Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 02:11 PM UTC

PDB ID	:	5B66 / pdb_00005b66
Title	:	Crystal structure analysis of Photosystem II complex
Authors	:	Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on	:	2016-05-25
Resolution	:	1.85 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:

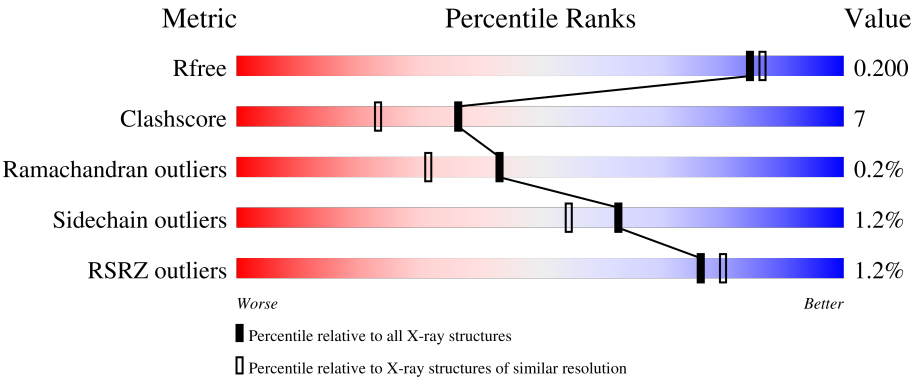
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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.



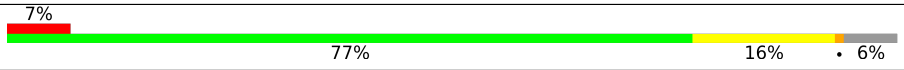
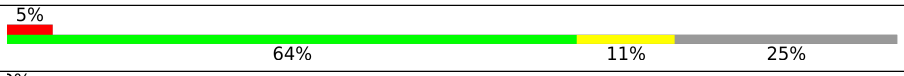
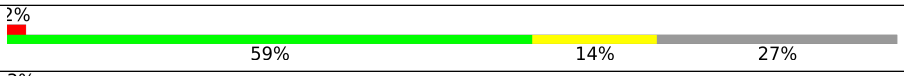
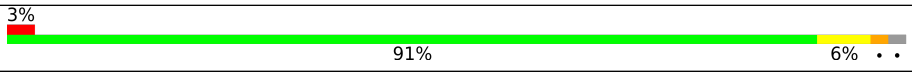
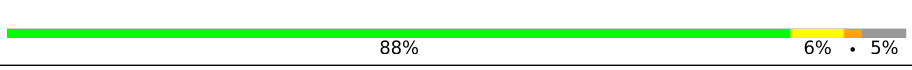
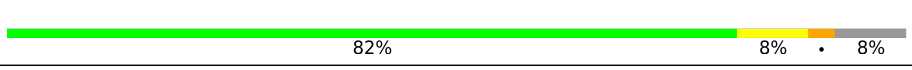
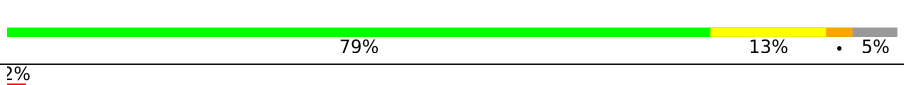
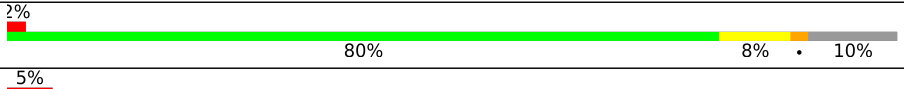
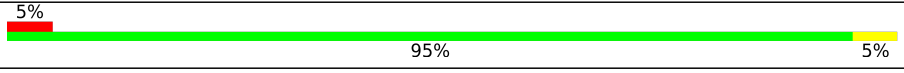
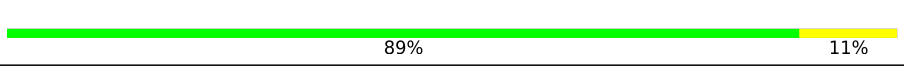
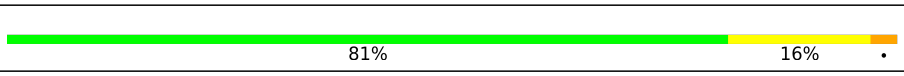
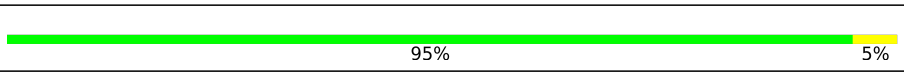
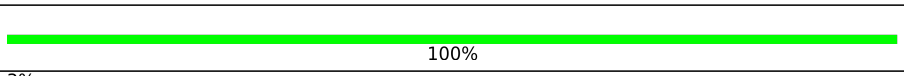
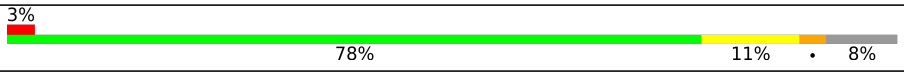
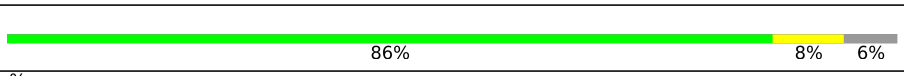
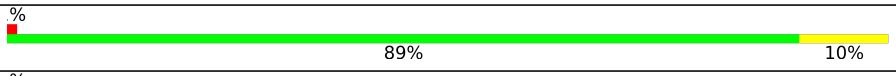
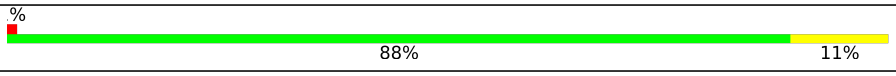
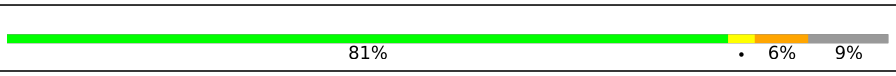
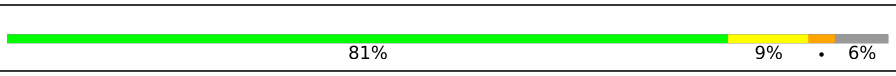
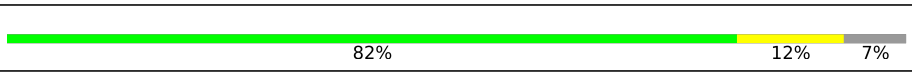
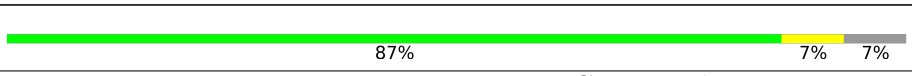
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	87% 10%
1	a	344	88% 9%
2	B	505	89% 10%
2	b	505	90% 8%
3	C	455	91% 8%

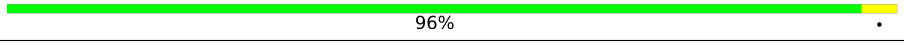
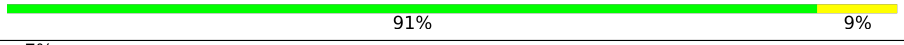
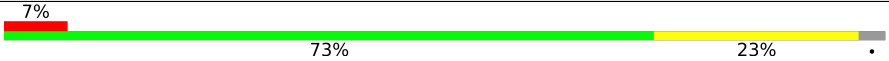
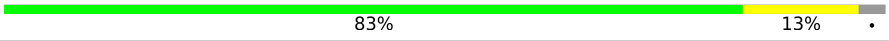
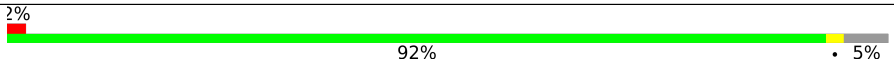
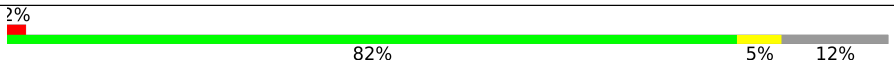
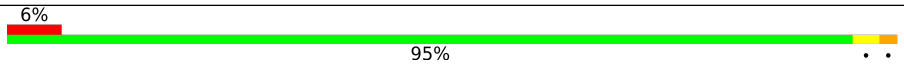
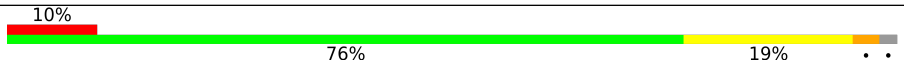
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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	401	X	-	-	-
20	CLA	B	601	X	-	-	-
20	CLA	B	602	X	-	-	-
20	CLA	B	603	X	-	-	-
20	CLA	B	604	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	607	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	613	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	B	616	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-
20	CLA	C	507	X	-	-	-
20	CLA	C	508	X	-	-	-
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	512	X	-	-	-
20	CLA	D	401	X	-	-	-
20	CLA	D	404	X	-	-	-
20	CLA	a	403	X	-	-	-
20	CLA	b	603	X	-	-	-
20	CLA	b	604	X	-	-	-
20	CLA	b	605	X	-	-	-
20	CLA	b	606	X	-	-	-
20	CLA	b	607	X	-	-	-
20	CLA	b	608	X	-	-	-
20	CLA	b	609	X	-	-	-
20	CLA	b	612	X	-	-	-
20	CLA	b	614	X	-	-	-
20	CLA	b	615	X	-	-	-
20	CLA	b	616	X	-	-	-
20	CLA	b	617	X	-	-	-
20	CLA	b	618	X	-	-	-
20	CLA	c	501	X	-	-	-
20	CLA	c	504	X	-	-	-
20	CLA	c	505	X	-	-	-
20	CLA	c	506	X	-	-	-
20	CLA	c	507	X	-	-	-
20	CLA	c	509	X	-	-	-
20	CLA	c	510	X	-	-	-
20	CLA	c	511	X	-	-	-
20	CLA	c	512	X	-	-	-
20	CLA	d	402	X	-	-	-
26	UNL	U	901	-	-	X	-
28	DMS	B	635	-	-	X	-
28	DMS	B	642	-	-	X	-
28	DMS	B	644	-	-	X	-
28	DMS	C	531	-	-	X	-
28	DMS	C	532	-	-	X	-
28	DMS	D	414	-	-	X	-
28	DMS	U	903[B]	-	-	X	-
28	DMS	b	631	-	-	X	-
28	DMS	b	639	-	-	X	-
28	DMS	c	530	-	-	X	-
28	DMS	c	536	-	-	X	-
28	DMS	d	414	-	-	X	-
28	DMS	i	104	-	-	X	-
28	DMS	o	302	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	DMS	o	303	-	-	X	-
28	DMS	o	306	-	-	X	-
28	DMS	v	206	-	-	X	-
31	BCT	A	421	-	-	X	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 54996 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
			2626	1721	430	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2622	1719	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	11	0
			4012	2632	668	699	13			
2	b	495	Total	C	N	O	S	0	4	0
			3884	2550	650	671	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	1	0
			3483	2280	582	608	13			
3	c	455	Total	C	N	O	S	0	1	0
			3523	2305	591	614	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2728	1808	446	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	78	Total	C	N	O	0	1	0
			632	413	101	118			
5	e	78	Total	C	N	O	0	2	0
			636	419	99	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	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	64	Total	C	N	O	S	0	1	0
			508	339	81	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total 284	C 194	N 45	O 44	S 1	0	0	0
8	i	36	Total 300	C 203	N 49	O 47	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total 251	C 171	N 37	O 42	S 1	0	0	0
9	j	40	Total 272	C 183	N 41	O 47	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 293	C 204	N 43	O 46	0	0	0
10	k	37	Total 285	C 199	N 42	O 44	0	0	0

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 302	C 203	N 48	O 51	0	1	0
11	l	37	Total 296	C 200	N 45	O 51	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 259	C 175	N 37	O 46	S 1	0	1	0

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	6	0
			1870	1172	309	384	5			
13	o	243	Total	C	N	O	S	0	2	0
			1838	1153	305	376	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	1	0
			257	181	35	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			766	486	128	152			
15	u	97	Total	C	N	O	0	0	0
			770	489	129	152			

- 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	3	0
			1080	685	181	210	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			212	139	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			213	140	37	33	3			

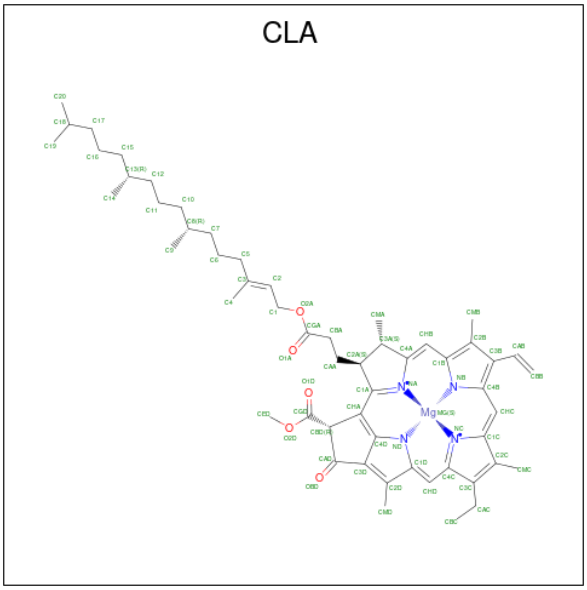
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			274	183	44	47			
18	x	35	Total	C	N	O	0	0	0
			252	171	38	43			

