C33
36	e	101	DGD	C4A-C5A-C6A-C7A
24	c	510	CLA	C6-C7-C8-C10
24	c	510	CLA	C11-C10-C8-C7
24	c	516	CLA	C11-C10-C8-C7
36	C	518	DGD	C4A-C5A-C6A-C7A
24	b	619	CLA	C16-C17-C18-C20
27	a	414	SQD	C12-C13-C14-C15
36	e	101	DGD	C6A-C7A-C8A-C9A
37	D	409	LHG	C28-C29-C30-C31
35	C	520	LMG	C31-C32-C33-C34
24	c	515	CLA	O1A-CGA-O2A-C1
29	M	105	LMT	C5-C6-C7-C8
35	a	415	LMG	C11-C10-O7-C8
35	j	101	LMG	C15-C16-C17-C18
24	a	409	CLA	C4C-C3C-CAC-CBC
37	D	408	LHG	C13-C14-C15-C16
36	e	101	DGD	C7B-C8B-C9B-CAB
37	d	407	LHG	C25-C26-C27-C28
24	A	405	CLA	C13-C15-C16-C17
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	C	511	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	b	625	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CAD-CBD-CGD-O2D
24	c	517	CLA	CAD-CBD-CGD-O2D
25	D	401	PHO	CAD-CBD-CGD-O2D
38	e	103	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
38	e	103	HEM	C2C-C3C-CAC-CBC
36	D	406	DGD	C5B-C6B-C7B-C8B
24	d	404	CLA	C15-C16-C17-C18
29	f	103	LMT	C9-C10-C11-C12
24	b	625	CLA	C4-C3-C5-C6
34	B	623	HTG	C3'-C4'-C5'-C6'
35	C	520	LMG	C29-C30-C31-C32
27	F	103	SQD	O5-C1-O6-C44
24	b	625	CLA	C2-C3-C5-C6
31	D	405	PL9	C9-C11-C12-C13
35	c	522	LMG	C36-C37-C38-C39
37	D	409	LHG	C24-C25-C26-C27
35	C	501	LMG	O1-C7-C8-C9
35	z	101	LMG	O1-C7-C8-C9
37	D	409	LHG	C2-C3-O3-P
37	d	409	LHG	C2-C3-O3-P
37	l	101	LHG	O6-C4-C5-O7
24	b	610	CLA	CAA-CBA-CGA-O2A
24	b	619	CLA	C2A-CAA-CBA-CGA
36	h	102	DGD	C6A-C7A-C8A-C9A
24	A	405	CLA	C16-C17-C18-C19
24	C	510	CLA	C16-C17-C18-C19
37	E	101	LHG	O9-C7-O7-C5
24	B	602	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	610	CLA	CHA-CBD-CGD-O2D
24	c	506	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D
27	A	411	SQD	C18-C19-C20-C21
24	B	602	CLA	O1A-CGA-O2A-C1
27	F	103	SQD	C33-C34-C35-C36
35	b	629	LMG	C39-C40-C41-C42
29	M	105	LMT	C2'-C1'-O1'-C1
27	L	102	SQD	O47-C45-C46-O48
35	C	501	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
35	a	415	LMG	O7-C8-C9-O8
35	c	522	LMG	O7-C8-C9-O8
36	D	406	DGD	O1G-C1G-C2G-O2G
36	e	101	DGD	O1G-C1G-C2G-O2G
37	E	101	LHG	O7-C5-C6-O8
35	b	629	LMG	C37-C38-C39-C40
37	l	101	LHG	C17-C18-C19-C20
24	b	610	CLA	C16-C17-C18-C19
28	B	629	GOL	O1-C1-C2-O2
28	V	203	GOL	O2-C2-C3-O3
28	b	606	GOL	O1-C1-C2-O2
28	f	101	GOL	O2-C2-C3-O3
28	v	202	GOL	O1-C1-C2-O2
24	B	616	CLA	C4-C3-C5-C6
24	A	406	CLA	C2C-C3C-CAC-CBC
27	A	411	SQD	C16-C17-C18-C19
35	C	501	LMG	C36-C37-C38-C39
36	e	101	DGD	C9B-CAB-CBB-CCB
36	C	518	DGD	C3B-C4B-C5B-C6B
36	c	520	DGD	CCB-CDB-CEB-CFB
34	b	607	HTG	C4'-C5'-C6'-C7'
36	c	521	DGD	O1A-C1A-O1G-C1G
24	B	613	CLA	C8-C10-C11-C12
27	F	103	SQD	C5-C6-S-O8
26	C	516	BCR	C11-C12-C13-C35
26	b	628	BCR	C37-C22-C23-C24
28	b	606	GOL	C1-C2-C3-O3
28	o	301	GOL	O1-C1-C2-C3
36	c	520	DGD	C6A-C7A-C8A-C9A
24	b	621	CLA	C1A-C2A-CAA-CBA
24	B	616	CLA	C5-C6-C7-C8
34	b	601	HTG	C3'-C4'-C5'-C6'
37	D	408	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O3
36	H	102	DGD	O2G-C1B-C2B-C3B
24	b	612	CLA	C5-C6-C7-C8
35	C	520	LMG	C12-C13-C14-C15
36	C	518	DGD	C5A-C6A-C7A-C8A
35	C	520	LMG	O10-C28-O8-C9
37	L	101	LHG	C4-O6-P-O5
27	F	103	SQD	C34-C35-C36-C37
24	B	612	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	b	621	CLA	C8-C10-C11-C12
24	c	513	CLA	C15-C16-C17-C18
31	a	416	PL9	C39-C41-C42-C43
37	d	407	LHG	C30-C31-C32-C33
29	M	105	LMT	C1-C2-C3-C4
35	M	101	LMG	C34-C35-C36-C37
37	d	407	LHG	C11-C10-C9-C8
36	c	520	DGD	C2B-C3B-C4B-C5B
24	b	619	CLA	C16-C17-C18-C19
27	a	405	SQD	C35-C36-C37-C38
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	b	610	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	508	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
27	A	415	SQD	O5-C5-C6-S
27	F	103	SQD	C5-C6-S-O9
27	f	102	SQD	C31-C32-C33-C34
35	C	520	LMG	C29-C28-O8-C9
24	A	407	CLA	C11-C10-C8-C7
24	A	409	CLA	C6-C7-C8-C10
24	B	612	CLA	C12-C13-C15-C16
24	B	616	CLA	C2-C3-C5-C6
24	B	617	CLA	C6-C7-C8-C10
24	a	410	CLA	C11-C10-C8-C7
24	b	623	CLA	C12-C13-C15-C16
24	c	513	CLA	C11-C10-C8-C7
34	V	206	HTG	C2-C1-S1-C1'
37	e	102	LHG	O6-C4-C5-O7
35	a	415	LMG	C19-C20-C21-C22
37	d	409	LHG	C9-C10-C11-C12
24	b	620	CLA	C8-C10-C11-C12
29	f	103	LMT	C2B-C1B-O1B-C4'
27	a	414	SQD	C27-C28-C29-C30
29	b	630	LMT	C6-C7-C8-C9
27	a	405	SQD	C24-C25-C26-C27
35	C	521	LMG	C14-C15-C16-C17
36	H	102	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
24	d	402	CLA	C2C-C3C-CAC-CBC
27	A	415	SQD	C24-C25-C26-C27
35	c	522	LMG	O1-C7-C8-C9
35	C	501	LMG	O1-C7-C8-O7
35	z	101	LMG	O1-C7-C8-O7
37	e	102	LHG	O7-C5-C6-O8
24	c	510	CLA	C10-C11-C12-C13
29	C	522	LMT	O1'-C1-C2-C3
34	B	623	HTG	C4'-C5'-C6'-C7'
36	e	101	DGD	CAA-CBA-CCA-CDA
36	C	518	DGD	C5D-C6D-O5D-C1E
24	B	614	CLA	C15-C16-C17-C18
24	C	510	CLA	C10-C11-C12-C13
24	C	510	CLA	C13-C15-C16-C17
24	C	502	CLA	C13-C15-C16-C17
31	d	406	PL9	C45-C44-C46-C47
29	B	622	LMT	C2B-C1B-O1B-C4'
31	d	406	PL9	C43-C44-C46-C47
29	F	102	LMT	C2-C3-C4-C5
24	D	403	CLA	C8-C10-C11-C12
24	B	612	CLA	C14-C13-C15-C16
35	a	415	LMG	C31-C32-C33-C34
24	C	514	CLA	C3-C5-C6-C7
29	a	404	LMT	C3-C4-C5-C6
24	d	402	CLA	C15-C16-C17-C18
27	L	102	SQD	C31-C32-C33-C34
35	C	520	LMG	C35-C36-C37-C38
36	D	406	DGD	C3B-C4B-C5B-C6B
37	D	407	LHG	C11-C10-C9-C8
24	A	409	CLA	C2B-C3B-CAB-CBB
24	B	603	CLA	C2B-C3B-CAB-CBB
24	B	616	CLA	C2B-C3B-CAB-CBB
24	c	505	CLA	C2B-C3B-CAB-CBB
29	A	416	LMT	O1'-C1-C2-C3
35	b	629	LMG	C17-C18-C19-C20
37	d	409	LHG	C30-C31-C32-C33
24	b	623	CLA	C15-C16-C17-C18
35	C	501	LMG	C18-C19-C20-C21
36	C	519	DGD	C9A-CAA-CBA-CCA
36	c	519	DGD	CBA-CCA-CDA-CEA
37	D	407	LHG	C33-C34-C35-C36
27	B	621	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	C46-C45-O47-C7
24	b	623	CLA	CBD-CGD-O2D-CED
24	c	505	CLA	C2A-CAA-CBA-CGA
24	C	512	CLA	C2-C1-O2A-CGA
24	b	622	CLA	C2-C1-O2A-CGA
40	V	205	HEC	C2B-C3B-CAB-CBB
27	a	414	SQD	C7-C8-C9-C10
37	D	407	LHG	C7-C8-C9-C10
37	d	407	LHG	C33-C34-C35-C36
24	C	510	CLA	C8-C10-C11-C12
24	a	412	CLA	O1A-CGA-O2A-C1
37	D	407	LHG	O10-C23-O8-C6
29	m	102	LMT	C11-C10-C9-C8
24	C	513	CLA	O1D-CGD-O2D-CED
31	D	405	PL9	C35-C34-C36-C37
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	D	404	BCR	C5-C6-C7-C8
26	b	626	BCR	C5-C6-C7-C8
37	E	101	LHG	C15-C16-C17-C18
24	b	624	CLA	C16-C17-C18-C19
36	C	517	DGD	O6E-C1E-O5D-C6D
24	B	611	CLA	C2A-CAA-CBA-CGA
29	M	104	LMT	C2'-C1'-O1'-C1
36	C	517	DGD	C2E-C1E-O5D-C6D
27	B	621	SQD	O47-C45-C46-O48
27	F	103	SQD	O47-C45-C46-O48
37	D	408	LHG	C4-O6-P-O3
37	e	102	LHG	C4-O6-P-O3
35	c	522	LMG	C39-C40-C41-C42
37	D	408	LHG	C11-C10-C9-C8
27	f	102	SQD	O6-C44-C45-C46
24	a	410	CLA	C12-C13-C15-C16
24	b	610	CLA	C11-C10-C8-C7
24	b	615	CLA	C11-C10-C8-C7
24	d	403	CLA	C11-C12-C13-C15
24	A	407	CLA	C11-C10-C8-C9
24	a	410	CLA	C11-C10-C8-C9
26	h	101	BCR	C9-C10-C11-C12
36	D	406	DGD	C2B-C3B-C4B-C5B
34	B	625	HTG	C2'-C3'-C4'-C5'
37	e	102	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
36	H	102	DGD	CCA-CDA-CEA-CFA
37	d	407	LHG	C34-C35-C36-C37
37	D	409	LHG	C25-C26-C27-C28
27	a	405	SQD	C24-C23-O48-C46
28	v	202	GOL	C1-C2-C3-O3
36	c	519	DGD	C1A-C2A-C3A-C4A
28	B	626	GOL	O2-C2-C3-O3
25	a	411	PHO	C2C-C3C-CAC-CBC
27	f	102	SQD	C34-C35-C36-C37
24	b	611	CLA	C16-C17-C18-C19
24	a	412	CLA	CBA-CGA-O2A-C1
27	a	405	SQD	O10-C23-O48-C46
24	A	409	CLA	C4B-C3B-CAB-CBB
24	B	603	CLA	C4B-C3B-CAB-CBB
24	B	612	CLA	C4B-C3B-CAB-CBB
24	c	505	CLA	C4B-C3B-CAB-CBB
36	c	519	DGD	O6E-C1E-O5D-C6D
26	k	101	BCR	C9-C10-C11-C12
29	C	522	LMT	C1-C2-C3-C4
29	f	103	LMT	C1-C2-C3-C4
31	A	418	PL9	C19-C21-C22-C23
27	a	405	SQD	C29-C30-C31-C32
34	B	624	HTG	C3'-C4'-C5'-C6'
35	J	101	LMG	C20-C21-C22-C23
38	e	103	HEM	C4B-C3B-CAB-CBB
24	B	605	CLA	C4-C3-C5-C6
24	B	607	CLA	C10-C11-C12-C13
24	b	618	CLA	C2-C3-C5-C6
37	d	409	LHG	O10-C23-O8-C6
37	E	101	LHG	C25-C26-C27-C28
24	B	602	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C2-C1-O2A-CGA
24	c	515	CLA	C2-C1-O2A-CGA
24	c	517	CLA	C2-C1-O2A-CGA
27	L	102	SQD	C11-C10-C9-C8
29	B	622	LMT	O1'-C1-C2-C3
27	a	414	SQD	C10-C11-C12-C13
24	B	614	CLA	C10-C11-C12-C13
36	h	102	DGD	CCB-CDB-CEB-CFB
24	B	610	CLA	C3A-C2A-CAA-CBA
37	D	407	LHG	C17-C18-C19-C20
29	M	104	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	d	409	LHG	C33-C34-C35-C36
40	v	205	HEC	C2B-C3B-CAB-CBB
29	C	522	LMT	C2B-C1B-O1B-C4'
25	d	401	PHO	C2C-C3C-CAC-CBC
24	B	615	CLA	C6-C7-C8-C9
24	C	505	CLA	C11-C12-C13-C14
24	b	616	CLA	C6-C7-C8-C9
24	c	514	CLA	C11-C12-C13-C14
24	b	624	CLA	C16-C17-C18-C20
38	E	102	HEM	C2A-CAA-CBA-CGA
29	B	622	LMT	C5-C6-C7-C8
35	C	501	LMG	C17-C18-C19-C20
35	Z	101	LMG	O1-C7-C8-C9
36	h	102	DGD	O1G-C1G-C2G-C3G
38	E	102	HEM	CAD-CBD-CGD-O2D
37	e	102	LHG	C18-C19-C20-C21
38	E	102	HEM	CAD-CBD-CGD-O1D
34	b	631	HTG	C4-C5-C6-O6
27	f	102	SQD	C30-C31-C32-C33
37	L	101	LHG	C23-C24-C25-C26
37	l	101	LHG	C13-C14-C15-C16
38	e	103	HEM	CAA-CBA-CGA-O1A
24	a	412	CLA	C4-C3-C5-C6
31	A	418	PL9	C45-C44-C46-C47
24	C	507	CLA	C1A-C2A-CAA-CBA
24	c	505	CLA	C1A-C2A-CAA-CBA
24	d	402	CLA	C1A-C2A-CAA-CBA
37	D	407	LHG	C24-C23-O8-C6
24	B	604	CLA	C11-C10-C8-C7
24	C	502	CLA	C11-C12-C13-C15
24	C	507	CLA	C12-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
24	a	410	CLA	C6-C7-C8-C10
24	b	625	CLA	C12-C13-C15-C16
24	C	511	CLA	C8-C10-C11-C12
34	C	524	HTG	C1'-C2'-C3'-C4'
24	C	513	CLA	C3-C5-C6-C7
36	H	102	DGD	O6E-C5E-C6E-O5E
24	d	402	CLA	C4C-C3C-CAC-CBC
35	J	101	LMG	C16-C17-C18-C19
37	d	407	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
24	b	612	CLA	C2A-CAA-CBA-CGA
24	A	409	CLA	C8-C10-C11-C12
24	B	605	CLA	C13-C15-C16-C17
35	j	101	LMG	C29-C30-C31-C32
37	L	101	LHG	C28-C29-C30-C31
35	C	520	LMG	C16-C17-C18-C19
35	C	521	LMG	C18-C19-C20-C21
24	a	410	CLA	C16-C17-C18-C20
24	c	517	CLA	C4-C3-C5-C6
31	A	418	PL9	C30-C29-C31-C32
27	a	414	SQD	C30-C31-C32-C33
35	a	415	LMG	C28-C29-C30-C31
24	B	610	CLA	C2-C3-C5-C6
25	a	411	PHO	C2-C3-C5-C6
35	z	101	LMG	C16-C17-C18-C19
40	V	205	HEC	CAD-CBD-CGD-O2D
35	a	415	LMG	C22-C23-C24-C25
27	A	411	SQD	O6-C44-C45-O47
35	c	523	LMG	O7-C8-C9-O8
37	d	408	LHG	O7-C5-C6-O8
37	D	408	LHG	C1-C2-C3-O3
37	d	407	LHG	C1-C2-C3-O3
35	J	101	LMG	C30-C31-C32-C33
24	c	516	CLA	C2-C1-O2A-CGA
24	a	412	CLA	C2-C3-C5-C6
31	A	418	PL9	C43-C44-C46-C47
31	D	405	PL9	C33-C34-C36-C37
24	A	409	CLA	O1A-CGA-O2A-C1
27	A	411	SQD	C15-C16-C17-C18
27	A	415	SQD	C17-C18-C19-C20
36	c	520	DGD	C7A-C8A-C9A-CAA
24	B	615	CLA	C16-C17-C18-C19
37	L	101	LHG	C33-C34-C35-C36
37	D	408	LHG	C33-C34-C35-C36
36	C	517	DGD	O1A-C1A-O1G-C1G
29	B	635	LMT	C7-C8-C9-C10
24	B	606	CLA	O1A-CGA-O2A-C1
26	T	103	BCR	C5-C6-C7-C8
26	c	518	BCR	C1-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
36	C	517	DGD	O2G-C1B-C2B-C3B
36	D	406	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
28	v	202	GOL	O1-C1-C2-C3
37	D	407	LHG	O1-C1-C2-C3
31	D	405	PL9	C45-C44-C46-C47
24	d	402	CLA	C13-C15-C16-C17
27	B	621	SQD	C34-C35-C36-C37
29	a	419	LMT	C7-C8-C9-C10
36	H	102	DGD	CBA-CCA-CDA-CEA
36	c	520	DGD	C9B-CAB-CBB-CCB
35	Z	101	LMG	C8-C7-O1-C1
36	c	519	DGD	C5D-C6D-O5D-C1E
27	L	102	SQD	C7-C8-C9-C10
36	C	517	DGD	C2A-C1A-O1G-C1G
24	B	602	CLA	CAA-CBA-CGA-O2A
35	C	501	LMG	O8-C28-C29-C30
24	b	618	CLA	C16-C17-C18-C19
37	D	409	LHG	C33-C34-C35-C36
38	e	103	HEM	CAD-CBD-CGD-O1D
24	d	404	CLA	CBD-CGD-O2D-CED
35	J	101	LMG	C34-C35-C36-C37
37	e	102	LHG	C28-C29-C30-C31
40	V	205	HEC	CAD-CBD-CGD-O1D
24	C	505	CLA	C12-C13-C15-C16
24	c	514	CLA	C12-C13-C15-C16
24	c	517	CLA	C2-C3-C5-C6
24	A	405	CLA	C15-C16-C17-C18
36	h	102	DGD	CDA-CEA-CFA-CGA
28	o	301	GOL	O2-C2-C3-O3
24	C	514	CLA	O1A-CGA-O2A-C1
29	B	622	LMT	C4B-C5B-C6B-O6B
35	a	415	LMG	C30-C31-C32-C33
24	b	611	CLA	C16-C17-C18-C20
40	v	205	HEC	CAD-CBD-CGD-O2D
34	B	623	HTG	C2'-C1'-S1-C1
34	V	206	HTG	O5-C1-S1-C1'
34	b	608	HTG	O5-C1-S1-C1'
24	C	513	CLA	CAA-CBA-CGA-O2A
24	C	507	CLA	C4-C3-C5-C6
31	A	418	PL9	C20-C19-C21-C22
31	A	418	PL9	C40-C39-C41-C42
37	D	407	LHG	C11-C12-C13-C14
31	A	418	PL9	C28-C29-C31-C32
36	C	519	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
24	A	409	CLA	C6-C7-C8-C9
24	B	607	CLA	C11-C12-C13-C14
24	C	507	CLA	C14-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C9
24	d	403	CLA	C11-C12-C13-C14
38	e	103	HEM	CAA-CBA-CGA-O2A
24	B	608	CLA	C3A-C2A-CAA-CBA
24	b	618	CLA	C3A-C2A-CAA-CBA
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	D	403	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	CAD-CBD-CGD-O2D
24	b	613	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	c	505	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CAD-CBD-CGD-O2D
24	c	516	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	C2-C1-O2A-CGA
24	b	623	CLA	C2-C1-O2A-CGA
37	E	101	LHG	C23-C24-C25-C26
27	f	102	SQD	O47-C7-C8-C9
35	Z	101	LMG	O7-C10-C11-C12
24	b	618	CLA	C4-C3-C5-C6
25	a	411	PHO	C4-C3-C5-C6
31	a	416	PL9	C30-C29-C31-C32
40	V	205	HEC	C4B-C3B-CAB-CBB
29	m	102	LMT	O5'-C1'-O1'-C1
36	D	406	DGD	O1G-C1A-C2A-C3A
37	d	407	LHG	O8-C23-C24-C25
37	e	102	LHG	O8-C23-C24-C25
29	M	102	LMT	C3-C4-C5-C6
26	b	628	BCR	C21-C22-C23-C24
35	j	101	LMG	C11-C12-C13-C14
36	H	102	DGD	C1G-C2G-C3G-O3G
36	D	406	DGD	CBA-CCA-CDA-CEA
37	D	408	LHG	C26-C27-C28-C29
24	B	605	CLA	O1D-CGD-O2D-CED
24	B	603	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	B	614	CLA	O2A-C1-C2-C3
24	b	611	CLA	O2A-C1-C2-C3
24	b	613	CLA	O2A-C1-C2-C3
24	d	404	CLA	O2A-C1-C2-C3
25	D	401	PHO	O2A-C1-C2-C3
25	a	411	PHO	O2A-C1-C2-C3
38	e	103	HEM	C4C-C3C-CAC-CBC
29	a	404	LMT	C4'-C5'-C6'-O6'
37	l	101	LHG	O7-C7-C8-C9
40	v	205	HEC	CAD-CBD-CGD-O1D
35	b	629	LMG	C20-C21-C22-C23
37	L	101	LHG	C18-C19-C20-C21
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	c	506	CLA	CHA-CBD-CGD-O2D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	d	402	CLA	CHA-CBD-CGD-O1D
24	d	402	CLA	CHA-CBD-CGD-O2D
24	c	516	CLA	CAA-CBA-CGA-O2A
37	L	101	LHG	C26-C27-C28-C29
24	A	405	CLA	C16-C17-C18-C20
36	c	520	DGD	O2G-C1B-C2B-C3B
37	E	101	LHG	O8-C23-C24-C25
36	c	521	DGD	O6D-C5D-C6D-O5D
24	B	614	CLA	CAA-CBA-CGA-O2A
37	L	101	LHG	O7-C7-C8-C9
24	c	514	CLA	CAA-CBA-CGA-O2A
35	M	101	LMG	O8-C28-C29-C30
27	a	405	SQD	C34-C35-C36-C37
29	f	103	LMT	O5B-C1B-O1B-C4'
37	d	407	LHG	C7-C8-C9-C10
37	l	101	LHG	C28-C29-C30-C31
24	c	508	CLA	C12-C13-C15-C16
27	A	411	SQD	O49-C7-O47-C45
24	c	510	CLA	C13-C15-C16-C17
35	z	101	LMG	O7-C10-C11-C12
36	e	101	DGD	O2G-C1B-C2B-C3B
24	B	604	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	b	625	CLA	C14-C13-C15-C16
24	B	612	CLA	C2B-C3B-CAB-CBB
24	C	505	CLA	C2B-C3B-CAB-CBB
24	d	402	CLA	C2B-C3B-CAB-CBB
29	C	522	LMT	O5B-C1B-O1B-C4'
36	C	517	DGD	C6A-C7A-C8A-C9A
27	F	103	SQD	C7-C8-C9-C10
37	d	409	LHG	C24-C23-O8-C6
27	a	405	SQD	C32-C33-C34-C35
36	c	521	DGD	CCA-CDA-CEA-CFA
37	D	408	LHG	C32-C33-C34-C35
27	A	411	SQD	C8-C7-O47-C45
38	e	103	HEM	CAD-CBD-CGD-O2D
24	C	511	CLA	CAA-CBA-CGA-O2A
38	E	102	HEM	CAA-CBA-CGA-O1A
36	D	406	DGD	O1A-C1A-C2A-C3A
37	d	409	LHG	C25-C26-C27-C28
37	e	102	LHG	C25-C26-C27-C28
28	B	629	GOL	C1-C2-C3-O3
31	D	405	PL9	C43-C44-C46-C47
29	M	105	LMT	C9-C10-C11-C12
35	J	101	LMG	C14-C15-C16-C17
24	C	513	CLA	CAA-CBA-CGA-O1A
26	K	101	BCR	C7-C8-C9-C10
26	d	405	BCR	C7-C8-C9-C10
27	A	415	SQD	C28-C29-C30-C31
24	A	409	CLA	CBA-CGA-O2A-C1
24	C	514	CLA	CBA-CGA-O2A-C1
37	d	409	LHG	C11-C10-C9-C8
24	B	610	CLA	C1A-C2A-CAA-CBA
24	C	514	CLA	C1A-C2A-CAA-CBA
24	c	510	CLA	C1A-C2A-CAA-CBA
27	f	102	SQD	C35-C36-C37-C38
36	C	518	DGD	CAA-CBA-CCA-CDA
29	B	622	LMT	C4-C5-C6-C7
29	M	105	LMT	C11-C10-C9-C8
35	a	415	LMG	C34-C35-C36-C37
36	c	521	DGD	CBB-CCB-CDB-CEB
36	h	102	DGD	C4E-C5E-C6E-O5E
37	d	409	LHG	O8-C23-C24-C25
36	c	521	DGD	C8A-C9A-CAA-CBA
24	a	409	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	b	611	CLA	C2A-CAA-CBA-CGA
37	d	408	LHG	C26-C27-C28-C29
24	A	407	CLA	C16-C17-C18-C20
37	d	407	LHG	O10-C23-C24-C25
24	B	609	CLA	C13-C15-C16-C17
25	a	411	PHO	C10-C11-C12-C13
36	C	517	DGD	CAA-CBA-CCA-CDA
37	D	407	LHG	C27-C28-C29-C30
36	C	518	DGD	O2G-C1B-C2B-C3B
35	z	101	LMG	O9-C10-C11-C12
27	B	621	SQD	C15-C16-C17-C18
36	c	519	DGD	C2E-C1E-O5D-C6D
34	b	607	HTG	C2'-C3'-C4'-C5'
35	c	522	LMG	C33-C34-C35-C36
24	A	407	CLA	C4B-C3B-CAB-CBB
24	B	616	CLA	C4B-C3B-CAB-CBB
24	C	505	CLA	C4B-C3B-CAB-CBB
37	D	408	LHG	C4-O6-P-O5
37	D	409	LHG	C4-O6-P-O4
37	D	409	LHG	C4-O6-P-O5
37	e	102	LHG	C4-O6-P-O5
24	B	612	CLA	C16-C17-C18-C19
35	C	521	LMG	C13-C14-C15-C16
24	c	516	CLA	CAA-CBA-CGA-O1A
27	f	102	SQD	O49-C7-C8-C9
37	e	102	LHG	O10-C23-C24-C25
26	c	518	BCR	C5-C6-C7-C8
26	t	101	BCR	C1-C6-C7-C8
24	a	409	CLA	C13-C15-C16-C17
27	f	102	SQD	C7-C8-C9-C10
36	c	520	DGD	O1B-C1B-C2B-C3B
37	l	101	LHG	O9-C7-C8-C9
40	v	205	HEC	C4B-C3B-CAB-CBB
36	e	101	DGD	C3A-C4A-C5A-C6A
36	e	101	DGD	O1B-C1B-C2B-C3B
37	L	101	LHG	O9-C7-C8-C9
37	D	409	LHG	C10-C11-C12-C13
37	E	101	LHG	C10-C11-C12-C13
35	C	520	LMG	C28-C29-C30-C31
37	E	101	LHG	O10-C23-C24-C25
40	v	205	HEC	C2C-C3C-CAC-CBC
38	E	102	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	B	608	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O1D
24	b	618	CLA	CAD-CBD-CGD-O1D
27	A	411	SQD	O5-C5-C6-S
35	Z	101	LMG	O9-C10-C11-C12
24	B	611	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
24	c	508	CLA	C14-C13-C15-C16
24	c	513	CLA	C11-C12-C13-C14
28	b	602	GOL	O1-C1-C2-O2
25	D	401	PHO	C10-C11-C12-C13
36	e	101	DGD	CAB-CBB-CCB-CDB
35	J	101	LMG	O7-C10-C11-C12
35	b	629	LMG	O8-C28-C29-C30
36	D	406	DGD	C6B-C7B-C8B-C9B
27	B	621	SQD	C12-C13-C14-C15
24	b	624	CLA	C13-C15-C16-C17
24	b	623	CLA	C2A-CAA-CBA-CGA
34	B	624	HTG	C4'-C5'-C6'-C7'
36	C	519	DGD	CBA-CCA-CDA-CEA
36	c	521	DGD	O1G-C1A-C2A-C3A
24	C	508	CLA	C5-C6-C7-C8
24	a	409	CLA	C15-C16-C17-C18
24	b	619	CLA	C15-C16-C17-C18
36	h	102	DGD	CDB-CEB-CFB-CGB
24	b	610	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
24	A	409	CLA	C10-C11-C12-C13
24	B	605	CLA	C2-C3-C5-C6
24	B	611	CLA	C12-C13-C15-C16
24	b	617	CLA	C11-C10-C8-C7
36	C	518	DGD	O1B-C1B-C2B-C3B
37	d	409	LHG	O10-C23-C24-C25
36	c	520	DGD	C8A-C9A-CAA-CBA
37	E	101	LHG	C14-C15-C16-C17
24	C	506	CLA	CAA-CBA-CGA-O2A
24	b	622	CLA	CAA-CBA-CGA-O2A
24	c	509	CLA	CAA-CBA-CGA-O2A
37	D	409	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	D	409	LHG	C19-C20-C21-C22
26	C	516	BCR	C11-C12-C13-C14
24	B	614	CLA	CAA-CBA-CGA-O1A
29	M	102	LMT	C2-C1-O1'-C1'
34	D	412	HTG	C1'-C2'-C3'-C4'
29	M	102	LMT	O5'-C1'-O1'-C1
24	C	505	CLA	C13-C15-C16-C17
24	b	615	CLA	C8-C10-C11-C12
24	b	615	CLA	C15-C16-C17-C18
24	C	511	CLA	CAA-CBA-CGA-O1A
36	c	521	DGD	O1A-C1A-C2A-C3A
24	B	606	CLA	CBA-CGA-O2A-C1
24	C	509	CLA	C13-C15-C16-C17
24	A	406	CLA	C4C-C3C-CAC-CBC
29	a	419	LMT	C5-C6-C7-C8
24	c	514	CLA	CAA-CBA-CGA-O1A
24	c	507	CLA	C2A-CAA-CBA-CGA
24	a	409	CLA	C16-C17-C18-C19
34	V	206	HTG	C2'-C3'-C4'-C5'
24	B	614	CLA	CBD-CGD-O2D-CED
24	C	506	CLA	CAA-CBA-CGA-O1A
24	B	610	CLA	C4-C3-C5-C6
35	C	501	LMG	O7-C10-C11-C12
29	M	104	LMT	C2B-C1B-O1B-C4'

There are no ring outliers.

161 monomers are involved in 342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	d	409	LHG	6	0
24	B	607	CLA	2	0
24	b	614	CLA	6	0
29	M	105	LMT	1	0
26	y	101	BCR	2	0
29	f	103	LMT	1	0
24	C	503	CLA	2	0
37	D	407	LHG	1	0
27	a	405	SQD	2	0
37	E	101	LHG	2	0
24	c	515	CLA	3	0
25	d	401	PHO	2	0
24	d	403	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	410	BCR	2	0
26	a	413	BCR	1	0
27	B	621	SQD	1	0
27	A	415	SQD	1	0
35	c	523	LMG	1	0
24	B	609	CLA	2	0
24	b	611	CLA	3	0
26	C	515	BCR	6	0
24	C	508	CLA	4	0
24	b	624	CLA	5	0
35	J	101	LMG	1	0
24	C	506	CLA	7	0
35	b	629	LMG	3	0
24	D	402	CLA	3	0
26	B	619	BCR	4	0
24	C	507	CLA	2	0
26	Y	101	BCR	3	0
24	a	410	CLA	3	0
29	M	102	LMT	3	0
37	e	102	LHG	4	0
24	C	510	CLA	3	0
24	A	407	CLA	1	0
24	A	406	CLA	4	0
37	l	101	LHG	2	0
24	a	409	CLA	4	0
24	c	513	CLA	1	0
24	B	604	CLA	2	0
24	c	506	CLA	2	0
36	C	517	DGD	4	0
36	c	519	DGD	2	0
26	H	101	BCR	4	0
24	B	612	CLA	3	0
24	b	625	CLA	2	0
24	c	512	CLA	6	0
35	c	522	LMG	3	0
24	B	611	CLA	2	0
29	b	630	LMT	3	0
35	j	101	LMG	2	0
24	C	514	CLA	9	0
24	B	610	CLA	3	0
37	L	101	LHG	2	0
28	B	630	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	b	631	HTG	1	0
35	C	521	LMG	1	0
35	C	501	LMG	6	0
24	C	511	CLA	1	0
35	a	415	LMG	1	0
24	b	619	CLA	1	0
37	d	408	LHG	1	0
28	A	413	GOL	1	0
29	B	622	LMT	1	0
26	B	620	BCR	3	0
31	A	418	PL9	5	0
26	C	516	BCR	5	0
24	c	508	CLA	1	0
24	B	614	CLA	4	0
24	C	513	CLA	6	0
24	b	622	CLA	2	0
38	e	103	HEM	2	0
36	e	101	DGD	9	0
24	C	502	CLA	1	0
28	T	102	GOL	2	0
24	c	509	CLA	7	0
35	M	101	LMG	2	0
24	b	623	CLA	1	0
24	c	505	CLA	2	0
24	C	509	CLA	2	0
37	D	409	LHG	8	0
24	B	613	CLA	1	0
26	k	101	BCR	1	0
24	B	603	CLA	1	0
24	C	512	CLA	4	0
34	b	632	HTG	1	0
26	h	101	BCR	4	0
24	b	610	CLA	2	0
26	d	405	BCR	3	0
24	A	409	CLA	4	0
28	f	101	GOL	1	0
29	a	404	LMT	3	0
34	B	623	HTG	2	0
24	c	507	CLA	3	0
34	D	412	HTG	2	0
28	b	604	GOL	1	0
29	m	102	LMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	c	520	DGD	2	0
25	A	408	PHO	3	0
24	c	510	CLA	2	0
28	T	101	GOL	1	0
24	B	602	CLA	1	0
34	d	412	HTG	3	0
24	B	616	CLA	7	0
24	B	606	CLA	3	0
24	c	511	CLA	4	0
26	c	527	BCR	4	0
27	A	411	SQD	6	0
38	E	102	HEM	3	0
36	C	518	DGD	1	0
24	b	620	CLA	2	0
31	d	406	PL9	1	0
28	a	402	GOL	1	0
24	b	621	CLA	1	0
24	c	517	CLA	6	0
24	d	404	CLA	2	0
27	a	414	SQD	2	0
34	b	601	HTG	1	0
35	C	520	LMG	1	0
24	d	402	CLA	3	0
24	c	516	CLA	2	0
24	b	616	CLA	1	0
26	K	101	BCR	3	0
34	V	206	HTG	2	0
26	B	618	BCR	1	0
25	D	401	PHO	1	0
24	b	615	CLA	1	0
29	a	419	LMT	1	0
24	A	405	CLA	3	0
26	b	628	BCR	3	0
37	d	407	LHG	2	0
26	b	627	BCR	3	0
24	B	605	CLA	3	0
31	D	405	PL9	2	0
24	B	608	CLA	2	0
28	v	201	GOL	1	0
24	D	403	CLA	1	0
24	b	618	CLA	1	0
26	D	404	BCR	1	0

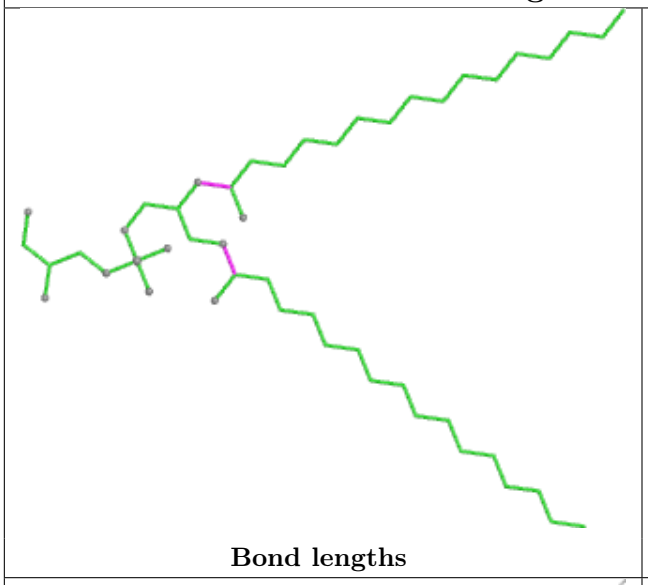
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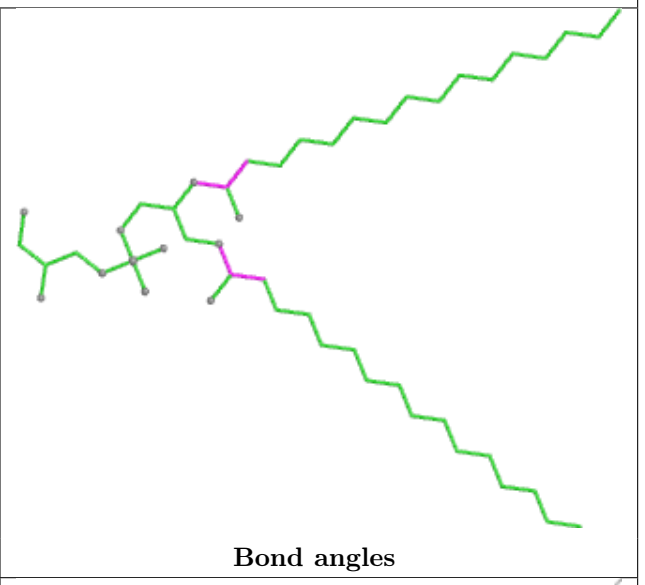
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	Z	101	LMG	1	0
29	C	522	LMT	2	0
28	c	502	GOL	2	0
26	t	101	BCR	6	0
29	A	416	LMT	2	0
31	a	416	PL9	6	0
26	T	103	BCR	6	0
27	L	102	SQD	2	0
27	F	103	SQD	1	0
24	b	613	CLA	2	0
26	b	626	BCR	2	0
27	f	102	SQD	2	1
24	B	615	CLA	4	0
36	D	406	DGD	2	0
24	b	617	CLA	1	0
24	c	514	CLA	2	0
26	c	518	BCR	1	0
25	a	411	PHO	2	0
35	z	101	LMG	4	0
24	B	617	CLA	8	0
24	b	612	CLA	1	0
24	C	504	CLA	3	0

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

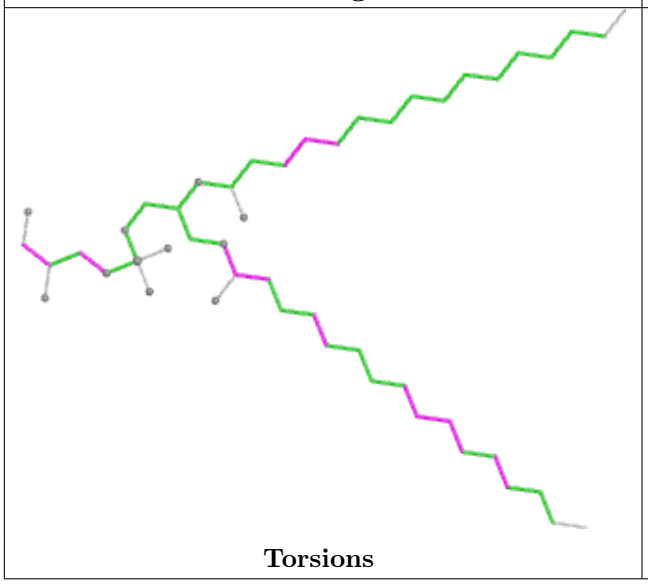
Ligand LHG d 409



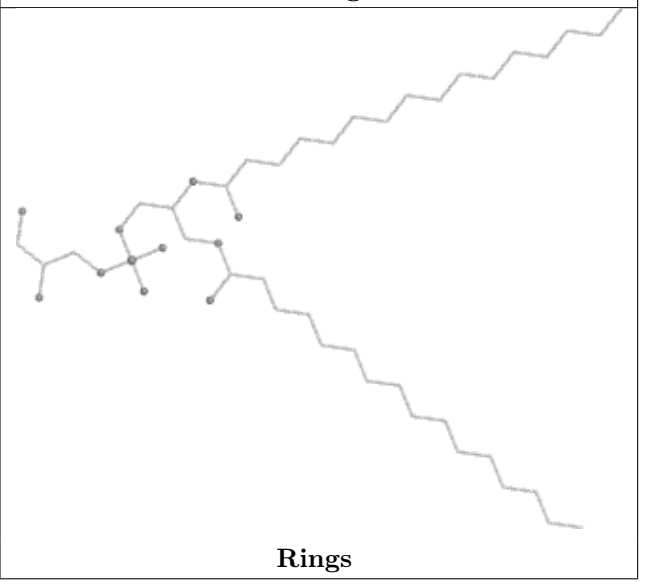
Bond lengths



Bond angles

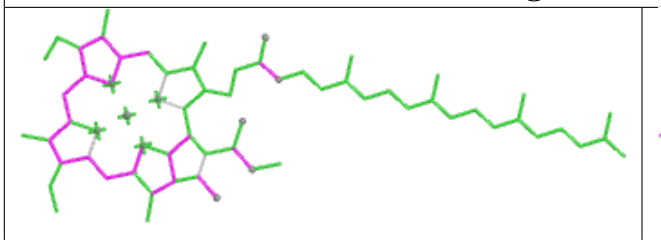


Torsions

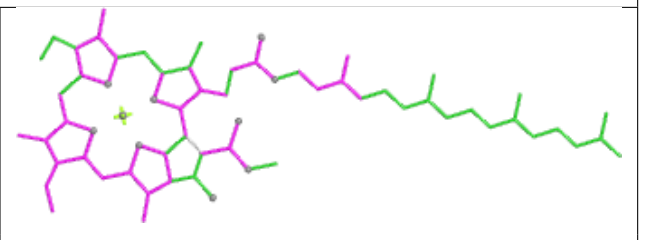


Rings

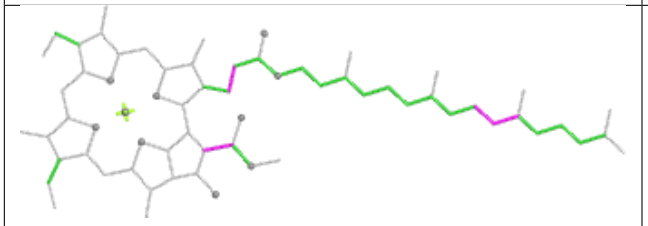
Ligand CLA B 607



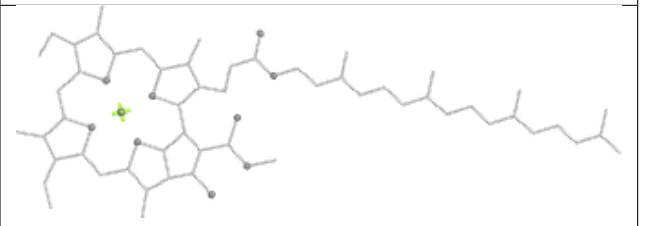
Bond lengths



Bond angles

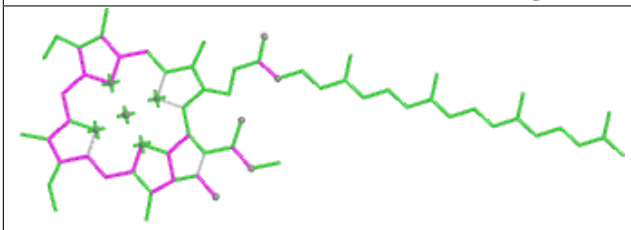


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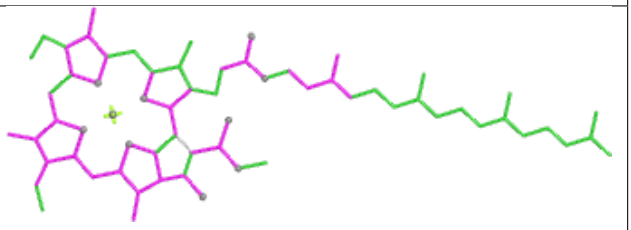


Rings

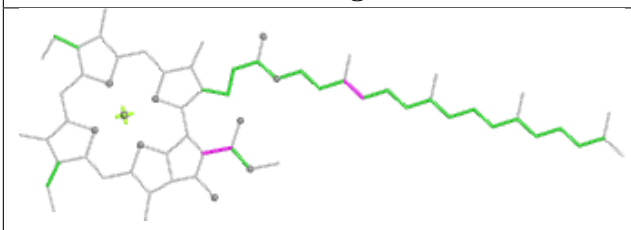
Ligand CLA b 614



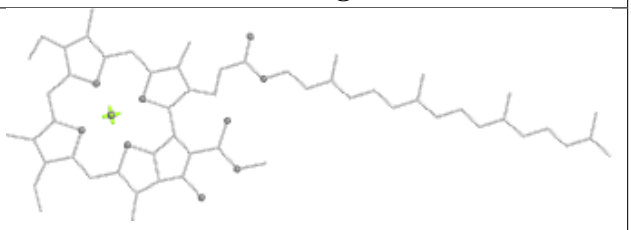
Bond lengths



Bond angles

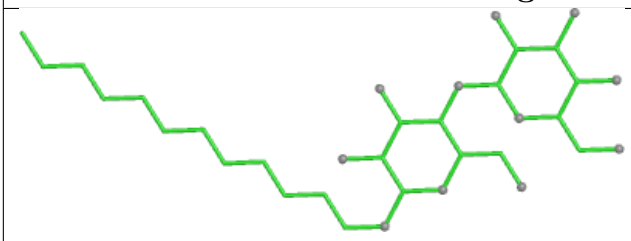


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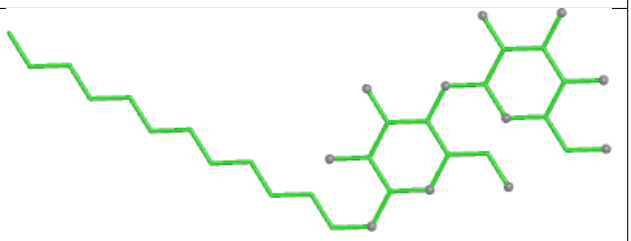


Rings

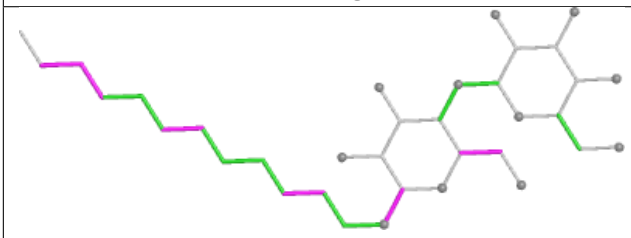
Ligand LMT M 105



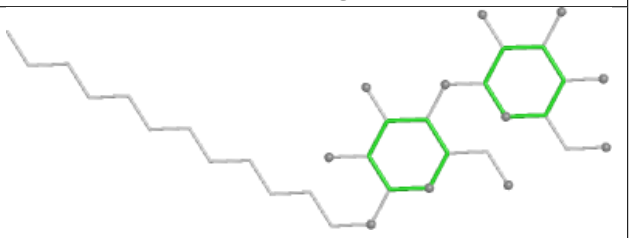
Bond lengths



Bond angles



Torsions

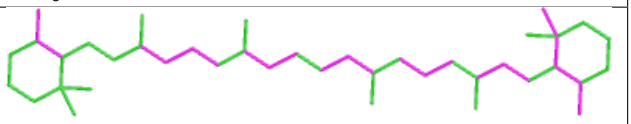


Rings

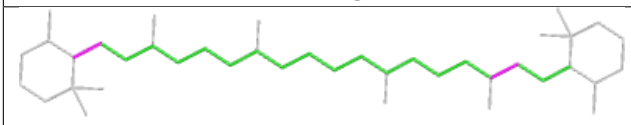
Ligand BCR y 101



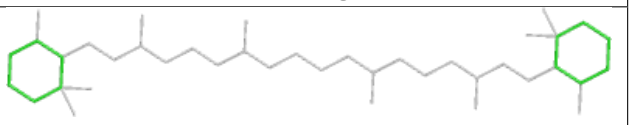
Bond lengths



Bond angles

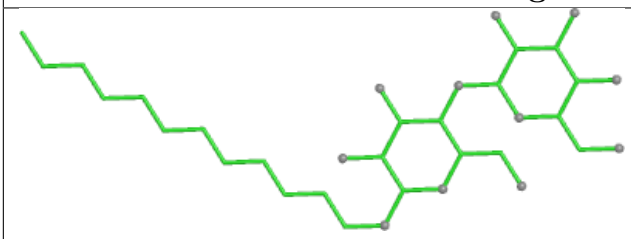


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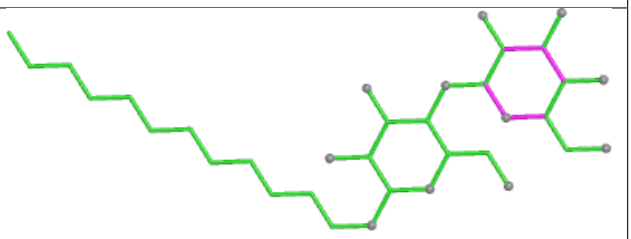


Rings

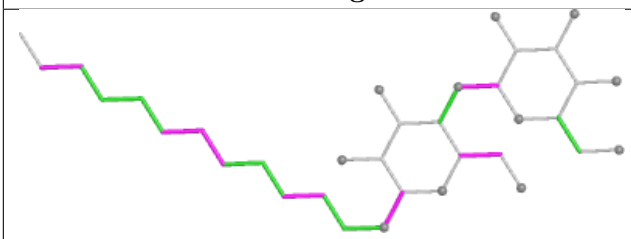
Ligand LMT f 103



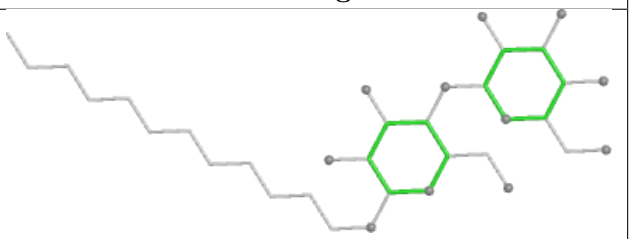
Bond lengths



Bond angles

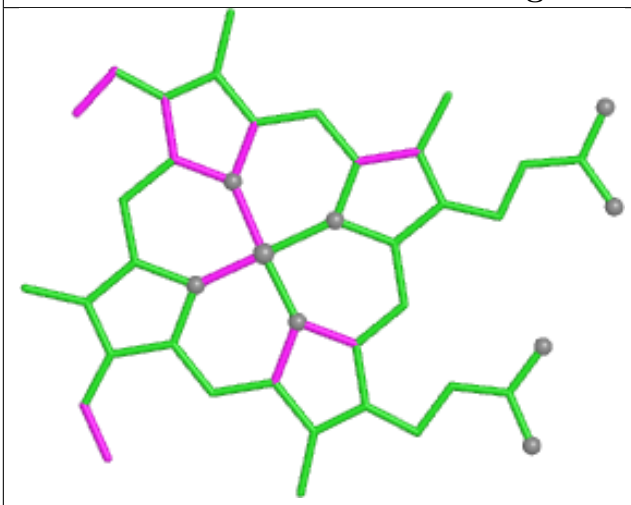


Torsions

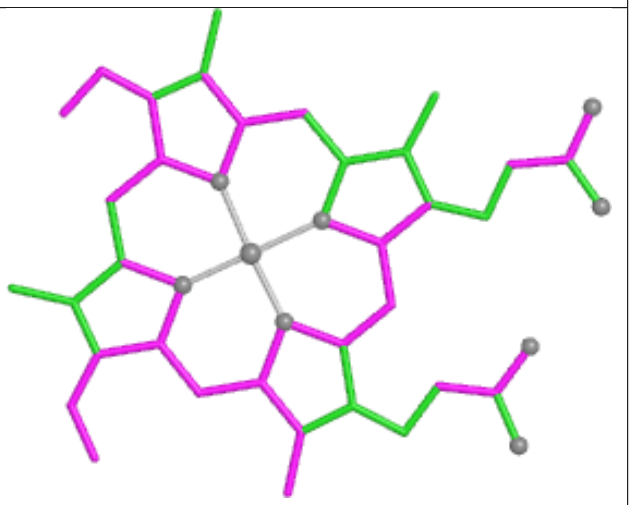


Rings

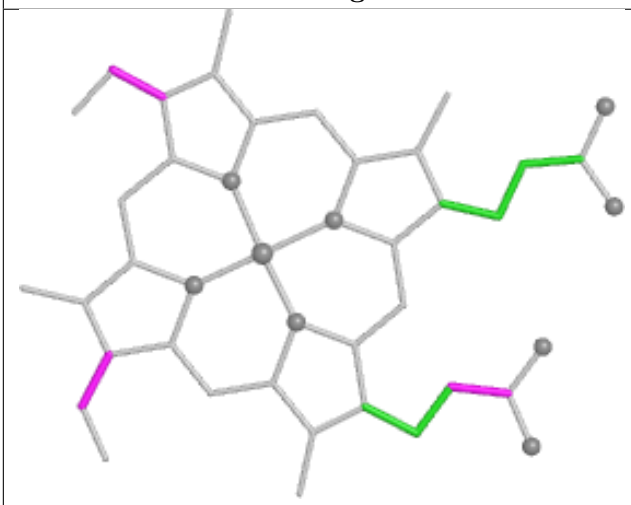
Ligand HEC v 205



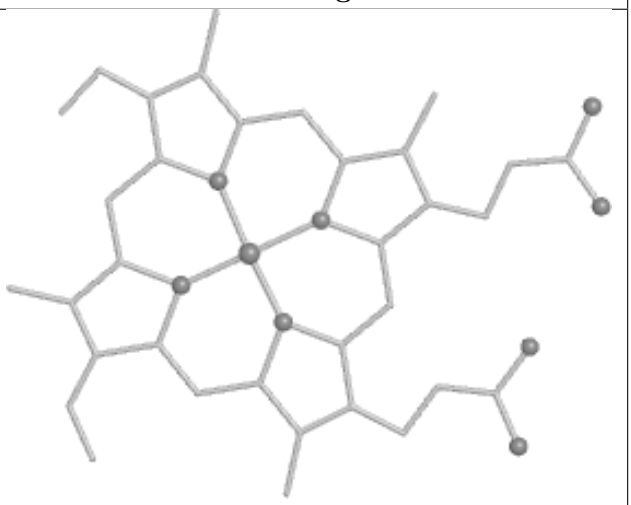
Bond lengths



Bond angles

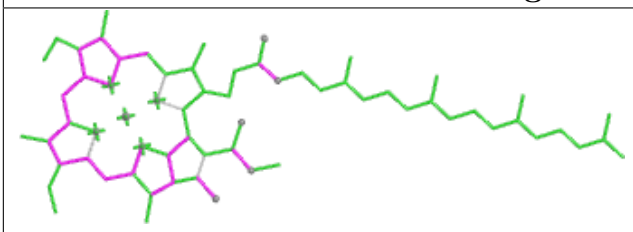


Torsions

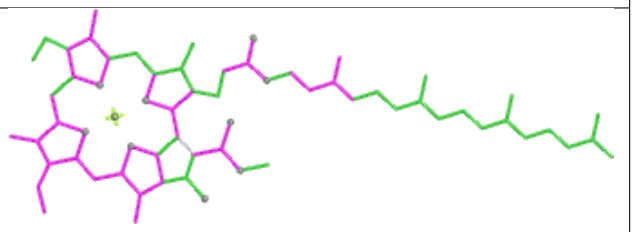


Rings

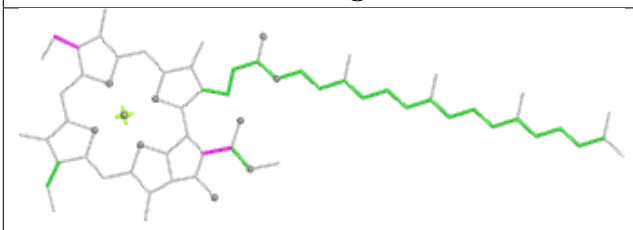
Ligand CLA C 503



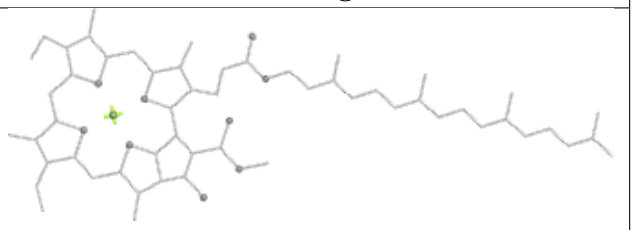
Bond lengths



Bond angles

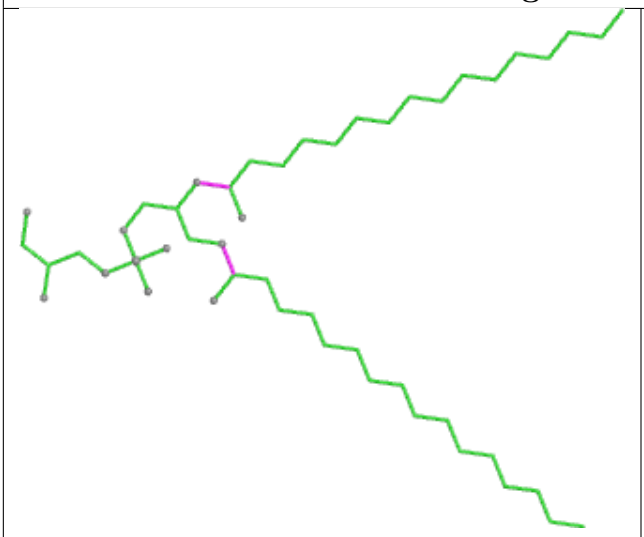


Torsions

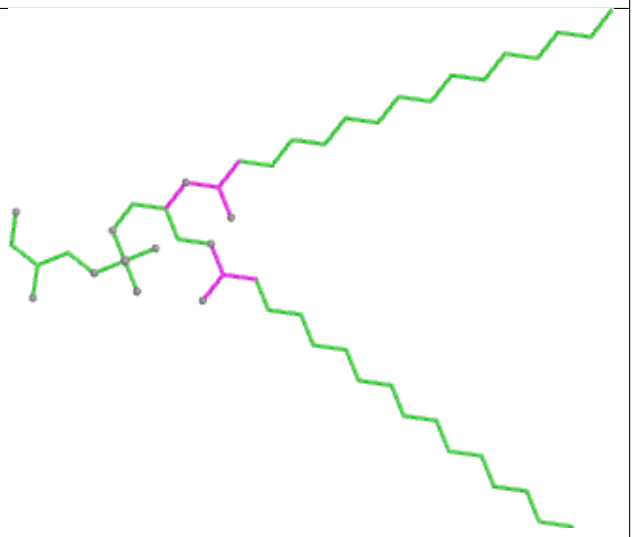


Rings

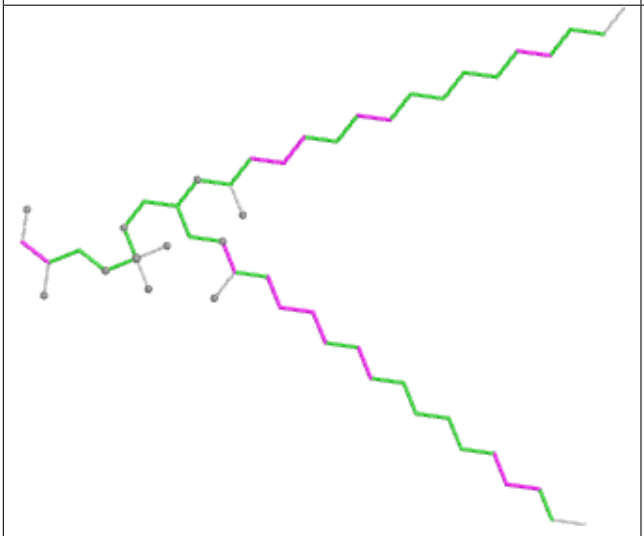
Ligand LHG D 407



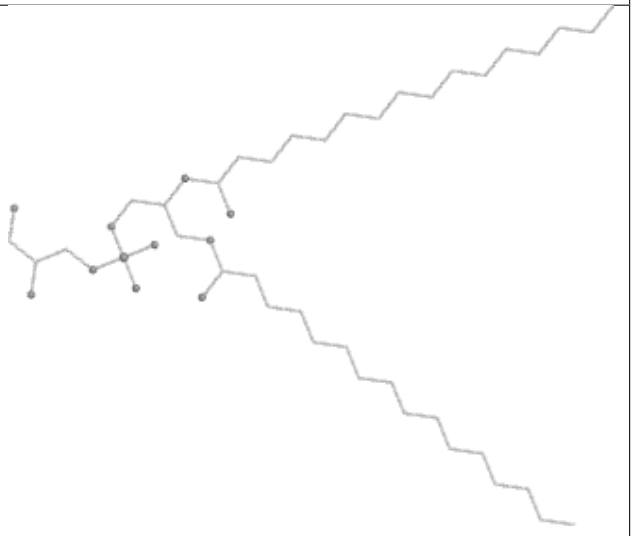
Bond lengths



Bond angles

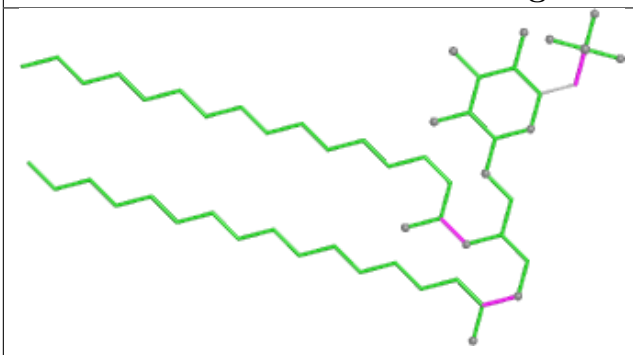


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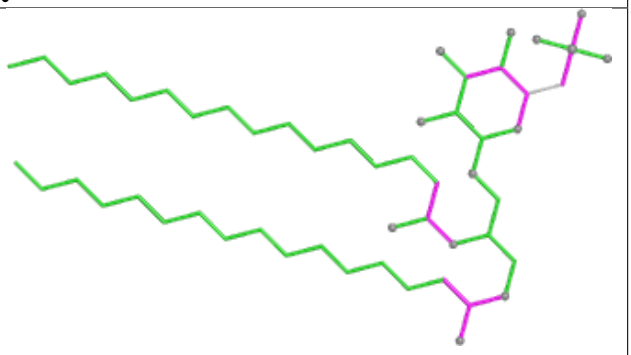


Rings

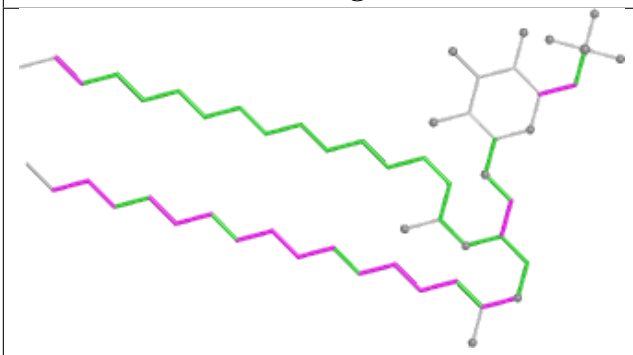
Ligand SQD a 405



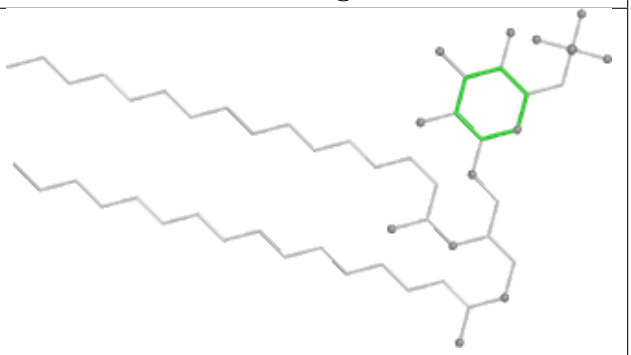
Bond lengths



Bond angles

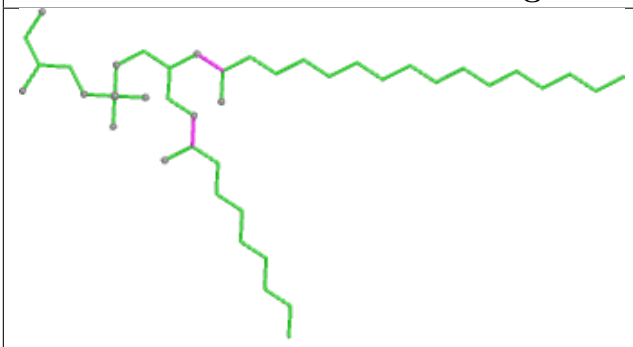


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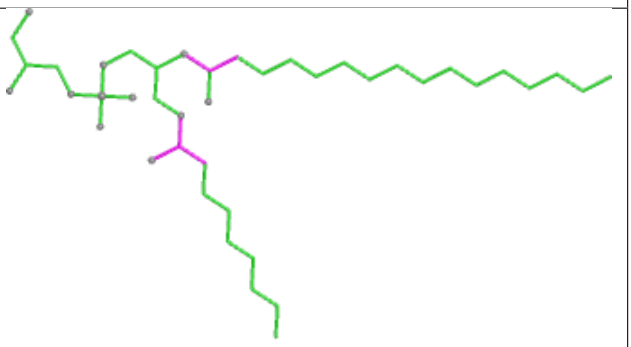


Rings

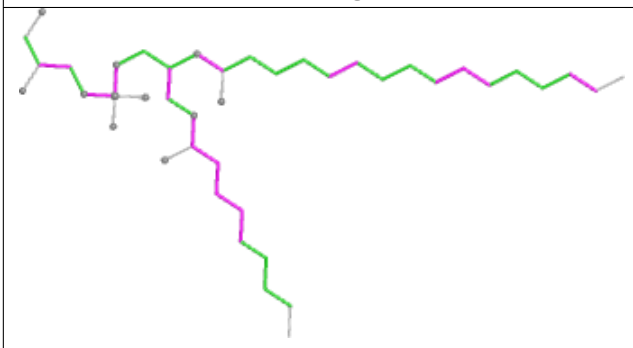
Ligand LHG E 101



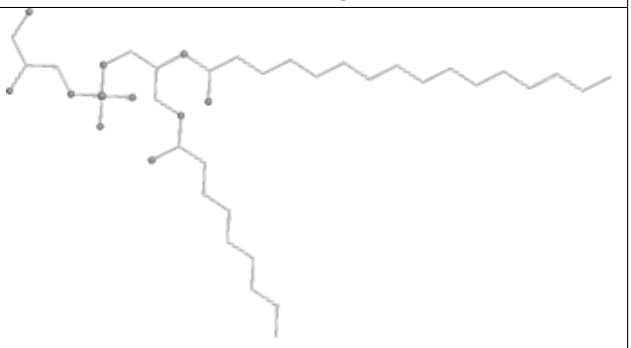
Bond lengths



Bond angles

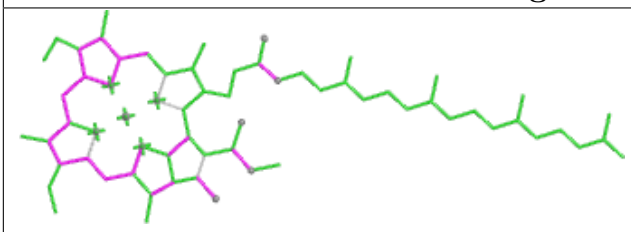


Torsions

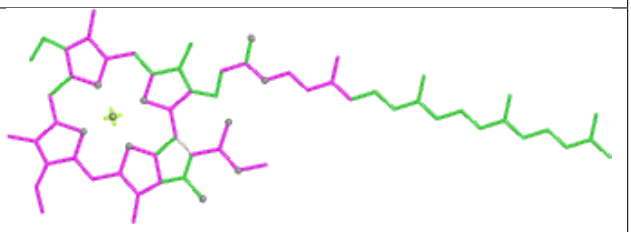


Rings

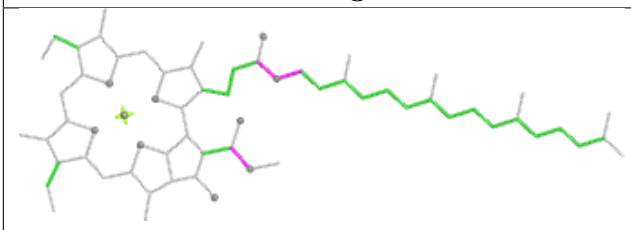
Ligand CLA c 515



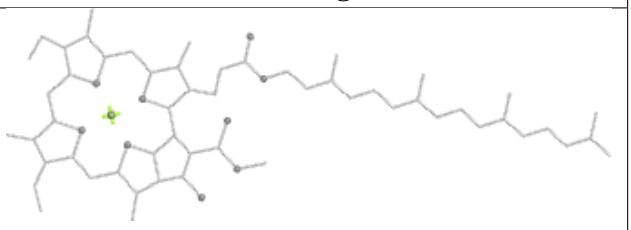
Bond lengths



Bond angles



Torsions

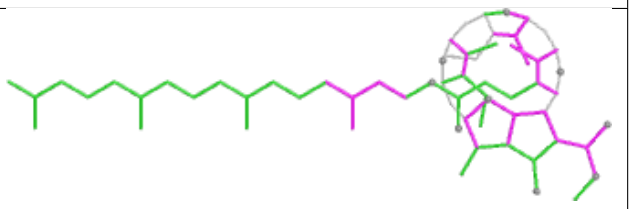


Rings

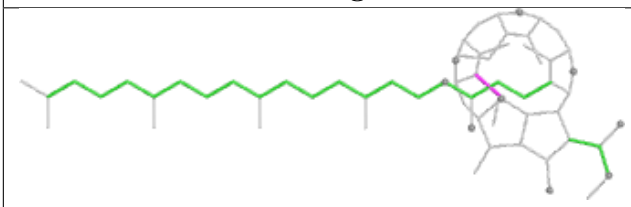
Ligand PHO d 401



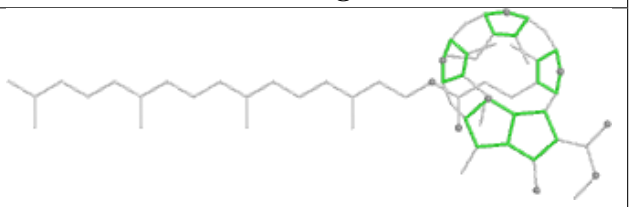
Bond lengths



Bond angles

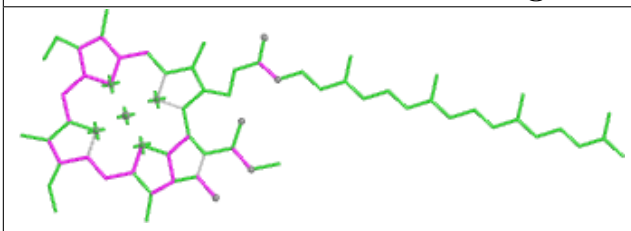


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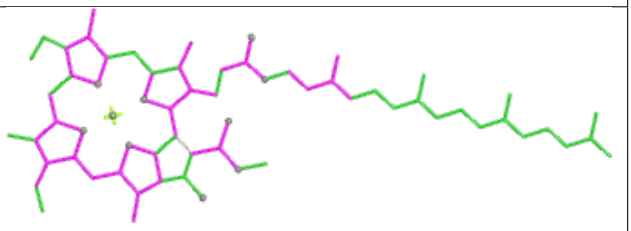


Rings

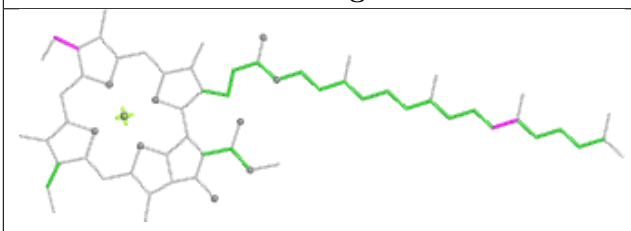
Ligand CLA d 403



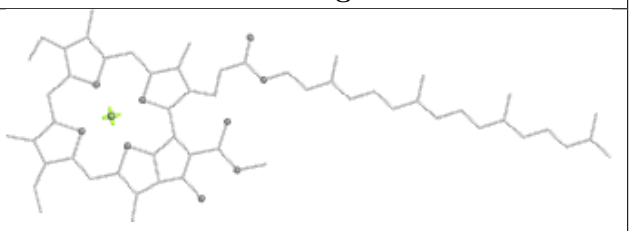
Bond lengths



Bond angles

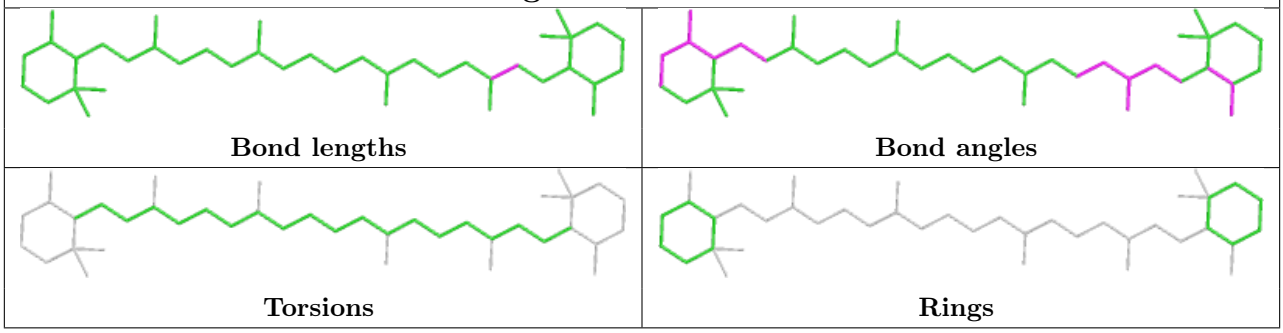


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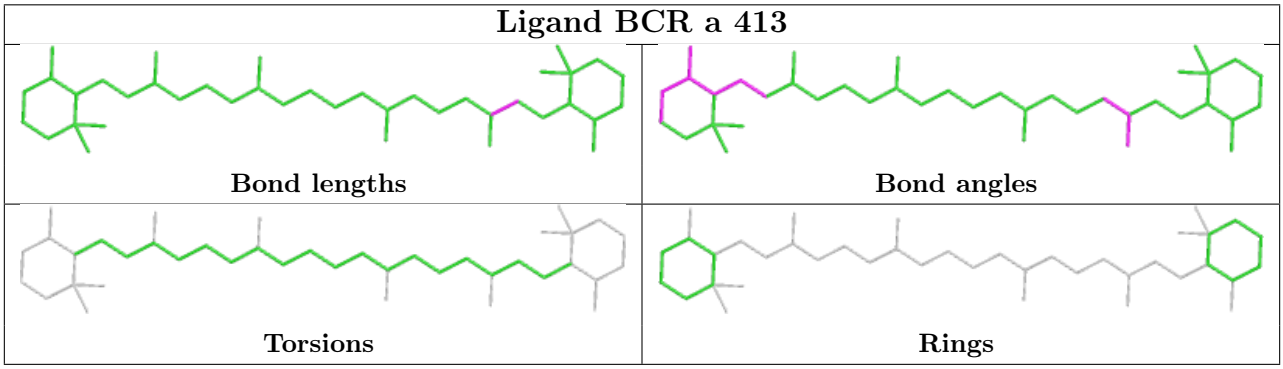


Rings

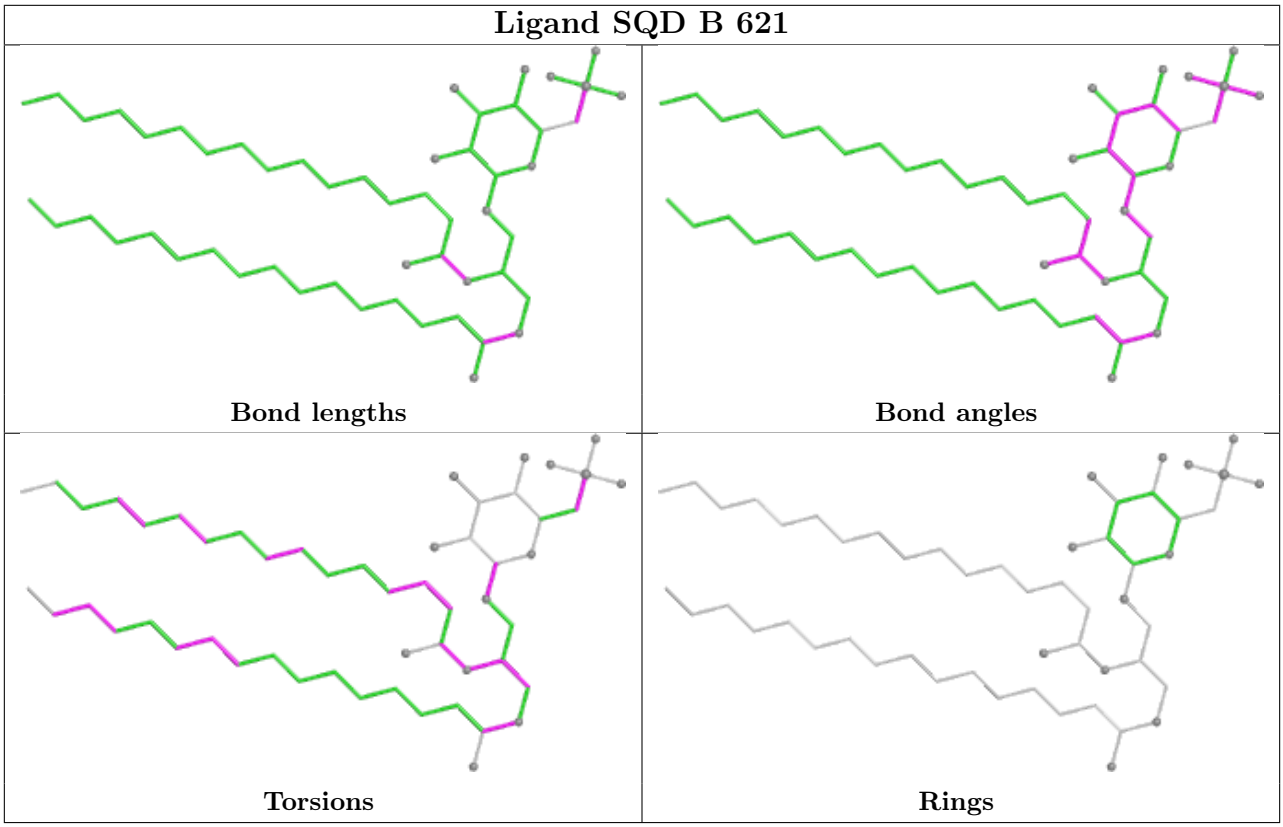
Ligand BCR A 410



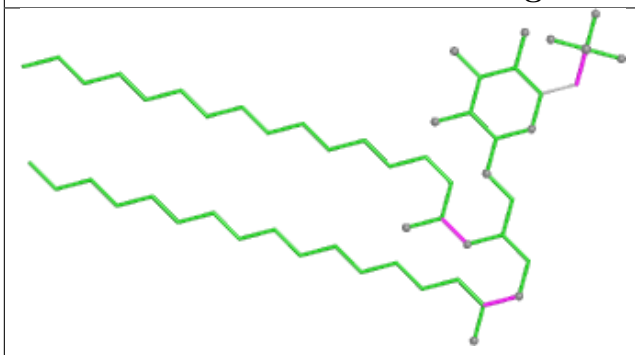
Ligand BCR a 413



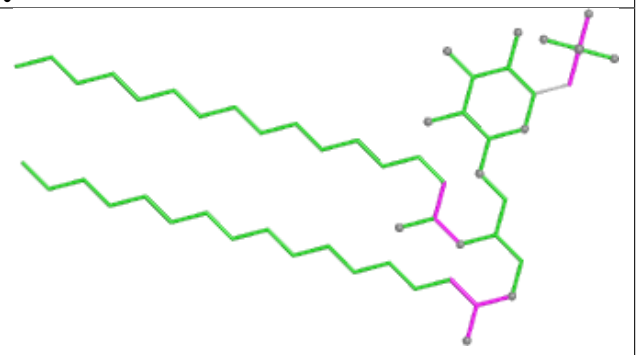
Ligand SQD B 621



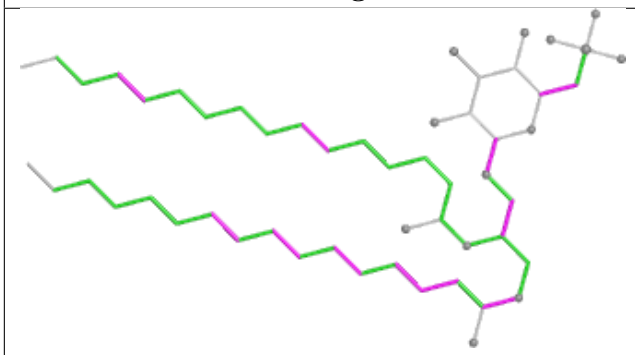
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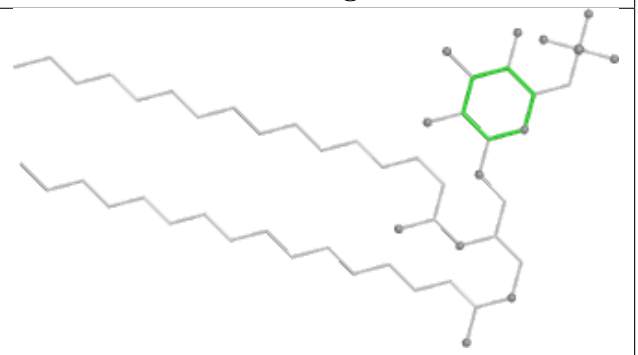
Bond lengths



Bond angles

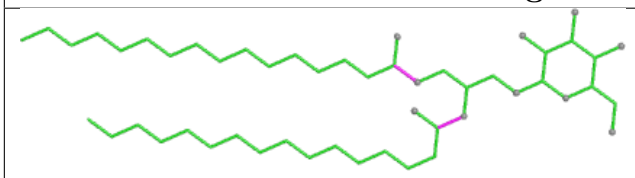


Torsions

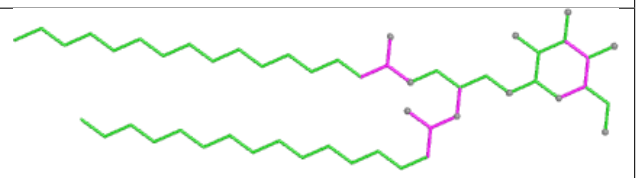


Rings

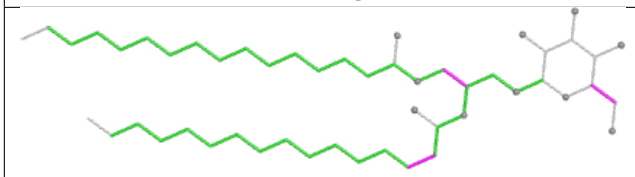
Ligand LMG c 523



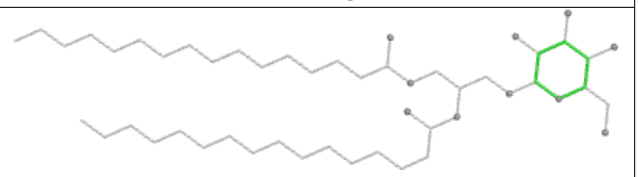
Bond lengths



Bond angles

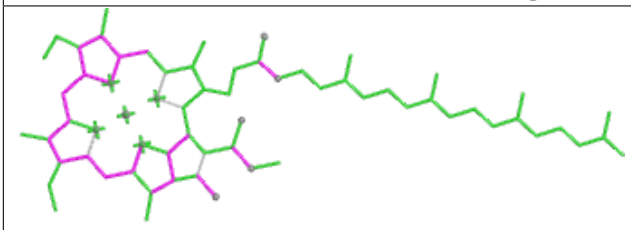


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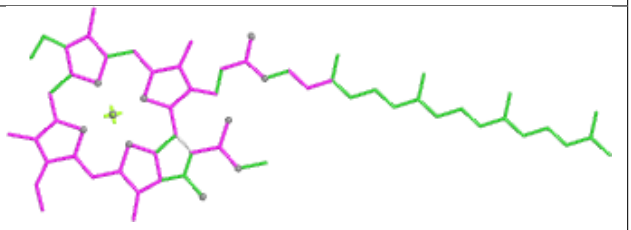


Rings

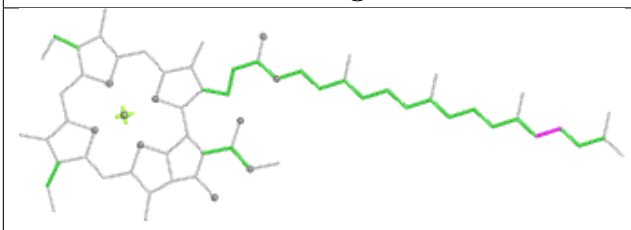
Ligand CLA B 609



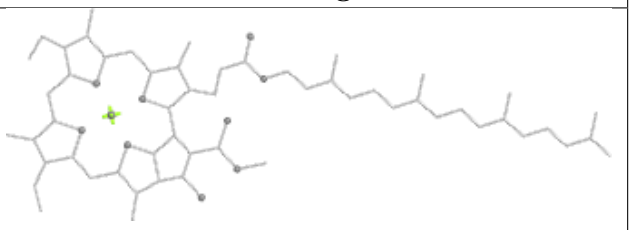
Bond lengths



Bond angles

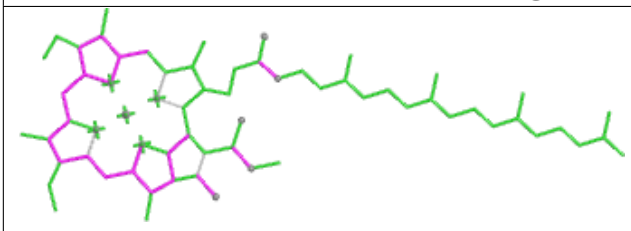


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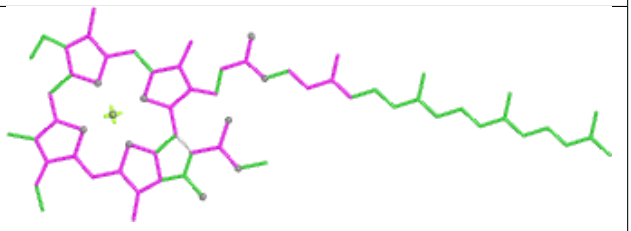


Rings

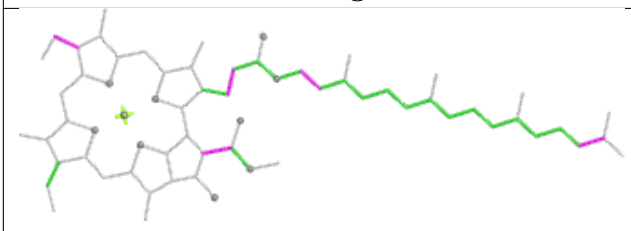
Ligand CLA b 611



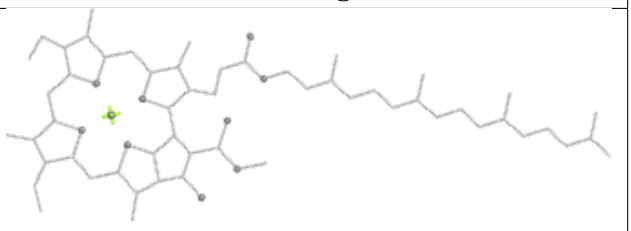
Bond lengths



Bond angles

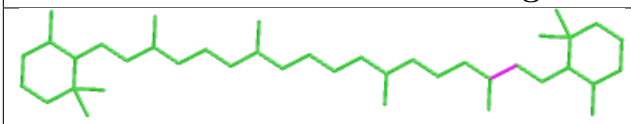


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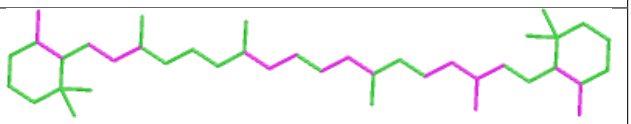


Rings

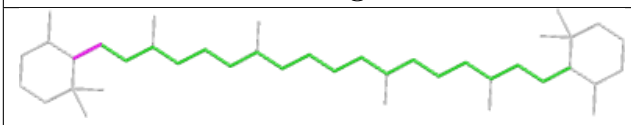
Ligand BCR C 515



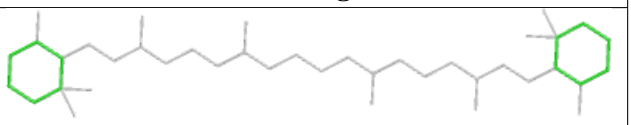
Bond lengths



Bond angles

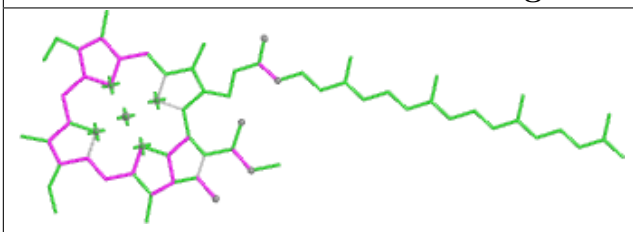


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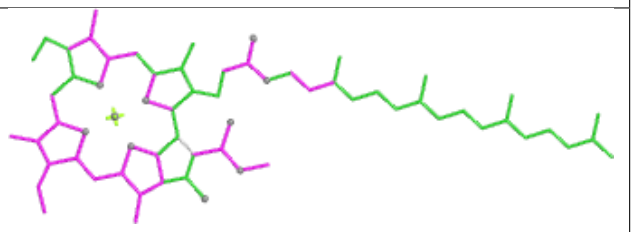


Rings

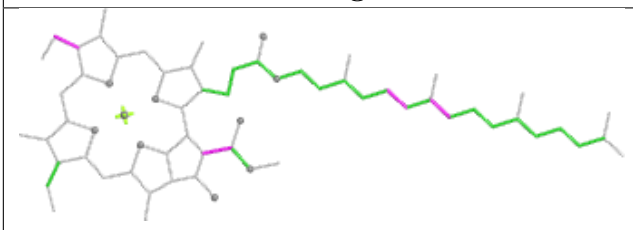
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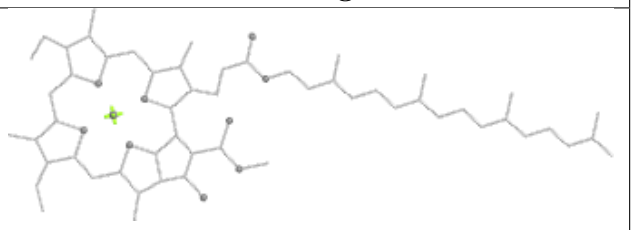
Bond lengths