- 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
			450	308	67	73	2			
19	z	61	Total	C	N	O	S	0	0	0
			433	297	66	69	1			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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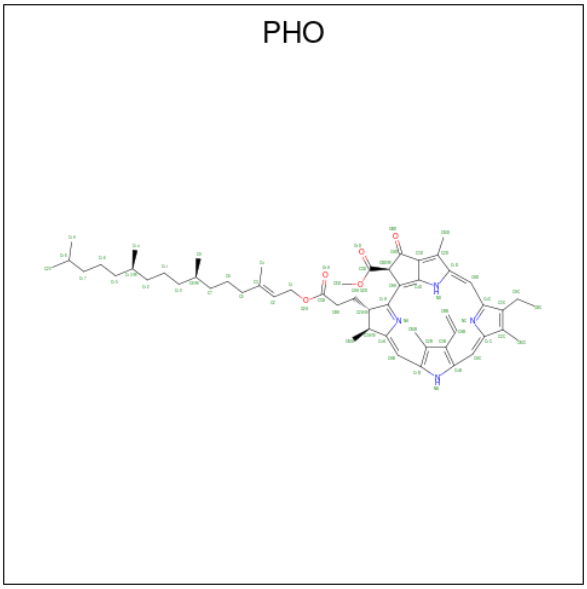
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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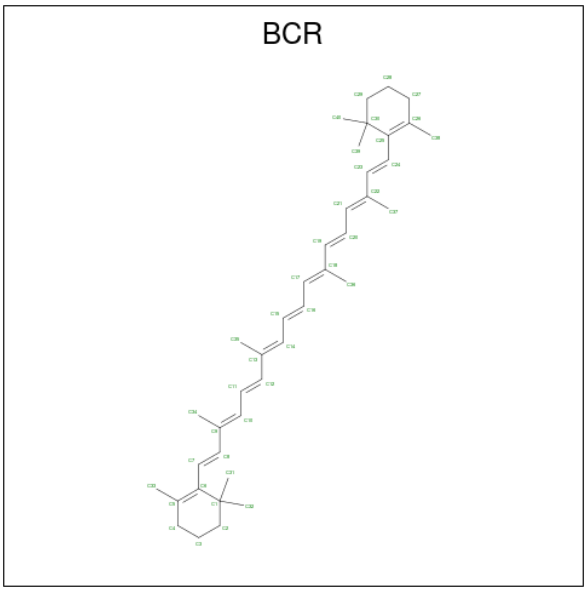
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



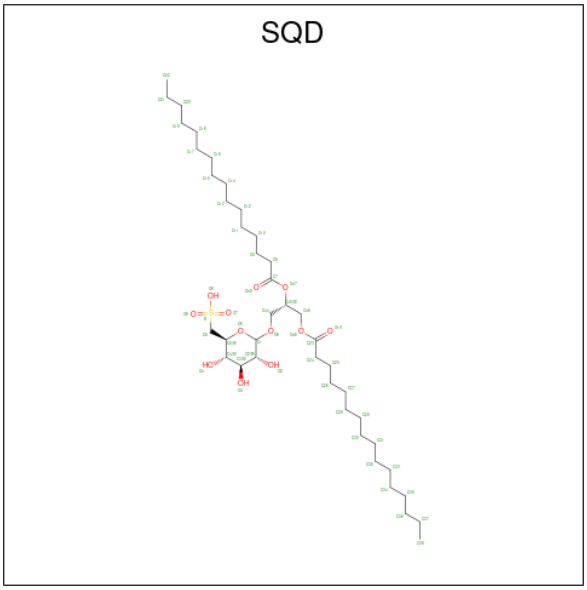
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	D	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	T	1	Total C 40 40	0	0
22	a	1	Total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

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

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



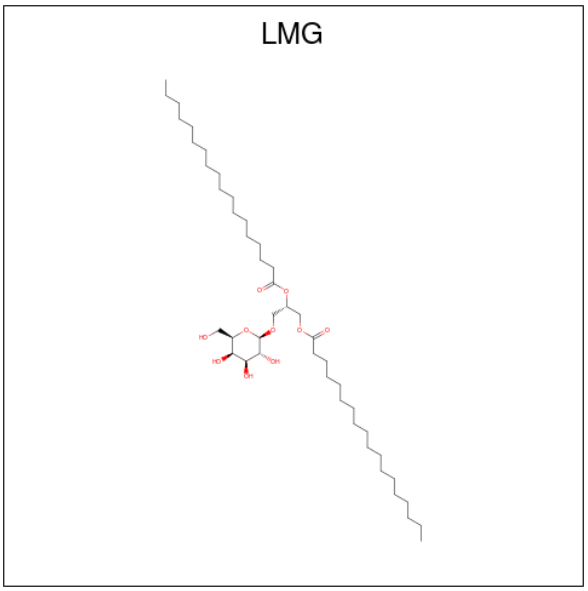
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O S 54 41 12 1	0	0
23	A	1	Total C O S 54 41 12 1	0	0
23	F	1	Total C O S 35 23 11 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	b	1	Total	C	O	S	0	0
			54	41	12	1		
23	f	1	Total	C	O	S	0	0
			40	27	12	1		
23	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			51	41	10		
24	B	1	Total	C	O	0	0
			51	41	10		
24	C	1	Total	C	O	0	0
			51	41	10		
24	C	1	Total	C	O	0	0
			45	35	10		
24	J	1	Total	C	O	0	0
			45	35	10		
24	a	1	Total	C	O	0	0
			51	41	10		
24	b	1	Total	C	O	0	0
			49	39	10		
24	c	1	Total	C	O	0	0
			51	41	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C O 51 41 10	0	0
24	j	1	Total C O 45 35 10	0	0

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

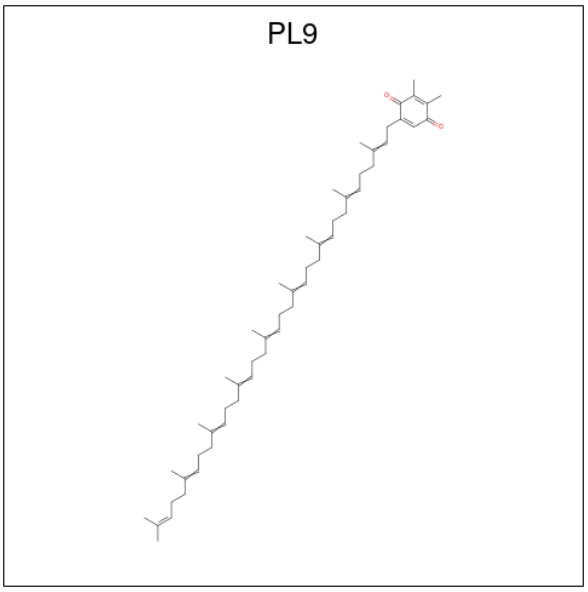
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	2	Total C O 40 35 5	0	0
26	B	6	Total C 84 84	0	0
26	C	1	Total C O 34 29 5	0	0
26	D	2	Total C O 53 48 5	0	0
26	E	1	Total C 15 15	0	0
26	H	2	Total C 10 10	0	0
26	I	5	Total C 61 61	0	0
26	J	4	Total C 33 33	0	0
26	L	1	Total C 14 14	0	0
26	M	1	Total C 12 12	0	0
26	T	1	Total C 13 13	0	0
26	U	1	Total C 14 14	0	0
26	X	1	Total C 16 16	0	0

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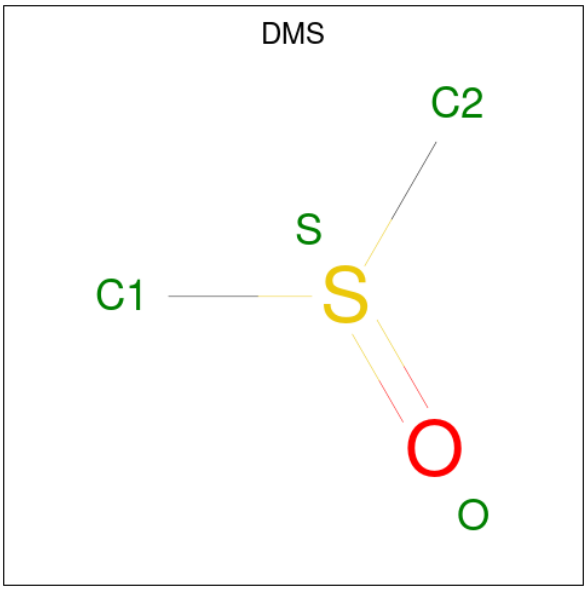
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	Z	1	Total C 4 4	0	0
26	a	3	Total C O 45 40 5	0	0
26	b	7	Total C 68 68	0	0
26	c	3	Total C O 48 43 5	0	0
26	d	3	Total C O 68 63 5	0	0
26	e	1	Total C 7 7	0	0
26	h	1	Total C 16 16	0	0
26	i	3	Total C 38 38	0	0
26	j	2	Total C 22 22	0	0
26	t	1	Total C 16 16	0	0
26	x	1	Total C 9 9	0	0
26	z	1	Total C 6 6	0	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 28 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			4	2	1	1		
28	A	1	Total	C	O	S	0	0
			4	2	1	1		
28	A	1	Total	C	O	S	0	0
			4	2	1	1		
28	A	1	Total	C	O	S	0	0
			4	2	1	1		
28	A	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	B	1	Total	C	O	S	0	0
			4	2	1	1		
28	C	1	Total	C	O	S	0	1
			8	4	2	2		
28	C	1	Total	C	O	S	0	0
			4	2	1	1		
28	C	1	Total	C	O	S	0	0
			4	2	1	1		
28	C	1	Total	C	O	S	0	0
			4	2	1	1		
28	C	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	C	1	Total	C	O	S	0	0
			4	2	1	1		
28	C	1	Total	C	O	S	0	0
			4	2	1	1		
28	C	1	Total	C	O	S	0	0
			4	2	1	1		
28	C	1	Total	C	O	S	0	0
			4	2	1	1		
28	D	1	Total	C	O	S	0	0
			4	2	1	1		
28	D	1	Total	C	O	S	0	0
			4	2	1	1		
28	D	1	Total	C	O	S	0	0
			4	2	1	1		
28	D	1	Total	C	O	S	0	0
			4	2	1	1		
28	F	1	Total	C	O	S	0	0
			4	2	1	1		
28	H	1	Total	C	O	S	0	0
			4	2	1	1		
28	O	1	Total	C	O	S	0	0
			4	2	1	1		
28	O	1	Total	C	O	S	0	0
			4	2	1	1		
28	O	1	Total	C	O	S	0	0
			4	2	1	1		
28	O	1	Total	C	O	S	0	0
			4	2	1	1		
28	O	1	Total	C	O	S	0	0
			4	2	1	1		
28	O	1	Total	C	O	S	0	0
			4	2	1	1		
28	O	1	Total	C	O	S	0	0
			4	2	1	1		
28	O	1	Total	C	O	S	0	0
			4	2	1	1		
28	U	1	Total	C	O	S	0	0
			4	2	1	1		
28	U	1	Total	C	O	S	0	1
			8	4	2	2		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	c	1	Total	C	O	S	0	0
			4	2	1	1		
28	c	1	Total	C	O	S	0	0
			4	2	1	1		
28	c	1	Total	C	O	S	0	0
			4	2	1	1		
28	c	1	Total	C	O	S	0	0
			4	2	1	1		
28	c	1	Total	C	O	S	0	0
			4	2	1	1		
28	c	1	Total	C	O	S	0	0
			4	2	1	1		
28	c	1	Total	C	O	S	0	0
			4	2	1	1		
28	d	1	Total	C	O	S	0	0
			4	2	1	1		
28	d	1	Total	C	O	S	0	0
			4	2	1	1		
28	d	1	Total	C	O	S	0	0
			4	2	1	1		
28	h	1	Total	C	O	S	0	0
			4	2	1	1		
28	i	1	Total	C	O	S	0	0
			4	2	1	1		
28	j	1	Total	C	O	S	0	0
			4	2	1	1		
28	o	1	Total	C	O	S	0	0
			4	2	1	1		
28	o	1	Total	C	O	S	0	0
			4	2	1	1		
28	o	1	Total	C	O	S	0	0
			4	2	1	1		
28	o	1	Total	C	O	S	0	0
			4	2	1	1		
28	o	1	Total	C	O	S	0	0
			4	2	1	1		
28	o	1	Total	C	O	S	0	0
			4	2	1	1		
28	o	1	Total	C	O	S	0	0
			4	2	1	1		
28	u	1	Total	C	O	S	0	0
			4	2	1	1		

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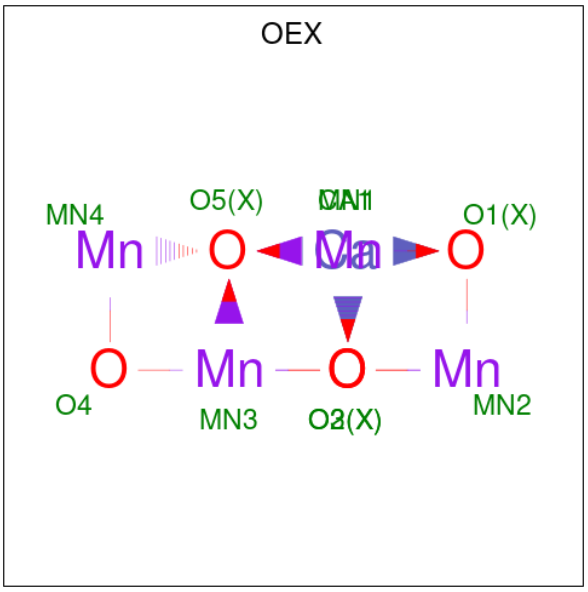
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	u	1	Total	C	O	S	0	0
			4	2	1	1		
28	u	1	Total	C	O	S	0	0
			4	2	1	1		
28	v	1	Total	C	O	S	0	0
			4	2	1	1		
28	v	1	Total	C	O	S	0	0
			4	2	1	1		
28	v	1	Total	C	O	S	0	0
			4	2	1	1		
28	v	1	Total	C	O	S	0	0
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

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

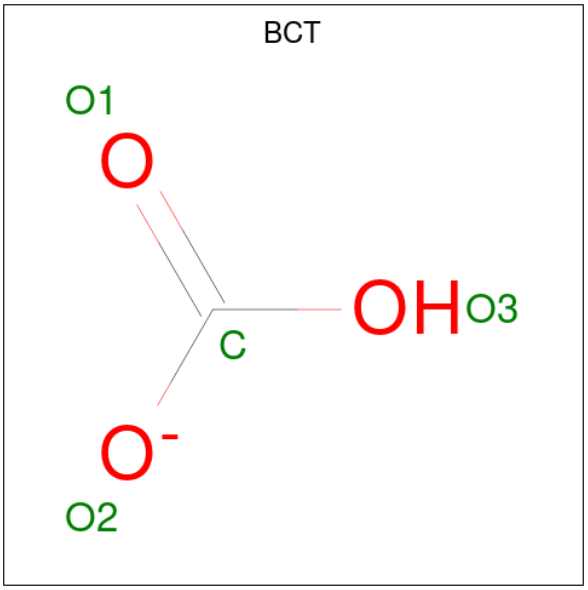
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	1	Total	Fe	0	0
			1	1		
29	a	1	Total	Fe	0	0
			1	1		

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



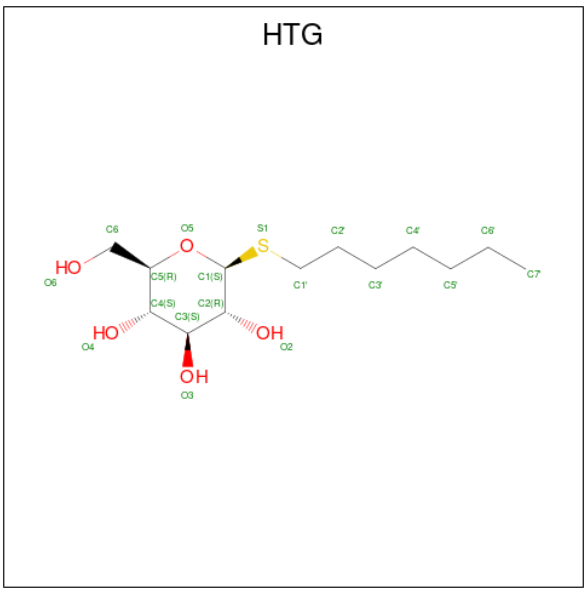
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	D	1	Total	C	O	S	0	0
			19	13	5	1		
32	O	1	Total	C	O	S	0	0
			19	13	5	1		
32	V	1	Total	C	O	S	0	0
			13	7	5	1		
32	b	1	Total	C	O	S	0	0
			19	13	5	1		

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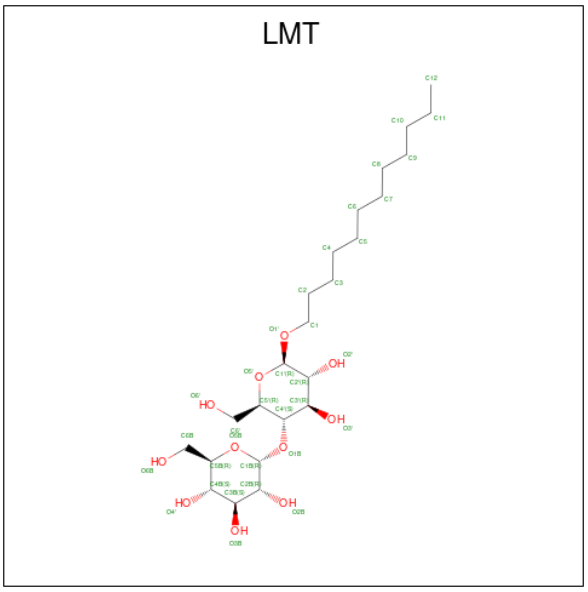
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	d	1	Total C O S 19 13 5 1	0	0
32	u	1	Total C S 8 7 1	0	0
32	v	1	Total C O S 14 8 5 1	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	O	1	Total Ca 1 1	0	0
33	V	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



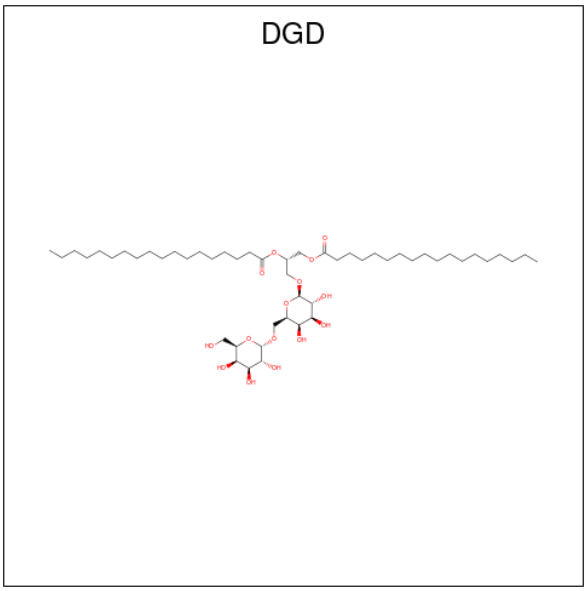
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			24	18	6		
34	B	1	Total	C	O	0	0
			24	18	6		
34	B	1	Total	C	O	0	0
			16	14	2		
34	E	1	Total	C	O	0	0
			24	18	6		
34	I	1	Total	C	O	0	0
			35	24	11		
34	J	1	Total	C	O	0	0
			24	18	6		
34	M	1	Total	C	O	0	0
			35	24	11		
34	T	1	Total	C	O	0	0
			24	18	6		
34	Z	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			32	21	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	c	1	Total	C	O	0	0
			35	24	11		
34	f	1	Total	C	O	0	0
			24	18	6		

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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



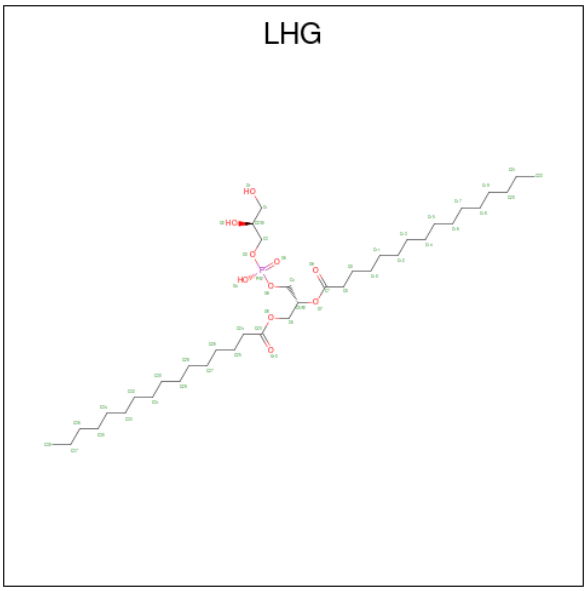
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 62 47 15	0	0
35	C	1	Total C O 55 40 15	0	0
35	C	1	Total C O 62 47 15	0	0
35	D	1	Total C O 51 41 10	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 57 42 15	0	0
35	c	1	Total C O 62 47 15	0	0

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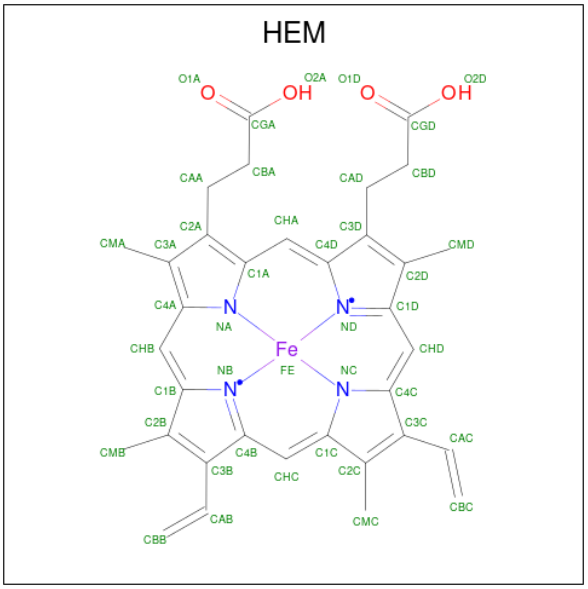
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	d	1	Total C O 51 41 10	0	0
35	h	1	Total C O 62 47 15	0	0

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



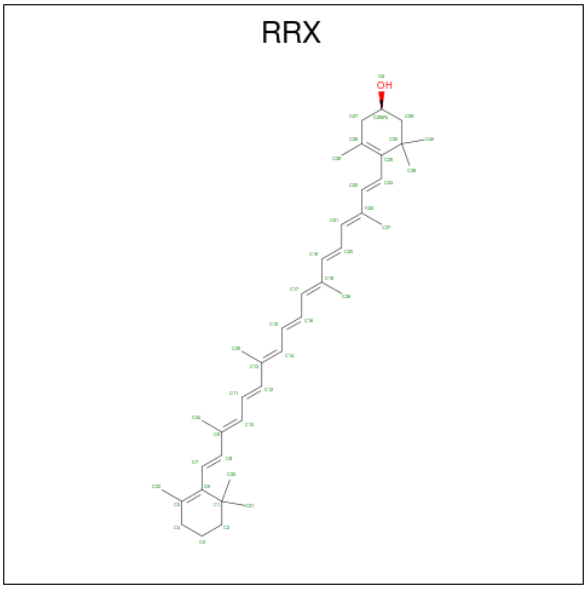
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	D	1	Total C O P 49 38 10 1	0	0
36	D	1	Total C O P 49 38 10 1	0	0
36	D	1	Total C O P 49 38 10 1	0	0
36	E	1	Total C O P 48 37 10 1	0	0
36	L	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	l	1	Total C O P 49 38 10 1	0	0

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



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).

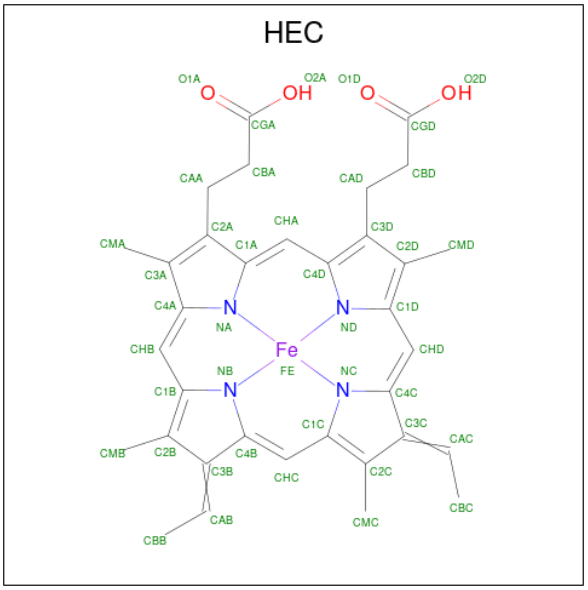


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	H	1	Total C O 41 40 1	0	0
38	x	1	Total C O 41 40 1	0	0

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	177	Total O 182 182	0	5

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	B	447	Total O 473 473	0	25
41	C	317	Total O 324 324	0	7
41	D	175	Total O 180 180	0	5
41	E	62	Total O 66 66	0	4
41	F	8	Total O 8 8	0	0
41	H	62	Total O 65 65	0	3
41	I	16	Total O 16 16	0	0
41	J	23	Total O 23 23	0	0
41	K	12	Total O 12 12	0	0
41	L	19	Total O 21 21	0	2
41	M	12	Total O 12 12	0	0
41	O	263	Total O 273 273	0	10
41	T	19	Total O 20 20	0	1
41	U	133	Total O 136 136	0	3
41	V	177	Total O 183 183	0	6
41	Y	7	Total O 7 7	0	0
41	X	22	Total O 22 22	0	0
41	Z	5	Total O 5 5	0	0
41	a	182	Total O 185 185	0	3
41	b	451	Total O 465 465	0	14
41	c	362	Total O 374 374	0	12

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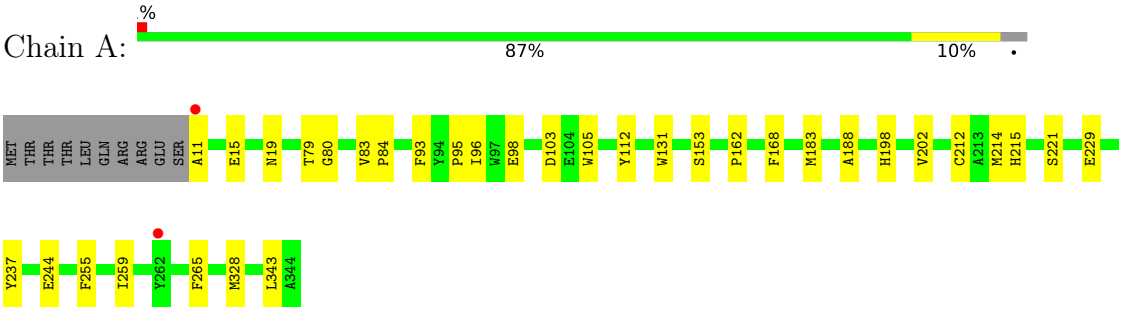
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	d	176	Total O 182 182	0	6
41	e	48	Total O 49 49	0	1
41	f	15	Total O 16 16	0	1
41	h	68	Total O 70 70	0	2
41	i	19	Total O 21 21	0	2
41	j	23	Total O 24 24	0	1
41	k	11	Total O 12 12	0	1
41	l	22	Total O 24 24	0	2
41	m	23	Total O 24 24	0	1
41	o	214	Total O 230 230	0	15
41	t	19	Total O 20 20	0	1
41	u	146	Total O 150 150	0	4
41	v	144	Total O 147 147	0	3
41	y	7	Total O 7 7	0	0
41	x	25	Total O 26 26	0	1
41	z	12	Total O 12 12	0	0

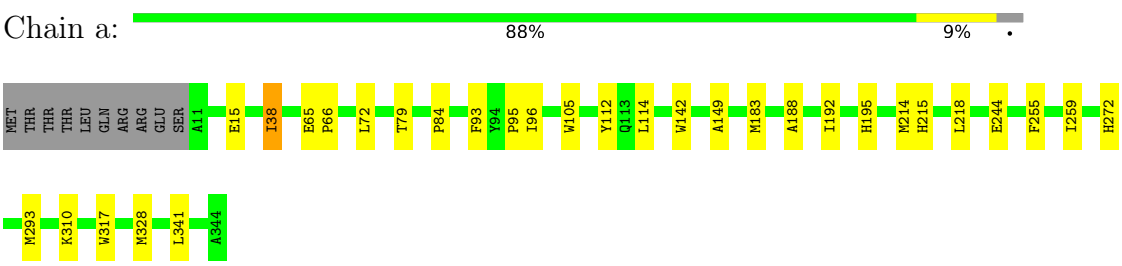
3 Residue-property plots

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

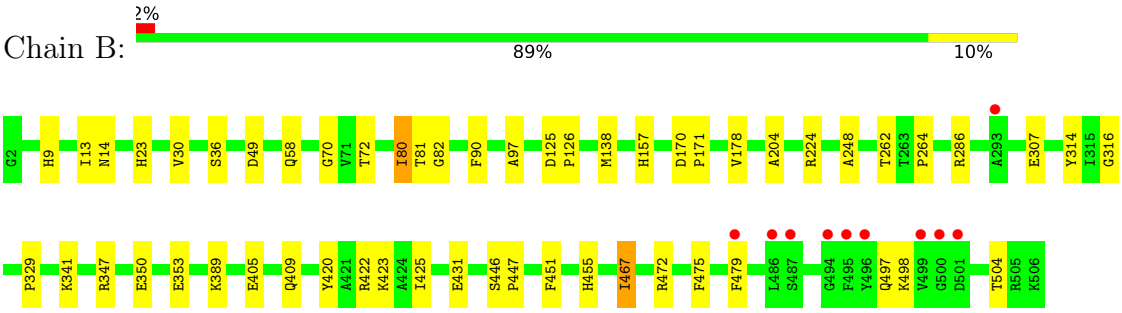
• Molecule 1: Photosystem II protein D1



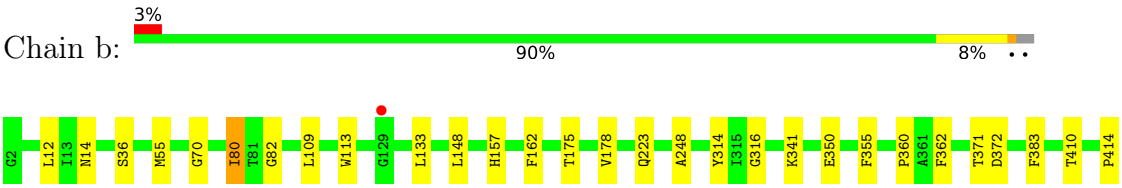
• Molecule 1: Photosystem II protein D1

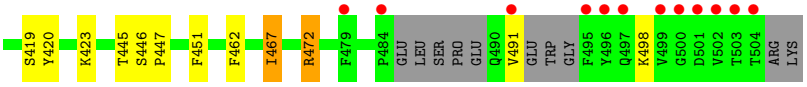


• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

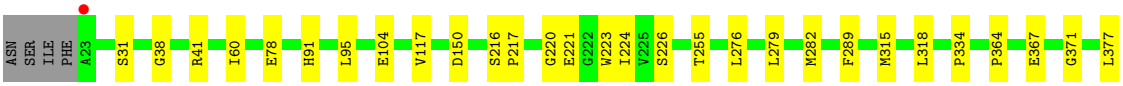


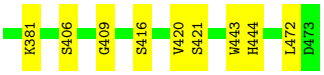


• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:





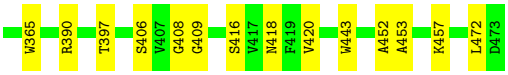


• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:







• Molecule 4: Photosystem II D2 protein

Chain D:







• Molecule 4: Photosystem II D2 protein

Chain d:



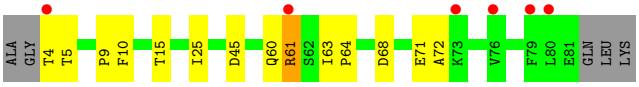




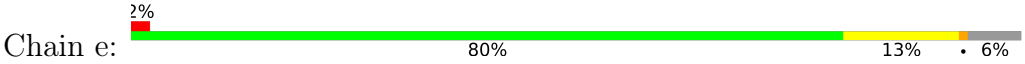
• Molecule 5: Cytochrome b559 subunit alpha

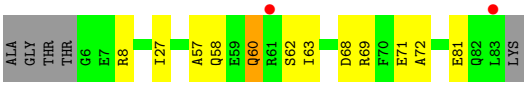
Chain E:





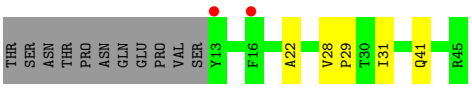
• Molecule 5: Cytochrome b559 subunit alpha





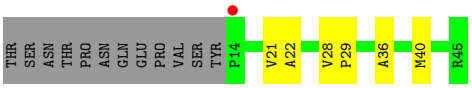
• Molecule 6: Cytochrome b559 subunit beta



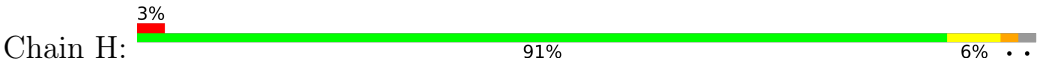


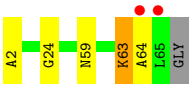
• Molecule 6: Cytochrome b559 subunit beta



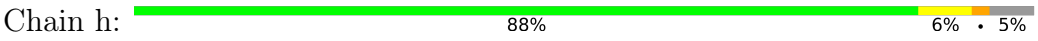


• Molecule 7: Photosystem II reaction center protein H



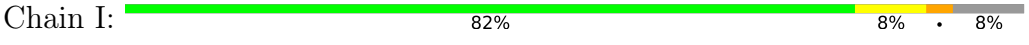


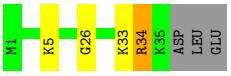
• Molecule 7: Photosystem II reaction center protein H





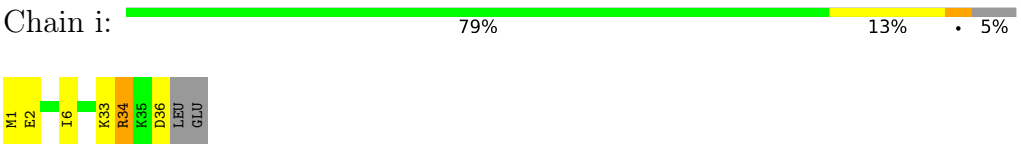
• Molecule 8: Photosystem II reaction center protein I





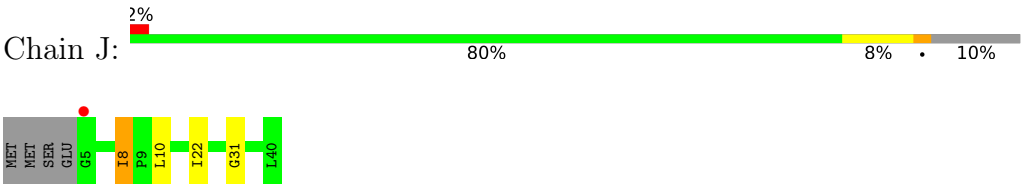
• Molecule 8: Photosystem II reaction center protein I

Chain i:



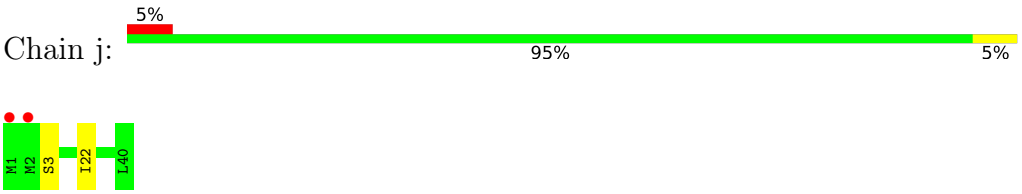
• Molecule 9: Photosystem II reaction center protein J

Chain J:



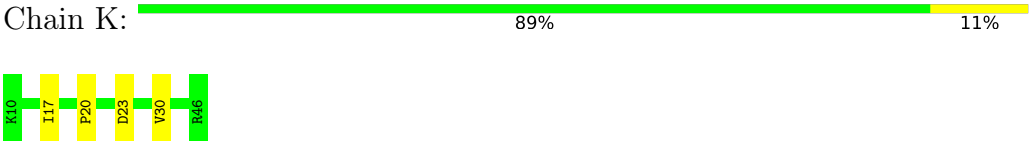
• Molecule 9: Photosystem II reaction center protein J

Chain j:



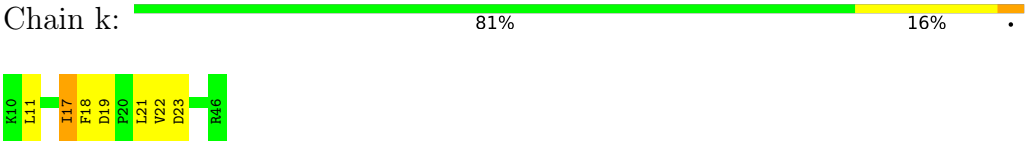
• Molecule 10: Photosystem II reaction center protein K

Chain K:



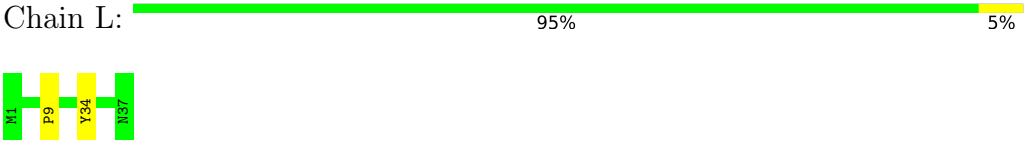
• Molecule 10: Photosystem II reaction center protein K

Chain k:



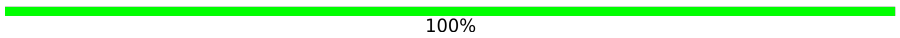
• Molecule 11: Photosystem II reaction center protein L

Chain L:



• Molecule 11: Photosystem II reaction center protein L

Chain l:

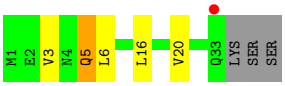


There are no outlier residues recorded for this chain.

• Molecule 12: Photosystem II reaction center protein M

Chain M:

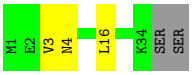




• Molecule 12: Photosystem II reaction center protein M

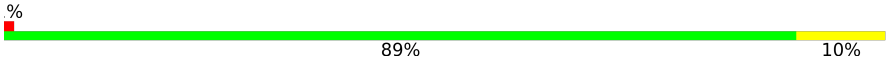
Chain m:

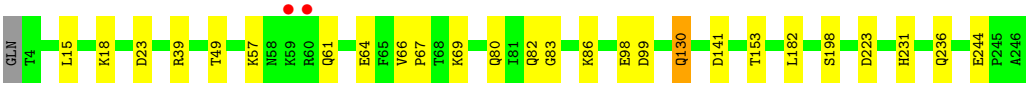




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

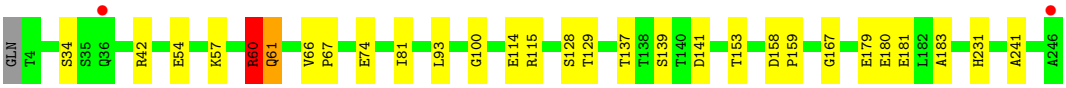




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

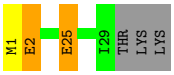




• Molecule 14: Photosystem II reaction center protein T

Chain T:





• Molecule 14: Photosystem II reaction center protein T

Chain t:

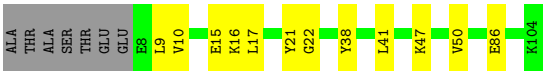




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

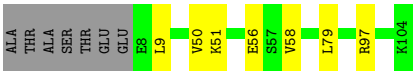




• Molecule 15: Photosystem II 12 kDa extrinsic protein

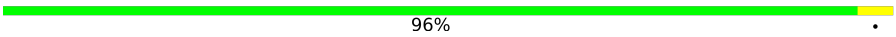
Chain u:

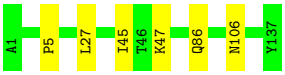




• Molecule 16: Cytochrome c-550

Chain V:

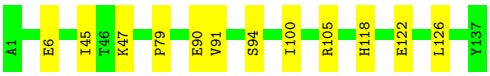




• Molecule 16: Cytochrome c-550

Chain v:

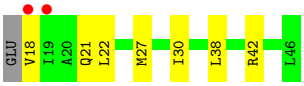




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:

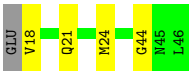




• Molecule 17: Photosystem II reaction center protein Ycf12

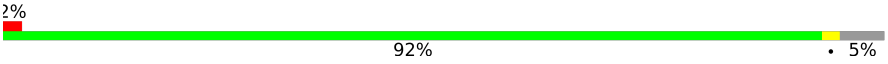
Chain y:

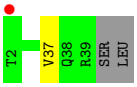




• Molecule 18: Photosystem II reaction center protein X

Chain X:

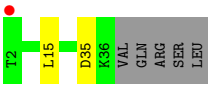




• Molecule 18: Photosystem II reaction center protein X

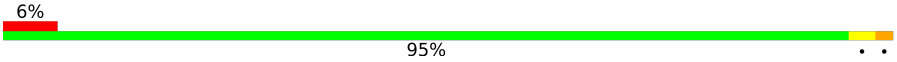
Chain x:

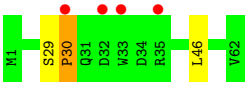




• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

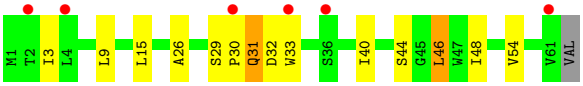




• Molecule 19: Photosystem II reaction center protein Z

Chain z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.47Å 228.18Å 286.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.85 19.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-1.85) 99.9 (19.99-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.201 0.162 , 0.200	Depositor DCC
R_{free} test set	33616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 65.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.19	3/2717 (0.1%)	0.98	2/3707 (0.1%)
1	a	1.15	3/2718 (0.1%)	1.02	3/3707 (0.1%)
2	B	1.10	4/4181 (0.1%)	0.96	1/5700 (0.0%)
2	b	1.13	1/4029 (0.0%)	0.96	1/5490 (0.0%)
3	C	1.06	2/3599 (0.1%)	0.95	1/4901 (0.0%)
3	c	1.03	1/3640 (0.0%)	0.96	1/4956 (0.0%)
4	D	1.17	3/2826 (0.1%)	0.99	6/3850 (0.2%)
4	d	1.15	3/2817 (0.1%)	0.94	0/3839
5	E	0.89	0/654	0.96	0/896
5	e	0.85	0/661	0.99	2/904 (0.2%)
6	F	0.93	0/278	0.82	0/379
6	f	0.98	0/265	0.93	0/360
7	H	0.95	0/524	0.94	0/715
7	h	0.97	0/517	0.91	0/704
8	I	0.86	0/281	0.93	1/380 (0.3%)
8	i	0.80	0/300	0.90	0/405
9	J	0.89	0/257	0.88	0/349
9	j	0.88	0/278	1.00	0/378
10	K	0.89	0/303	0.95	0/416
10	k	0.85	0/295	0.91	0/407
11	L	0.98	1/312 (0.3%)	0.95	0/425
11	l	1.02	0/306	1.00	0/418
12	M	0.87	0/265	1.02	0/362
12	m	0.84	0/270	0.97	0/369
13	O	0.95	0/1919	0.98	0/2607
13	o	0.91	0/1875	0.98	0/2548
14	T	0.92	0/259	1.11	4/352 (1.1%)
14	t	0.95	0/257	0.98	0/349
15	U	0.99	0/777	0.91	0/1055
15	u	0.94	0/781	0.91	0/1059
16	V	1.05	0/1110	0.99	0/1506