Bond angles

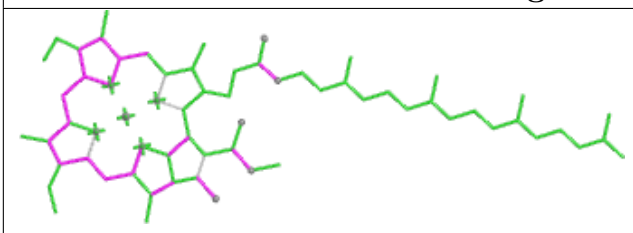


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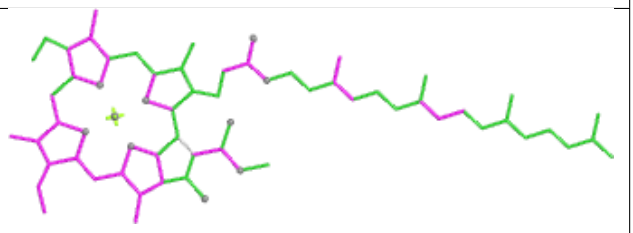


Rings

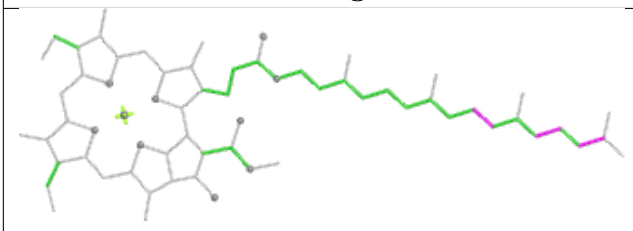
Ligand CLA b 624



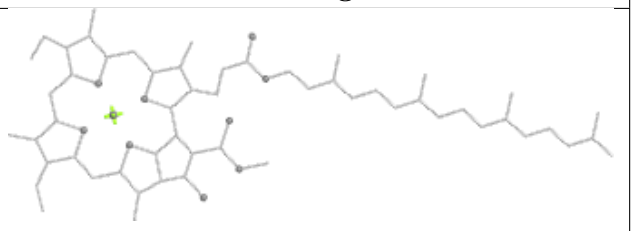
Bond lengths



Bond angles

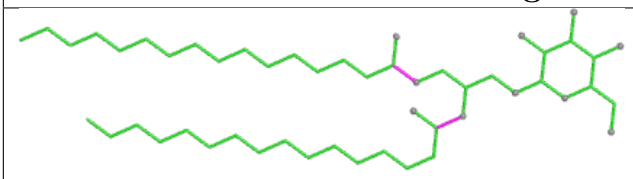


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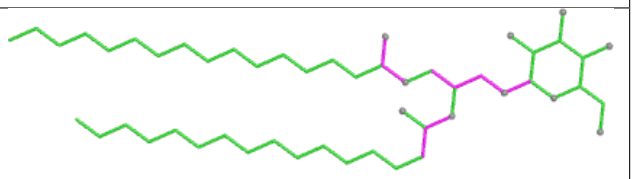


Rings

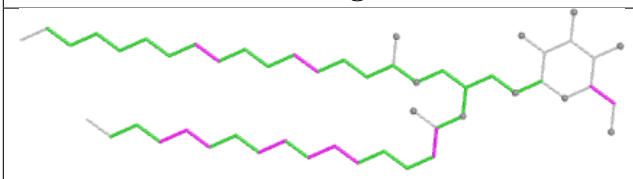
Ligand LMG J 101



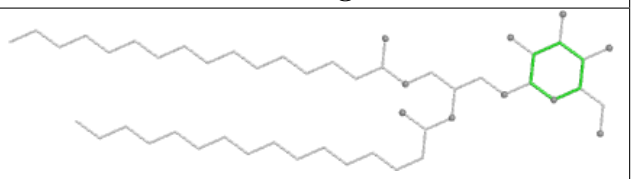
Bond lengths



Bond angles

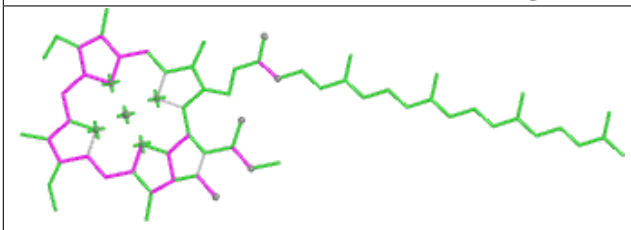


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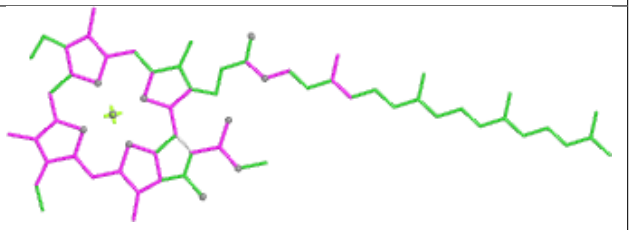


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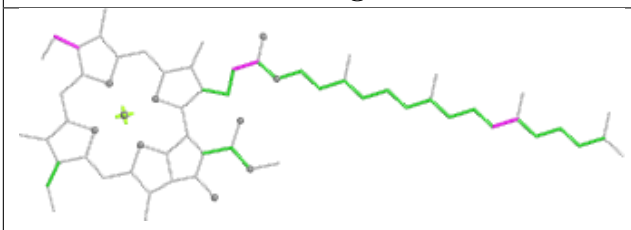
Ligand CLA C 506



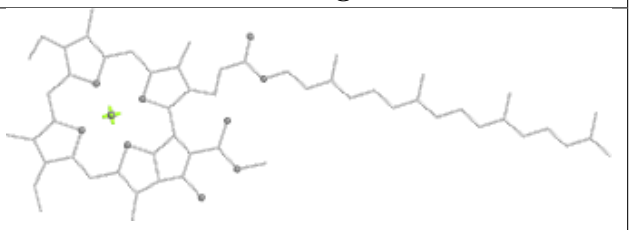
Bond lengths



Bond angles

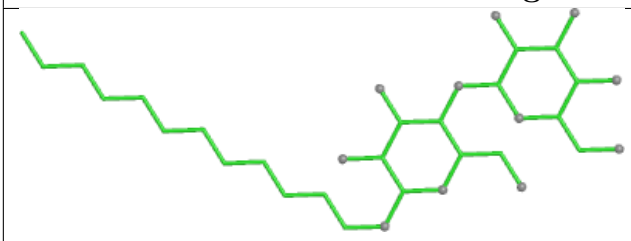


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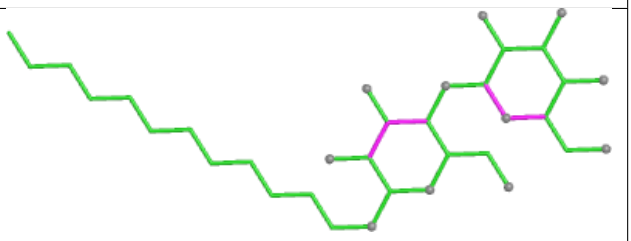


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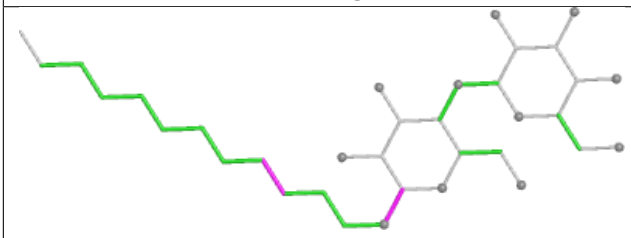
Ligand LMT F 102



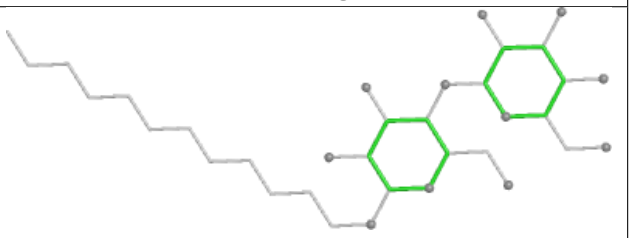
Bond lengths



Bond angles

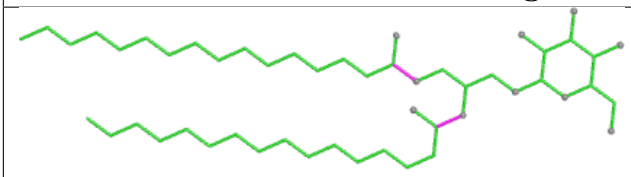


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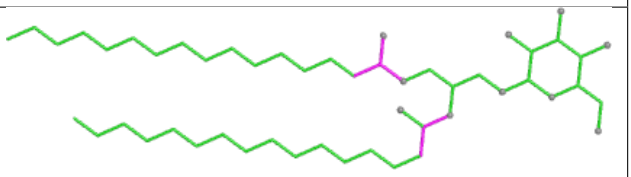


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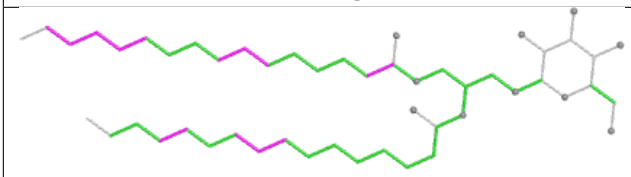
Ligand LMG b 629



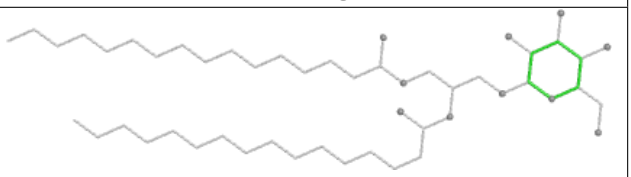
Bond lengths



Bond angles

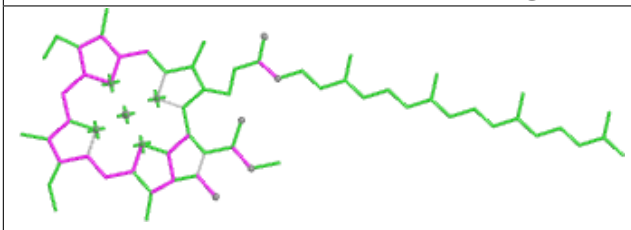


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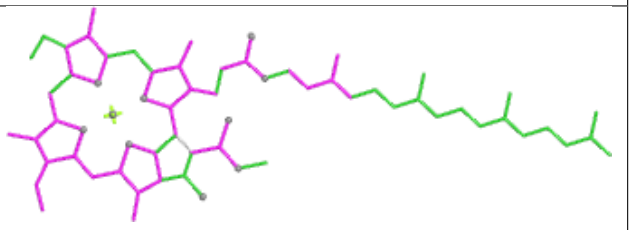


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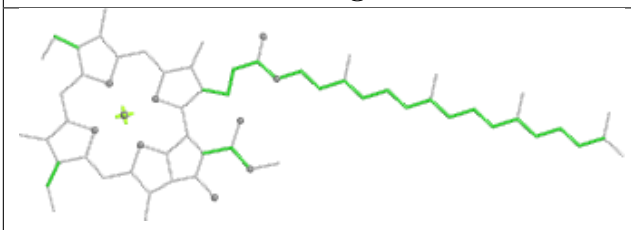
Ligand CLA D 402



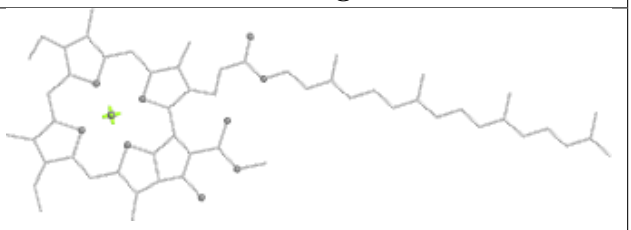
Bond lengths



Bond angles



Torsions

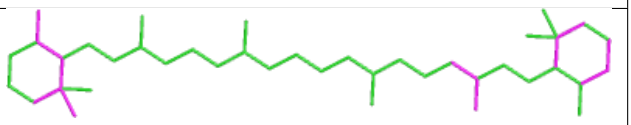


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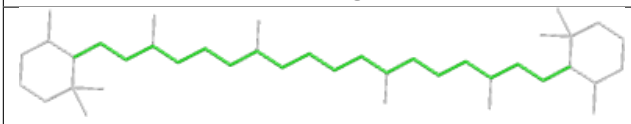
Ligand BCR B 619



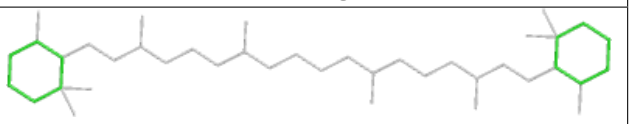
Bond lengths



Bond angles

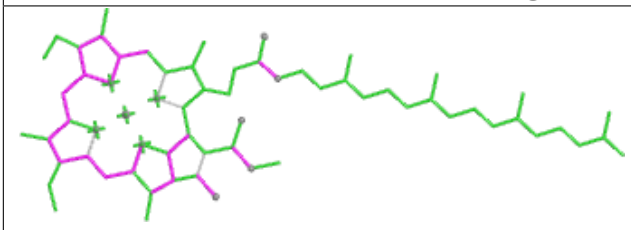


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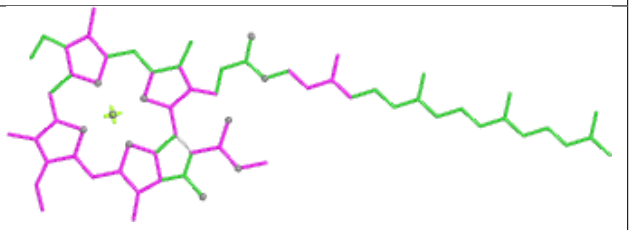


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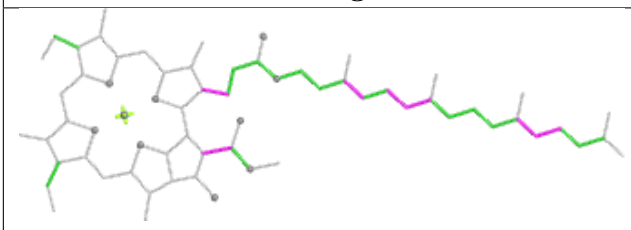
Ligand CLA C 507



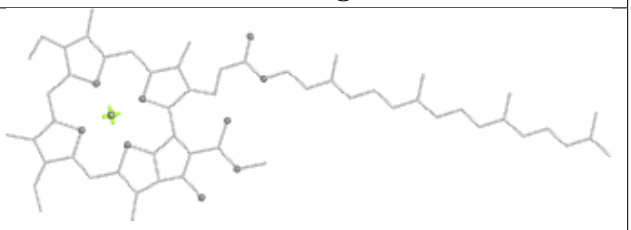
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Bond angles

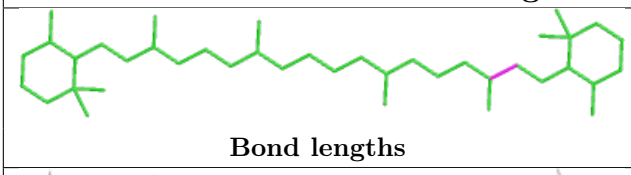


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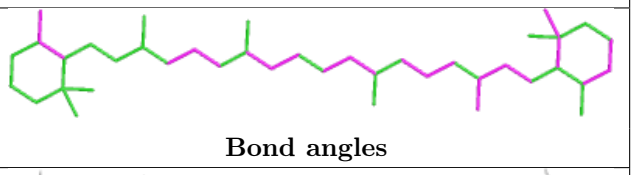


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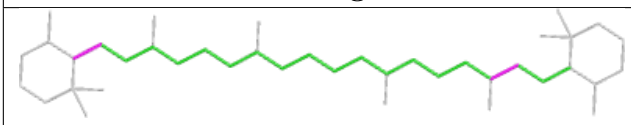
Ligand BCR Y 101



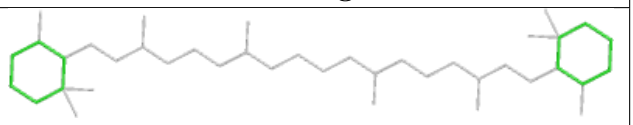
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Bond angles

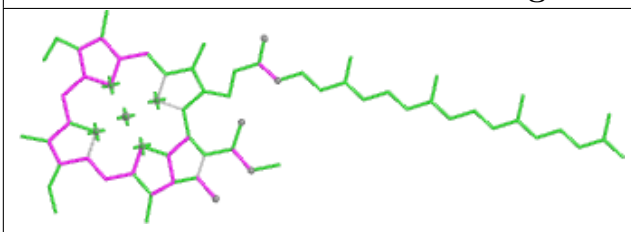


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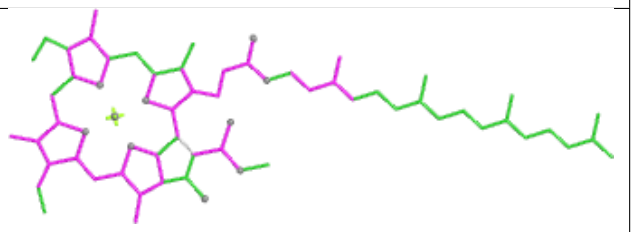


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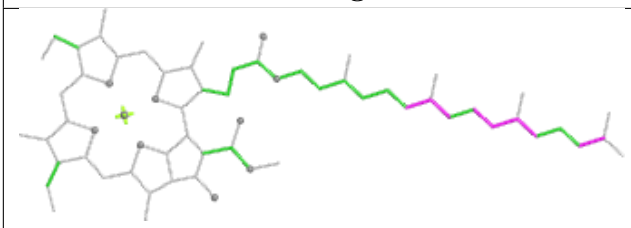
Ligand CLA a 410



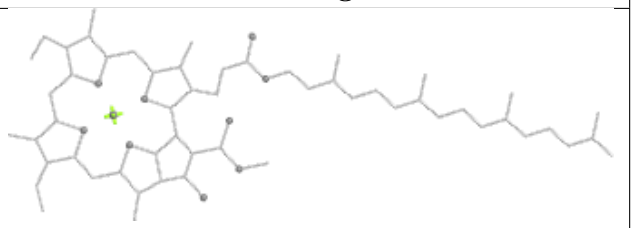
Bond lengths



Bond angles

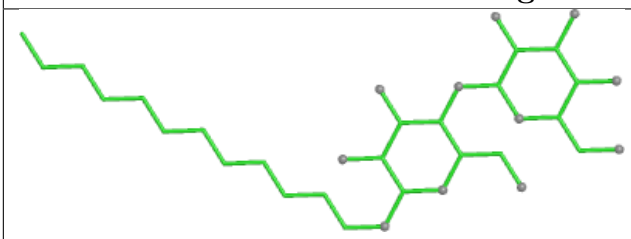


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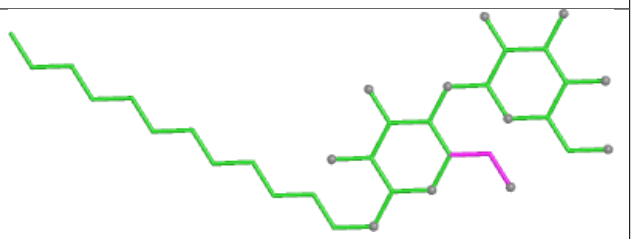


Rings

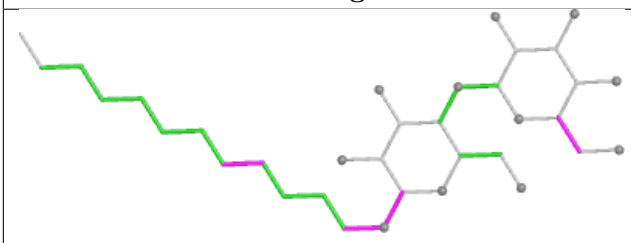
Ligand LMT M 102



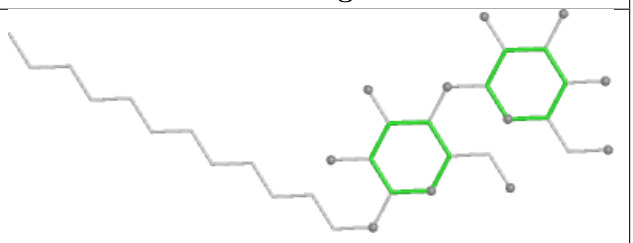
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Bond angles

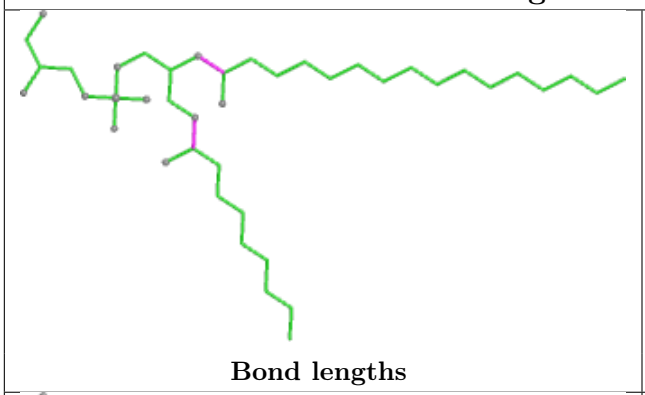


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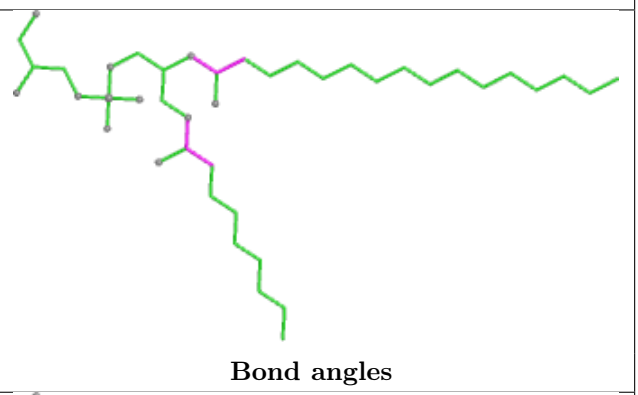


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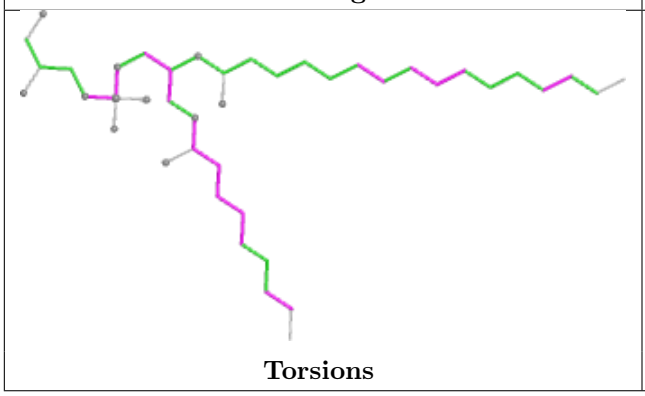
Ligand LHG e 102



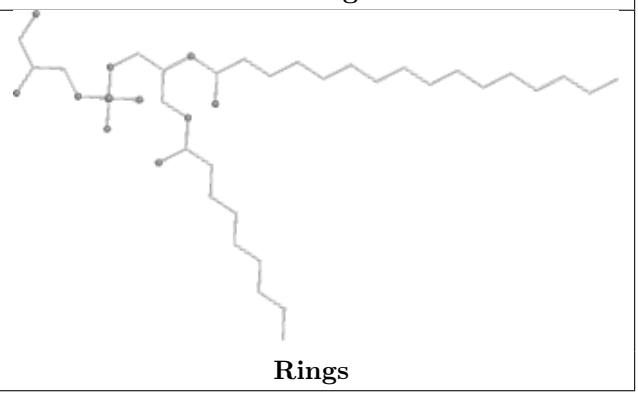
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Bond angles

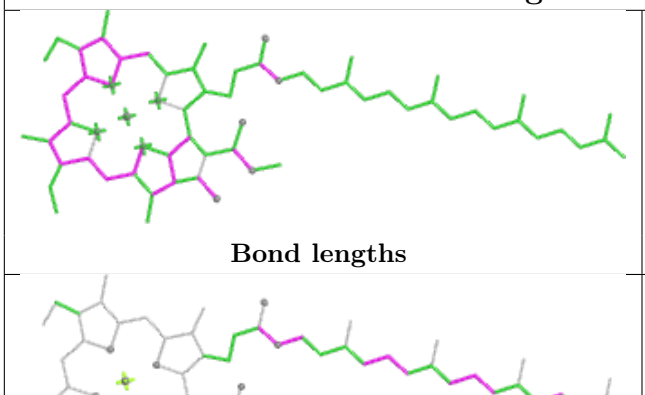


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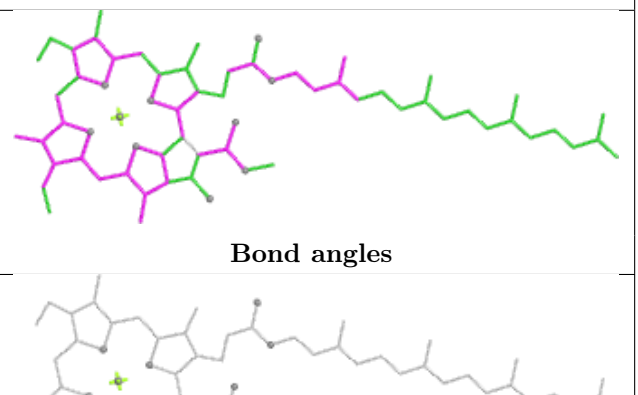


Rings

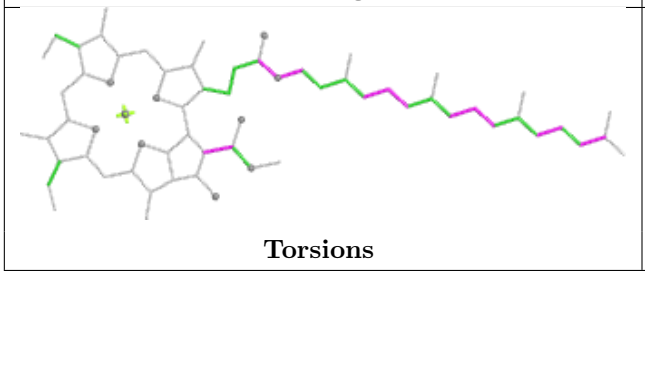
Ligand CLA C 510



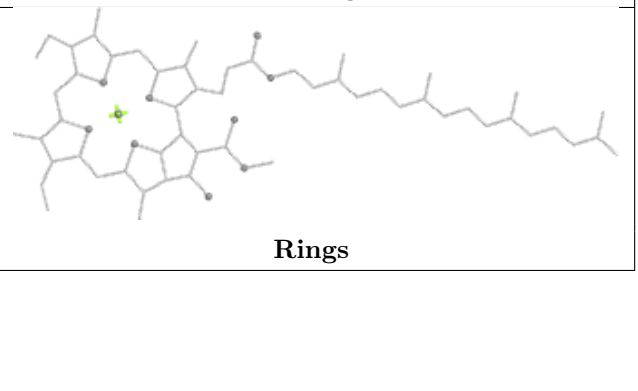
Bond lengths



Bond angles

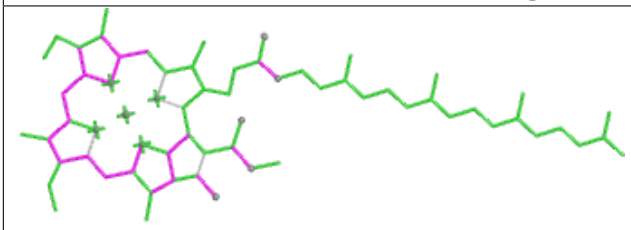


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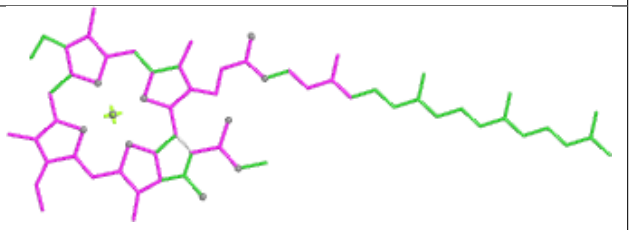


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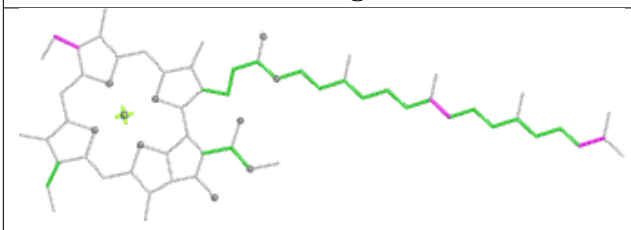
Ligand CLA A 407



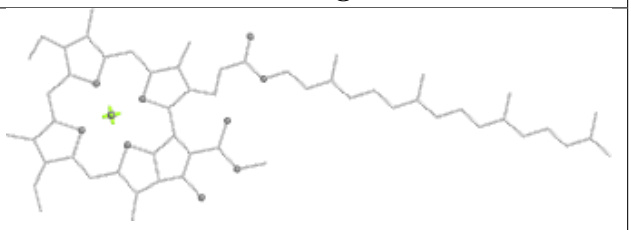
Bond lengths



Bond angles

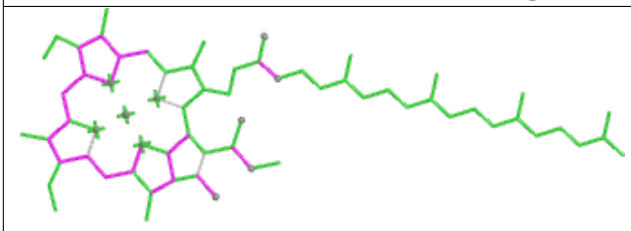


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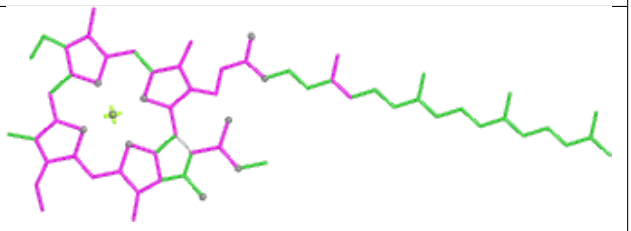


Rings

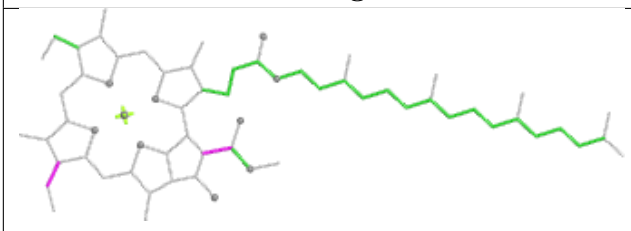
Ligand CLA A 406



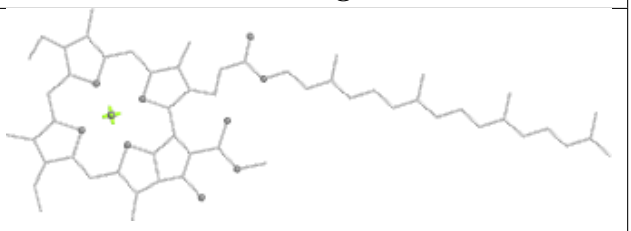
Bond lengths



Bond angles

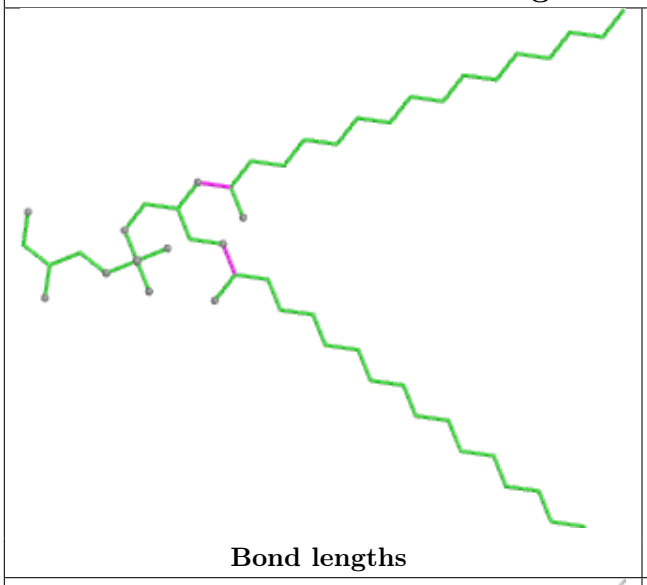


Torsions

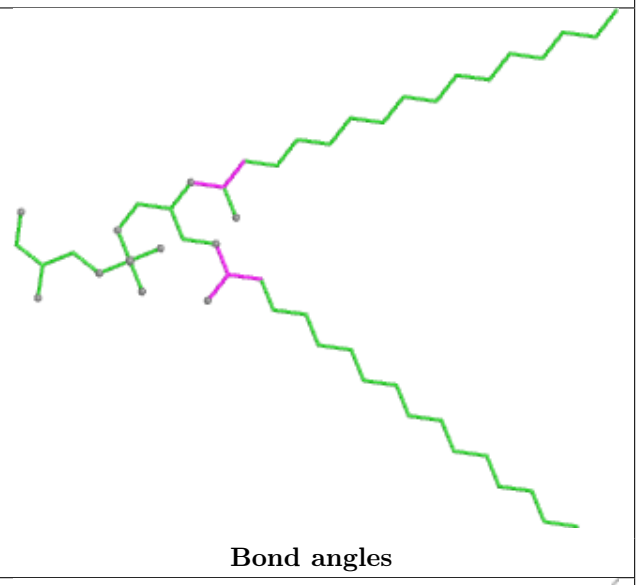


Rings

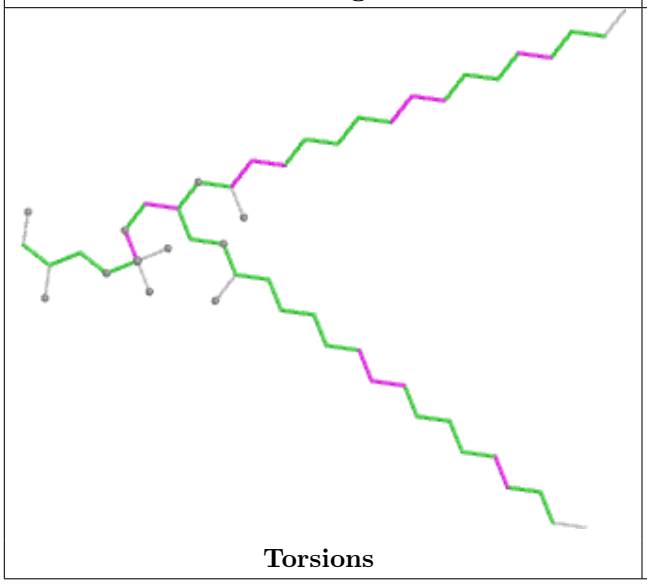
Ligand LHG l 101



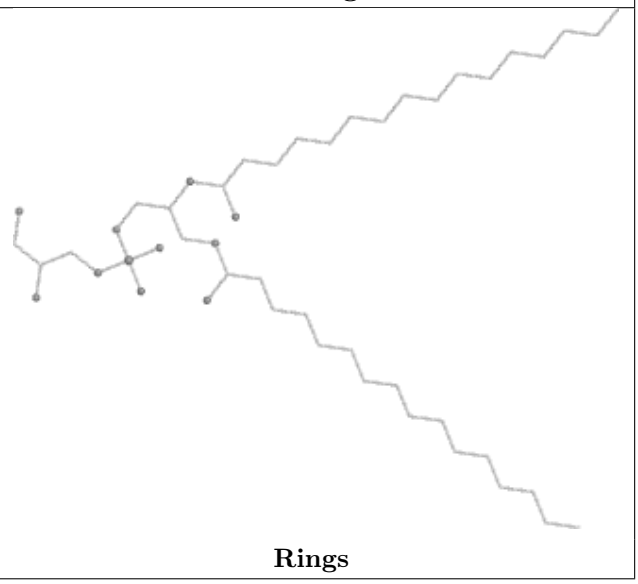
Bond lengths



Bond angles

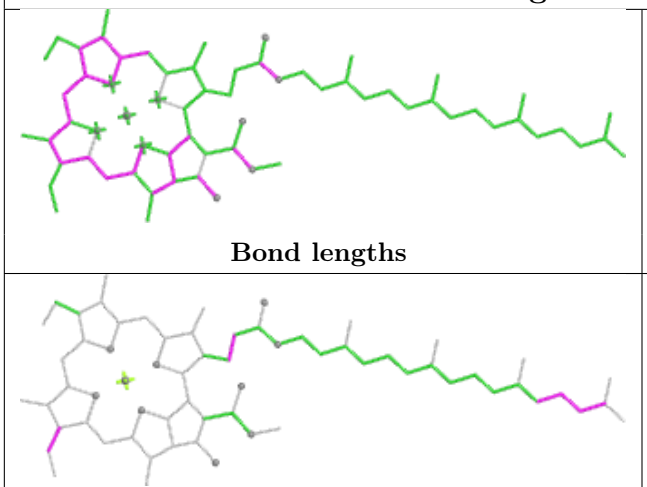


Torsions

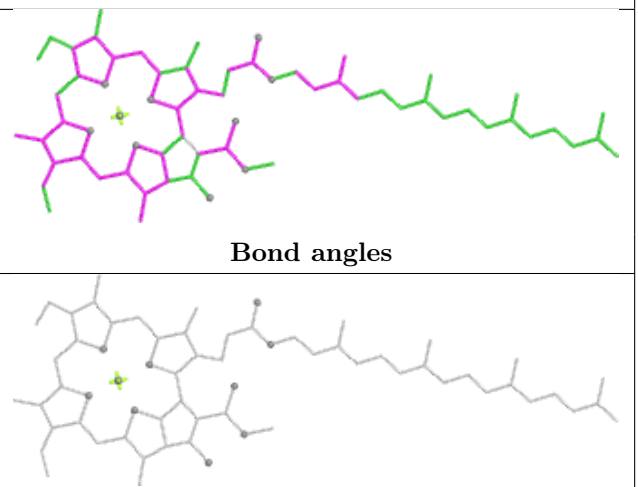


Rings

Ligand CLA a 409



Bond lengths

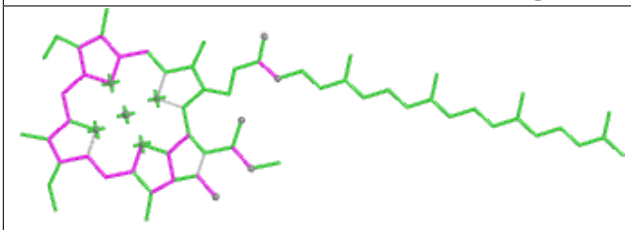


Bond angles

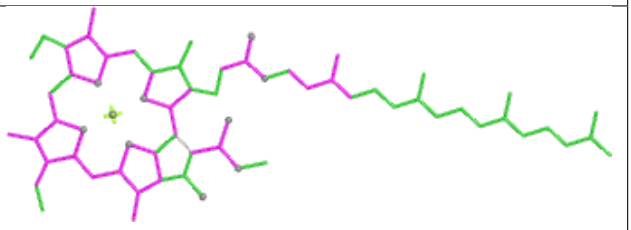
Torsions

Rings

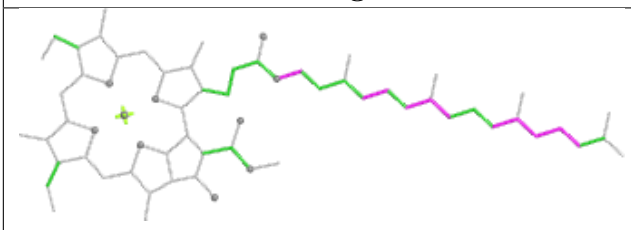
Ligand CLA c 513



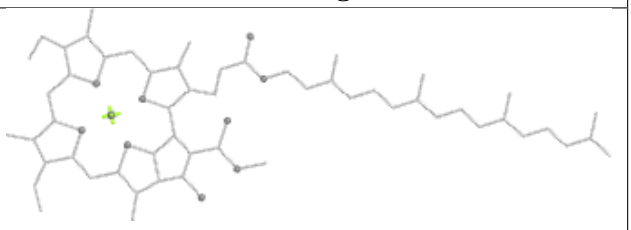
Bond lengths



Bond angles

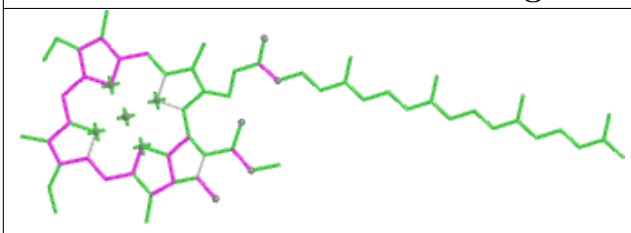


Torsions

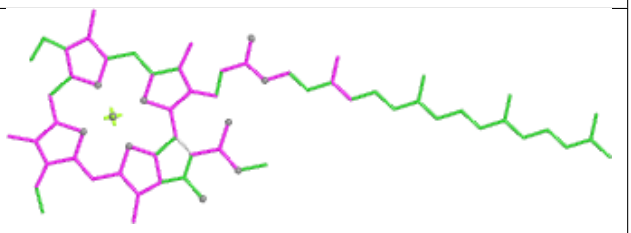


Rings

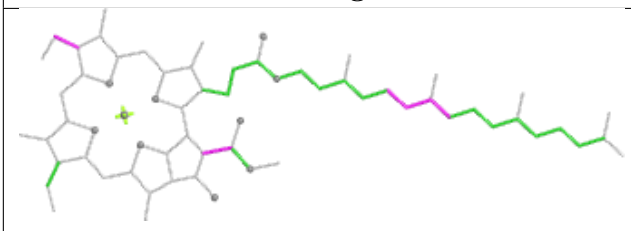
Ligand CLA B 604



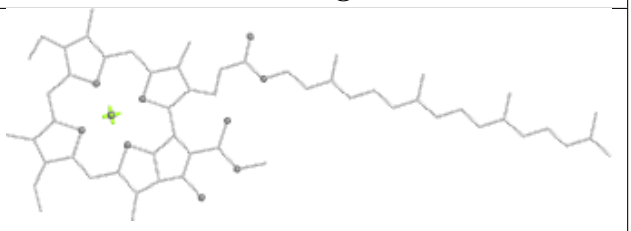
Bond lengths



Bond angles

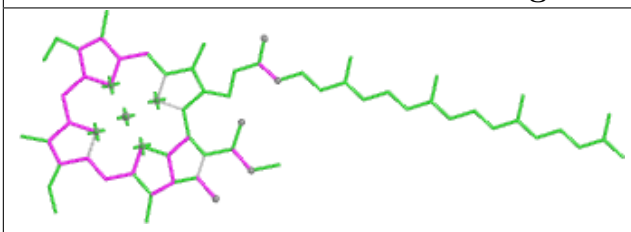


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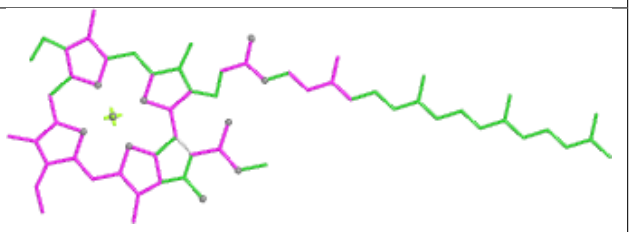


Rings

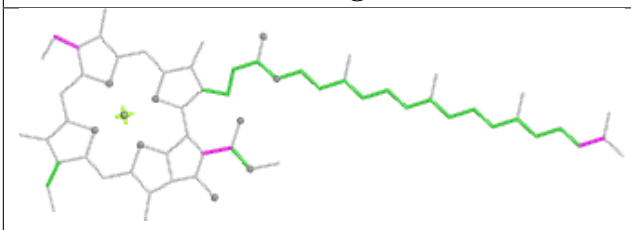
Ligand CLA c 506



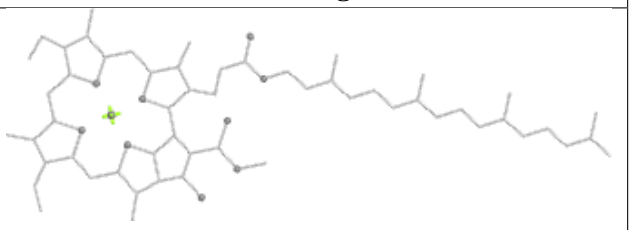
Bond lengths



Bond angles

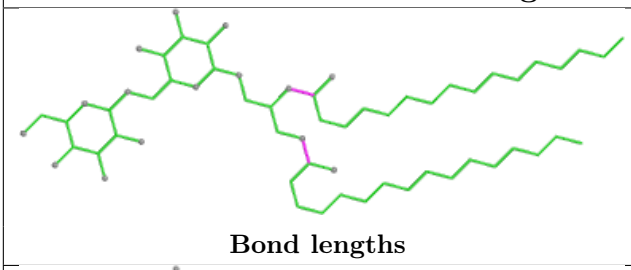


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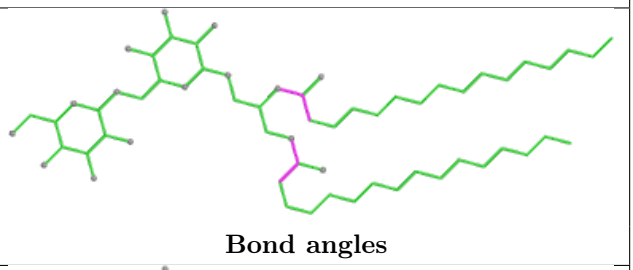


Rings

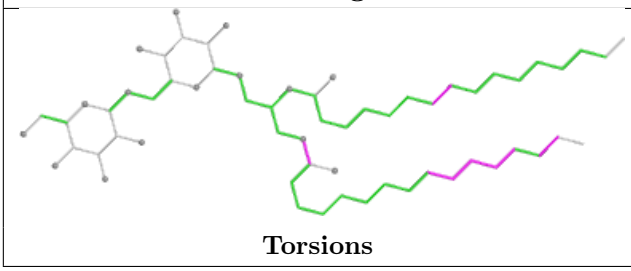
Ligand DGD C 519



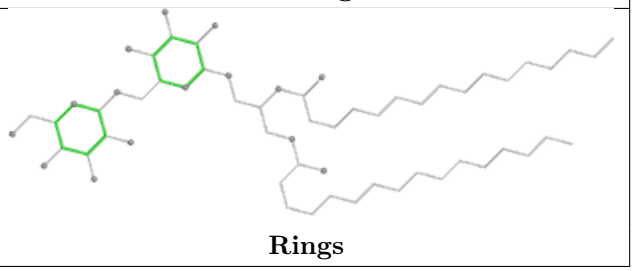
Bond lengths



Bond angles

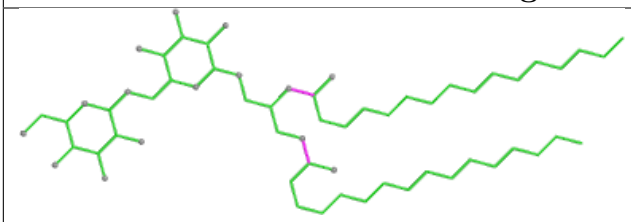


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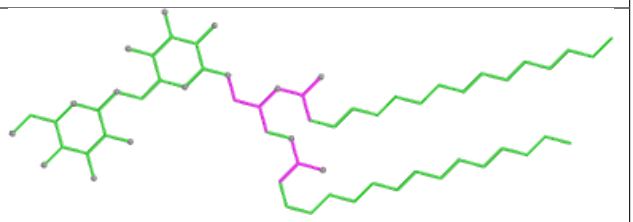


Rings

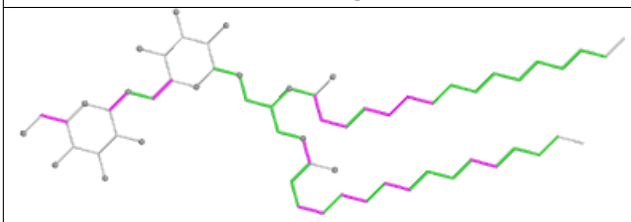
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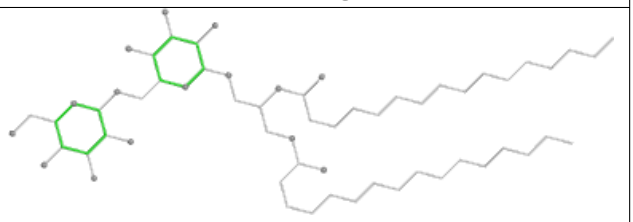
Bond lengths



Bond angles

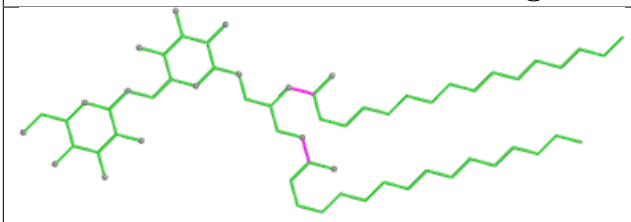


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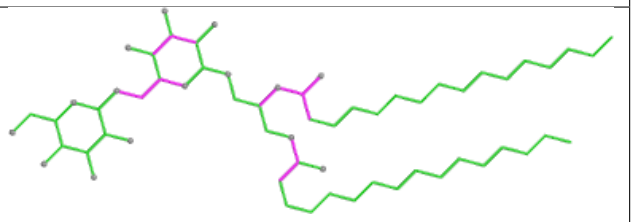


Rings

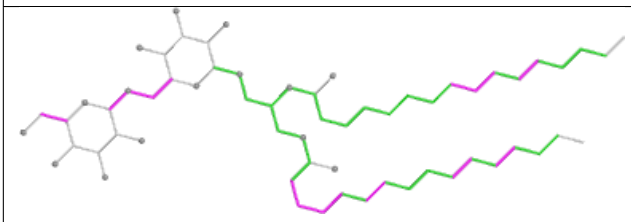
Ligand DGD c 519



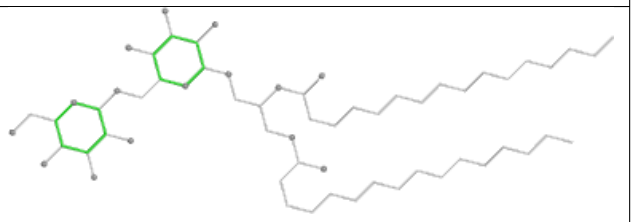
Bond lengths



Bond angles

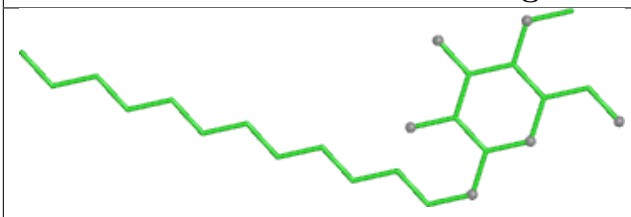


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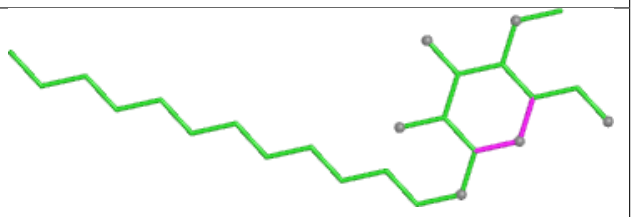


Rings

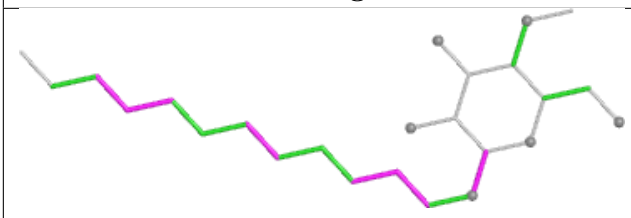
Ligand LMT T 104



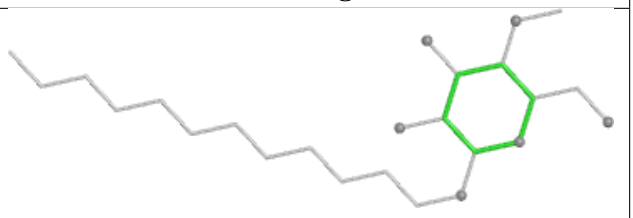
Bond lengths



Bond angles



Torsions

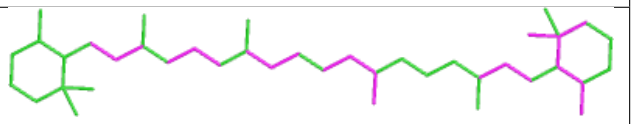


Rings

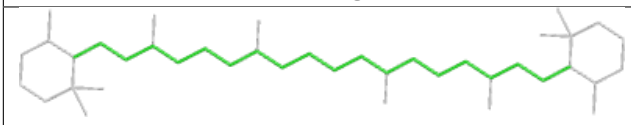
Ligand BCR H 101



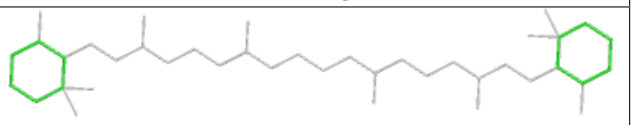
Bond lengths



Bond angles

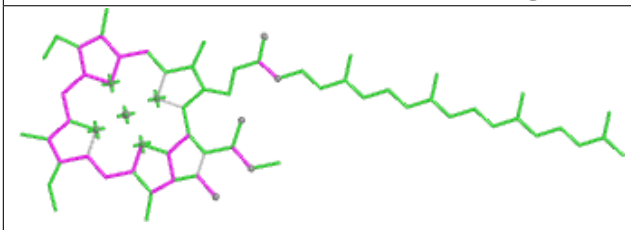


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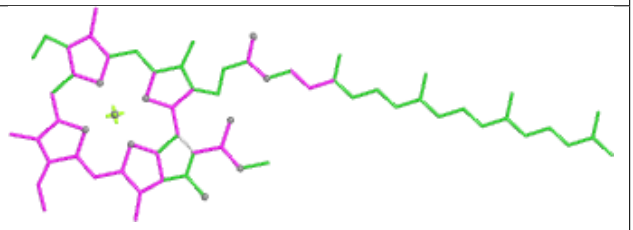


Rings

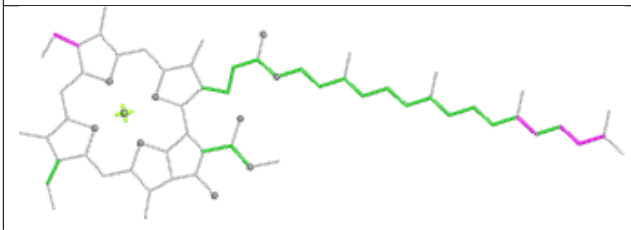
Ligand CLA B 612



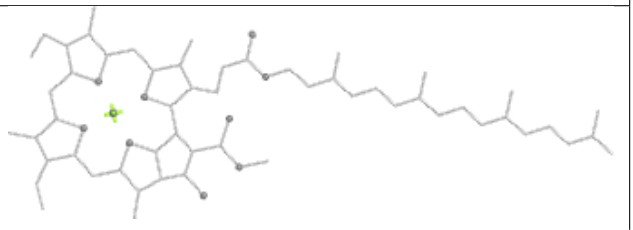
Bond lengths



Bond angles

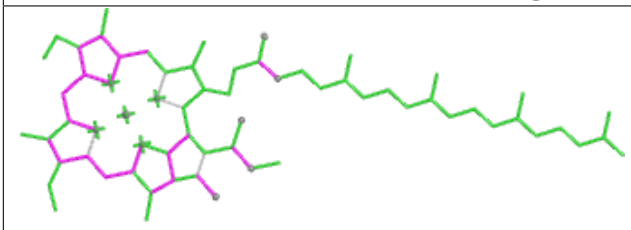


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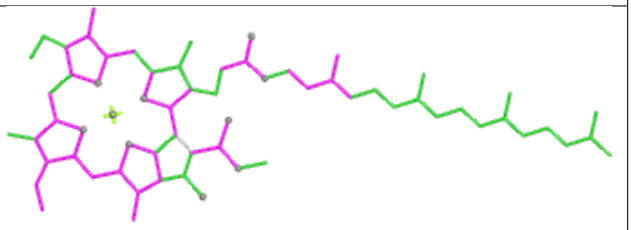


Rings

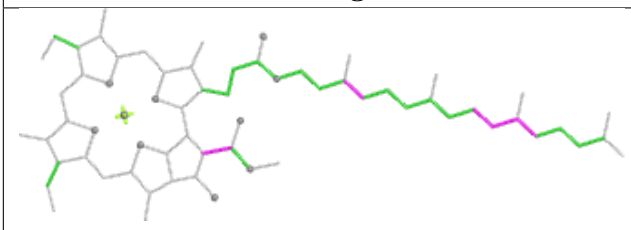
Ligand CLA b 625



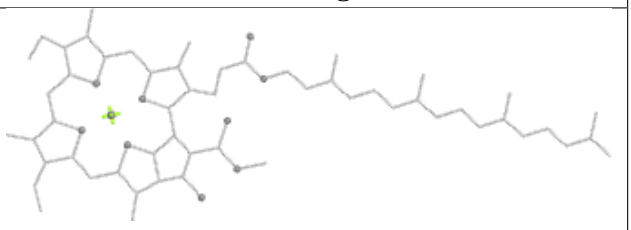
Bond lengths



Bond angles

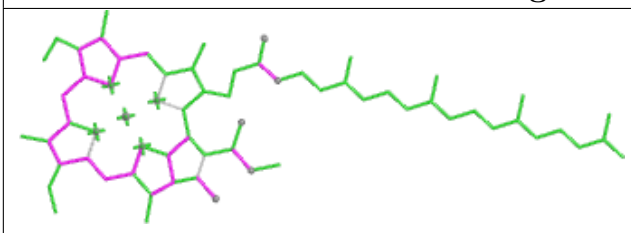


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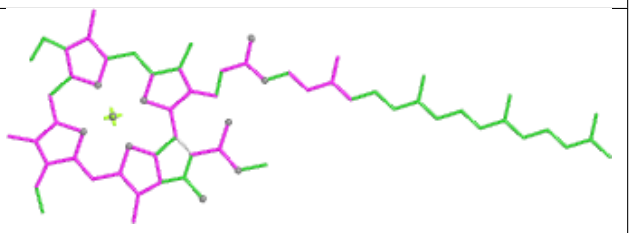


Rings

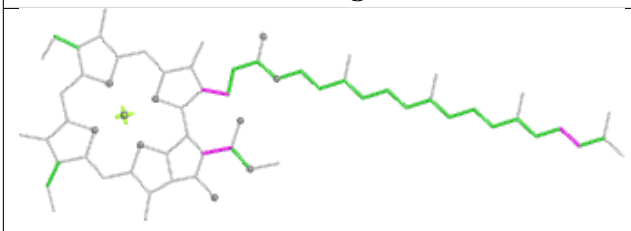
Ligand CLA c 512



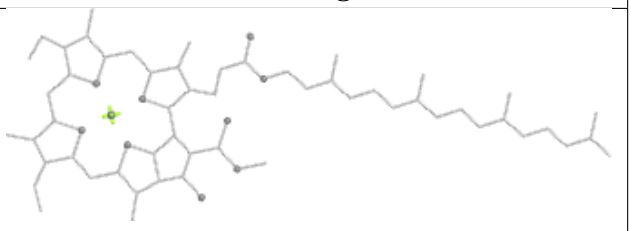
Bond lengths



Bond angles

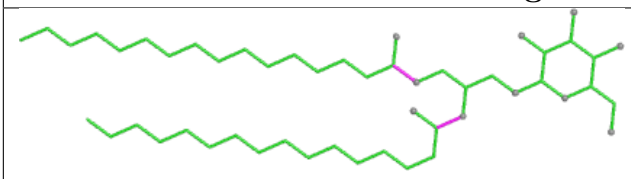


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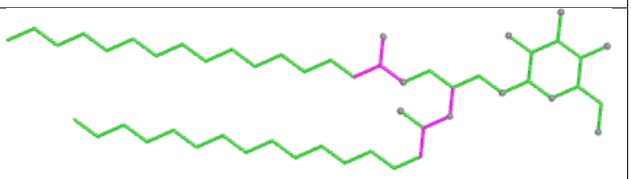


Rings

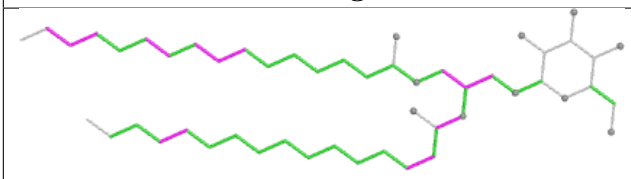
Ligand LMG c 522



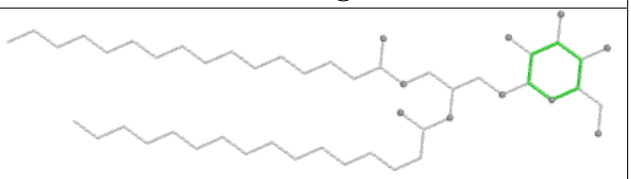
Bond lengths



Bond angles

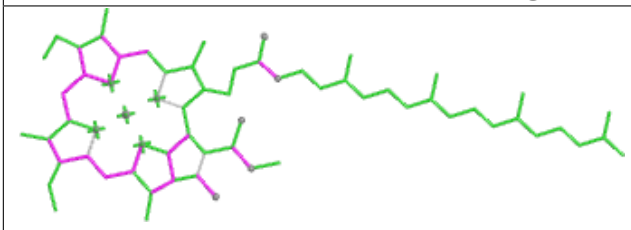


Torsions

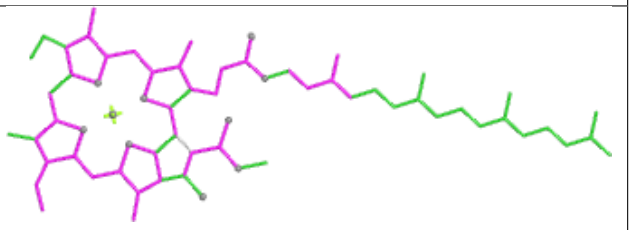


Rings

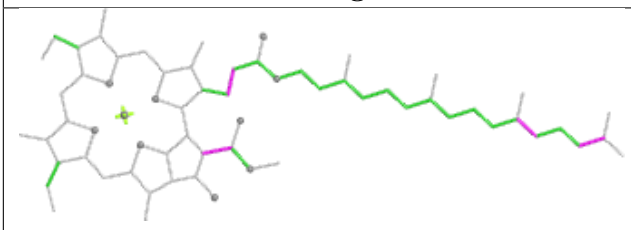
Ligand CLA B 611



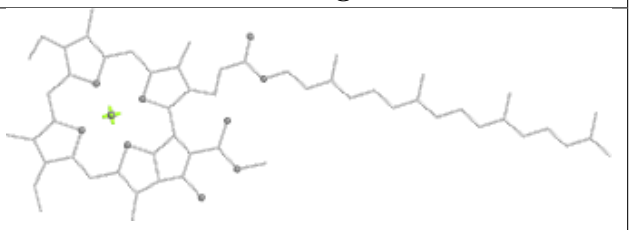
Bond lengths



Bond angles



Torsions

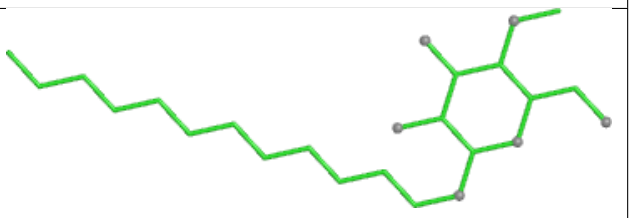


Rings

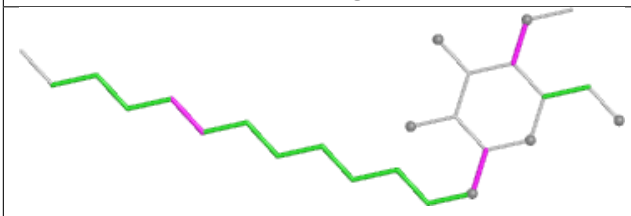
Ligand LMT b 630



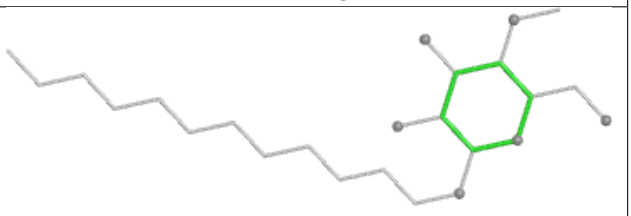
Bond lengths



Bond angles

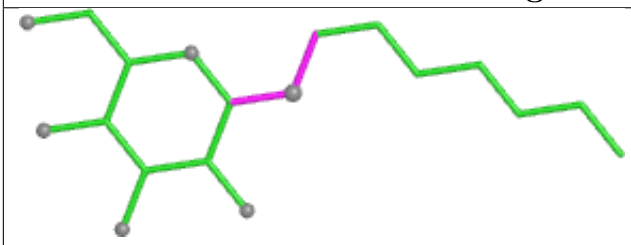


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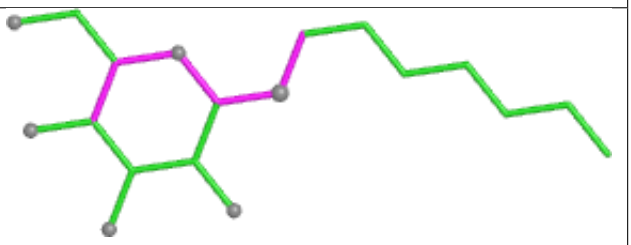


Rings

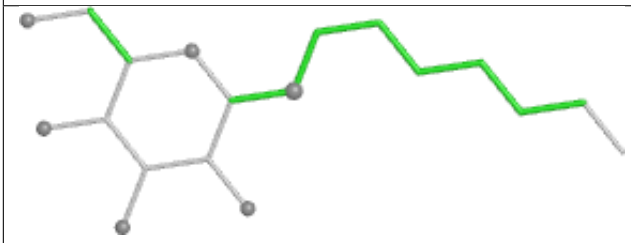
Ligand HTG c 525



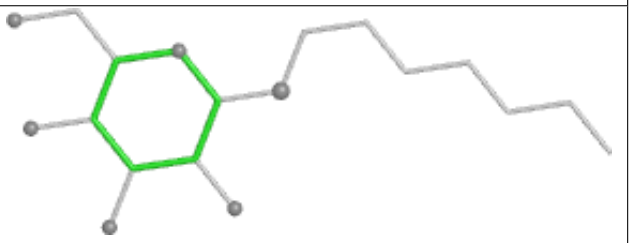
Bond lengths



Bond angles

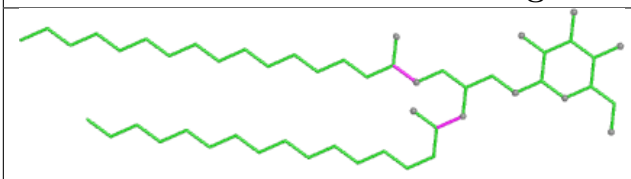


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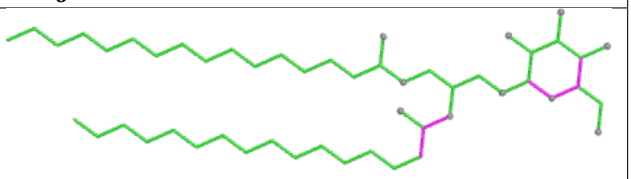


Rings

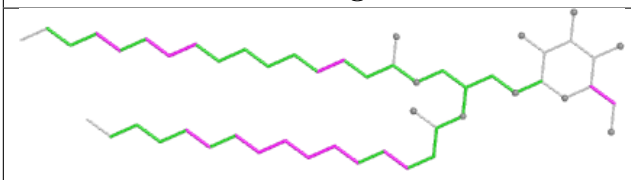
Ligand LMG j 101



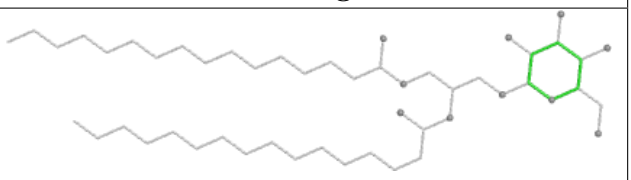
Bond lengths



Bond angles

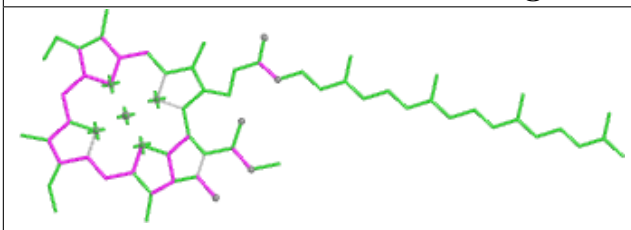


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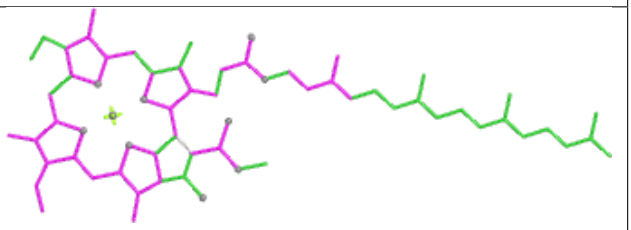


Rings

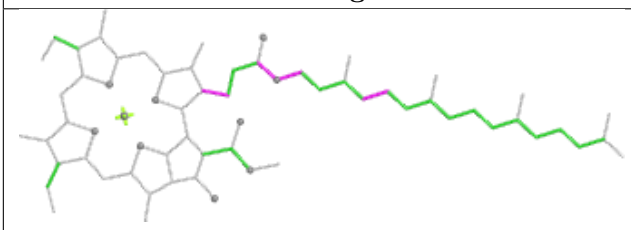
Ligand CLA C 514



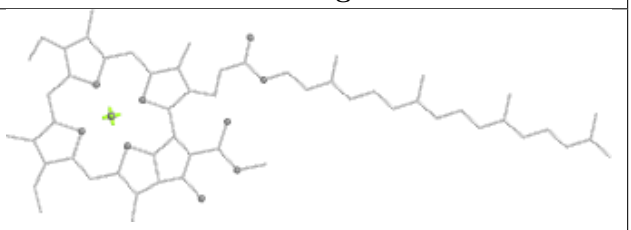
Bond lengths



Bond angles

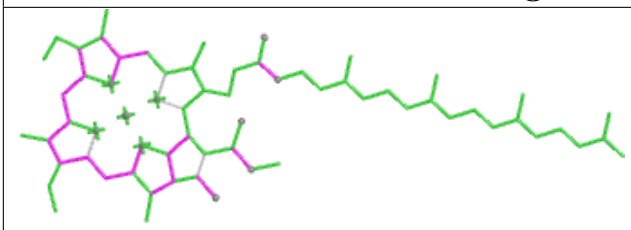


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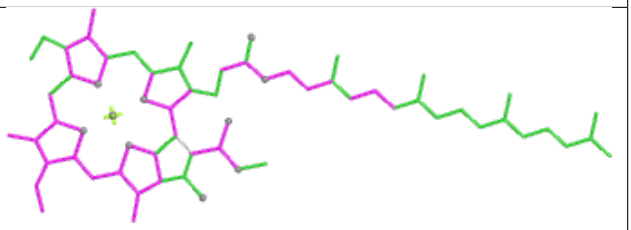


Rings

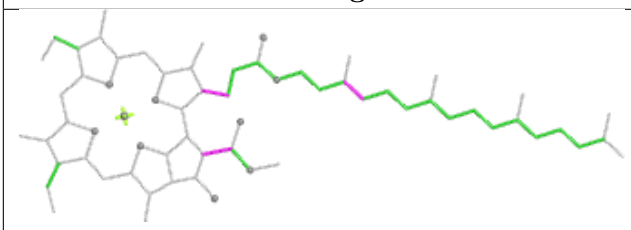
Ligand CLA B 610



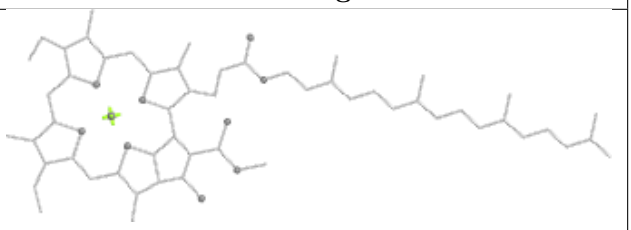
Bond lengths



Bond angles

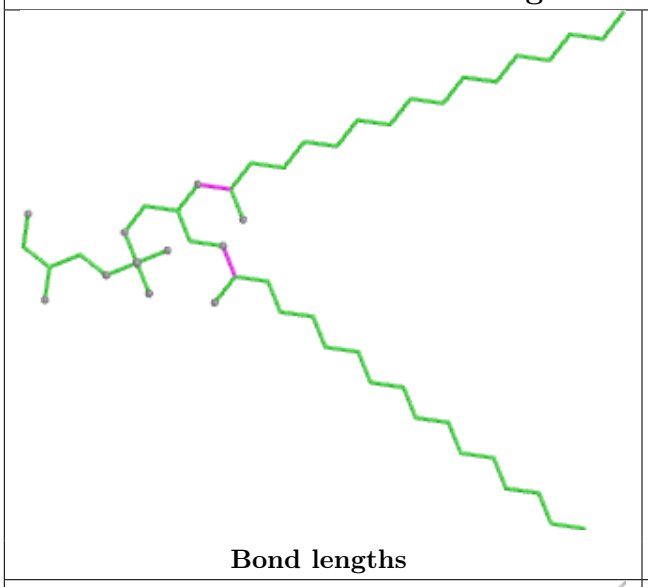


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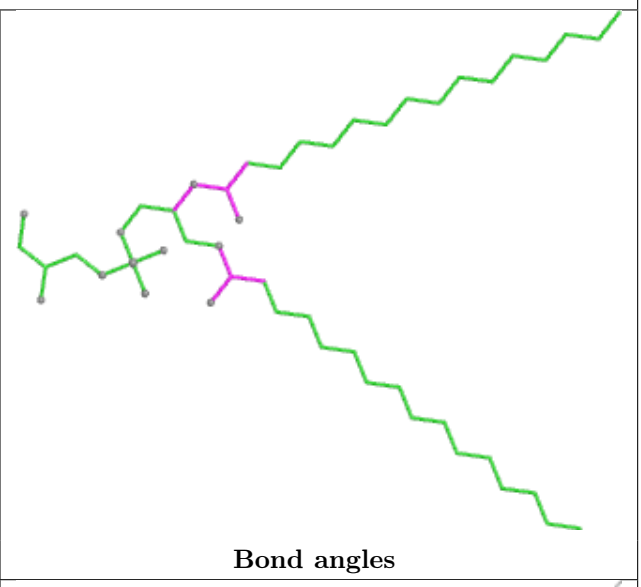


Rings

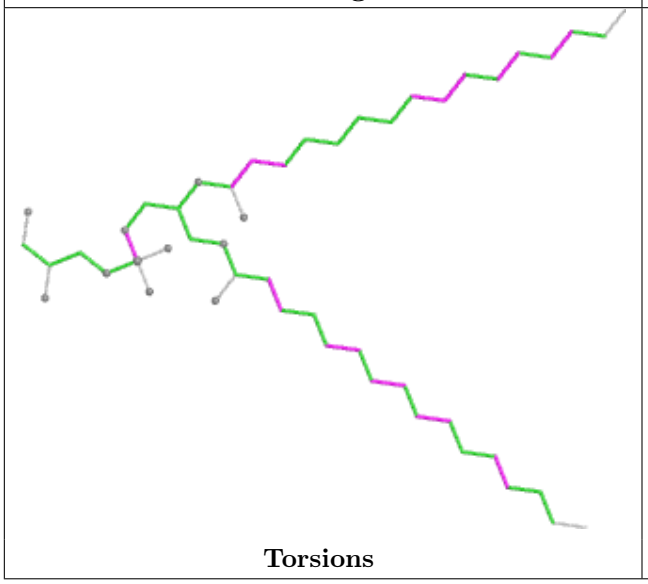
Ligand LHG L 101



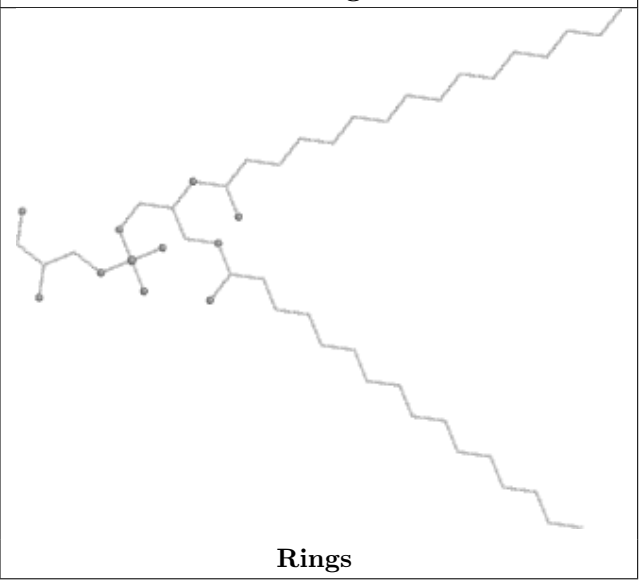
Bond lengths



Bond angles

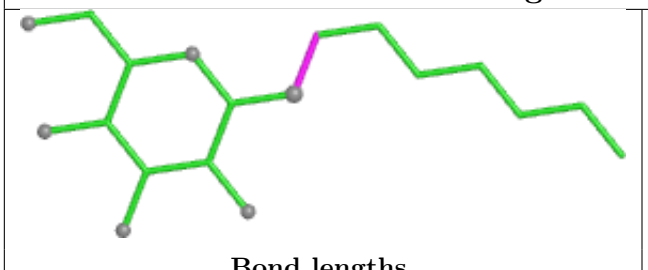


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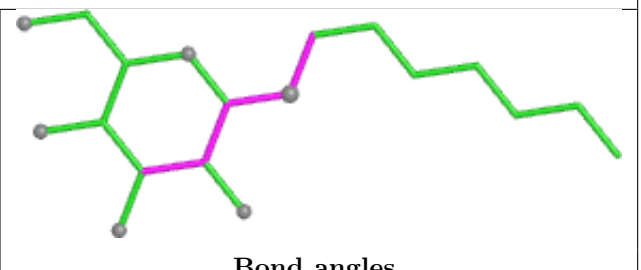


Rings

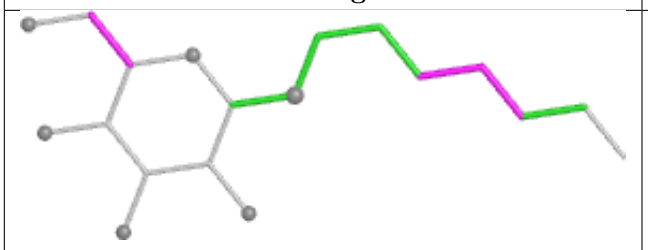
Ligand HTG b 631



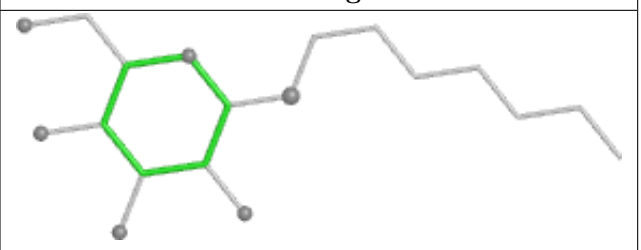
Bond lengths



Bond angles

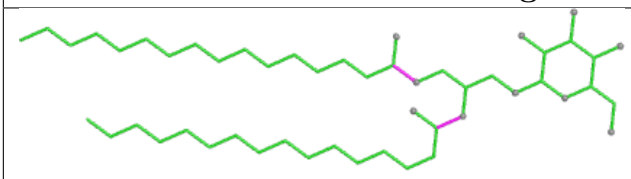


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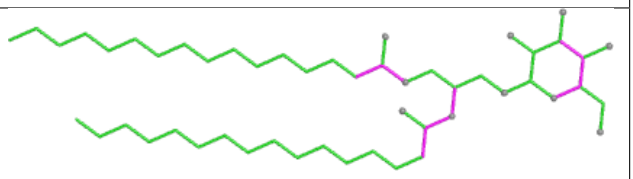


Rings

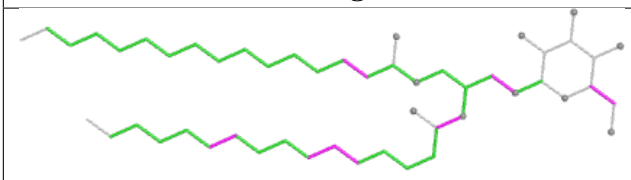
Ligand LMG C 521



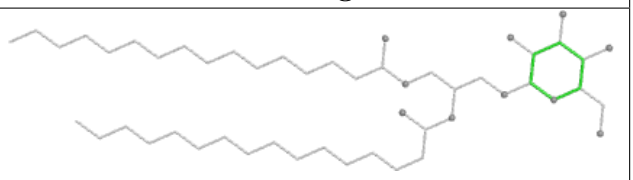
Bond lengths



Bond angles

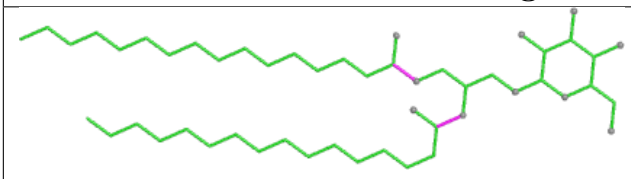


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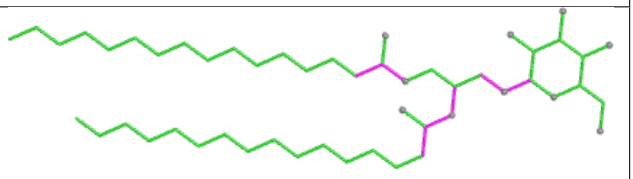


Rings

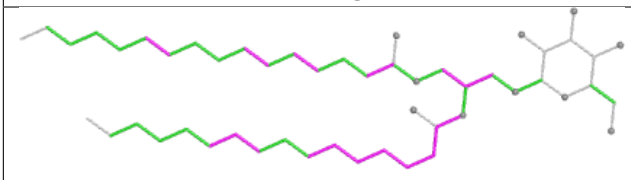
Ligand LMG C 501



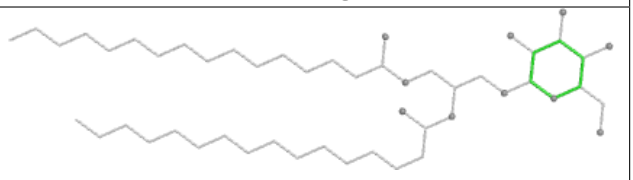
Bond lengths



Bond angles

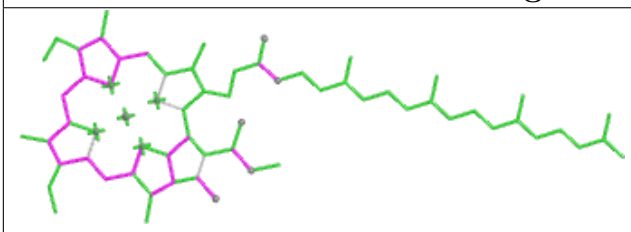


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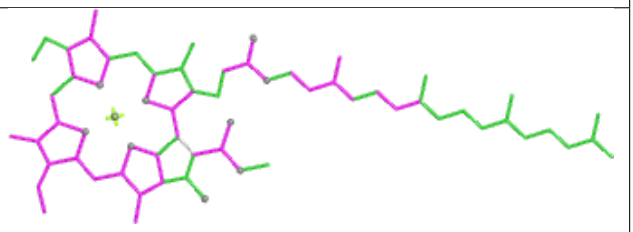


Rings

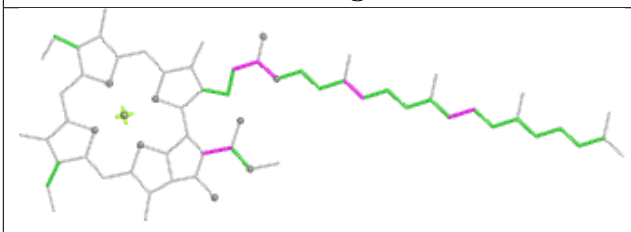
Ligand CLA C 511



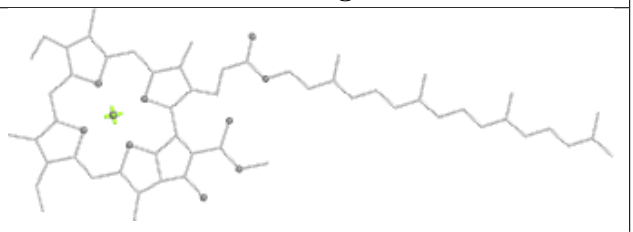
Bond lengths



Bond angles

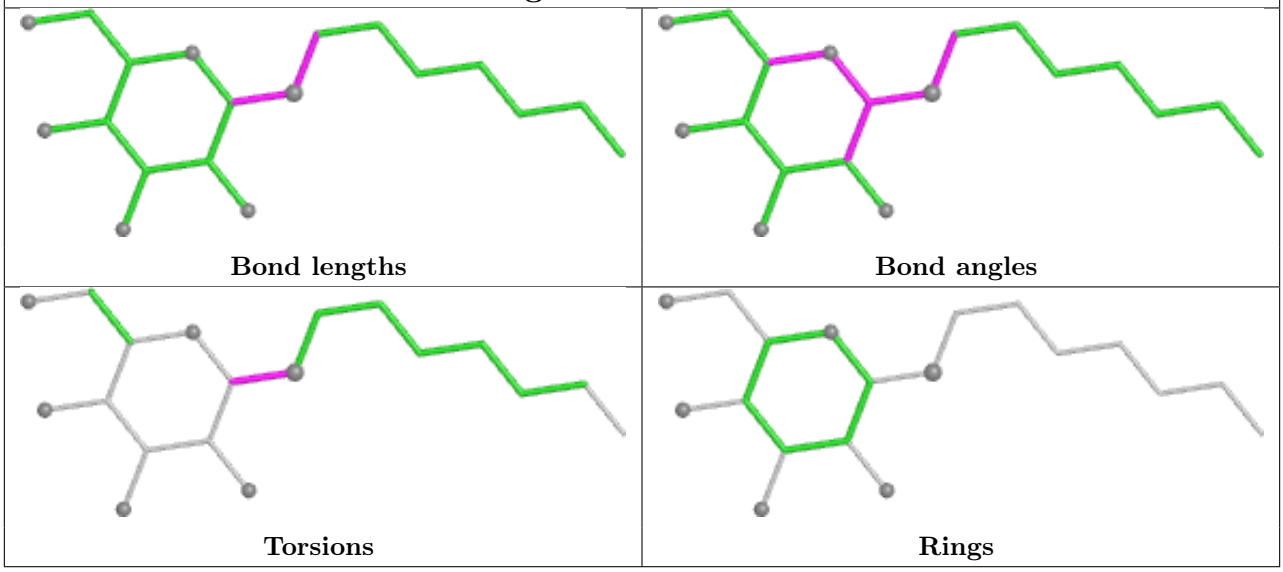


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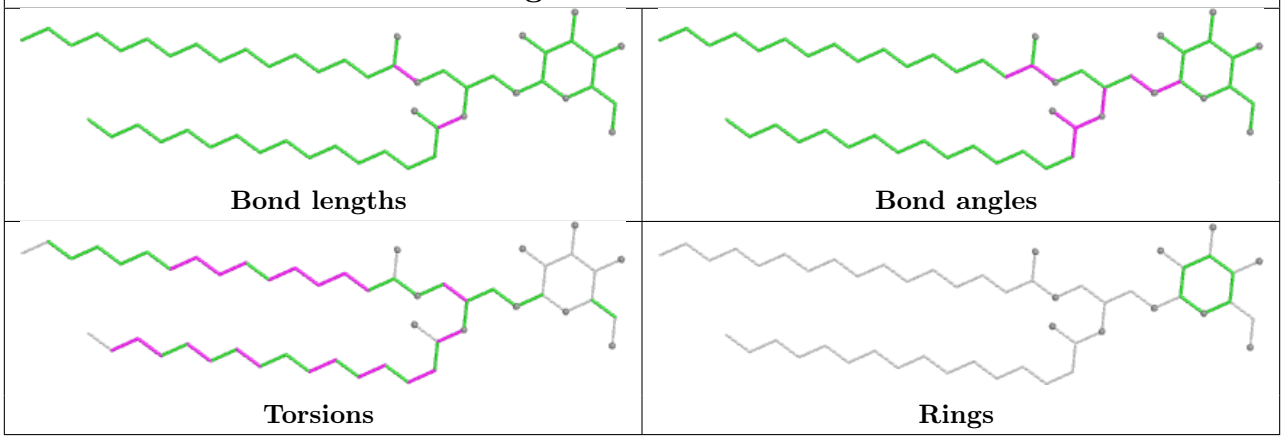