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.94	0/1073	0.94	1/1461 (0.1%)
17	Y	0.72	0/213	0.96	0/285
17	y	0.63	0/214	0.97	0/286
18	X	0.75	0/277	1.07	0/375
18	x	0.77	0/255	0.92	0/345
19	Z	0.78	0/461	0.95	0/632
19	z	0.68	0/444	1.03	0/611
All	All	1.05	21/42208 (0.0%)	0.97	23/57488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	LEU	C-N	11.57	1.49	1.33
2	b	414	PRO	CA-C	6.43	1.58	1.52
4	D	87	HIS	CG-CD2	6.31	1.42	1.35
4	d	330	ALA	C-O	-6.04	1.18	1.24
4	d	117	HIS	ND1-CE1	5.87	1.38	1.32
2	B	9	HIS	ND1-CE1	5.84	1.38	1.32
1	a	38	ILE	CA-CB	5.72	1.57	1.54
4	D	87	HIS	ND1-CE1	5.50	1.38	1.32
1	a	149	ALA	CA-C	5.50	1.58	1.52
2	B	9	HIS	CG-CD2	5.46	1.41	1.35
2	B	23	HIS	CG-CD2	5.37	1.41	1.35
1	A	198	HIS	ND1-CE1	5.32	1.37	1.32
3	C	444	HIS	CG-CD2	5.20	1.41	1.35
2	B	97	ALA	N-CA	5.20	1.52	1.46
3	C	91	HIS	CG-CD2	5.14	1.41	1.35
1	a	195	HIS	CG-CD2	5.13	1.41	1.35
11	L	34	TYR	N-CA	5.07	1.52	1.46
1	A	80	GLY	N-CA	5.06	1.52	1.45
4	D	197	HIS	CE1-NE2	5.06	1.37	1.32
3	c	365	TRP	CD2-CE2	5.03	1.50	1.41
4	d	248	THR	CA-C	5.03	1.59	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	139	ARG	CA-C-N	-7.16	114.42	121.65
4	D	139	ARG	C-N-CA	-7.16	114.42	121.65
14	T	25[A]	GLU	CA-C-N	-6.25	113.94	120.38
14	T	25[A]	GLU	C-N-CA	-6.25	113.94	120.38
14	T	25[B]	GLU	CA-C-N	-6.25	113.94	120.38
14	T	25[B]	GLU	C-N-CA	-6.25	113.94	120.38
4	D	170	ALA	CA-C-N	-6.17	113.59	119.76
4	D	170	ALA	C-N-CA	-6.17	113.59	119.76
1	a	142	TRP	N-CA-C	6.04	120.35	112.92
1	A	83	VAL	N-CA-C	5.87	113.68	108.63
1	a	65	GLU	CA-C-N	-5.81	113.71	119.99
1	a	65	GLU	C-N-CA	-5.81	113.71	119.99
5	e	63	ILE	N-CA-C	5.80	114.42	109.02
1	A	131	TRP	CA-CB-CG	-5.26	103.61	113.60
4	D	94	GLY	CA-C-N	5.18	125.26	119.87
4	D	94	GLY	C-N-CA	5.18	125.26	119.87
2	b	175	THR	CB-CA-C	-5.17	102.57	111.45
3	C	421	SER	N-CA-C	5.15	115.52	109.60
8	I	34	ARG	N-CA-C	5.10	117.05	109.25
2	B	23	HIS	N-CA-C	5.06	116.79	111.28
3	c	408	GLY	N-CA-C	-5.04	105.31	112.37
5	e	58	GLN	N-CA-C	5.02	116.75	111.28
16	v	105	ARG	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	60	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2626	0	2515	26	0
1	a	2622	0	2529	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4012	0	3860	58	0
2	b	3884	0	3743	50	0
3	C	3483	0	3397	33	0
3	c	3523	0	3439	39	0
4	D	2728	0	2636	35	0
4	d	2722	0	2623	27	0
5	E	632	0	605	16	0
5	e	636	0	612	9	0
6	F	269	0	277	4	0
6	f	257	0	269	4	0
7	H	508	0	524	6	0
7	h	501	0	526	4	0
8	I	284	0	303	6	0
8	i	300	0	320	2	0
9	J	251	0	257	3	0
9	j	272	0	271	2	0
10	K	293	0	305	4	0
10	k	285	0	290	4	0
11	L	302	0	316	1	0
11	l	296	0	305	0	0
12	M	259	0	281	32	0
12	m	264	0	283	26	0
13	O	1870	0	1836	29	0
13	o	1838	0	1789	30	0
14	T	257	0	260	1	0
14	t	258	0	261	3	0
15	U	766	0	758	21	0
15	u	770	0	769	6	0
16	V	1080	0	1097	9	0
16	v	1052	0	1040	14	0
17	Y	212	0	237	4	0
17	y	213	0	239	4	0
18	X	274	0	297	1	0
18	x	252	0	277	2	0
19	Z	450	0	455	1	0
19	z	433	0	422	7	0
20	A	189	0	202	8	0
20	B	1040	0	1152	22	0
20	C	830	0	900	25	0
20	D	195	0	216	4	0
20	a	172	0	166	5	0
20	b	1040	0	1152	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	c	840	0	923	29	0
20	d	195	0	216	4	0
21	A	64	0	74	1	0
21	D	64	0	74	1	0
21	a	128	0	148	2	0
22	A	40	0	56	5	0
22	B	120	0	168	6	0
22	C	80	0	112	3	0
22	D	40	0	56	3	0
22	K	80	0	112	3	0
22	T	40	0	56	4	0
22	a	40	0	56	1	0
22	b	120	0	168	5	0
22	c	40	0	56	1	0
22	d	40	0	56	3	0
22	j	40	0	56	5	0
22	k	80	0	112	6	0
22	t	40	0	56	4	0
23	A	108	0	156	5	0
23	F	35	0	40	1	0
23	a	108	0	156	9	0
23	b	54	0	78	3	0
23	f	40	0	47	2	0
23	l	54	0	78	2	0
24	A	51	0	72	4	0
24	B	51	0	72	0	0
24	C	96	0	132	5	0
24	J	45	0	60	0	0
24	a	51	0	72	4	0
24	b	49	0	68	2	0
24	c	102	0	144	0	0
24	j	45	0	60	0	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	40	0	0	0	0
26	B	84	0	0	3	0
26	C	34	0	0	0	0
26	D	53	0	0	0	0
26	E	15	0	0	0	0
26	H	10	0	0	0	0
26	I	61	0	0	0	0
26	J	33	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	L	14	0	0	0	0
26	M	12	0	0	0	0
26	T	13	0	0	0	0
26	U	14	0	0	3	0
26	X	16	0	0	0	0
26	Z	4	0	0	0	0
26	a	45	0	0	1	0
26	b	68	0	0	2	0
26	c	48	0	0	0	0
26	d	68	0	0	0	0
26	e	7	0	0	0	0
26	h	16	0	0	0	0
26	i	38	0	0	0	0
26	j	22	0	0	0	0
26	t	16	0	0	0	0
26	x	9	0	0	0	0
26	z	6	0	0	0	0
27	A	55	0	80	11	0
27	D	55	0	80	0	0
27	a	55	0	80	10	0
27	d	55	0	80	0	0
28	A	20	0	30	8	0
28	B	48	0	72	24	0
28	C	40	0	60	15	0
28	D	16	0	24	12	0
28	F	4	0	6	3	0
28	H	4	0	6	0	0
28	O	36	0	54	7	0
28	U	16	0	24	16	0
28	V	24	0	36	5	0
28	b	44	0	66	27	0
28	c	40	0	60	16	0
28	d	12	0	18	8	0
28	h	4	0	6	0	0
28	i	4	0	6	4	0
28	j	4	0	6	0	0
28	o	28	0	42	22	0
28	u	12	0	18	3	0
28	v	32	0	48	4	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	10	0	0	0	0
31	A	4	0	0	5	0
31	a	4	0	0	0	0
32	B	95	0	130	17	0
32	C	76	0	104	2	0
32	D	19	0	26	3	0
32	O	19	0	26	0	0
32	V	13	0	11	0	0
32	b	76	0	104	6	0
32	c	38	0	52	1	0
32	d	19	0	26	0	0
32	u	8	0	15	0	0
32	v	14	0	13	1	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	V	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	64	0	95	4	0
34	E	24	0	35	0	0
34	I	35	0	46	2	0
34	J	24	0	35	1	0
34	M	35	0	46	0	0
34	T	24	0	35	0	0
34	Z	35	0	46	0	0
34	a	35	0	46	10	0
34	b	57	0	72	3	0
34	c	35	0	46	2	0
34	f	24	0	35	0	0
34	m	70	0	92	1	0
34	z	35	0	46	5	0
35	C	179	0	232	0	0
35	D	51	0	71	5	0
35	H	62	0	82	2	0
35	c	181	0	236	3	0
35	d	51	0	71	2	0
35	h	62	0	82	1	0
36	D	147	0	222	19	0
36	E	48	0	71	6	0
36	L	49	0	74	0	0
36	d	147	0	222	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	l	49	0	74	1	0
37	E	43	0	30	1	0
37	e	43	0	30	3	0
38	H	41	0	56	0	0
38	x	41	0	56	3	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	182	0	0	3	0
41	B	473	0	0	18	0
41	C	324	0	0	9	0
41	D	180	0	0	1	0
41	E	66	0	0	1	0
41	F	8	0	0	0	0
41	H	65	0	0	2	0
41	I	16	0	0	1	0
41	J	23	0	0	0	0
41	K	12	0	0	0	0
41	L	21	0	0	0	0
41	M	12	0	0	1	0
41	O	273	0	0	10	0
41	T	20	0	0	0	0
41	U	136	0	0	4	0
41	V	183	0	0	4	0
41	X	22	0	0	1	0
41	Y	7	0	0	0	0
41	Z	5	0	0	0	0
41	a	185	0	0	6	0
41	b	465	0	0	8	0
41	c	374	0	0	4	0
41	d	182	0	0	5	0
41	e	49	0	0	0	0
41	f	16	0	0	0	0
41	h	70	0	0	1	0
41	i	21	0	0	2	0
41	j	24	0	0	0	0
41	k	12	0	0	0	0
41	l	24	0	0	1	0
41	m	24	0	0	0	0
41	o	230	0	0	10	0
41	t	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	u	150	0	0	0	0
41	v	147	0	0	2	0
41	x	26	0	0	1	0
41	y	7	0	0	1	0
41	z	12	0	0	1	0
All	All	54996	0	51554	741	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (741) 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)
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:CD2	1.18	1.58
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:HD22	1.43	1.45
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:HD11	1.55	1.32
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CD2	2.06	1.19
3:c:362:ARG:HD3	28:c:530:DMS:H11	1.21	1.19
32:B:621:HTG:H5	34:a:418:LMT:O2'	1.42	1.18
2:B:347[B]:ARG:NH1	41:B:1031[B]:HOH:O	1.81	1.14
2:b:350:GLU:HG3	28:b:639:DMS:H12	1.29	1.13
15:U:22:GLY:HA2	28:U:903[B]:DMS:H13	1.30	1.12
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:HD21	1.80	1.12
12:M:16[B]:LEU:HD22	12:m:16[B]:LEU:CD1	1.79	1.12
12:M:16[B]:LEU:HD13	12:m:16[B]:LEU:HD13	1.30	1.12
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:HD21	1.14	1.11
1:A:214:MET:HG2	27:A:411:PL9:H102	1.10	1.10
36:D:409:LHG:H382	36:D:409:LHG:H132	1.25	1.09
36:D:409:LHG:H382	36:D:409:LHG:C13	1.81	1.09
5:E:61:ARG:NH2	41:E:201:HOH:O	1.83	1.08
5:e:57:ALA:HB3	5:e:60[A]:GLN:HE22	1.15	1.06
20:c:510:CLA:H41	36:d:408:LHG:H383	1.37	1.05
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:CD2	1.88	1.02
15:U:86:GLU:HG2	26:U:901:UNL:C16	1.88	1.02
4:d:233:ARG:HG2	4:d:233:ARG:HH11	1.23	1.02
2:B:178:VAL:H	28:B:642:DMS:H22	1.25	1.02
36:D:409:LHG:H342	36:D:409:LHG:H302	1.36	1.02
15:U:22:GLY:HA2	28:U:903[B]:DMS:C1	1.90	1.02
13:o:115:ARG:HH11	28:o:302:DMS:H11	1.20	1.01
36:d:408:LHG:H132	36:d:408:LHG:C37	1.91	1.00
28:o:302:DMS:H12	41:o:600:HOH:O	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:362:ARG:HH11	28:c:530:DMS:H12	1.27	1.00
13:O:141:ASP:HB2	28:O:310:DMS:H11	1.43	0.99
15:U:17:LEU:HD23	28:U:903[B]:DMS:H11	1.44	0.99
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CD1	2.37	0.98
34:a:418:LMT:H6E	41:a:540:HOH:O	1.63	0.98
1:a:214:MET:HG2	27:a:415:PL9:H102	1.40	0.97
16:V:5:PRO:HD3	28:V:206:DMS:H21	1.50	0.93
2:b:350:GLU:HG3	28:b:639:DMS:C1	1.98	0.93
41:B:980:HOH:O	28:D:414:DMS:H21	1.67	0.93
16:v:90:GLU:HB2	28:v:206:DMS:C1	1.98	0.93
3:C:364:PRO:HA	28:C:531:DMS:H23	1.48	0.93
2:B:405:GLU:HG2	41:B:1060:HOH:O	1.68	0.93
36:D:409:LHG:H132	36:D:409:LHG:C38	1.99	0.93
31:A:421:BCT:O1	4:D:264[A]:LYS:NZ	2.03	0.92
13:O:130[A]:GLN:H	13:O:130[A]:GLN:HE21	1.17	0.91
28:c:536:DMS:H11	16:v:47:LYS:NZ	1.86	0.90
16:v:90:GLU:HB2	28:v:206:DMS:H11	1.52	0.90
3:c:362:ARG:NH1	28:c:530:DMS:H12	1.87	0.89
1:A:214:MET:CG	27:A:411:PL9:H102	2.02	0.89
1:A:214:MET:HG2	27:A:411:PL9:C10	1.99	0.89
20:c:510:CLA:H41	36:d:408:LHG:C38	2.04	0.88
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:HD21	1.54	0.88
20:C:510:CLA:H41	36:D:409:LHG:H381	1.56	0.88
12:M:16[B]:LEU:HD13	12:m:16[B]:LEU:CD1	2.03	0.87
28:c:536:DMS:H11	16:v:47:LYS:HZ3	1.39	0.87
28:c:530:DMS:H13	41:o:417:HOH:O	1.72	0.87
32:B:621:HTG:H5	34:a:418:LMT:H2O2	1.36	0.87
12:M:16[B]:LEU:CG	12:m:16[B]:LEU:HD21	2.04	0.86
3:c:362:ARG:HD3	28:c:530:DMS:C1	2.05	0.86
4:D:140:PRO:HD2	28:D:414:DMS:H22	1.57	0.86
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CD1	2.53	0.86
1:a:66:PRO:HG2	28:o:302:DMS:H13	1.57	0.85
20:C:504:CLA:H201	36:D:409:LHG:H352	1.58	0.85
5:e:57:ALA:HB3	5:e:60[A]:GLN:NE2	1.92	0.84
13:o:115:ARG:HH11	28:o:302:DMS:C1	1.90	0.84
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:HD13	2.07	0.84
22:b:621:BCR:H331	22:b:621:BCR:C8	2.08	0.83
15:U:9:LEU:HA	28:U:904:DMS:S	2.19	0.83
2:B:389:LYS:HE3	41:B:987:HOH:O	1.79	0.83
31:A:421:BCT:C	4:D:264[A]:LYS:NZ	2.42	0.82
41:C:745:HOH:O	8:I:33:LYS:HE2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:214:MET:HG2	27:a:415:PL9:C10	2.09	0.82
12:M:16[B]:LEU:HD22	12:m:16[B]:LEU:HD11	0.83	0.82
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.60	0.81
36:E:103:LHG:H271	36:E:103:LHG:H321	1.61	0.81
20:d:404:CLA:HBB1	20:d:404:CLA:HMB3	1.63	0.80
36:d:408:LHG:H132	36:d:408:LHG:H372	1.62	0.80
13:o:180:GLU:O	28:o:303:DMS:H21	1.81	0.79
36:d:408:LHG:H372	36:d:408:LHG:H332	1.65	0.79
13:O:49[A]:THR:HG22	41:O:613:HOH:O	1.82	0.79
3:c:362:ARG:HH11	28:c:530:DMS:C1	1.95	0.78
36:D:409:LHG:H302	36:D:409:LHG:C34	2.14	0.78
41:a:511:HOH:O	4:d:139:ARG:HD2	1.82	0.78
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:CG	2.14	0.78
20:A:401:CLA:HBB1	20:A:401:CLA:HMB3	1.65	0.77
31:A:421:BCT:C	4:D:264[A]:LYS:HZ3	1.97	0.77
13:o:74[B]:GLU:OE1	41:o:401:HOH:O	2.00	0.77
20:C:508:CLA:HBC2	36:D:409:LHG:H371	1.65	0.77
1:a:72:LEU:HD11	34:a:418:LMT:H52	1.65	0.77
13:O:64:GLU:HG3	41:O:595:HOH:O	1.83	0.77
2:b:350:GLU:H	28:b:639:DMS:C1	1.99	0.76
3:C:367:GLU:HB2	28:C:531:DMS:H21	1.66	0.76
2:B:423:LYS:HG3	32:B:622:HTG:H1'2	1.66	0.76
12:M:16[B]:LEU:CG	12:m:16[B]:LEU:CD2	2.63	0.76
36:D:409:LHG:H342	36:D:409:LHG:C30	2.16	0.75
2:b:472:ARG:HG2	28:d:414:DMS:H12	1.67	0.75
13:O:231:HIS:HD2	41:O:568:HOH:O	1.70	0.75
10:k:21:LEU:HB2	17:y:24:MET:HE3	1.66	0.75
15:U:22:GLY:CA	28:U:903[B]:DMS:H13	2.12	0.75
28:o:306:DMS:H23	41:o:607:HOH:O	1.86	0.74
28:B:642:DMS:H23	41:B:755:HOH:O	1.86	0.74
2:b:423:LYS:HE2	41:o:444:HOH:O	1.86	0.74
5:E:68:ASP:OD1	5:E:71:GLU:HB2	1.86	0.74
23:a:409:SQD:H381	9:j:22:ILE:HD11	1.70	0.73
35:D:406:DGD:HD4	5:E:45:ASP:HB3	1.71	0.73
28:o:307:DMS:H21	41:o:515:HOH:O	1.87	0.73
36:D:409:LHG:H382	36:D:409:LHG:H131	1.69	0.73
4:D:12:ARG:HG3	4:D:13:GLY:N	2.04	0.72
15:U:17:LEU:HD23	28:U:903[B]:DMS:C1	2.19	0.72
2:B:178:VAL:H	28:B:642:DMS:C2	2.00	0.72
15:U:17:LEU:CD2	28:U:903[B]:DMS:H11	2.19	0.72
32:B:621:HTG:H1	34:a:418:LMT:H11	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:621:BCR:H331	22:b:621:BCR:HC8	1.70	0.71
28:b:631:DMS:H12	41:d:537:HOH:O	1.89	0.71
28:i:104:DMS:H22	41:i:206:HOH:O	1.91	0.71
2:b:350:GLU:H	28:b:639:DMS:H11	1.55	0.71
4:d:233:ARG:HG2	4:d:233:ARG:NH1	1.98	0.71
4:D:144:ILE:CD1	28:D:414:DMS:O	2.39	0.71
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CD2	2.54	0.71
12:M:16[A]:LEU:HD23	23:b:622:SQD:H381	1.72	0.70
5:E:61:ARG:HG3	28:V:208:DMS:H21	1.72	0.70
2:b:410:THR:H	28:b:640:DMS:H23	1.57	0.70
13:O:57:LYS:HD2	41:b:755:HOH:O	1.92	0.70
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:CG	2.22	0.70
2:b:360:PRO:HA	28:b:631:DMS:H11	1.74	0.69
28:A:418:DMS:H12	5:E:63:ILE:HD11	1.72	0.69
3:c:362:ARG:CD	28:c:530:DMS:H11	2.13	0.69
2:B:423:LYS:CG	32:B:622:HTG:H1'2	2.23	0.69
13:O:130[A]:GLN:H	13:O:130[A]:GLN:NE2	1.90	0.69
7:h:63:LYS:HG3	41:h:257:HOH:O	1.93	0.69
13:O:198:SER:OG	28:O:306:DMS:H23	1.93	0.69
28:C:532:DMS:H22	16:V:47:LYS:HE3	1.74	0.69
2:B:82:GLY:O	28:o:308:DMS:S	2.50	0.68
36:d:408:LHG:H132	36:d:408:LHG:H371	1.74	0.68
31:A:421:BCT:O3	4:D:264[A]:LYS:NZ	2.27	0.68
4:D:12:ARG:HG3	4:D:13:GLY:H	1.56	0.68
28:c:536:DMS:C1	16:v:47:LYS:NZ	2.57	0.68
13:O:49[A]:THR:HG23	41:O:437:HOH:O	1.93	0.68
28:C:527:DMS:H23	41:C:797:HOH:O	1.93	0.67
28:C:532:DMS:H21	41:C:603:HOH:O	1.93	0.67
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.74	0.67
20:C:508:CLA:CBC	36:D:409:LHG:H371	2.25	0.67
20:c:508:CLA:HBC2	36:d:408:LHG:H361	1.77	0.67
7:H:59:ASN:HD22	7:H:64:ALA:HB3	1.60	0.67
2:B:409:GLN:HE21	28:B:644:DMS:C1	2.08	0.66
20:c:513:CLA:HBB1	20:c:513:CLA:HMB3	1.77	0.66
13:O:15:LEU:HD23	13:O:18:LYS:HD2	1.76	0.66
13:o:115:ARG:HD3	28:o:302:DMS:H11	1.76	0.66
15:U:17:LEU:CD2	28:U:903[B]:DMS:C1	2.74	0.66
28:B:641:DMS:H11	41:B:931:HOH:O	1.95	0.65
2:B:341:LYS:NZ	32:B:622:HTG:S1	2.62	0.65
2:B:472:ARG:HG2	28:D:414:DMS:C1	2.26	0.65
2:b:371:THR:OG1	28:b:638:DMS:H13	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:GLU:OE1	2:B:431[A]:GLU:OE1	2.14	0.65
16:v:90:GLU:CB	28:v:206:DMS:C1	2.73	0.65
20:B:601:CLA:HED2	20:B:601:CLA:H43	1.79	0.65
20:B:602:CLA:H42	41:B:1029:HOH:O	1.97	0.65
3:C:367:GLU:HB2	28:C:531:DMS:C2	2.26	0.64
28:b:631:DMS:H13	41:d:541:HOH:O	1.95	0.64
36:D:409:LHG:H152	36:D:409:LHG:H362	1.80	0.64
5:E:15:THR:HB	9:J:8:ILE:O	1.97	0.64
28:d:413:DMS:H11	41:d:586[A]:HOH:O	1.98	0.64
20:B:606:CLA:C14	20:B:611:CLA:HED2	2.28	0.63
23:a:401:SQD:H442	41:a:667:HOH:O	1.96	0.63
13:O:130[A]:GLN:HG3	28:O:310:DMS:H12	1.79	0.63
22:T:101:BCR:H321	22:T:101:BCR:HC8	1.80	0.63
28:o:307:DMS:H22	41:o:488:HOH:O	1.97	0.63
5:E:10:PHE:H	36:E:103:LHG:HC32	1.64	0.63
3:C:117:VAL:CG1	24:C:524:LMG:H202	2.28	0.63
28:A:418:DMS:H23	5:E:63:ILE:HD12	1.81	0.63
4:d:342:PRO:HA	28:d:413:DMS:H12	1.81	0.63
15:U:10:VAL:H	28:U:904:DMS:H21	1.64	0.62
4:d:123:ILE:HD11	35:h:101:DGD:HAW2	1.80	0.62
32:v:210:HTG:H1'1	41:v:439:HOH:O	1.98	0.62
20:B:616:CLA:HBB1	20:B:616:CLA:HMB3	1.81	0.62
3:C:364:PRO:O	28:C:531:DMS:H12	1.98	0.62
28:c:536:DMS:C1	16:v:47:LYS:HZ1	2.13	0.62
22:t:101:BCR:HC8	22:t:101:BCR:H311	1.81	0.62
3:c:201:ASN:HB2	41:c:844:HOH:O	1.99	0.62
13:o:115:ARG:NH1	28:o:302:DMS:H11	2.04	0.62
1:A:98[A]:GLU:OE2	41:A:501:HOH:O	2.11	0.62
22:B:618:BCR:H331	22:B:618:BCR:C8	2.29	0.62
13:o:231:HIS:HD2	28:o:306:DMS:O	1.83	0.62
1:A:265:PHE:HE2	27:A:411:PL9:H122	1.64	0.61
36:D:409:LHG:C34	36:D:409:LHG:C30	2.75	0.61
34:a:418:LMT:C6'	41:a:540:HOH:O	2.36	0.61
20:B:601:CLA:H201	26:B:628:UNL:C15	2.31	0.61
2:b:248:ALA:HA	20:b:605:CLA:H42	1.81	0.61
2:b:341:LYS:NZ	32:b:625:HTG:S1	2.66	0.61
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CG	2.77	0.61
28:F:102:DMS:C1	16:V:27:LEU:HD21	2.31	0.60
13:O:49[B]:THR:HG23	13:O:236:GLN:HB2	1.81	0.60
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.36	0.60
1:a:66:PRO:CG	28:o:302:DMS:H13	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:404:CLA:HBB1	20:d:404:CLA:CMB	2.31	0.60
24:A:407:LMG:C25	24:A:407:LMG:H422	2.31	0.60
15:U:86:GLU:H	26:U:901:UNL:C16	2.15	0.60
2:b:341:LYS:NZ	32:b:625:HTG:O2	2.21	0.60
28:F:102:DMS:H12	16:V:27:LEU:HD21	1.84	0.60
15:u:56:GLU:N	28:u:203:DMS:O	2.23	0.60
20:C:506:CLA:H92	34:I:101:LMT:H111	1.84	0.60
28:b:634:DMS:H23	41:b:1015:HOH:O	2.02	0.60
13:O:231:HIS:CD2	41:O:568:HOH:O	2.50	0.59
41:a:511:HOH:O	4:d:139:ARG:CD	2.45	0.59
15:U:22:GLY:HA2	28:U:903[B]:DMS:H12	1.83	0.59
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.35	0.59
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.84	0.59
28:V:204:DMS:H21	41:V:474:HOH:O	2.02	0.59
2:b:341:LYS:HZ1	32:b:625:HTG:C2	2.14	0.59
37:E:104:HEM:HMC2	6:F:31:ILE:HG13	1.84	0.59
13:o:115:ARG:CD	28:o:302:DMS:H11	2.32	0.59
27:A:411:PL9:H162	36:E:103:LHG:H322	1.84	0.59
34:B:626:LMT:H5'	34:a:418:LMT:O6'	2.03	0.59
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.85	0.59
32:B:621:HTG:H1'1	28:B:643:DMS:H22	1.83	0.59
20:C:504:CLA:C20	36:D:409:LHG:H352	2.30	0.59
2:b:350:GLU:N	28:b:639:DMS:C1	2.64	0.59
19:z:44:SER:O	19:z:48:ILE:HG13	2.03	0.59
3:C:117:VAL:HG12	24:C:524:LMG:H202	1.84	0.58
4:D:144:ILE:HD11	28:D:414:DMS:O	2.01	0.58
7:H:59:ASN:HD22	7:H:64:ALA:CB	2.16	0.58
20:B:611:CLA:H151	20:B:611:CLA:H203	1.84	0.58
5:E:9:PRO:HA	36:E:103:LHG:HC32	1.84	0.58
20:B:605:CLA:H43	20:B:606:CLA:H2	1.85	0.58
20:b:617:CLA:H2	20:b:618:CLA:HBB2	1.86	0.58
13:o:42:ARG:O	13:o:241:ALA:HA	2.03	0.58
2:b:472:ARG:CG	28:d:414:DMS:H12	2.32	0.58
27:A:411:PL9:H502	4:D:39:PRO:HG3	1.86	0.57
23:A:406:SQD:C12	23:A:406:SQD:H162	2.34	0.57
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.87	0.57
20:c:501:CLA:H192	20:c:506:CLA:C1B	2.35	0.57
1:A:103:ASP:OD2	28:A:415:DMS:H22	2.05	0.57
16:V:106[A]:ASN:OD1	41:V:301:HOH:O	2.17	0.57
2:B:224[B]:ARG:NH2	41:B:702:HOH:O	2.37	0.57
16:v:91:VAL:HG13	28:v:206:DMS:H12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:635:DMS:H11	41:B:902:HOH:O	2.03	0.57
3:c:182:PHE:HA	32:c:520:HTG:H61	1.85	0.57
12:M:16[A]:LEU:CD2	23:b:622:SQD:H381	2.34	0.56
34:b:628:LMT:H6E	4:d:19:ASP:OD2	2.05	0.56
22:B:619:BCR:H331	22:B:619:BCR:C8	2.34	0.56
34:J:103:LMT:H123	26:J:107:UNL:C3	2.35	0.56
1:a:183:MET:HA	20:a:403:CLA:HMD1	1.86	0.56