Rings

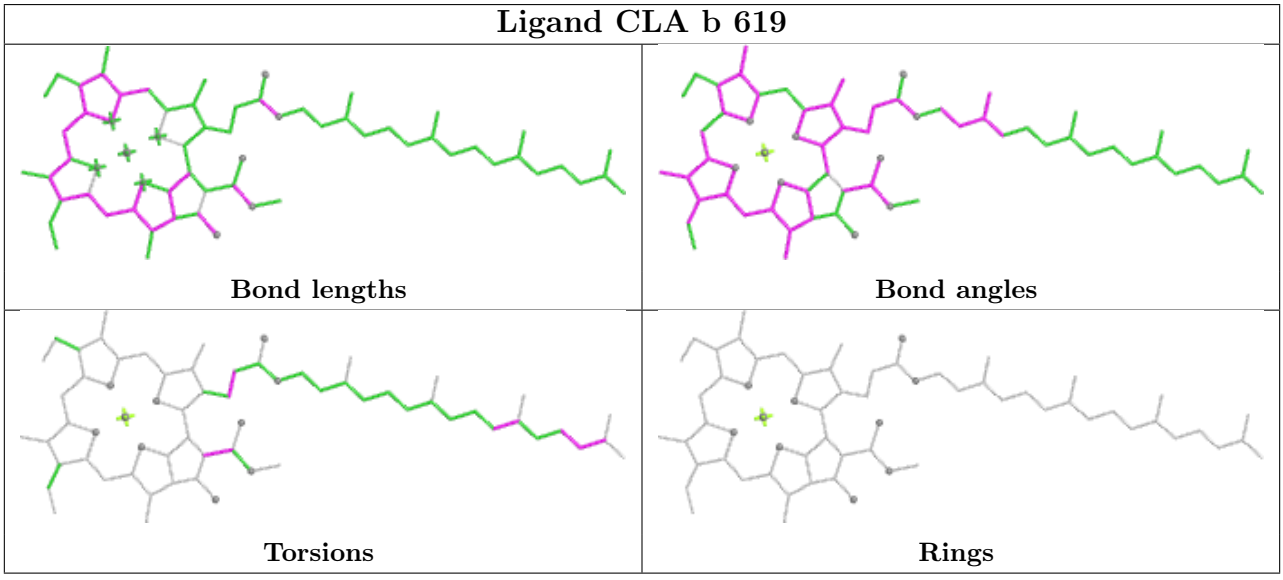
Ligand HTG b 608



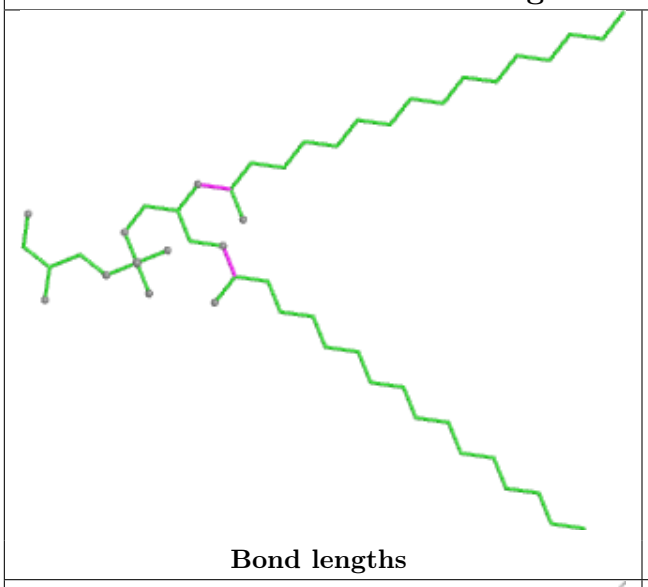
Ligand LMG a 415



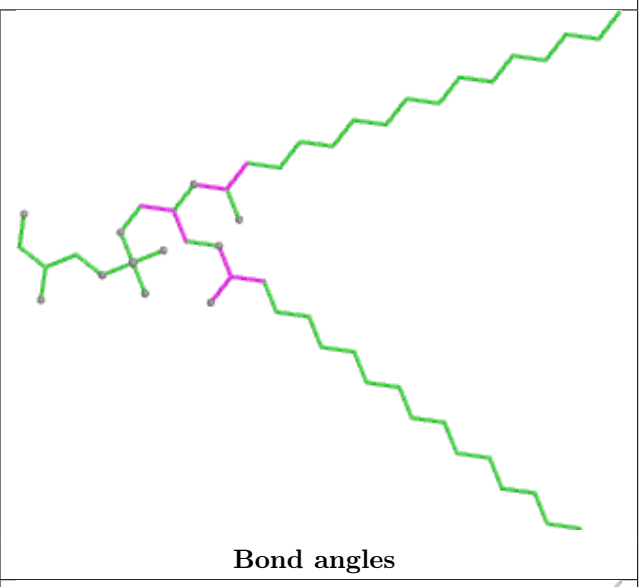
Ligand CLA b 619



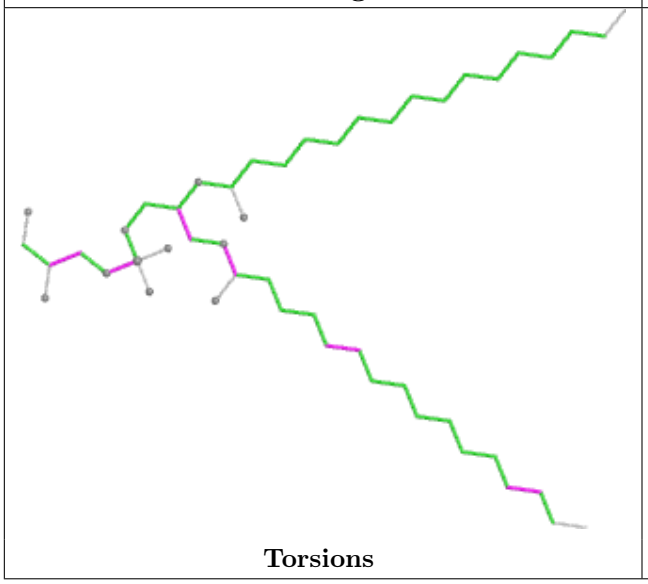
Ligand LHG d 408



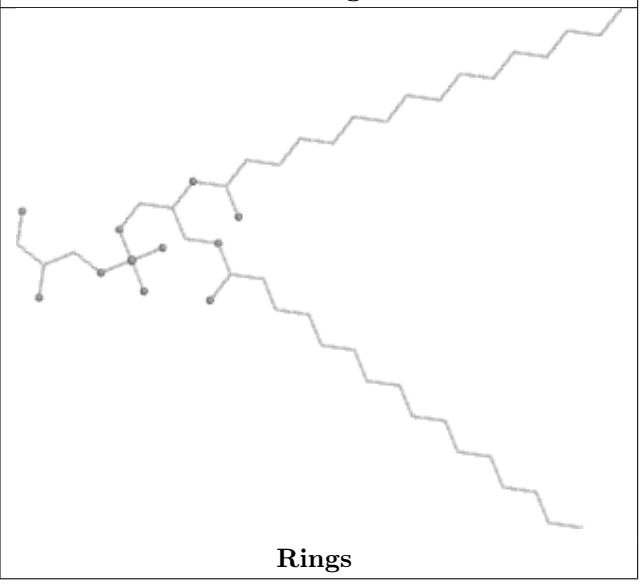
Bond lengths



Bond angles

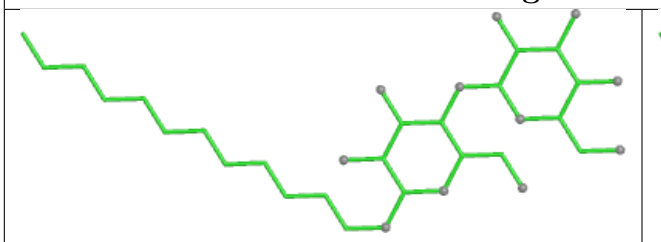


Torsions

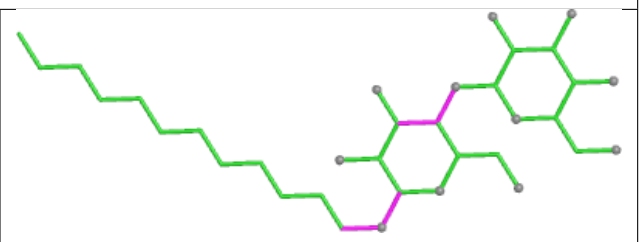


Rings

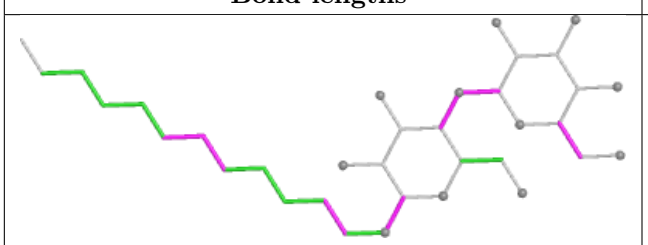
Ligand LMT B 622



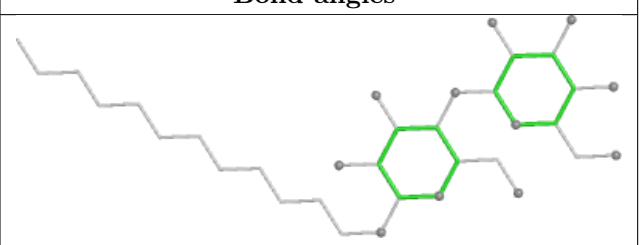
Bond lengths



Bond angles

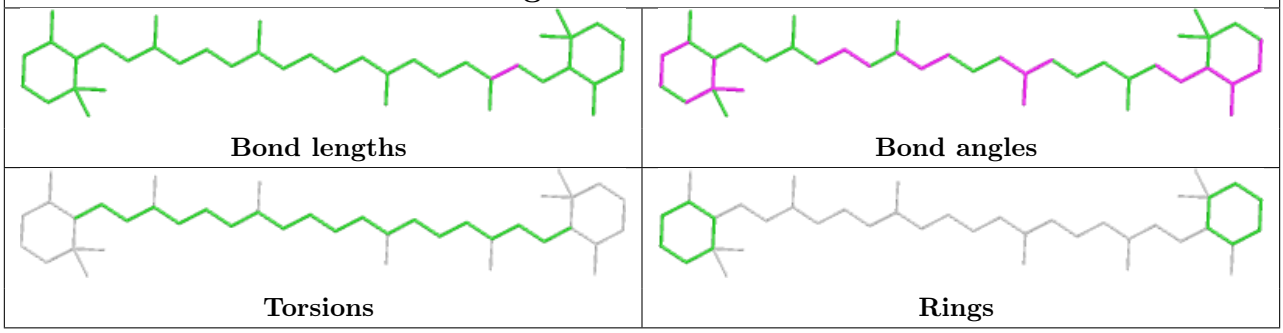


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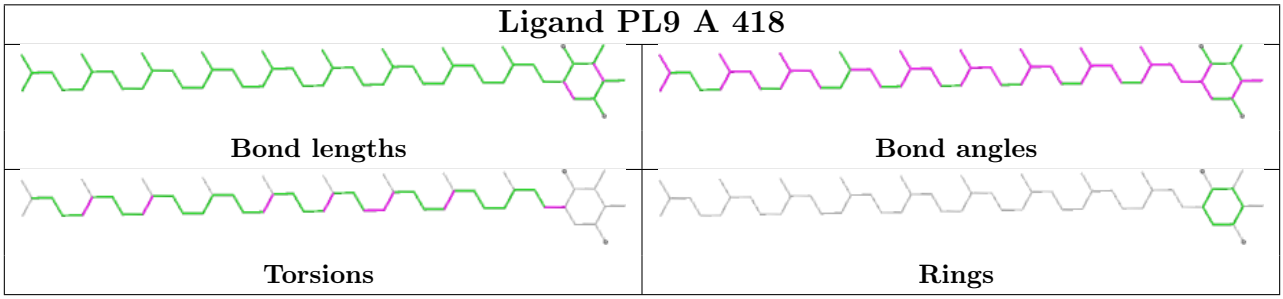


Rings

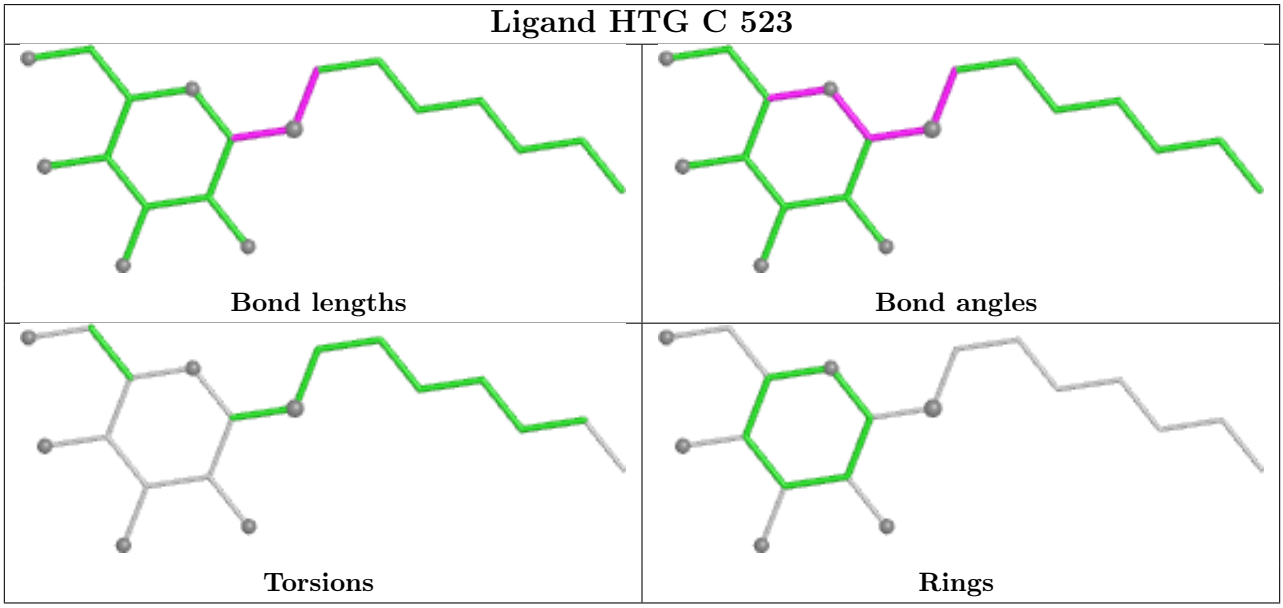
Ligand BCR B 620



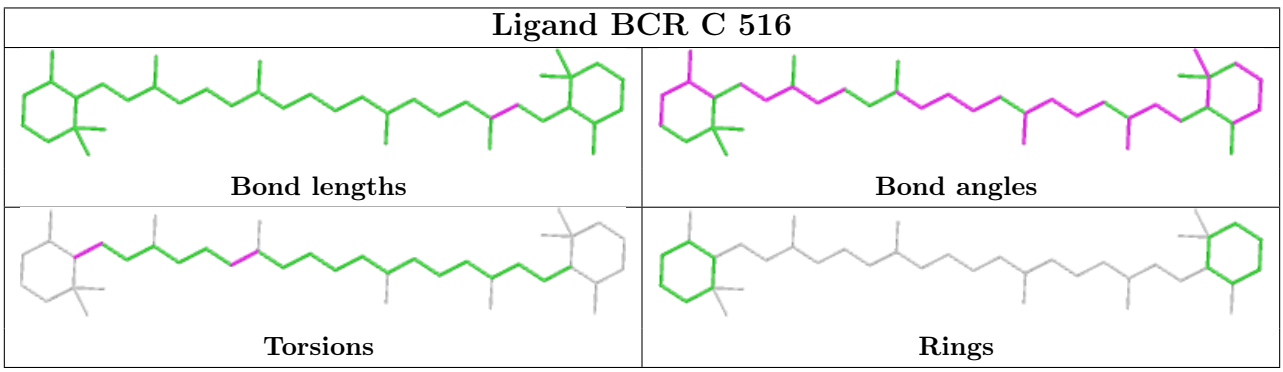
Ligand PL9 A 418



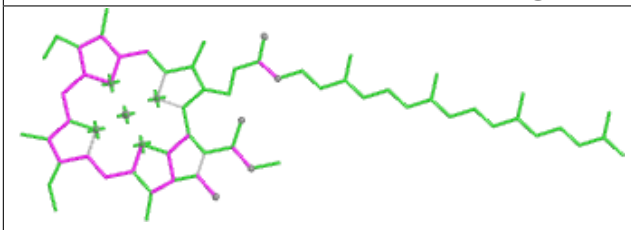
Ligand HTG C 523



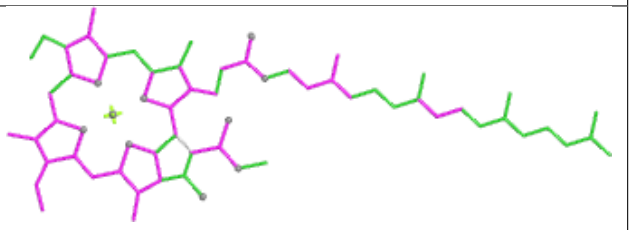
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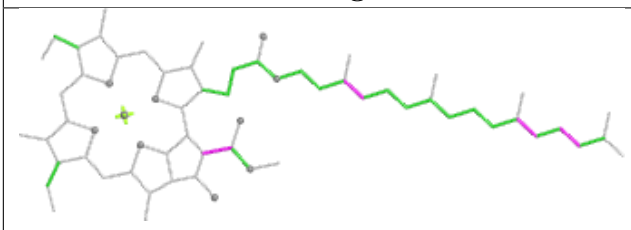
Ligand CLA c 508



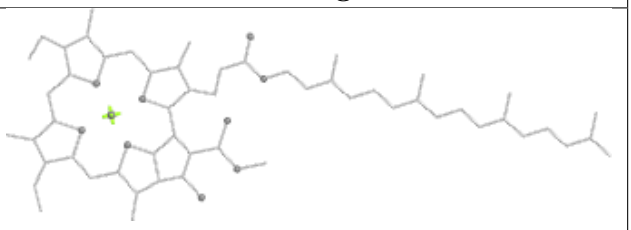
Bond lengths



Bond angles

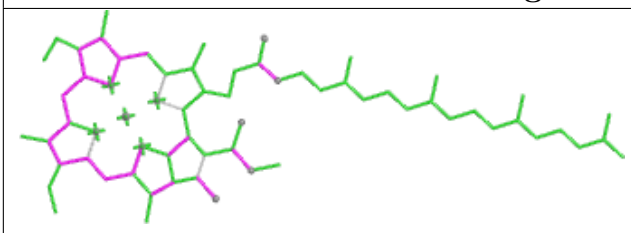


Torsions

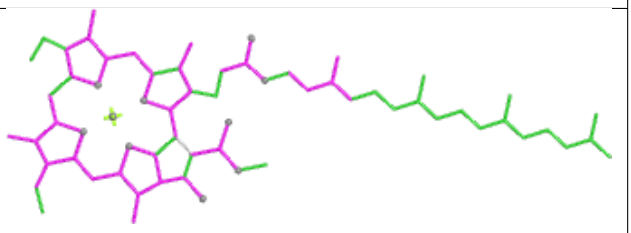


Rings

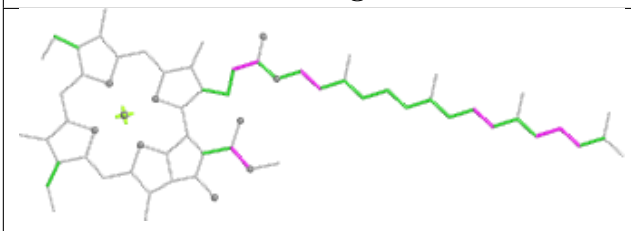
Ligand CLA B 614



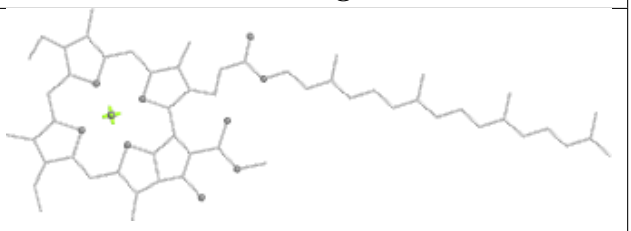
Bond lengths



Bond angles

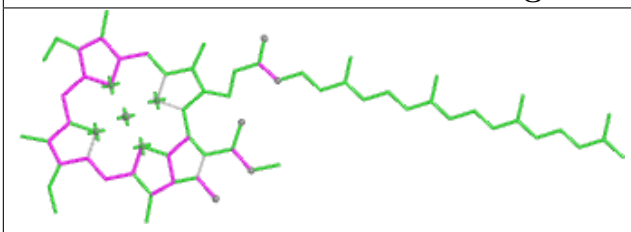


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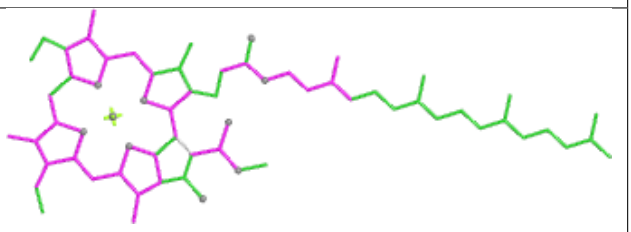


Rings

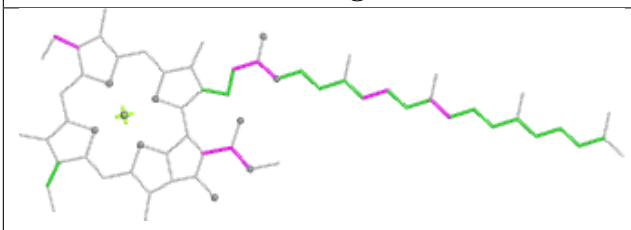
Ligand CLA C 513



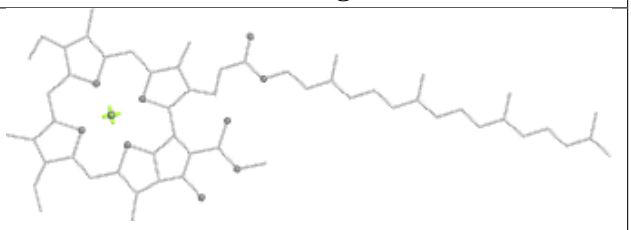
Bond lengths



Bond angles

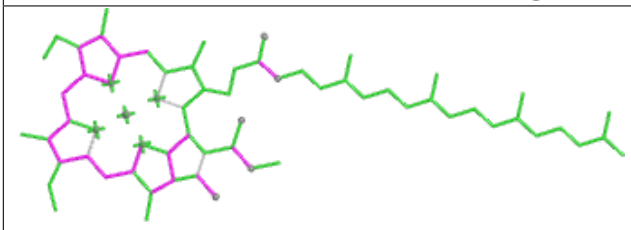


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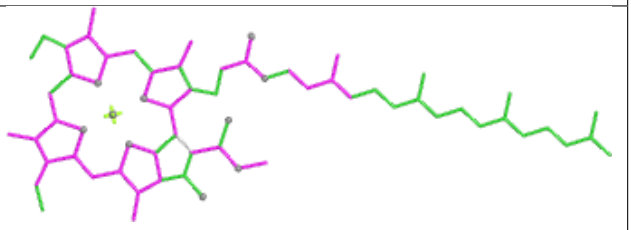


Rings

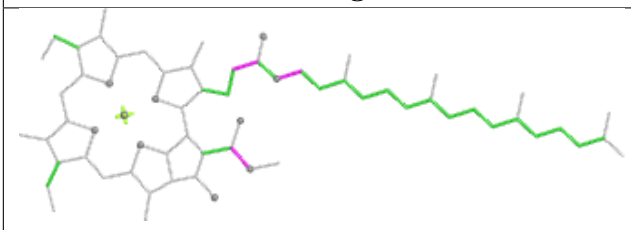
Ligand CLA b 622



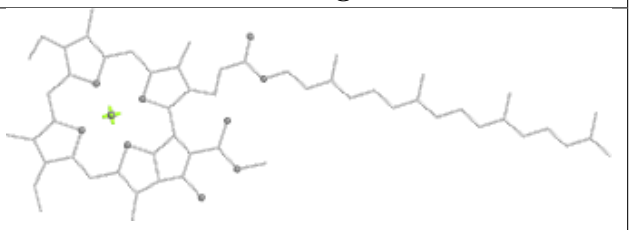
Bond lengths



Bond angles

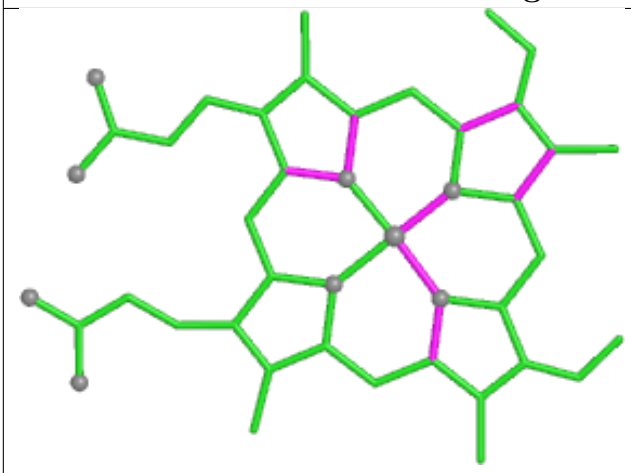


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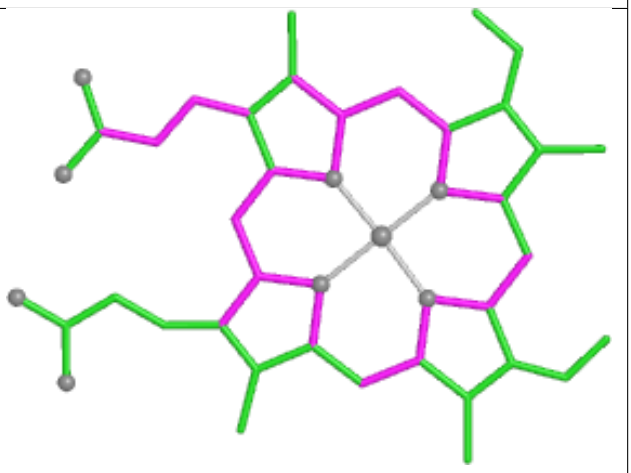


Rings

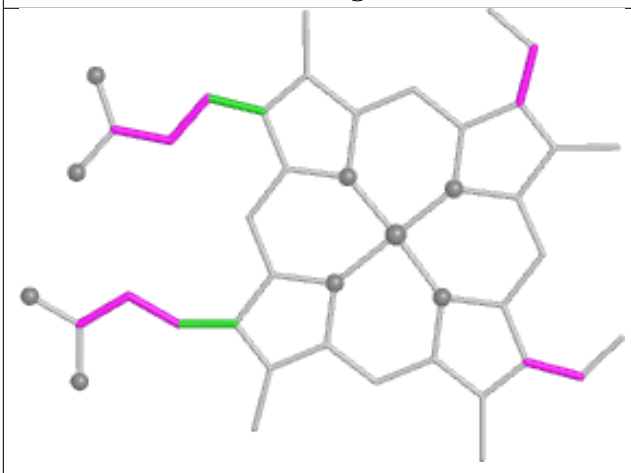
Ligand HEM e 103



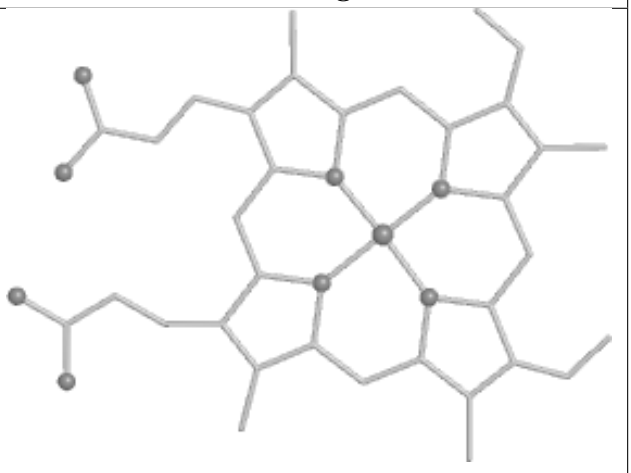
Bond lengths



Bond angles

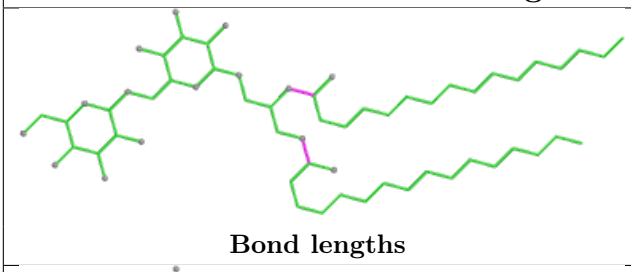


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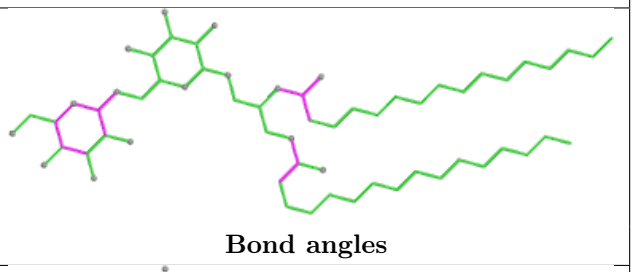


Rings

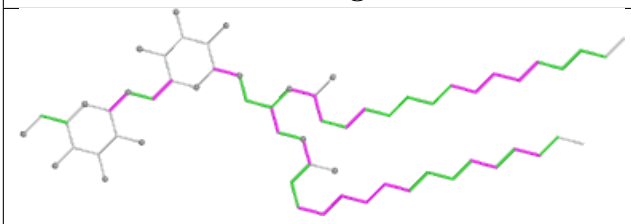
Ligand DGD e 101



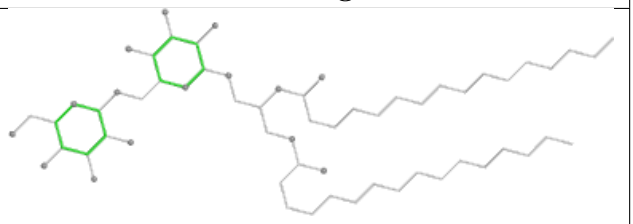
Bond lengths



Bond angles

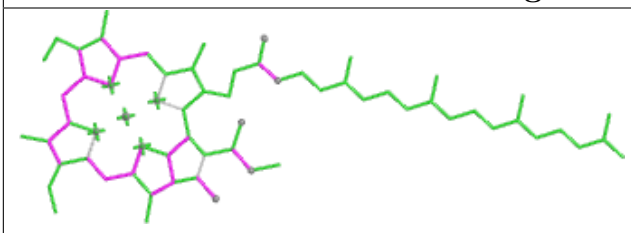


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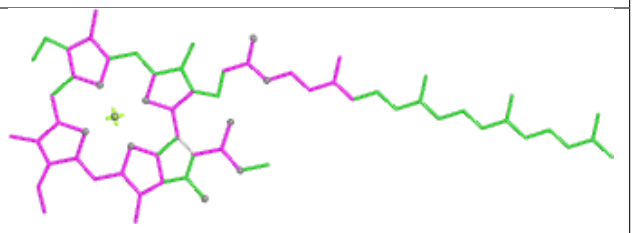


Rings

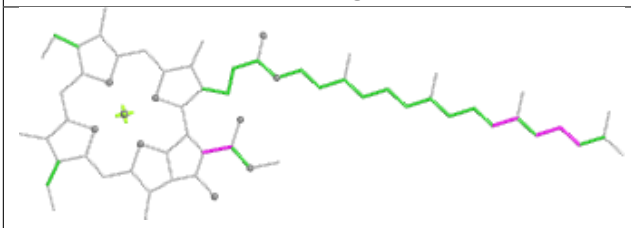
Ligand CLA C 502



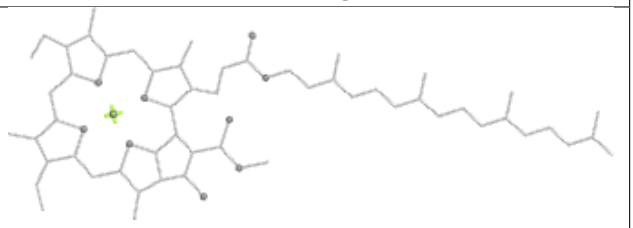
Bond lengths



Bond angles

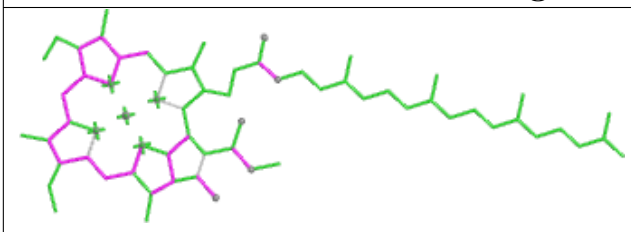


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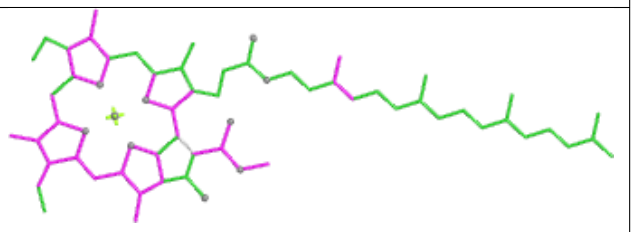


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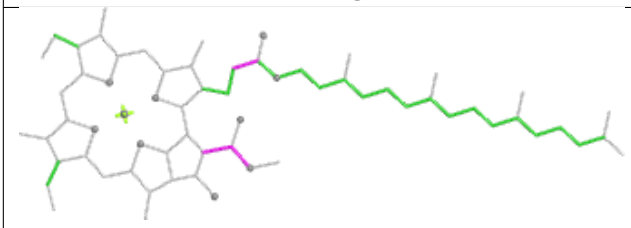
Ligand CLA c 509



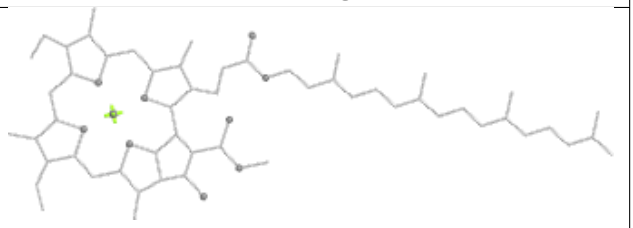
Bond lengths



Bond angles

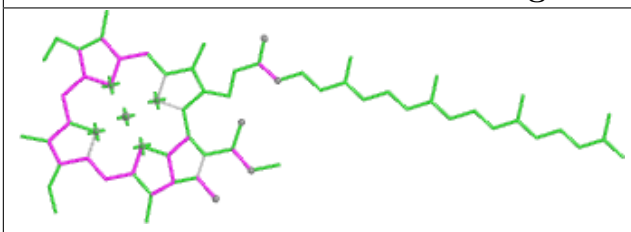


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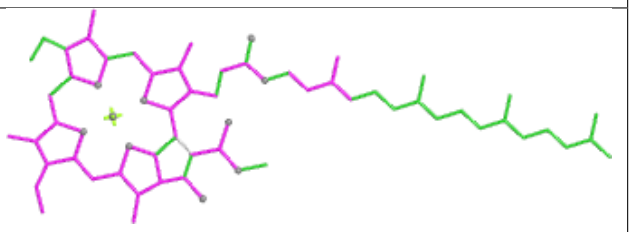


Rings

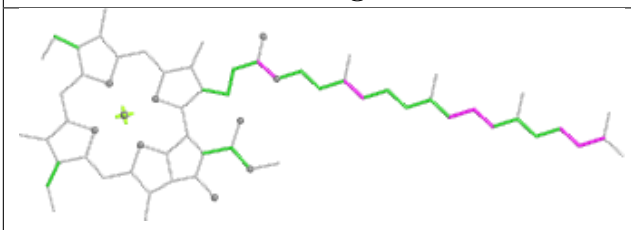
Ligand CLA a 412



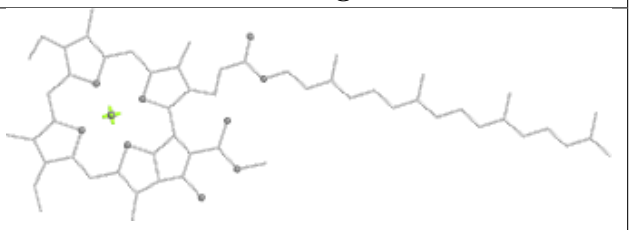
Bond lengths



Bond angles

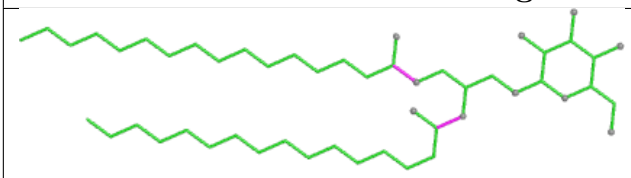


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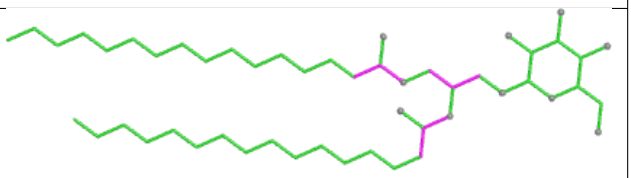


Rings

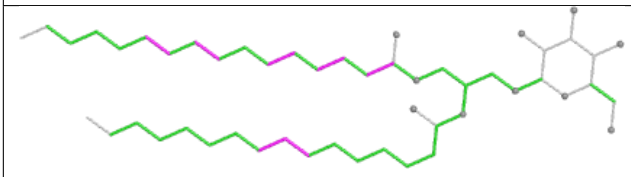
Ligand LMG M 101



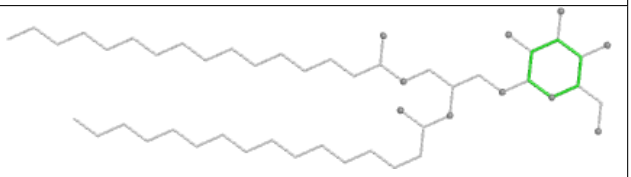
Bond lengths



Bond angles

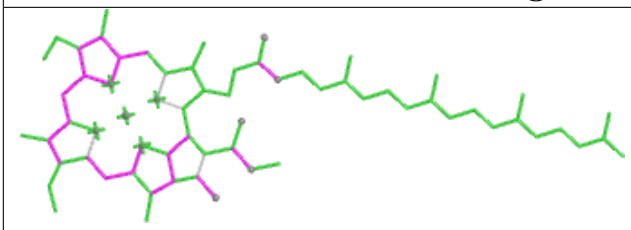


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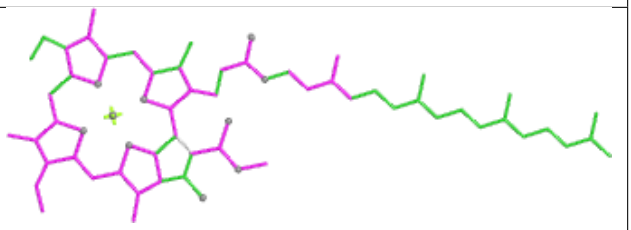


Rings

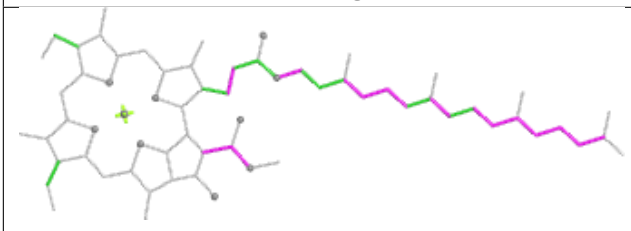
Ligand CLA b 623



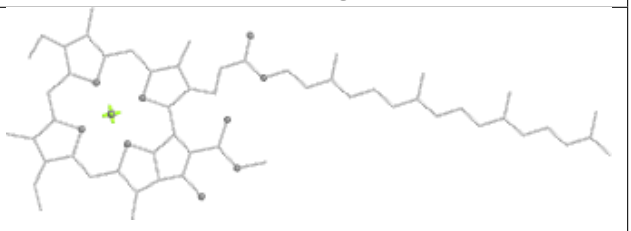
Bond lengths



Bond angles

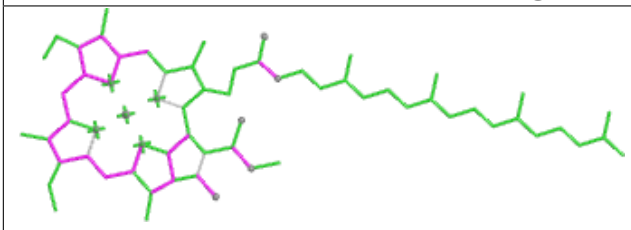


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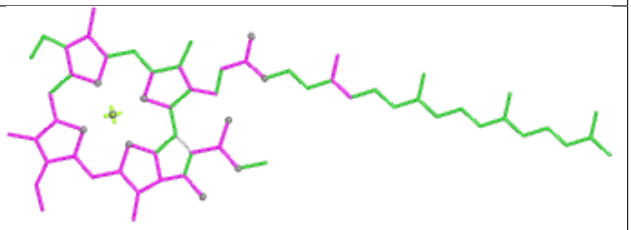


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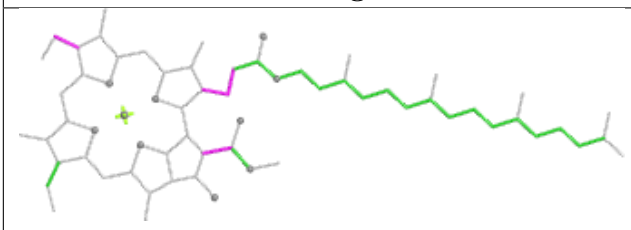
Ligand CLA c 505



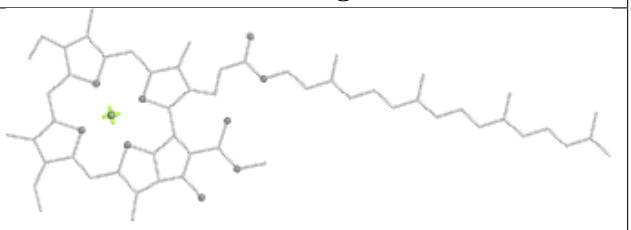
Bond lengths



Bond angles

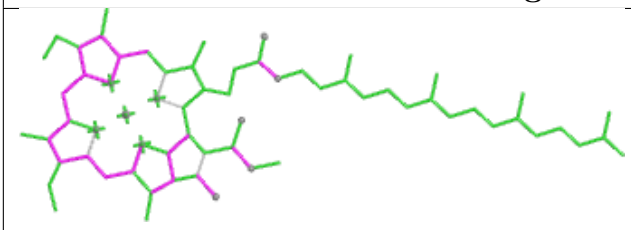


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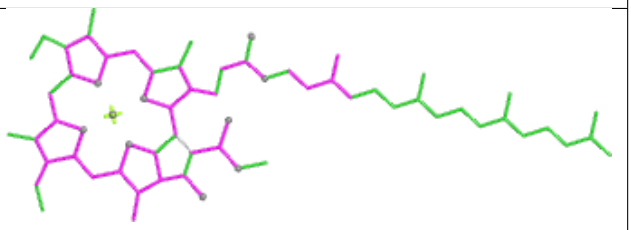


Rings

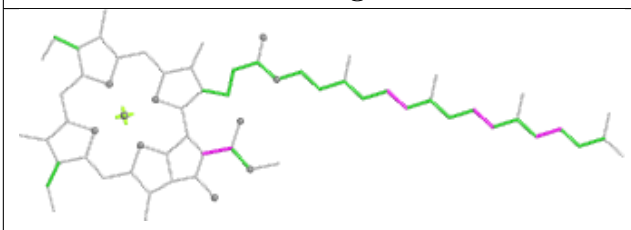
Ligand CLA C 509



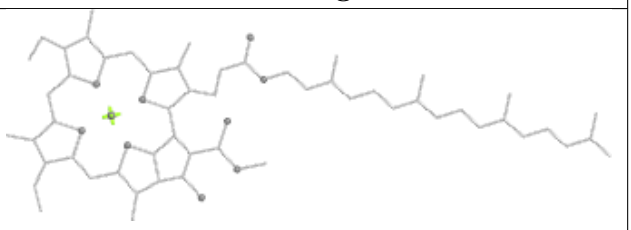
Bond lengths



Bond angles

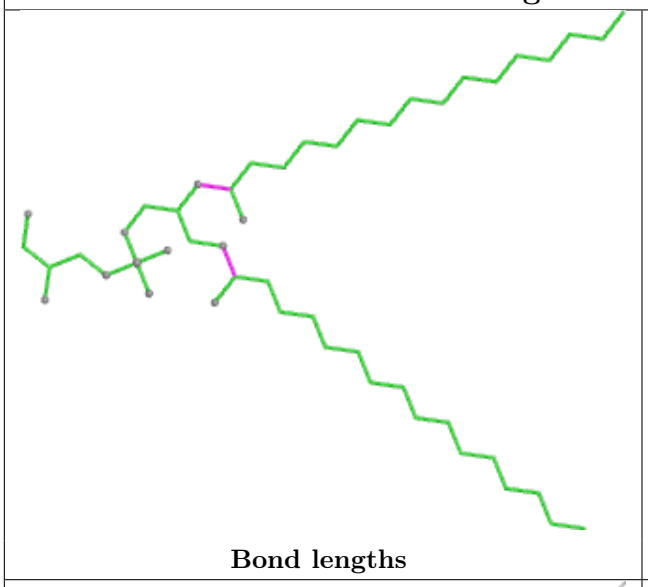


Torsions

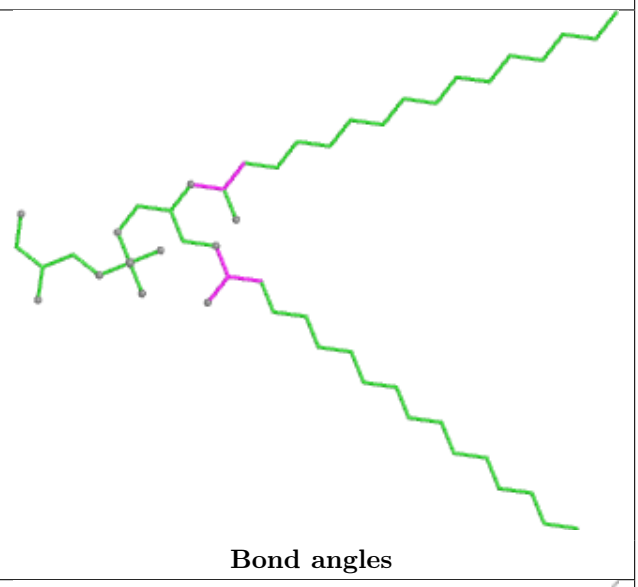


Rings

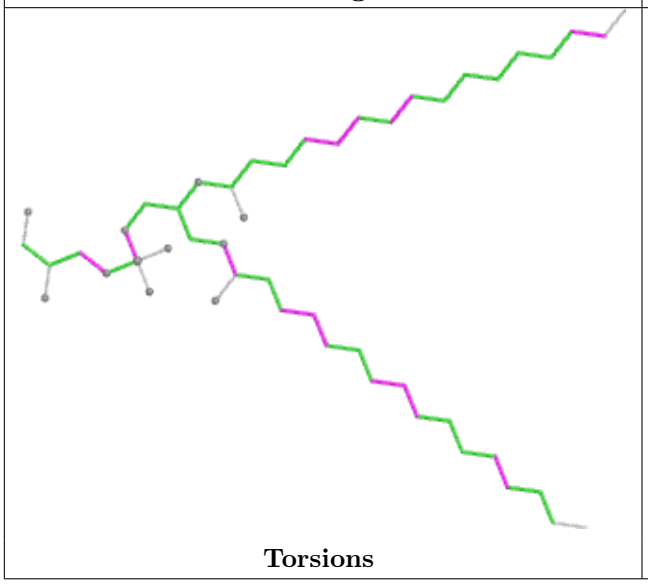
Ligand LHG D 409



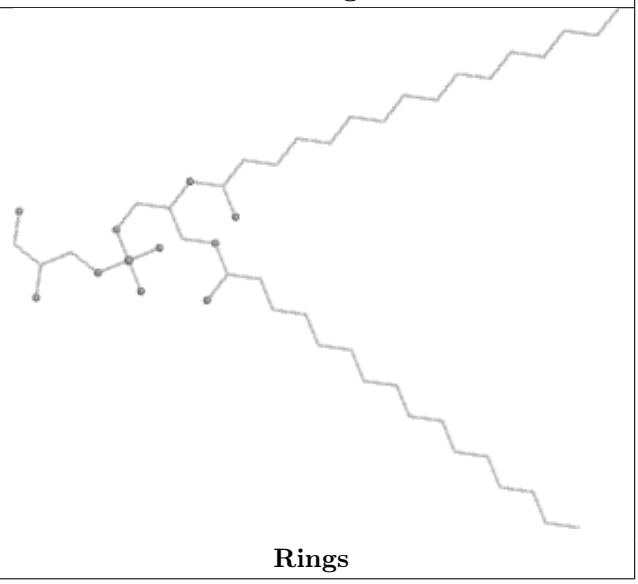
Bond lengths



Bond angles

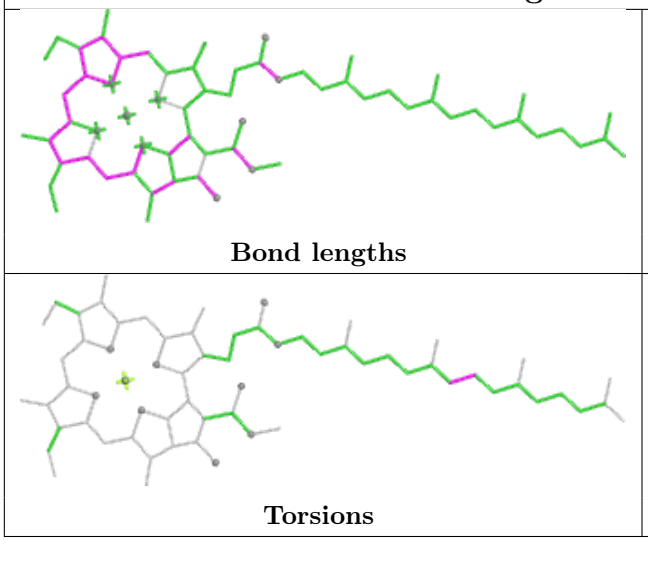


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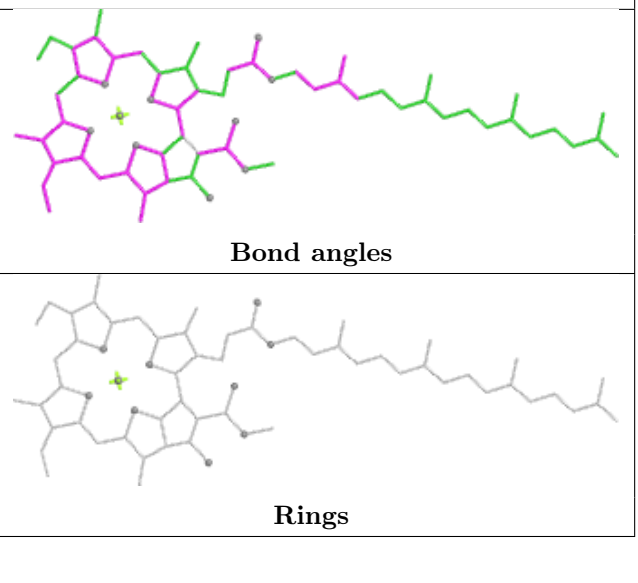


Rings

Ligand CLA B 613



Bond lengths

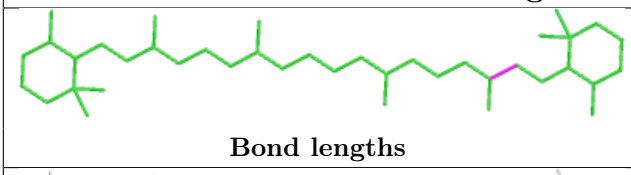


Bond angles

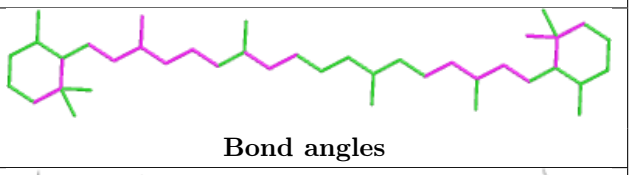
Torsions

Rings

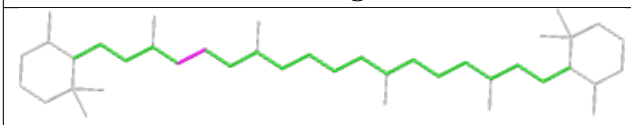
Ligand BCR k 101



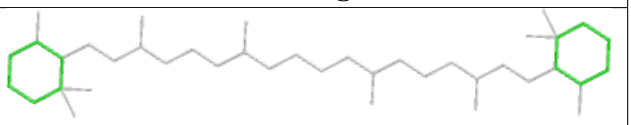
Bond lengths



Bond angles

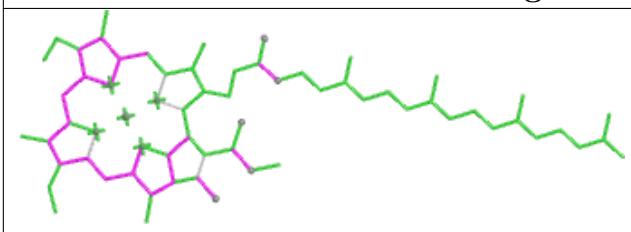


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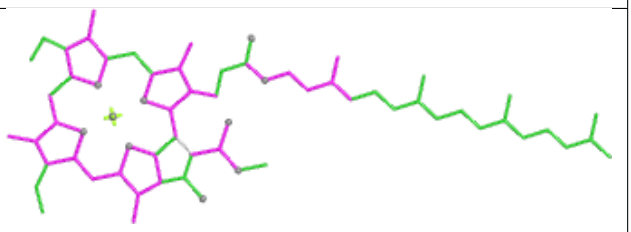


Rings

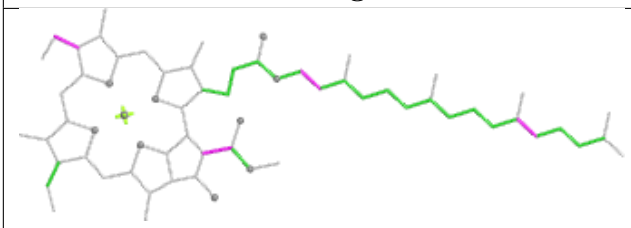
Ligand CLA B 603



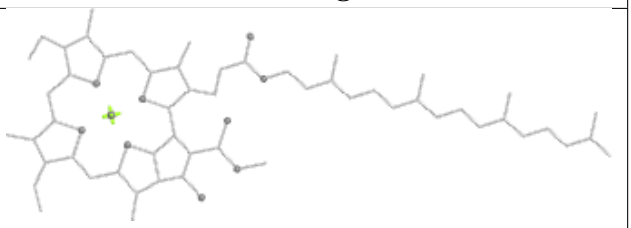
Bond lengths



Bond angles

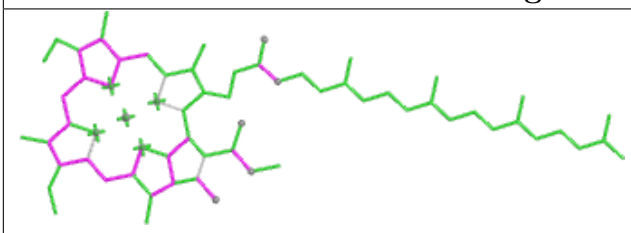


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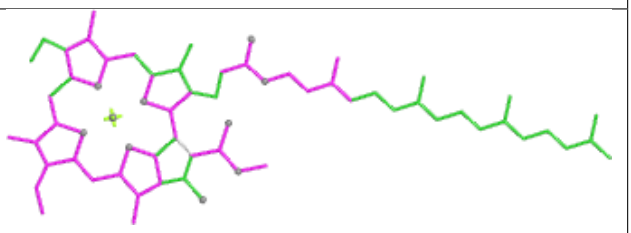


Rings

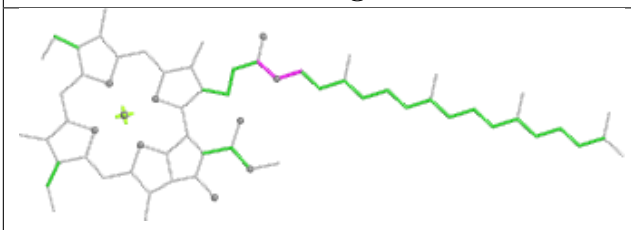
Ligand CLA C 512



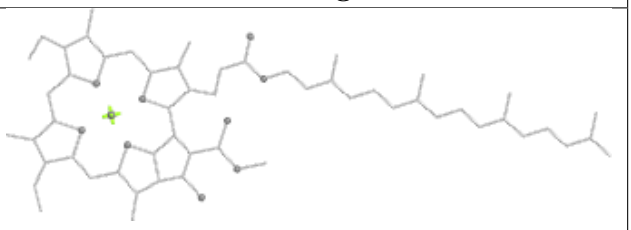
Bond lengths



Bond angles

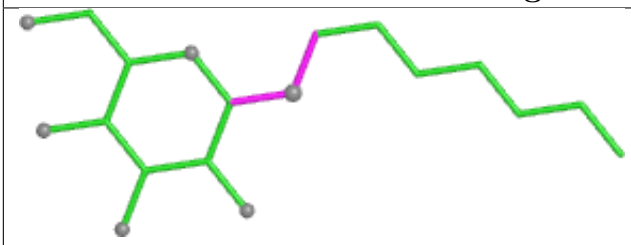


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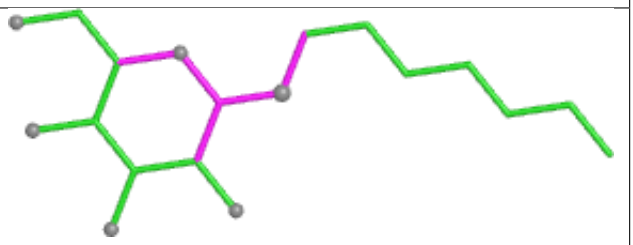


Rings

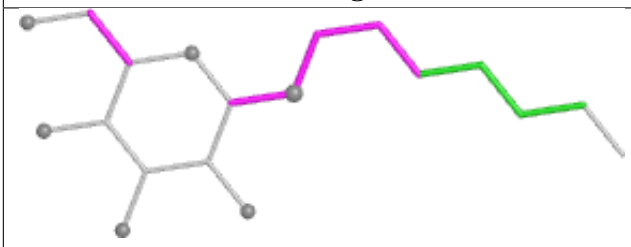
Ligand HTG b 632



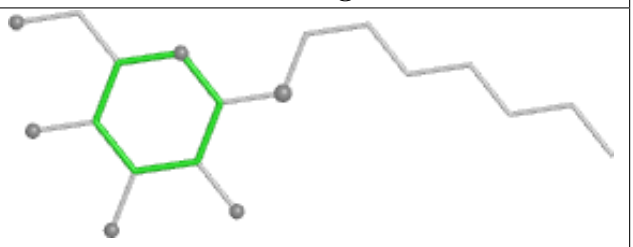
Bond lengths



Bond angles



Torsions

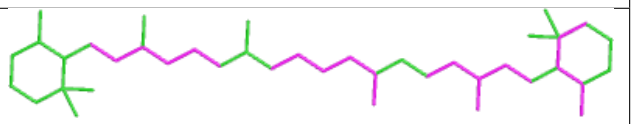


Rings

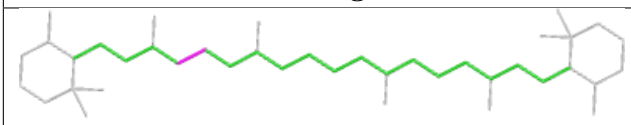
Ligand BCR h 101



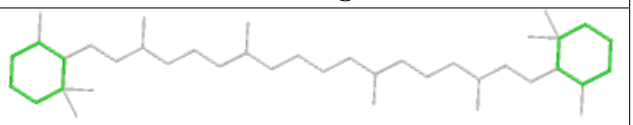
Bond lengths



Bond angles

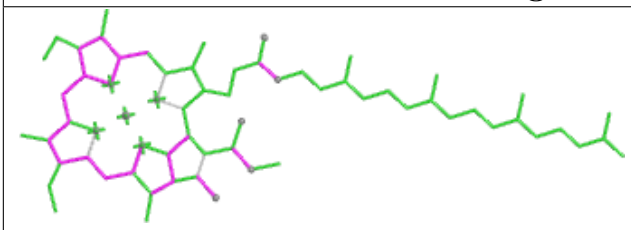


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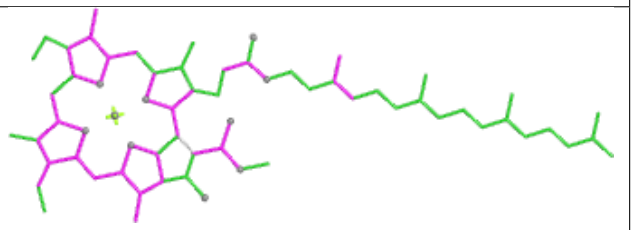


Rings

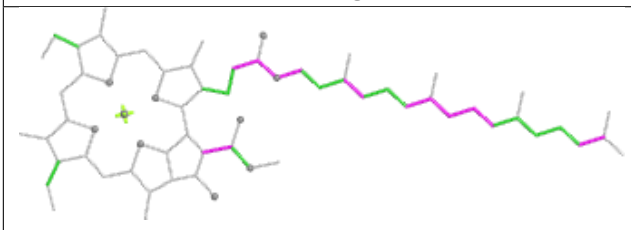
Ligand CLA b 610



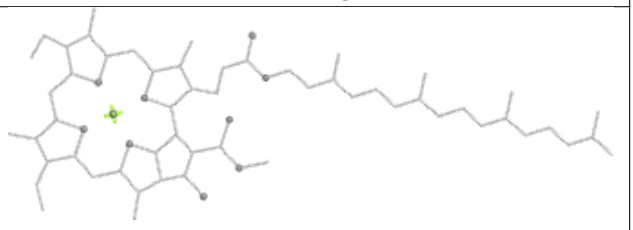
Bond lengths



Bond angles

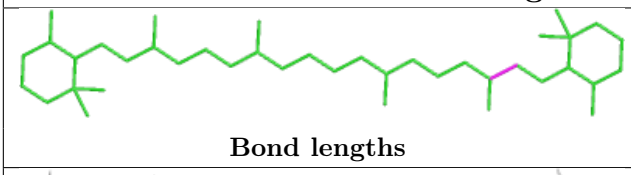


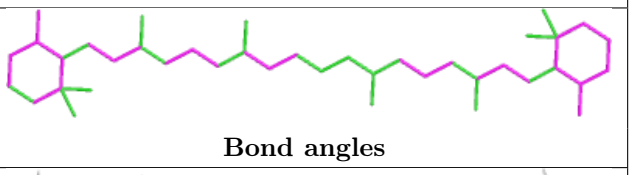
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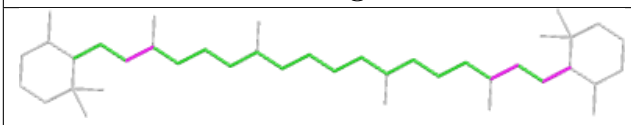


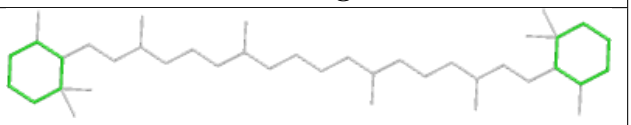
Rings

Ligand BCR d 405

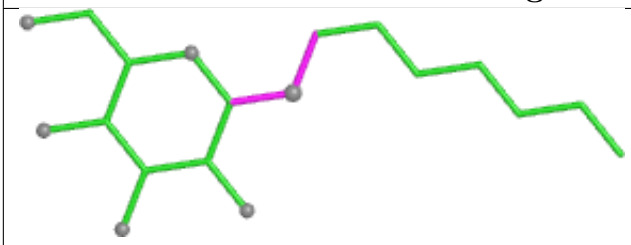

Bond lengths

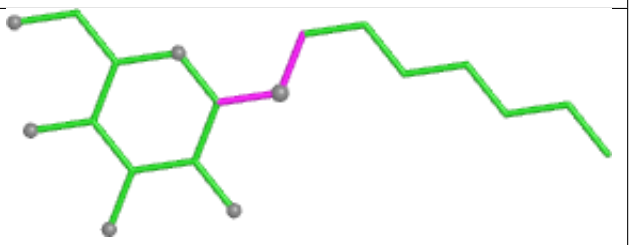

Bond angles

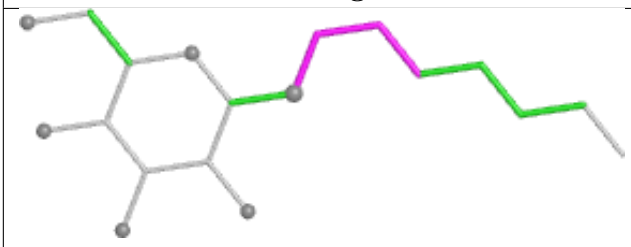

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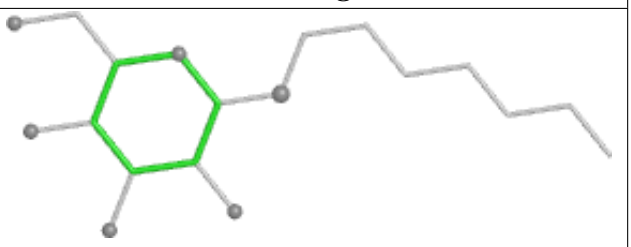

Rings

Ligand HTG c 524

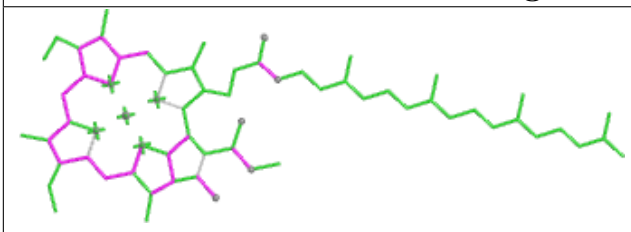

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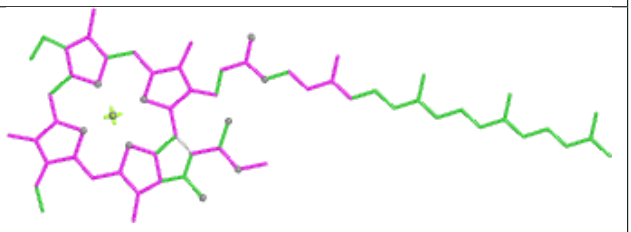

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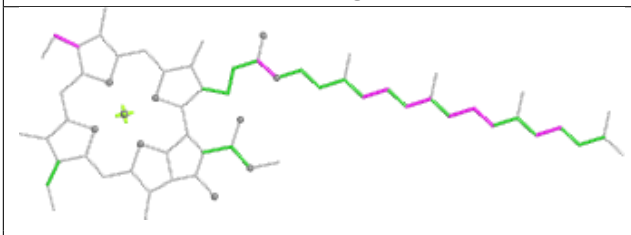

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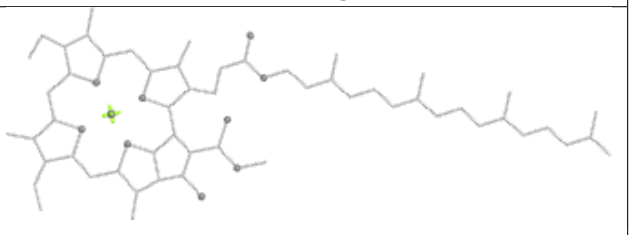

Rings

Ligand CLA A 409

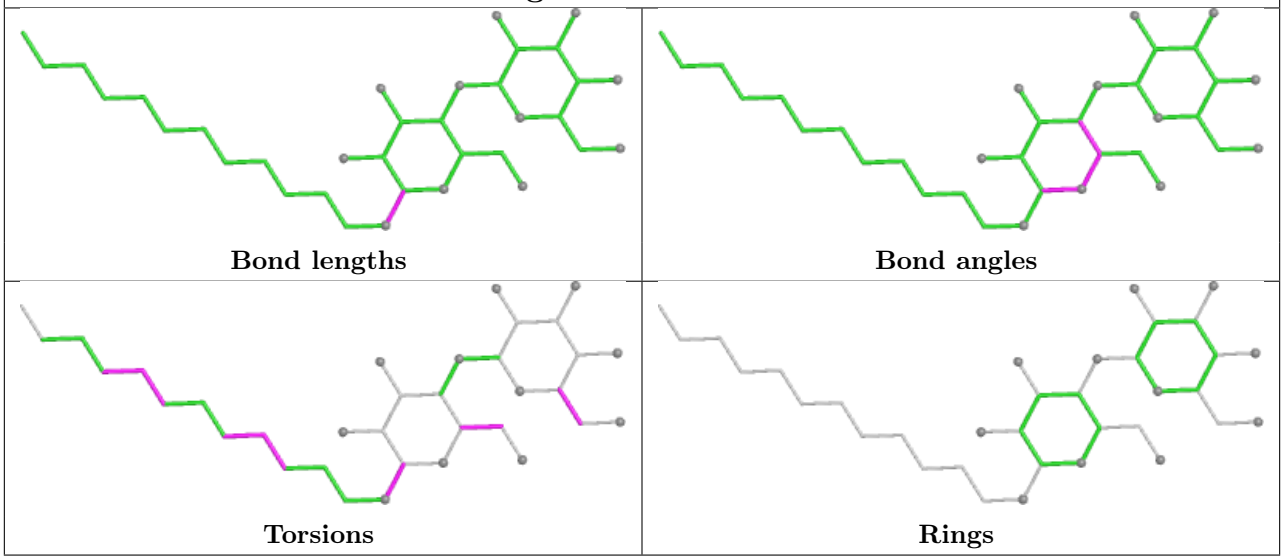

Bond lengths


Bond angles

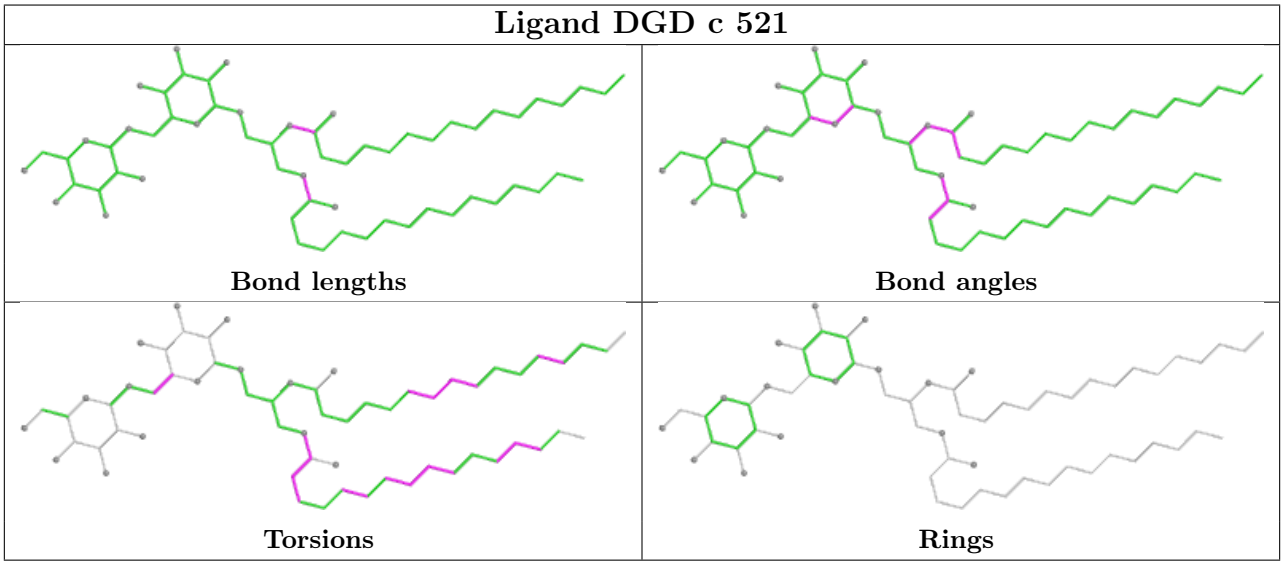

Torsions


Rings

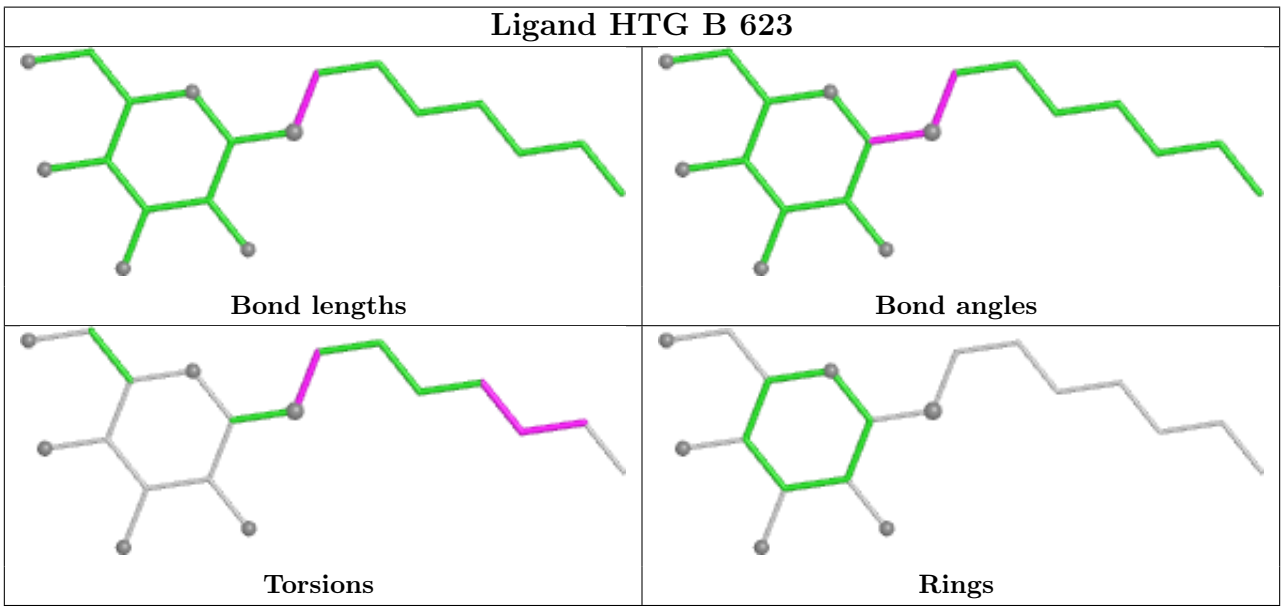
Ligand LMT a 404



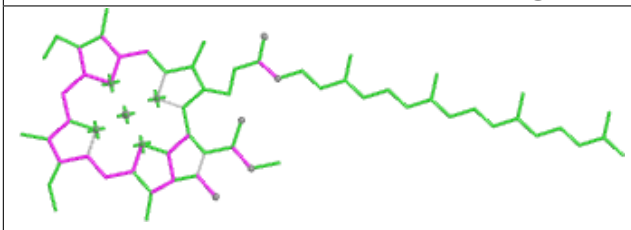
Ligand DGD c 521



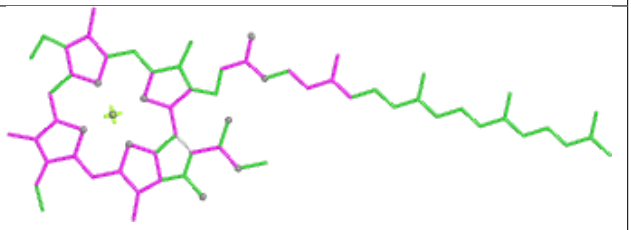
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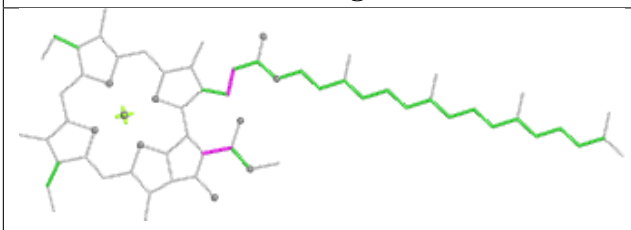
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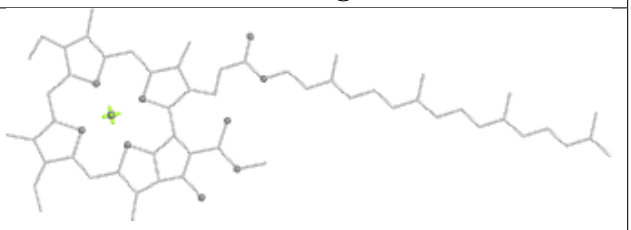
Bond lengths



Bond angles

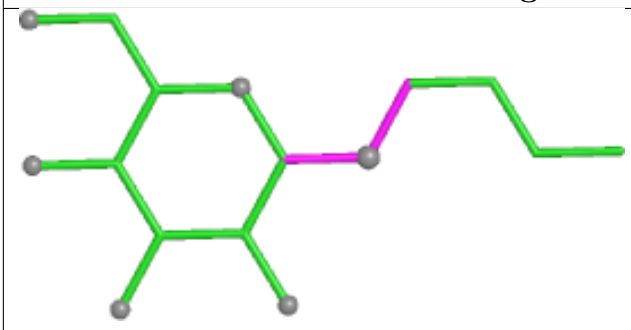


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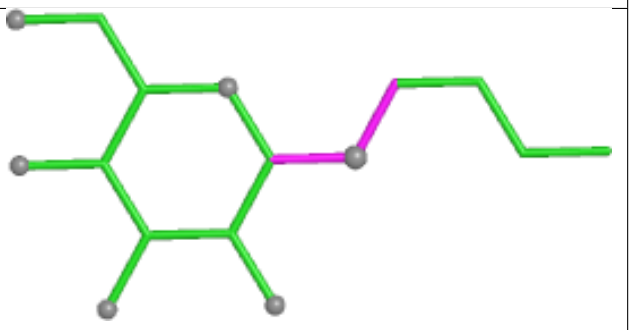


Rings

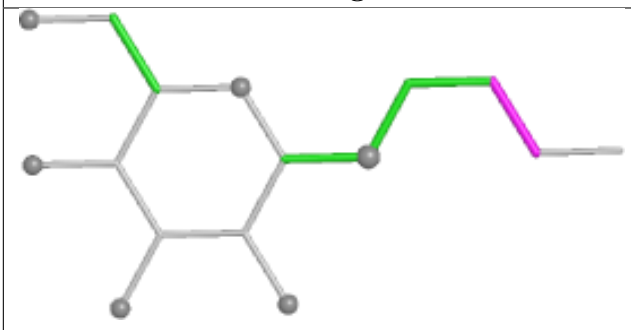
Ligand HTG D 412



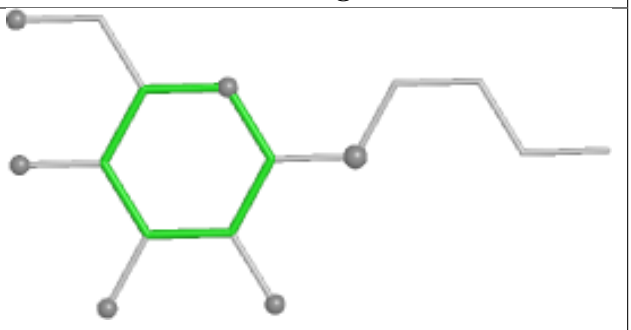
Bond lengths



Bond angles

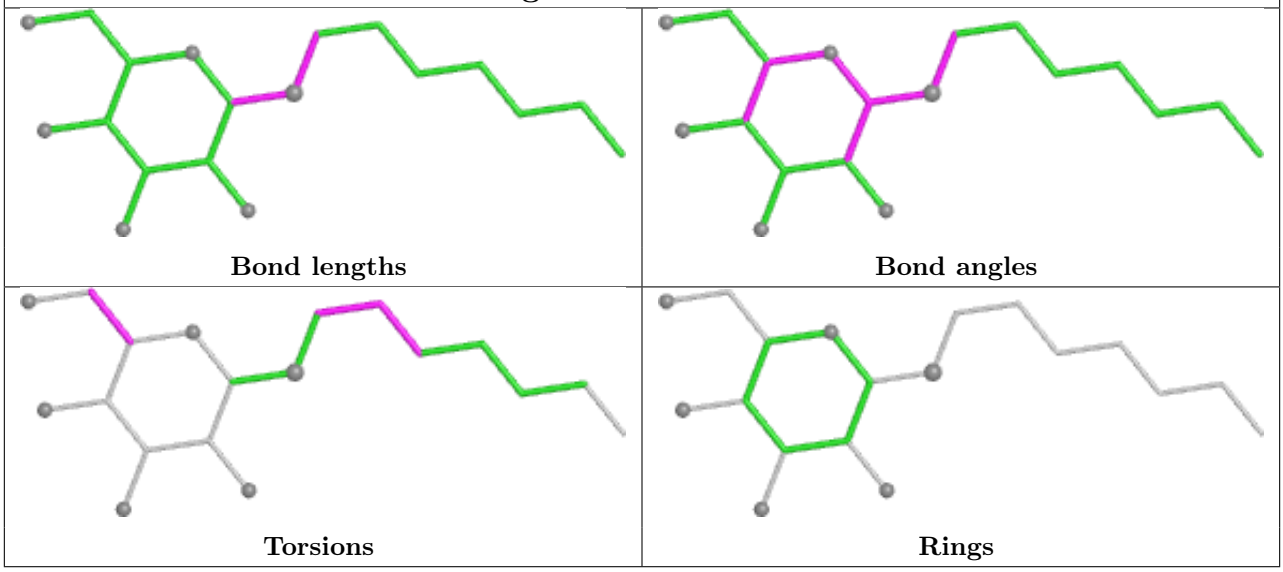


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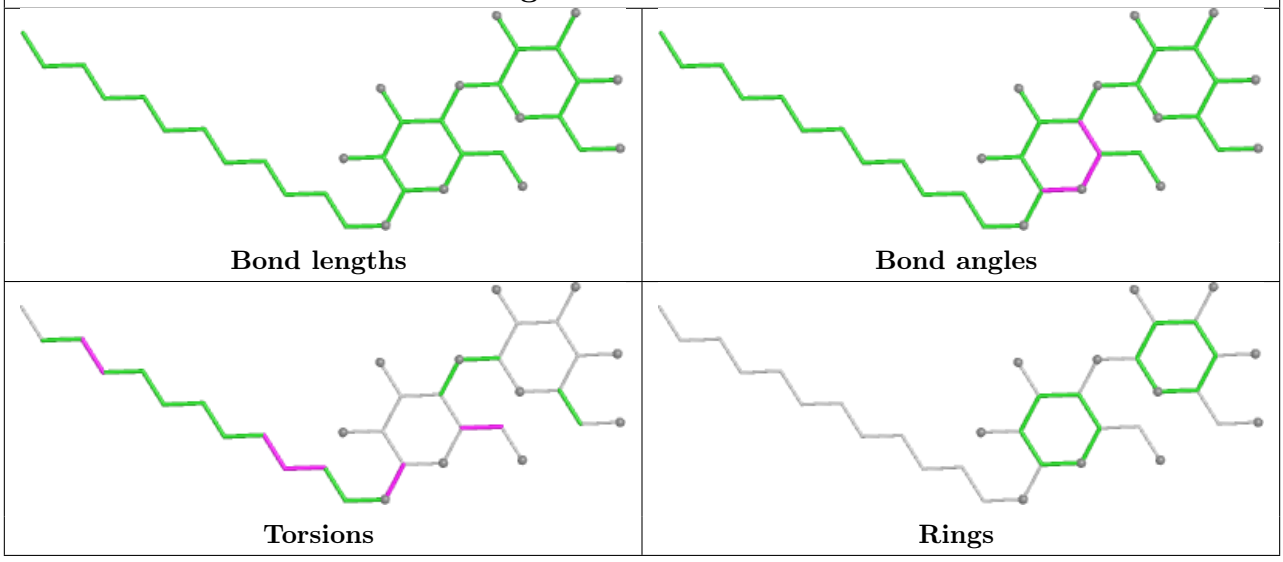


Rings

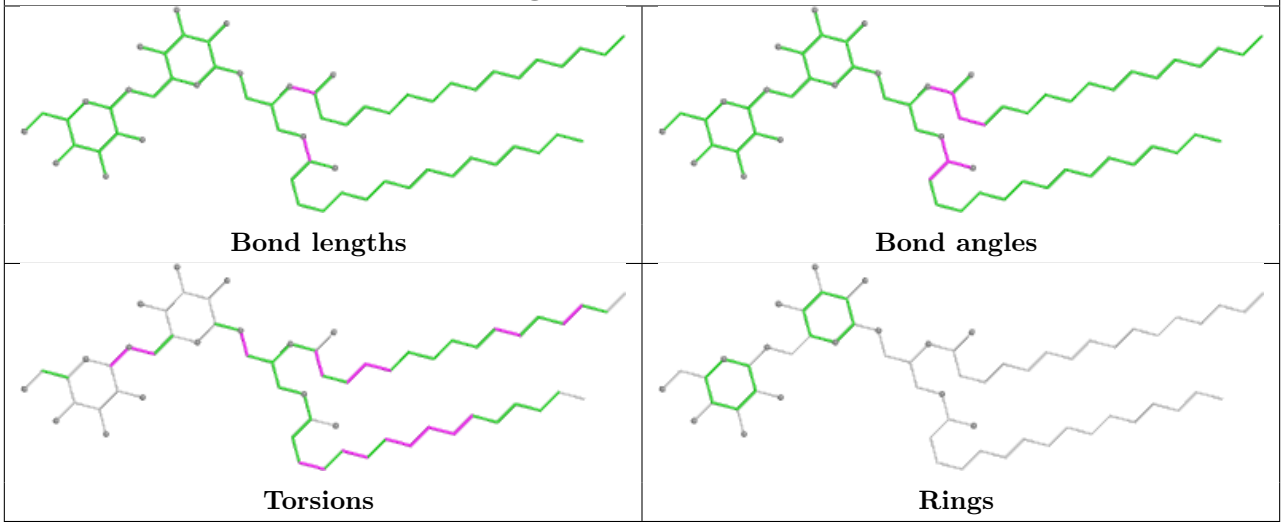
Ligand HTG C 524



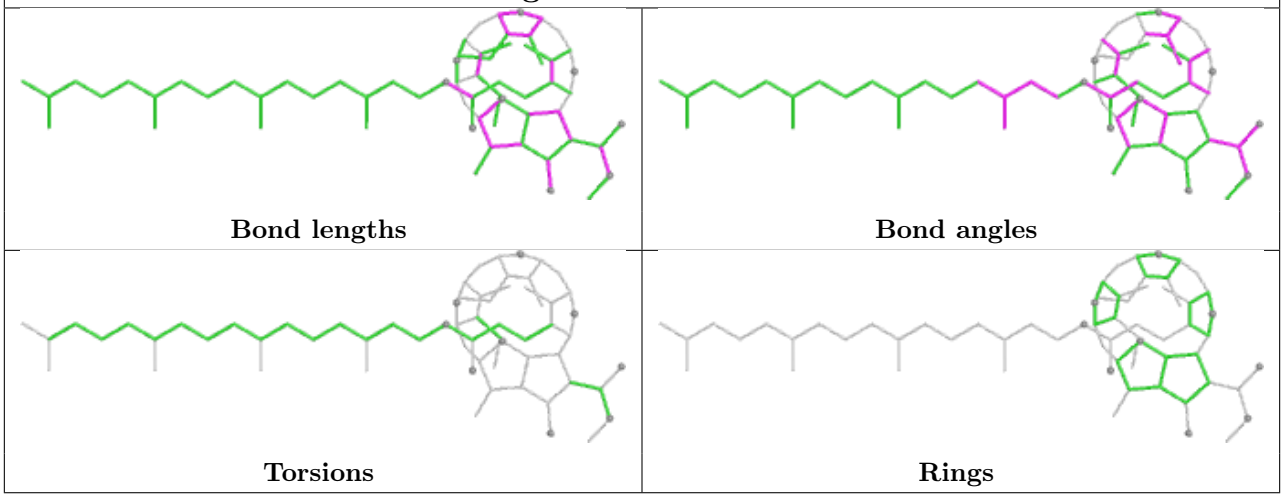
Ligand LMT m 102



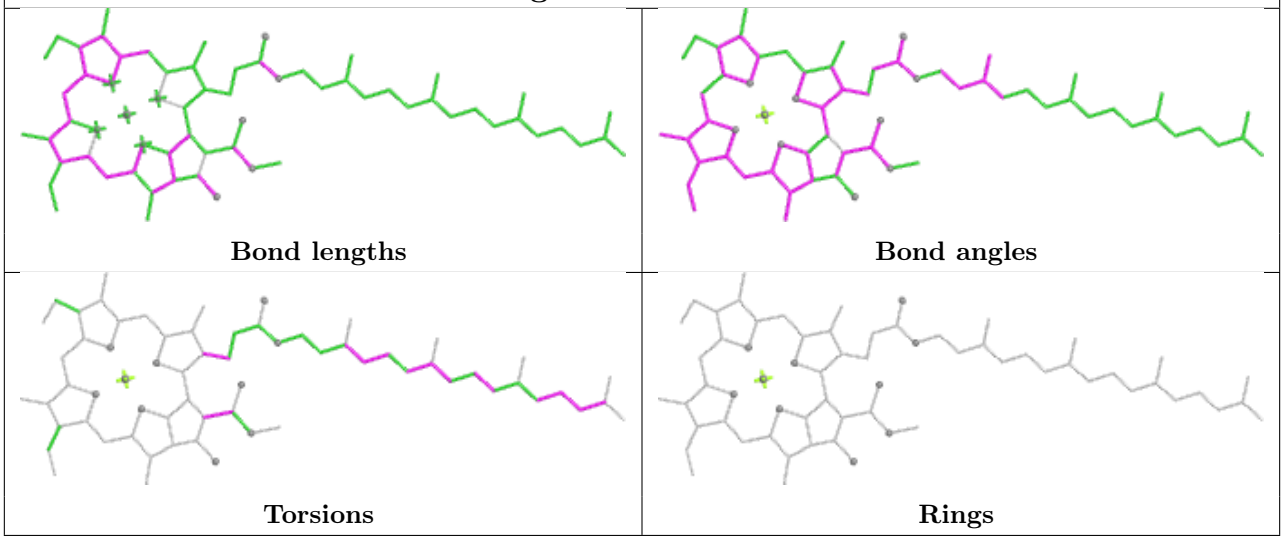
Ligand DGD c 520



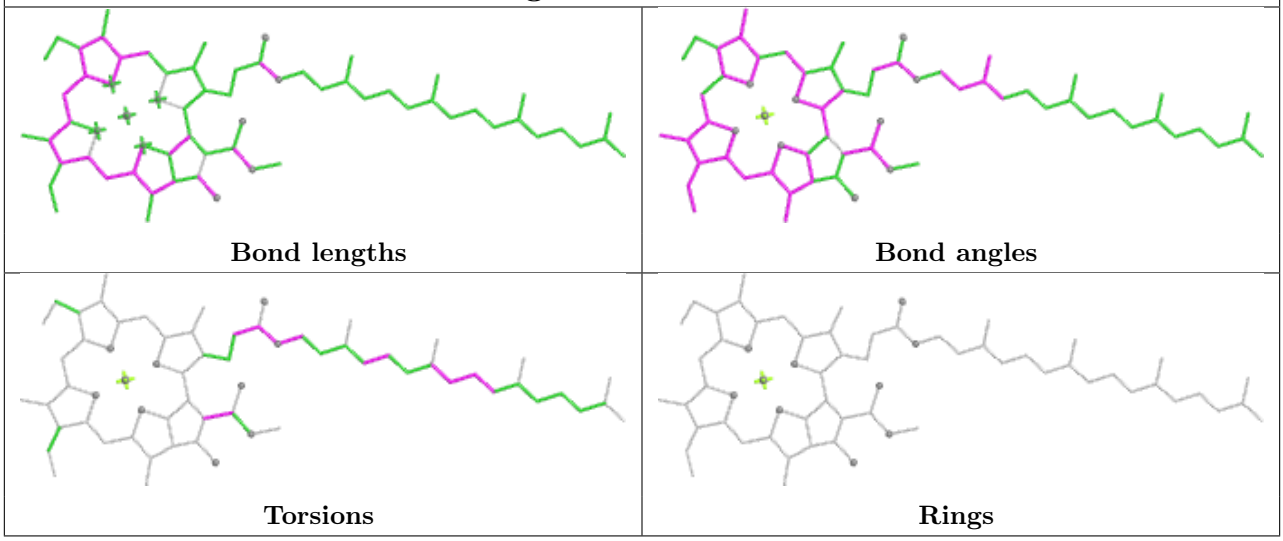
Ligand PHO A 408



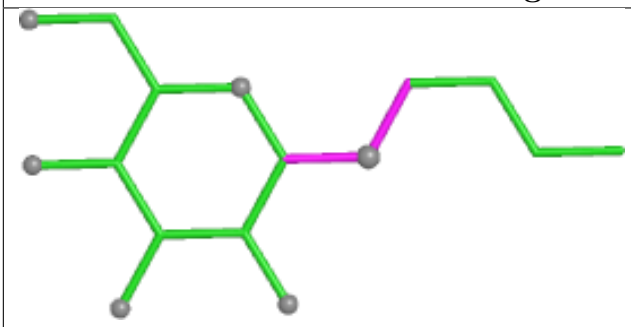
Ligand CLA c 510



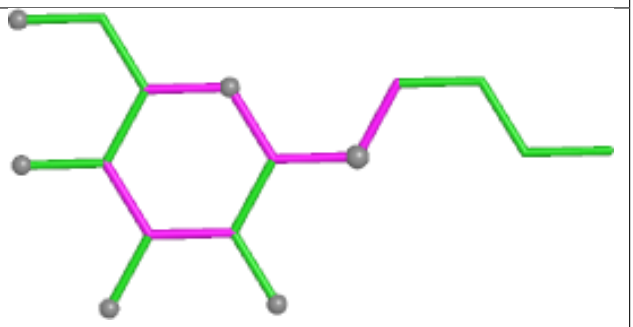
Ligand CLA B 602



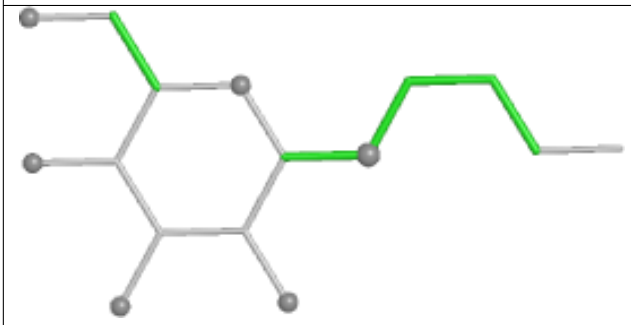
Ligand HTG d 412



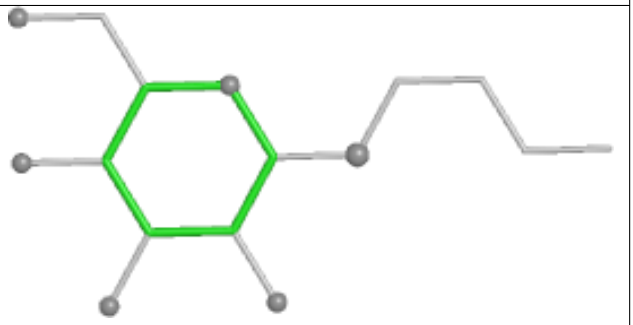
Bond lengths



Bond angles

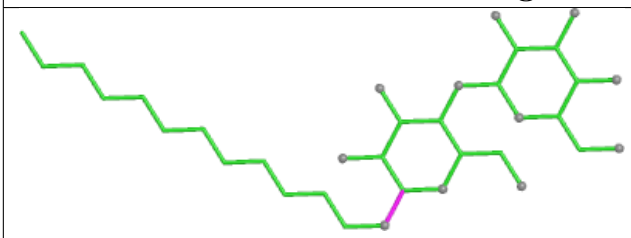


Torsions

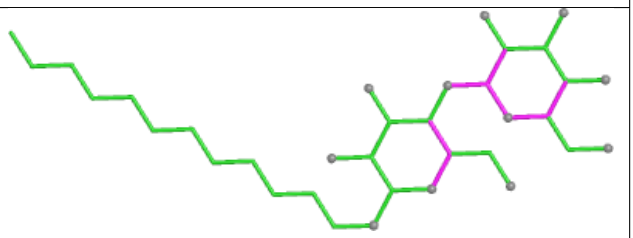


Rings

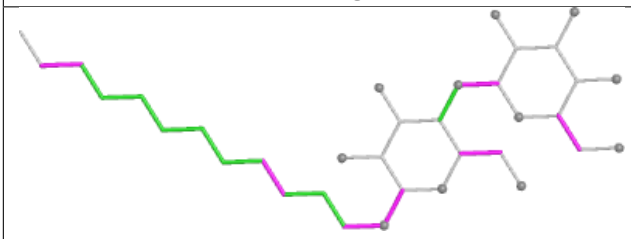
Ligand LMT M 104



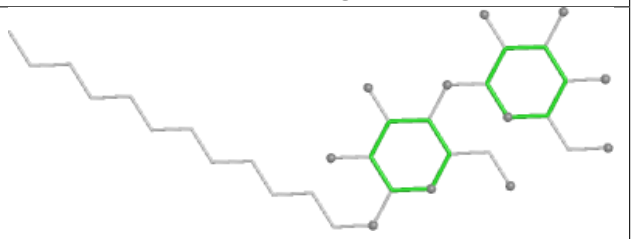
Bond lengths



Bond angles

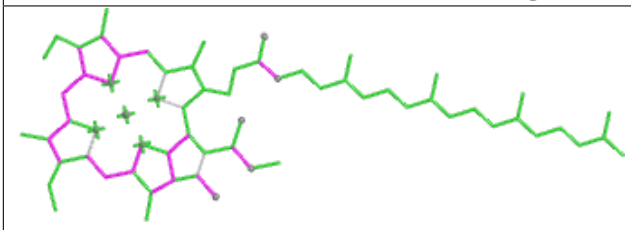


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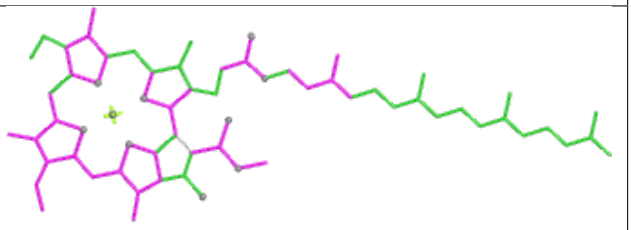