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.40	0.56
35:c:516:DGD:HAT2	35:c:517:DGD:HBH2	1.86	0.56
20:B:601:CLA:C20	26:B:628:UNL:C15	2.83	0.56
34:z:102:LMT:H6'2	34:z:102:LMT:H2B	1.87	0.56
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CG	2.80	0.56
15:u:50:VAL:O	28:u:202:DMS:H23	2.04	0.56
20:b:609:CLA:H2	24:b:623:LMG:H152	1.87	0.56
36:d:408:LHG:H132	36:d:408:LHG:C38	2.36	0.56
24:C:519:LMG:H221	10:K:30:VAL:HG11	1.87	0.56
13:o:179:GLU:HG2	41:o:420:HOH:O	2.06	0.56
28:C:531:DMS:H22	41:C:878:HOH:O	2.06	0.55
23:F:101:SQD:H461	41:X:201:HOH:O	2.07	0.55
3:c:409:GLY:HA2	28:c:536:DMS:S	2.46	0.55
1:a:38:ILE:HG12	23:a:401:SQD:H142	1.87	0.55
22:C:515:BCR:H331	22:C:515:BCR:C8	2.36	0.55
2:b:355:PHE:HB2	28:b:638:DMS:H11	1.88	0.55
2:B:409:GLN:HE21	28:B:644:DMS:H12	1.71	0.55
20:b:611:CLA:NC	38:x:101:RRX:H56	2.21	0.55
2:B:13:ILE:O	28:B:645:DMS:H11	2.06	0.55
28:B:641:DMS:H13	41:B:1079:HOH:O	2.07	0.55
24:C:519:LMG:H242	9:J:22:ILE:HD13	1.88	0.55
22:D:405:BCR:H313	35:D:406:DGD:HAW2	1.88	0.55
5:e:57:ALA:CB	5:e:60[A]:GLN:HE22	2.05	0.55
41:l:211[B]:HOH:O	12:m:4:ASN:ND2	2.39	0.55
3:C:279:LEU:HD12	3:C:282:MET:CE	2.37	0.54
13:o:183:ALA:HB3	28:o:303:DMS:H22	1.88	0.54
13:O:39:ARG:HH11	13:O:82:GLN:HE21	1.54	0.54
28:A:418:DMS:H12	5:E:63:ILE:CD1	2.37	0.54
15:U:10:VAL:H	28:U:904:DMS:C2	2.20	0.54
22:b:621:BCR:HC8	22:b:621:BCR:C33	2.38	0.54
7:H:2:ALA:N	41:H:201:HOH:O	2.41	0.54
22:d:405:BCR:H331	22:d:405:BCR:C8	2.38	0.54
2:B:171:PRO:HB3	7:H:63:LYS:HA	1.90	0.54
28:C:532:DMS:H22	16:V:47:LYS:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.89	0.54
3:c:452:ALA:O	28:i:104:DMS:H13	2.08	0.54
20:a:404:CLA:HBB1	20:a:404:CLA:HMB1	1.89	0.54
3:c:127:PHE:CE1	34:z:102:LMT:H21	2.43	0.54
3:C:409:GLY:HA2	28:C:532:DMS:S	2.48	0.54
23:A:406:SQD:H162	23:A:406:SQD:H122	1.90	0.53
20:c:509:CLA:HMB1	20:c:509:CLA:HBB1	1.90	0.53
41:C:745:HOH:O	8:I:33:LYS:CE	2.47	0.53
7:H:59:ASN:ND2	7:H:64:ALA:HB3	2.23	0.53
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.53
27:A:411:PL9:H151	36:E:103:LHG:H331	1.90	0.53
28:C:532:DMS:C2	41:C:603:HOH:O	2.55	0.53
11:L:9:PRO:HA	34:m:102:LMT:H6D	1.90	0.53
28:U:903[A]:DMS:H23	41:U:1017:HOH:O	2.08	0.53
20:b:616:CLA:H161	20:b:616:CLA:H111	1.89	0.53
5:e:60[B]:GLN:NE2	5:e:62:SER:O	2.40	0.53
1:a:215:HIS:HA	27:a:415:PL9:O1	2.08	0.53
4:d:272:LEU:C	4:d:272:LEU:HD23	2.33	0.53
1:A:237:TYR:CZ	4:D:264[B]:LYS:HG3	2.44	0.53
15:U:47:LYS:NZ	41:U:1002:HOH:O	2.42	0.53
20:B:604:CLA:C4D	20:B:606:CLA:H43	2.38	0.53
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.44	0.53
19:z:3:ILE:HA	41:z:201:HOH:O	2.08	0.53
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.43	0.53
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.91	0.53
3:C:150:ASP:OD2	41:C:601:HOH:O	2.19	0.53
2:B:36[A]:SER:OG	22:B:618:BCR:H362	2.08	0.52
28:B:635:DMS:H22	28:D:413:DMS:C1	2.40	0.52
20:b:607:CLA:HHC	20:b:607:CLA:HBB1	1.91	0.52
1:A:183:MET:HA	20:A:401:CLA:HMD1	1.91	0.52
28:b:631:DMS:H11	41:b:764:HOH:O	2.10	0.52
28:b:639:DMS:H12	41:b:1051:HOH:O	2.10	0.52
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.43	0.52
3:C:371:GLY:HA3	41:C:622:HOH:O	2.10	0.52
20:c:513:CLA:HBB1	20:c:513:CLA:CMB	2.39	0.52
13:o:129:THR:HA	13:o:141:ASP:O	2.08	0.52
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.90	0.52
28:i:104:DMS:C2	41:i:206:HOH:O	2.55	0.52
31:A:421:BCT:C	4:D:264[A]:LYS:HZ1	2.12	0.52
3:C:318:LEU:C	3:C:318:LEU:HD23	2.34	0.52
4:D:13:GLY:HA3	32:D:417:HTG:H62	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:618:CLA:H203	20:b:618:CLA:H143	1.91	0.52
13:o:231:HIS:HE1	41:o:498:HOH:O	1.93	0.52
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.40	0.52
2:B:14[B]:ASN:HA	28:B:645:DMS:H21	1.91	0.52
20:c:506:CLA:HMC2	20:c:507:CLA:H102	1.92	0.52
26:B:647:UNL:C13	23:a:401:SQD:H302	2.40	0.52
20:c:508:CLA:CBC	36:d:408:LHG:H361	2.39	0.52
2:B:472:ARG:HG2	28:D:414:DMS:H12	1.92	0.51
3:c:126:GLY:O	3:c:130:VAL:HG23	2.10	0.51
20:c:502:CLA:H61	20:c:512:CLA:H42	1.91	0.51
15:U:50:VAL:O	28:U:902:DMS:H23	2.11	0.51
3:c:179:ALA:O	3:c:184:GLY:HA2	2.11	0.51
22:T:101:BCR:H382	22:T:101:BCR:H23C	1.92	0.51
20:C:504:CLA:H202	36:D:409:LHG:H361	1.92	0.51
15:U:21:TYR:O	28:U:903[B]:DMS:H13	2.11	0.51
23:l:101:SQD:H192	22:t:101:BCR:H351	1.93	0.51
4:D:99:GLY:O	35:D:406:DGD:HA21	2.10	0.51
2:b:472:ARG:CG	28:d:414:DMS:C1	2.89	0.51
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.93	0.51
17:y:18:VAL:N	41:y:101:HOH:O	2.44	0.51
16:V:5:PRO:CD	28:V:206:DMS:H21	2.34	0.51
27:a:415:PL9:H502	4:d:39:PRO:HG3	1.93	0.51
2:b:410:THR:H	28:b:640:DMS:C2	2.22	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.51
2:B:409:GLN:NE2	28:B:644:DMS:H13	2.26	0.51
3:c:38:GLY:HA3	20:c:511:CLA:HMD2	1.93	0.50
13:o:114:GLU:OE2	28:o:306:DMS:H12	2.11	0.50
22:d:405:BCR:H313	35:d:416:DGD:HAT2	1.94	0.50
23:A:412:SQD:H442	41:A:661:HOH:O	2.11	0.50
2:B:423:LYS:HE2	41:B:886:HOH:O	2.10	0.50
2:b:372:ASP:O	28:b:638:DMS:H12	2.12	0.50
1:A:215:HIS:HA	27:A:411:PL9:O1	2.11	0.50
20:a:403:CLA:HBB1	20:a:403:CLA:HMB1	1.94	0.50
4:d:236:ASN:O	4:d:239:GLN:HG2	2.12	0.50
7:h:12:ARG:HB3	7:h:13:PRO:HD3	1.94	0.50
24:a:410:LMG:C25	24:a:410:LMG:C43	2.90	0.50
4:D:304:ARG:HH12	34:b:627:LMT:H6'1	1.76	0.50
4:D:12:ARG:CG	4:D:13:GLY:H	2.18	0.50
2:b:148[B]:LEU:HD23	20:b:606:CLA:H202	1.93	0.50
20:b:607:CLA:C14	20:b:612:CLA:HED2	2.42	0.50
20:c:504:CLA:H191	36:d:408:LHG:H362	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:406:SQD:H142	36:D:409:LHG:H161	1.94	0.49
2:B:409:GLN:HE21	28:B:644:DMS:H13	1.77	0.49
3:C:279:LEU:HA	3:C:282:MET:HE3	1.94	0.49
15:U:16:LYS:NZ	41:U:1004:HOH:O	2.45	0.49
2:b:350:GLU:CG	28:b:639:DMS:C1	2.84	0.49
28:B:635:DMS:H22	28:D:413:DMS:H11	1.94	0.49
20:C:506:CLA:HMC2	20:C:507:CLA:H102	1.93	0.49
2:B:224[B]:ARG:HH11	34:B:625:LMT:H2'	1.76	0.49
17:Y:18:VAL:O	17:Y:22:LEU:HD12	2.12	0.49
35:c:517:DGD:HBF1	36:d:408:LHG:H223	1.95	0.49
12:M:5:GLN:H	12:M:5:GLN:HE21	1.60	0.49
17:Y:38:LEU:O	17:Y:42:ARG:HD3	2.13	0.49
2:b:341:LYS:NZ	32:b:625:HTG:C2	2.75	0.49
2:B:350:GLU:HG3	28:B:637:DMS:O	2.12	0.49
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.49
15:u:97:ARG:NH1	28:u:202:DMS:O	2.38	0.49
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.94	0.49
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.78	0.49
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.95	0.49
20:C:510:CLA:H41	36:D:409:LHG:C38	2.35	0.49
5:E:10:PHE:H	36:E:103:LHG:C3	2.24	0.49
4:D:272:LEU:C	4:D:272:LEU:HD23	2.38	0.49
2:B:178:VAL:N	28:B:642:DMS:H22	2.10	0.49
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.95	0.48
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.94	0.48
16:v:122:GLU:HG3	16:v:126:LEU:HD12	1.95	0.48
1:A:229:GLU:HG2	41:A:577:HOH:O	2.13	0.48
22:d:405:BCR:HC22	35:d:416:DGD:HA82	1.95	0.48
2:B:409:GLN:NE2	28:B:644:DMS:C1	2.76	0.48
22:D:405:BCR:C8	22:D:405:BCR:H331	2.44	0.48
28:o:307:DMS:C2	41:o:488:HOH:O	2.57	0.48
21:A:403:PHO:NC	21:A:403:PHO:ND	2.62	0.48
24:A:407:LMG:H231	24:A:407:LMG:H201	1.56	0.48
20:c:508:CLA:HMB3	20:c:508:CLA:HBB1	1.96	0.48
23:A:412:SQD:H272	2:b:109:LEU:HD13	1.96	0.48
20:C:510:CLA:H52	36:D:409:LHG:H372	1.95	0.48
4:D:13:GLY:HA3	32:D:417:HTG:C6	2.43	0.48
1:A:215:HIS:ND1	27:A:411:PL9:O1	2.39	0.48
2:B:90:PHE:H	32:B:632:HTG:H62	1.78	0.48
4:D:209:LEU:HD23	4:D:209:LEU:C	2.39	0.48
7:h:3[B]:ARG:HG2	7:h:3[B]:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:44:GLY:HA2	19:z:30:PRO:HD3	1.95	0.48
27:A:411:PL9:H403	6:F:22:ALA:HB2	1.96	0.48
32:B:621:HTG:H2'2	34:a:418:LMT:H21	1.96	0.48
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.95	0.48
2:b:162:PHE:O	20:b:608:CLA:HHD	2.14	0.48
2:b:472:ARG:HG3	28:d:414:DMS:C1	2.44	0.48
20:b:615:CLA:H18	36:d:406:LHG:H202	1.96	0.48
23:b:622:SQD:H311	23:b:622:SQD:H342	1.39	0.48
20:c:506:CLA:H51	34:c:523:LMT:H102	1.96	0.48
19:z:15:LEU:HD22	19:z:46:LEU:HD23	1.94	0.48
3:C:60:ILE:HG22	20:C:503:CLA:HHD	1.95	0.48
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.96	0.48
20:A:401:CLA:CBD	20:D:402:CLA:HAC2	2.44	0.47
3:C:104:GLU:HB2	28:C:527:DMS:H22	1.95	0.47
22:j:102:BCR:H321	22:j:102:BCR:HC8	1.96	0.47
13:o:231:HIS:CD2	28:o:306:DMS:O	2.66	0.47
20:B:614:CLA:HBB1	20:B:614:CLA:HMB1	1.95	0.47
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:CD1	2.33	0.47
13:O:244:GLU:HG2	28:O:307:DMS:C1	2.43	0.47
14:t:25:GLU:OE1	14:t:25:GLU:HA	2.13	0.47
36:d:408:LHG:H372	36:d:408:LHG:C33	2.41	0.47
2:B:248:ALA:HA	20:B:604:CLA:H42	1.96	0.47
23:a:409:SQD:H272	36:d:408:LHG:H142	1.97	0.47
20:B:605:CLA:H93	20:B:606:CLA:HAB	1.96	0.47
20:C:502:CLA:H193	32:C:520:HTG:H3'1	1.95	0.47
5:E:68:ASP:O	5:E:72:ALA:HB2	2.15	0.47
1:a:341:LEU:HD13	28:c:536:DMS:H12	1.97	0.47
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.96	0.47
28:c:536:DMS:H13	16:v:47:LYS:HZ1	1.77	0.47
20:C:509:CLA:CMB	20:C:509:CLA:HBB1	2.45	0.47
20:C:509:CLA:HBB1	20:C:509:CLA:HMB3	1.95	0.47
20:C:513:CLA:C4B	22:C:514:BCR:H383	2.43	0.47
20:b:609:CLA:C1D	24:b:623:LMG:H111	2.45	0.47