Rings

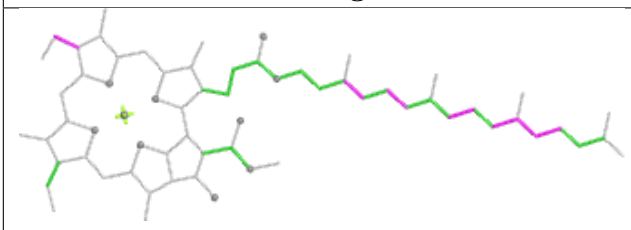
Ligand CLA B 616



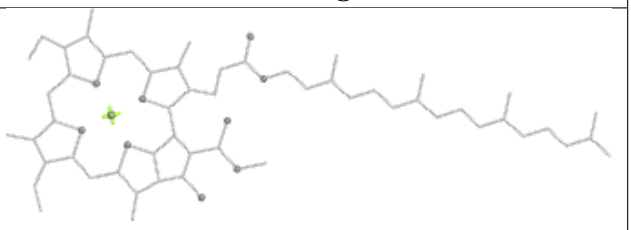
Bond lengths



Bond angles

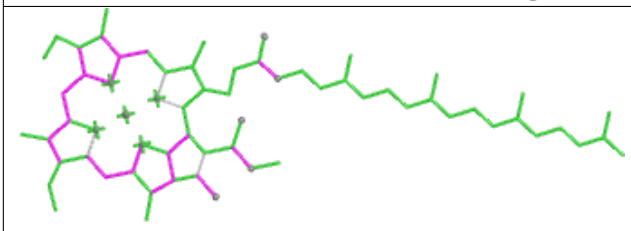


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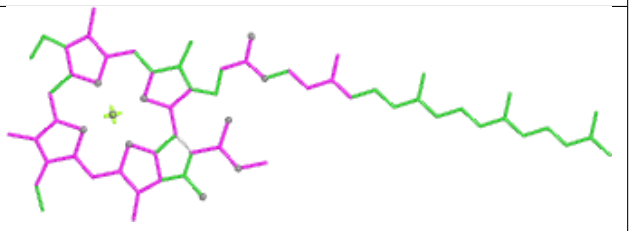


Rings

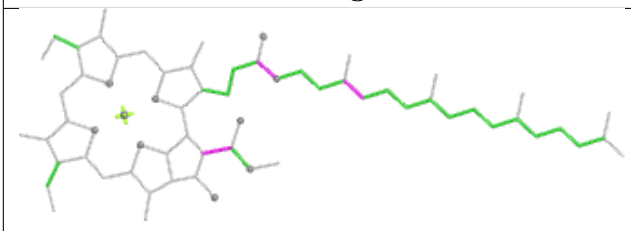
Ligand CLA B 606



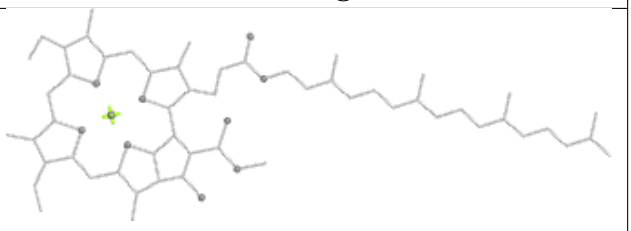
Bond lengths



Bond angles

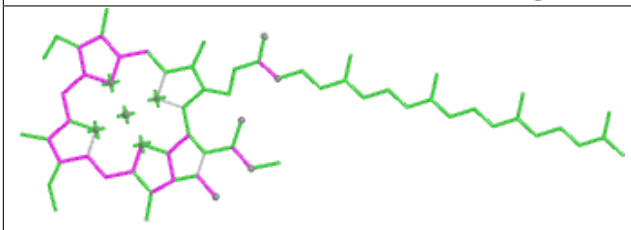


Torsions

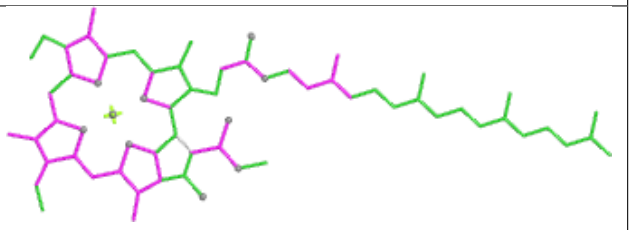


Rings

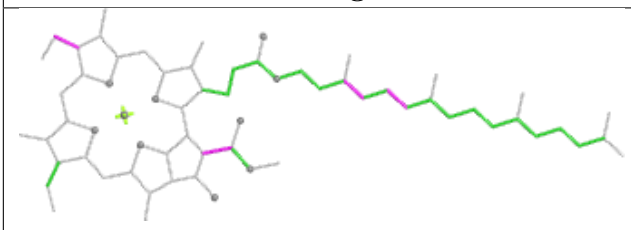
Ligand CLA c 511



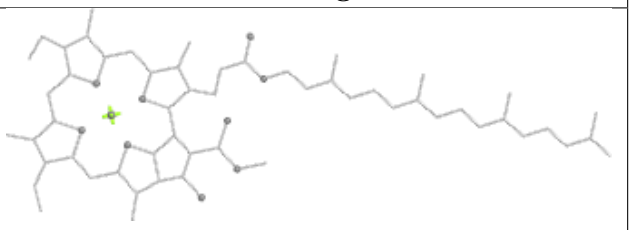
Bond lengths



Bond angles

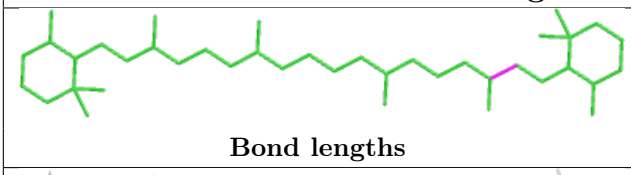


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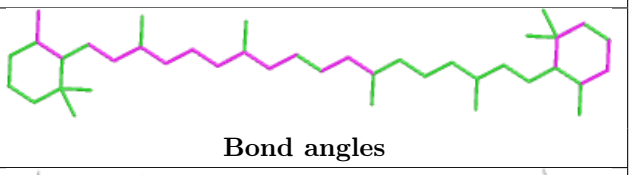


Rings

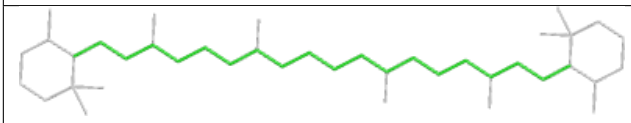
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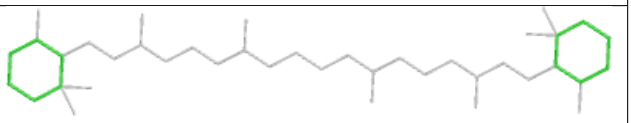
Bond lengths



Bond angles

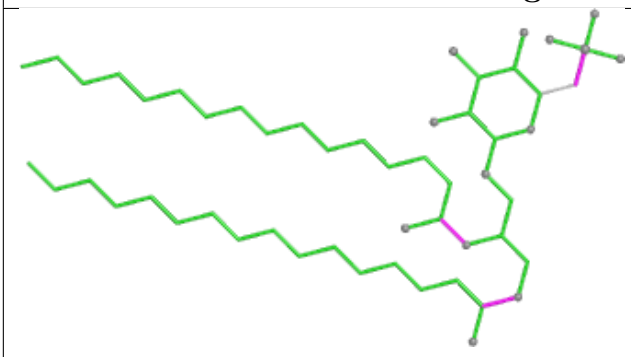


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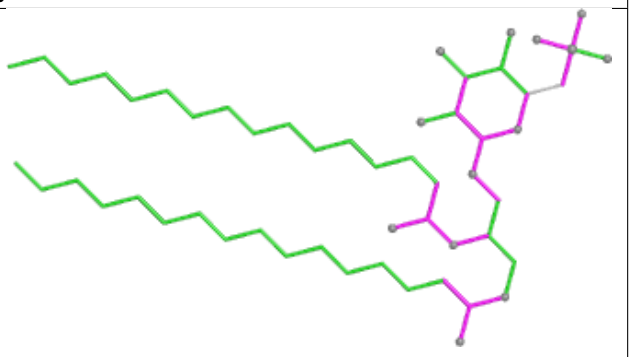


Rings

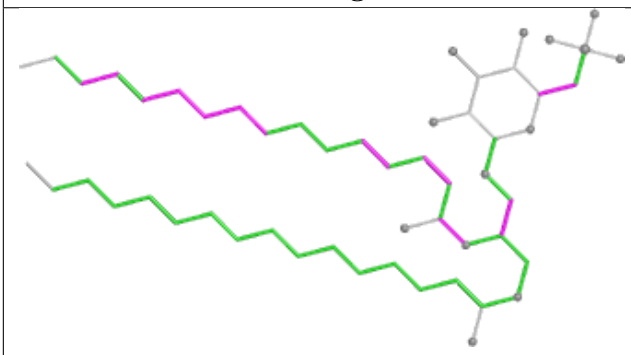
Ligand SQD A 411



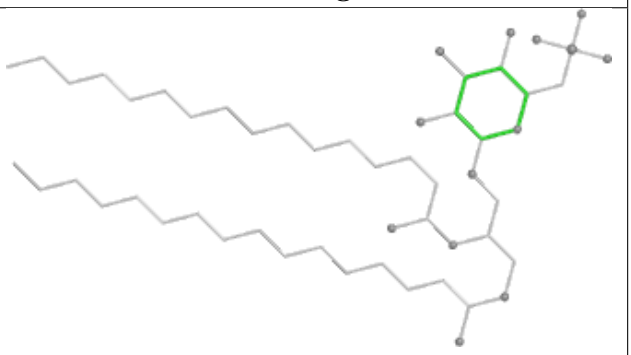
Bond lengths



Bond angles

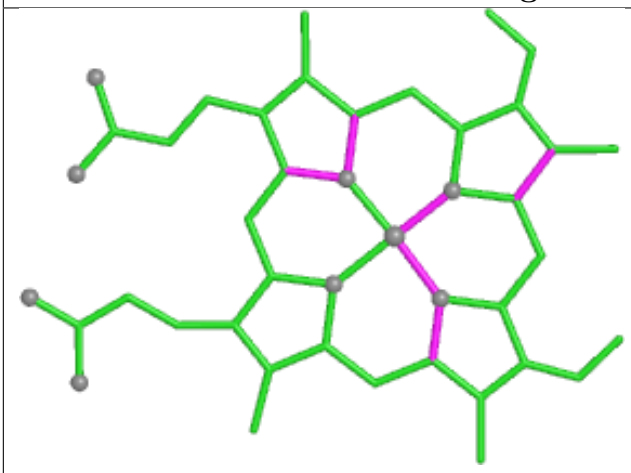


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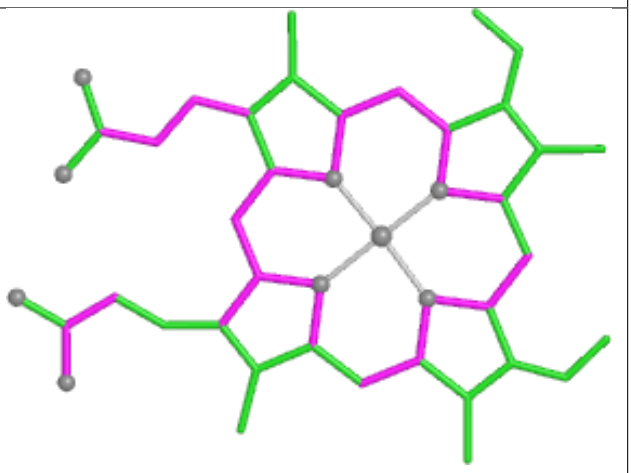


Rings

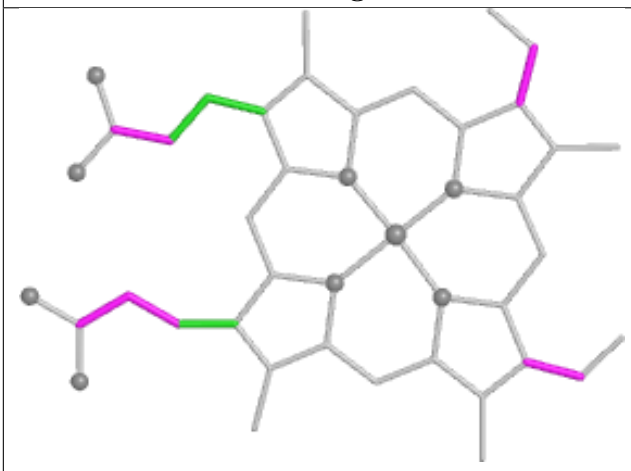
Ligand HEM E 102



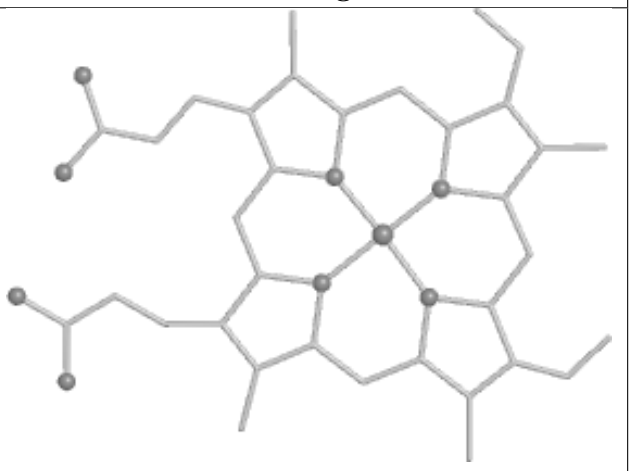
Bond lengths



Bond angles

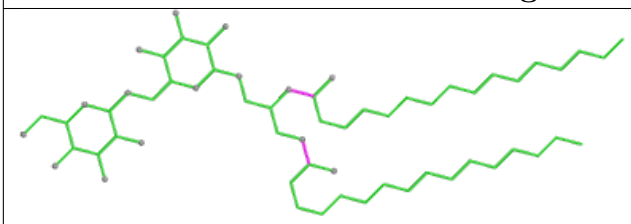


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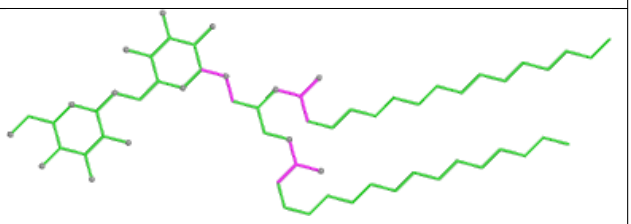


Rings

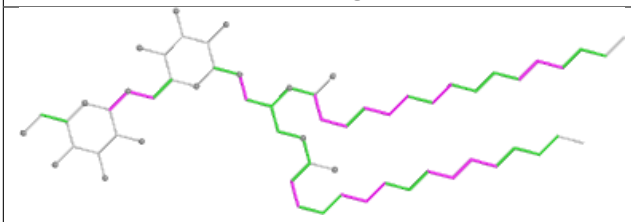
Ligand DGD C 518



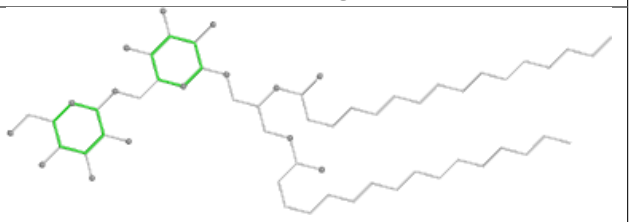
Bond lengths



Bond angles

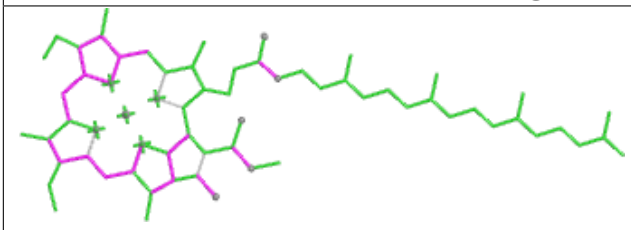


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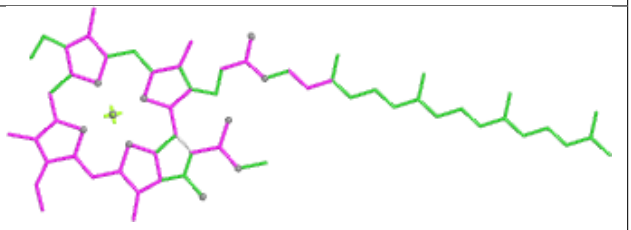


Rings

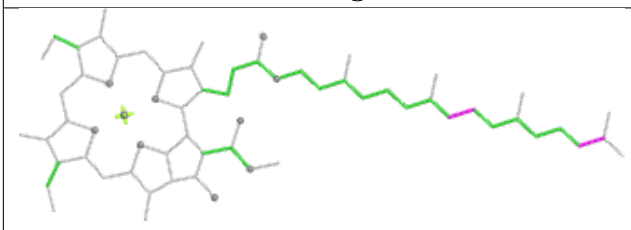
Ligand CLA b 620



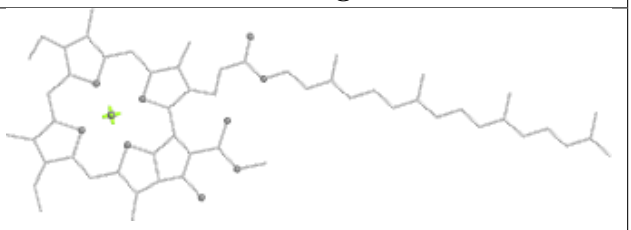
Bond lengths



Bond angles

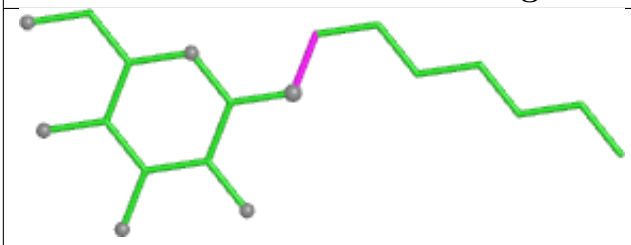


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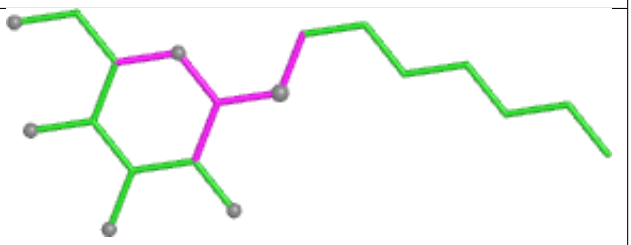


Rings

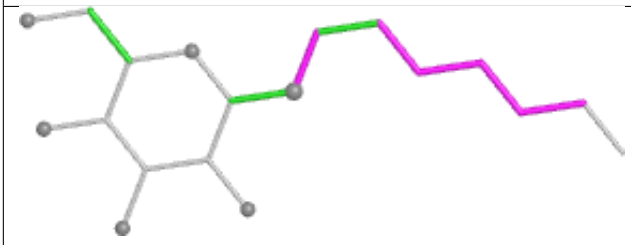
Ligand HTG B 624



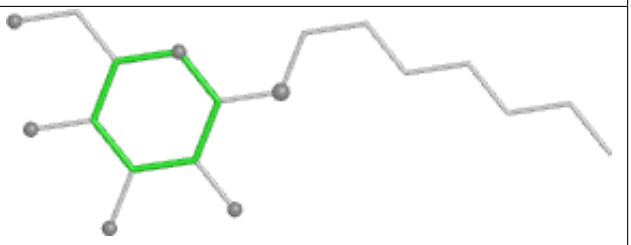
Bond lengths



Bond angles

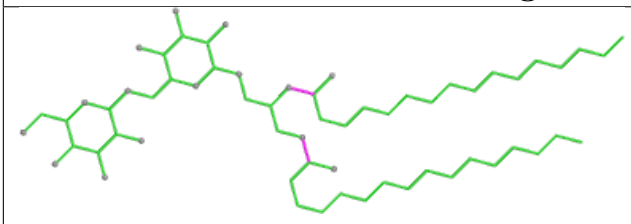


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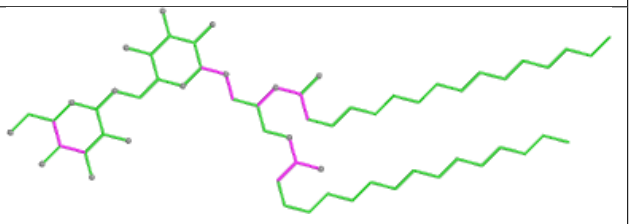


Rings

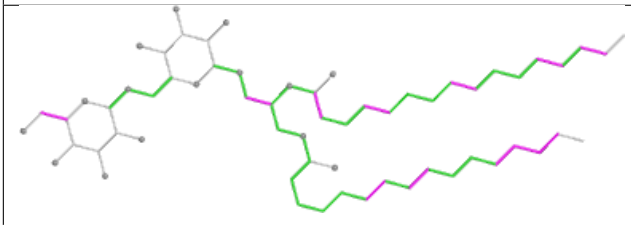
Ligand DGD H 102



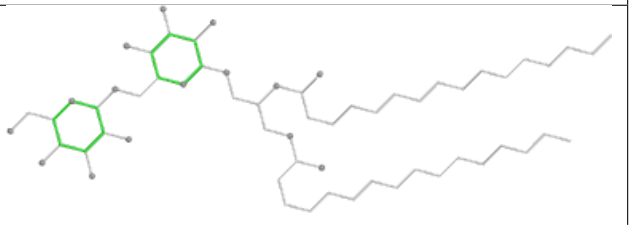
Bond lengths



Bond angles

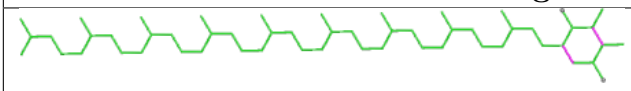


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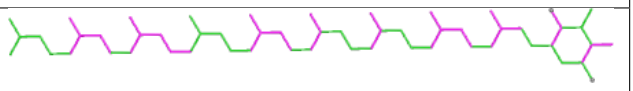


Rings

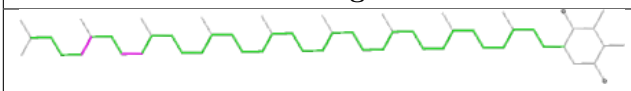
Ligand PL9 d 406



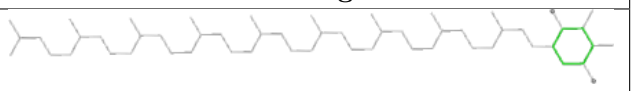
Bond lengths



Bond angles

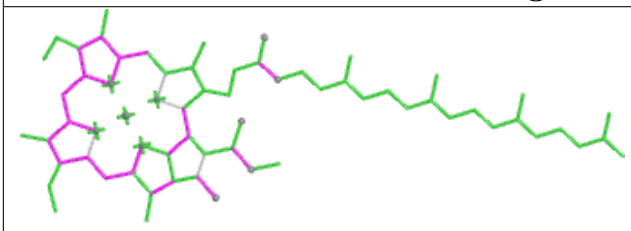


Torsions

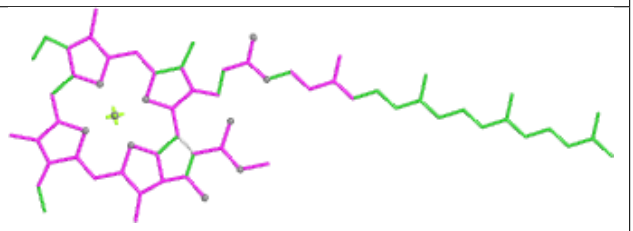


Rings

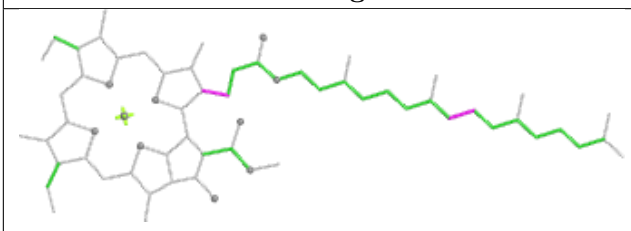
Ligand CLA b 621



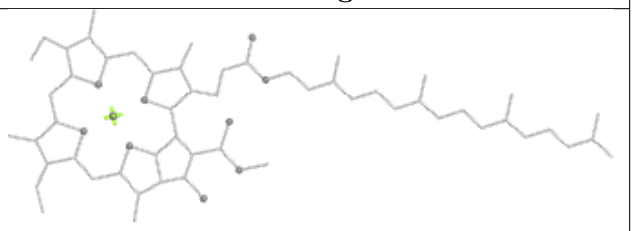
Bond lengths



Bond angles

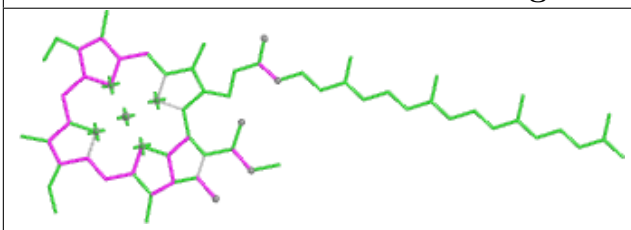


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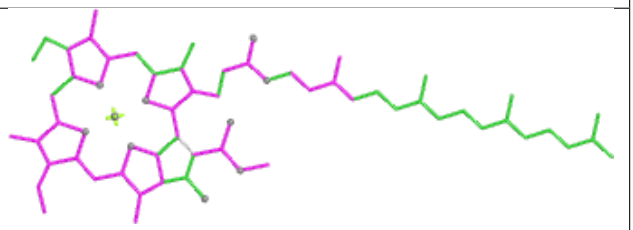


Rings

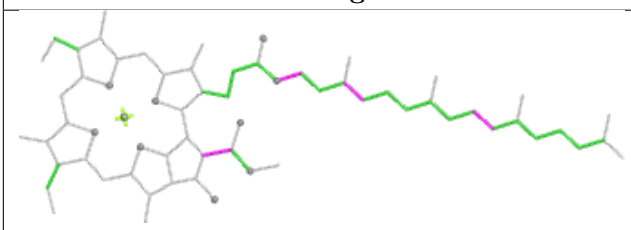
Ligand CLA c 517



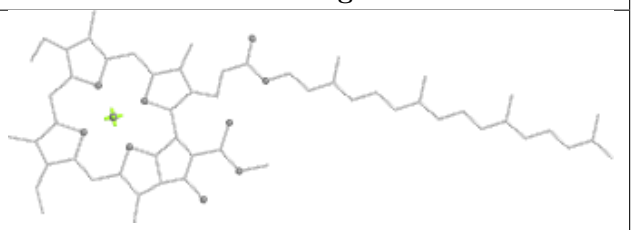
Bond lengths



Bond angles

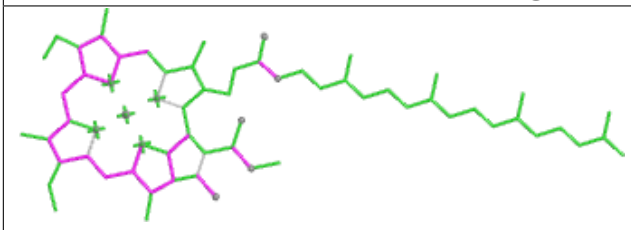


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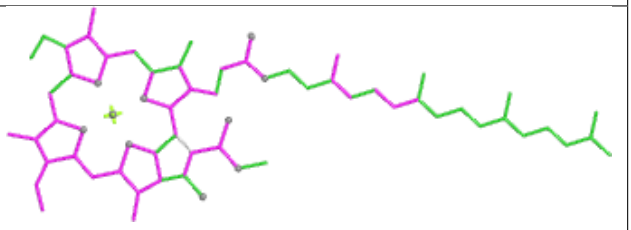


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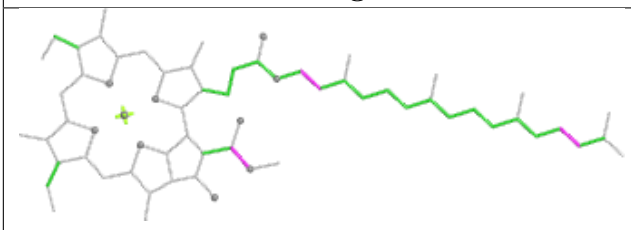
Ligand CLA d 404



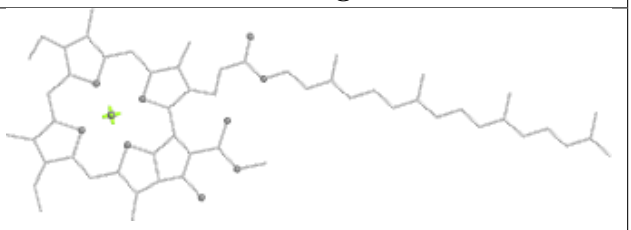
Bond lengths



Bond angles

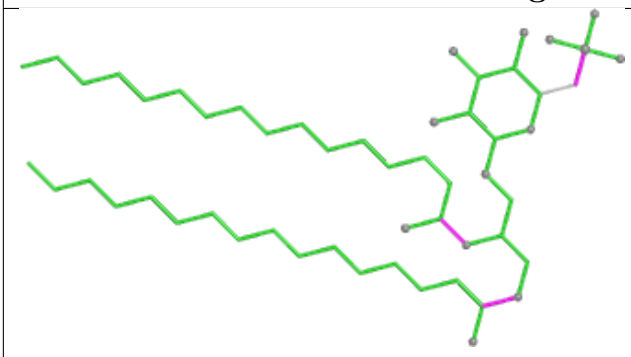


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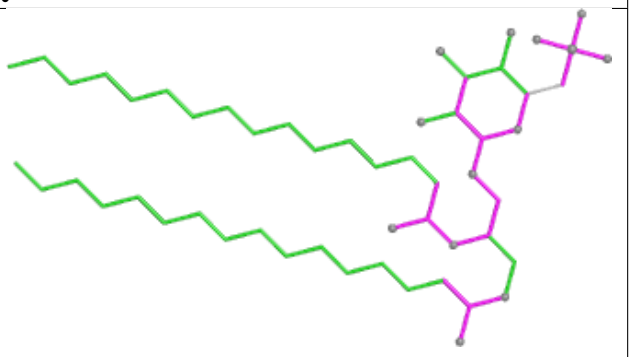


Rings

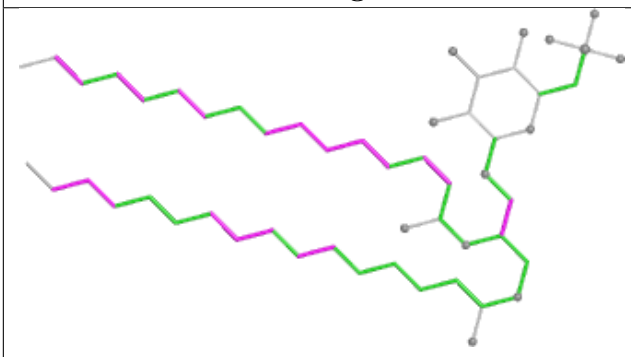
Ligand SQD a 414



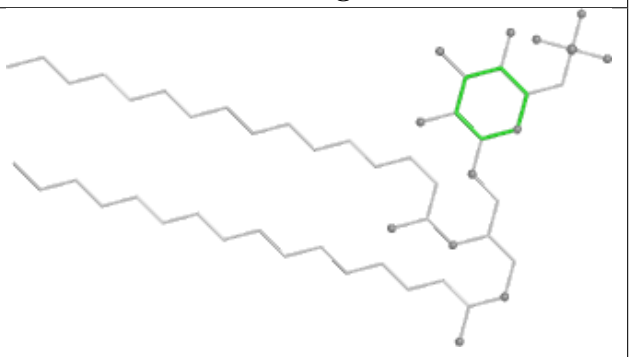
Bond lengths



Bond angles

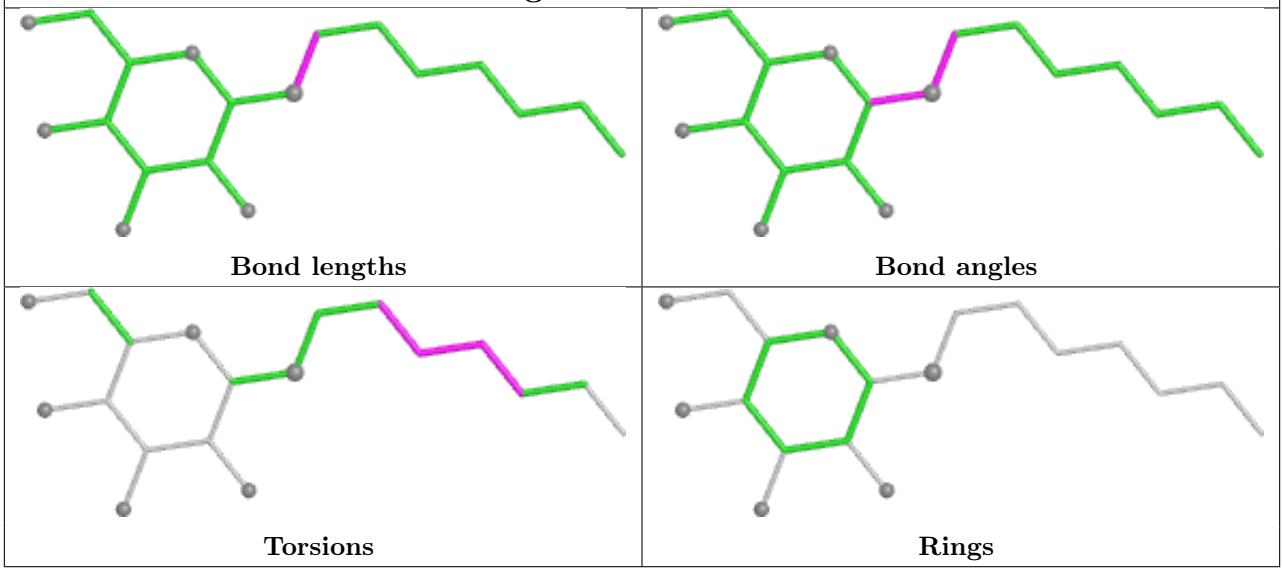


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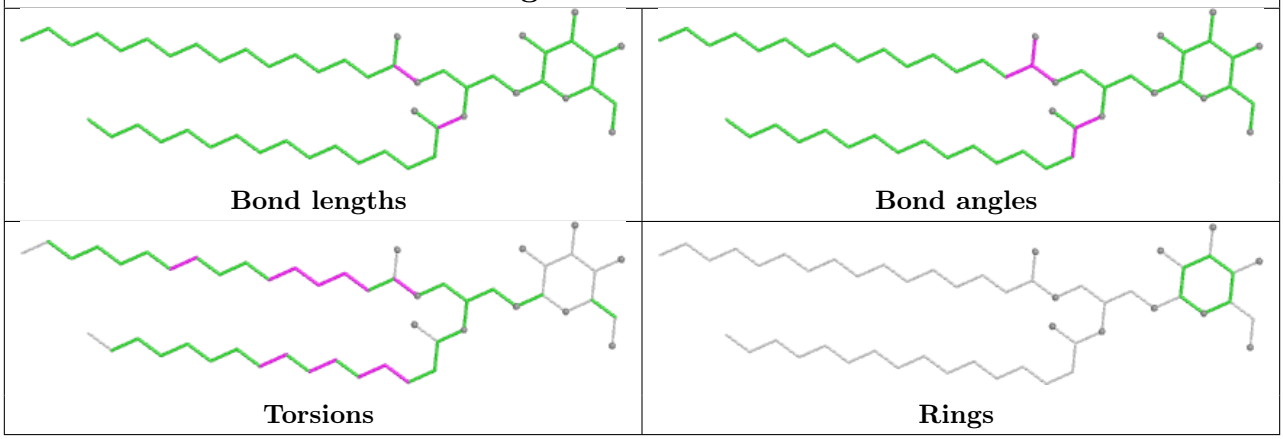


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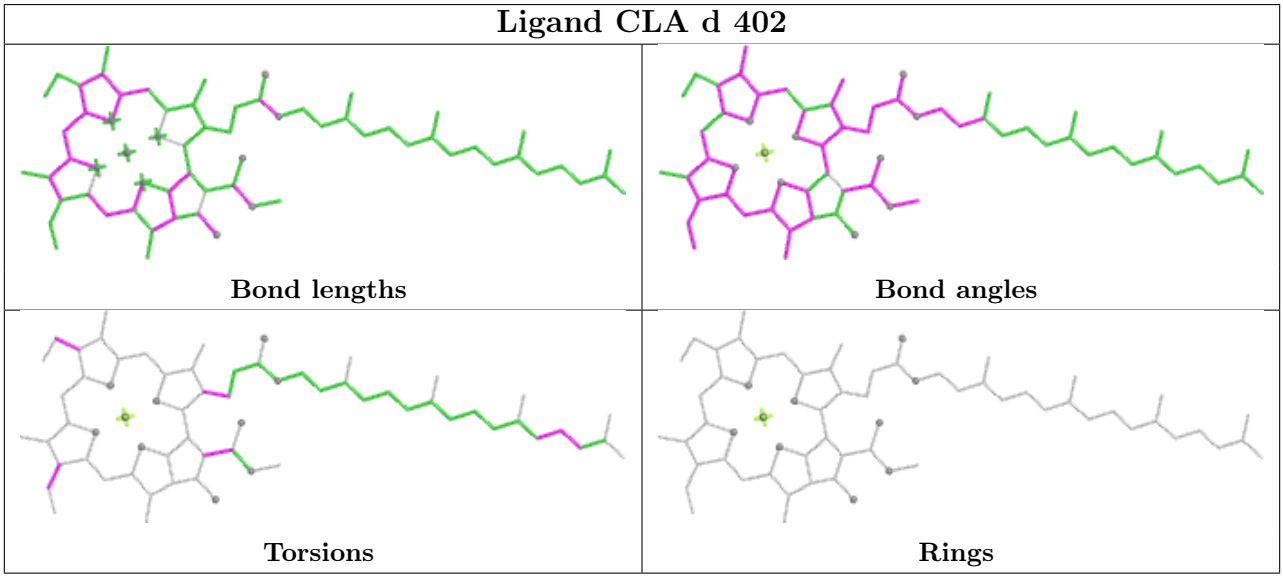
Ligand HTG b 601



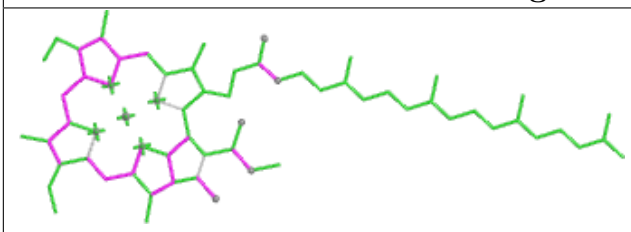
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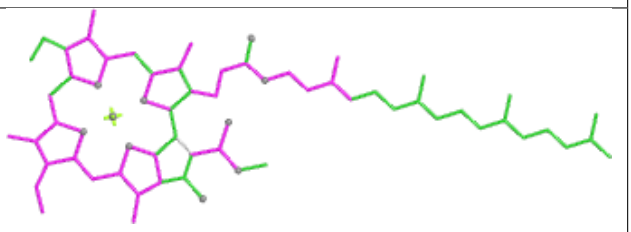
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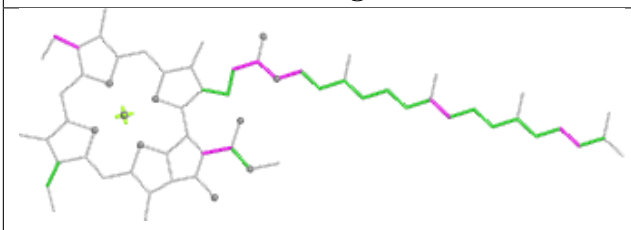
Ligand CLA c 516



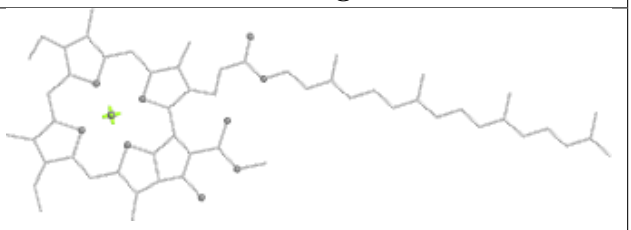
Bond lengths



Bond angles

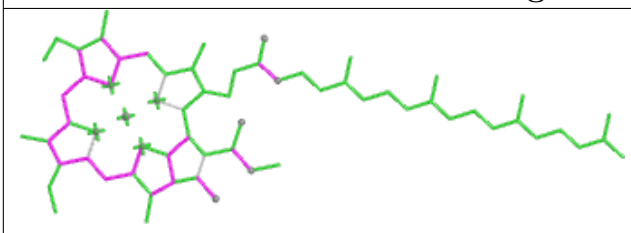


Torsions

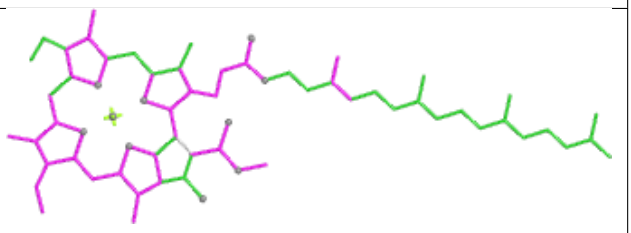


Rings

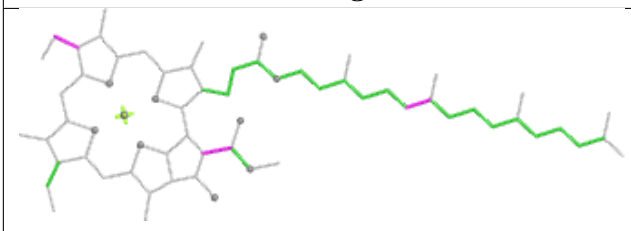
Ligand CLA b 616



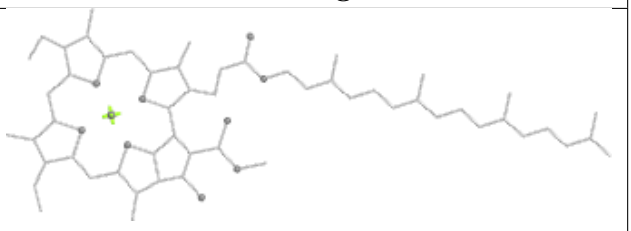
Bond lengths



Bond angles

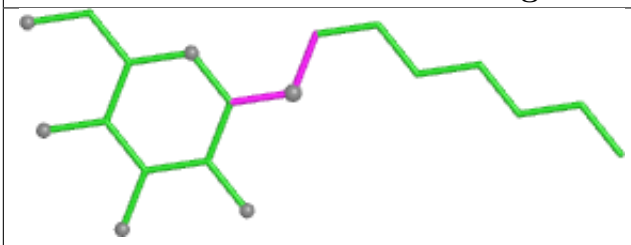


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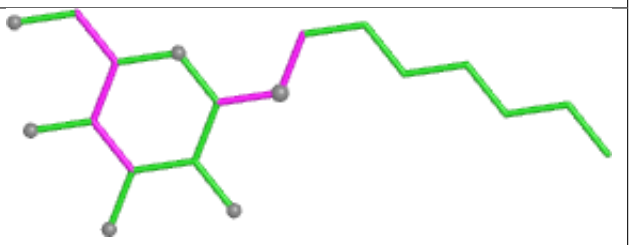


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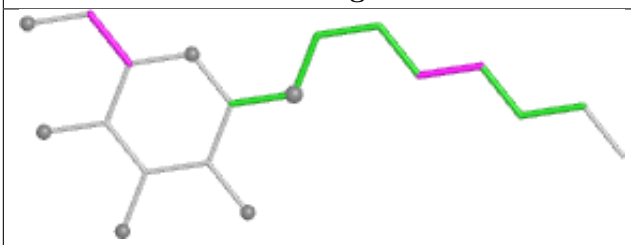
Ligand HTG B 632



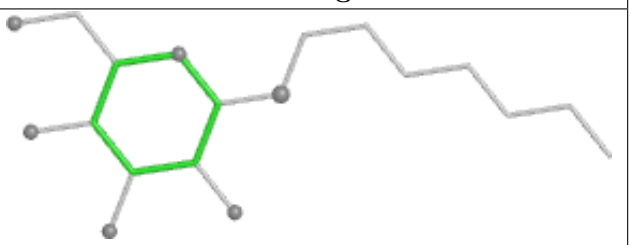
Bond lengths



Bond angles

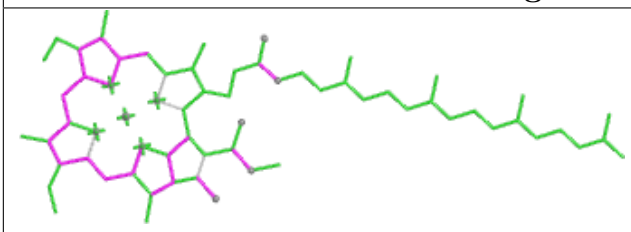


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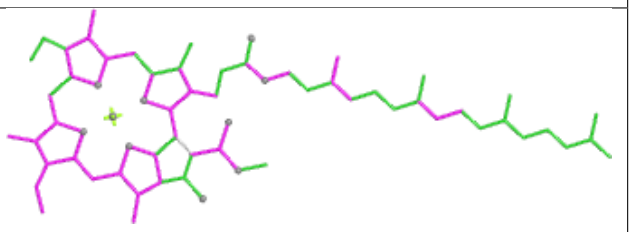


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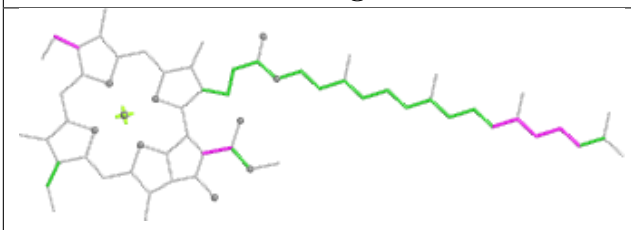
Ligand CLA C 505



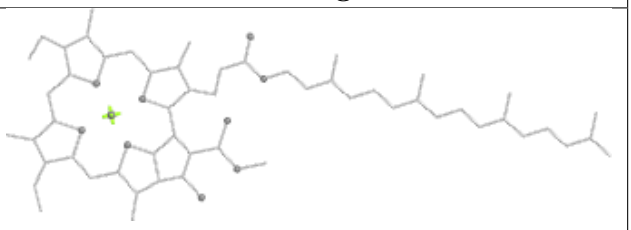
Bond lengths



Bond angles



Torsions

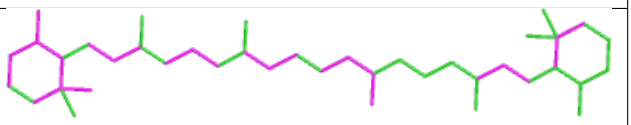


Rings

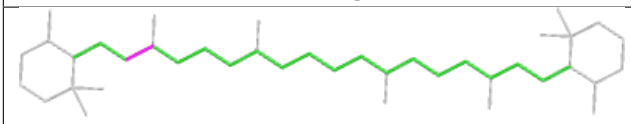
Ligand BCR K 101



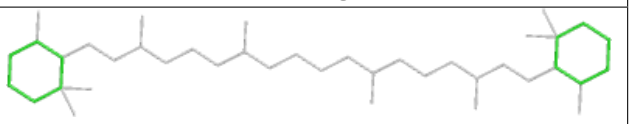
Bond lengths



Bond angles

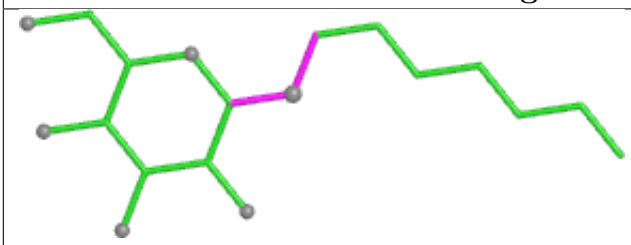


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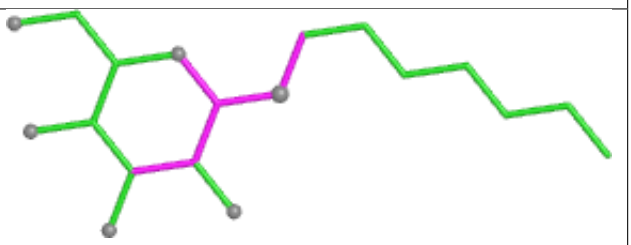


Rings

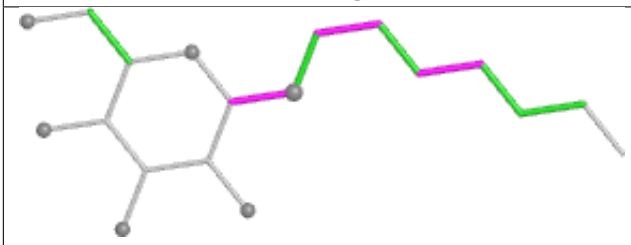
Ligand HTG V 206



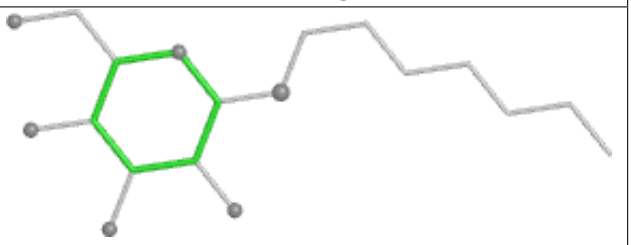
Bond lengths



Bond angles

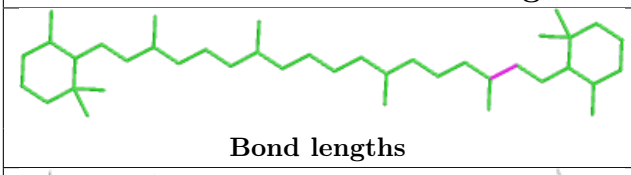


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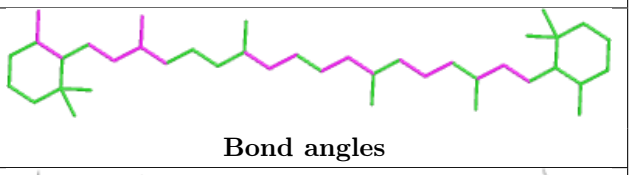


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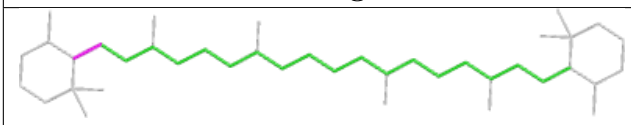
Ligand BCR B 618



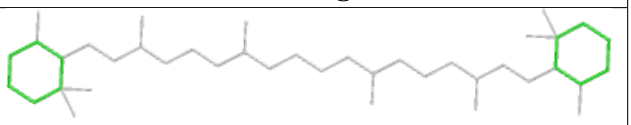
Bond lengths



Bond angles



Torsions

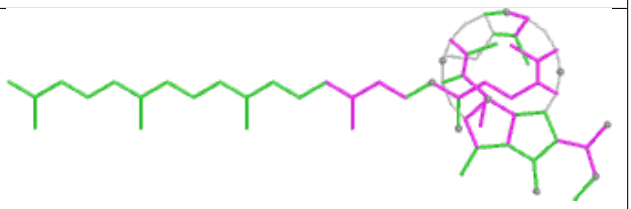


Rings

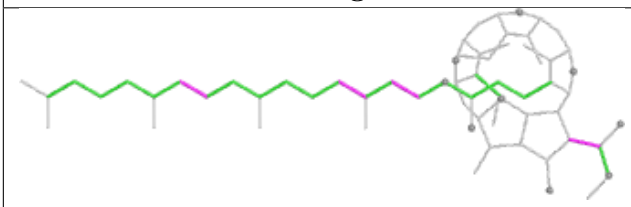
Ligand PHO D 401



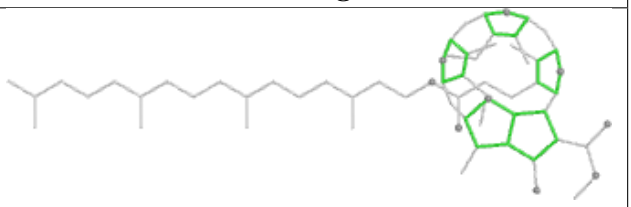
Bond lengths



Bond angles

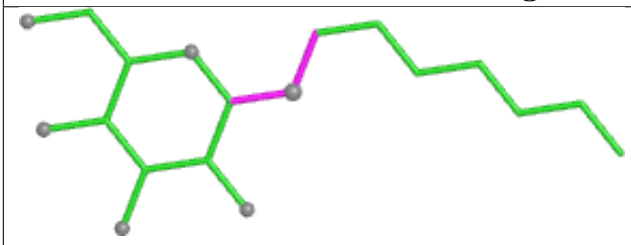


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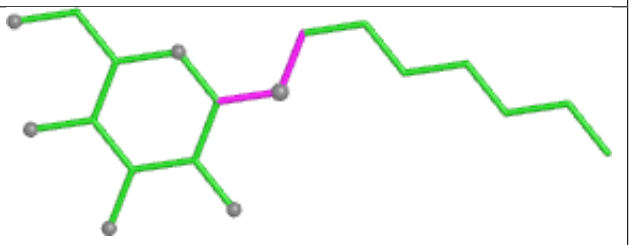


Rings

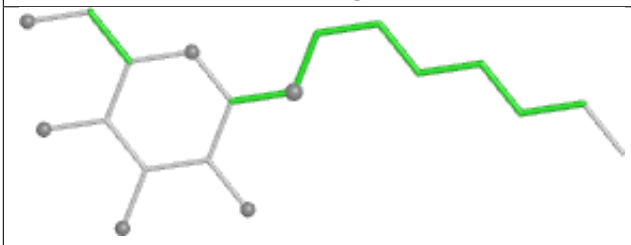
Ligand HTG B 633



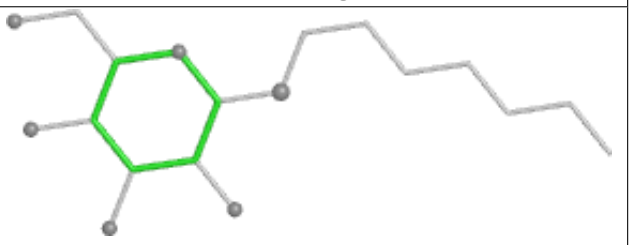
Bond lengths



Bond angles

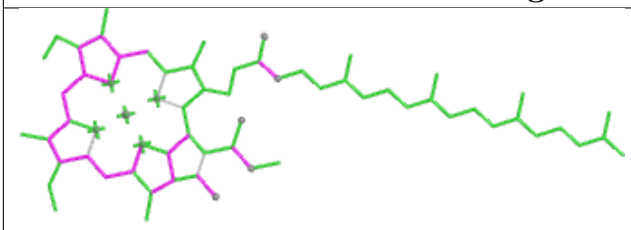


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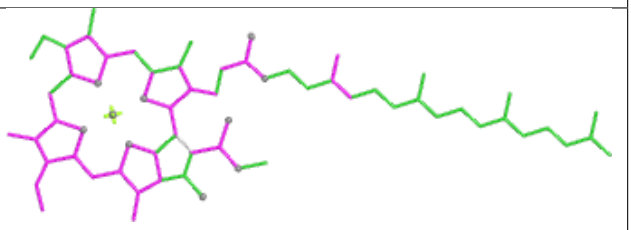


Rings

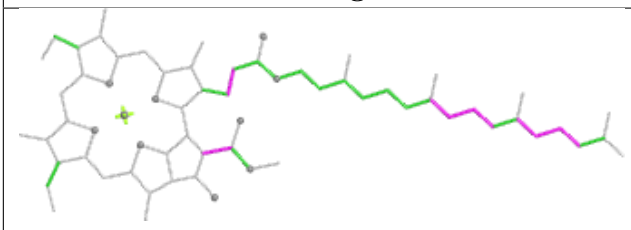
Ligand CLA b 615



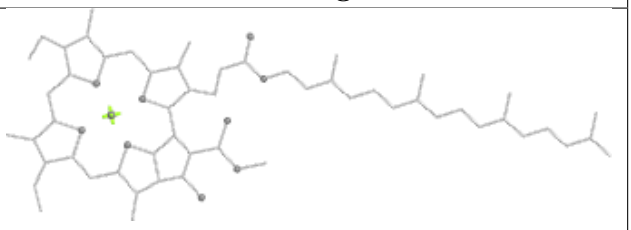
Bond lengths



Bond angles

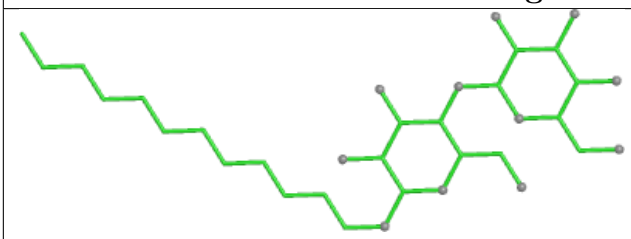


Torsions

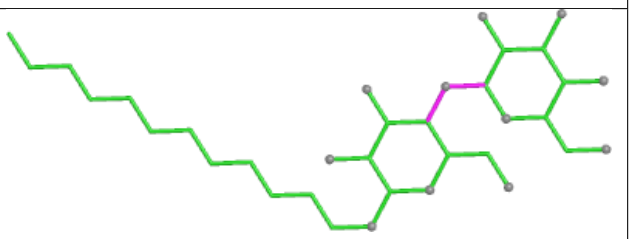


Rings

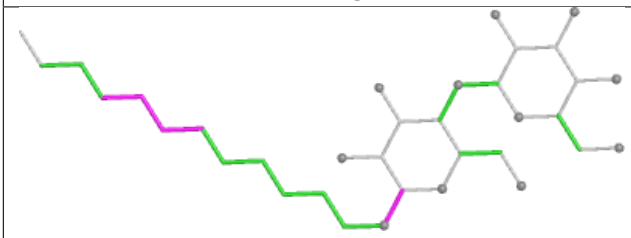
Ligand LMT a 419



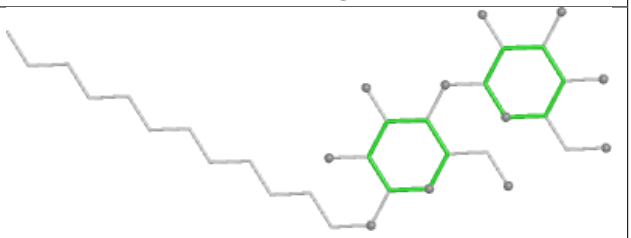
Bond lengths



Bond angles



Torsions

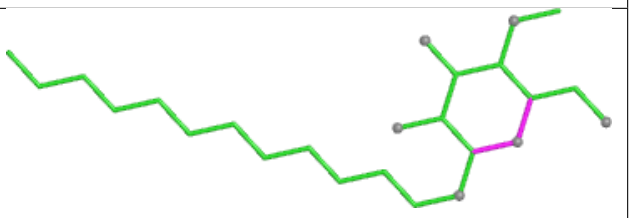


Rings

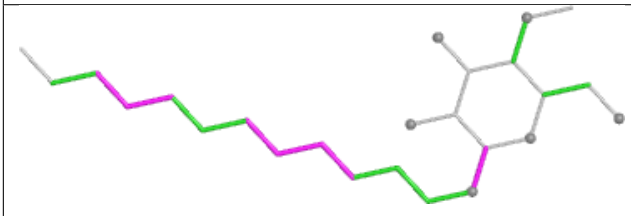
Ligand LMT B 635



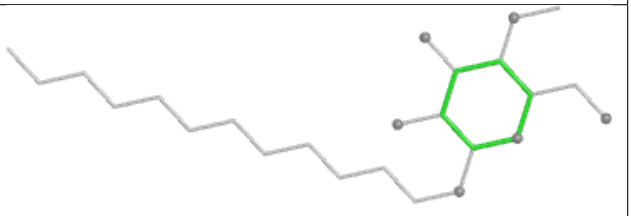
Bond lengths



Bond angles

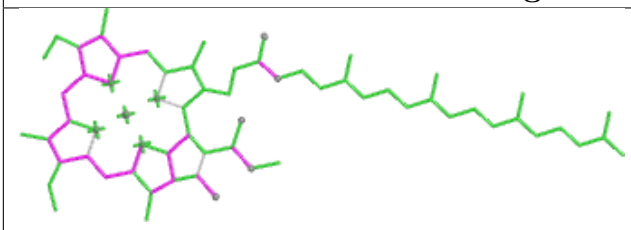


Torsions

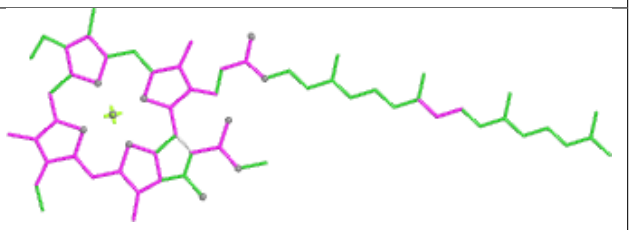


Rings

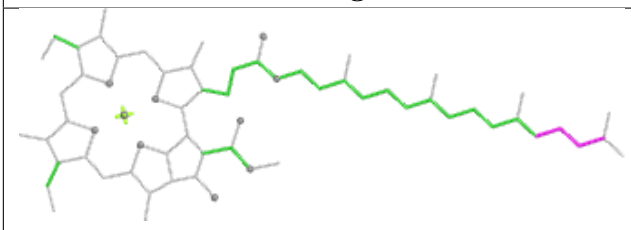
Ligand CLA A 405



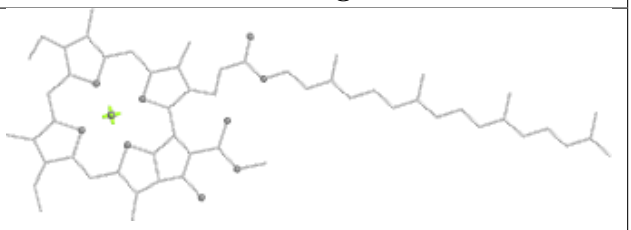
Bond lengths



Bond angles

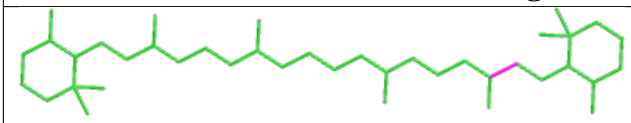


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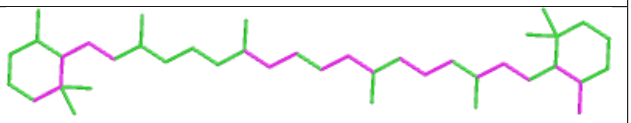


Rings

Ligand BCR b 628



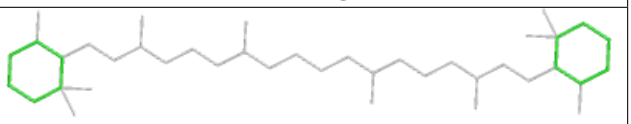
Bond lengths



Bond angles

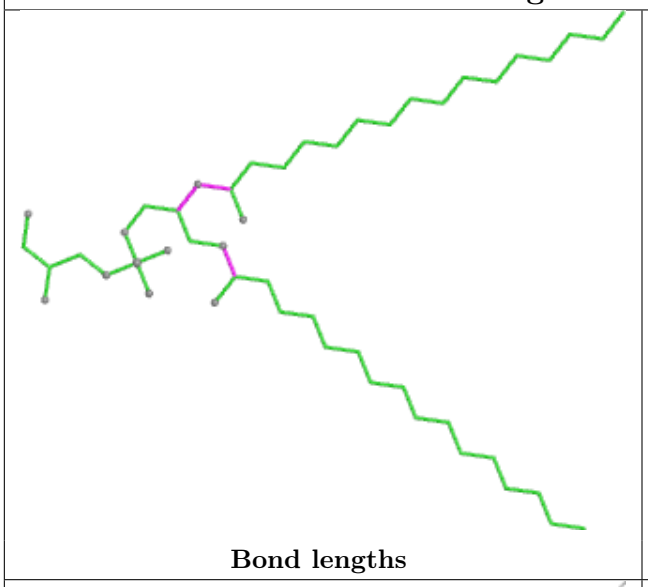


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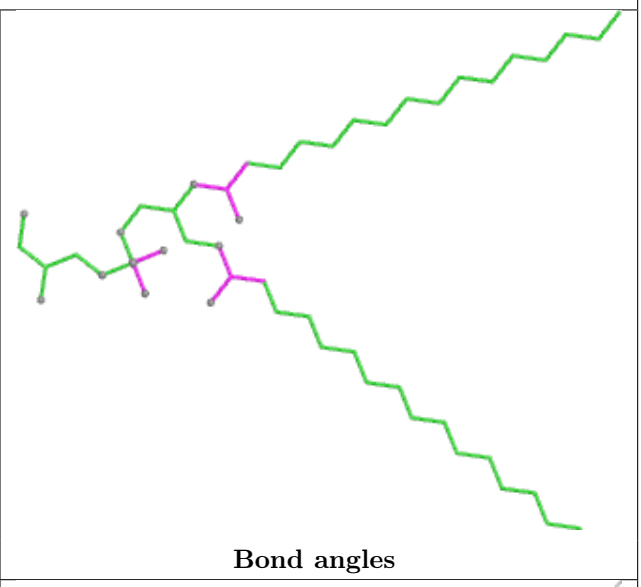


Rings

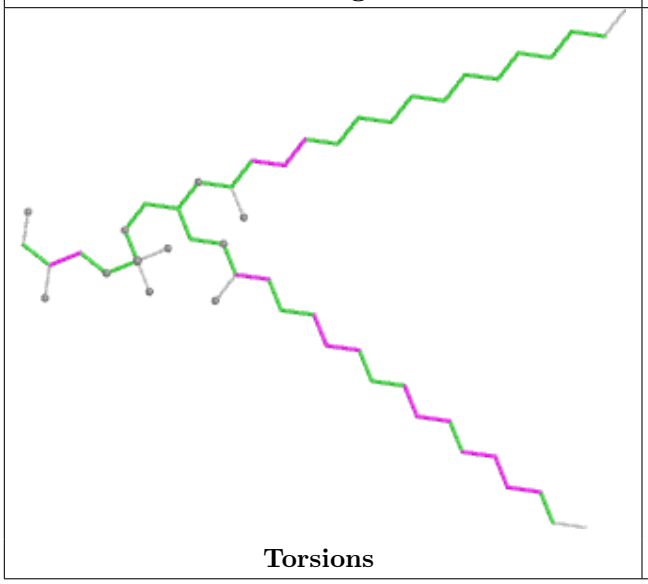
Ligand LHG d 407



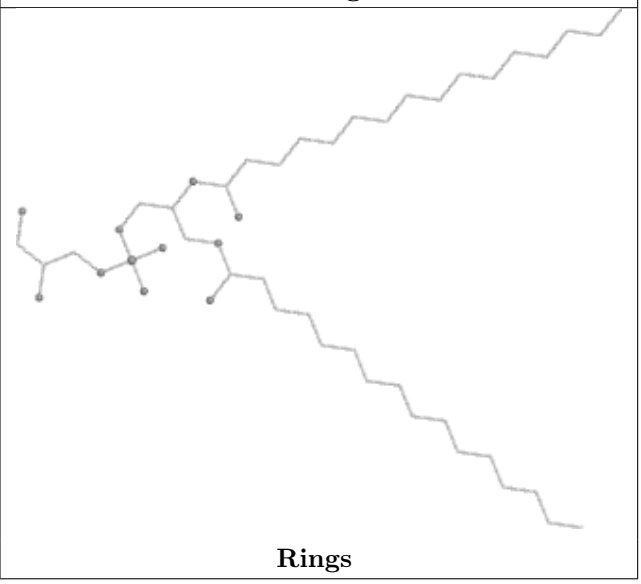
Bond lengths



Bond angles



Torsions

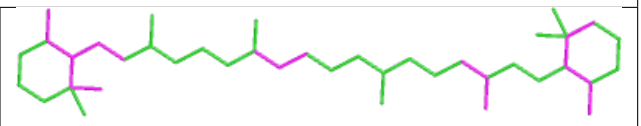


Rings

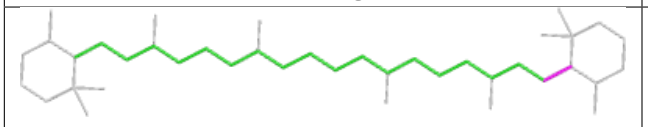
Ligand BCR b 627



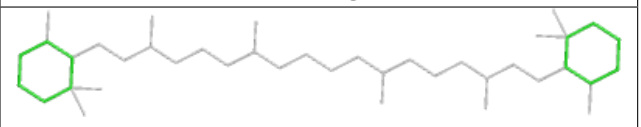
Bond lengths



Bond angles

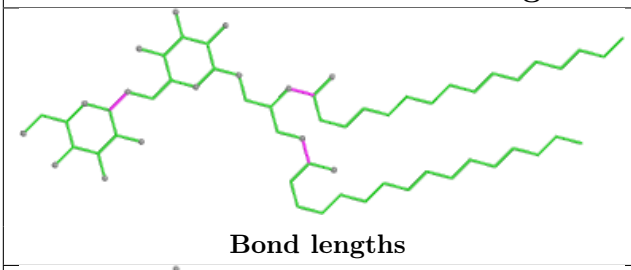


Torsions

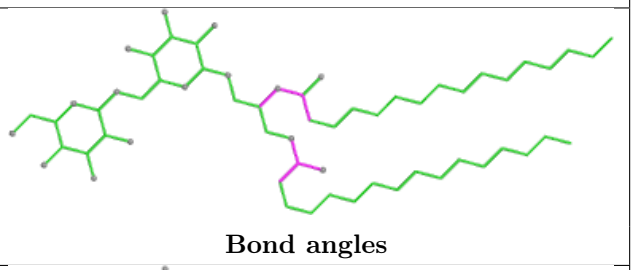


Rings

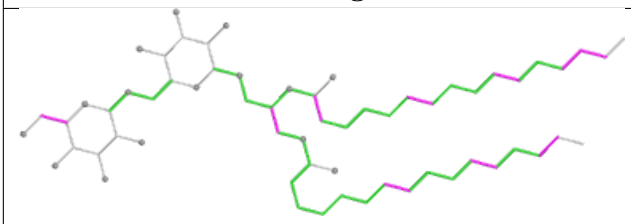
Ligand DGD h 102



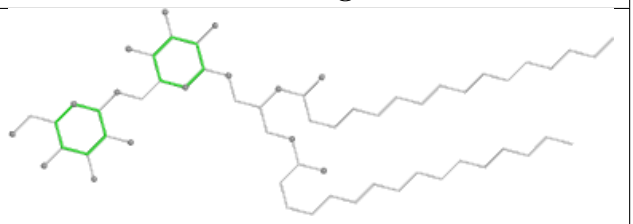
Bond lengths



Bond angles

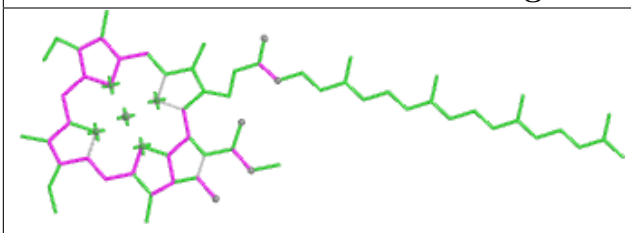


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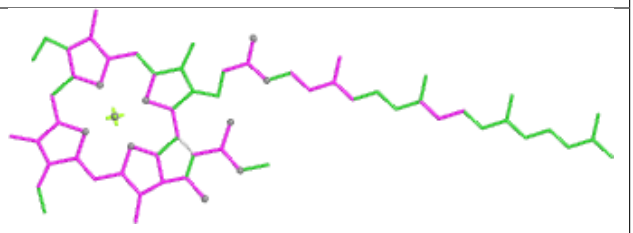


Rings

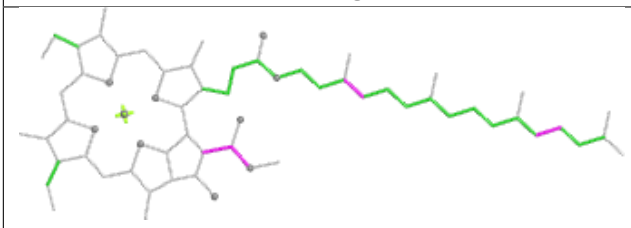
Ligand CLA B 605



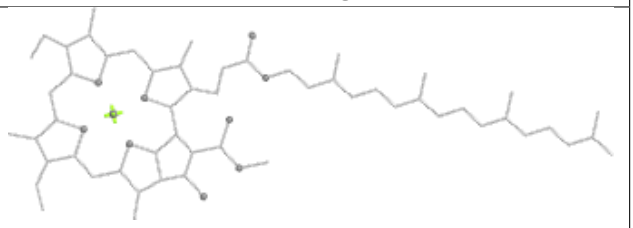
Bond lengths



Bond angles

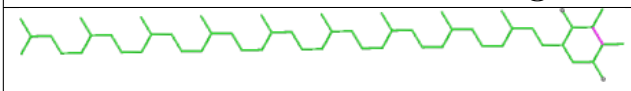


Torsions

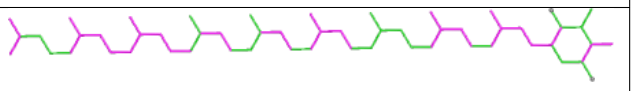


Rings

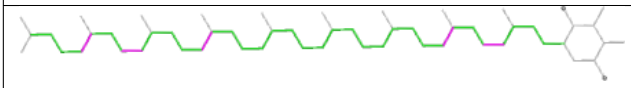
Ligand PL9 D 405



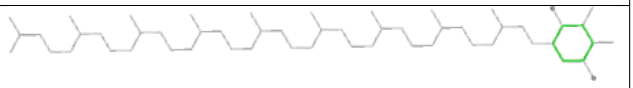
Bond lengths



Bond angles

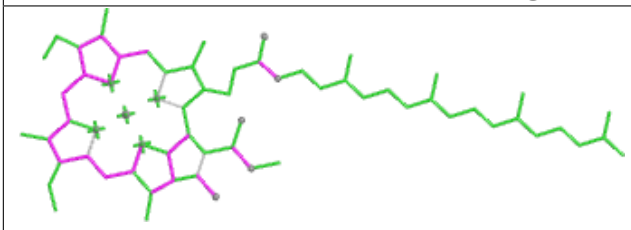


Torsions

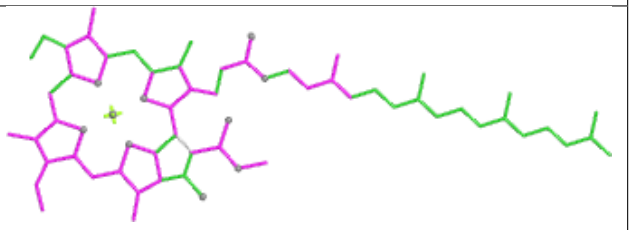


Rings

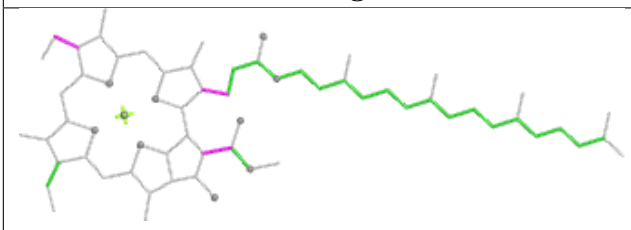
Ligand CLA B 608



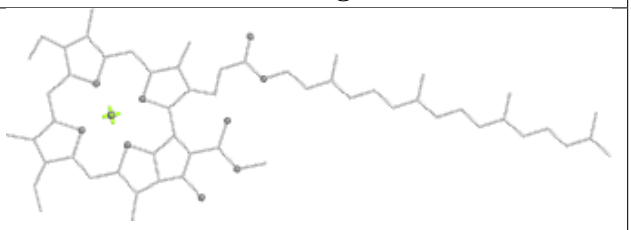
Bond lengths



Bond angles

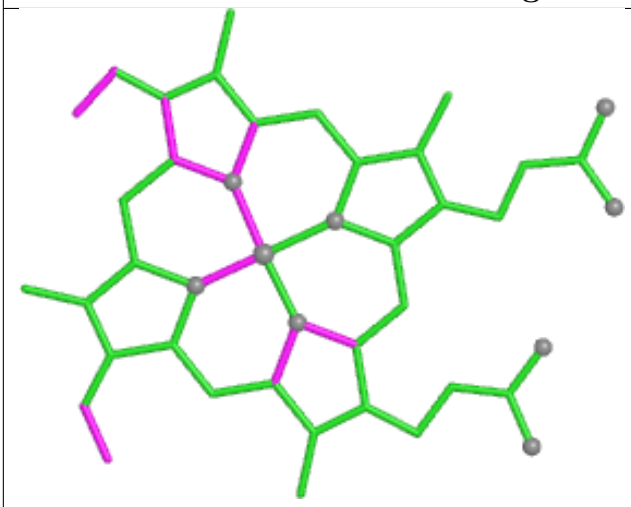


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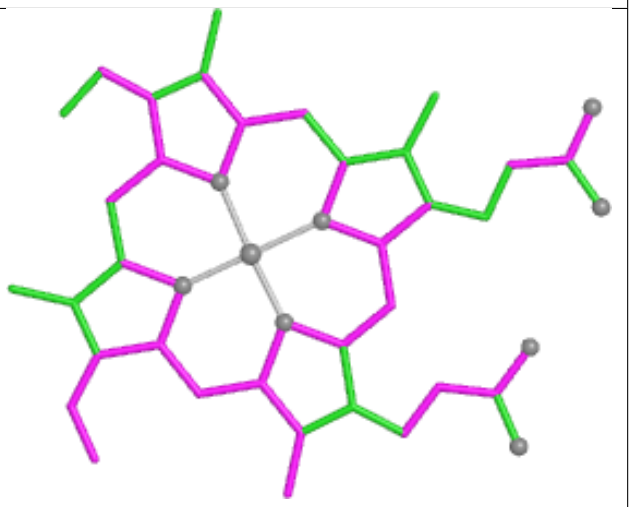


Rings

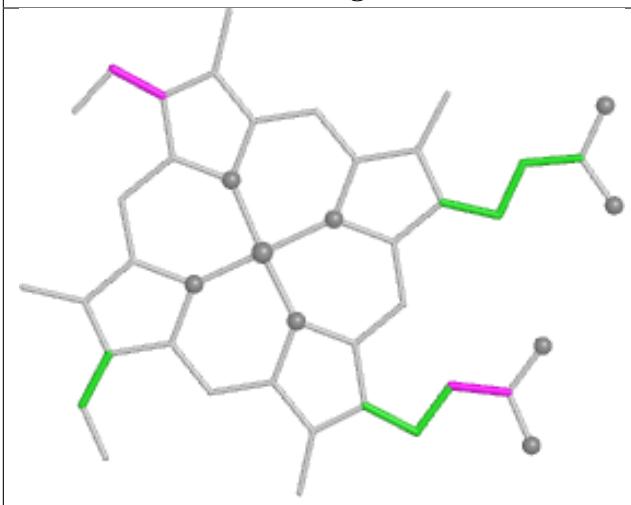
Ligand HEC V 205



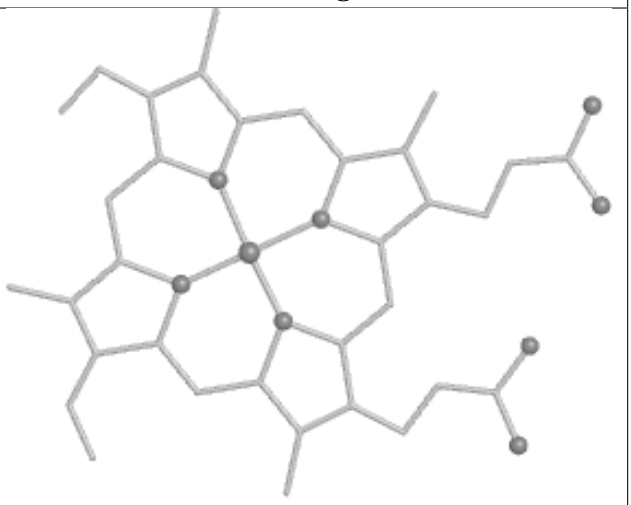
Bond lengths



Bond angles

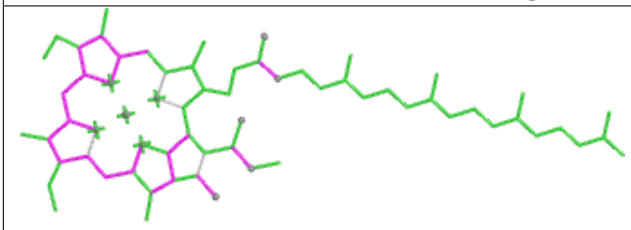


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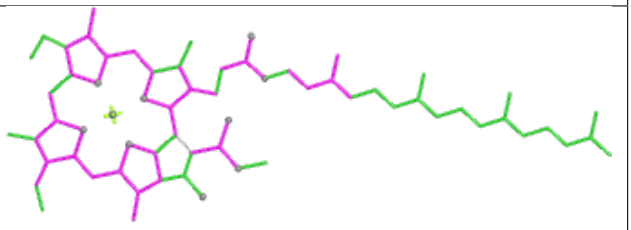


Rings

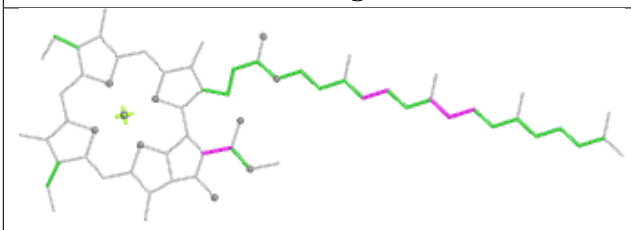
Ligand CLA D 403



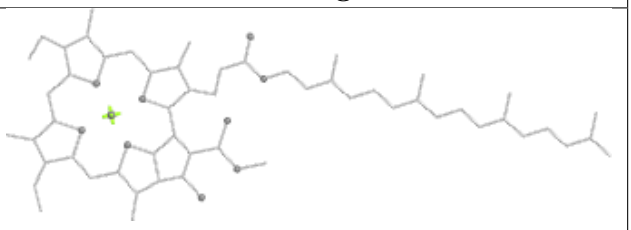
Bond lengths



Bond angles

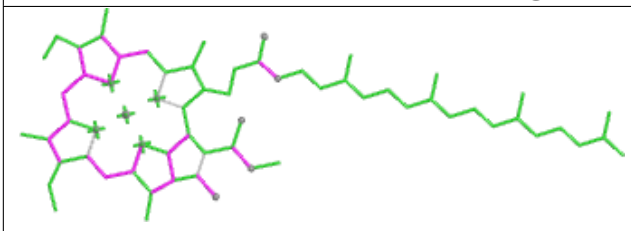


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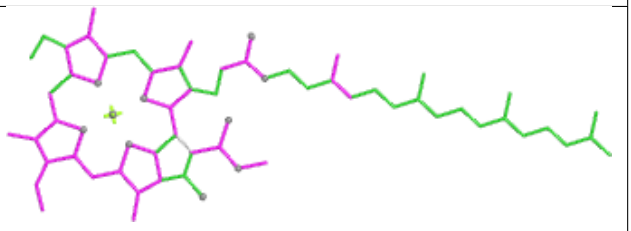


Rings

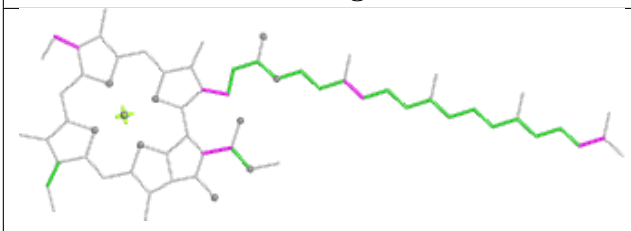
Ligand CLA b 618



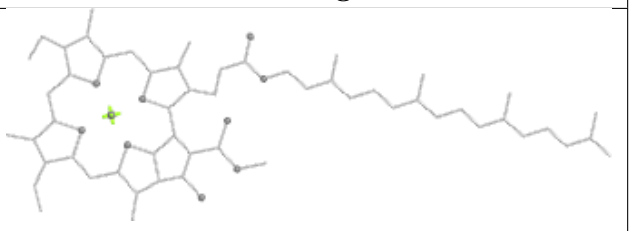
Bond lengths



Bond angles

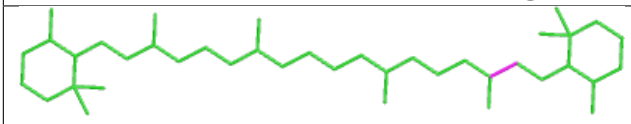


Torsions

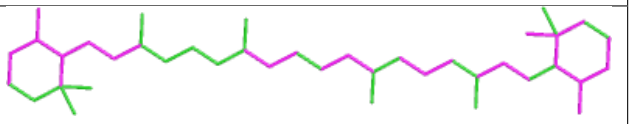


Rings

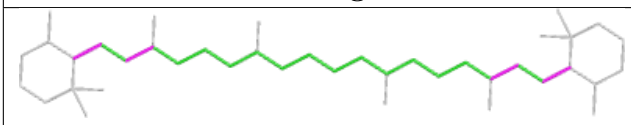
Ligand BCR D 404



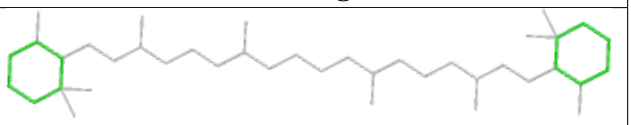
Bond lengths



Bond angles

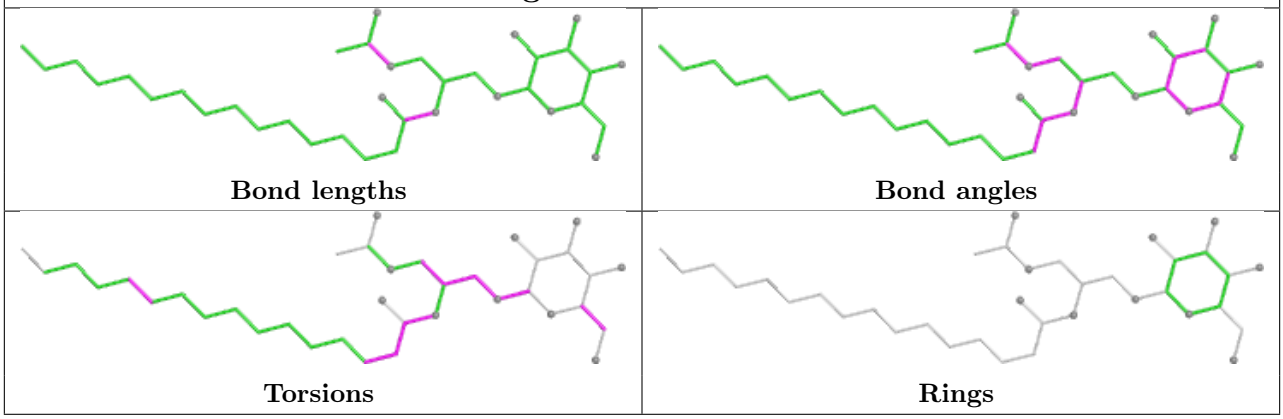


Torsions

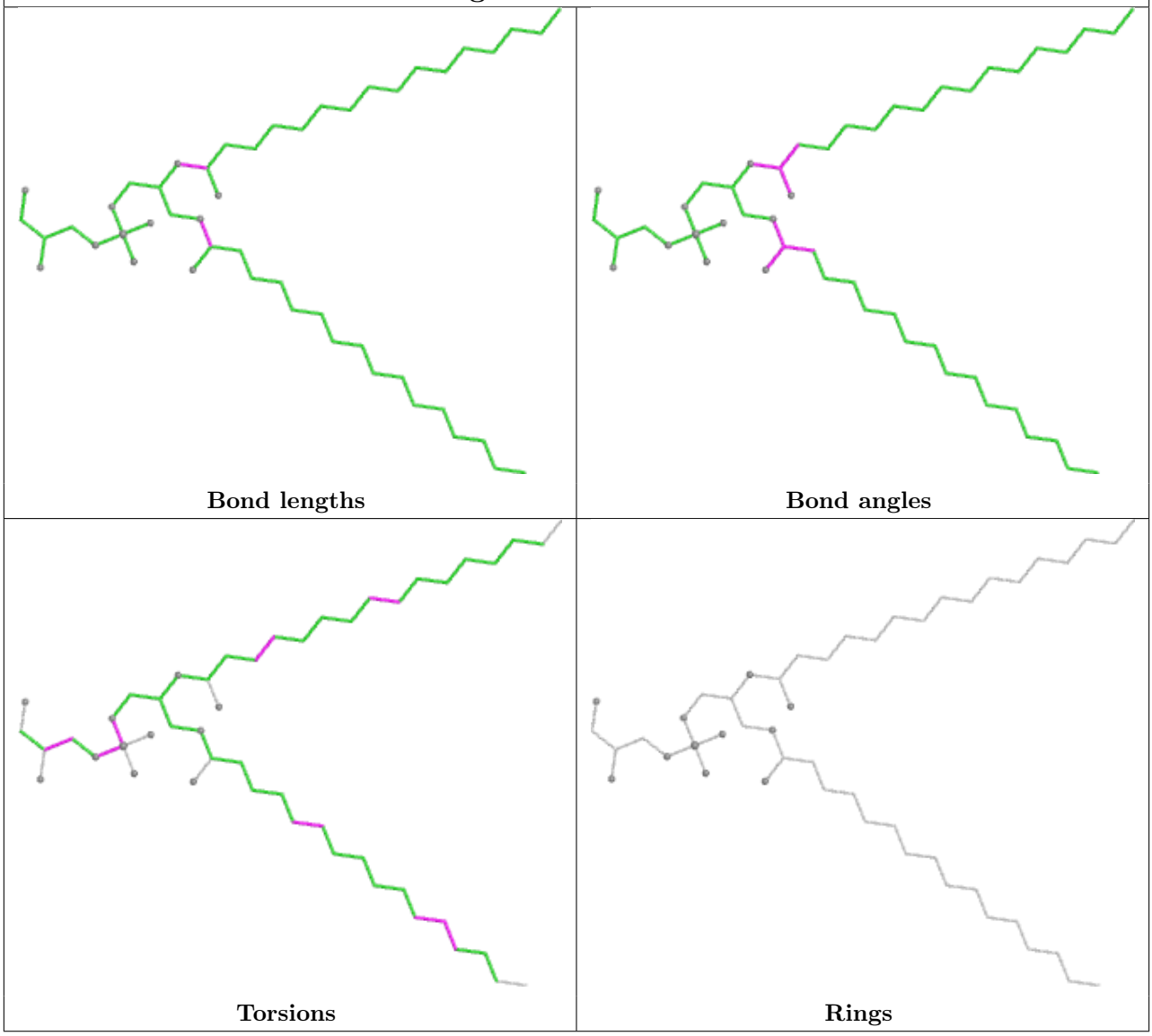


Rings

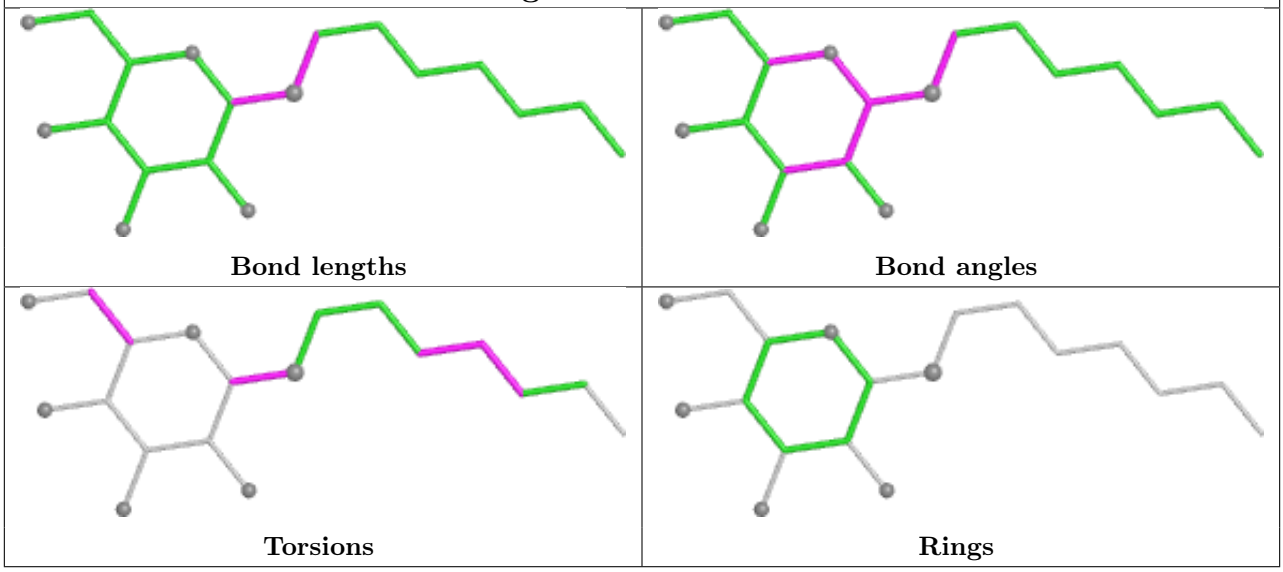
Ligand LMG Z 101



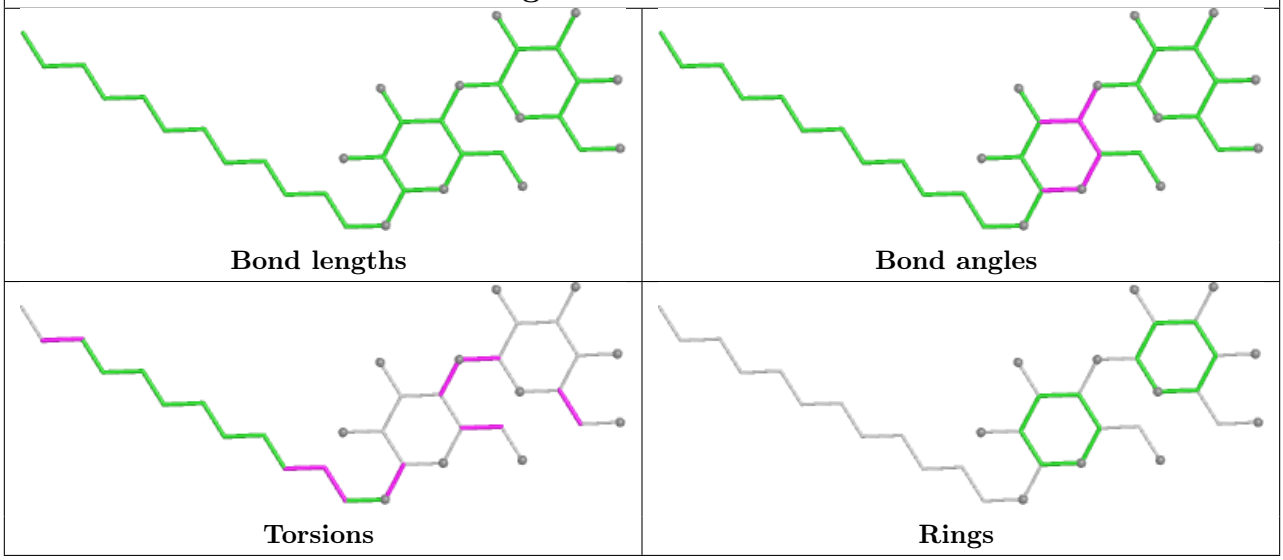
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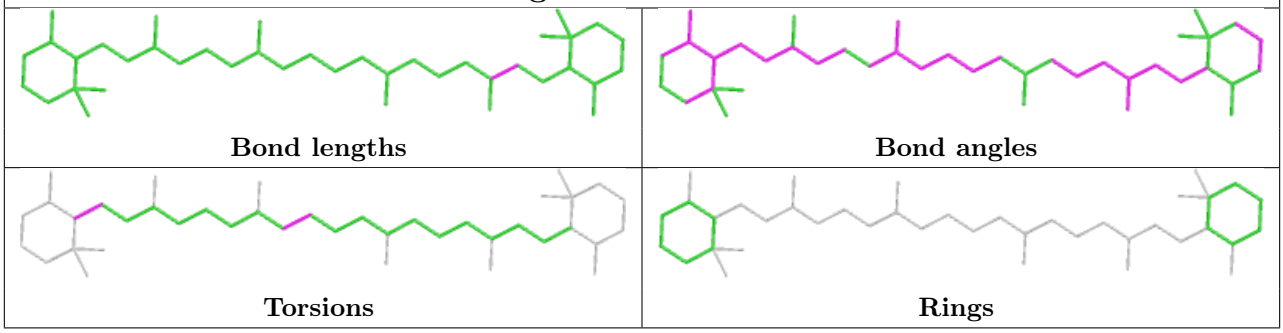
Ligand HTG B 625



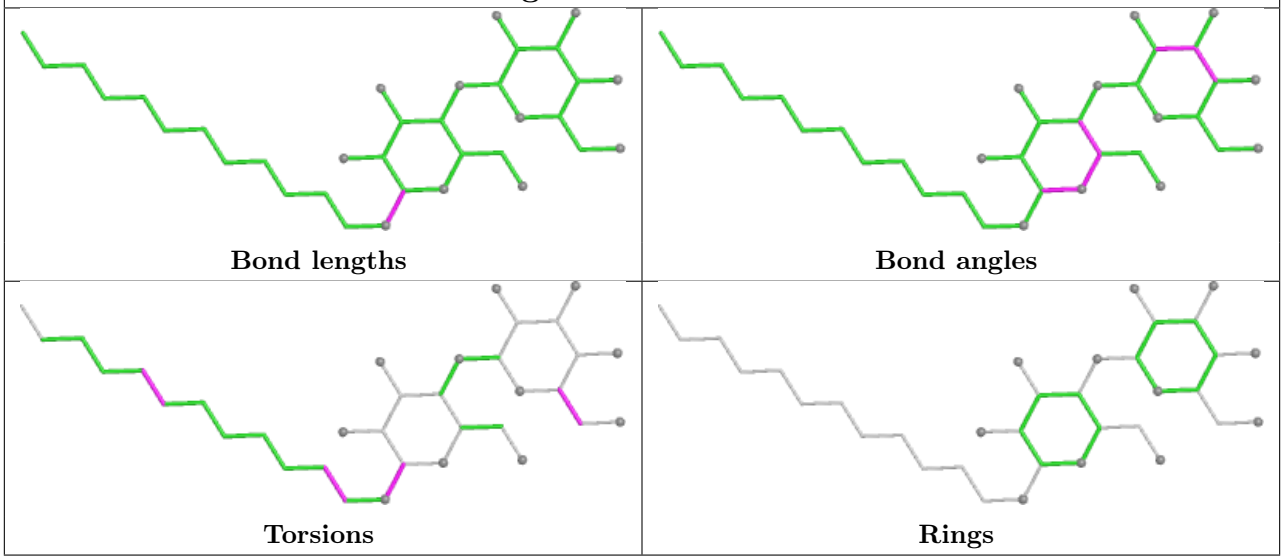
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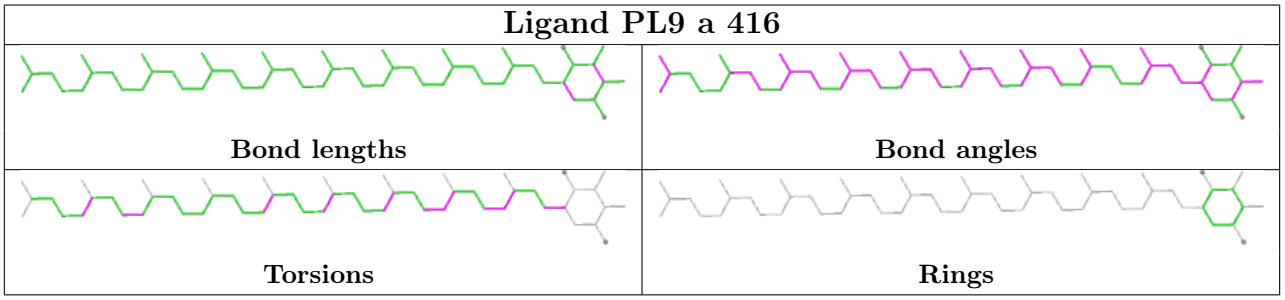
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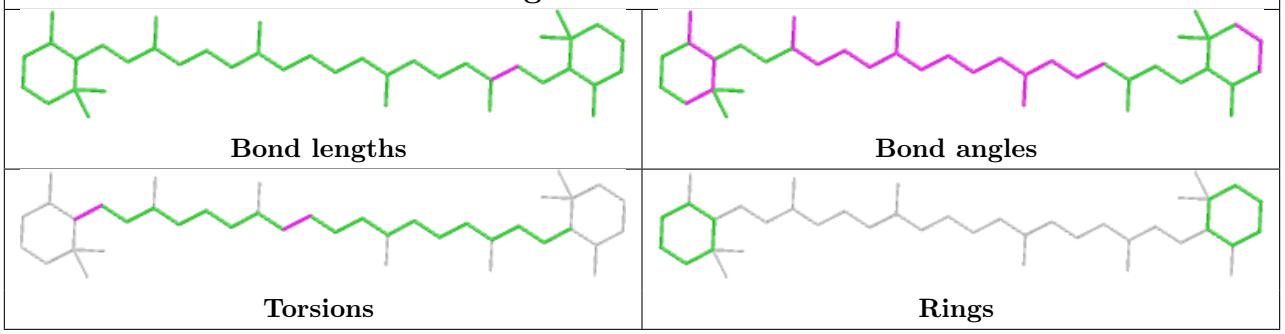
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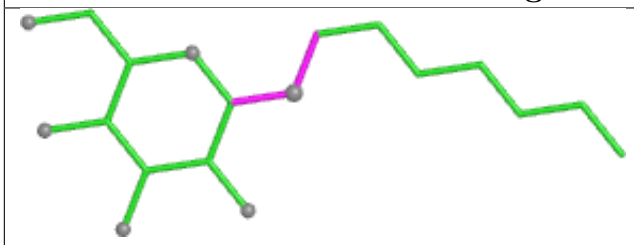
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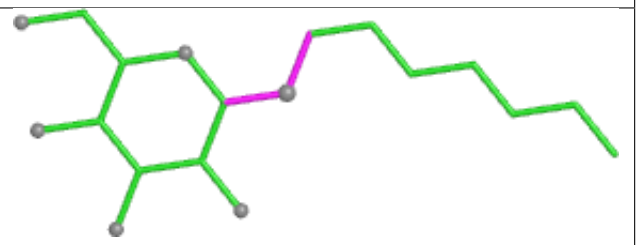
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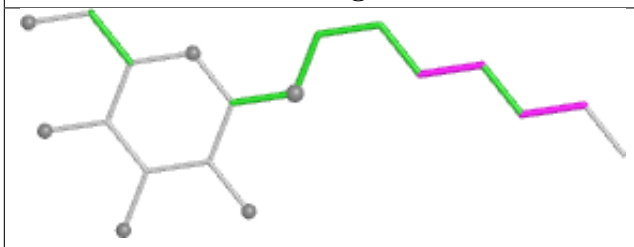
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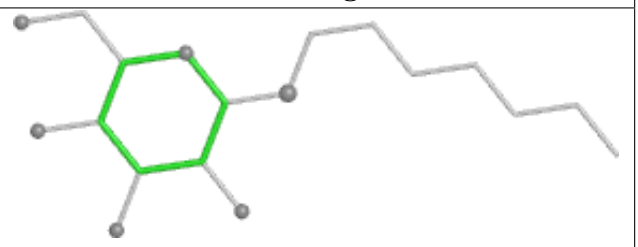
Bond lengths



Bond angles

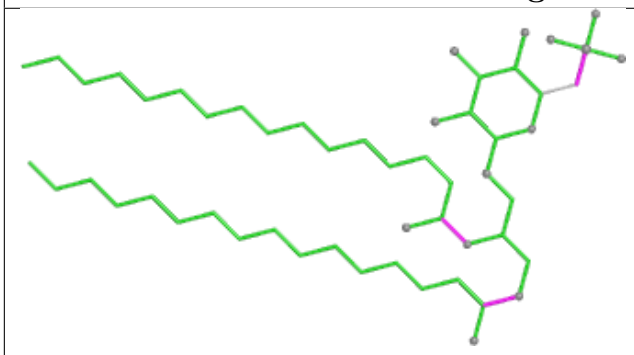


Torsions

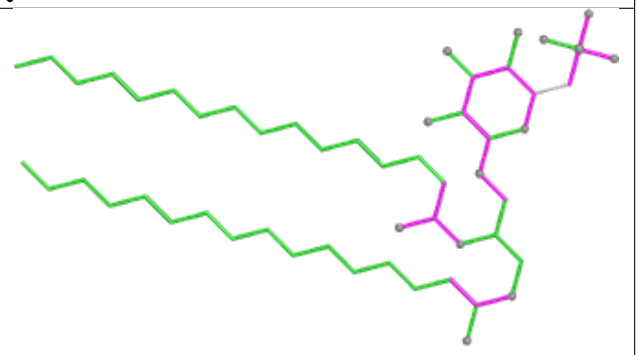


Rings

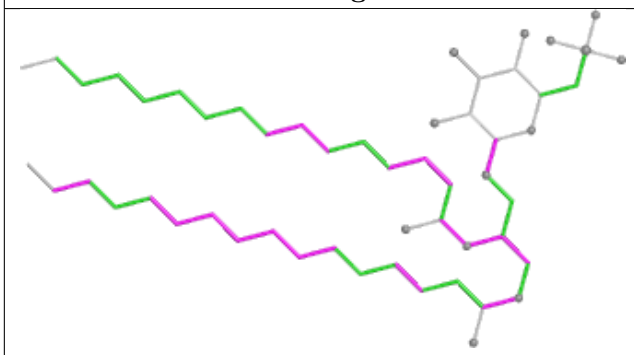
Ligand SQD L 102



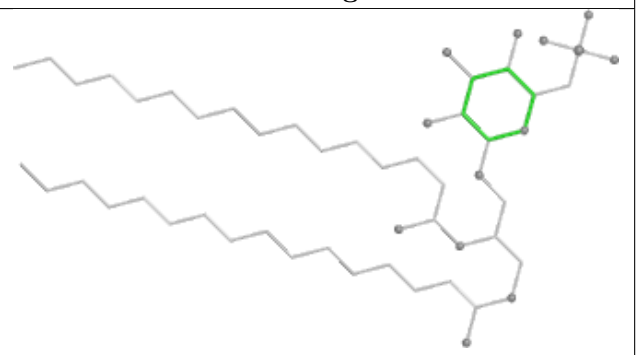
Bond lengths



Bond angles

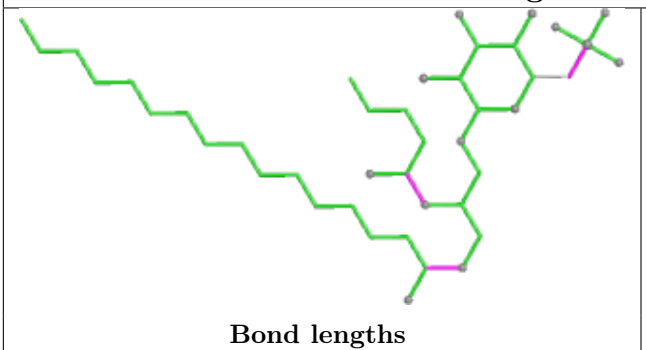


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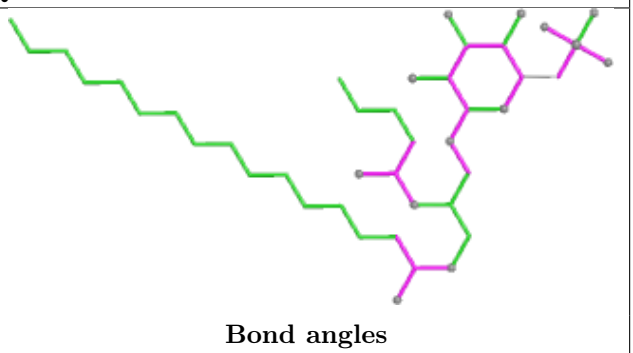


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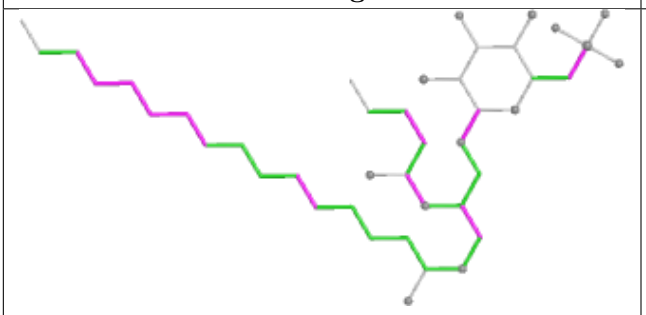
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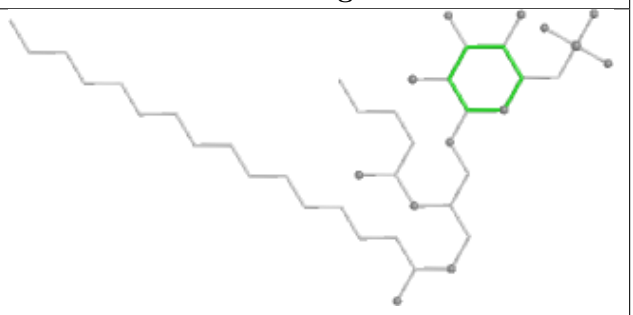
Bond lengths



Bond angles

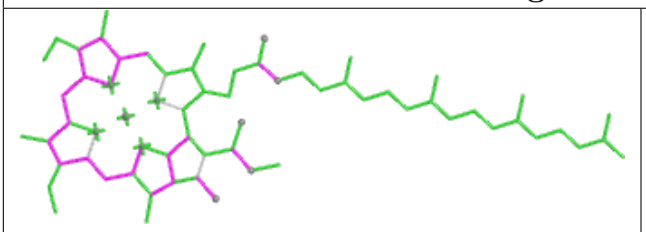


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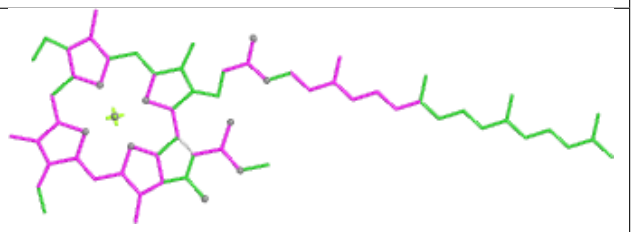


Rings

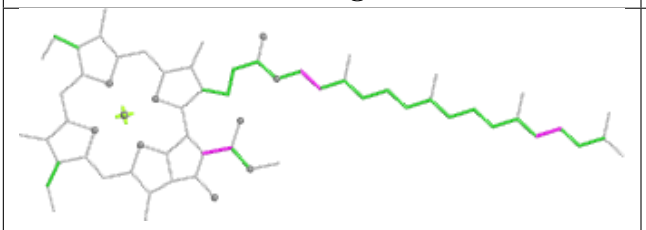
Ligand CLA b 613



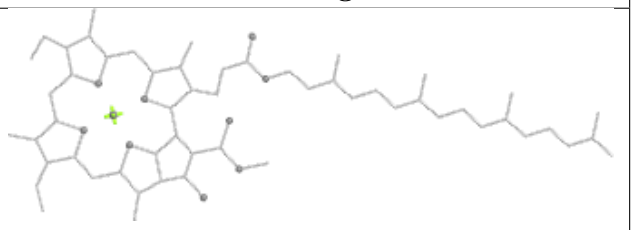
Bond lengths



Bond angles

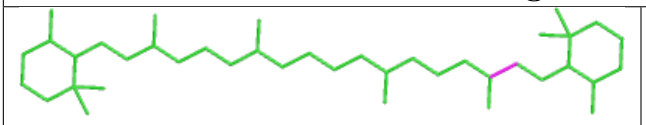


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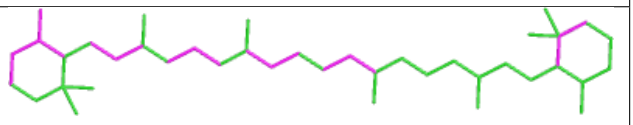


Rings

Ligand BCR b 626



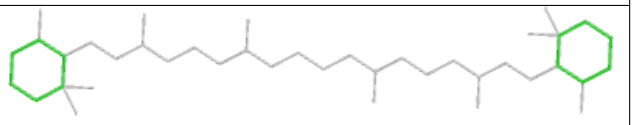
Bond lengths



Bond angles

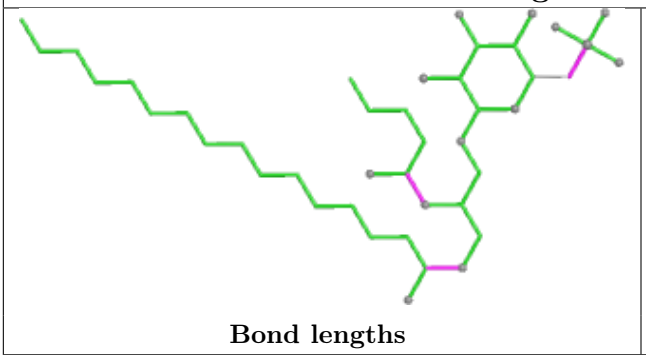


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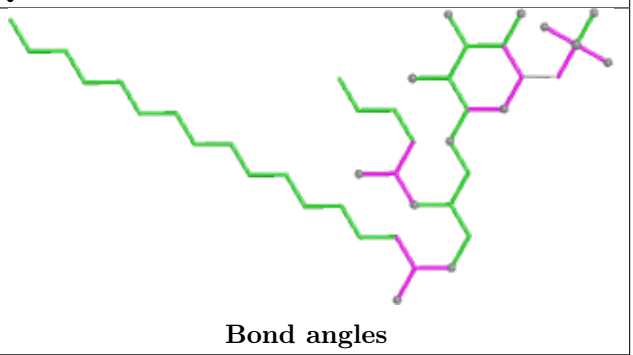


Rings

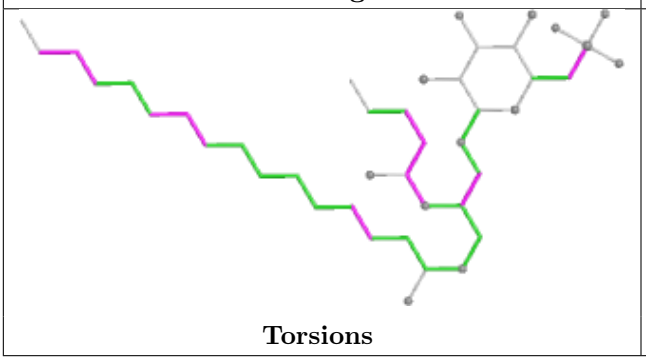
Ligand SQD f 102



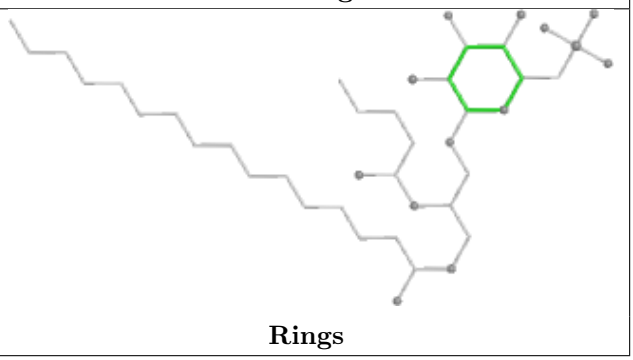
Bond lengths



Bond angles

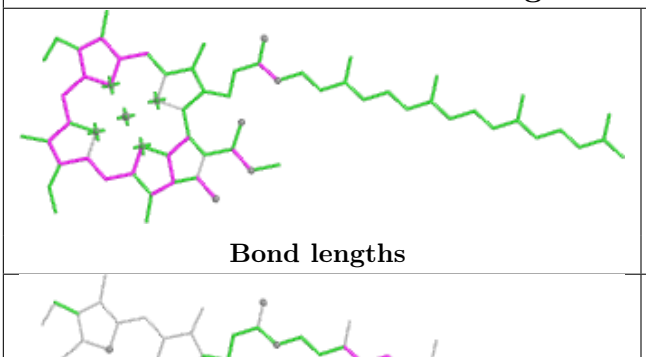


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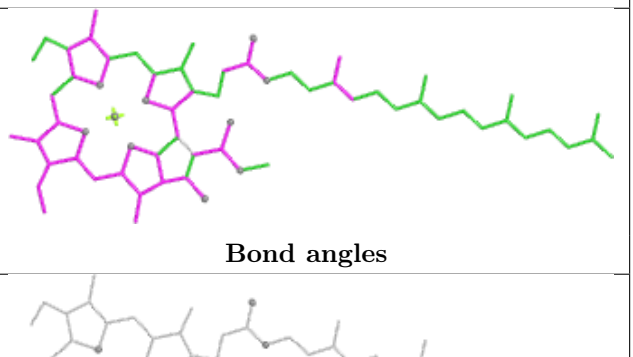


Rings

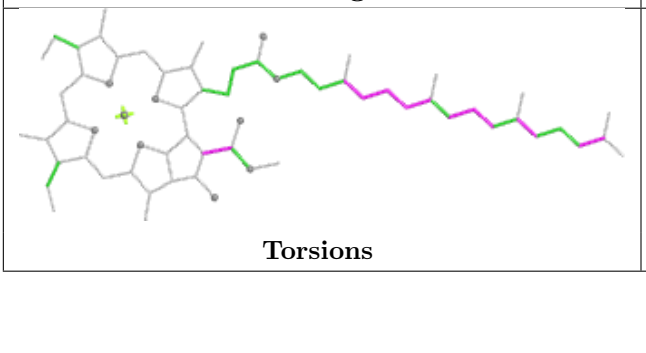
Ligand CLA B 615



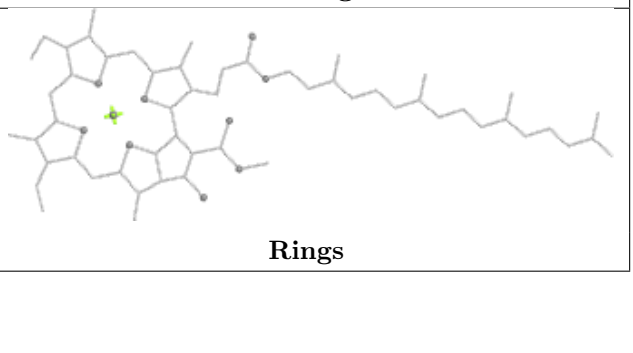
Bond lengths



Bond angles

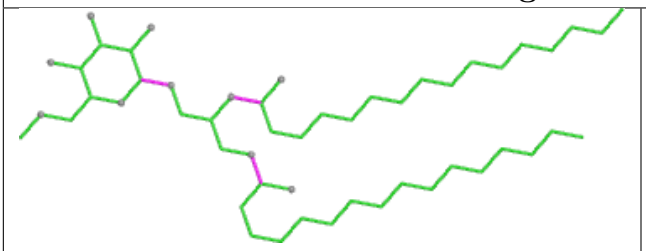


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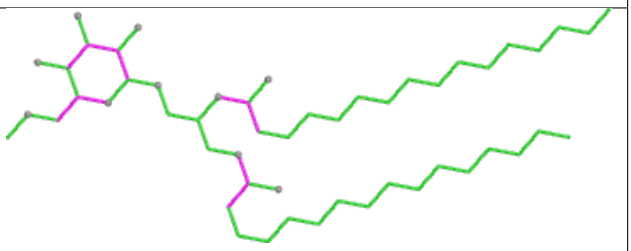


Rings

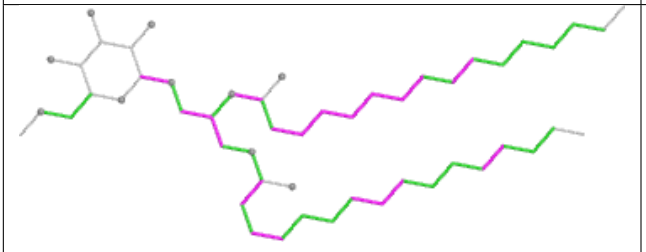
Ligand DGD D 406



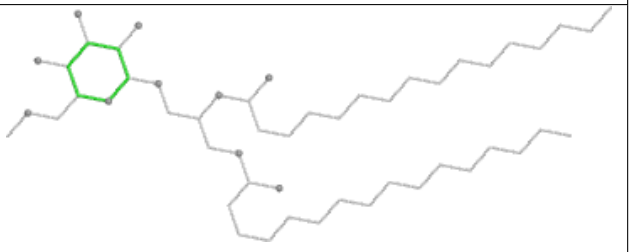
Bond lengths



Bond angles

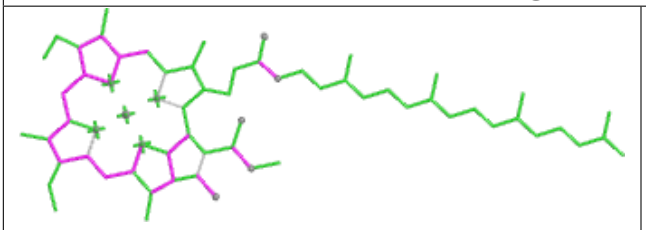


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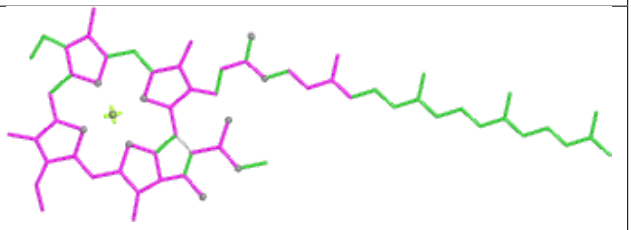


Rings

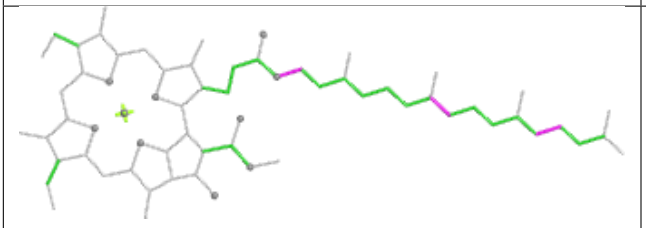
Ligand CLA b 617



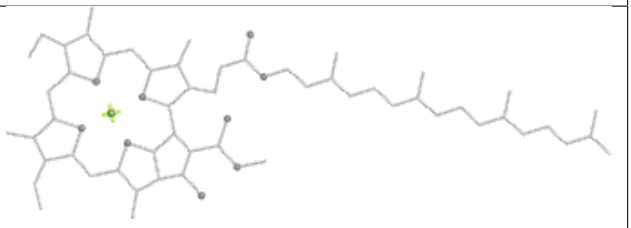
Bond lengths



Bond angles

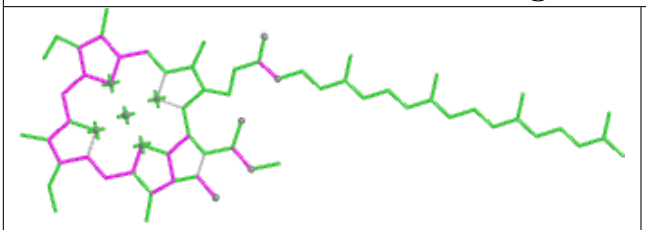


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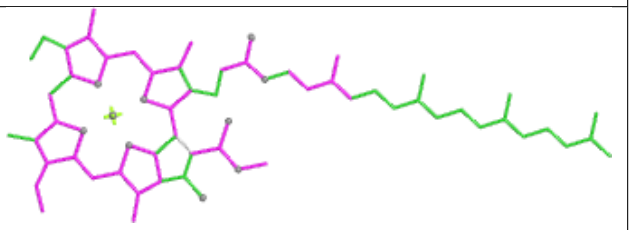


Rings

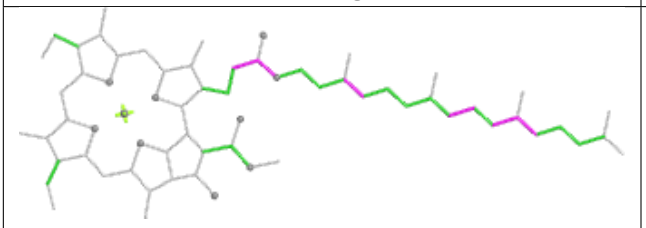
Ligand CLA c 514



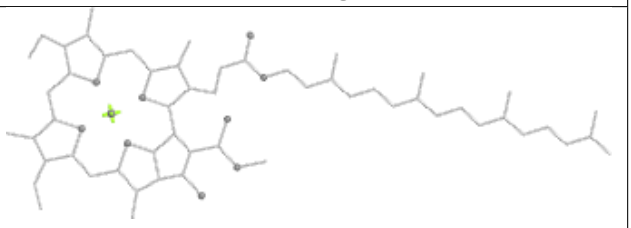
Bond lengths



Bond angles

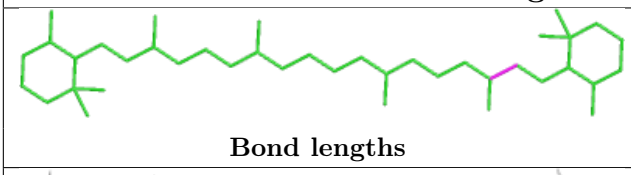


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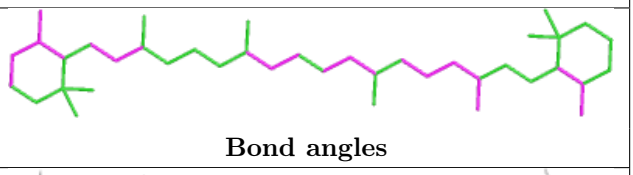


Rings

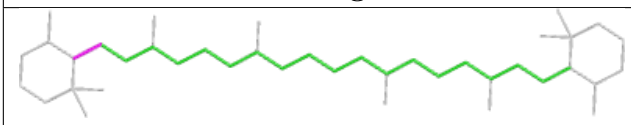
Ligand BCR c 518



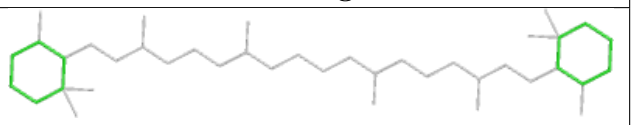
Bond lengths



Bond angles



Torsions

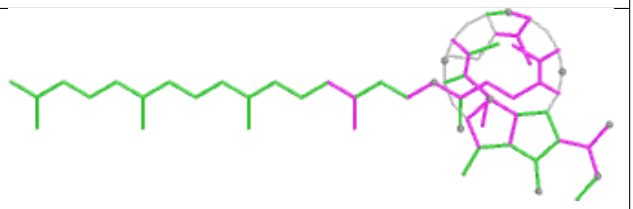


Rings

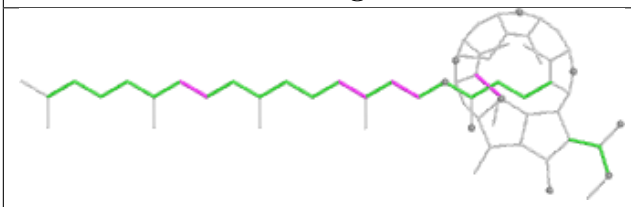
Ligand PHO a 411



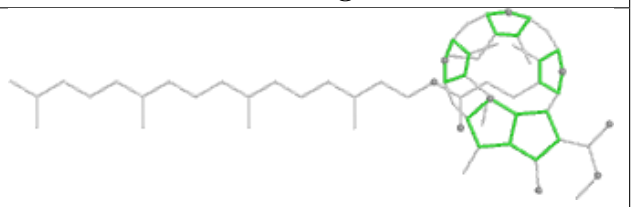
Bond lengths



Bond angles

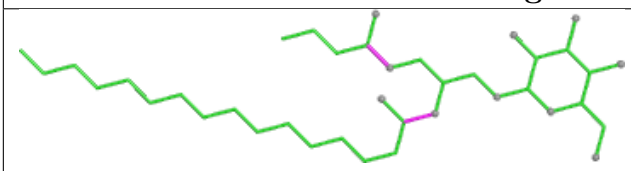


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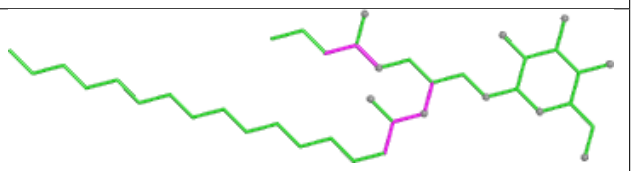


Rings

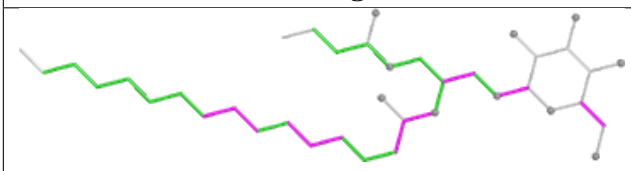
Ligand LMG z 101



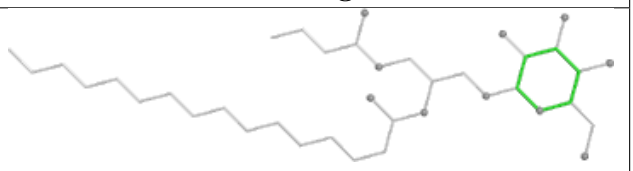
Bond lengths



Bond angles

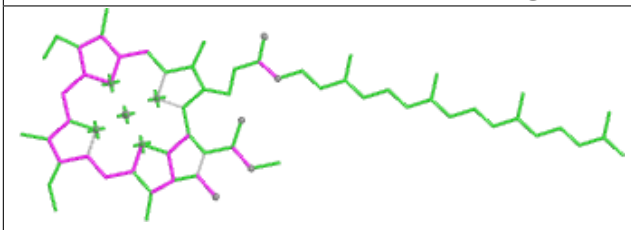


Torsions

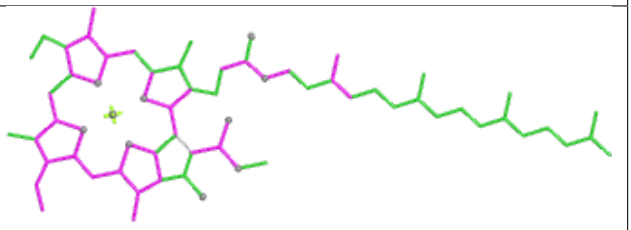


Rings

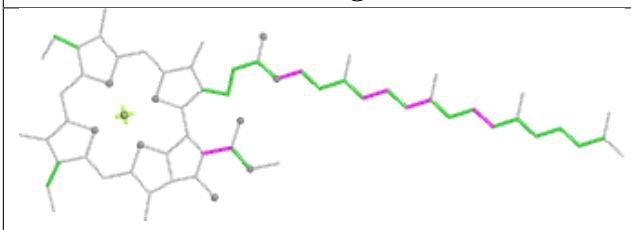
Ligand CLA B 617



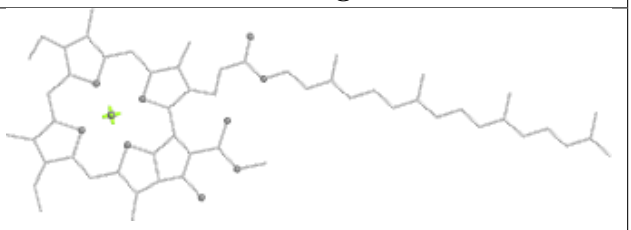
Bond lengths



Bond angles

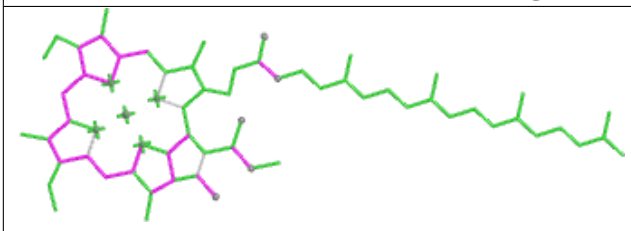


Torsions

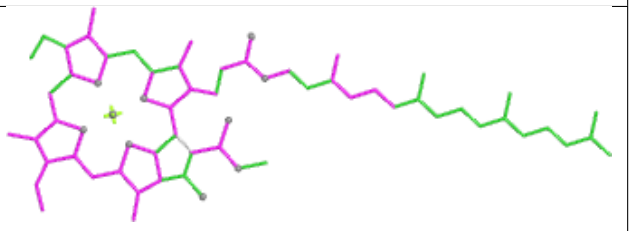


Rings

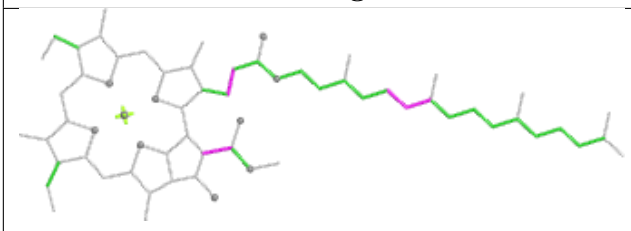
Ligand CLA b 612



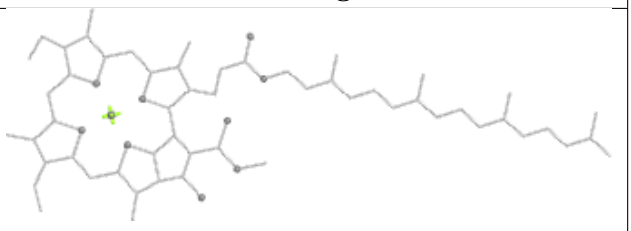
Bond lengths



Bond angles

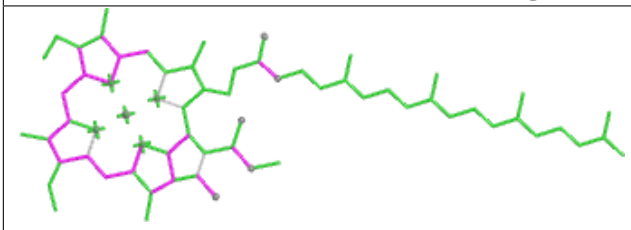


Torsions

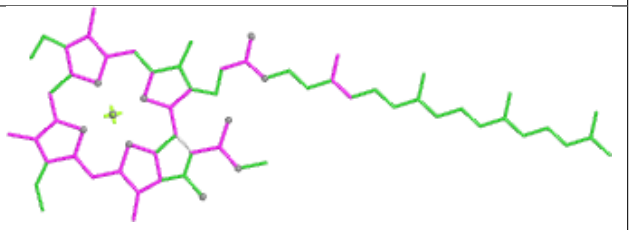


Rings

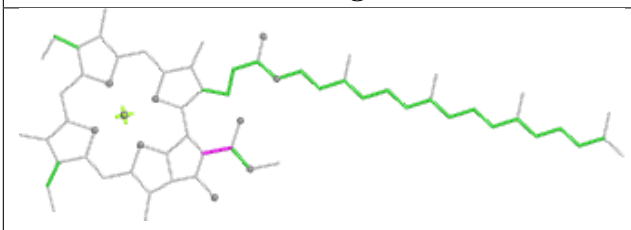
Ligand CLA C 504



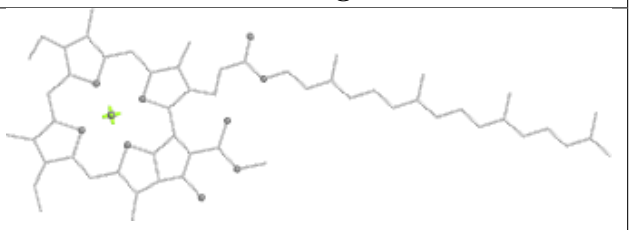
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.70	0 100 100	25, 39, 69, 112	3 (0%)
1	a	334/344 (97%)	-0.69	1 (0%) 90 91	24, 40, 74, 141	6 (1%)
2	B	504/505 (99%)	-0.61	2 (0%) 88 90	22, 44, 78, 119	10 (1%)
2	b	503/505 (99%)	-0.52	6 (1%) 76 79	26, 44, 81, 174	12 (2%)
3	C	451/455 (99%)	-0.54	0 100 100	31, 51, 70, 120	4 (0%)
3	c	455/455 (100%)	-0.52	0 100 100	25, 53, 71, 124	6 (1%)
4	D	341/342 (99%)	-0.74	0 100 100	22, 41, 64, 131	1 (0%)
4	d	341/342 (99%)	-0.73	1 (0%) 90 91	24, 42, 65, 122	1 (0%)
5	E	81/84 (96%)	-0.16	1 (1%) 76 79	32, 63, 95, 127	2 (2%)
5	e	81/84 (96%)	0.01	2 (2%) 58 62	35, 65, 118, 172	2 (2%)
6	F	34/44 (77%)	-0.27	0 100 100	46, 57, 91, 98	0
6	f	32/44 (72%)	-0.21	1 (3%) 51 55	47, 57, 115, 139	0
7	H	65/65 (100%)	-0.37	2 (3%) 51 55	34, 53, 71, 154	1 (1%)
7	h	65/65 (100%)	-0.43	2 (3%) 51 55	43, 56, 77, 165	0
8	I	37/38 (97%)	-0.27	0 100 100	43, 53, 107, 152	0
8	i	37/38 (97%)	-0.28	1 (2%) 56 60	42, 53, 100, 129	0
9	J	38/39 (97%)	-0.01	2 (5%) 32 36	44, 61, 133, 171	0
9	j	39/39 (100%)	-0.10	1 (2%) 57 61	48, 61, 130, 168	0
10	K	37/37 (100%)	-0.27	0 100 100	53, 62, 77, 105	0
10	k	37/37 (100%)	-0.34	0 100 100	53, 62, 80, 105	0
11	L	37/37 (100%)	-0.63	0 100 100	18, 37, 101, 123	1 (2%)
11	l	37/37 (100%)	-0.64	0 100 100	22, 36, 99, 122	1 (2%)
12	M	33/36 (91%)	-0.66	0 100 100	23, 38, 63, 116	1 (3%)
12	m	33/36 (91%)	-0.65	0 100 100	33, 38, 71, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.58	1 (0%)	88	90	25, 49, 95, 134	8 (3%)
13	o	243/244 (99%)	-0.50	2 (0%)	82	84	27, 50, 102, 167	5 (2%)
14	T	29/32 (90%)	-0.71	1 (3%)	48	52	31, 37, 65, 135	1 (3%)
14	t	29/32 (90%)	-0.69	1 (3%)	48	52	31, 38, 66, 135	1 (3%)
15	U	97/104 (93%)	-0.65	0	100	100	37, 48, 75, 118	0
15	u	97/104 (93%)	-0.60	0	100	100	41, 49, 72, 118	0
16	V	137/137 (100%)	-0.54	0	100	100	26, 49, 78, 121	1 (0%)
16	v	137/137 (100%)	-0.56	1 (0%)	84	85	40, 55, 82, 123	0
17	Y	29/30 (96%)	0.66	2 (6%)	23	26	64, 77, 135, 141	0
17	y	29/30 (96%)	0.32	2 (6%)	23	26	67, 80, 135, 142	0
18	X	39/40 (97%)	0.04	1 (2%)	57	61	53, 62, 114, 138	0
18	x	38/40 (95%)	0.22	2 (5%)	32	36	53, 62, 110, 130	0
19	Z	62/62 (100%)	0.23	4 (6%)	25	28	65, 77, 122, 164	0
19	z	62/62 (100%)	0.36	2 (3%)	50	54	68, 79, 122, 165	0
20	R	18/34 (52%)	2.72	13 (72%)	0	0	106, 139, 173, 174	0
All	All	5275/5384 (97%)	-0.51	54 (1%)	79	82	18, 48, 91, 174	67 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	4.7
20	R	13	LEU	4.3
20	R	3	TRP	4.2
2	b	486	LEU	3.9
20	R	9	LEU	3.8
17	Y	18	VAL	3.7
19	z	3	ILE	3.7
7	h	65	LEU	3.5
2	b	499	VAL	3.5
14	t	30	THR	3.4
20	R	10	LEU	3.3
5	e	5	THR	3.3
7	H	66	GLY	3.3
20	R	14	LEU	3.3
18	x	2	THR	3.2
20	R	12	VAL	3.2
2	B	479	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
20	R	5	VAL	3.1
20	R	6	LEU	3.1
5	e	4	THR	3.1
2	b	495	PHE	3.0
9	j	1	MET	2.8
2	b	502	VAL	2.8
2	B	495	PHE	2.7
7	H	65	LEU	2.7
18	x	37	VAL	2.7
20	R	7	VAL	2.6
9	J	2	SER	2.6
20	R	18	TRP	2.6
17	y	18	VAL	2.5
9	J	5	GLY	2.5
19	Z	61	VAL	2.5
19	z	62	VAL	2.5
2	b	493	TRP	2.5
6	f	14	PRO	2.4
7	h	66	GLY	2.4
20	R	16	ALA	2.4
13	o	58	ASN	2.4
19	Z	62	VAL	2.4
5	E	4	THR	2.4
17	Y	20	ALA	2.3
18	X	37	VAL	2.3
8	i	37	LEU	2.3
17	y	20	ALA	2.2
14	T	30	THR	2.2
4	d	12	ARG	2.2
1	a	263	ALA	2.1
2	b	479	PHE	2.1
20	R	19	ALA	2.1
16	v	106	ASN	2.1
13	O	4	THR	2.1
19	Z	3	ILE	2.1
13	o	4	THR	2.0
19	Z	33	TRP	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
14	FME	T	1	10/11	0.95	0.07	33,38,60,72	0
12	FME	m	1	10/11	0.96	0.09	35,47,107,124	0
12	FME	M	1	10/11	0.97	0.07	33,52,85,91	0
14	FME	t	1	10/11	0.97	0.05	28,40,49,83	0
8	FME	I	1	10/11	0.98	0.06	36,49,53,57	0
8	FME	i	1	10/11	0.98	0.06	39,51,57,61	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	DGD	D	406	52/66	0.69	0.15	62,106,145,154	0
36	DGD	e	101	62/66	0.69	0.16	68,115,177,183	0
37	LHG	e	102	42/49	0.71	0.12	68,134,167,175	0
29	LMT	F	102	35/35	0.74	0.15	81,117,147,150	0
28	GOL	V	201	6/6	0.74	0.15	69,78,89,95	0
27	SQD	f	102	43/54	0.75	0.14	86,119,144,148	0
29	LMT	C	522	35/35	0.75	0.14	83,119,152,161	0
33	CA	b	609	1/1	0.77	0.13	137,137,137,137	0
29	LMT	b	630	25/35	0.77	0.13	70,95,151,153	0
32	UNL	m	101	10/-	0.77	0.15	54,59,86,88	0
33	CA	B	601	1/1	0.77	0.09	143,143,143,143	0
29	LMT	M	104	35/35	0.78	0.14	44,96,137,144	0
29	LMT	f	103	35/35	0.78	0.13	74,122,151,156	0
32	UNL	a	403	30/-	0.78	0.14	69,90,128,130	0
34	HTG	D	412	16/19	0.79	0.14	70,142,157,160	0
32	UNL	A	419	28/-	0.79	0.13	63,86,104,104	0
32	UNL	M	103	10/-	0.79	0.12	48,61,72,79	0
29	LMT	a	419	35/35	0.79	0.13	86,112,130,132	0
32	UNL	j	102	10/-	0.80	0.13	64,78,93,97	0
32	UNL	i	101	40/-	0.80	0.14	49,77,144,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	HTG	c	525	19/19	0.81	0.12	56,109,121,130	0
32	UNL	C	528	34/-	0.81	0.13	68,109,132,133	0
34	HTG	B	625	19/19	0.81	0.12	72,118,144,148	0
32	UNL	I	101	40/-	0.81	0.14	41,84,148,161	0
29	LMT	A	416	35/35	0.82	0.12	40,84,106,133	0
32	UNL	J	102	10/-	0.82	0.14	47,71,94,97	0
32	UNL	D	411	40/-	0.82	0.12	56,80,133,139	0
34	HTG	b	608	19/19	0.83	0.11	56,113,148,151	0
28	GOL	O	301	6/6	0.83	0.10	68,79,81,88	0
34	HTG	d	412	16/19	0.83	0.12	64,114,125,129	0
32	UNL	c	526	32/-	0.83	0.13	63,98,133,141	0
29	LMT	B	622	35/35	0.83	0.12	62,118,148,153	0
37	LHG	E	101	42/49	0.83	0.12	67,98,120,121	0
34	HTG	V	206	19/19	0.83	0.12	61,91,114,204	0
35	LMG	c	523	51/55	0.84	0.11	49,107,130,130	0
35	LMG	z	101	39/55	0.84	0.14	63,116,139,159	0
34	HTG	b	632	19/19	0.84	0.12	66,115,147,147	0
34	HTG	B	633	19/19	0.84	0.11	53,105,137,170	0
29	LMT	a	404	35/35	0.84	0.12	44,83,115,132	0
35	LMG	C	521	51/55	0.84	0.12	55,109,128,136	0
27	SQD	B	621	54/54	0.85	0.12	52,88,144,153	0
28	GOL	c	502	6/6	0.85	0.16	75,86,99,108	0
32	UNL	B	634	33/-	0.85	0.13	57,82,136,141	0
35	LMG	Z	101	37/55	0.85	0.14	50,111,133,137	0
32	UNL	b	633	33/-	0.85	0.14	41,94,159,162	0
28	GOL	C	525	6/6	0.86	0.13	54,60,75,81	0
27	SQD	F	103	43/54	0.86	0.11	75,102,123,134	0
31	PL9	A	418	55/55	0.86	0.13	56,99,114,133	0
31	PL9	a	416	55/55	0.86	0.14	64,103,126,128	0
32	UNL	d	411	36/-	0.86	0.11	54,77,132,138	0
28	GOL	T	101	6/6	0.86	0.18	51,78,96,104	0
34	HTG	C	524	19/19	0.86	0.10	82,92,128,134	0
27	SQD	L	102	54/54	0.87	0.10	46,74,126,143	0
27	SQD	a	405	54/54	0.87	0.10	43,78,123,126	0
29	LMT	B	635	25/35	0.87	0.12	42,86,138,141	0
27	SQD	A	415	54/54	0.87	0.10	48,74,114,132	0
28	GOL	A	414	6/6	0.87	0.12	53,77,82,88	0
28	GOL	B	630	6/6	0.87	0.12	51,67,75,83	0
34	HTG	b	631	19/19	0.87	0.12	58,68,84,96	0
28	GOL	t	102	6/6	0.87	0.15	54,82,93,98	0
34	HTG	B	624	19/19	0.87	0.12	48,66,92,98	0
29	LMT	m	102	35/35	0.88	0.10	35,98,128,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	HTG	c	524	19/19	0.88	0.09	89,95,108,128	0
28	GOL	a	402	6/6	0.88	0.11	73,83,89,92	0
28	GOL	b	606	6/6	0.88	0.12	63,79,87,89	0
29	LMT	M	105	35/35	0.89	0.10	41,84,106,116	0
28	GOL	v	201	6/6	0.89	0.13	71,93,96,100	0
28	GOL	T	102	6/6	0.90	0.12	106,113,118,120	0
29	LMT	M	102	35/35	0.90	0.10	41,85,110,112	0
34	HTG	C	523	19/19	0.90	0.09	72,86,102,106	0
29	LMT	T	104	25/35	0.90	0.12	34,84,134,140	0
33	CA	f	104	1/1	0.91	0.06	104,104,104,104	0
35	LMG	a	415	51/55	0.91	0.10	57,82,99,102	0
35	LMG	c	522	51/55	0.91	0.09	51,86,112,114	0
32	UNL	X	101	18/-	0.91	0.11	56,75,101,102	0
32	UNL	d	410	17/-	0.91	0.11	48,69,97,101	0
28	GOL	B	636	6/6	0.91	0.10	48,57,65,65	0
35	LMG	C	501	51/55	0.91	0.09	49,84,108,116	0
35	LMG	C	520	51/55	0.91	0.09	50,77,108,118	0
28	GOL	B	626	6/6	0.91	0.10	44,52,59,85	0
24	CLA	C	514	65/65	0.92	0.08	51,65,99,109	0
24	CLA	c	517	65/65	0.92	0.08	57,80,96,104	0
22	CL	U	201	1/1	0.92	0.11	92,92,92,92	0
28	GOL	b	605	6/6	0.92	0.14	67,80,108,110	0
32	UNL	d	413	18/-	0.92	0.11	52,71,109,110	0
28	GOL	v	202	6/6	0.92	0.10	74,80,100,114	0
28	GOL	o	301	6/6	0.93	0.10	71,80,88,106	0
27	SQD	A	411	54/54	0.93	0.09	45,78,99,103	0
28	GOL	B	628	6/6	0.93	0.10	52,71,84,87	0
35	LMG	b	629	51/55	0.93	0.08	41,51,73,89	0
28	GOL	B	629	6/6	0.93	0.12	48,57,63,72	0
24	CLA	B	602	65/65	0.93	0.09	43,60,100,128	0
24	CLA	b	610	65/65	0.93	0.08	43,69,104,133	0
34	HTG	B	632	19/19	0.93	0.08	48,69,99,103	0
28	GOL	A	413	6/6	0.93	0.14	51,54,63,67	0
37	LHG	D	409	49/49	0.93	0.09	36,54,115,128	0
24	CLA	C	507	65/65	0.93	0.08	46,64,107,116	0
28	GOL	f	101	6/6	0.93	0.08	76,84,86,91	0
24	CLA	c	510	65/65	0.94	0.07	44,63,92,115	0
24	CLA	C	505	65/65	0.94	0.07	34,48,82,94	0
26	BCR	C	515	40/40	0.94	0.07	49,65,78,83	0
35	LMG	J	101	51/55	0.94	0.10	38,58,111,127	0
35	LMG	M	101	51/55	0.94	0.07	35,52,78,95	0
28	GOL	v	203	6/6	0.94	0.10	47,53,61,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	D	404	40/40	0.94	0.07	38,51,93,99	0
27	SQD	a	414	54/54	0.94	0.08	49,79,106,110	0
26	BCR	b	627	40/40	0.94	0.06	31,41,60,69	0
26	BCR	c	527	40/40	0.94	0.08	57,74,86,89	0
35	LMG	j	101	51/55	0.94	0.08	46,58,105,117	0
26	BCR	d	405	40/40	0.94	0.07	40,55,77,83	0
26	BCR	t	101	40/40	0.94	0.06	31,46,62,64	0
32	UNL	D	410	17/-	0.94	0.08	37,68,83,91	0
26	BCR	y	101	40/40	0.94	0.07	44,61,74,84	0
23	BCT	a	418	4/4	0.94	0.08	60,63,70,83	0
24	CLA	b	625	65/65	0.94	0.08	35,54,102,112	0
24	CLA	C	508	65/65	0.95	0.07	42,54,68,76	0
28	GOL	B	631	6/6	0.95	0.08	40,73,74,83	0
26	BCR	H	101	40/40	0.95	0.06	36,51,67,73	0
26	BCR	K	101	40/40	0.95	0.07	43,55,63,69	0
28	GOL	F	101	6/6	0.95	0.07	70,74,77,77	0
26	BCR	T	103	40/40	0.95	0.06	28,47,64,68	0
26	BCR	Y	101	40/40	0.95	0.07	44,60,69,71	0
34	HTG	b	607	19/19	0.95	0.06	46,75,81,82	0
24	CLA	C	513	65/65	0.95	0.07	46,63,85,92	0
24	CLA	B	615	65/65	0.95	0.07	27,41,91,103	0
28	GOL	V	204	6/6	0.95	0.09	68,81,85,94	0
24	CLA	a	412	65/65	0.95	0.08	32,48,114,123	0
26	BCR	k	101	40/40	0.95	0.07	45,62,73,75	0
24	CLA	B	617	65/65	0.95	0.09	36,52,114,120	0
24	CLA	b	615	65/65	0.95	0.07	31,45,89,103	0
24	CLA	b	618	65/65	0.95	0.06	36,48,60,71	0
24	CLA	b	623	65/65	0.95	0.07	27,41,88,115	0
24	CLA	C	502	65/65	0.95	0.07	38,51,77,91	0
24	CLA	c	507	65/65	0.95	0.07	41,53,65,83	0
24	CLA	c	508	65/65	0.95	0.06	38,55,73,80	0
23	BCT	A	404	4/4	0.95	0.08	52,54,73,86	0
24	CLA	c	511	65/65	0.95	0.07	42,55,70,76	0
24	CLA	c	516	65/65	0.95	0.06	47,65,83,91	0
28	GOL	A	412	6/6	0.95	0.07	43,50,53,61	0
24	CLA	C	506	65/65	0.95	0.07	36,48,70,73	0
24	CLA	d	404	65/65	0.95	0.07	37,52,101,114	0
36	DGD	C	518	62/66	0.95	0.07	37,55,95,113	0
26	BCR	A	410	40/40	0.95	0.06	30,39,45,50	0
36	DGD	H	102	62/66	0.95	0.07	32,49,69,79	0
36	DGD	c	520	62/66	0.95	0.07	38,55,107,128	0
36	DGD	c	521	62/66	0.95	0.07	38,52,94,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	CA	F	104	1/1	0.95	0.05	84,84,84,84	0
37	LHG	D	407	49/49	0.95	0.07	31,49,67,73	0
28	GOL	B	627	6/6	0.95	0.09	47,62,83,99	0
26	BCR	B	620	40/40	0.95	0.06	32,46,59,65	0
37	LHG	d	409	49/49	0.95	0.09	34,55,108,115	0
24	CLA	B	607	65/65	0.95	0.07	31,43,93,105	0
24	CLA	D	403	65/65	0.96	0.07	38,52,104,119	0
24	CLA	B	614	65/65	0.96	0.06	26,37,63,84	0
26	BCR	c	518	40/40	0.96	0.06	40,55,67,69	0
24	CLA	C	509	65/65	0.96	0.06	36,50,110,126	0
24	CLA	c	512	65/65	0.96	0.06	36,49,116,129	0
26	BCR	h	101	40/40	0.96	0.06	42,56,70,74	0
24	CLA	c	513	65/65	0.96	0.07	42,54,74,88	0
24	CLA	c	514	65/65	0.96	0.06	41,53,63,77	0
24	CLA	c	515	65/65	0.96	0.07	43,54,75,87	0
24	CLA	C	510	65/65	0.96	0.07	41,54,76,80	0
24	CLA	b	616	65/65	0.96	0.06	24,36,48,52	0
24	CLA	C	511	65/65	0.96	0.06	39,49,62,82	0
28	GOL	V	202	6/6	0.96	0.08	40,47,51,59	0
28	GOL	V	203	6/6	0.96	0.08	59,61,61,68	0
24	CLA	b	620	65/65	0.96	0.06	28,40,52,59	0
26	BCR	B	619	40/40	0.96	0.05	29,41,56,60	0
36	DGD	C	517	62/66	0.96	0.07	32,47,94,98	0
28	GOL	b	602	6/6	0.96	0.09	56,60,69,93	0
36	DGD	C	519	62/66	0.96	0.06	36,48,73,86	0
31	PL9	D	405	55/55	0.96	0.06	26,38,51,69	0
28	GOL	b	603	6/6	0.96	0.07	47,56,83,87	0
36	DGD	c	519	62/66	0.96	0.06	38,48,98,105	0
24	CLA	b	622	65/65	0.96	0.05	26,39,55,61	0
24	CLA	C	512	65/65	0.96	0.06	41,57,68,83	0
26	BCR	C	516	40/40	0.96	0.05	39,54,64,65	0
36	DGD	h	102	62/66	0.96	0.07	34,50,68,82	0
24	CLA	A	409	65/65	0.96	0.07	33,47,119,128	0
34	HTG	b	601	19/19	0.96	0.07	40,50,74,83	0
24	CLA	c	505	65/65	0.96	0.06	42,55,66,70	0
37	LHG	d	407	49/49	0.96	0.06	37,51,64,71	0
24	CLA	c	506	65/65	0.96	0.06	39,54,67,74	0
24	CLA	C	504	65/65	0.96	0.06	39,50,60,64	0
24	CLA	B	603	65/65	0.97	0.05	33,44,51,54	0
26	BCR	a	413	40/40	0.97	0.05	30,41,52,56	0
26	BCR	b	626	40/40	0.97	0.05	30,42,49,49	0
24	CLA	B	604	65/65	0.97	0.05	34,44,53,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	PL9	d	406	55/55	0.97	0.05	26,38,48,58	0
26	BCR	b	628	40/40	0.97	0.05	39,50,66,77	0
24	CLA	C	503	65/65	0.97	0.05	37,46,61,71	0
24	CLA	a	409	65/65	0.97	0.05	28,35,51,55	0
28	GOL	a	401	6/6	0.97	0.08	51,66,70,85	0
24	CLA	c	509	65/65	0.97	0.06	36,47,70,78	0
24	CLA	a	410	65/65	0.97	0.06	31,41,105,116	0
24	CLA	A	407	65/65	0.97	0.06	28,40,98,118	0
28	GOL	b	604	6/6	0.97	0.07	60,73,79,90	0
24	CLA	B	608	65/65	0.97	0.05	24,36,50,55	0
24	CLA	b	611	65/65	0.97	0.06	33,45,55,59	0
24	CLA	b	612	65/65	0.97	0.05	34,44,57,62	0
24	CLA	b	613	65/65	0.97	0.06	26,38,73,79	0
24	CLA	b	614	65/65	0.97	0.06	29,39,49,58	0
24	CLA	B	609	65/65	0.97	0.05	32,43,56,58	0
24	CLA	d	402	65/65	0.97	0.05	27,35,43,55	0
24	CLA	B	610	65/65	0.97	0.05	34,47,56,66	0
25	PHO	A	408	64/64	0.97	0.05	29,42,52,56	0
25	PHO	D	401	64/64	0.97	0.05	25,35,41,43	0
25	PHO	a	411	64/64	0.97	0.04	28,36,44,47	0
25	PHO	d	401	64/64	0.97	0.05	29,42,50,56	0
24	CLA	b	617	65/65	0.97	0.05	34,45,55,58	0
26	BCR	B	618	40/40	0.97	0.04	27,40,47,52	0
34	HTG	B	623	19/19	0.97	0.06	40,54,75,76	0
24	CLA	B	611	65/65	0.97	0.06	36,47,54,68	0
24	CLA	b	619	65/65	0.97	0.06	36,46,56,60	0
24	CLA	B	613	65/65	0.97	0.05	28,38,48,55	0
37	LHG	D	408	49/49	0.97	0.06	27,42,64,86	0
24	CLA	b	621	65/65	0.97	0.05	29,42,50,56	0
22	CL	v	204	1/1	0.97	0.06	94,94,94,94	0
37	LHG	L	101	49/49	0.97	0.06	31,44,56,61	0
24	CLA	A	405	65/65	0.97	0.05	25,33,49,67	0
37	LHG	d	408	49/49	0.97	0.06	32,41,57,86	0
24	CLA	b	624	65/65	0.97	0.05	34,46,60,73	0
24	CLA	B	616	65/65	0.97	0.06	34,47,65,76	0
37	LHG	l	101	49/49	0.97	0.06	37,46,58,66	0
38	HEM	e	103	43/43	0.97	0.09	55,78,123,153	0
24	CLA	B	612	65/65	0.98	0.05	26,37,51,59	0
28	GOL	c	501	6/6	0.98	0.05	43,45,47,48	0
28	GOL	C	526	6/6	0.98	0.05	33,42,47,49	0
22	CL	A	403	1/1	0.98	0.07	35,35,35,35	0
24	CLA	B	605	65/65	0.98	0.05	26,37,70,75	0

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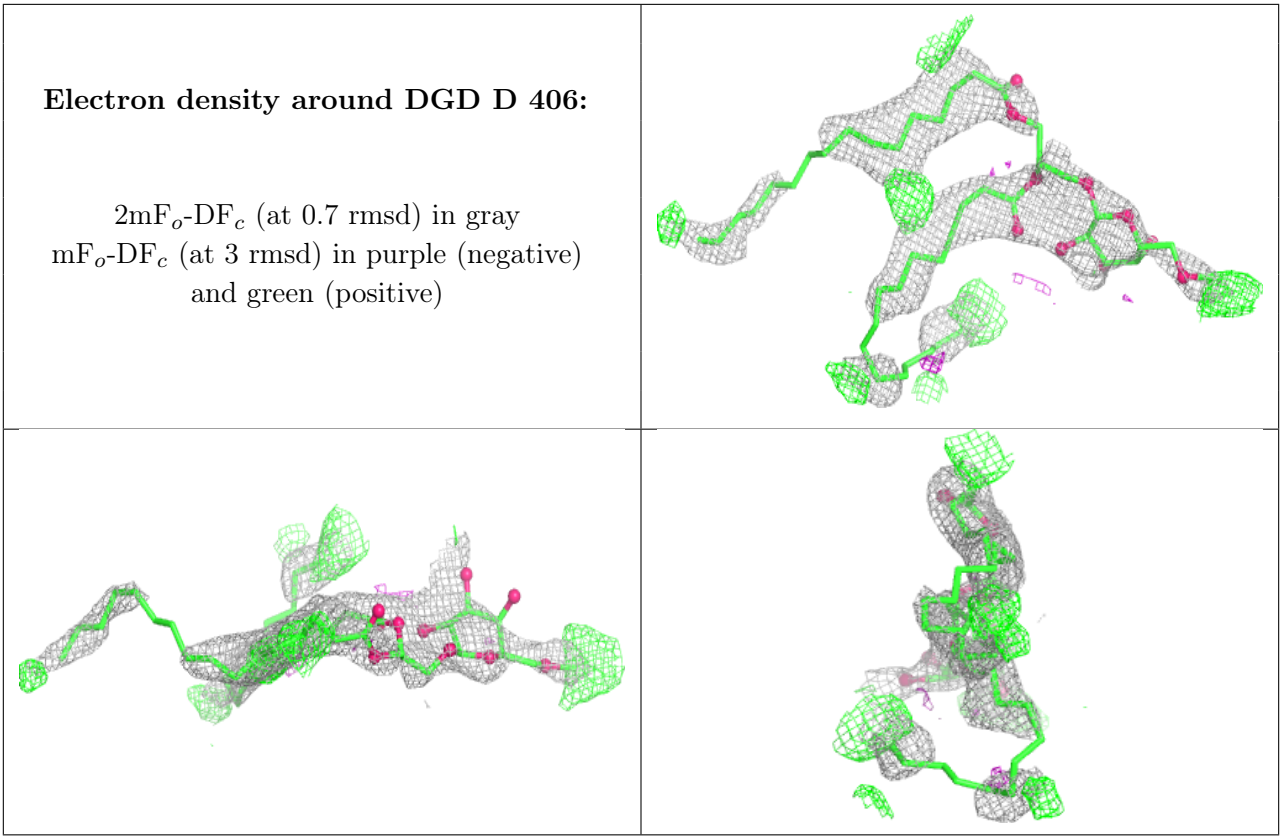
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	d	403	65/65	0.98	0.05	27,38,59,62	0
24	CLA	B	606	65/65	0.98	0.05	29,40,53,64	0
24	CLA	D	402	65/65	0.98	0.05	24,35,54,58	0
38	HEM	E	102	43/43	0.98	0.06	44,64,81,93	0
24	CLA	A	406	65/65	0.98	0.04	24,34,44,58	0
39	MG	j	103	1/1	0.98	0.07	57,57,57,57	0
33	CA	c	503	1/1	0.99	0.08	66,66,66,66	0
33	CA	c	504	1/1	0.99	0.03	74,74,74,74	0
33	CA	C	527	1/1	0.99	0.07	67,67,67,67	0
33	CA	o	302	1/1	0.99	0.04	91,91,91,91	0
22	CL	a	408	1/1	0.99	0.03	41,41,41,41	0
33	CA	O	302	1/1	0.99	0.02	84,84,84,84	0
39	MG	J	103	1/1	0.99	0.02	53,53,53,53	0
22	CL	a	407	1/1	0.99	0.05	36,36,36,36	0
40	HEC	V	205	43/43	0.99	0.04	35,41,50,53	0
40	HEC	v	205	43/43	0.99	0.05	42,52,61,62	0
22	CL	A	402	1/1	1.00	0.02	32,32,32,32	0
21	FE2	A	401	1/1	1.00	0.04	51,51,51,51	0
30	OEX	A	417	10/10	1.00	0.03	33,36,47,71	0
30	OEX	a	417	10/10	1.00	0.03	32,40,64,67	0
21	FE2	a	406	1/1	1.00	0.06	49,49,49,49	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.

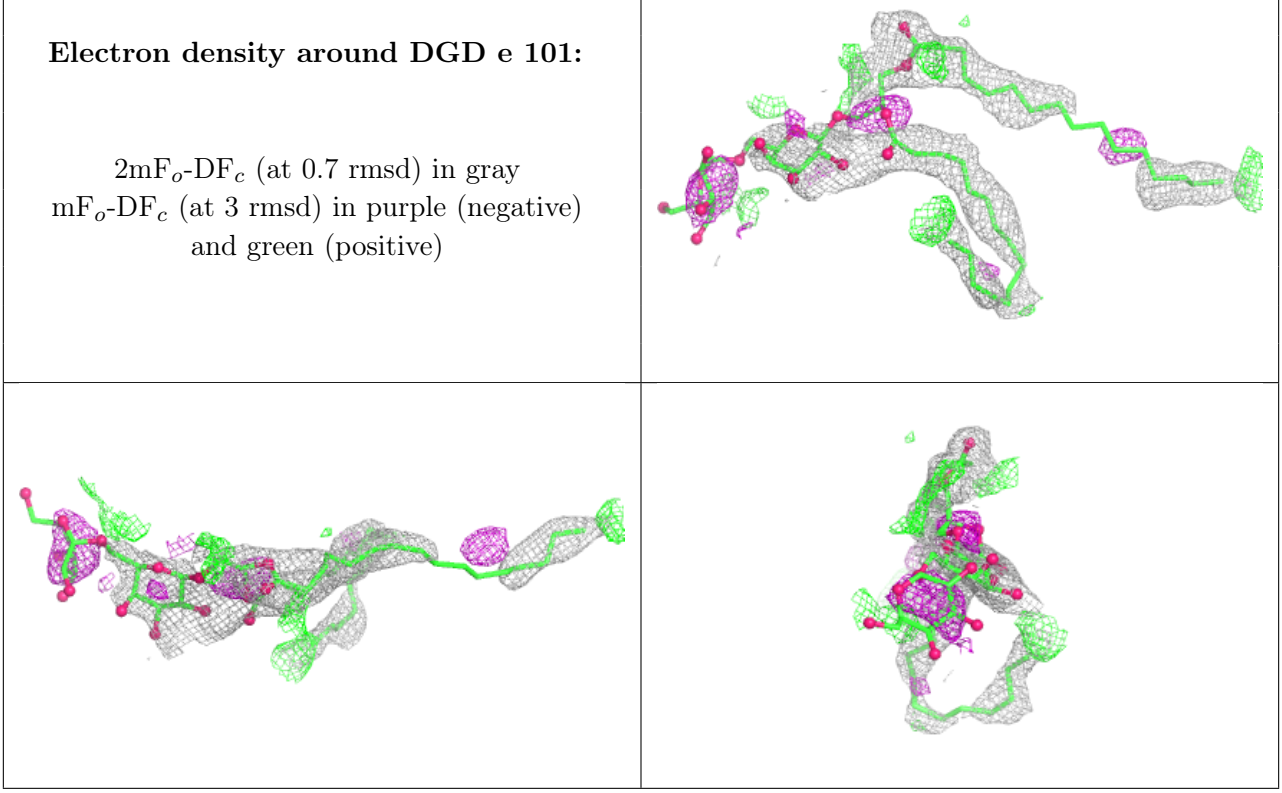
Electron density around DGD D 406:

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



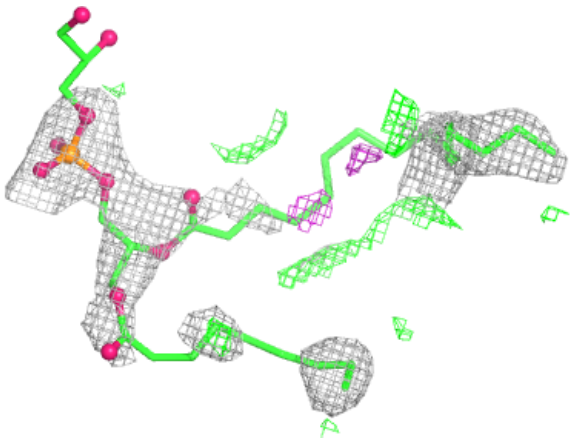
Electron density around DGD e 101:

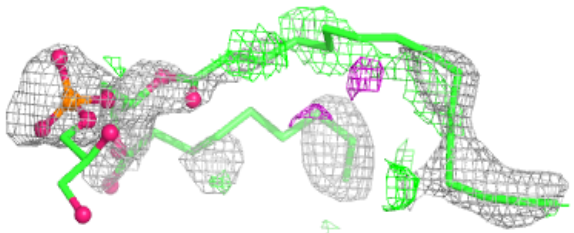
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

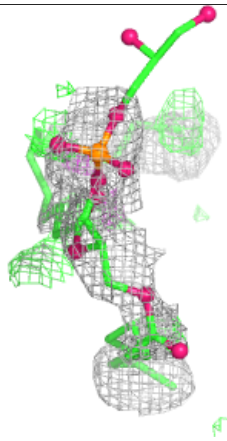


Electron density around LHG e 102:

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

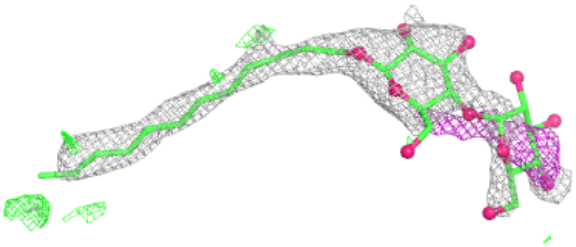


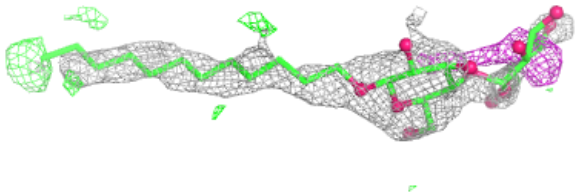


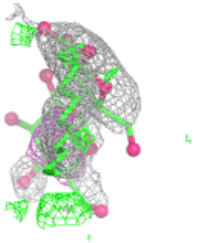


Electron density around LMT F 102:

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

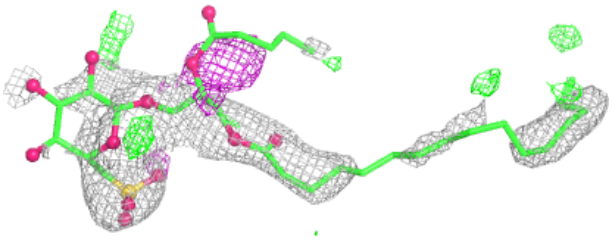


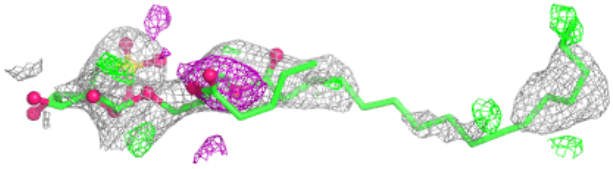


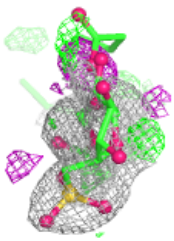


Electron density around SQD f 102:

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

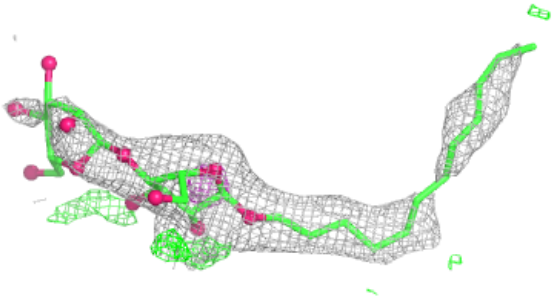


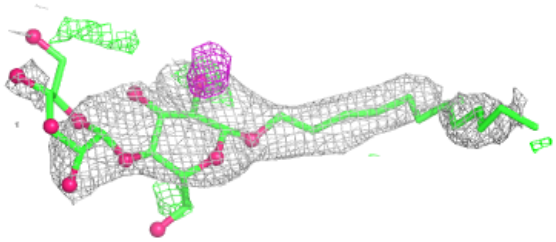


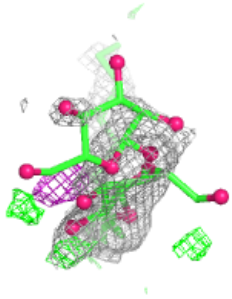


Electron density around LMT C 522:

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

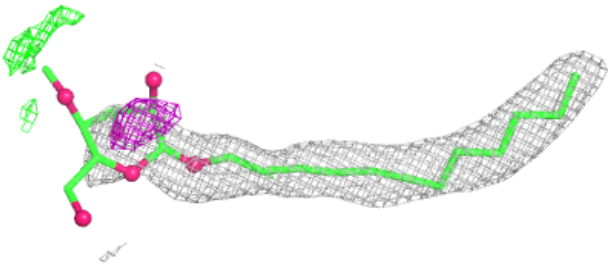


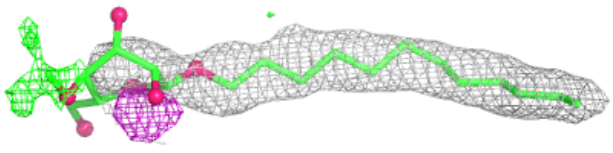


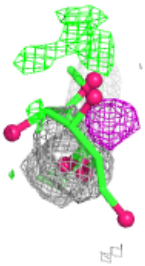


Electron density around LMT b 630:

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

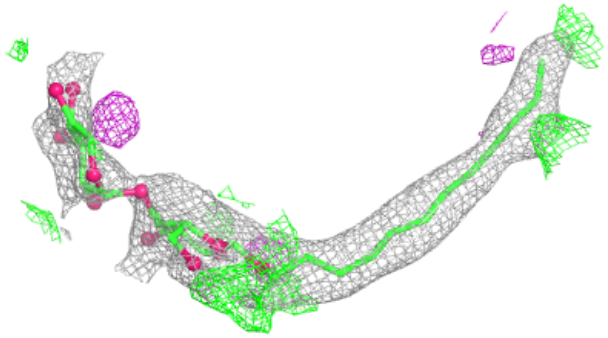


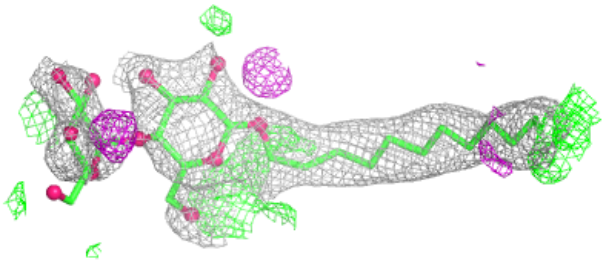


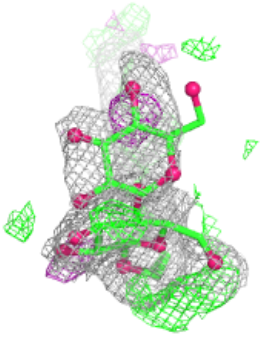


Electron density around LMT M 104:

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

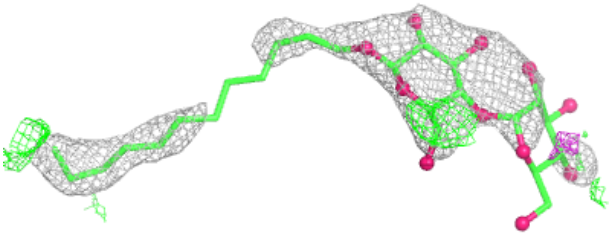


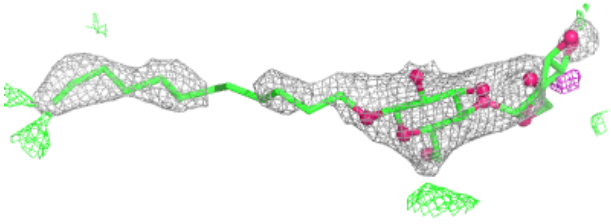


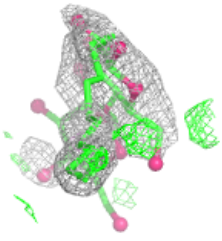


Electron density around LMT f 103:

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

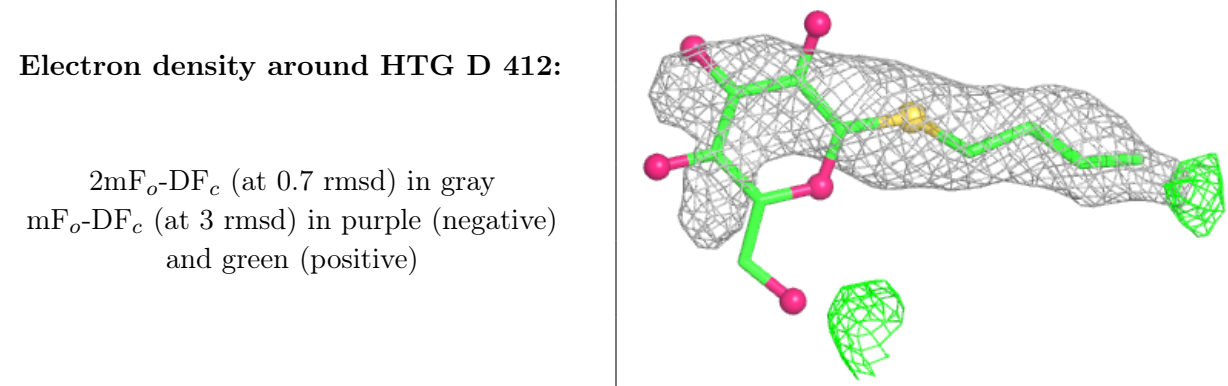






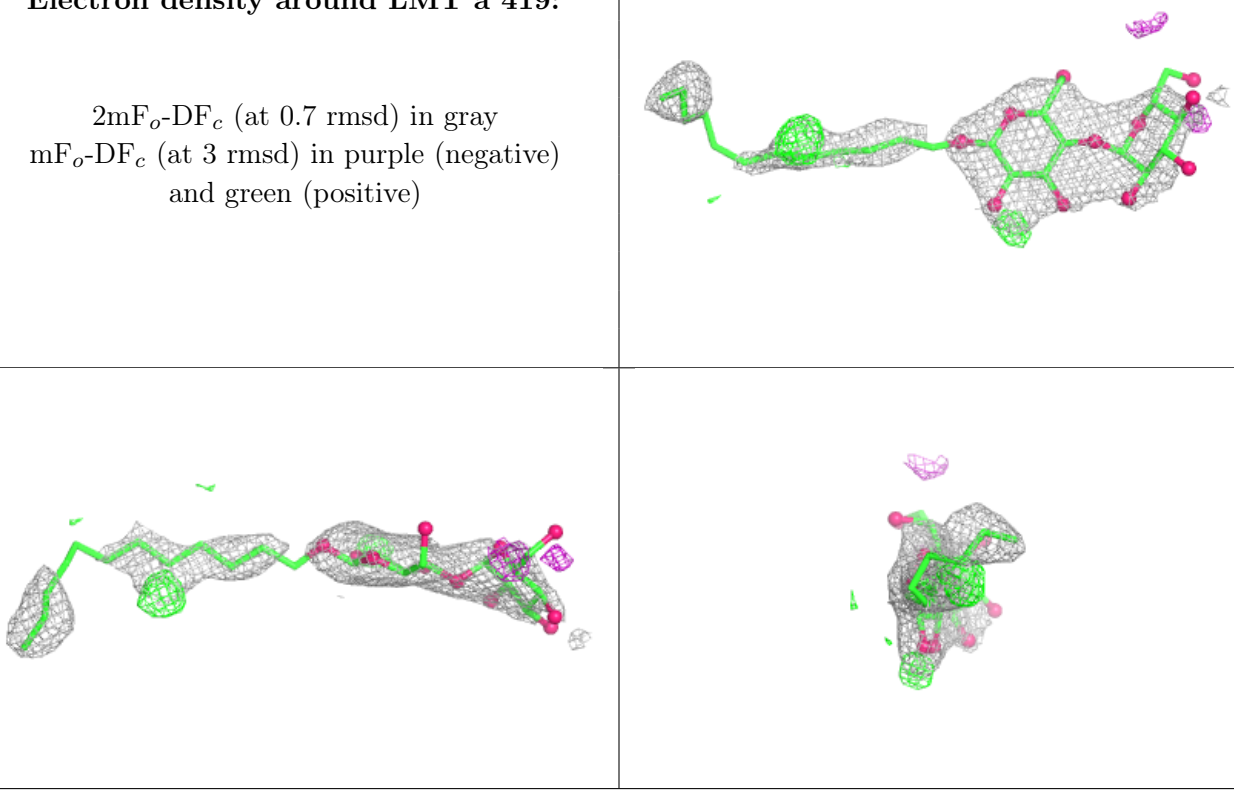
Electron density around HTG D 412:

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



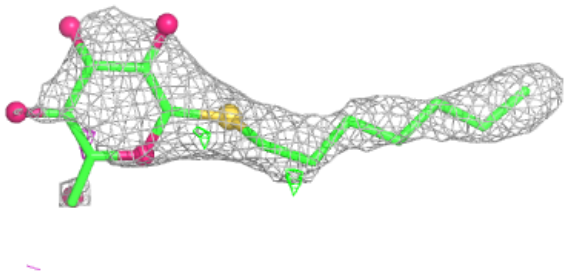
Electron density around LMT a 419:

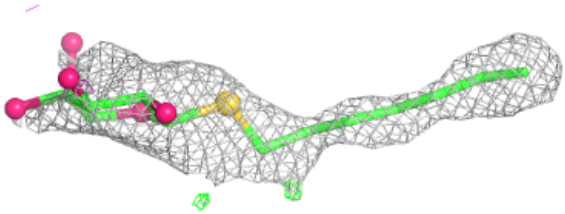
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

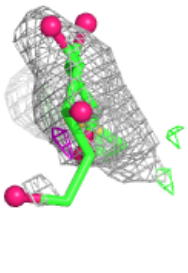


Electron density around HTG c 525:

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

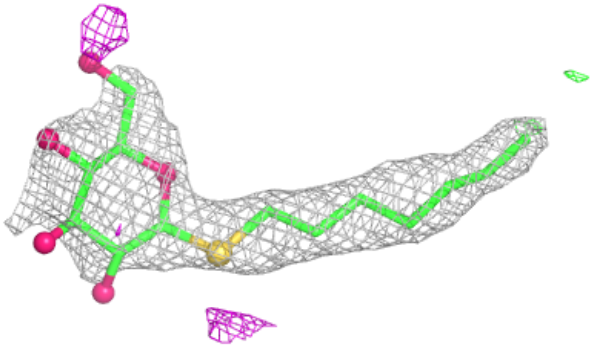


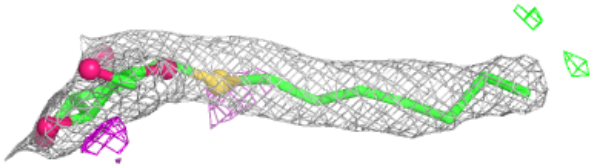


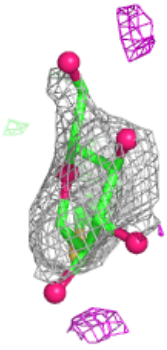


Electron density around HTG B 625:

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

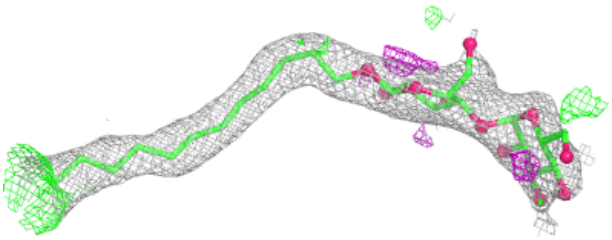


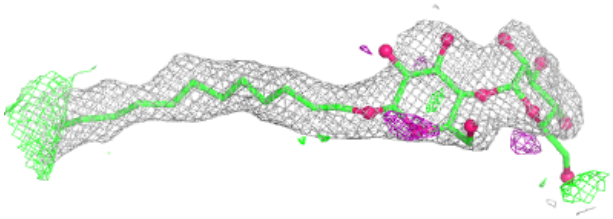


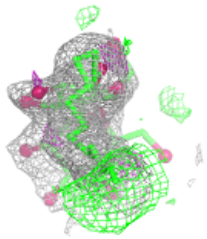


Electron density around LMT A 416:

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

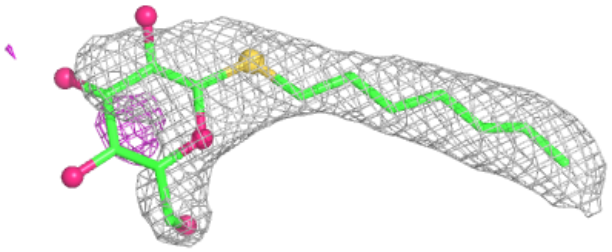


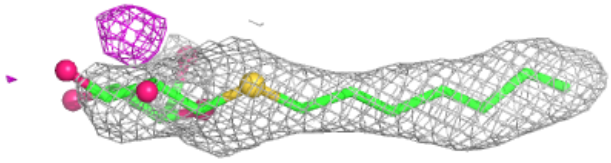


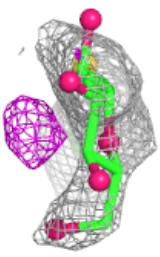


Electron density around HTG b 608:

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

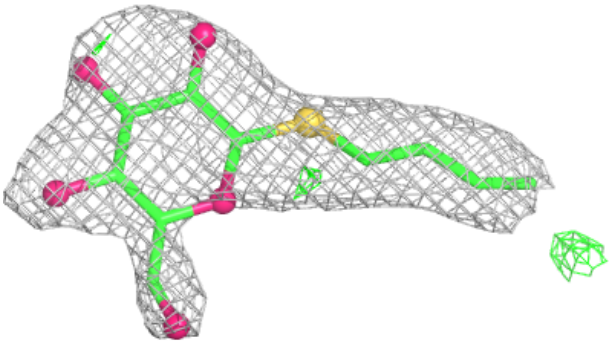


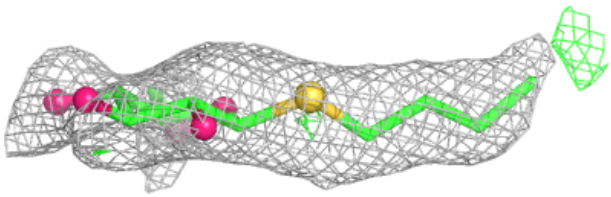


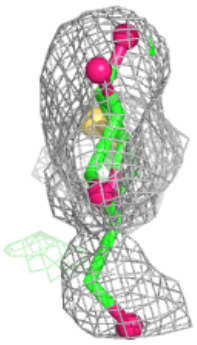


Electron density around HTG d 412:

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

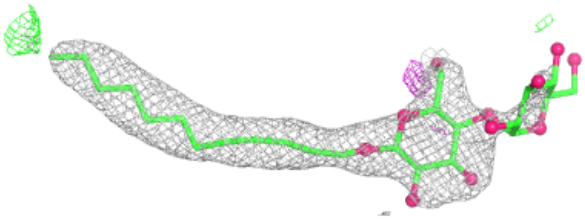


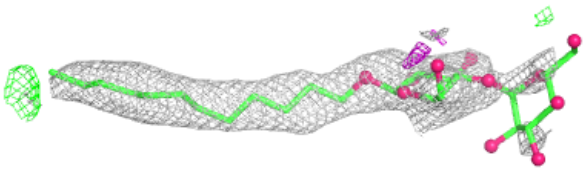


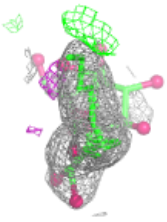


Electron density around LMT B 622:

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

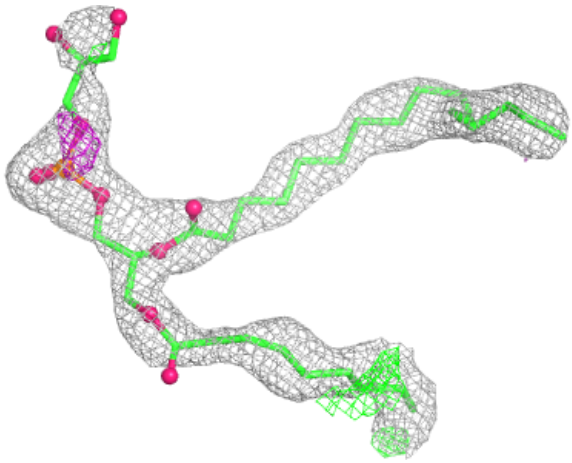


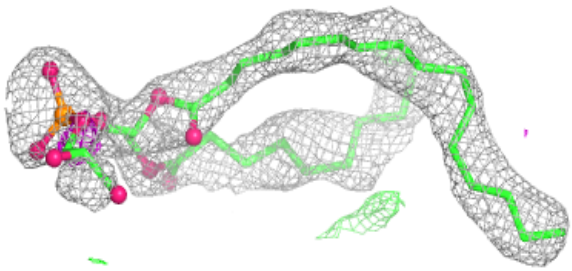




Electron density around LHG E 101:

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

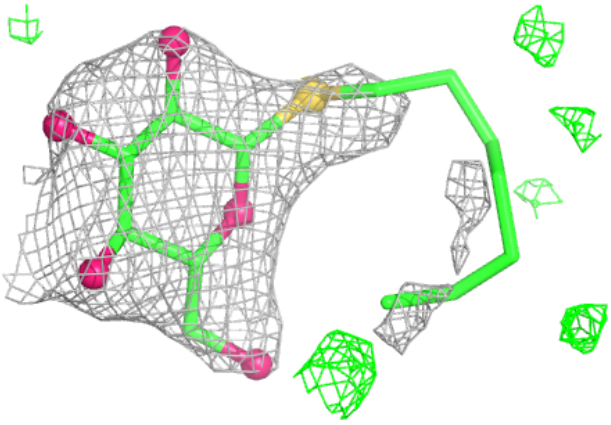


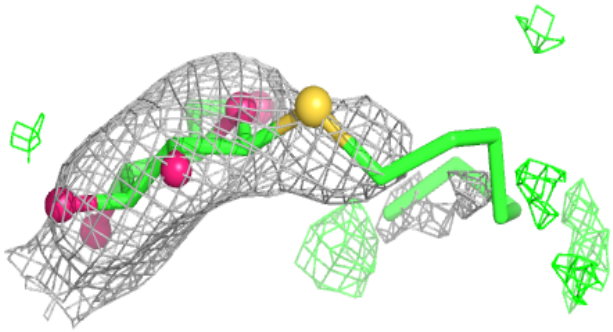


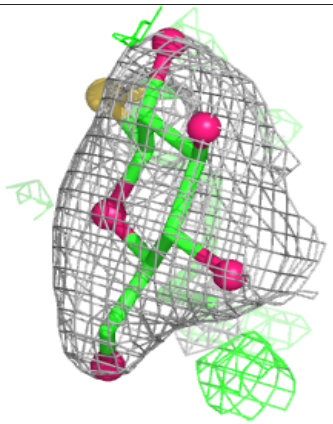


Electron density around HTG V 206:

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

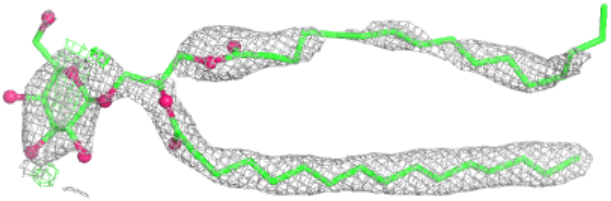


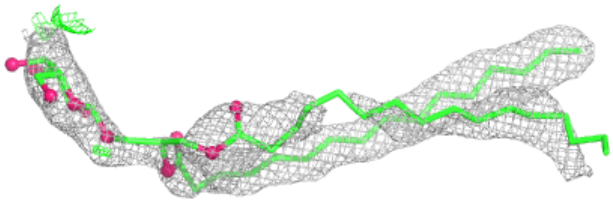


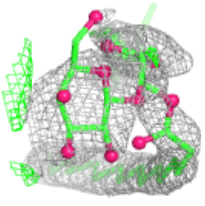


Electron density around LMG c 523:

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

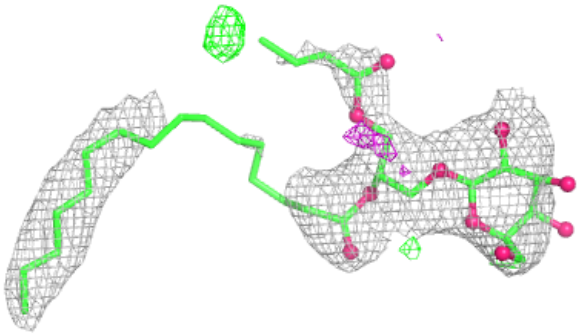


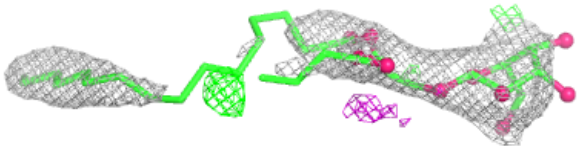




Electron density around LMG z 101:

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

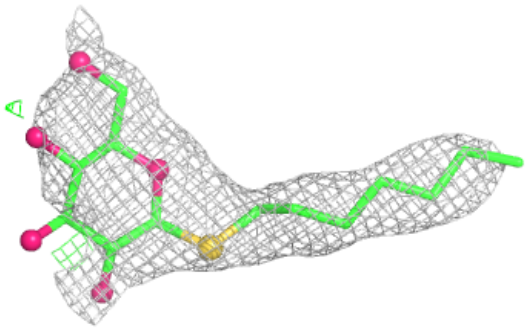


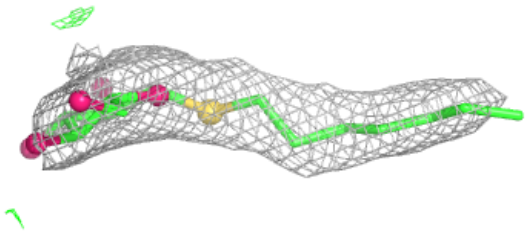


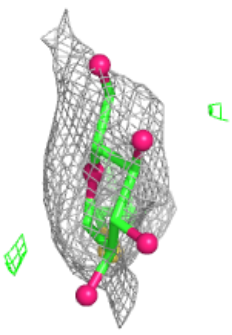


Electron density around HTG b 632:

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

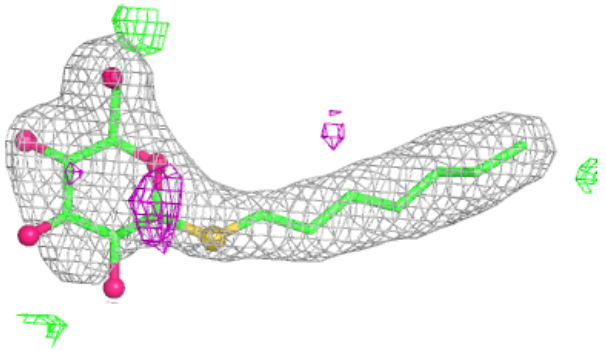


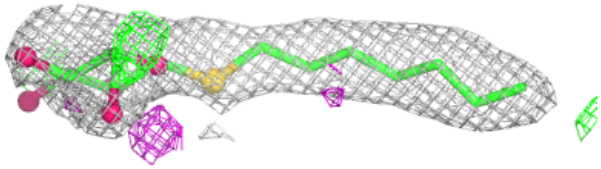


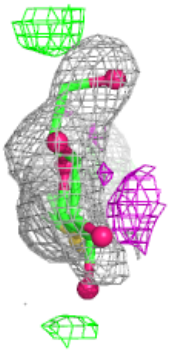


Electron density around HTG B 633:

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

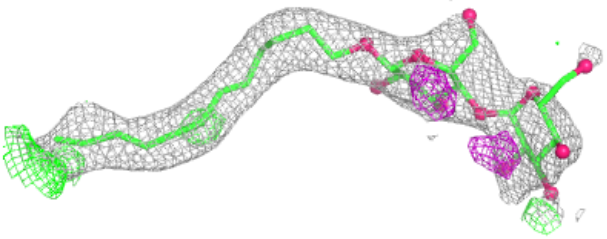


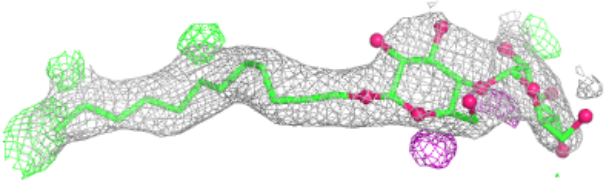


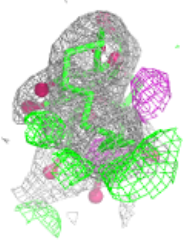


Electron density around LMT a 404:

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

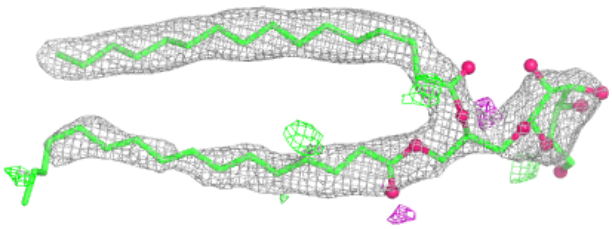


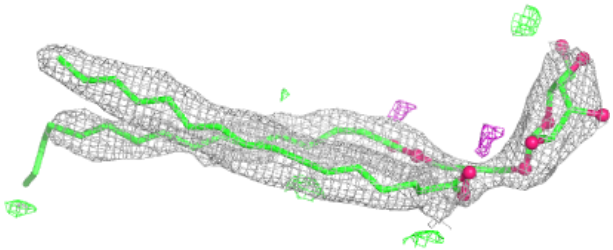


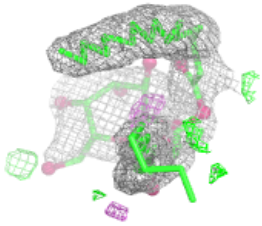


Electron density around LMG C 521:

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

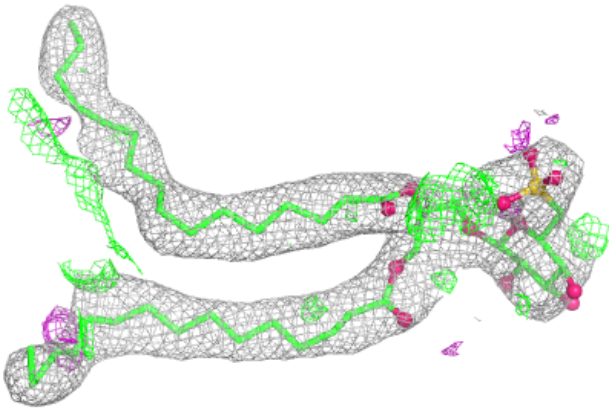


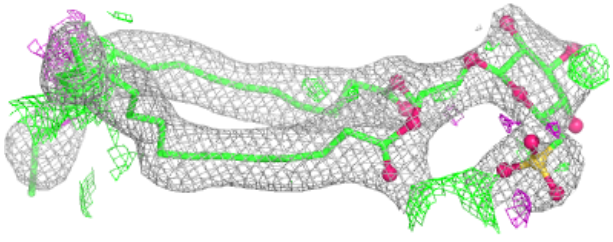


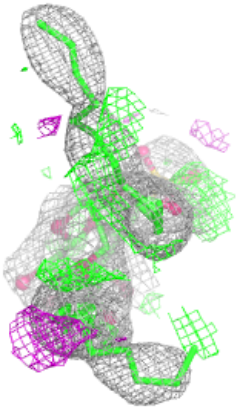


Electron density around SQD B 621:

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

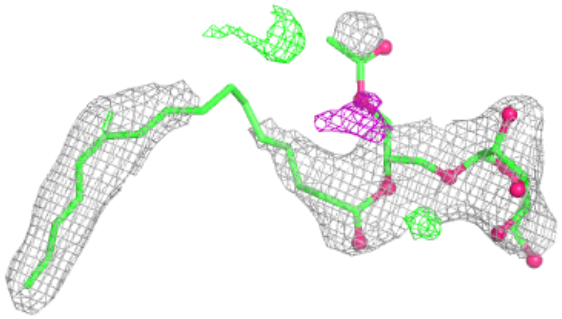


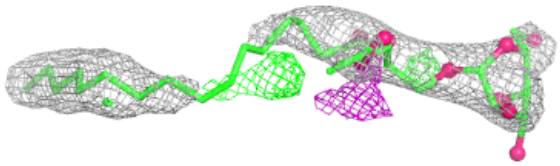


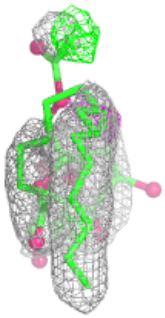


Electron density around LMG Z 101:

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

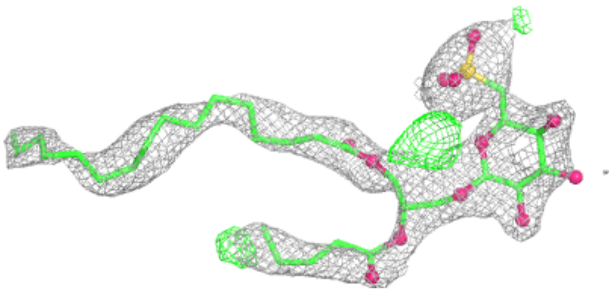


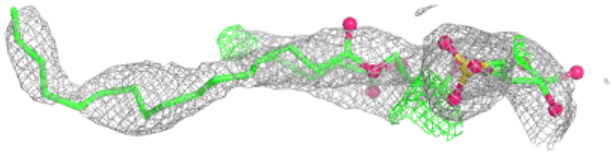


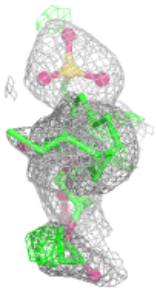


Electron density around SQD F 103:

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

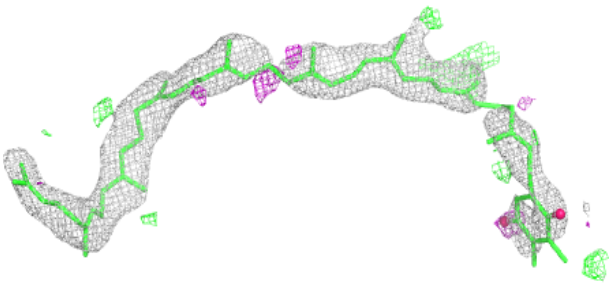


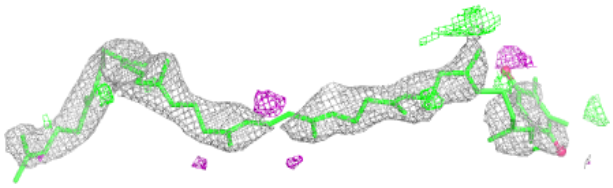


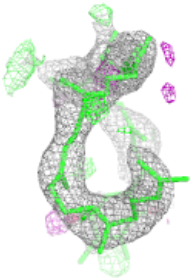


Electron density around PL9 A 418:

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

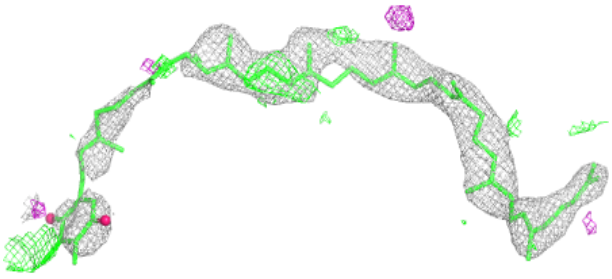


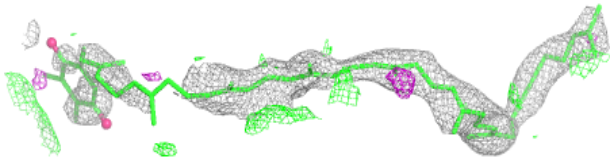


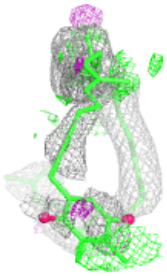


Electron density around PL9 a 416:

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

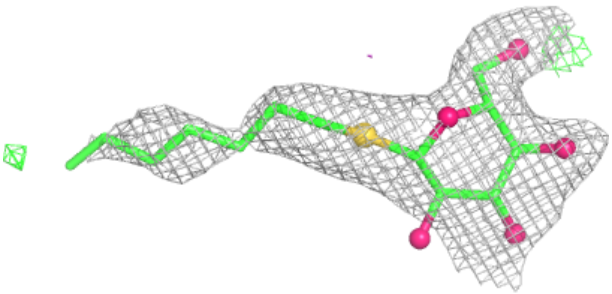


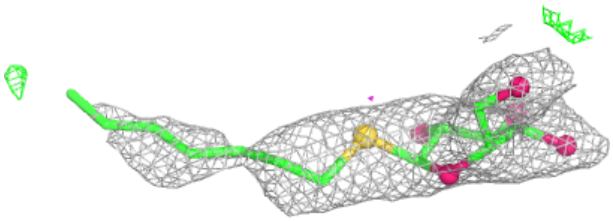


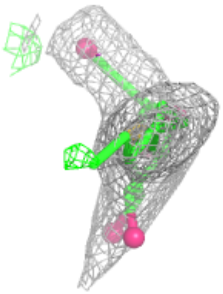


Electron density around HTG C 524:

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

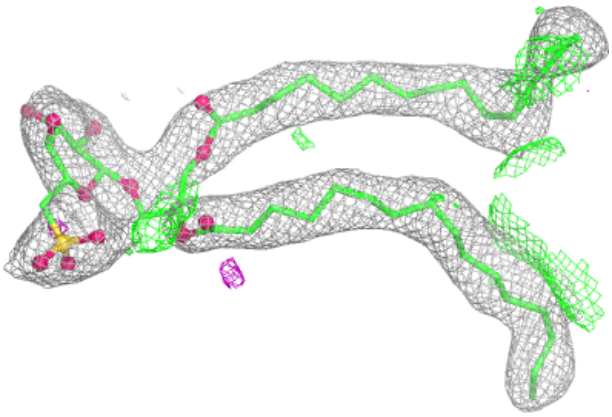


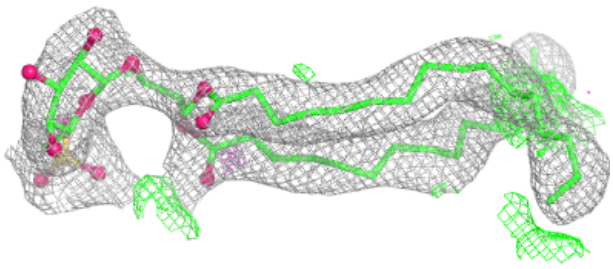


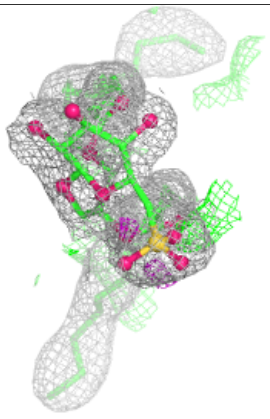


Electron density around SQD L 102:

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

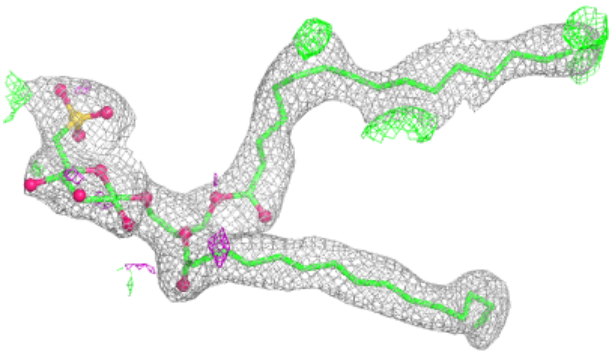


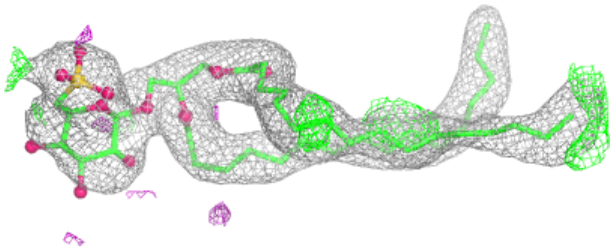


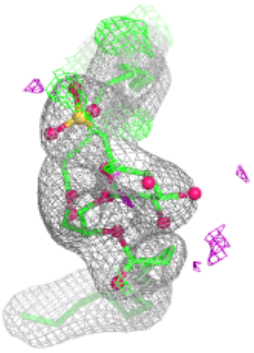


Electron density around SQD a 405:

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

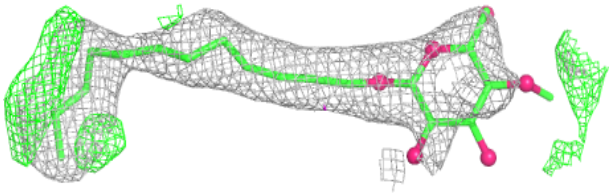


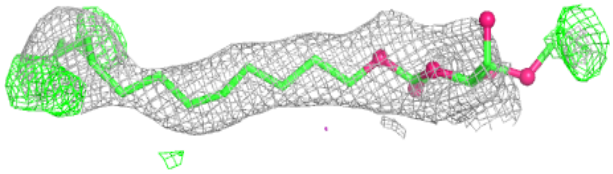


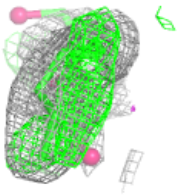


Electron density around LMT B 635:

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

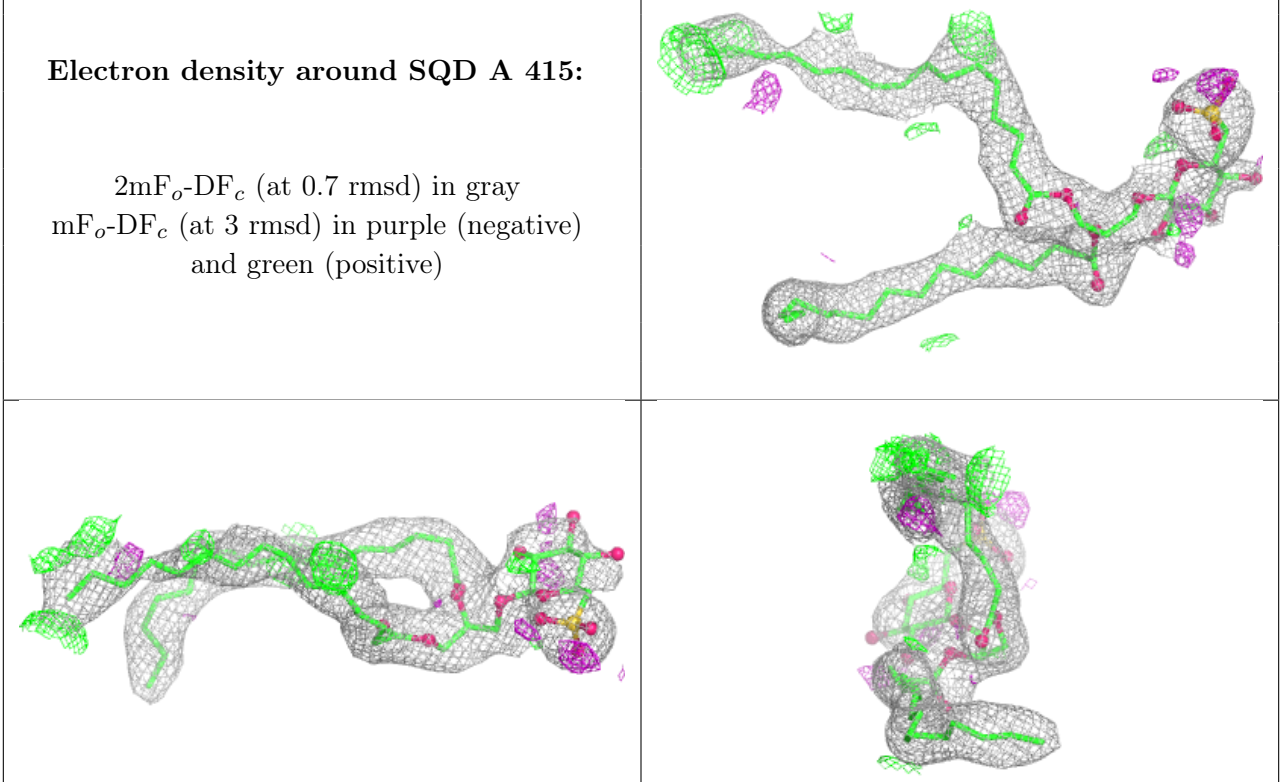






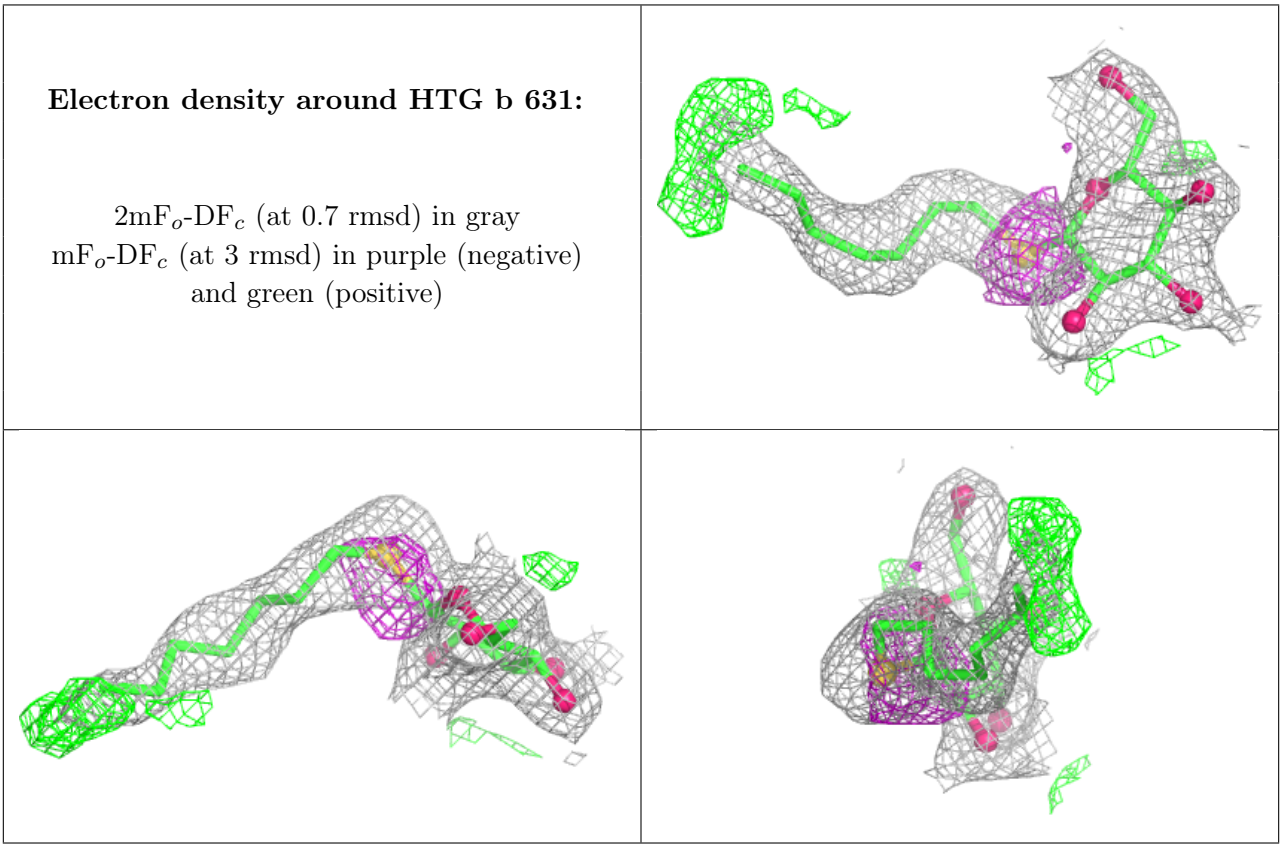
Electron density around SQD A 415:

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



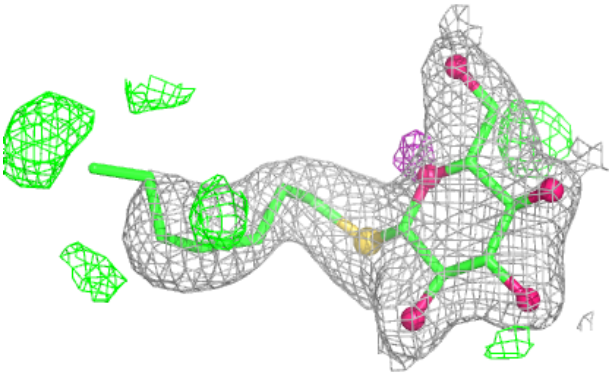
Electron density around HTG b 631:

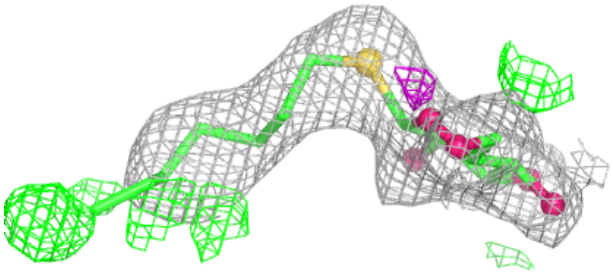
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

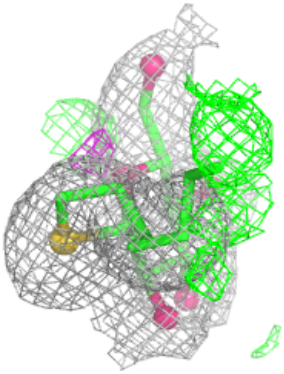


Electron density around HTG B 624:

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

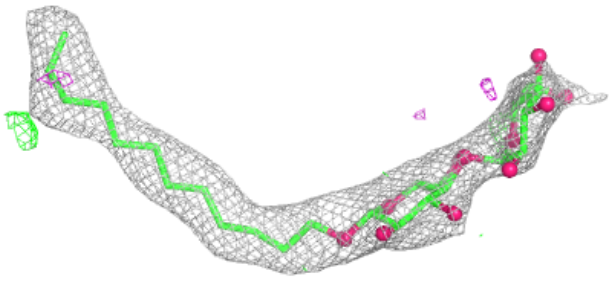


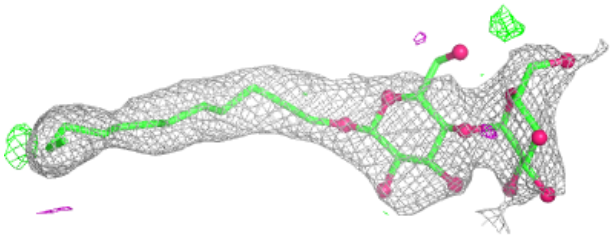


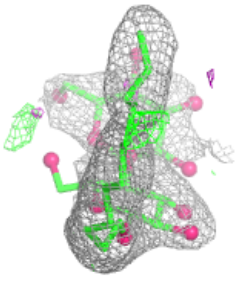


Electron density around LMT m 102:

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

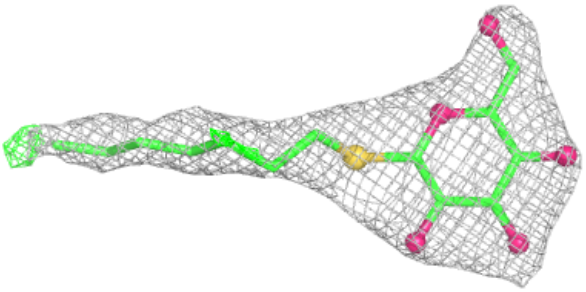


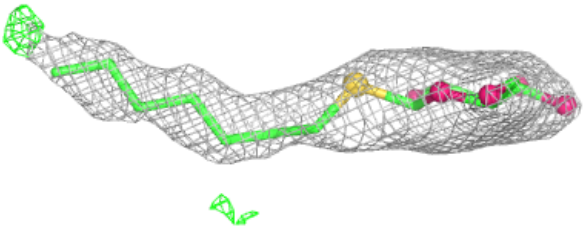


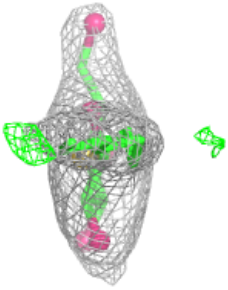


Electron density around HTG c 524:

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

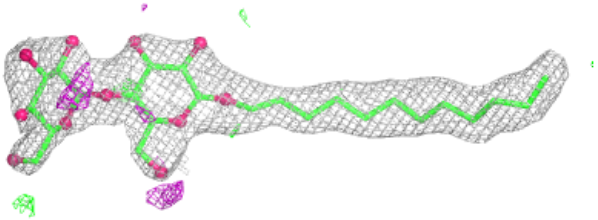


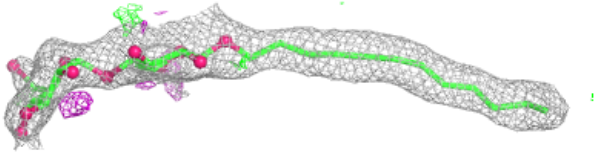




Electron density around LMT M 105:

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

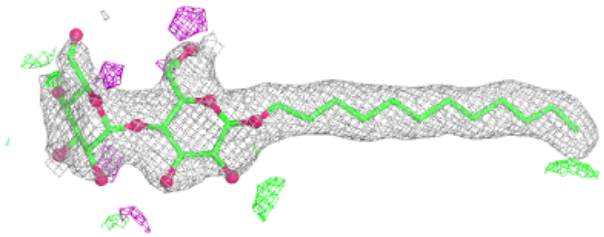


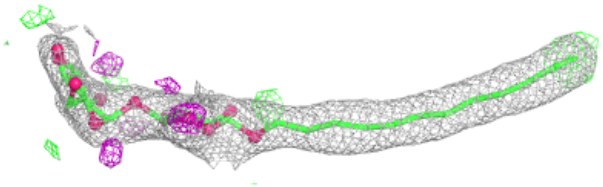




Electron density around LMT M 102:

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

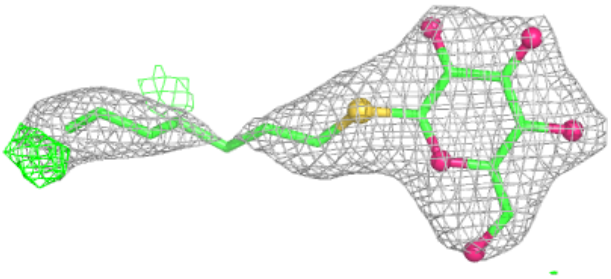


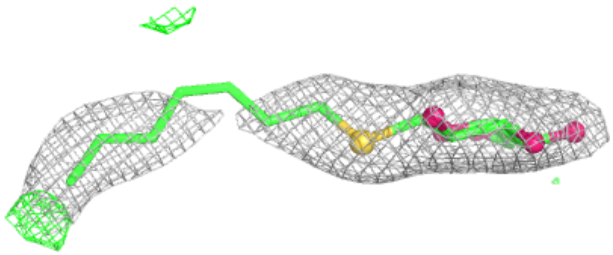


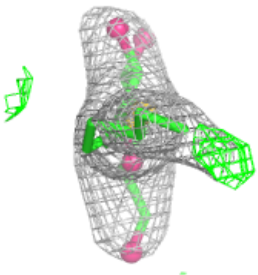


Electron density around HTG C 523:

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

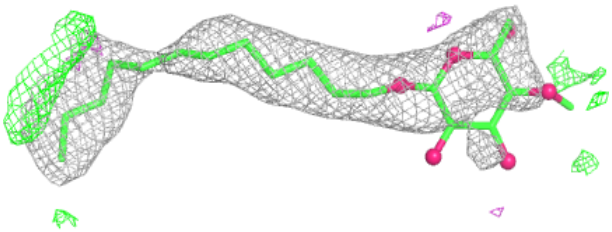


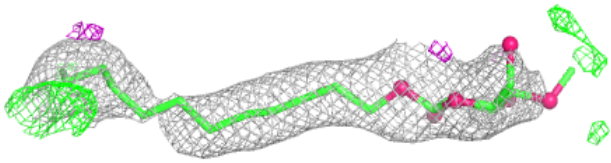


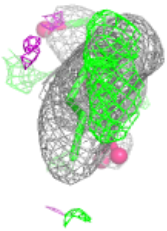


Electron density around LMT T 104:

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

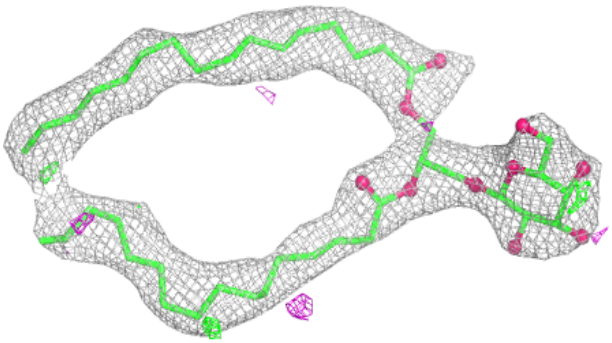


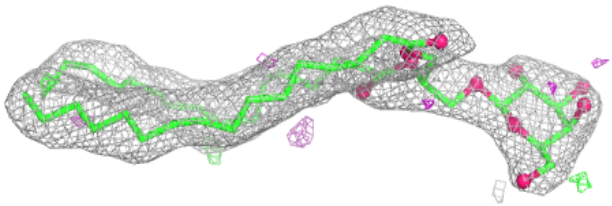


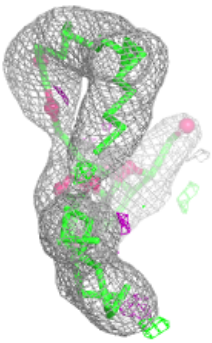


Electron density around LMG a 415:

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

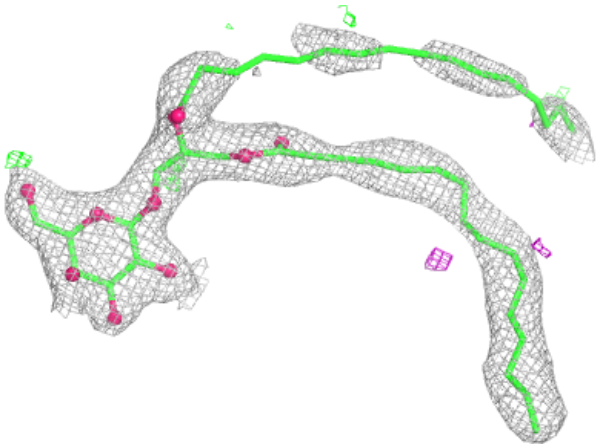


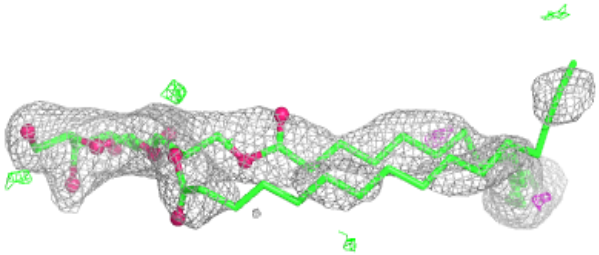


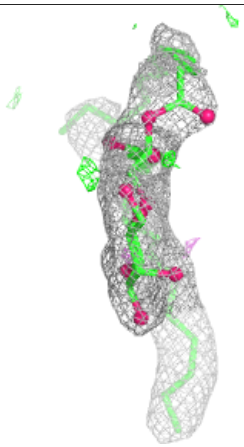


Electron density around LMG c 522:

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

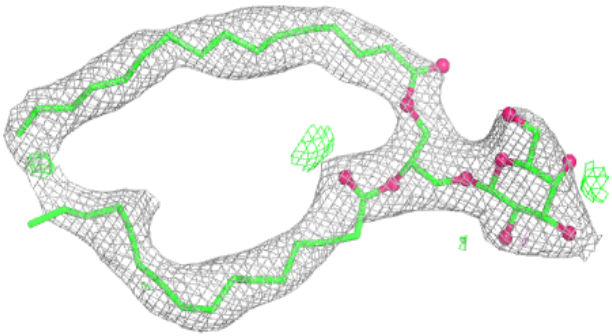


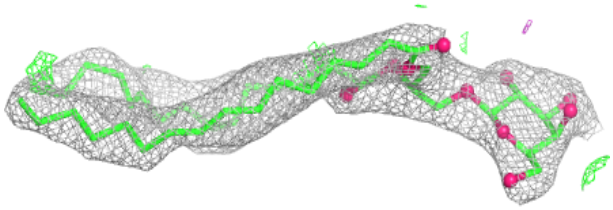


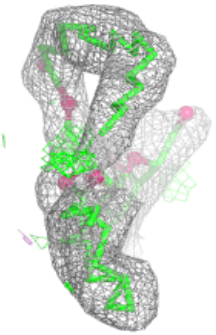


Electron density around LMG C 501:

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

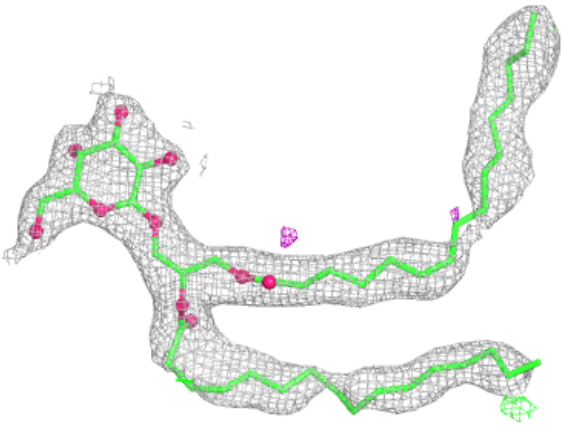


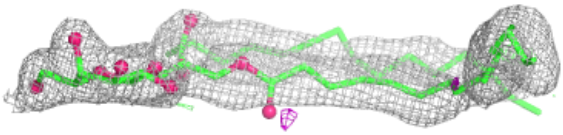


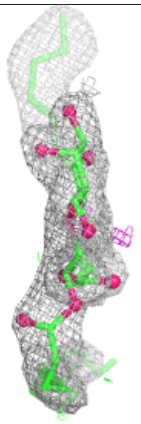


Electron density around LMG C 520:

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

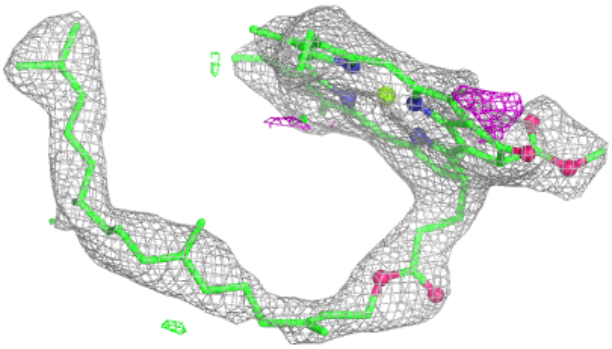


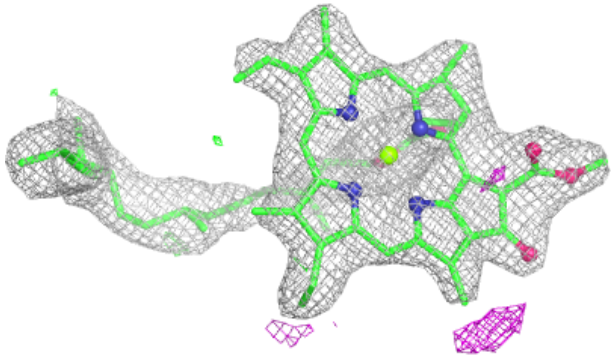


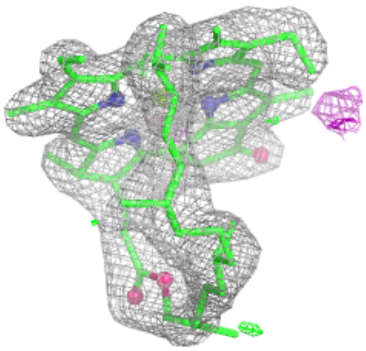


Electron density around CLA C 514:

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

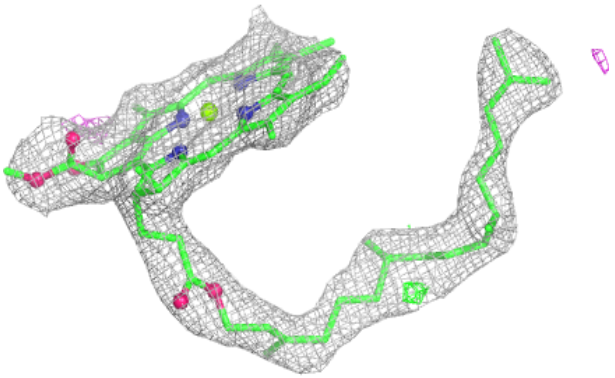


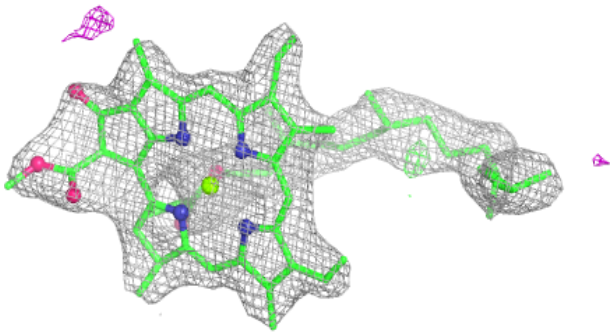


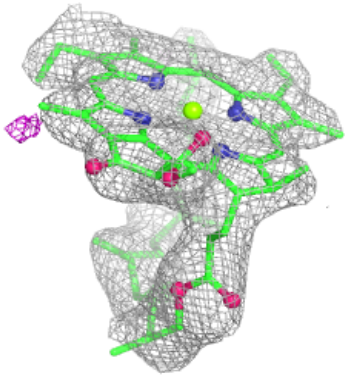


Electron density around CLA c 517:

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

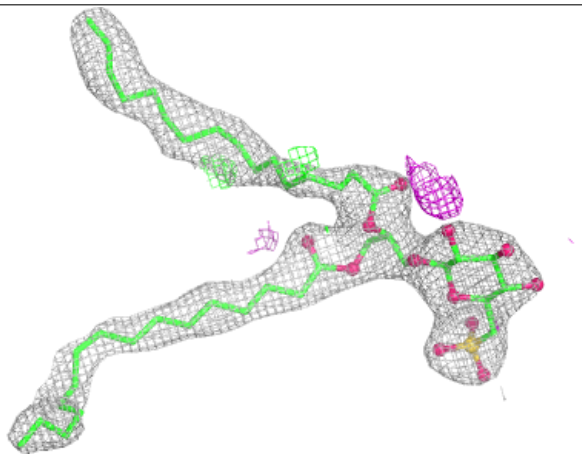


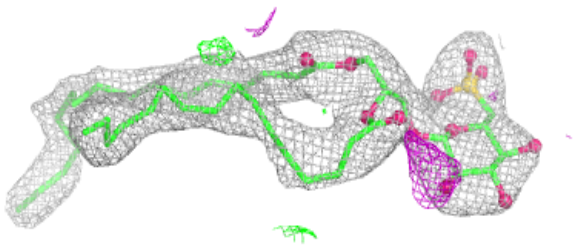


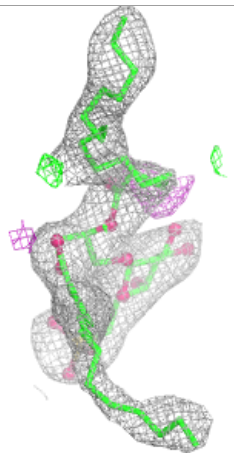


Electron density around SQD A 411:

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

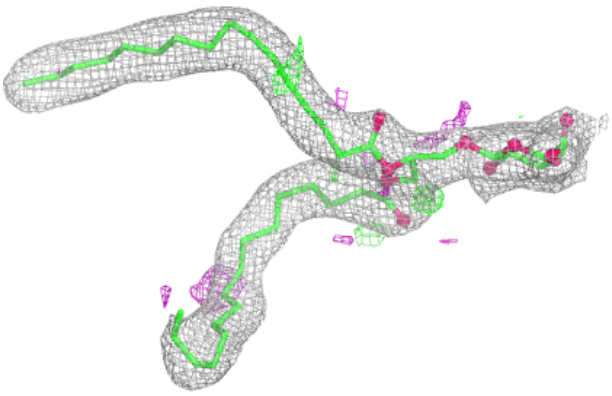


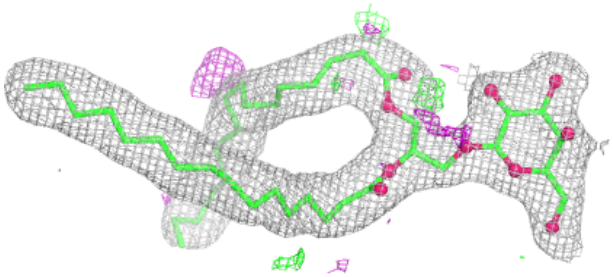


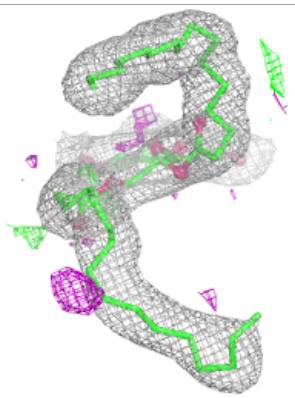


Electron density around LMG b 629:

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

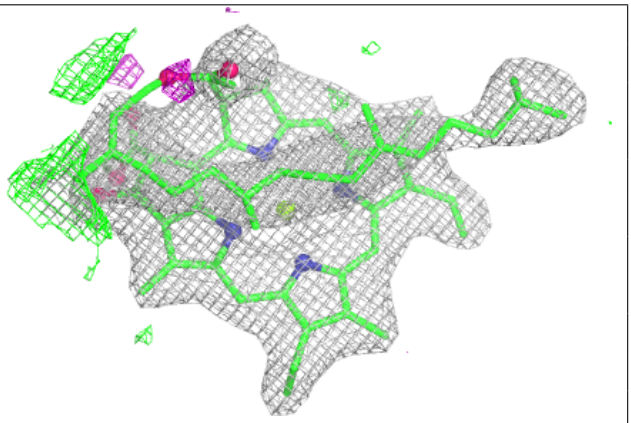


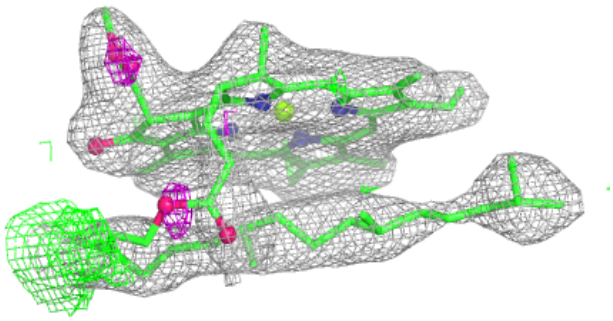


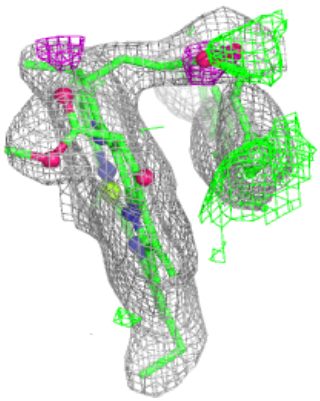


Electron density around CLA B 602:

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

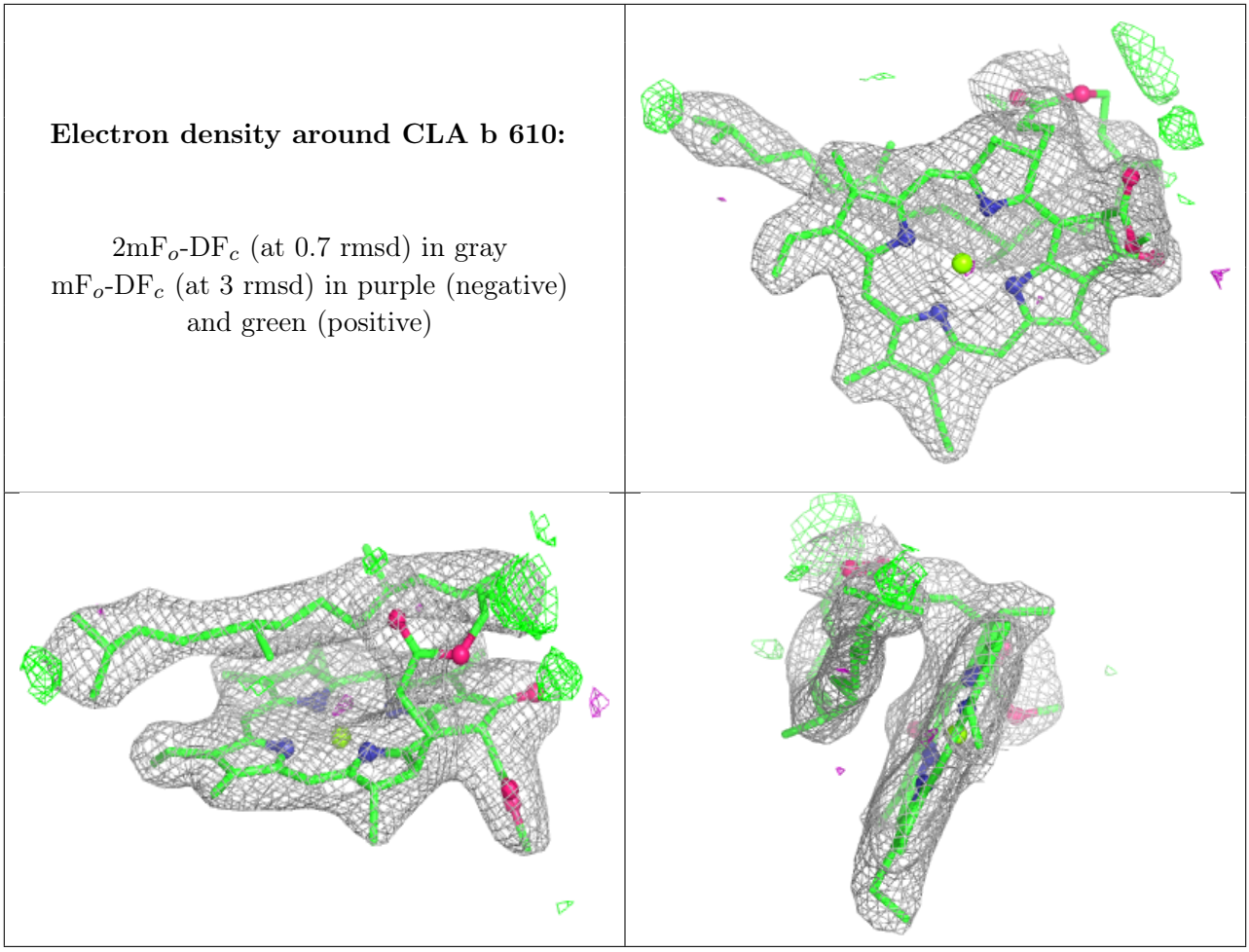






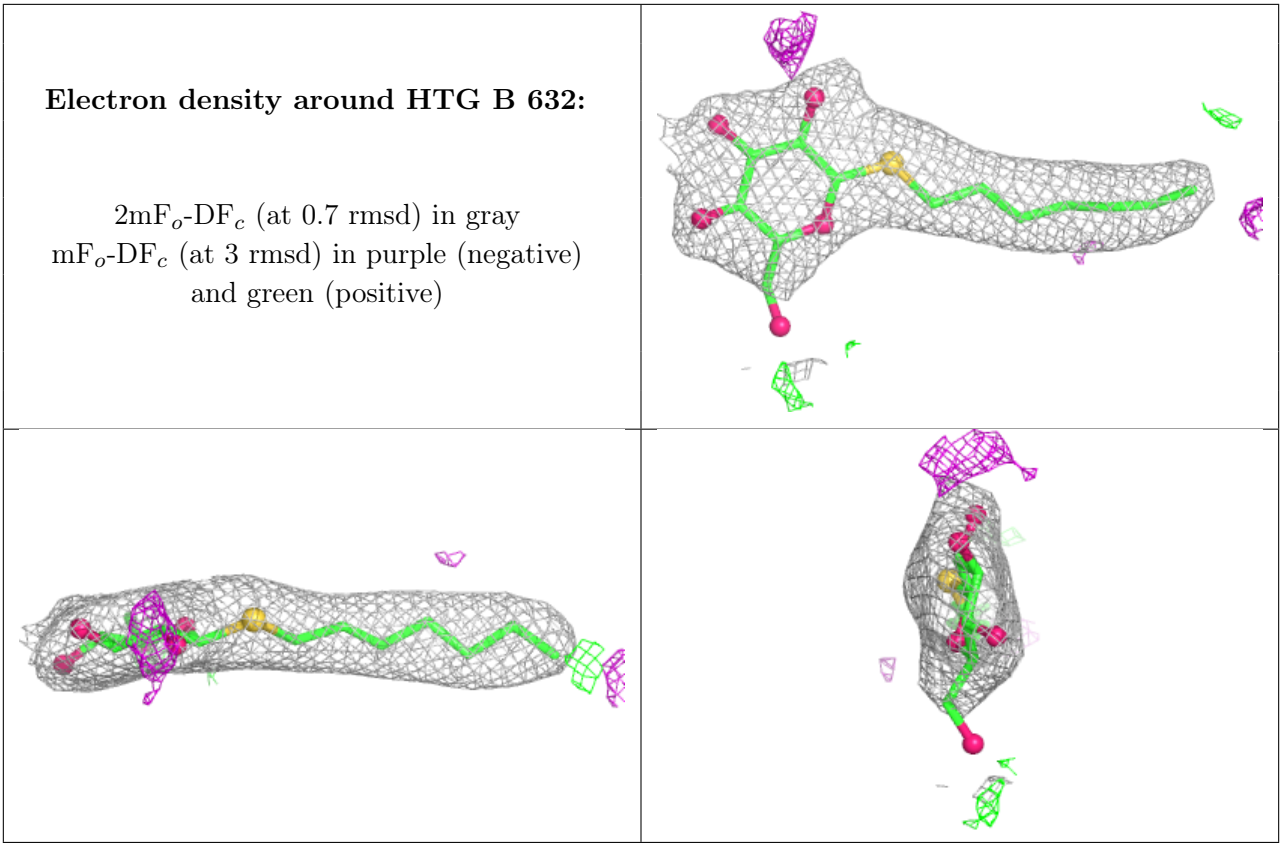
Electron density around CLA b 610:

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



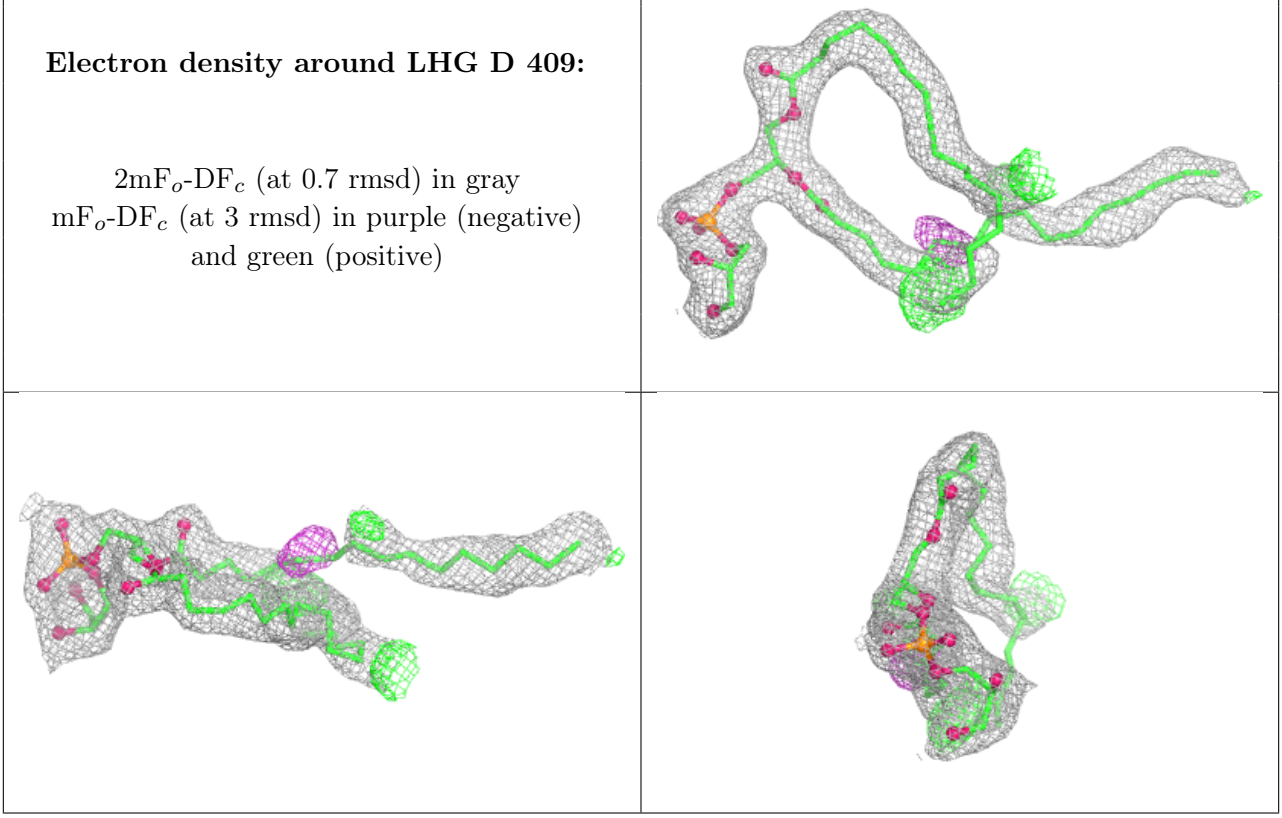
Electron density around HTG B 632:

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



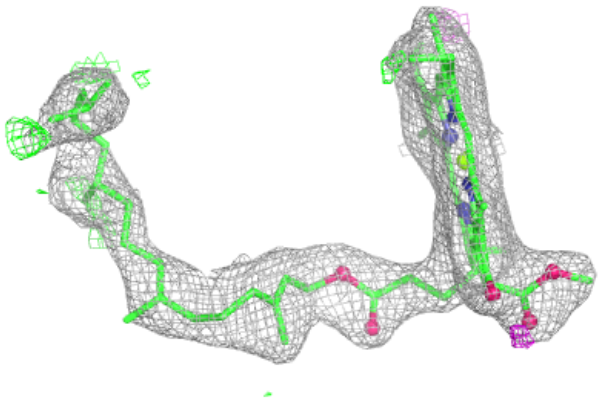
Electron density around LHG D 409:

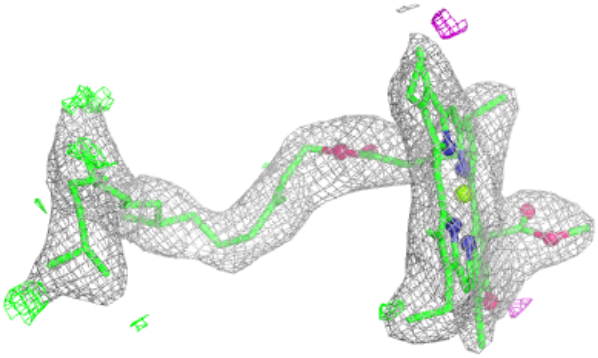
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

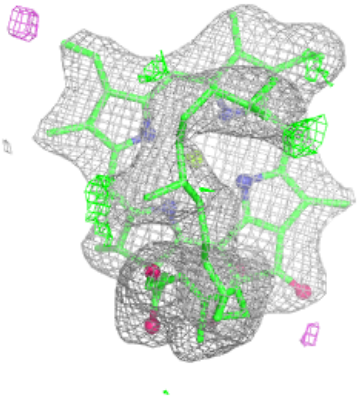


Electron density around CLA C 507:

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

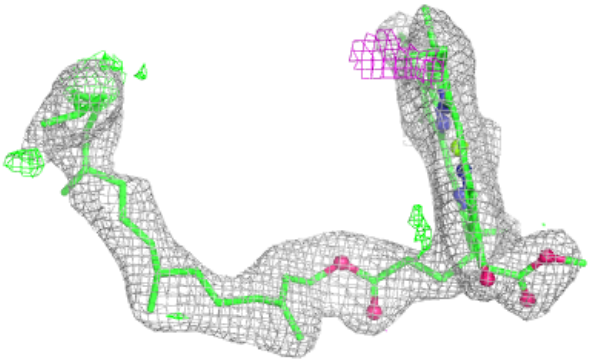


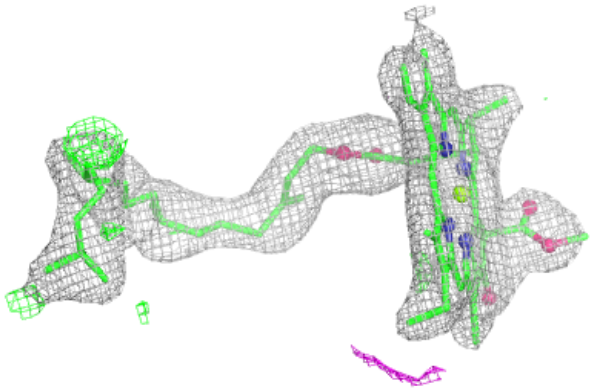


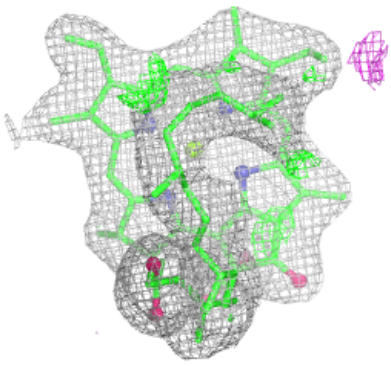


Electron density around CLA c 510:

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

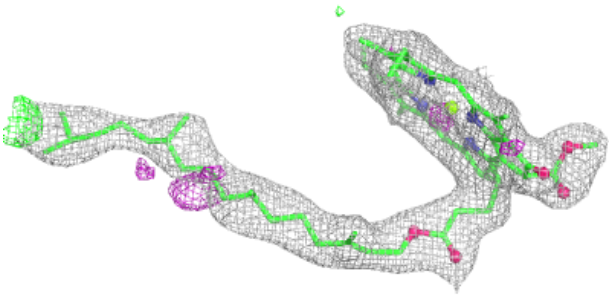


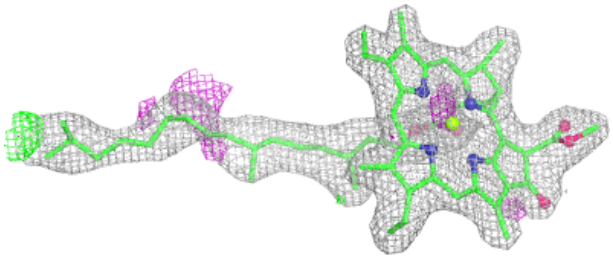


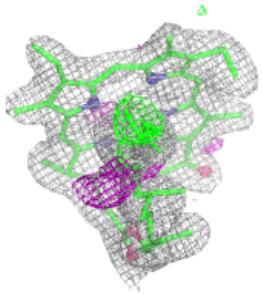


Electron density around CLA C 505:

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

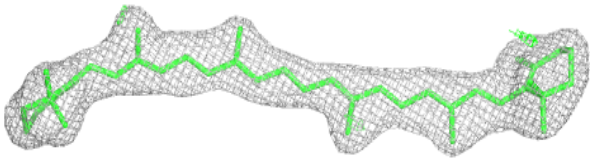


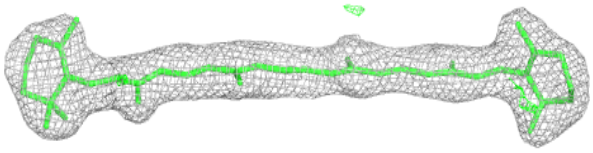


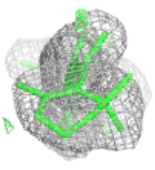


Electron density around BCR C 515:

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

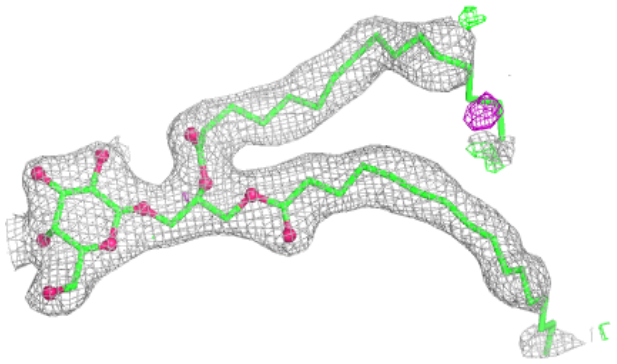


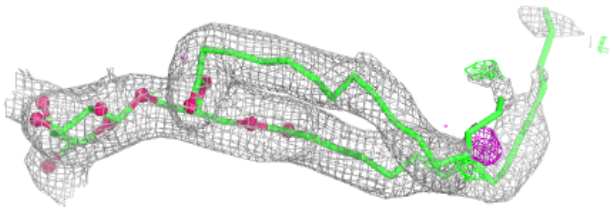


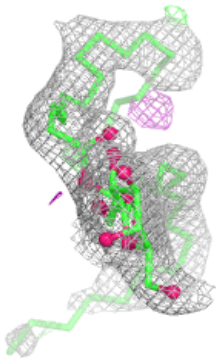


Electron density around LMG J 101:

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

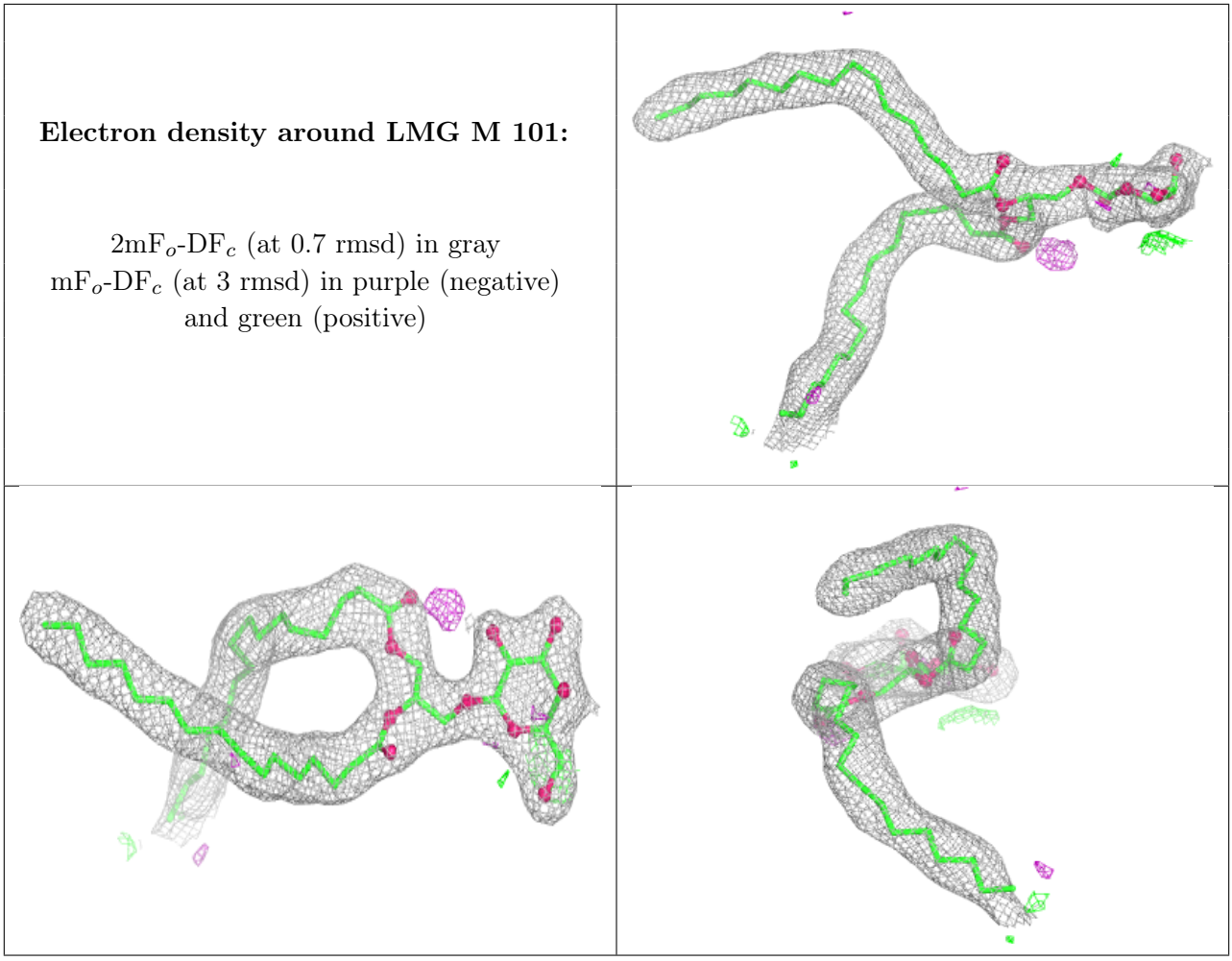






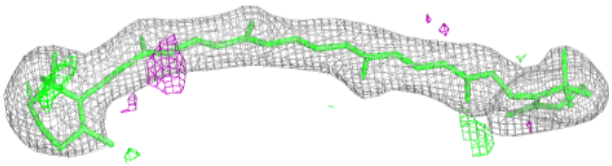
Electron density around LMG M 101:

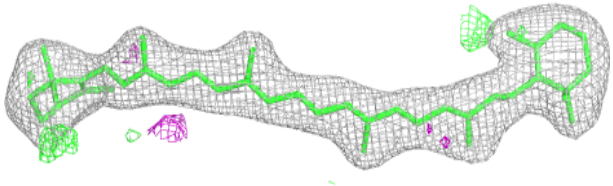
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

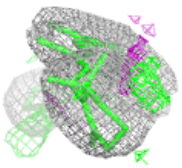


Electron density around BCR D 404:

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

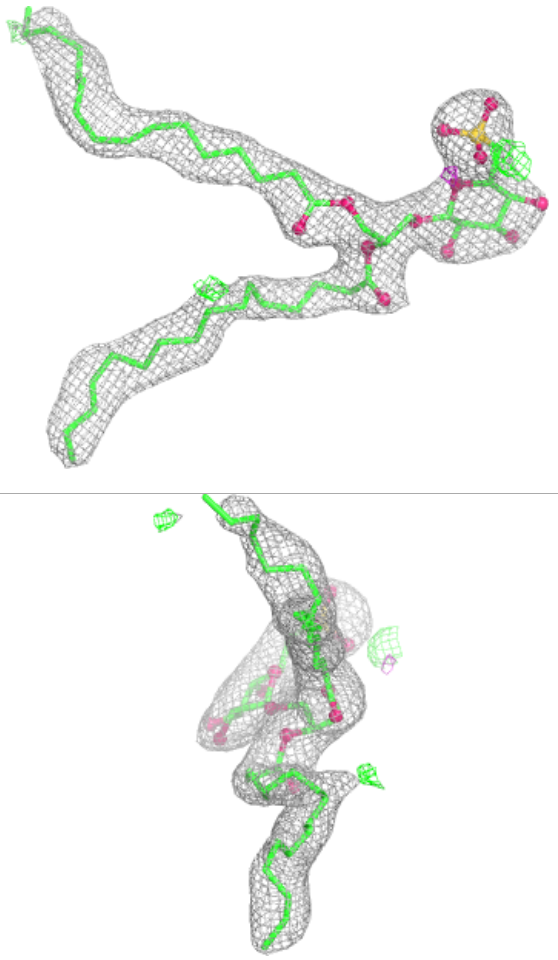


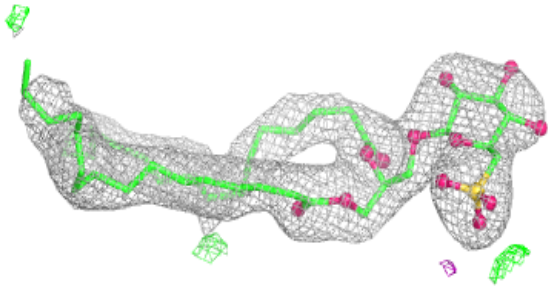




Electron density around SQD a 414:

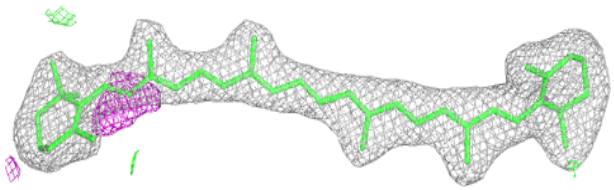
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

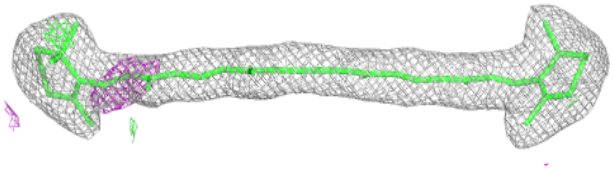


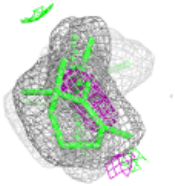


Electron density around BCR b 627:

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

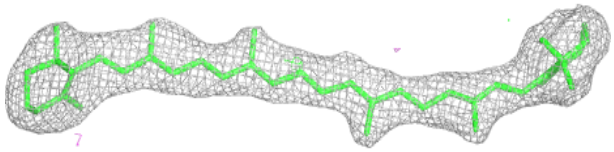


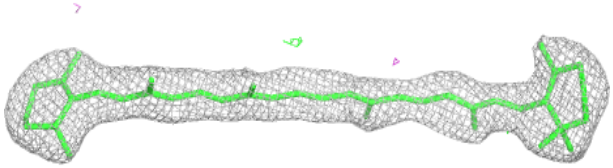


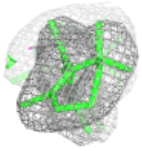


Electron density around BCR c 527:

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

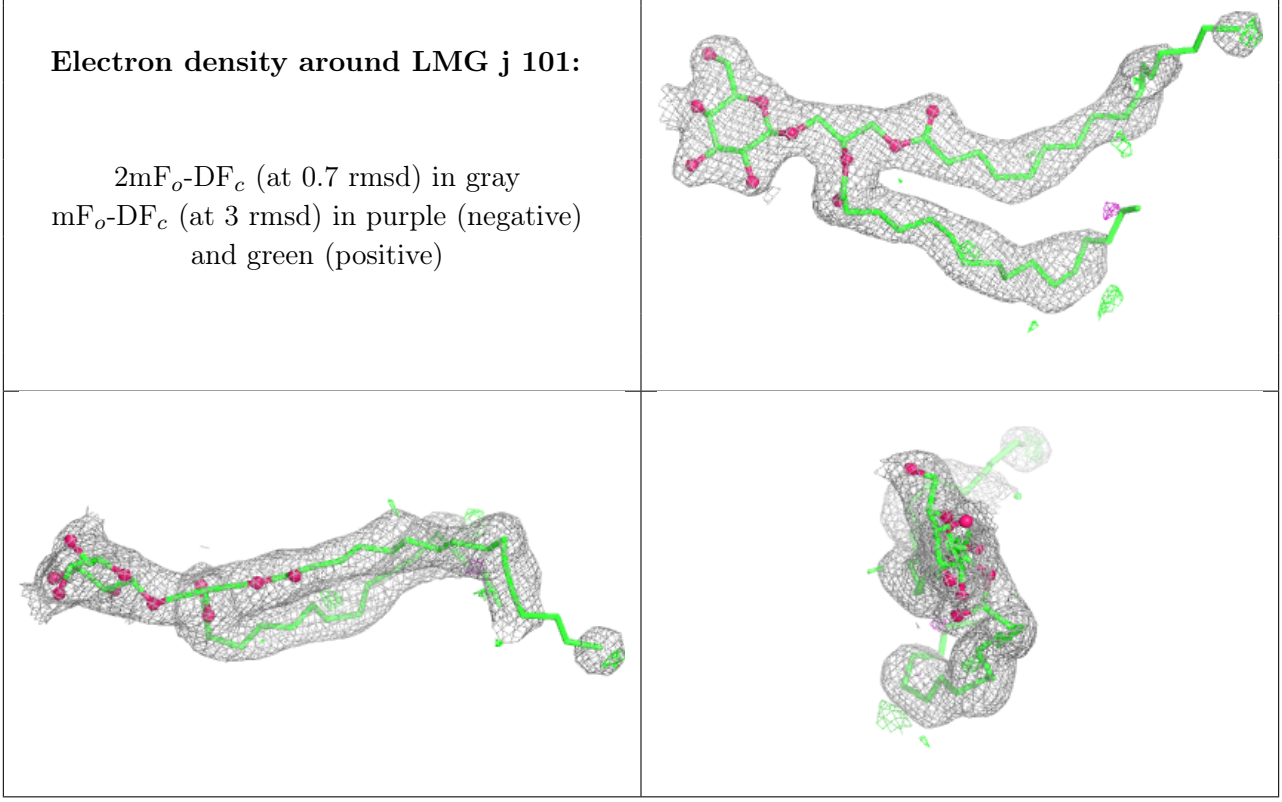






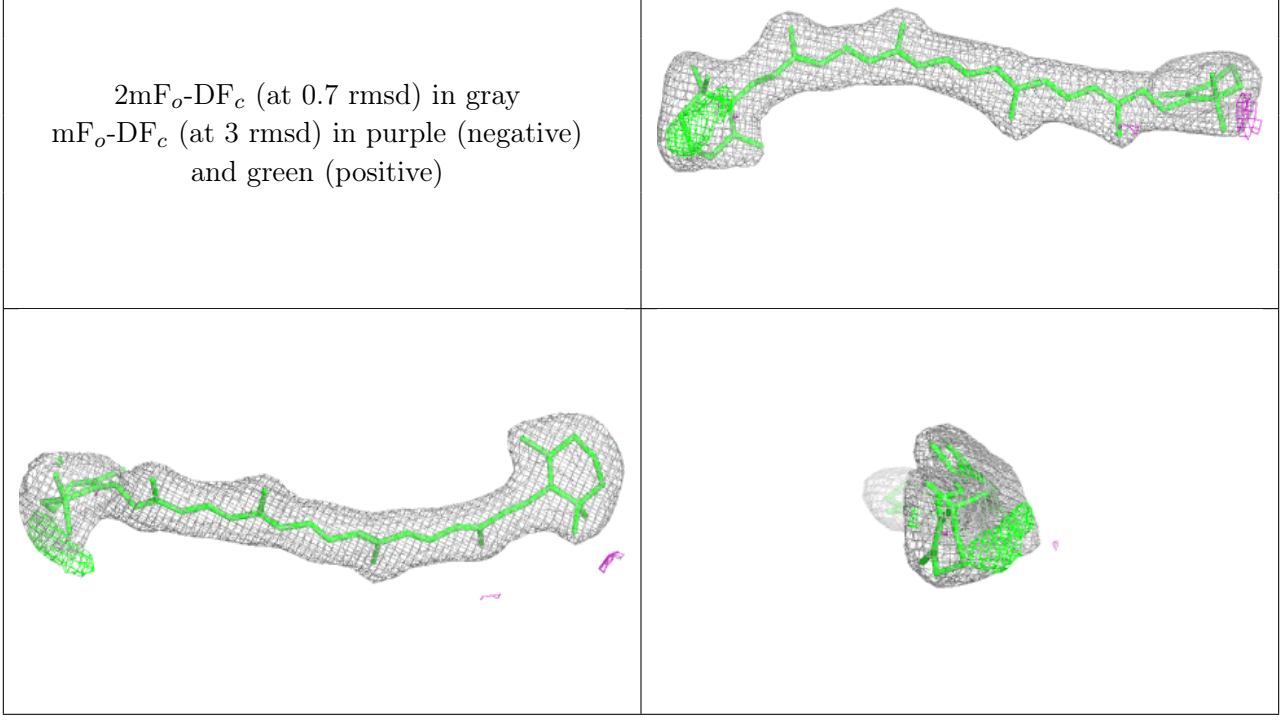
Electron density around LMG j 101:

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



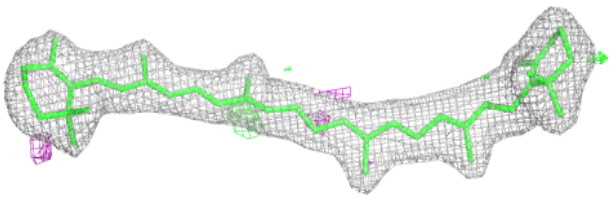
Electron density around BCR d 405:

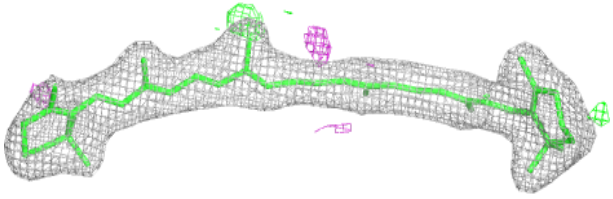
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

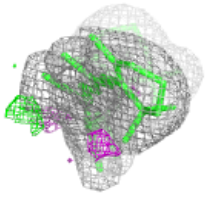


Electron density around BCR t 101:

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

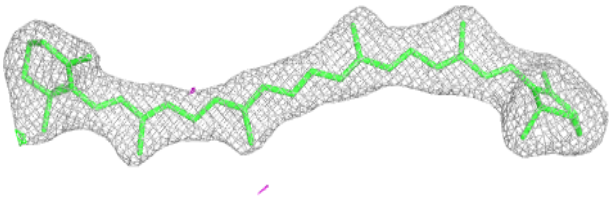


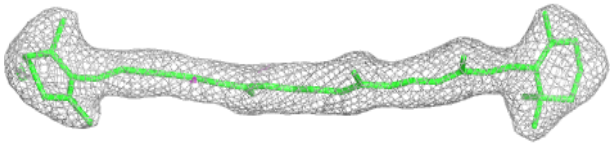


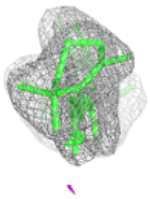


Electron density around BCR y 101:

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

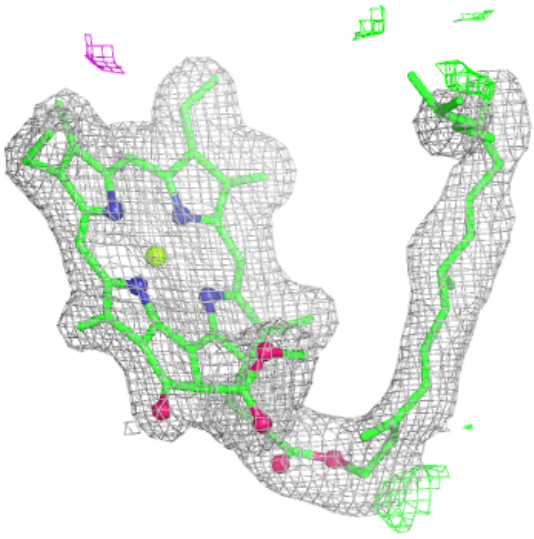


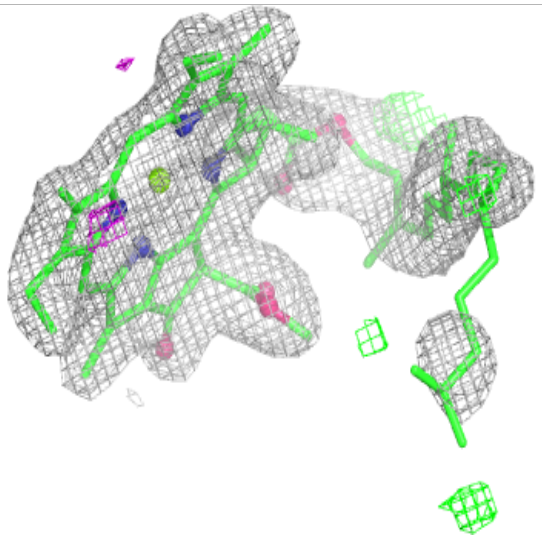


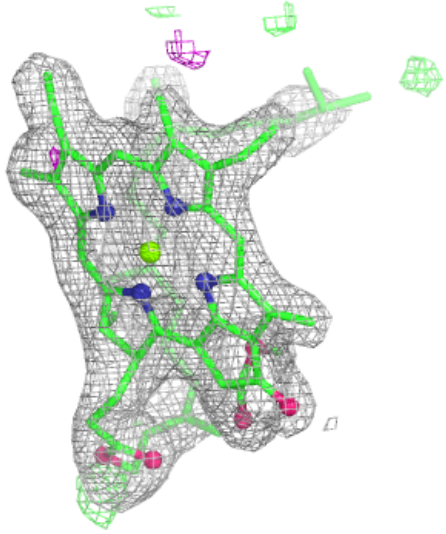


Electron density around CLA b 625:

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

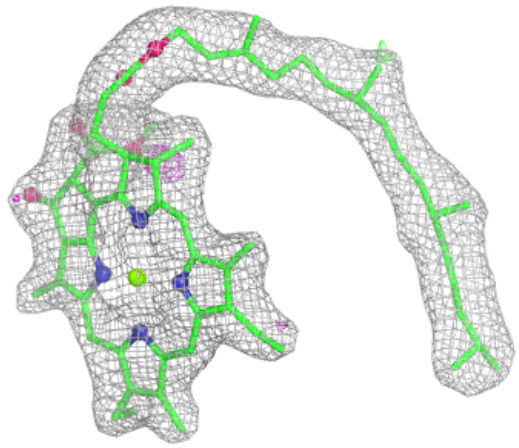


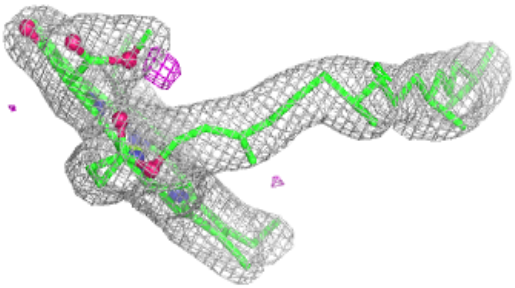


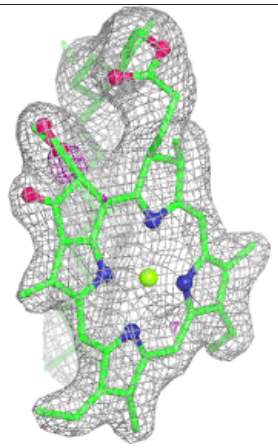


Electron density around CLA C 508:

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

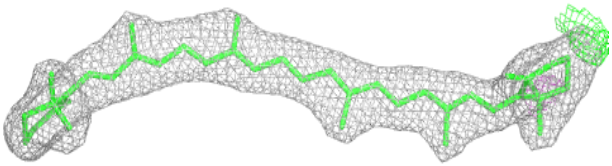


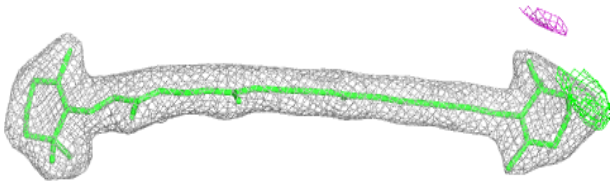


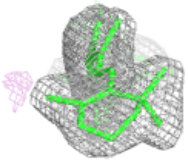


Electron density around BCR H 101:

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

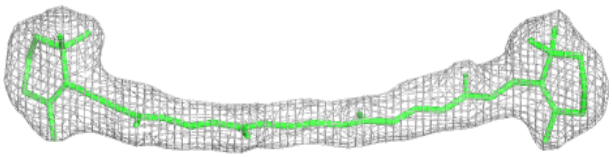


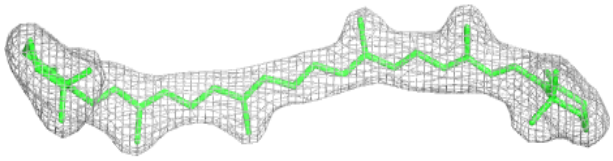


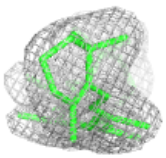


Electron density around BCR K 101:

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

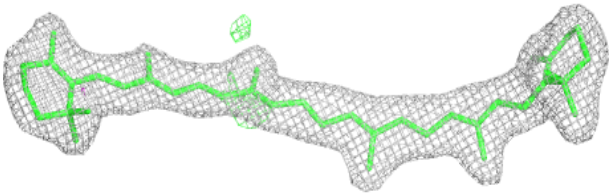


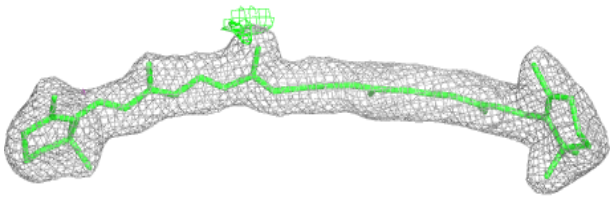


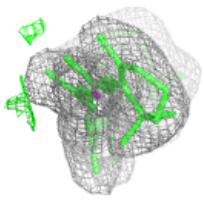


Electron density around BCR T 103:

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

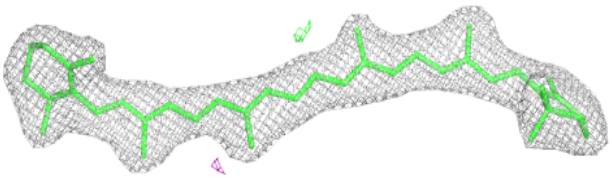


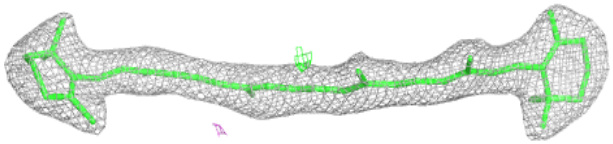


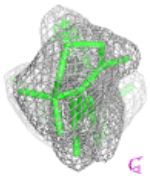


Electron density around BCR Y 101:

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

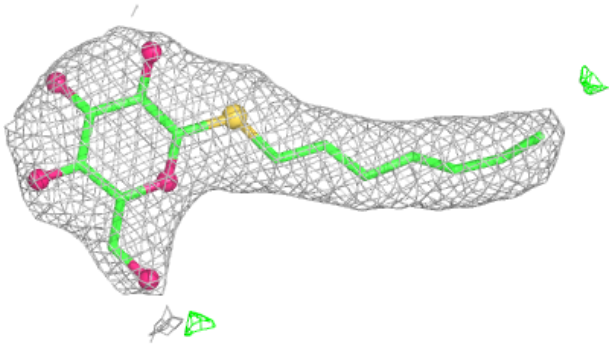


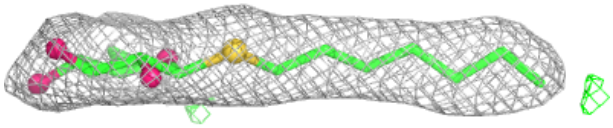


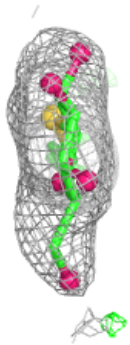


Electron density around HTG b 607:

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

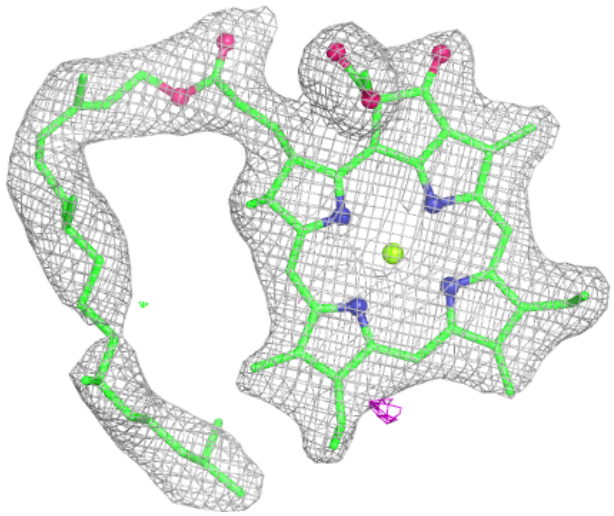


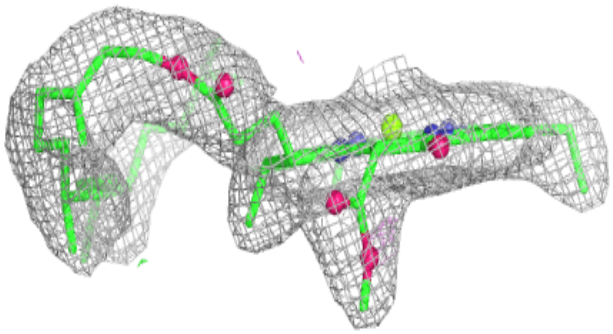


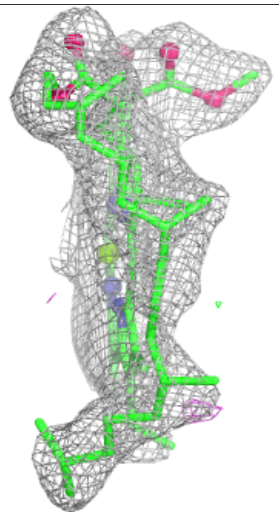


Electron density around CLA C 513:

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

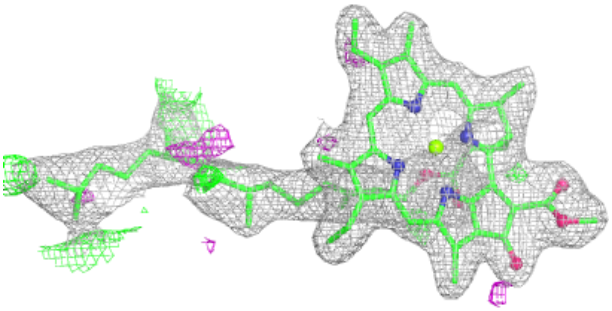


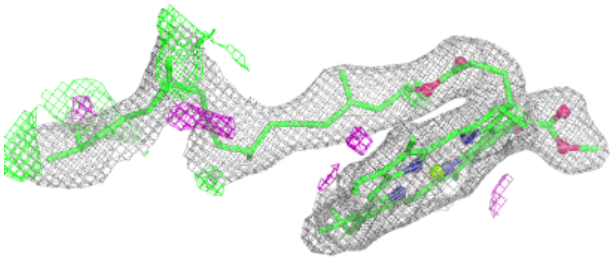


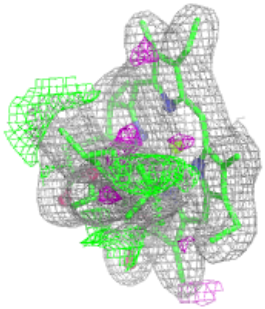


Electron density around CLA B 615:

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

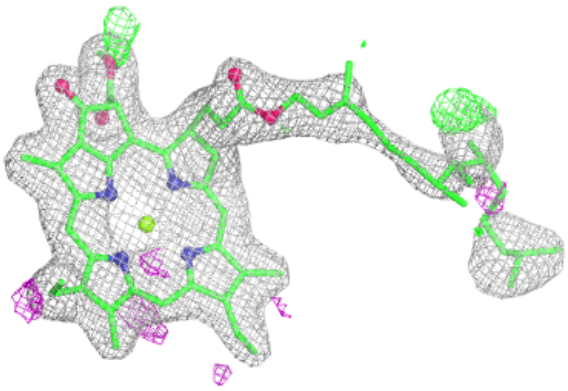


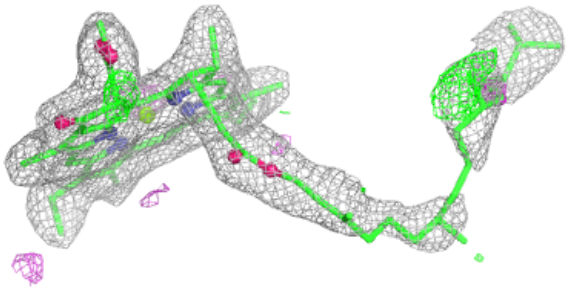


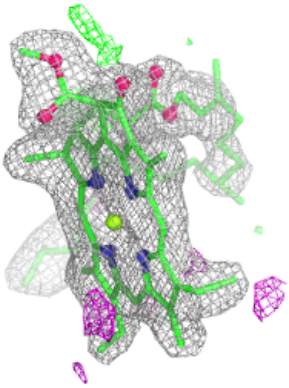


Electron density around CLA a 412:

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

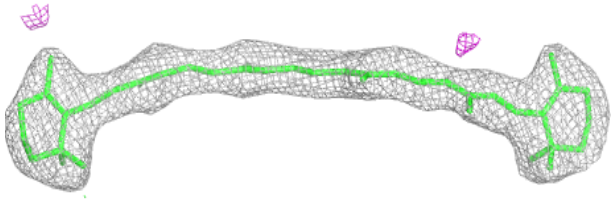


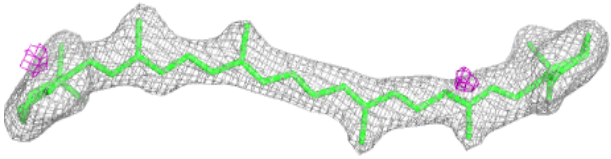


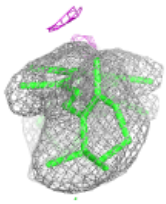


Electron density around BCR k 101:

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

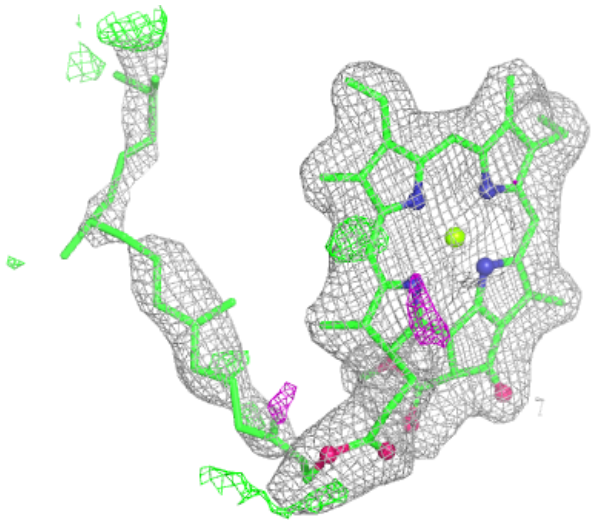


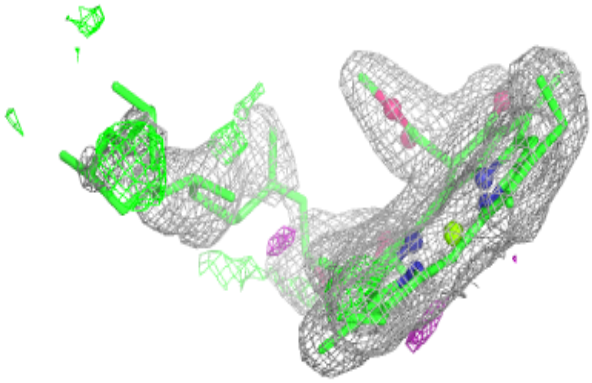




Electron density around CLA B 617:

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

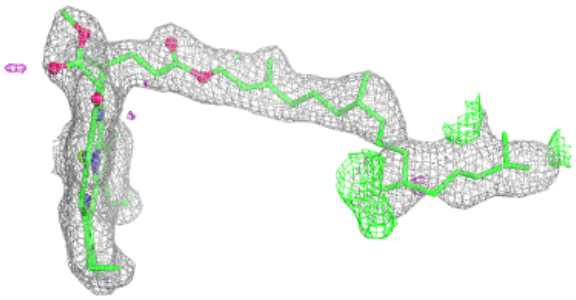


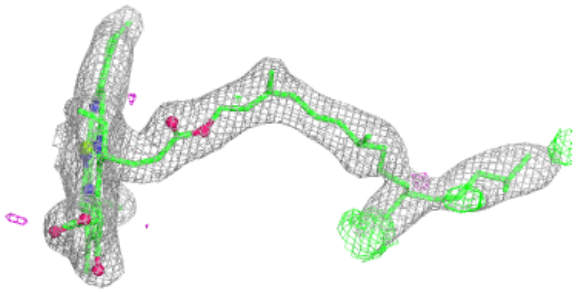


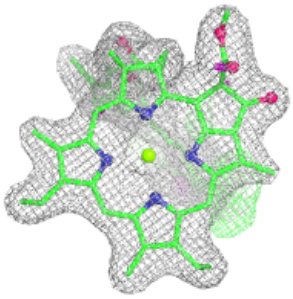


Electron density around CLA b 615:

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

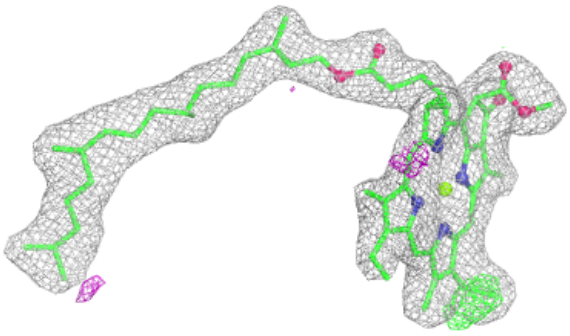


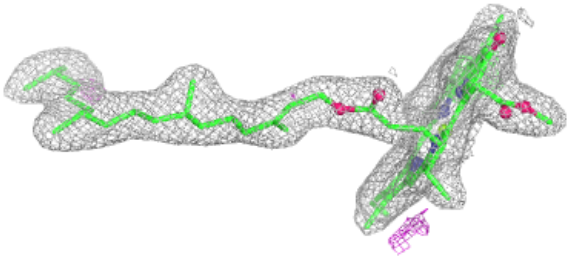


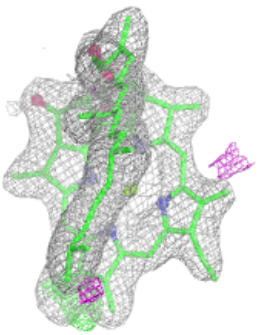


Electron density around CLA b 618:

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

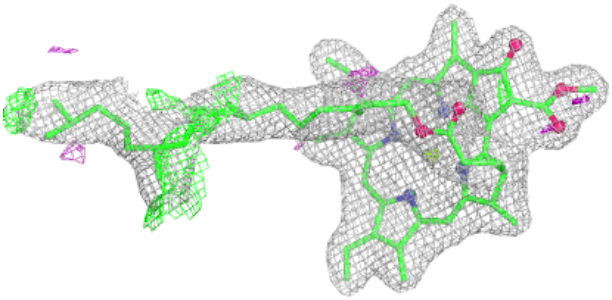


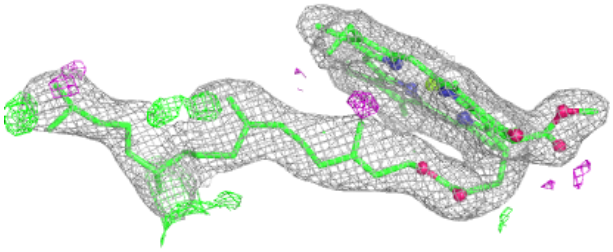




Electron density around CLA b 623:

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

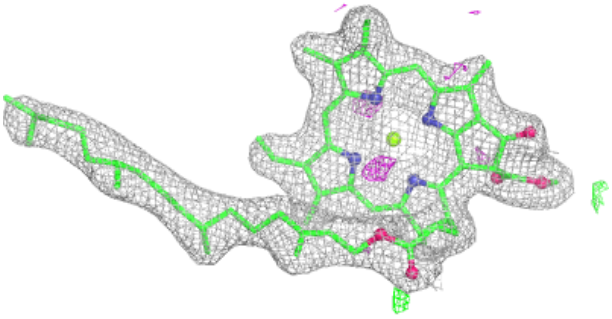


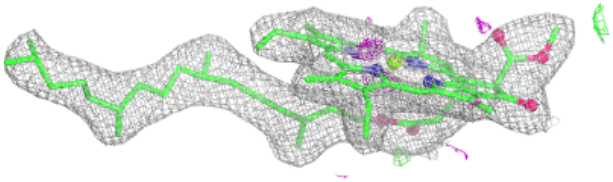


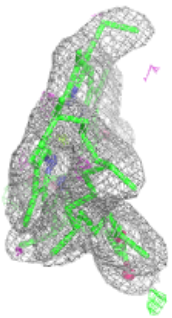


Electron density around CLA C 502:

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

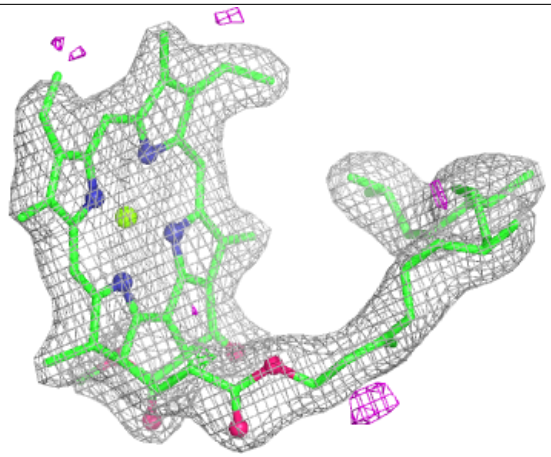


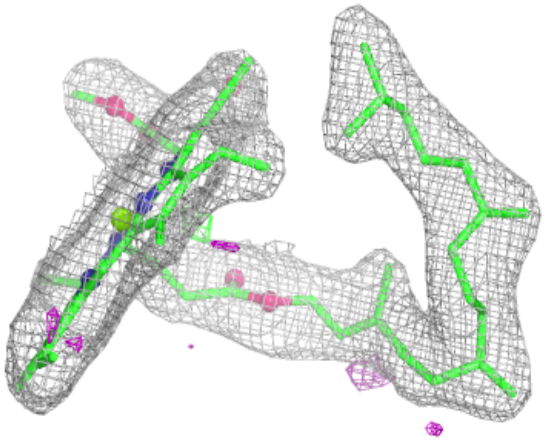


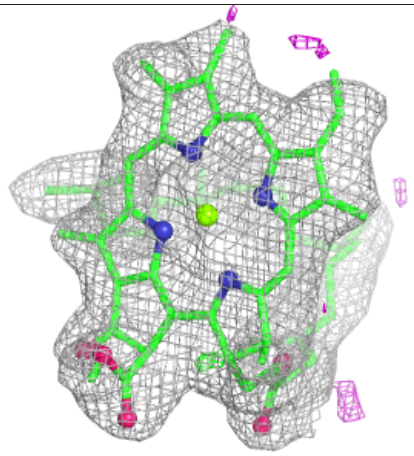


Electron density around CLA c 507:

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

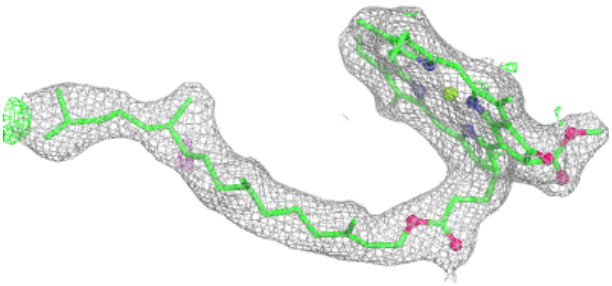


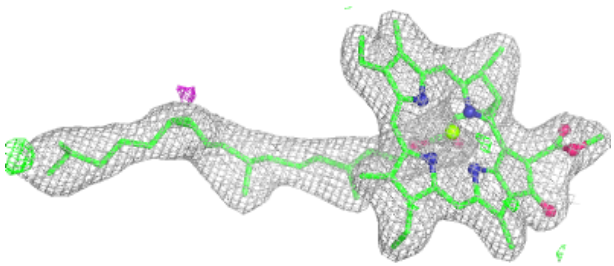


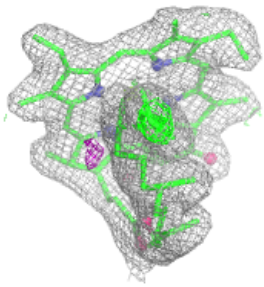


Electron density around CLA c 508:

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

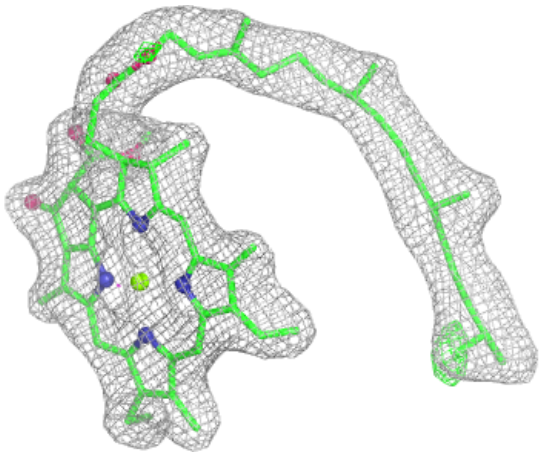


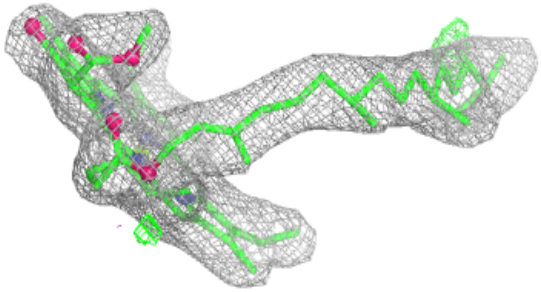


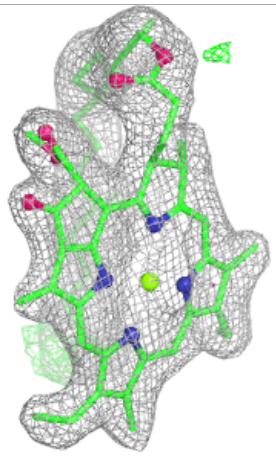


Electron density around CLA c 511:

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

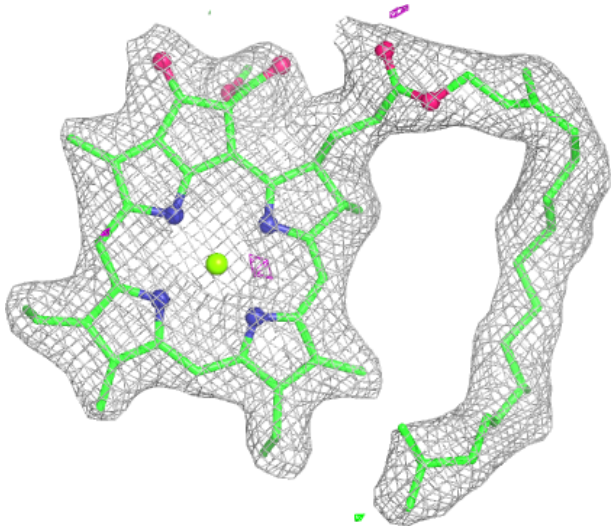


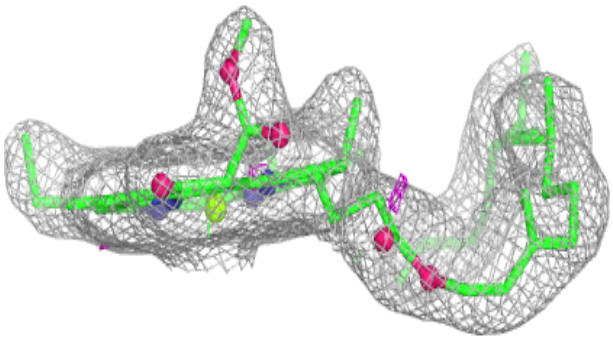


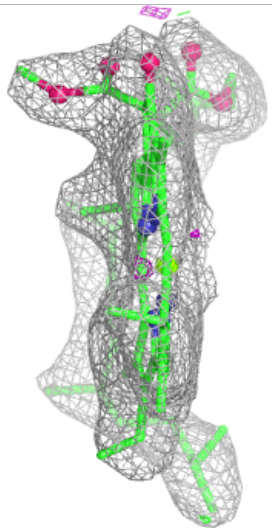


Electron density around CLA c 516:

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

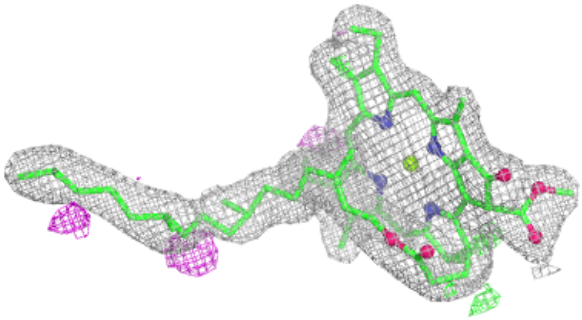


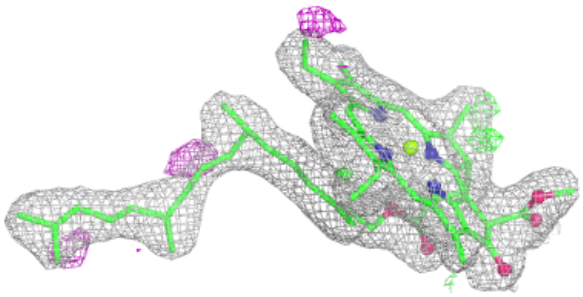


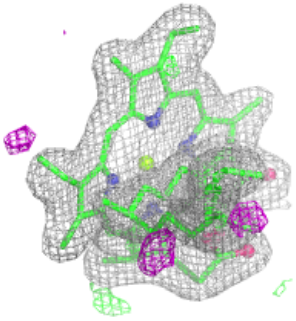


Electron density around CLA C 506:

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

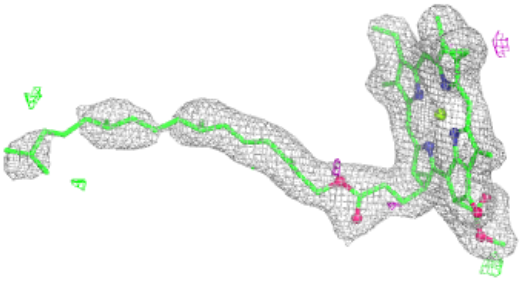


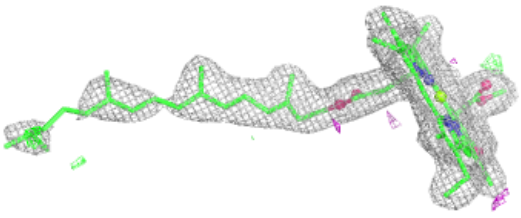


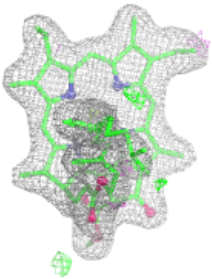


Electron density around CLA d 404:

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

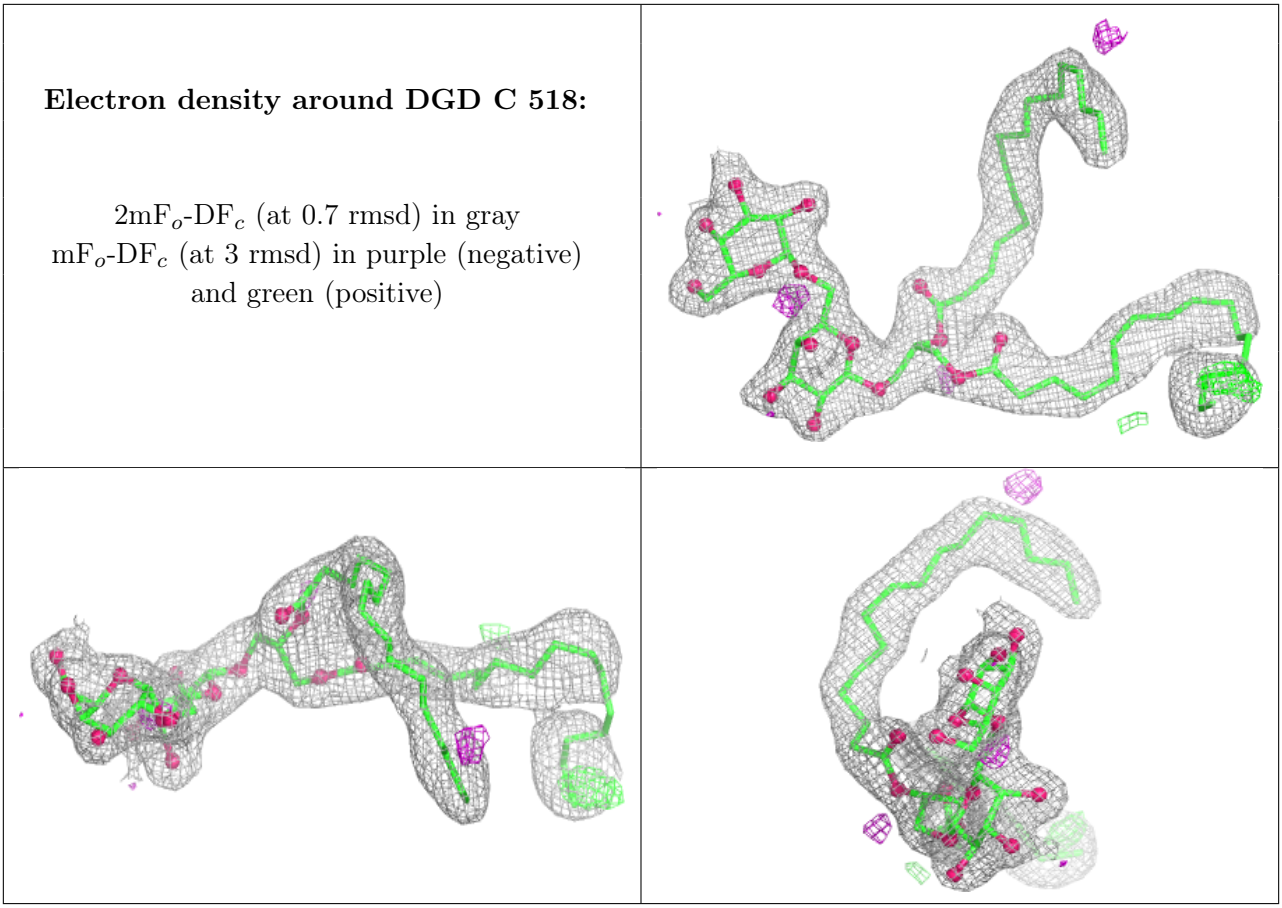






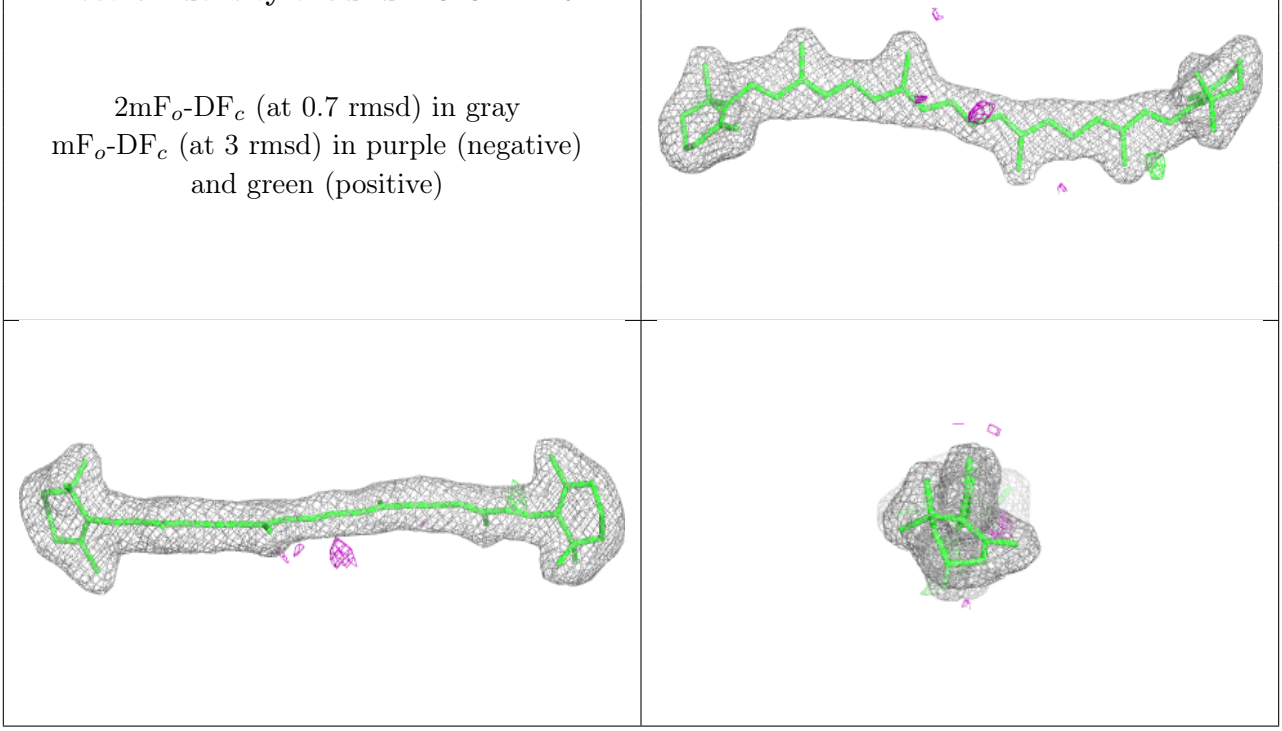
Electron density around DGD C 518:

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



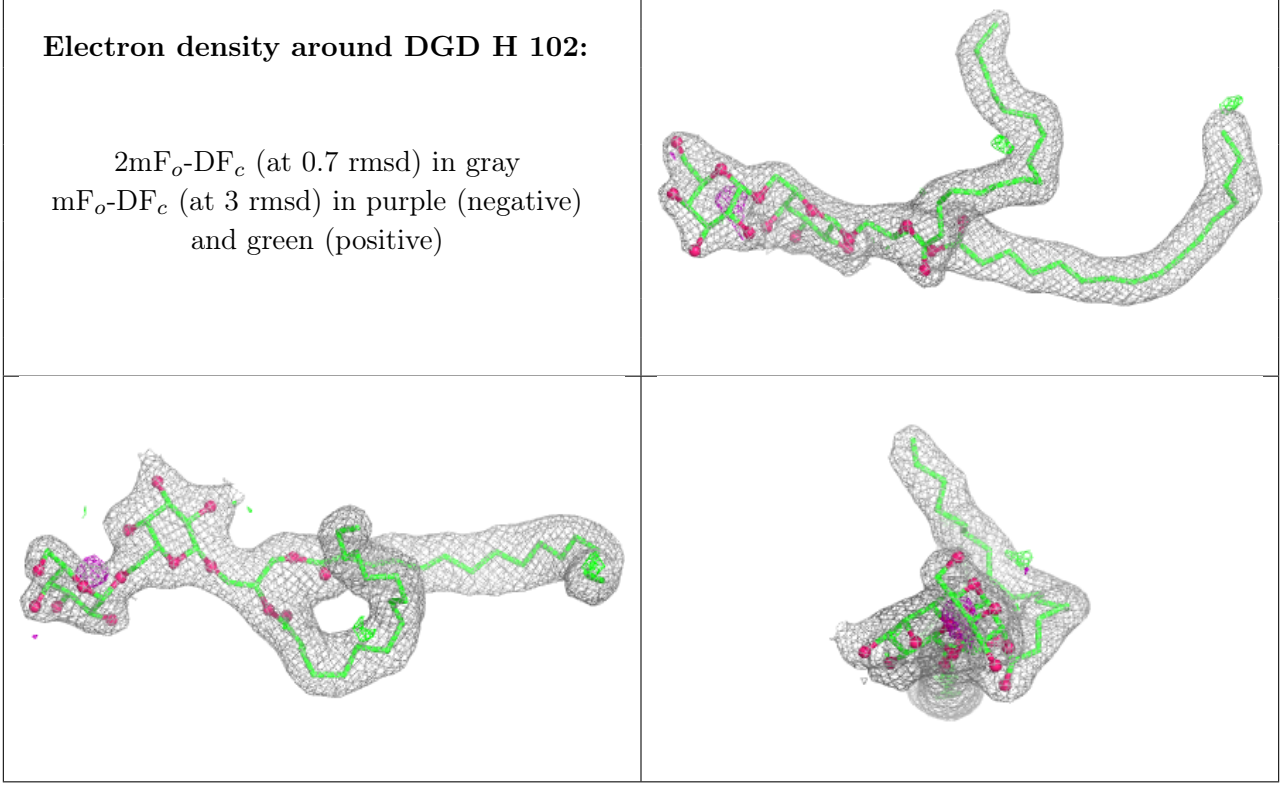
Electron density around BCR A 410:

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



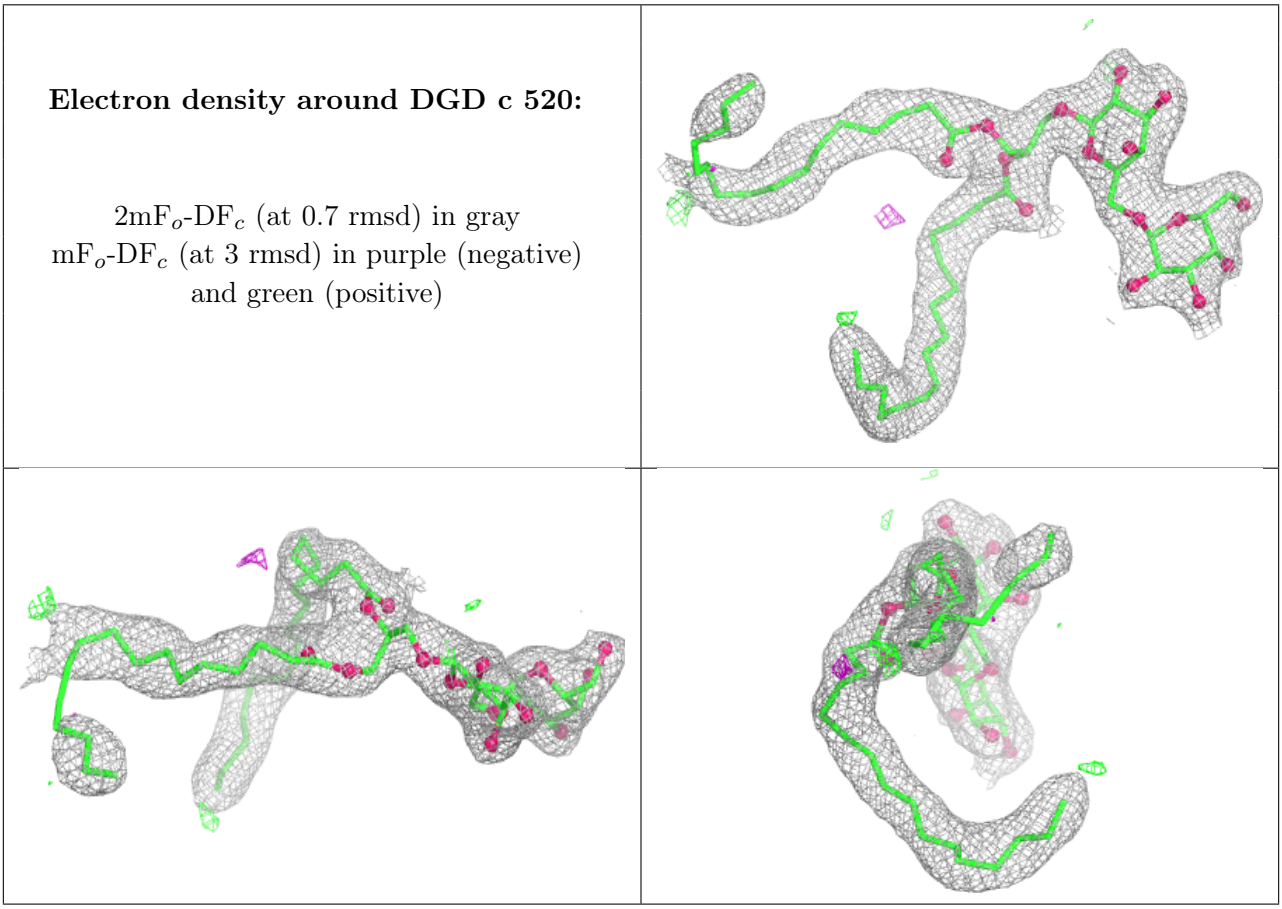
Electron density around DGD H 102:

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



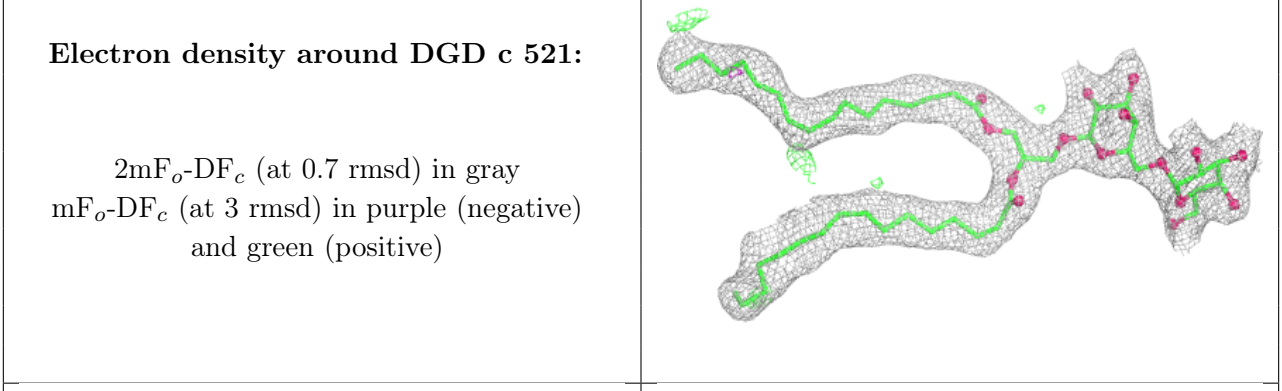
Electron density around DGD c 520:

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



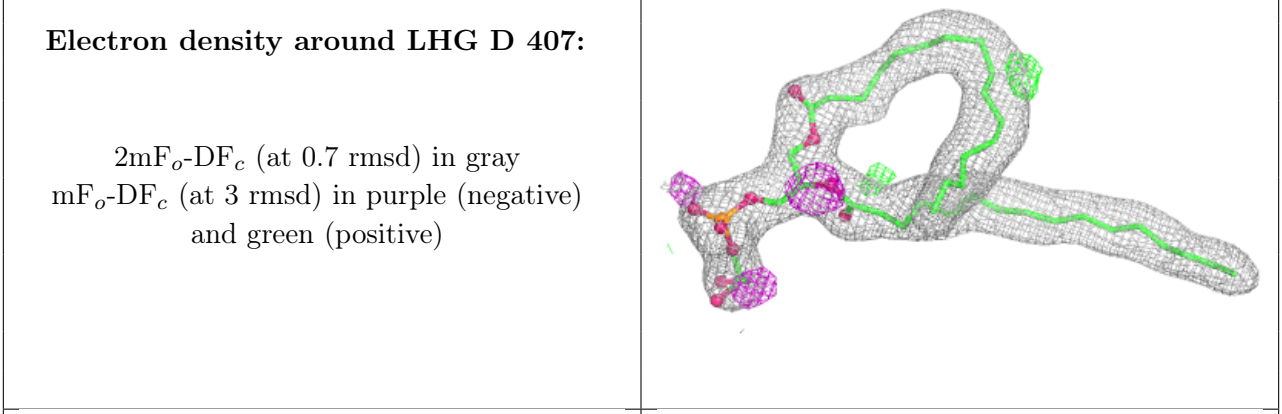
Electron density around DGD c 521:

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



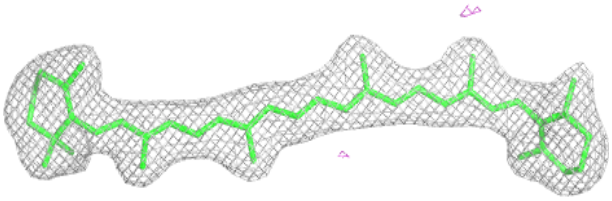
Electron density around LHG D 407:

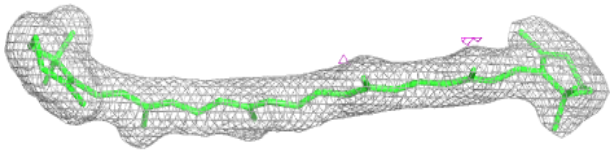
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

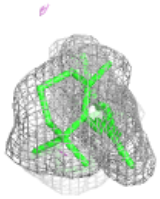


Electron density around BCR B 620:

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

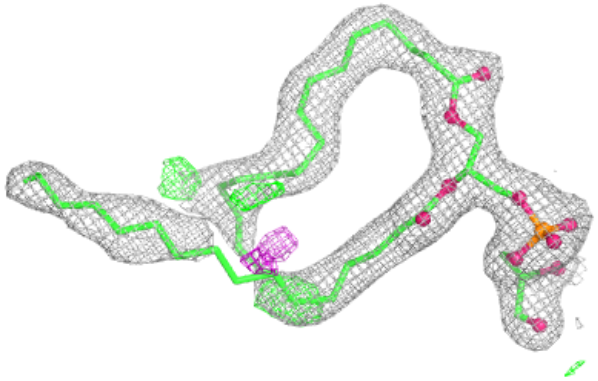


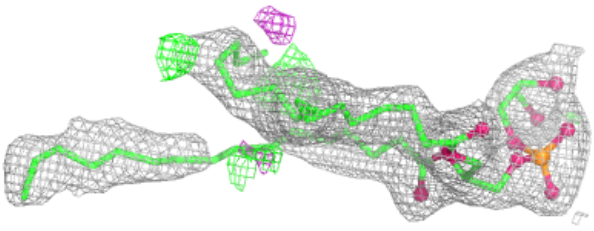


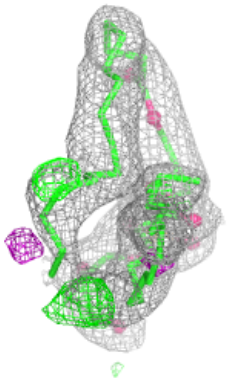


Electron density around LHG d 409:

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

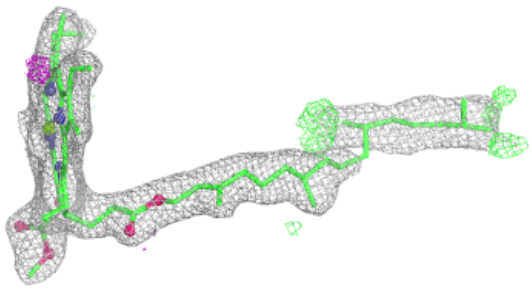


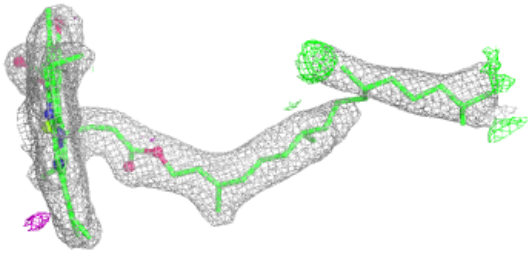


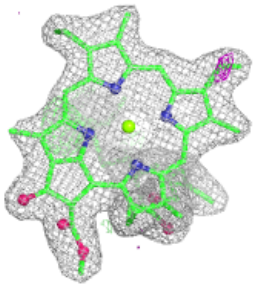


Electron density around CLA B 607:

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

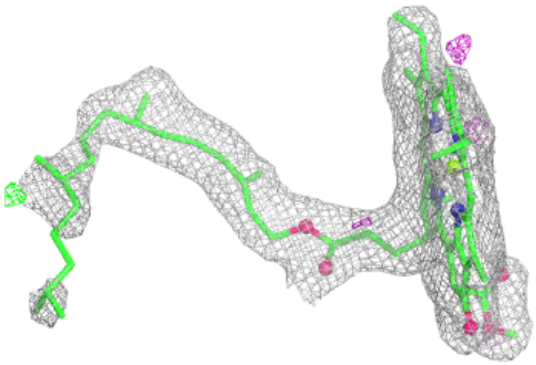


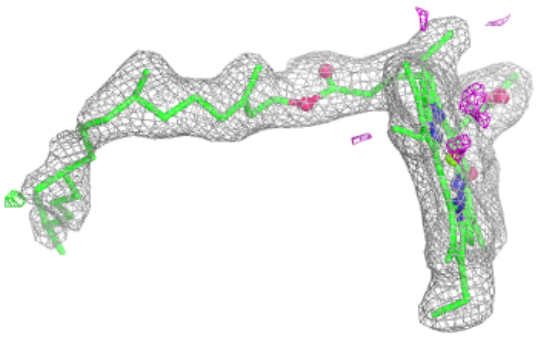


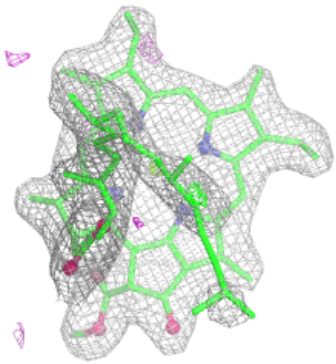


Electron density around CLA D 403:

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

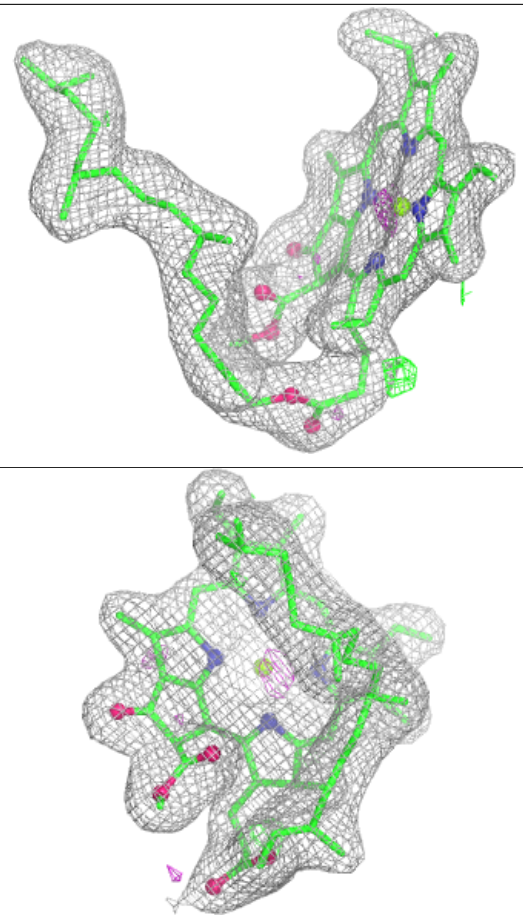






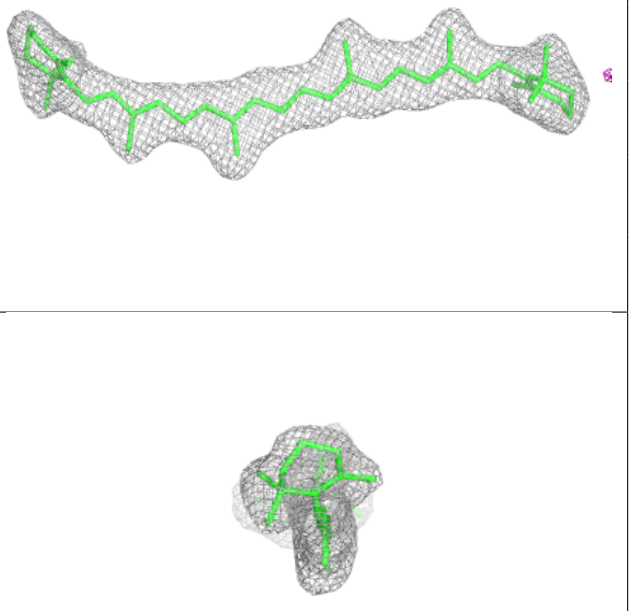
Electron density around CLA B 614:

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



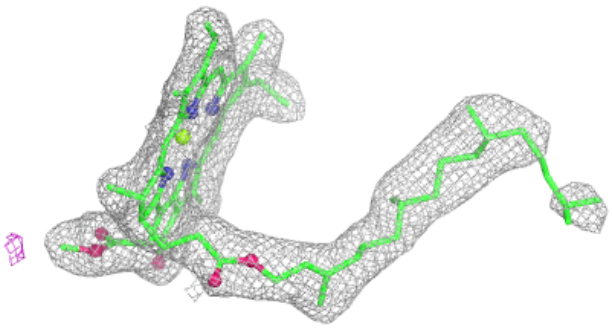
Electron density around BCR c 518:

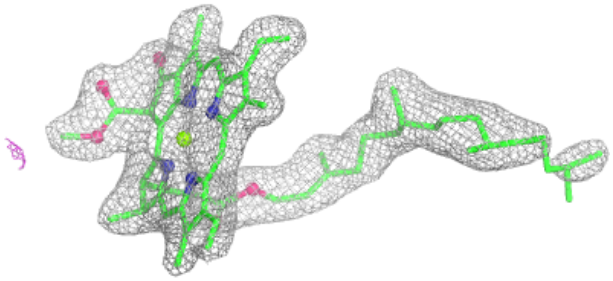
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

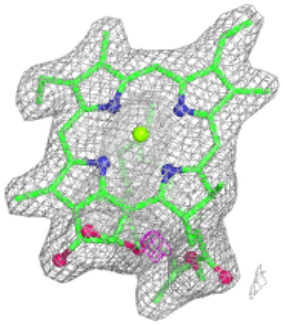


Electron density around CLA C 509:

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

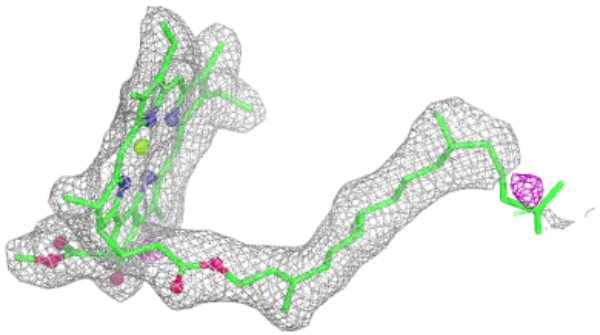


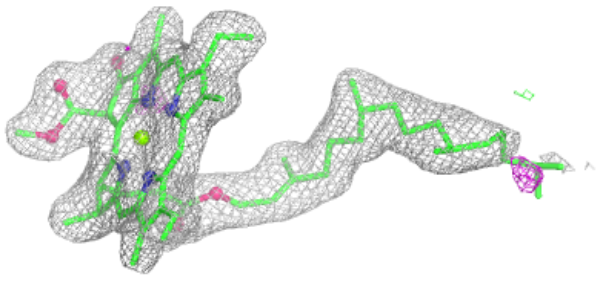


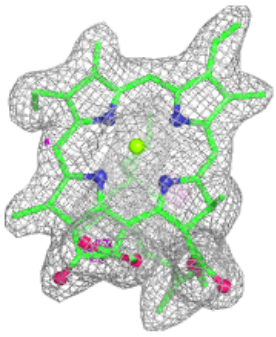


Electron density around CLA c 512:

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

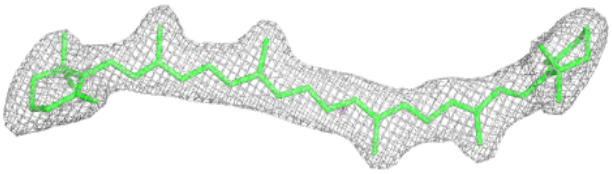


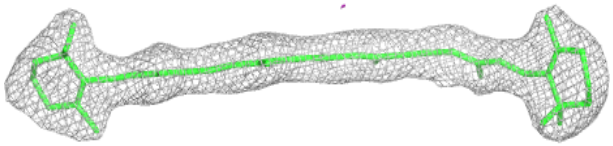


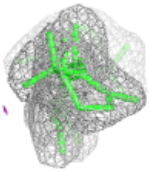


Electron density around BCR h 101:

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

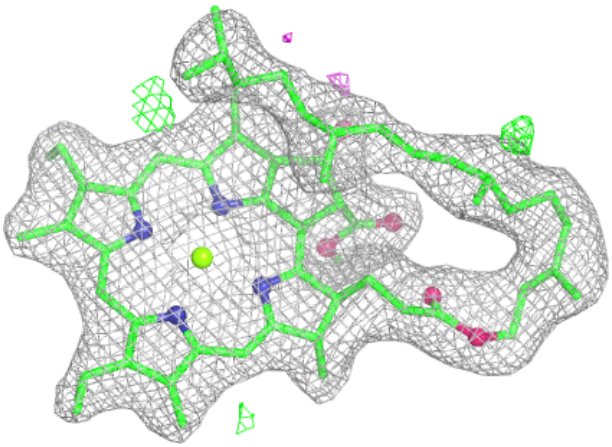


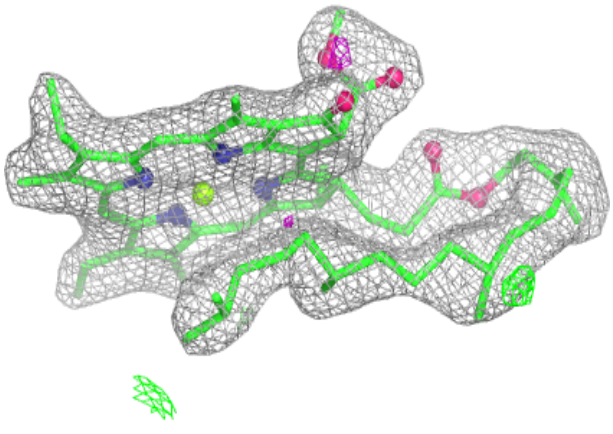


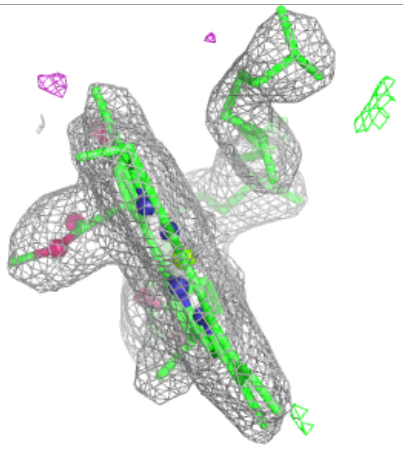


Electron density around CLA c 513:

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

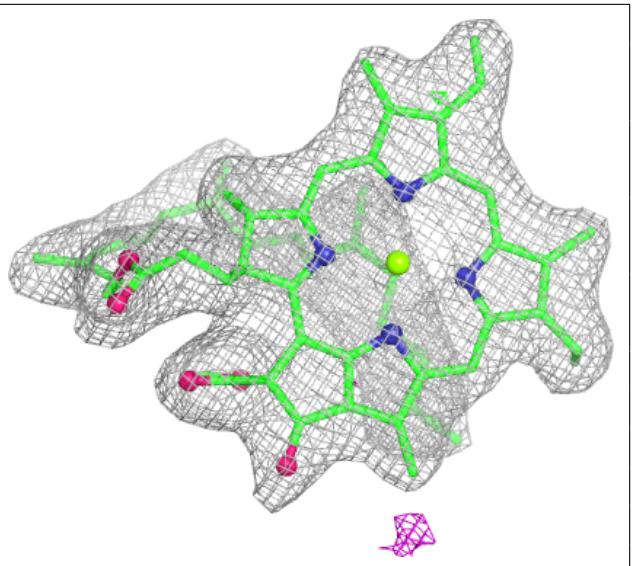


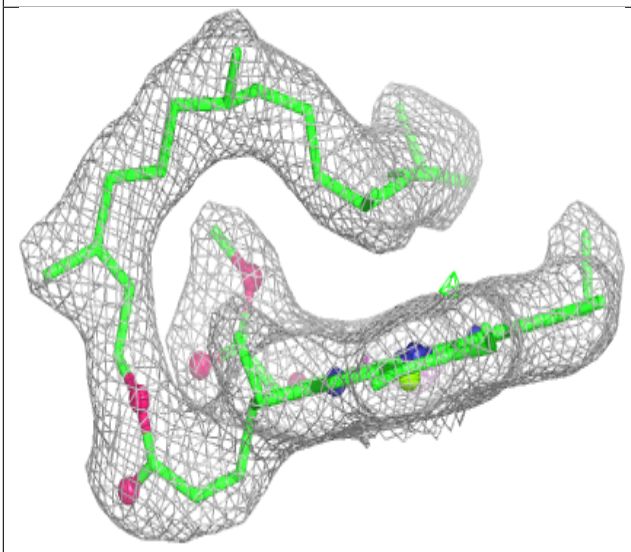


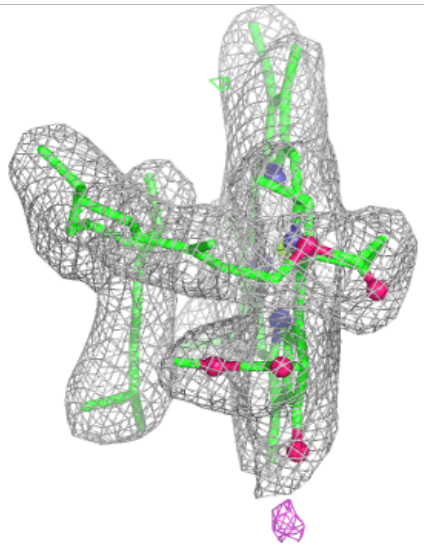


Electron density around CLA c 514:

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

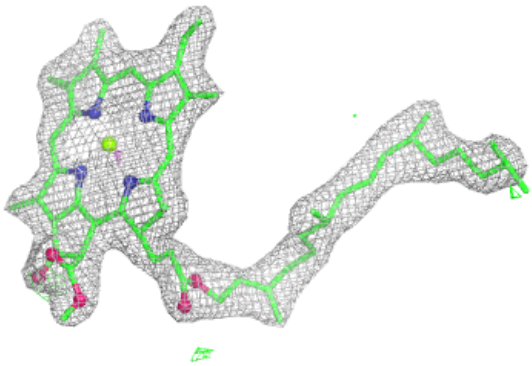


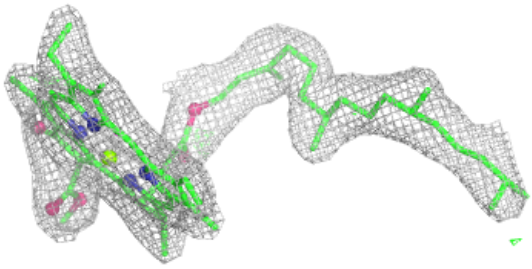


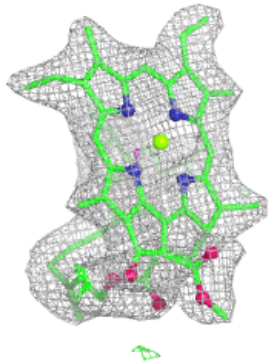


Electron density around CLA c 515:

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

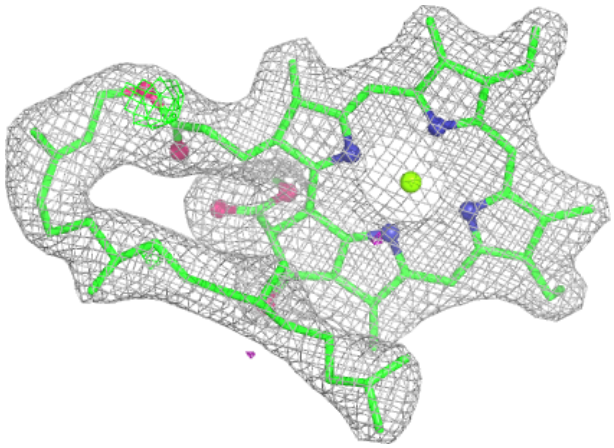


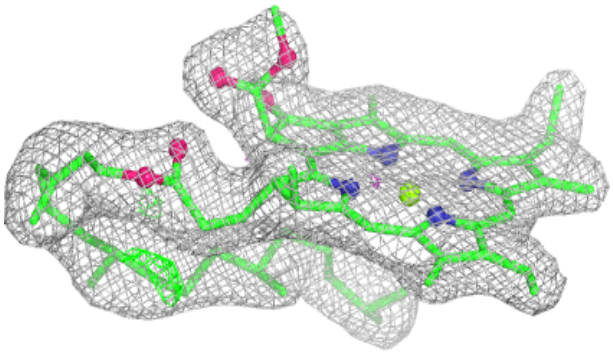


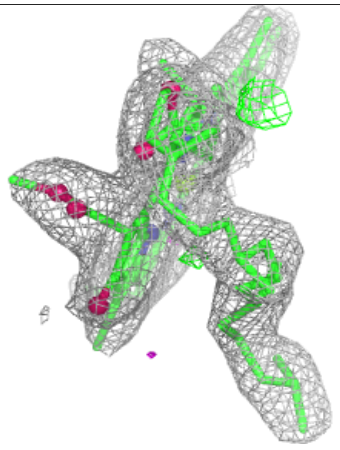


Electron density around CLA C 510:

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

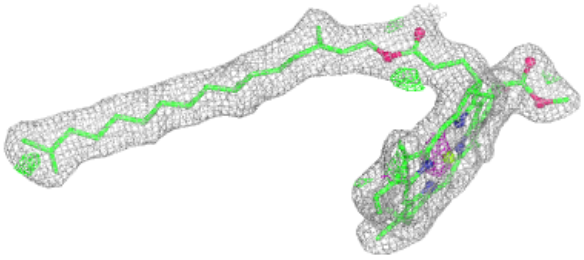


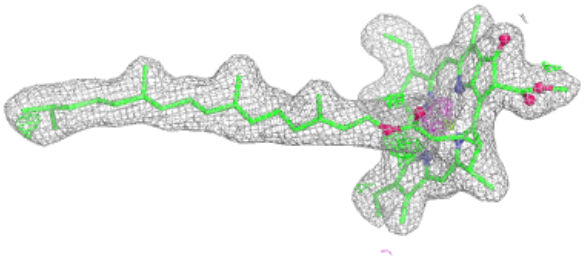


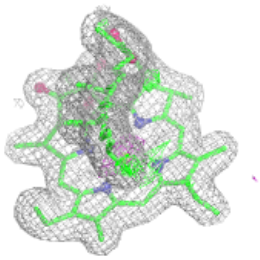


Electron density around CLA b 616:

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

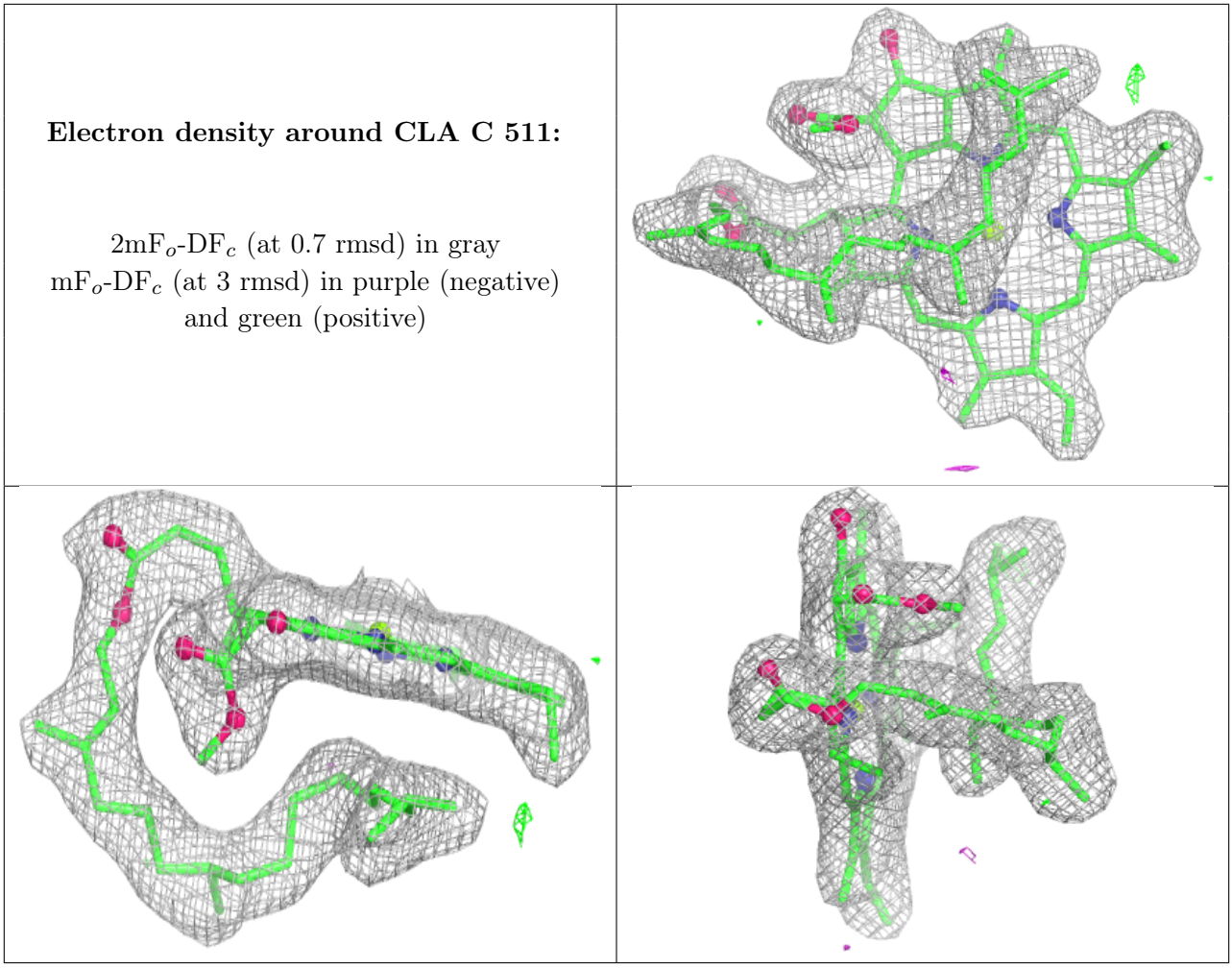






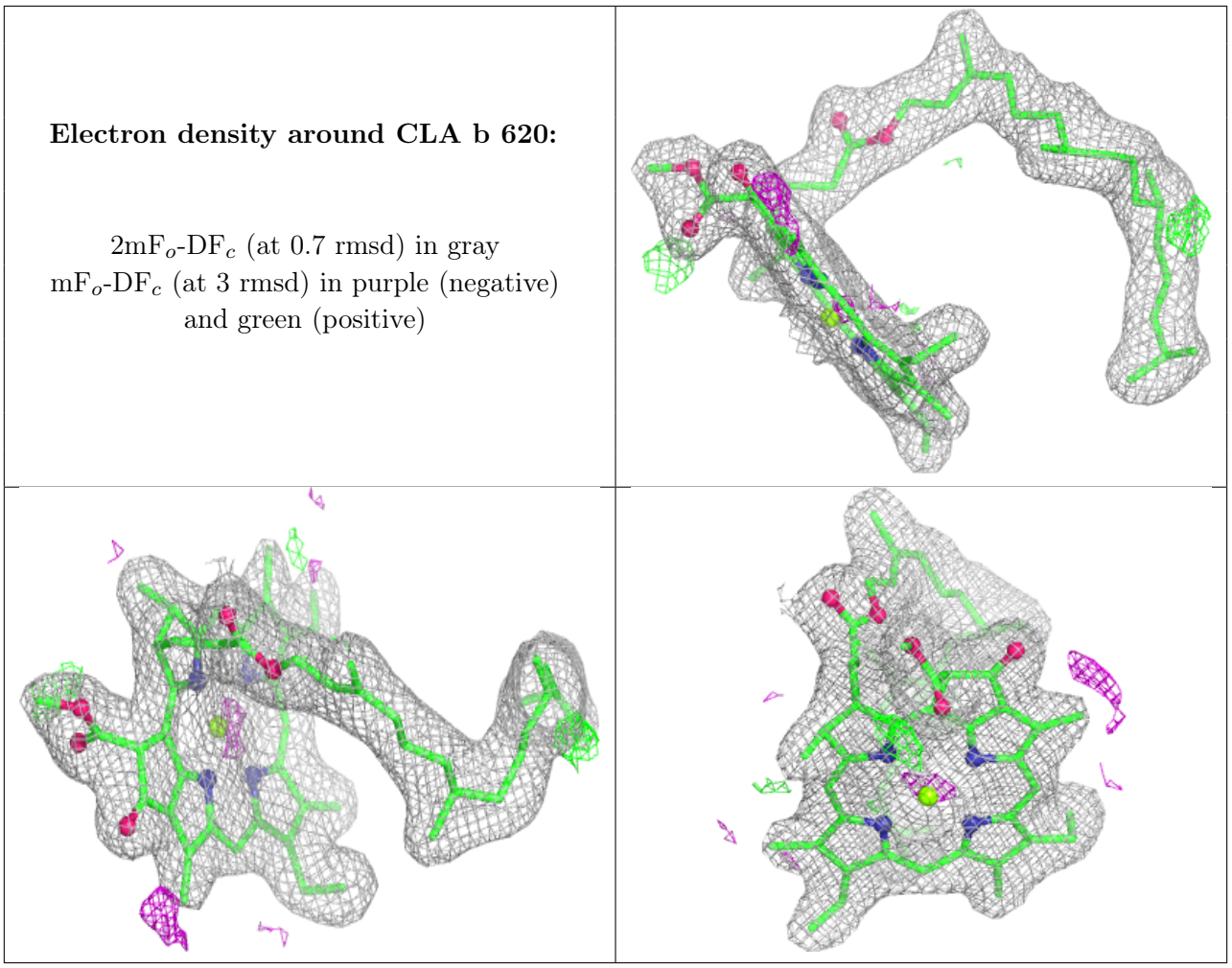
Electron density around CLA C 511:

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



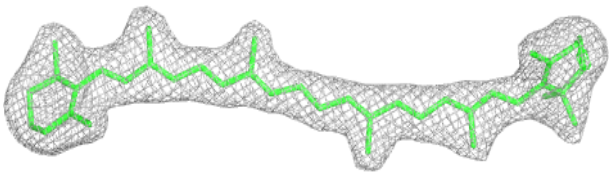
Electron density around CLA b 620:

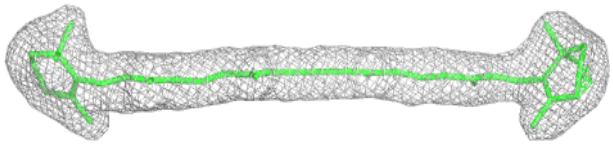
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

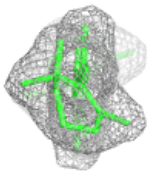


Electron density around BCR B 619:

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

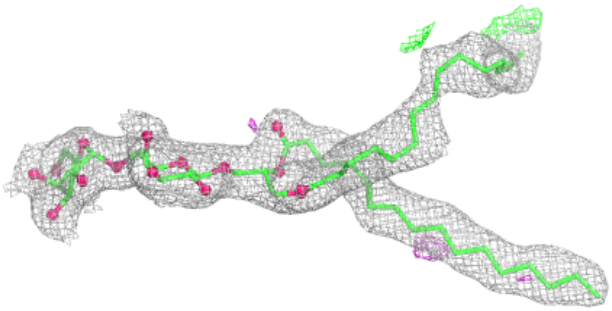


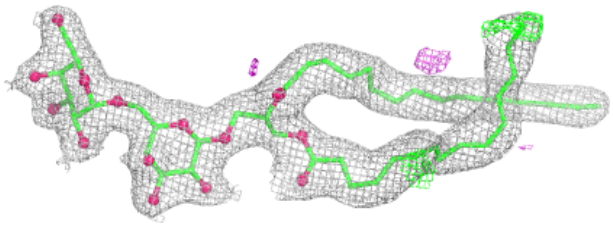


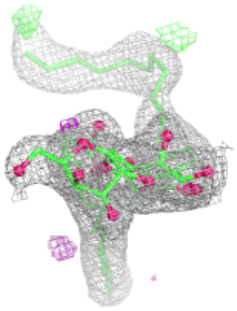


Electron density around DGD C 517:

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

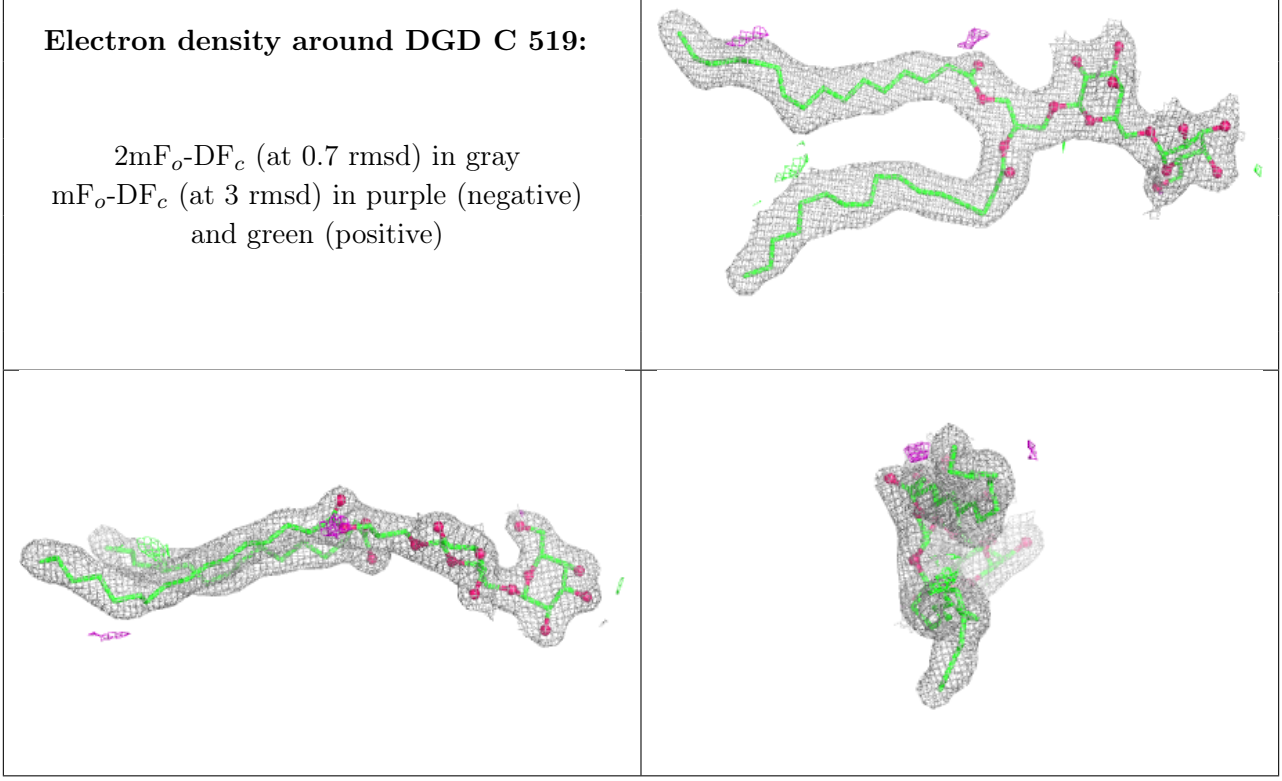






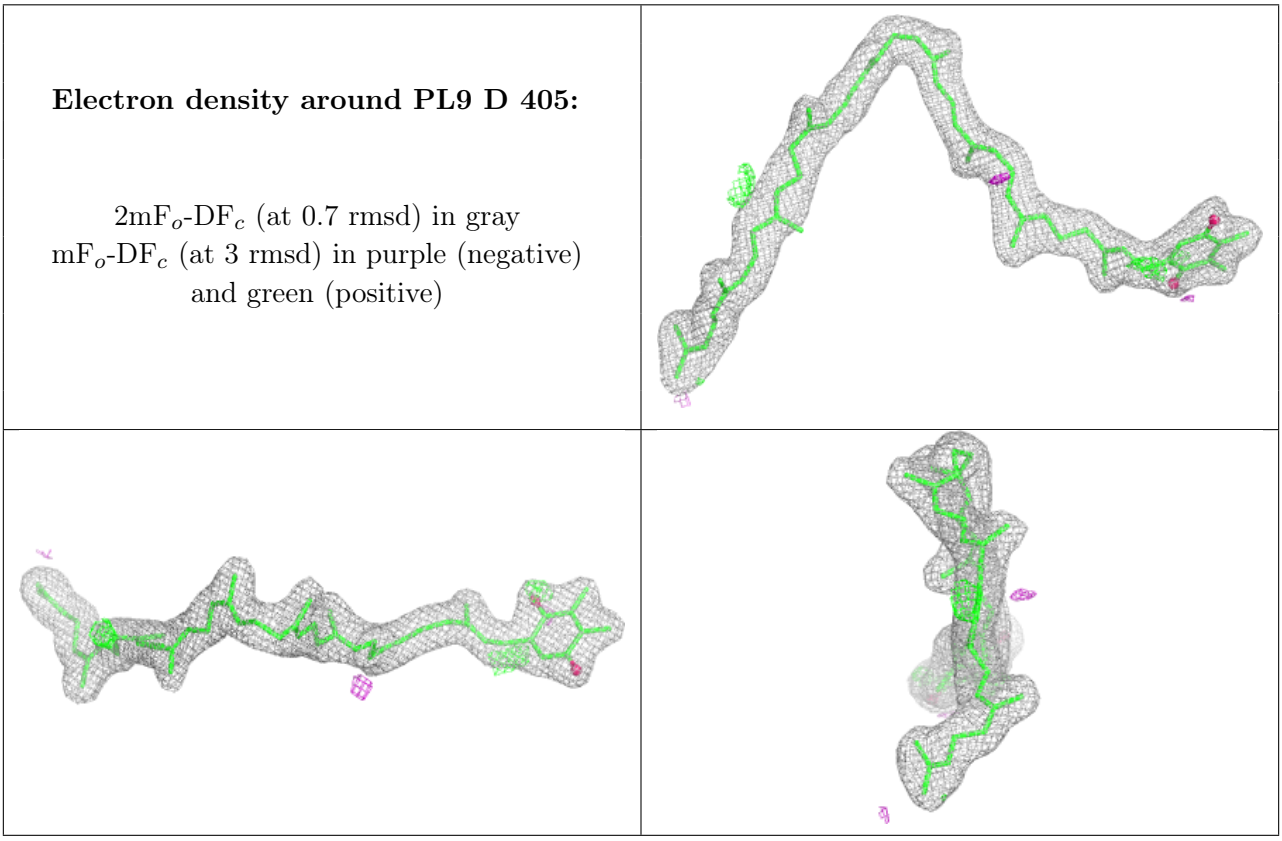
Electron density around DGD C 519:

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



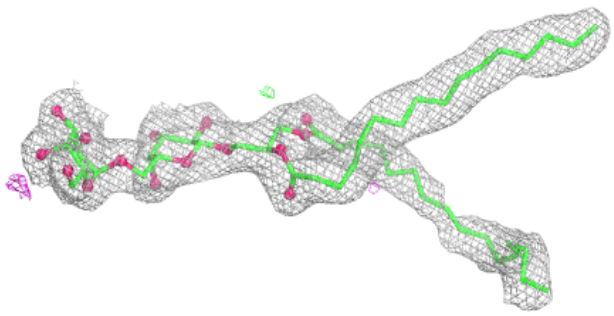
Electron density around PL9 D 405:

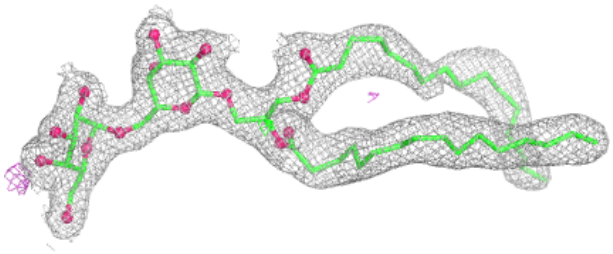
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

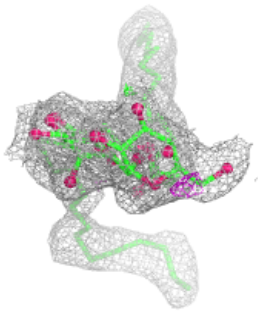


Electron density around DGD c 519:

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

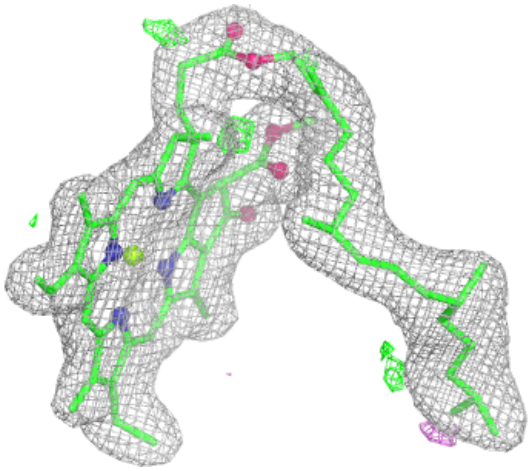


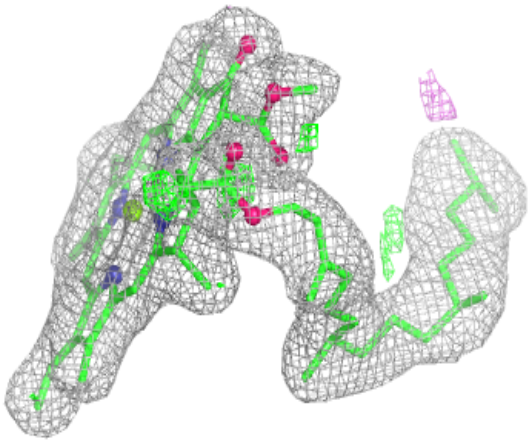


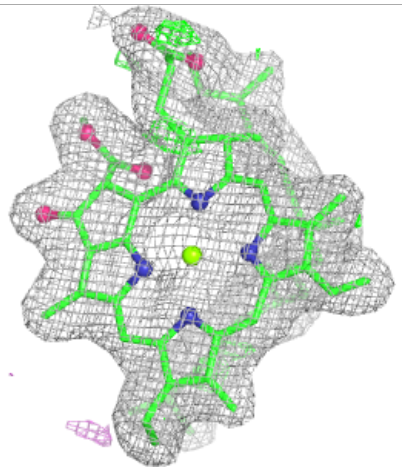


Electron density around CLA b 622:

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

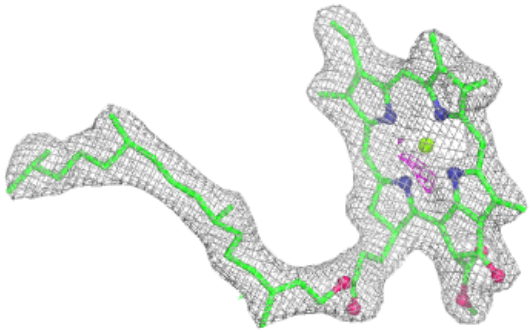


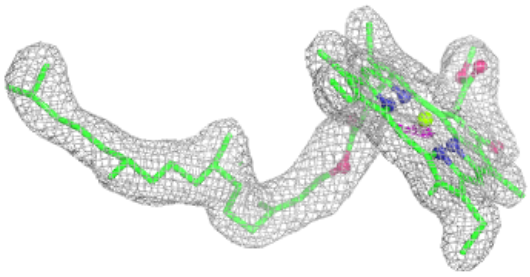


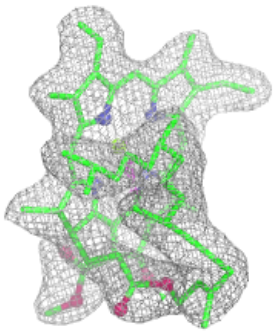


Electron density around CLA C 512:

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

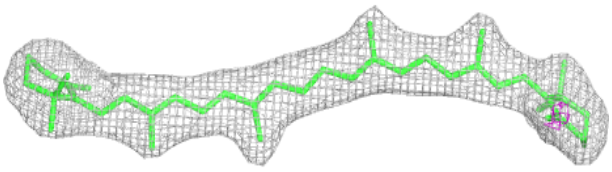


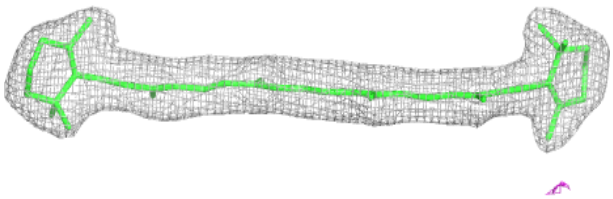


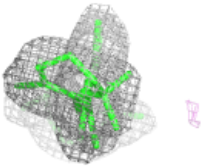


Electron density around BCR C 516:

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

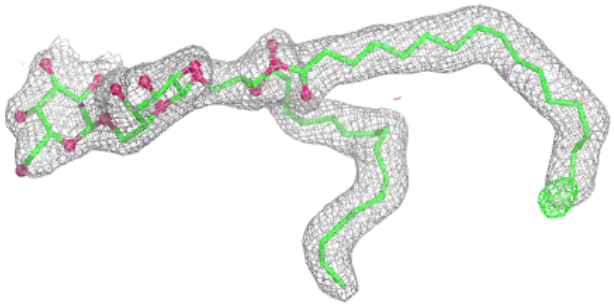


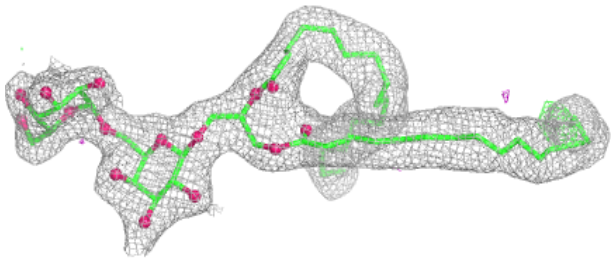


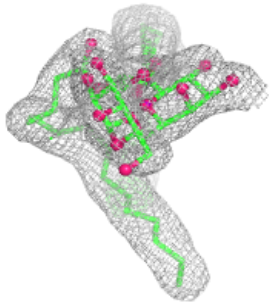


Electron density around DGD h 102:

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

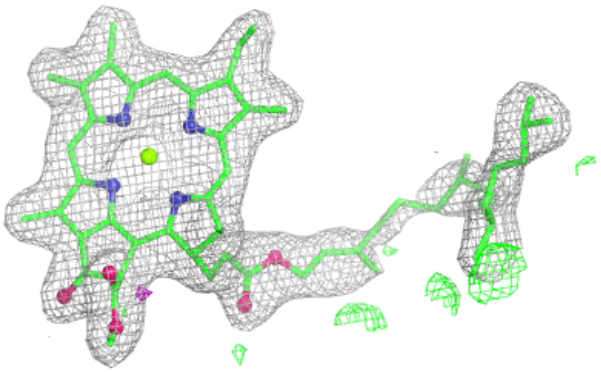


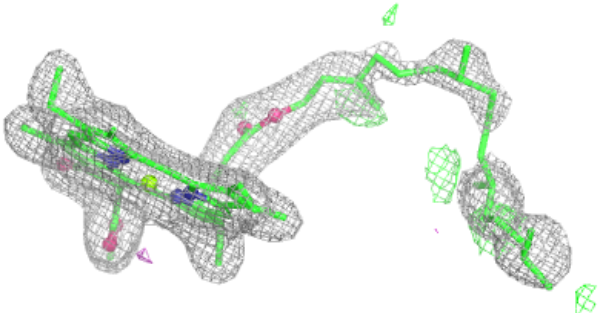


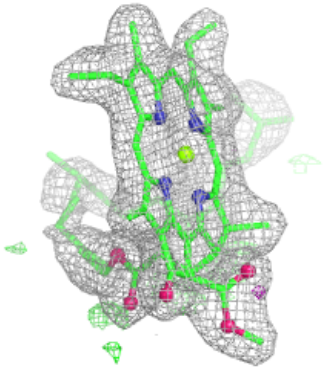


Electron density around CLA A 409:

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

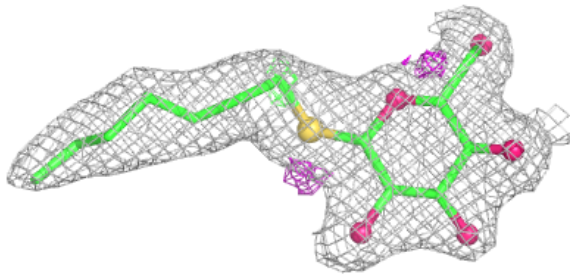


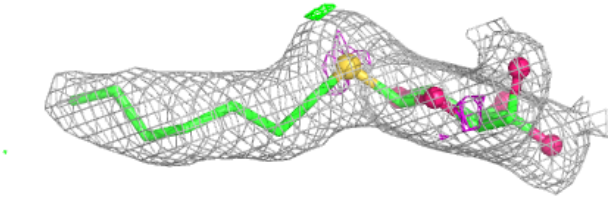


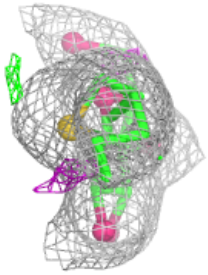


Electron density around HTG b 601:

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

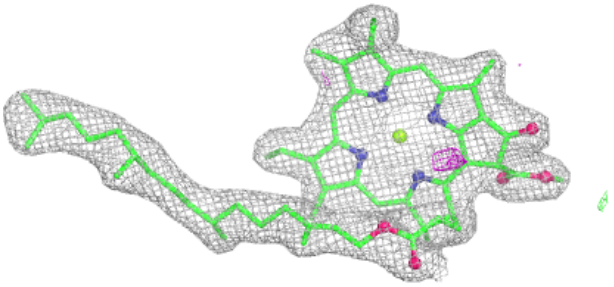


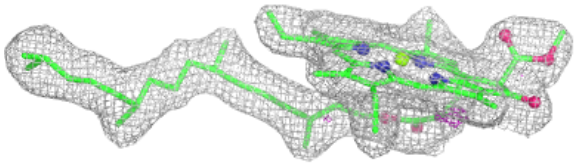


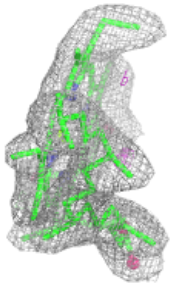


Electron density around CLA c 505:

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

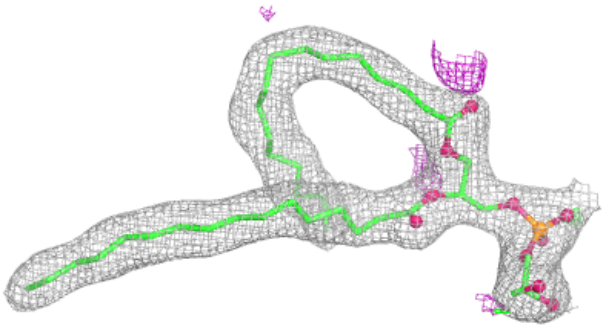


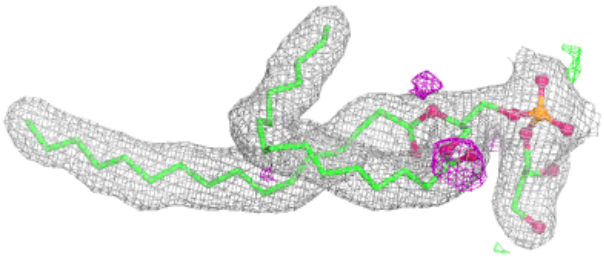


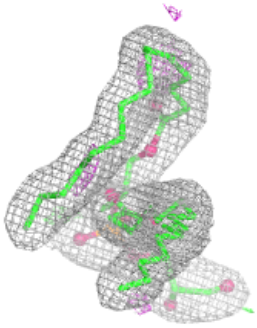


Electron density around LHG d 407:

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

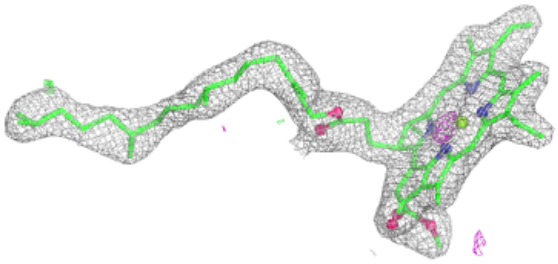


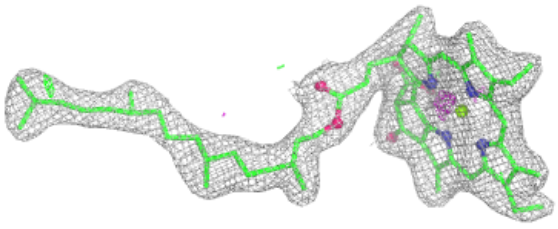


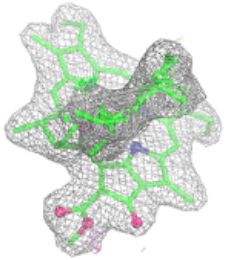


Electron density around CLA c 506:

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

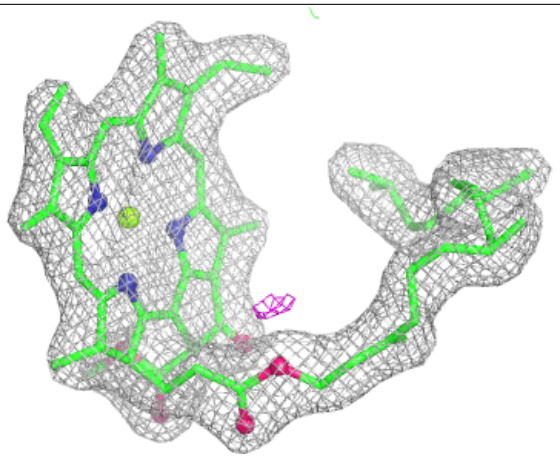


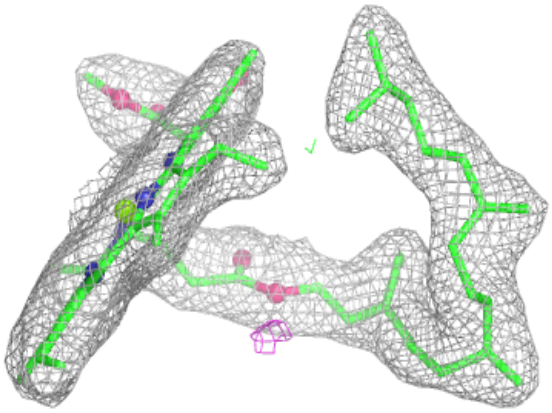


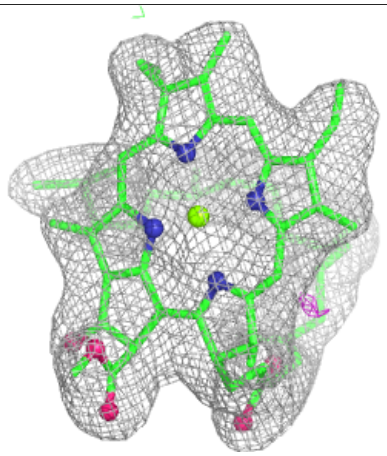


Electron density around CLA C 504:

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

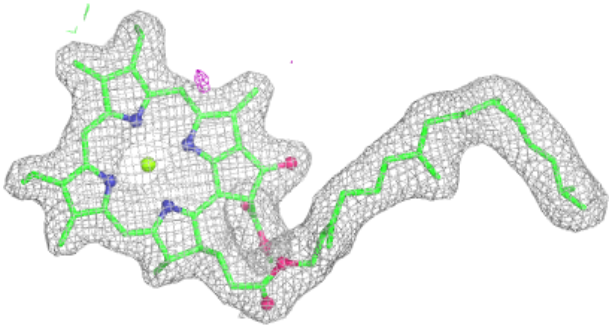


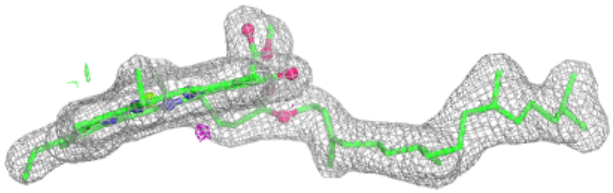


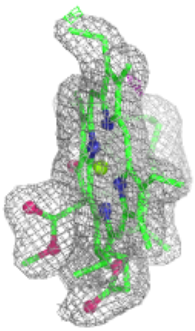


Electron density around CLA B 603:

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

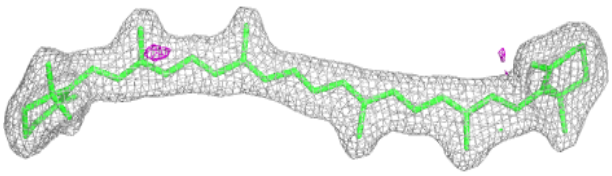


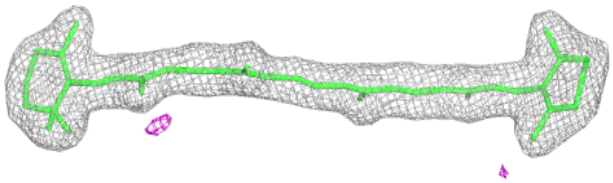


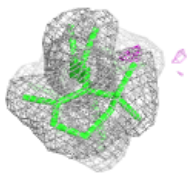


Electron density around BCR a 413:

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

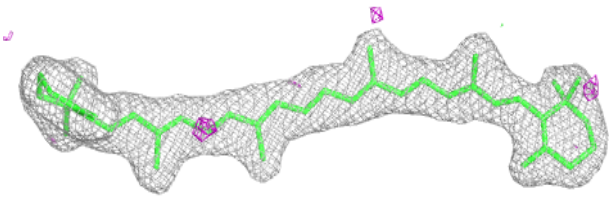


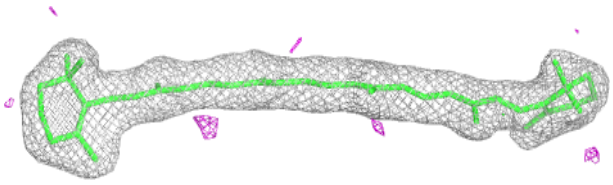


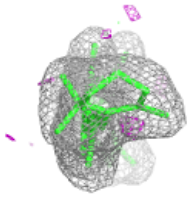


Electron density around BCR b 626:

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

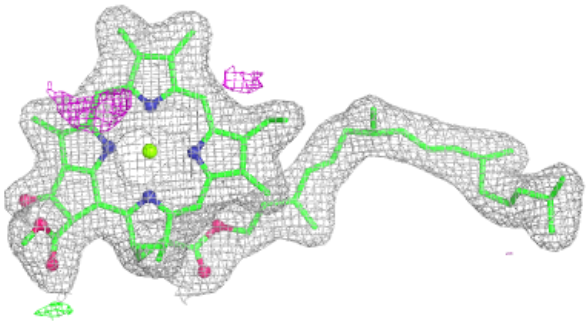


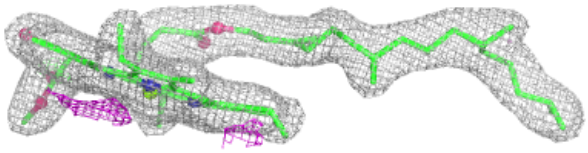


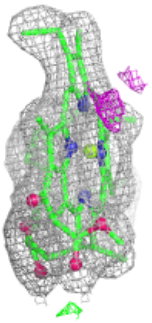


Electron density around CLA B 604:

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

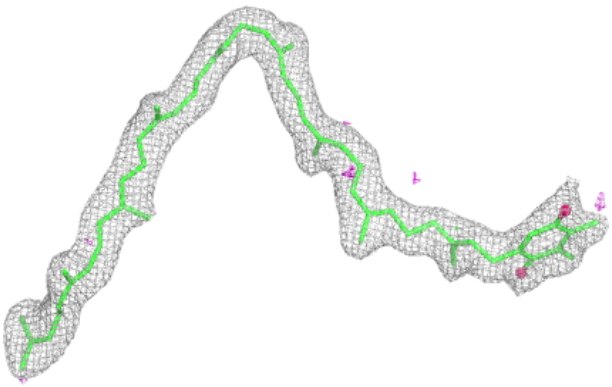


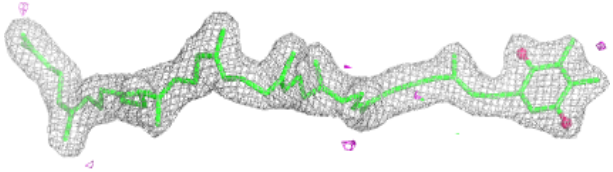


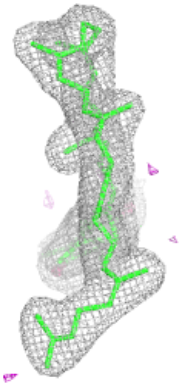


Electron density around PL9 d 406:

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

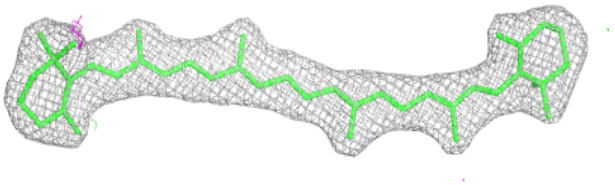


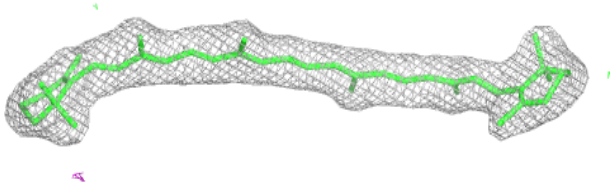


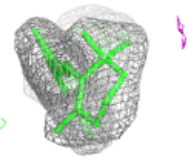


Electron density around BCR b 628:

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

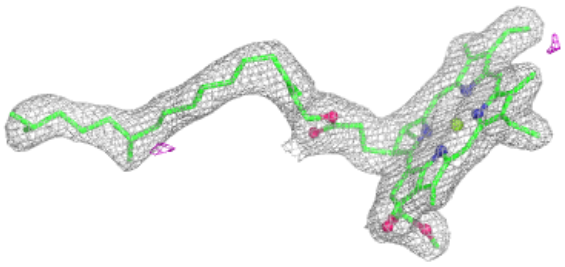


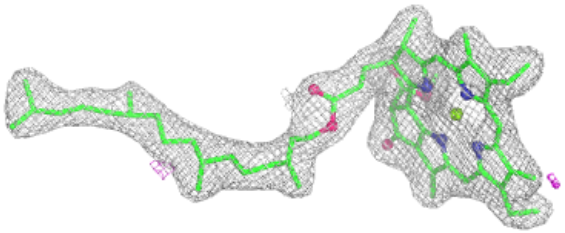


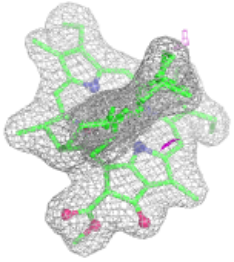


Electron density around CLA C 503:

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

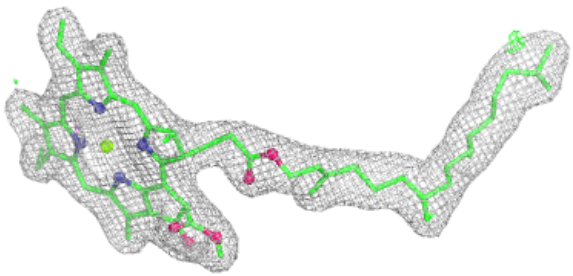


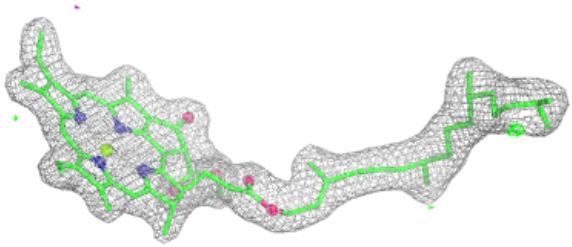


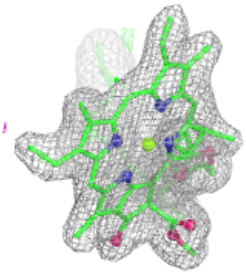


Electron density around CLA a 409:

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

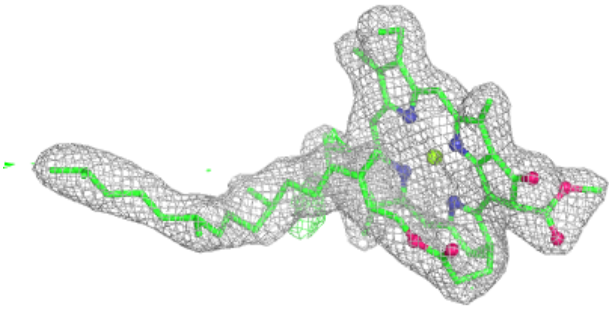


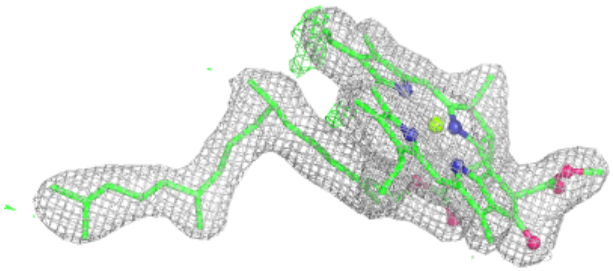


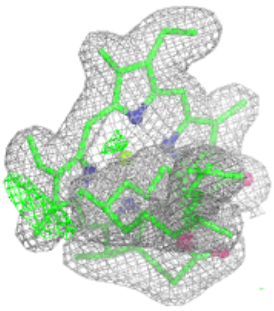


Electron density around CLA c 509:

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

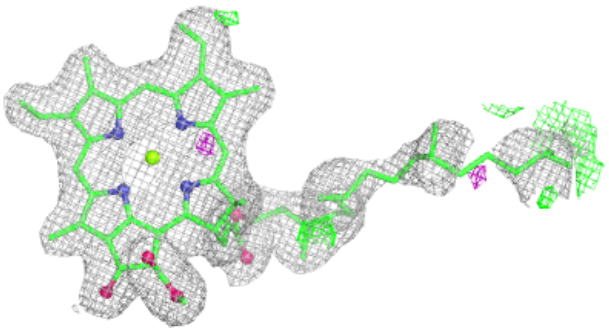


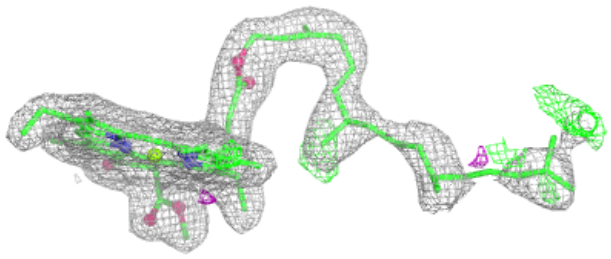


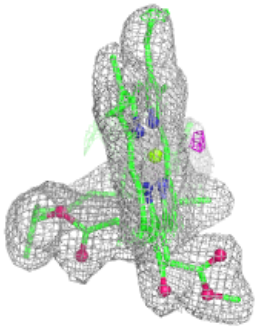


Electron density around CLA a 410:

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

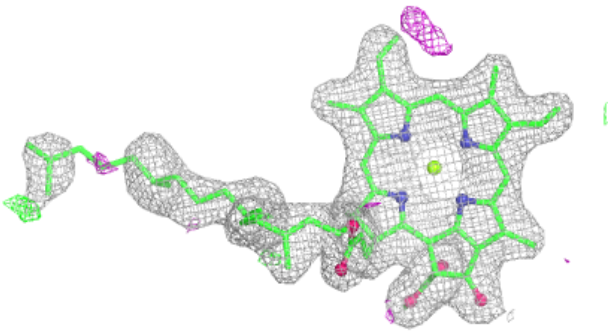


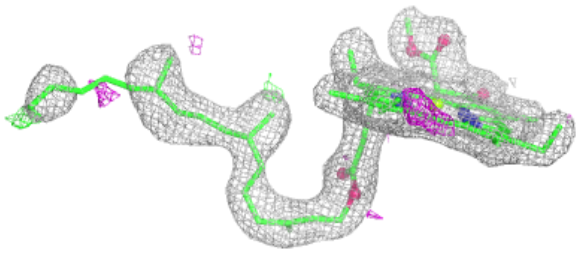


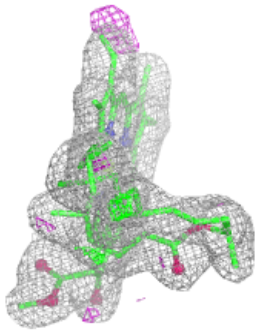


Electron density around CLA A 407:

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

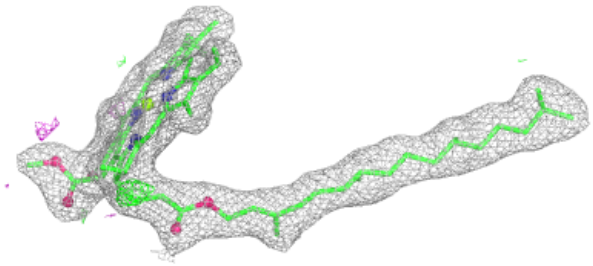


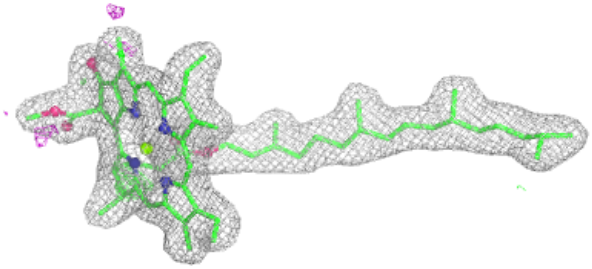


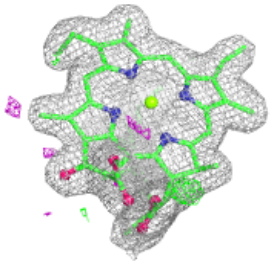


Electron density around CLA B 608:

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

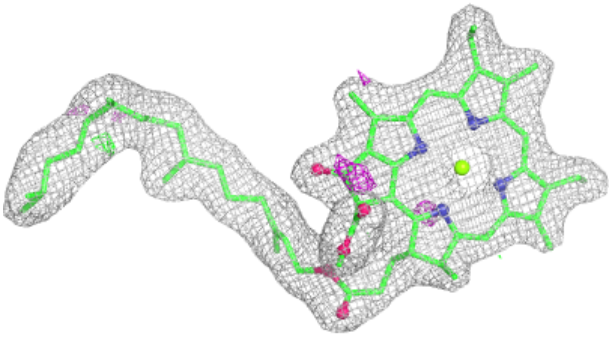


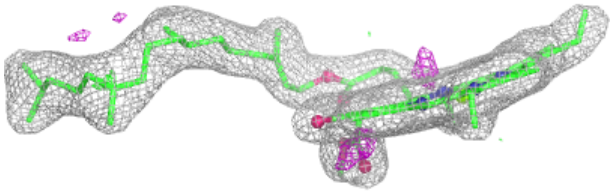


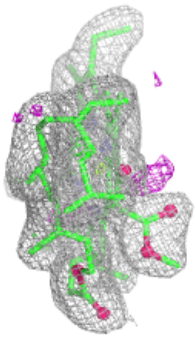


Electron density around CLA b 611:

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

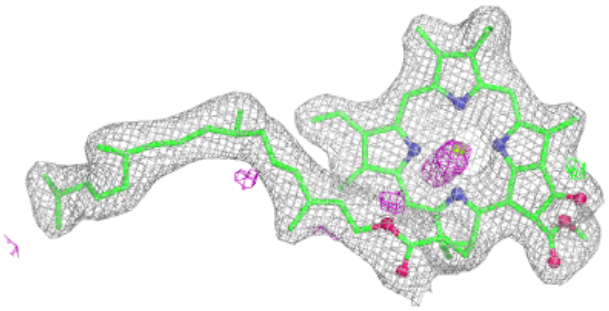


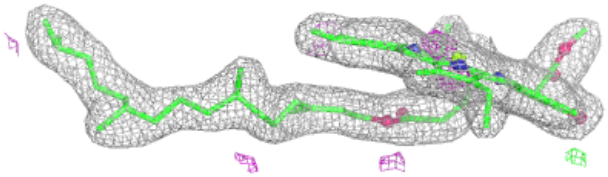


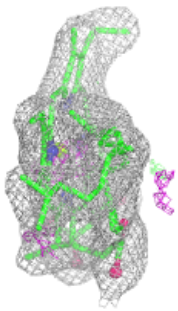


Electron density around CLA b 612:

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

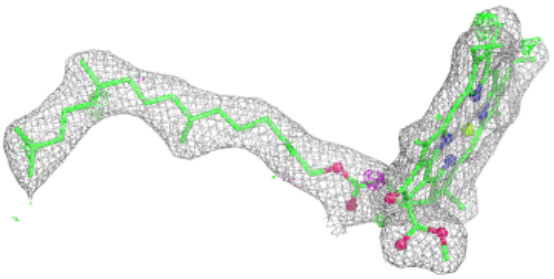


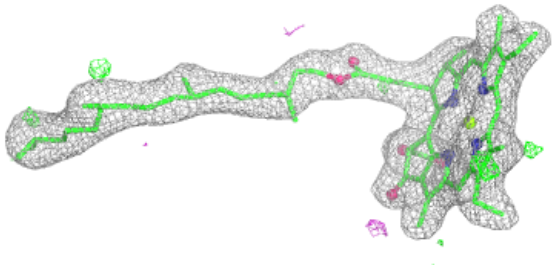


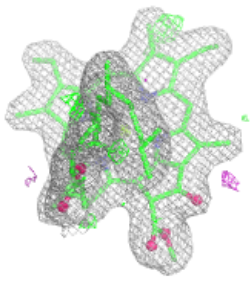


Electron density around CLA b 613:

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

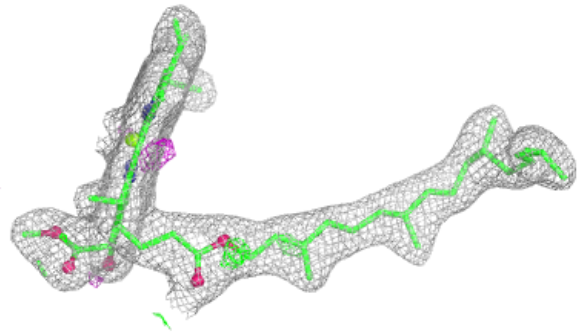


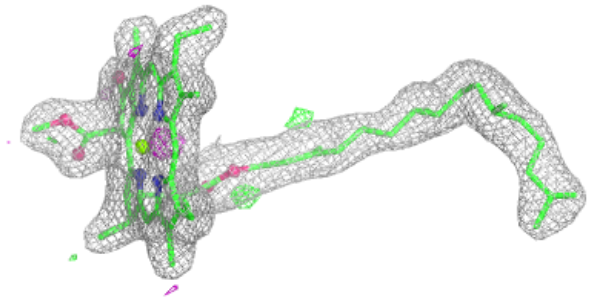


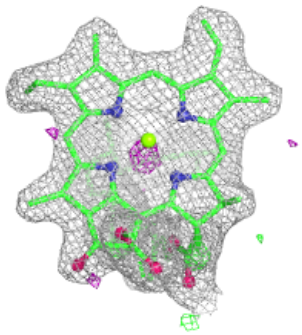


Electron density around CLA b 614:

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

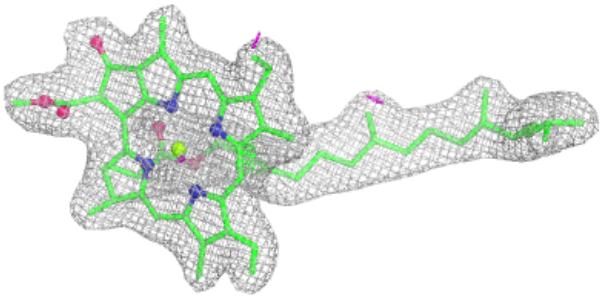


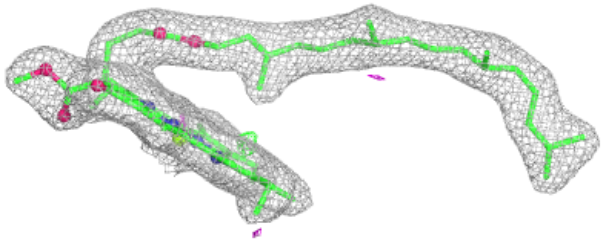


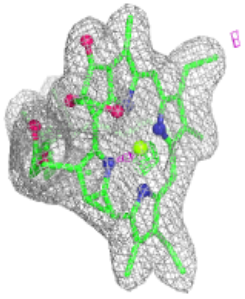


Electron density around CLA B 609:

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

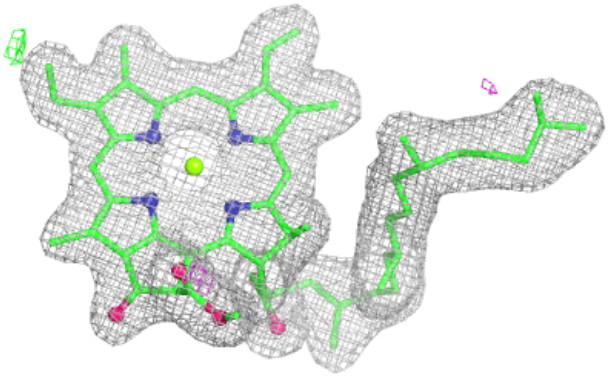


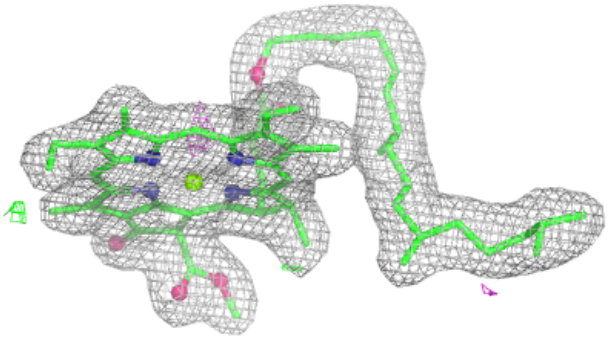


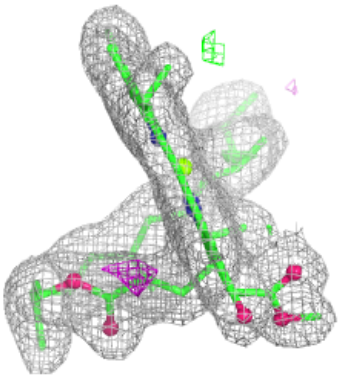


Electron density around CLA d 402:

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

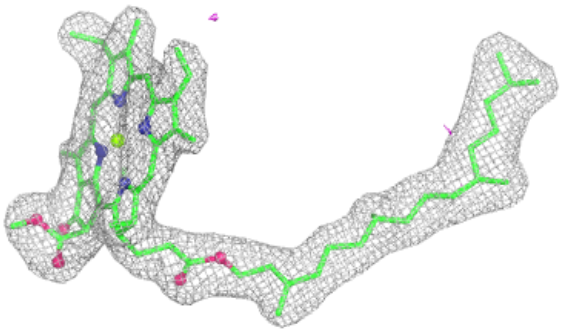


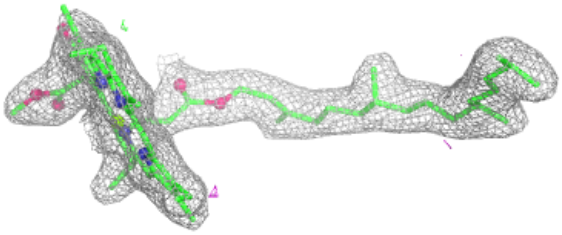


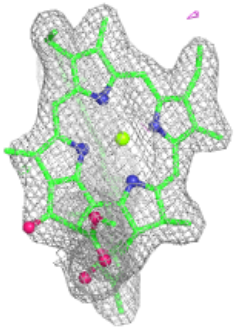


Electron density around CLA B 610:

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

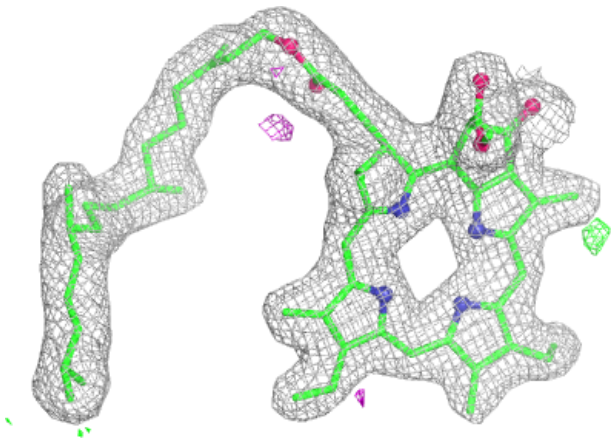


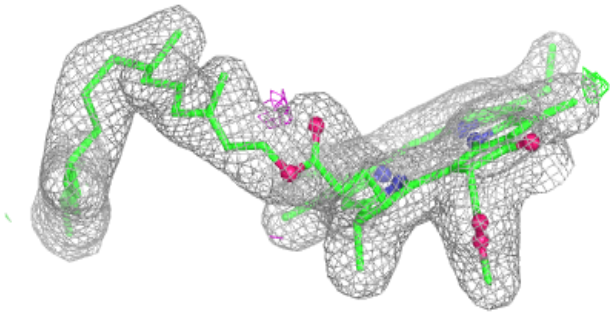


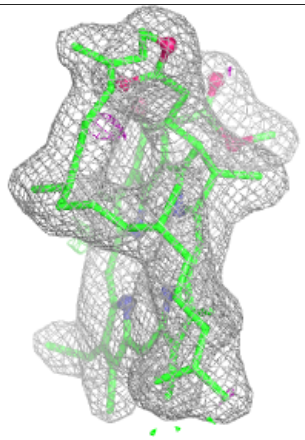


Electron density around PHO A 408:

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

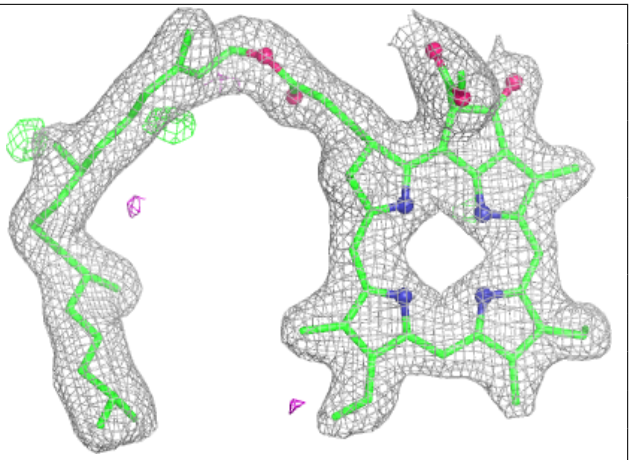


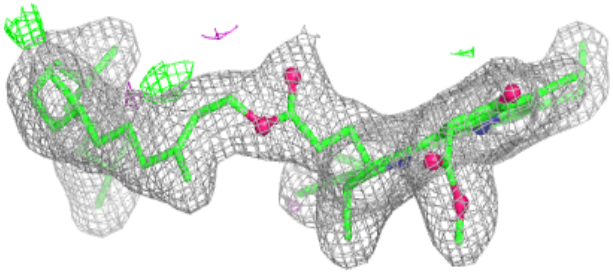


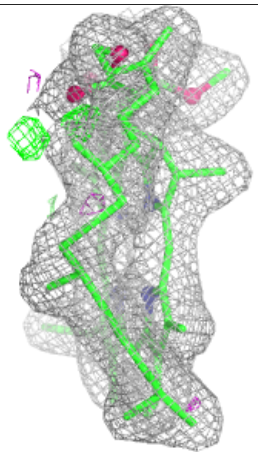


Electron density around PHO D 401:

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

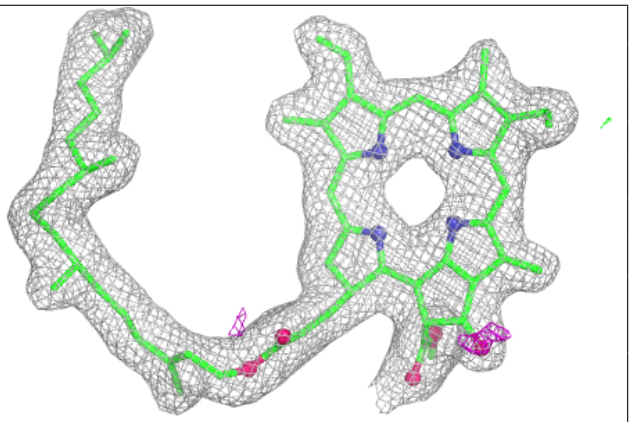


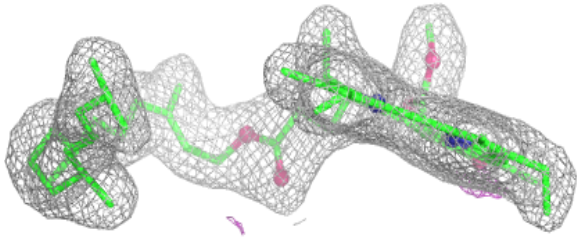


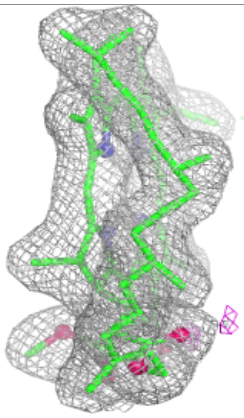


Electron density around PHO a 411:

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

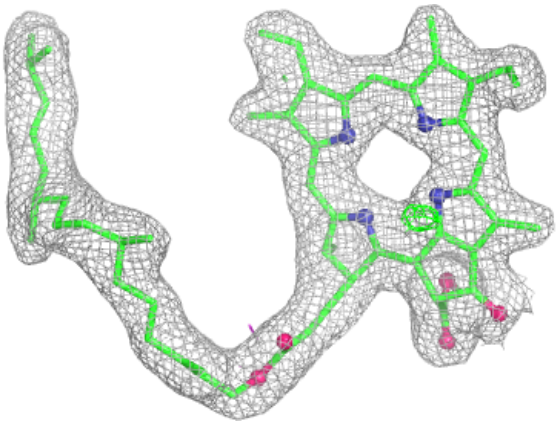


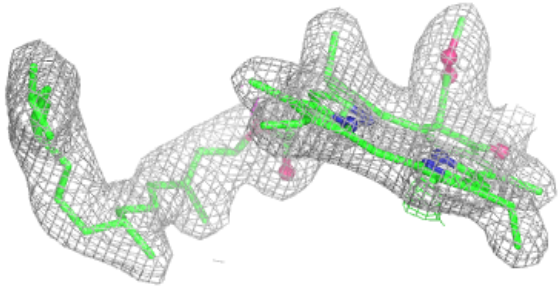


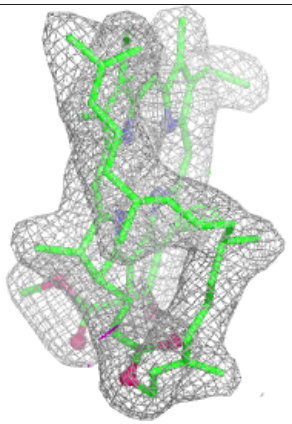


Electron density around PHO d 401:

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

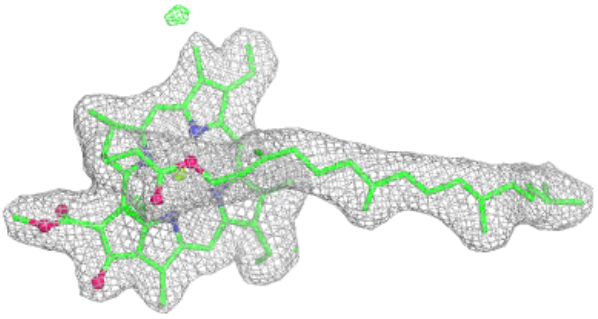


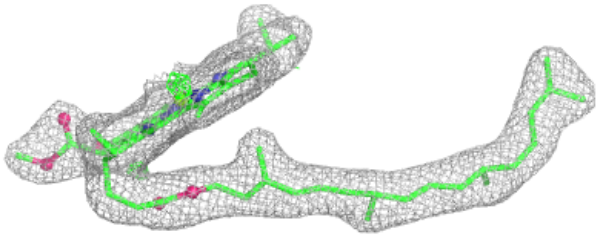




Electron density around CLA b 617:

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

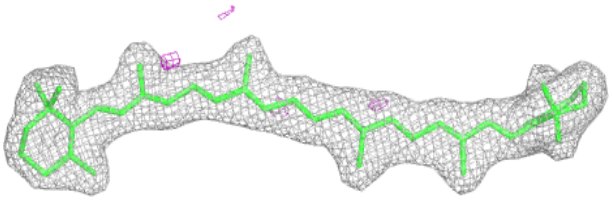


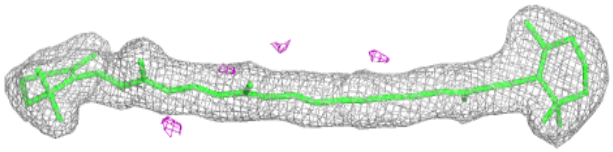


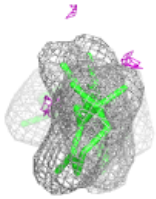


Electron density around BCR B 618:

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

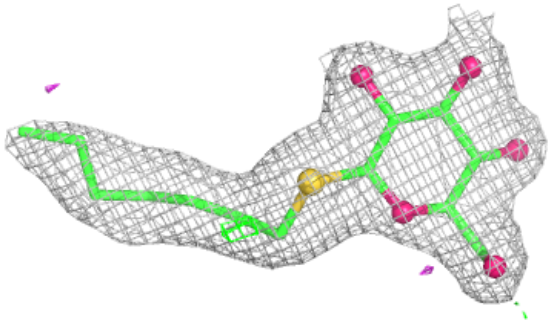


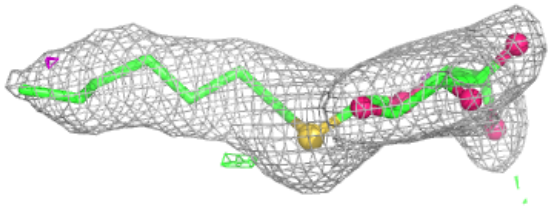


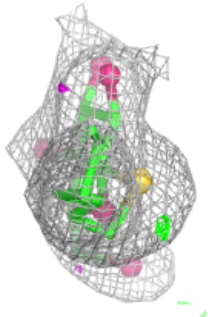


Electron density around HTG B 623:

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

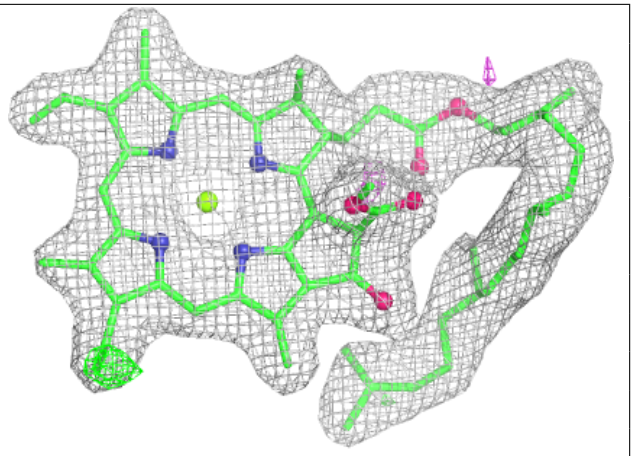


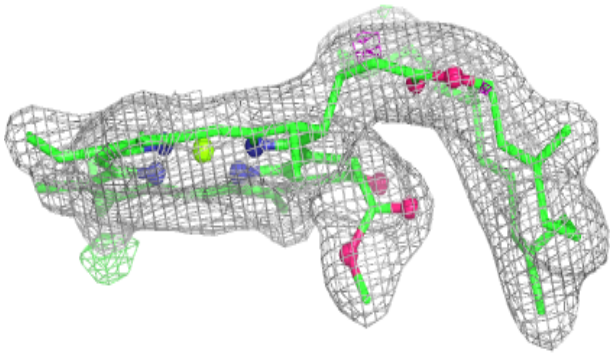


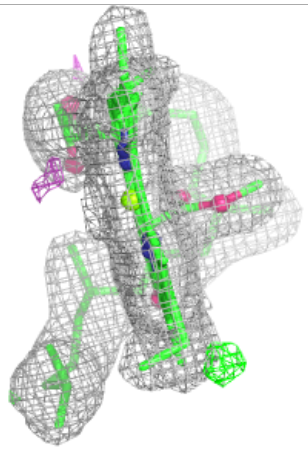


Electron density around CLA B 611:

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

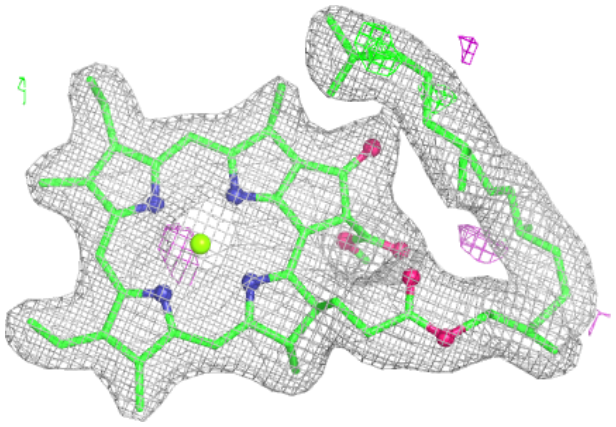


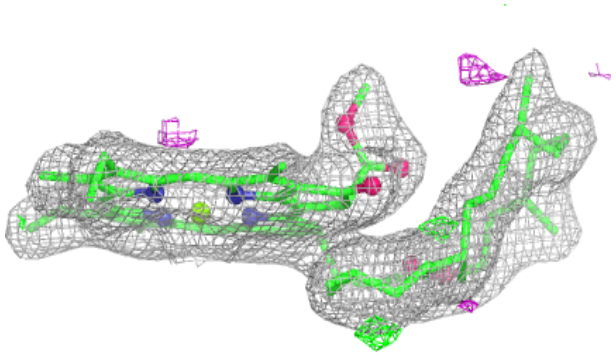


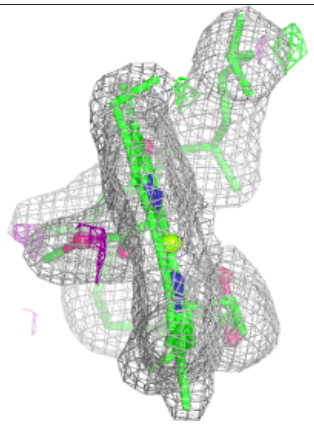


Electron density around CLA b 619:

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

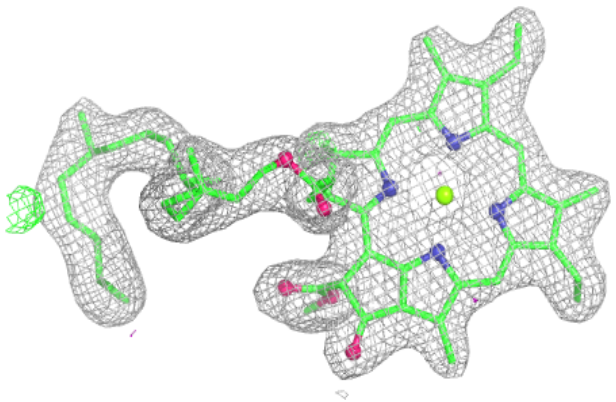


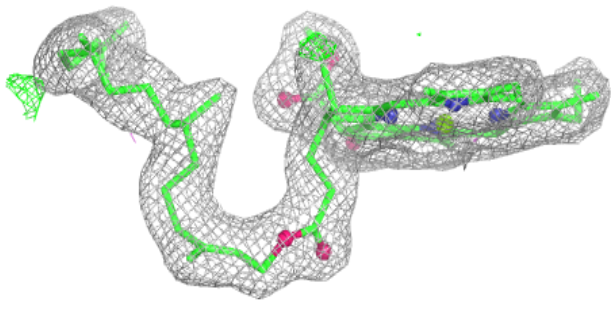


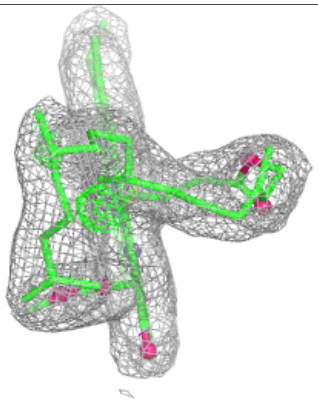


Electron density around CLA B 613:

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

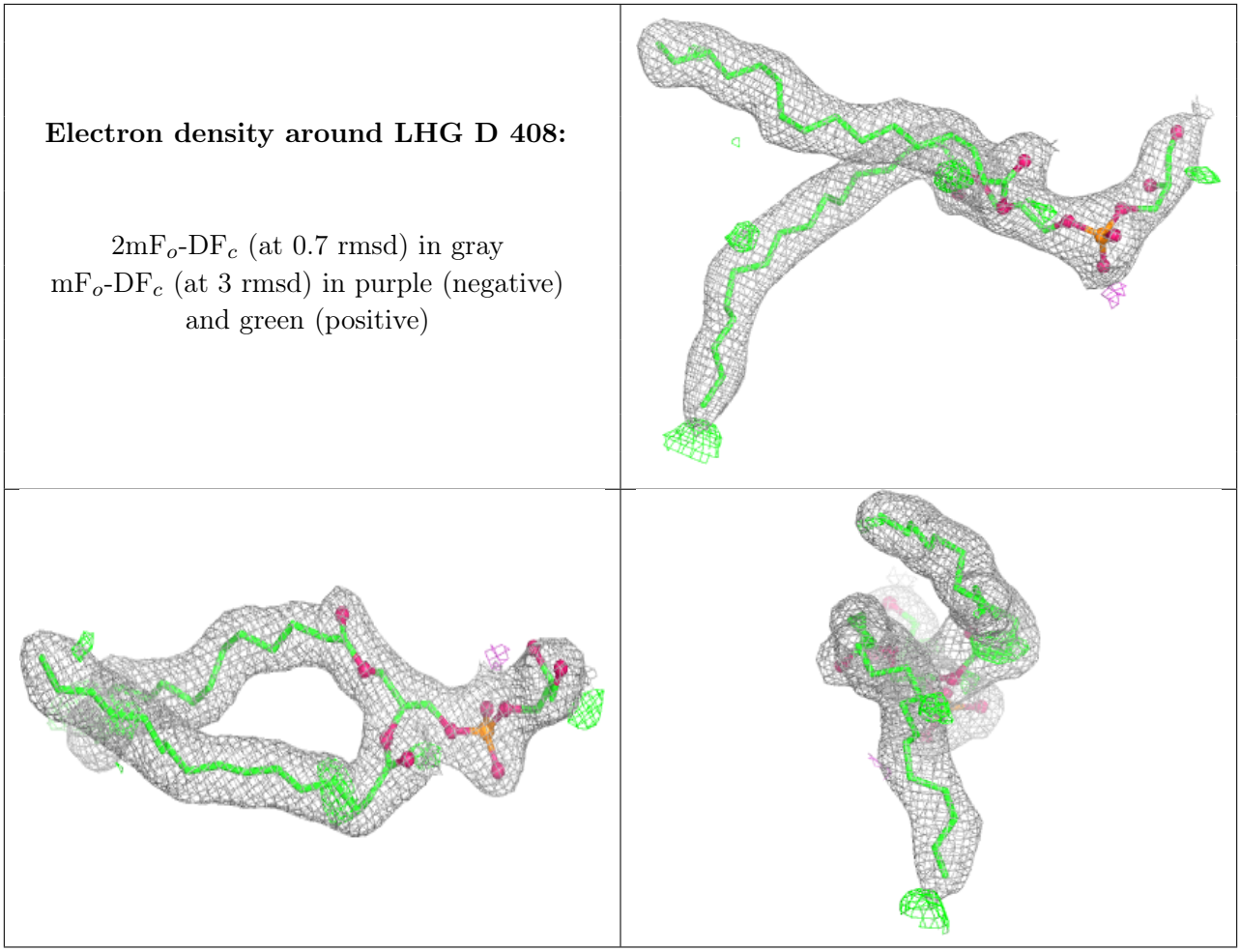






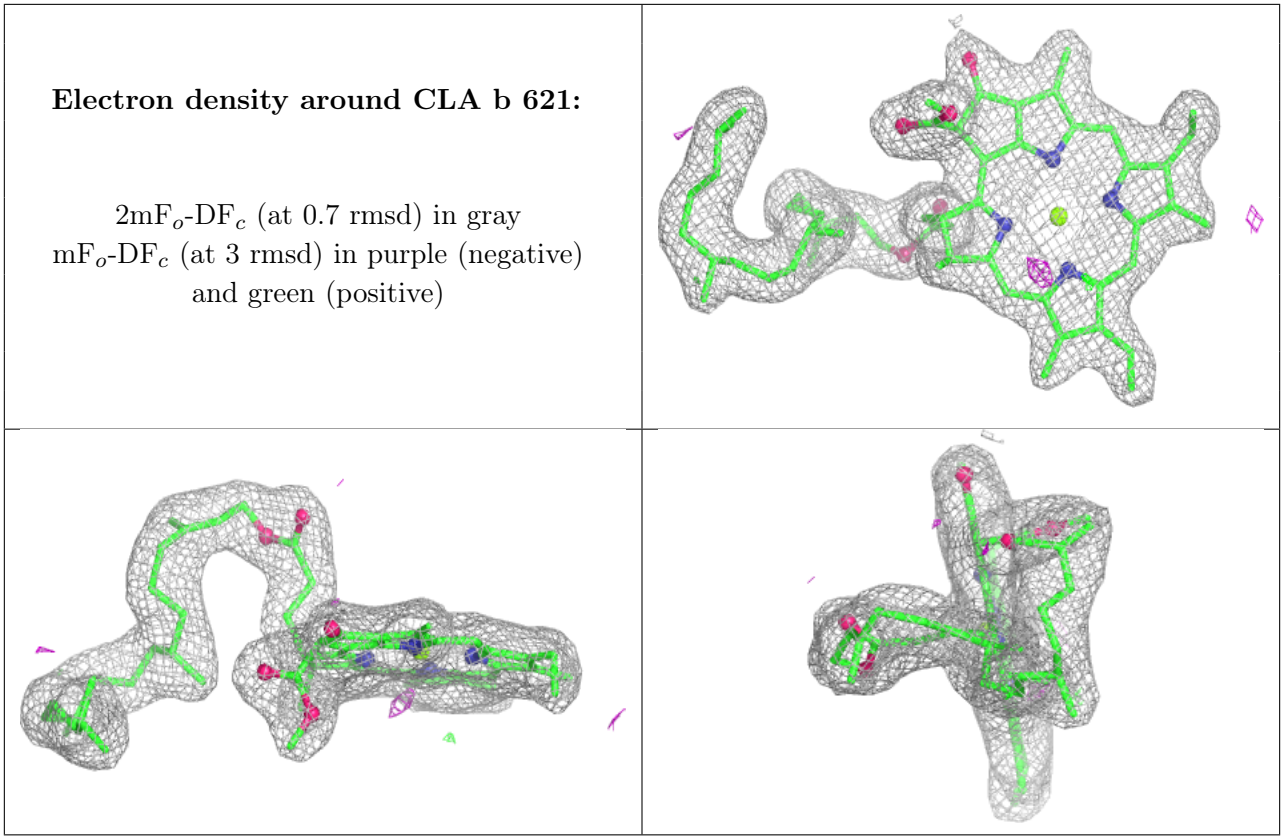
Electron density around LHG D 408:

$2mF_o$-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 621:

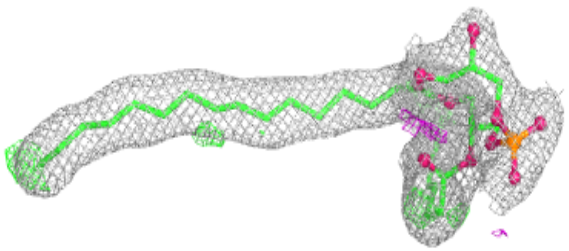
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

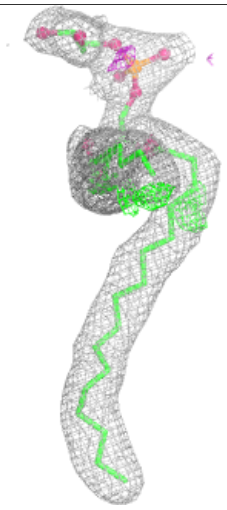


Electron density around LHG L 101:

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

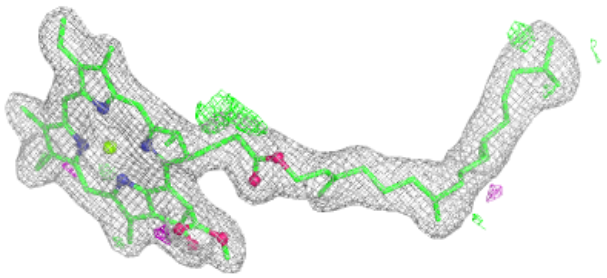


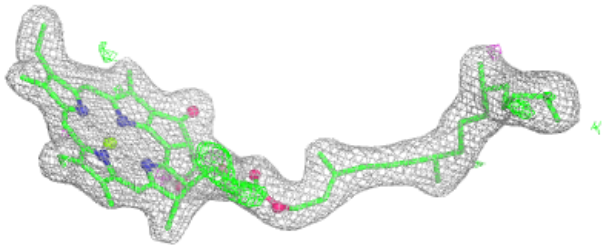




Electron density around CLA A 405:

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

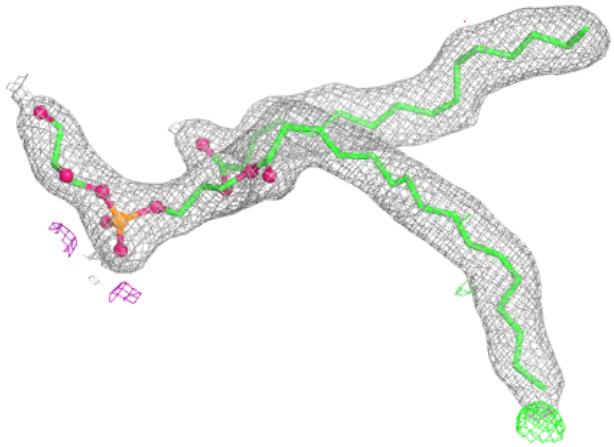


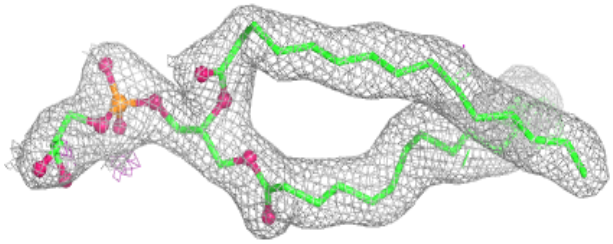


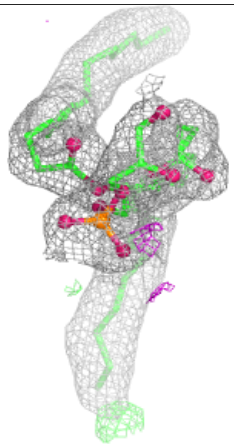


Electron density around LHG d 408:

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

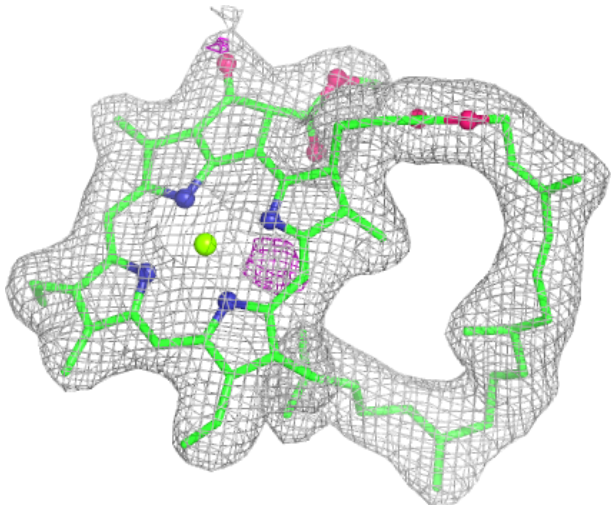


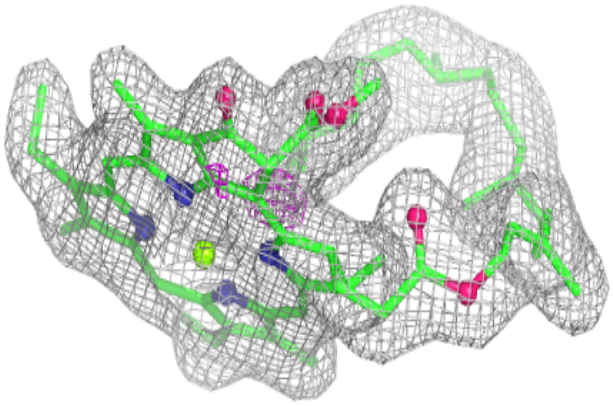


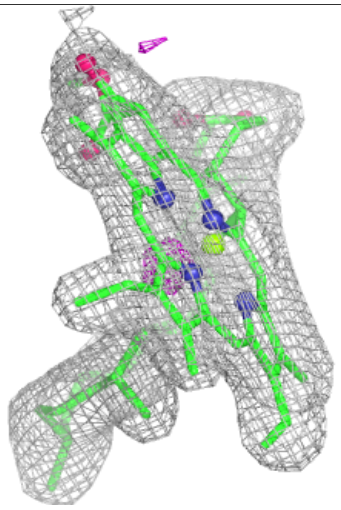


Electron density around CLA b 624:

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

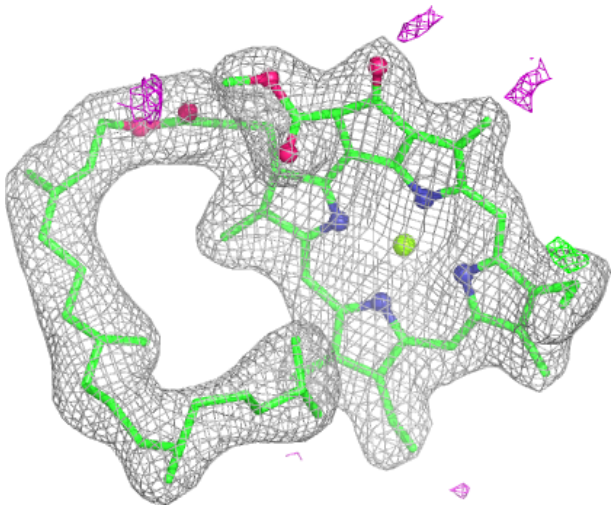


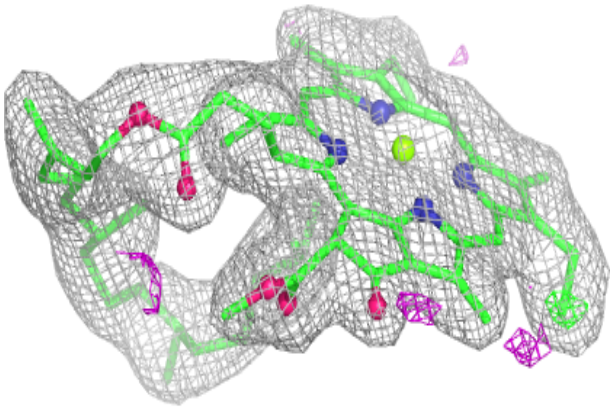


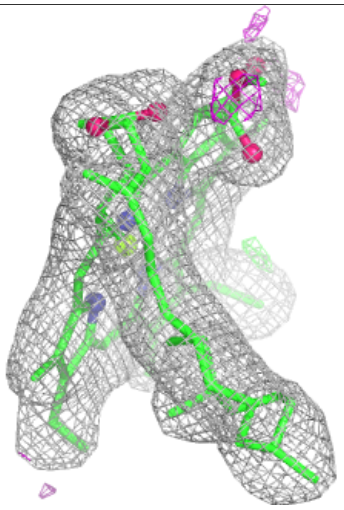


Electron density around CLA B 616:

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



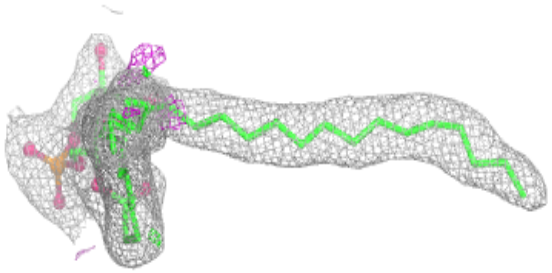


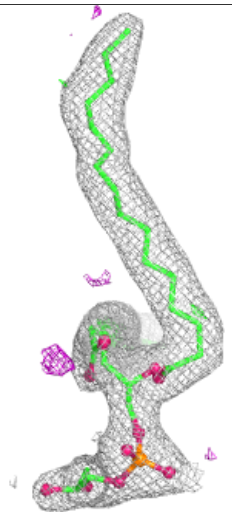


Electron density around LHG l 101:

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

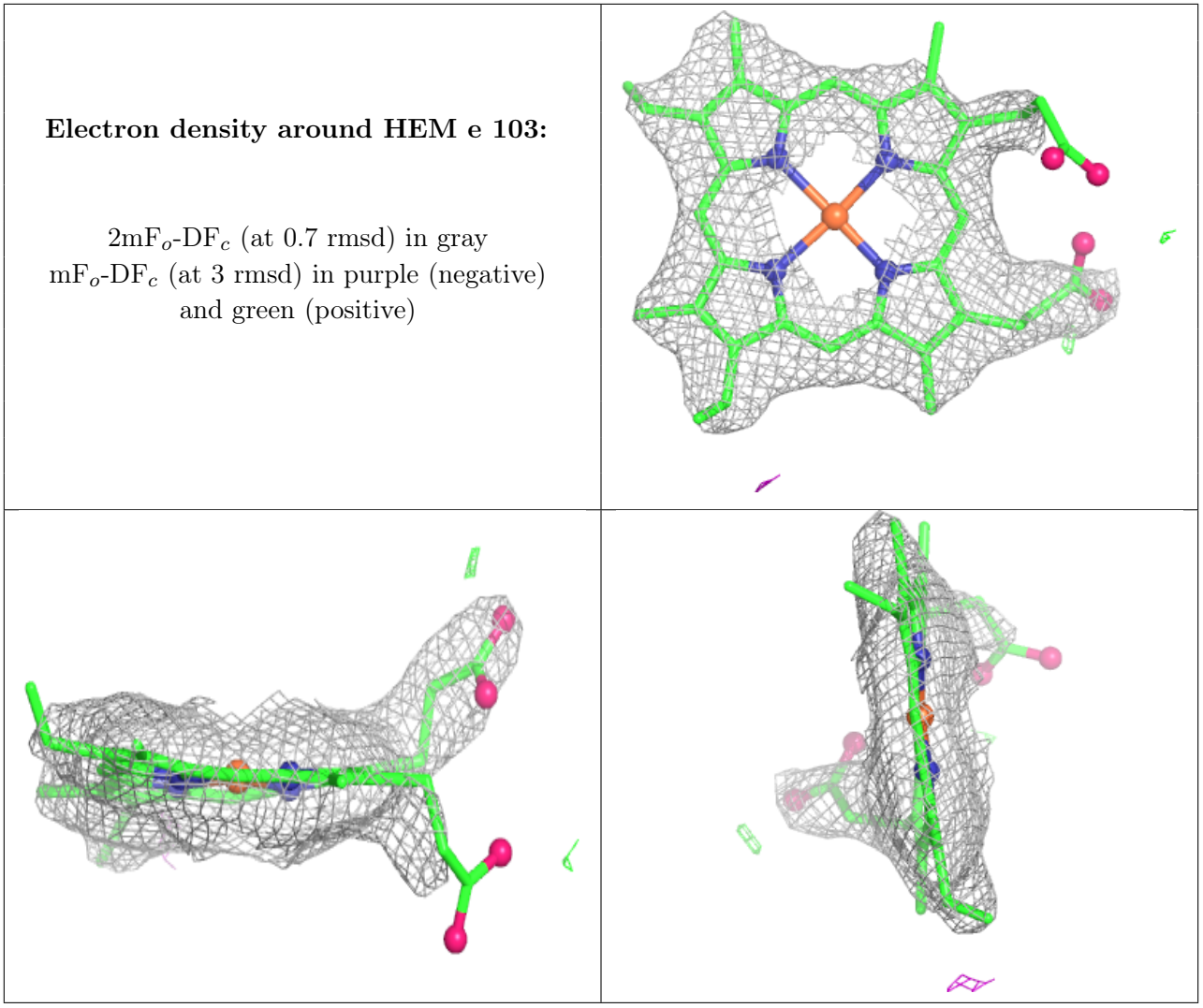






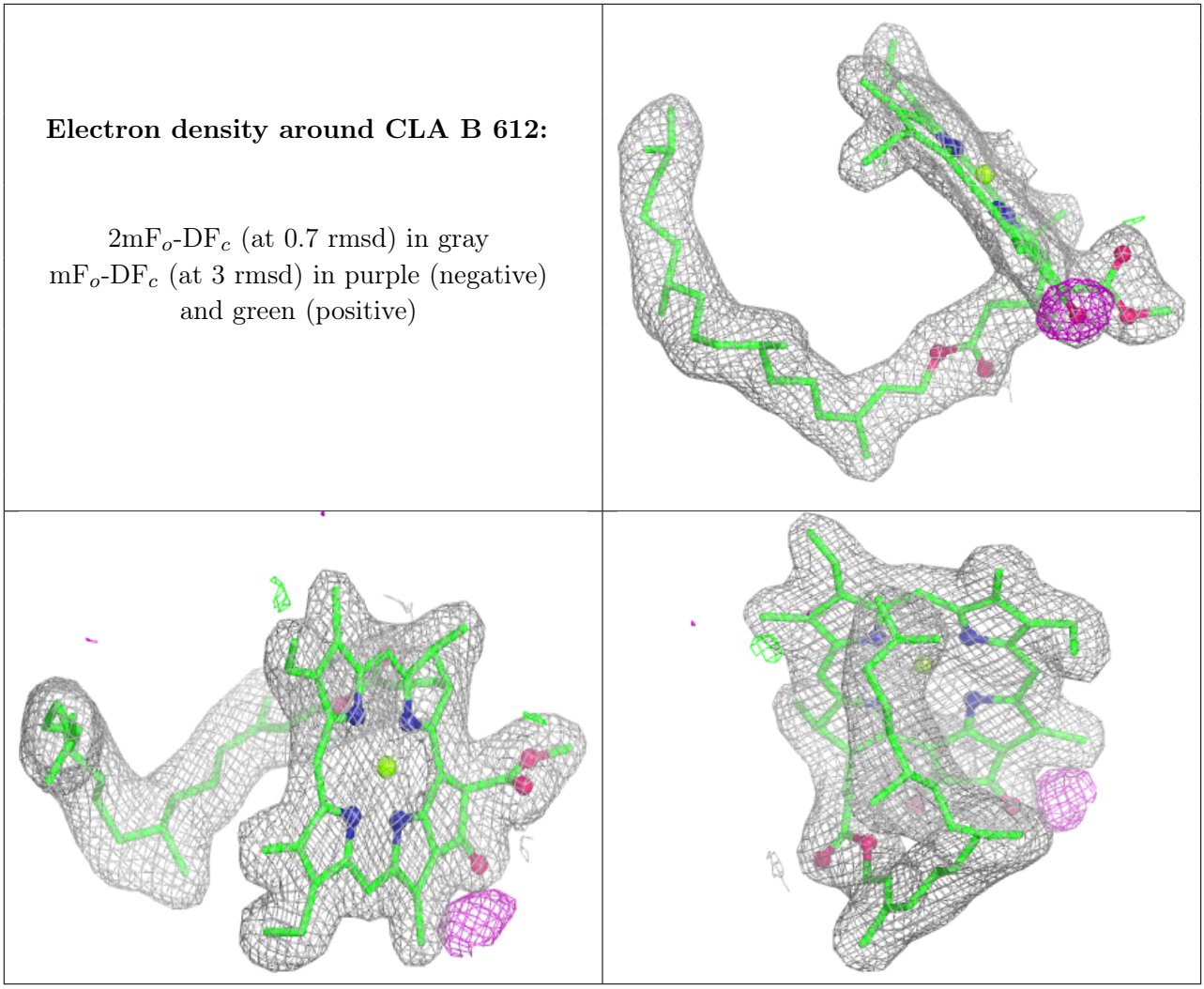
Electron density around HEM e 103:

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



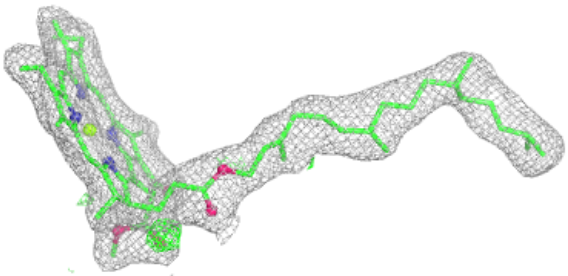
Electron density around CLA B 612:

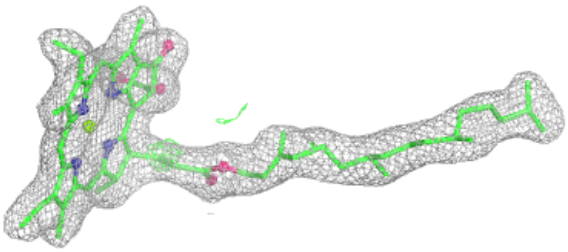
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

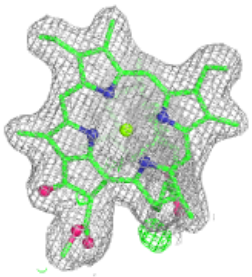


Electron density around CLA B 605:

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

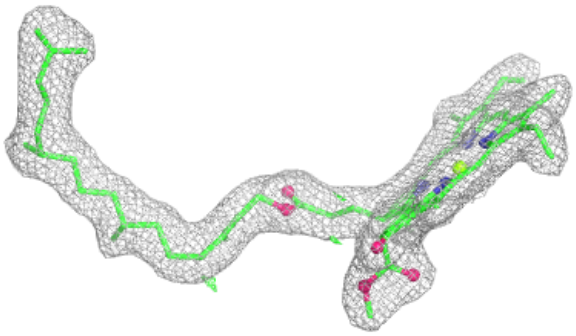


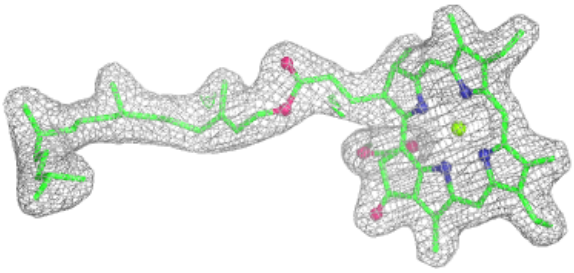


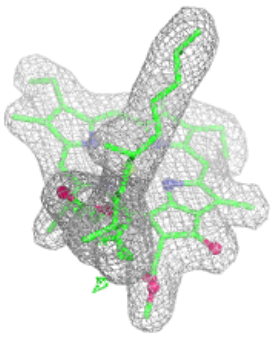


Electron density around CLA d 403:

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

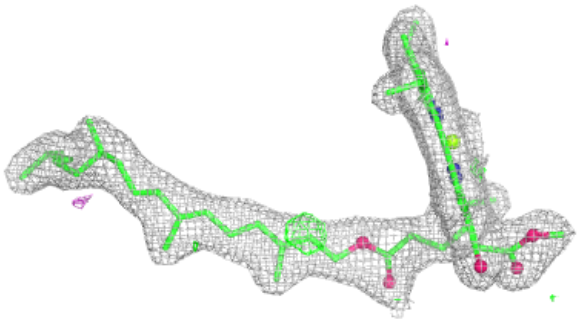


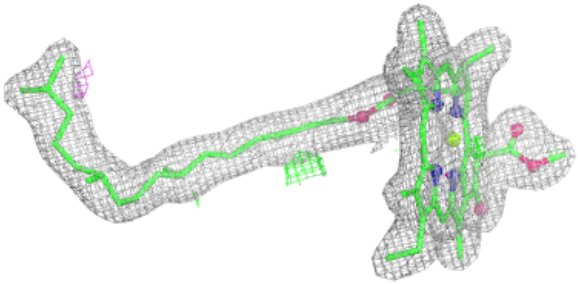


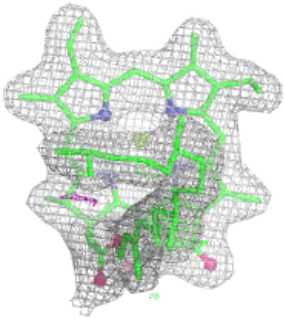


Electron density around CLA B 606:

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

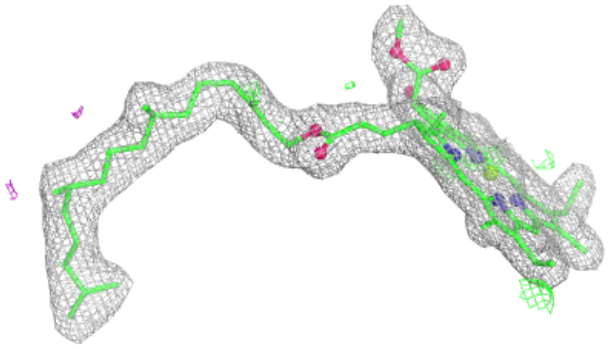


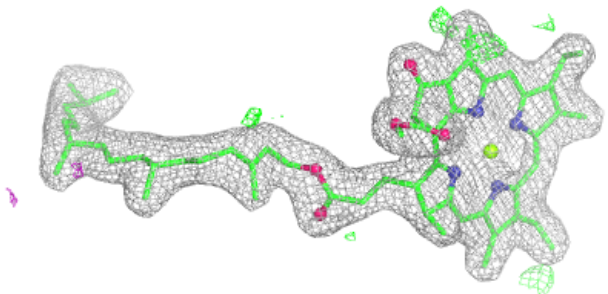


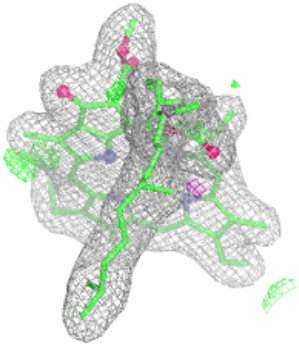


Electron density around CLA D 402:

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

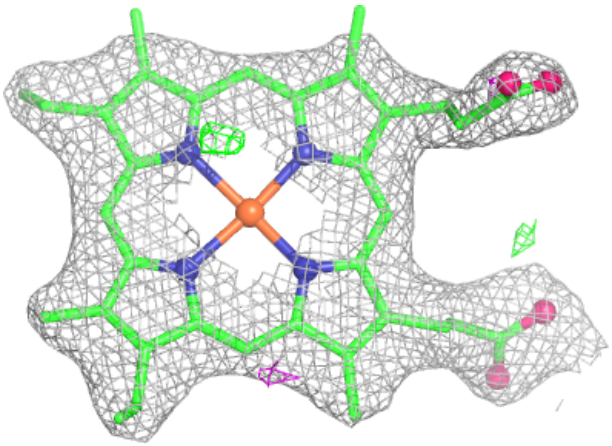


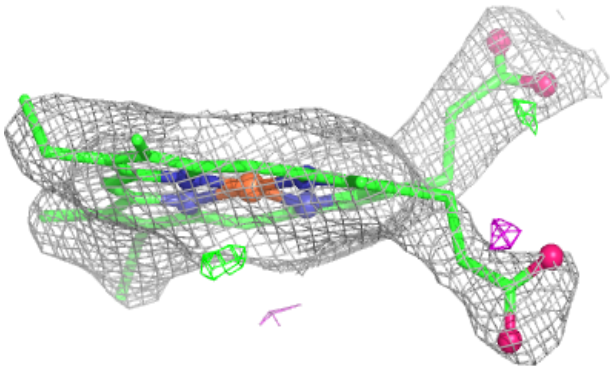


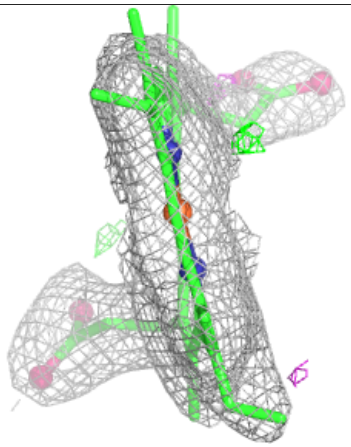


Electron density around HEM E 102:

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

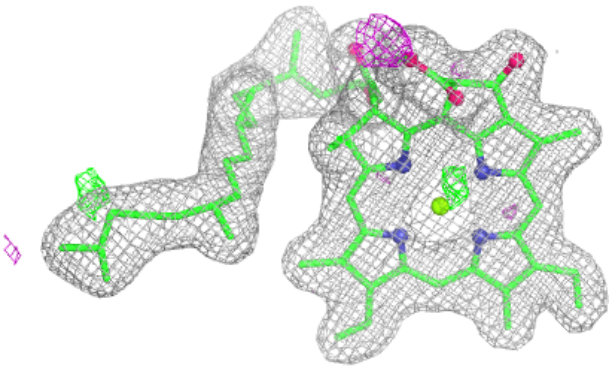


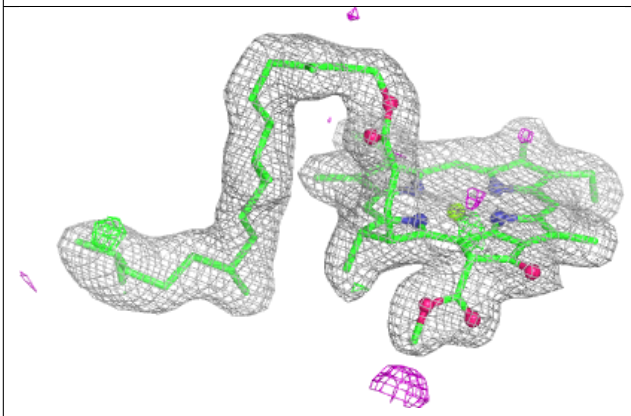


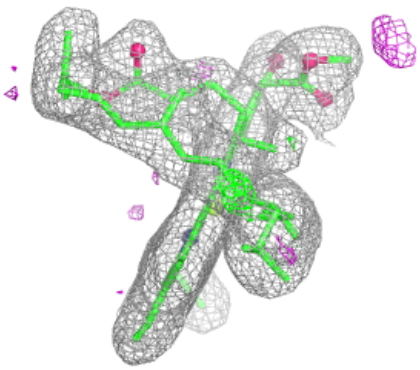


Electron density around CLA A 406:

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

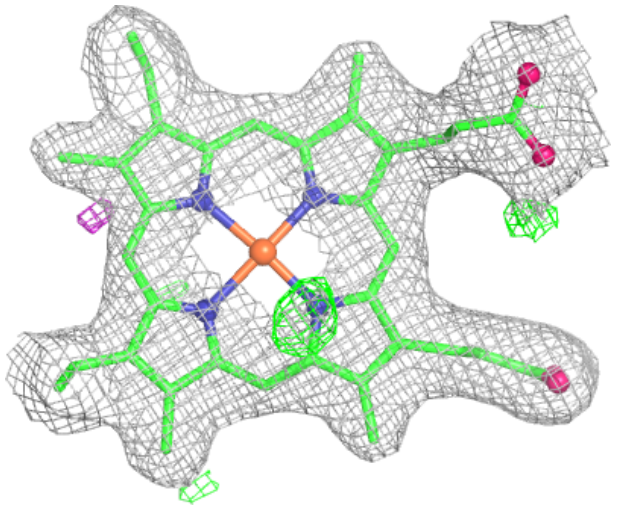


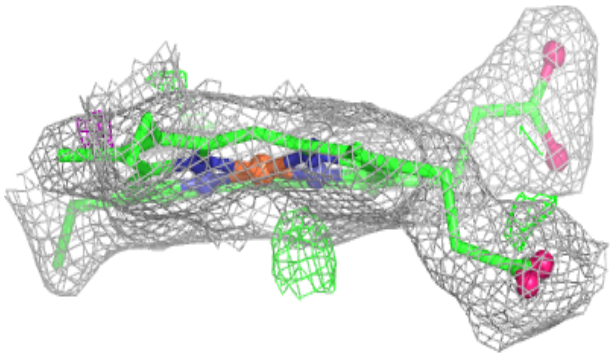




Electron density around HEC V 205:

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

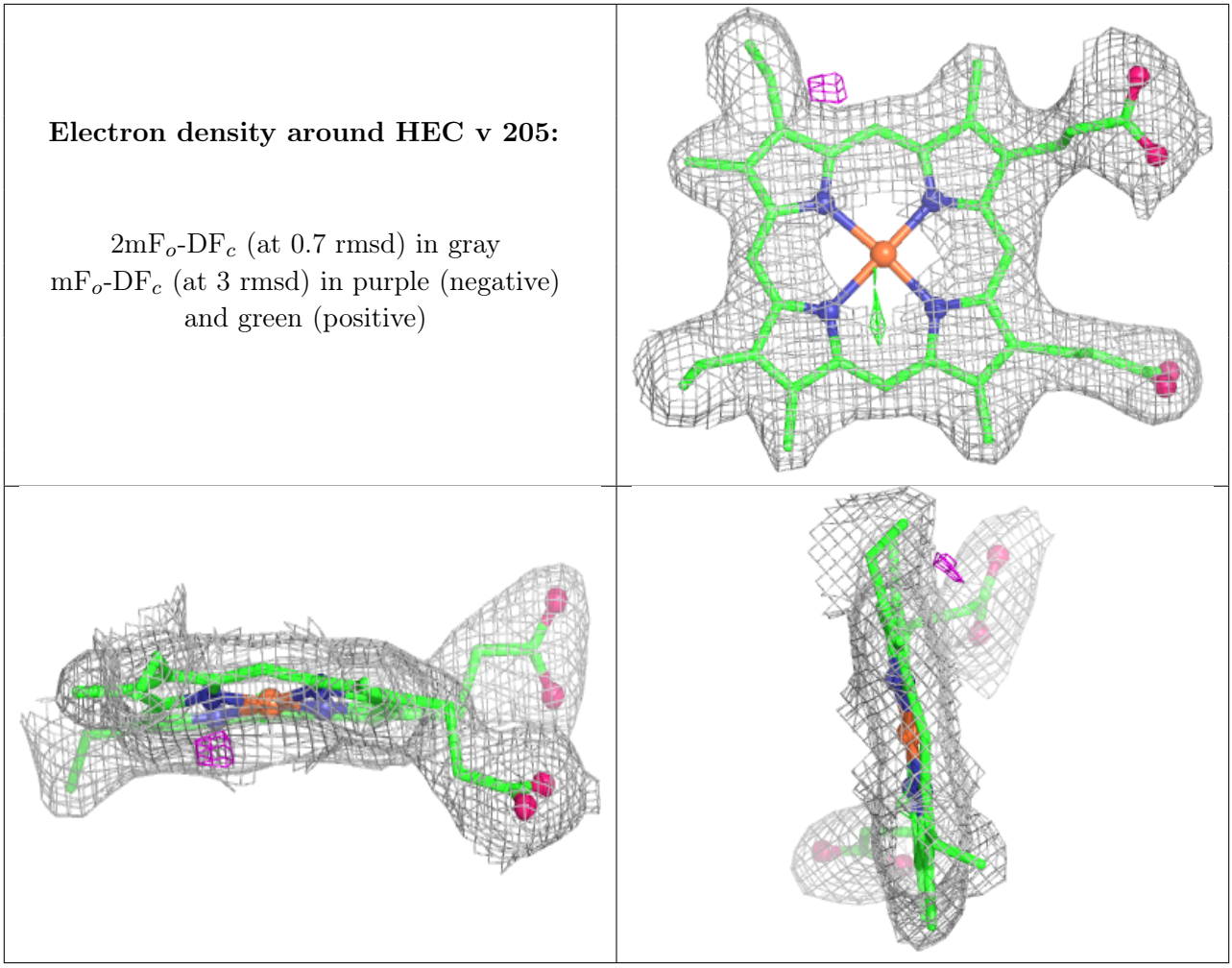






Electron density around HEC v 205:

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



6.5 Other polymers (i)

There are no such residues in this entry.