28:A:416:DMS:H13	8:I:5:LYS:HZ3	1.78	0.47
20:b:603:CLA:H91	38:x:101:RRX:H25	1.97	0.47
3:c:443:TRP:CE2	20:c:508:CLA:HMD2	2.50	0.47
7:h:38:PHE:HB2	38:x:101:RRX:C10	2.44	0.47
18:x:15:LEU:HD23	41:x:214:HOH:O	2.14	0.47
1:a:310:LYS:NZ	41:a:505:HOH:O	2.46	0.47
2:b:467:ILE:HG12	4:d:126:MET:HE1	1.97	0.47
13:o:54:GLU:HA	28:o:306:DMS:H22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:14:ASN:HA	28:b:632:DMS:H11	1.96	0.47
2:b:350:GLU:N	28:b:639:DMS:H13	2.29	0.47
20:c:504:CLA:C19	36:d:408:LHG:H362	2.45	0.47
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.50	0.46
22:A:405:BCR:H382	22:A:405:BCR:H23C	1.97	0.46
13:O:39:ARG:HH11	13:O:82:GLN:NE2	2.13	0.46
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.97	0.46
28:A:416:DMS:H13	8:I:5:LYS:NZ	2.30	0.46
20:b:604:CLA:CMB	20:b:604:CLA:HBB1	2.46	0.46
36:d:408:LHG:H161	36:d:408:LHG:H331	1.97	0.46
2:B:157:HIS:C	2:B:157:HIS:CD2	2.94	0.46
22:T:101:BCR:H382	22:T:101:BCR:C23	2.45	0.46
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.97	0.46
28:A:416:DMS:H22	28:A:417:DMS:H22	1.96	0.46
20:B:611:CLA:CBB	20:B:611:CLA:HHC	2.44	0.46
3:C:334:PRO:HA	13:O:153:THR:OG1	2.16	0.46
13:O:49[B]:THR:CG2	13:O:236:GLN:HB2	2.46	0.46
23:a:401:SQD:H382	26:a:402:UNL:C16	2.46	0.46
20:c:512:CLA:C1B	22:k:102:BCR:H401	2.46	0.46
2:B:30:VAL:HG12	20:B:606:CLA:HHD	1.98	0.46
2:B:286:ARG:HG2	2:B:286:ARG:HH11	1.80	0.46
13:o:158:ASP:HB2	13:o:159:PRO:CD	2.46	0.46
32:B:621:HTG:C5	34:a:418:LMT:H2O2	2.19	0.46
20:A:401:CLA:CAD	20:D:402:CLA:HAC2	2.46	0.46
28:B:642:DMS:C2	41:B:755:HOH:O	2.53	0.46
4:d:52:THR:O	4:d:66:SER:HA	2.16	0.46
26:U:901:UNL:C15	41:U:1118:HOH:O	2.63	0.46
13:o:115:ARG:HD3	28:o:302:DMS:C1	2.45	0.46
2:B:420:TYR:CD1	32:B:622:HTG:H1'1	2.50	0.46
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.51	0.46
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.97	0.46
22:k:101:BCR:H331	22:k:101:BCR:C8	2.46	0.46
13:O:223:ASP:OD2	28:O:305:DMS:H12	2.16	0.46
1:a:218:LEU:HD12	27:a:415:PL9:C3	2.46	0.46
2:b:157:HIS:C	2:b:157:HIS:CD2	2.93	0.46
28:b:634:DMS:H22	28:b:640:DMS:H11	1.98	0.46
2:b:36:SER:OG	22:b:620:BCR:H362	2.17	0.45
2:b:462:PHE:CE1	20:b:615:CLA:HMB3	2.51	0.45
20:b:612:CLA:HHC	20:b:612:CLA:HBB1	1.97	0.45
15:U:10:VAL:HG11	15:U:15:GLU:OE1	2.16	0.45
28:b:631:DMS:C1	41:b:764:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:84:PRO:HA	1:a:112:TYR:CG	2.52	0.45
27:a:415:PL9:H403	6:f:22:ALA:HB2	1.98	0.45
37:e:102:HEM:HMC1	37:e:102:HEM:HBC2	1.99	0.45
2:B:138:MET:HE3	20:B:616:CLA:CHD	2.46	0.45
4:D:103:ARG:O	4:D:107:LEU:HG	2.17	0.45
1:a:214:MET:CG	27:a:415:PL9:H102	2.29	0.45
23:a:409:SQD:H252	36:d:408:LHG:H142	1.97	0.45
3:c:318:LEU:C	3:c:318:LEU:HD23	2.41	0.45
16:v:45:ILE:C	16:v:45:ILE:HD12	2.41	0.45
22:A:405:BCR:H24C	22:A:405:BCR:H371	1.78	0.45
2:B:204:ALA:CB	20:B:603:CLA:HAB	2.47	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.45
4:D:246:MET:HB2	4:D:264[B]:LYS:HE2	1.99	0.45
8:I:26:GLY:HA3	34:I:101:LMT:H6'1	1.99	0.45
21:a:406:PHO:HBC2	21:a:406:PHO:HHD	1.99	0.45
2:b:55:MET:CE	2:b:80:ILE:HG12	2.47	0.45
3:c:60:ILE:HG22	20:c:503:CLA:HHD	1.99	0.45
34:B:626:LMT:H123	14:t:8:PHE:HA	1.99	0.45
13:O:86:LYS:HD3	41:O:449:HOH:O	2.17	0.45
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.99	0.45
24:C:519:LMG:H221	10:K:30:VAL:CG1	2.46	0.45
22:A:405:BCR:H401	28:A:415:DMS:H12	1.98	0.45
34:a:418:LMT:H6'1	4:d:304:ARG:HH12	1.82	0.45
28:b:631:DMS:C1	41:d:541:HOH:O	2.59	0.45
20:c:504:CLA:H42	35:c:516:DGD:HB31	1.99	0.45
22:K:101:BCR:HC7	22:K:101:BCR:H331	1.67	0.44
20:A:402:CLA:HAB	20:A:402:CLA:HHC	1.82	0.44
32:B:631:HTG:C6	41:B:829:HOH:O	2.64	0.44
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.53	0.44
22:c:514:BCR:H11C	22:c:514:BCR:H341	1.87	0.44
22:j:102:BCR:H311	22:j:102:BCR:C8	2.47	0.44
13:o:181:GLU:HA	28:o:303:DMS:H11	1.99	0.44
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:HD22	0.48	0.44
19:z:31:GLN:O	19:z:33:TRP:N	2.51	0.44
22:A:405:BCR:H382	22:A:405:BCR:C23	2.48	0.44
2:B:497:GLN:HB2	2:B:504:THR:HB	2.00	0.44
4:D:140:PRO:CD	28:D:414:DMS:H22	2.37	0.44
19:z:26:ALA:HB3	19:z:40:ILE:HD11	2.00	0.44
1:A:15:GLU:HG3	41:I:201:HOH:O	2.16	0.44
20:d:403:CLA:H203	20:d:403:CLA:H162	1.70	0.44
23:f:101:SQD:O10	23:f:101:SQD:H262	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:180:GLU:CD	13:o:180:GLU:H	2.26	0.44
20:B:606:CLA:H62	20:B:606:CLA:H41	1.79	0.44
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.53	0.44
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.98	0.44
20:b:610:CLA:H161	20:b:610:CLA:H141	1.85	0.44
20:b:611:CLA:CBB	20:b:611:CLA:HHC	2.48	0.44
28:b:635:DMS:C2	41:b:731:HOH:O	2.66	0.44
15:U:22:GLY:HA2	28:U:903[A]:DMS:H21	1.99	0.44
36:d:408:LHG:H122	36:d:408:LHG:H381	1.99	0.44
5:e:60[A]:GLN:HE21	5:e:60[A]:GLN:HB3	1.49	0.44
8:i:2:GLU:O	8:i:6:ILE:HG12	2.18	0.44
22:j:102:BCR:H382	22:j:102:BCR:H23C	2.00	0.44
13:o:60:ARG:O	13:o:61:GLN:CB	2.65	0.44
28:B:642:DMS:H12	41:B:719:HOH:O	2.17	0.44
3:C:276:LEU:HD23	20:C:509:CLA:HED1	2.00	0.44
4:D:304:ARG:HH22	34:b:627:LMT:H4B	1.82	0.44
12:M:5:GLN:HE21	12:M:5:GLN:N	2.14	0.44
1:a:15:GLU:HB2	34:c:523:LMT:H6'1	1.99	0.44
27:a:415:PL9:H172	27:a:415:PL9:H13	1.47	0.44
20:b:612:CLA:C15	20:b:612:CLA:H203	2.48	0.44
36:d:408:LHG:H132	36:d:408:LHG:H381	1.99	0.44
20:A:401:CLA:HBB1	20:A:401:CLA:CMB	2.40	0.43
28:C:527:DMS:C2	41:C:797:HOH:O	2.61	0.43
35:H:102:DGD:HAW2	35:H:102:DGD:HAN2	1.89	0.43
20:b:618:CLA:H61	20:b:618:CLA:H41	1.78	0.43
24:A:407:LMG:H292	3:C:216:SER:HA	2.00	0.43
20:b:606:CLA:H43	20:b:607:CLA:H2	2.00	0.43
24:A:407:LMG:H321	3:C:217:PRO:HD3	2.01	0.43
3:C:31:SER:CB	3:C:41:ARG:HG2	2.48	0.43
4:D:26:ARG:HA	5:E:5:THR:HB	1.99	0.43
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.01	0.43
4:D:244:TYR:OH	4:D:264[A]:LYS:NZ	2.46	0.43
4:d:85:MET:CE	4:d:96:GLU:HG2	2.48	0.43
28:d:413:DMS:C1	41:d:586[A]:HOH:O	2.61	0.43
6:f:21:VAL:HG21	23:f:101:SQD:H241	2.00	0.43
3:C:95:LEU:HD21	20:C:501:CLA:OBD	2.18	0.43
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.43
21:D:403:PHO:HBC2	21:D:403:PHO:HHD	2.00	0.43
2:b:472:ARG:HG2	28:d:414:DMS:C1	2.44	0.43
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.01	0.43
3:C:221:GLU:O	3:C:226:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:417:HTG:H61	41:D:591:HOH:O	2.18	0.43
13:O:39:ARG:HB2	13:O:83:GLY:O	2.19	0.43
3:C:220:GLY:O	28:C:530:DMS:H21	2.18	0.43
3:C:409:GLY:HA2	28:C:532:DMS:C1	2.49	0.43
3:C:443:TRP:CE2	20:C:508:CLA:HMD2	2.54	0.43
22:a:408:BCR:H20C	22:a:408:BCR:H361	1.89	0.43
41:c:937:HOH:O	15:u:51:LYS:HD2	2.17	0.43
16:V:45:ILE:HG12	41:V:469:HOH:O	2.18	0.43
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.01	0.43
2:B:49:ASP:OD1	13:o:57:LYS:NZ	2.51	0.43
20:B:611:CLA:HHC	20:B:611:CLA:HBB1	2.00	0.43
21:a:405:PHO:NC	21:a:405:PHO:ND	2.66	0.43
20:b:605:CLA:CMD	20:b:608:CLA:HMB1	2.49	0.43
20:b:606:CLA:H201	26:b:630:UNL:C16	2.49	0.43
36:d:406:LHG:O9	36:l:102:LHG:HC81	2.19	0.43
37:e:102:HEM:HBC2	37:e:102:HEM:CMC	2.49	0.43
15:u:51:LYS:HB2	15:u:51:LYS:HE3	1.66	0.43
41:B:732:HOH:O	13:o:57:LYS:HD2	2.19	0.42
20:a:403:CLA:HBB1	20:a:403:CLA:CMB	2.49	0.42
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.54	0.42
22:B:619:BCR:C23	22:B:619:BCR:H383	2.49	0.42
23:a:409:SQD:H302	20:c:508:CLA:H93	2.01	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.42
2:B:467:ILE:HG13	4:D:126:MET:HE1	2.01	0.42
2:B:479:PHE:HA	41:B:980:HOH:O	2.19	0.42
32:B:622:HTG:H6'2	32:B:622:HTG:H3'2	1.28	0.42
22:T:101:BCR:C23	22:T:101:BCR:C38	2.97	0.42
3:c:48:LYS:HG2	3:c:133:ALA:O	2.18	0.42
3:c:472:LEU:HD11	4:d:255:GLN:HG3	2.01	0.42
4:d:24:ARG:NH2	18:x:35:ASP:O	2.52	0.42
28:F:102:DMS:H11	16:V:27:LEU:HD21	2.01	0.42
23:a:409:SQD:H192	36:d:408:LHG:H212	2.00	0.42
24:a:410:LMG:H391	3:c:281:MET:HG3	1.99	0.42
20:b:607:CLA:HHC	20:b:607:CLA:CBB	2.49	0.42
3:c:443:TRP:CD2	20:c:508:CLA:HMD2	2.54	0.42
2:B:341:LYS:NZ	32:B:622:HTG:O2	2.37	0.42
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.08	0.42
13:O:244:GLU:HG2	28:O:307:DMS:H13	2.02	0.42
2:b:82:GLY:O	28:b:641:DMS:O	2.38	0.42
2:b:350:GLU:H	28:b:639:DMS:H13	1.78	0.42
22:k:102:BCR:H11C	22:k:102:BCR:H341	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:137:THR:C	13:o:139:SER:H	2.27	0.42
20:B:601:CLA:H41	20:B:601:CLA:H62	1.46	0.42
22:B:618:BCR:H382	22:t:101:BCR:H11C	2.01	0.42
1:a:218:LEU:HD12	27:a:415:PL9:C4	2.49	0.42
24:a:410:LMG:H232	20:c:505:CLA:H92	2.02	0.42
2:b:498:LYS:HA	4:d:24:ARG:HA	2.00	0.42
22:b:621:BCR:H361	22:b:621:BCR:H20C	1.80	0.42
3:C:279:LEU:HD22	20:C:509:CLA:HED2	2.01	0.42
3:C:381:LYS:NZ	13:O:99:ASP:OD1	2.45	0.42
1:a:215:HIS:ND1	27:a:415:PL9:O1	2.41	0.42
2:b:133:LEU:HD12	28:b:632:DMS:H22	2.02	0.42
28:b:641:DMS:H22	41:b:706:HOH:O	2.19	0.42
3:c:31:SER:CB	3:c:41:ARG:HG2	2.50	0.42
3:c:286:ALA:HB2	20:c:502:CLA:HMD2	2.01	0.42
20:B:602:CLA:H143	20:B:602:CLA:H161	1.89	0.42
3:c:153:ASP:HA	28:c:533:DMS:H12	2.02	0.42
3:c:266:TRP:CZ3	20:c:507:CLA:HAC2	2.55	0.42
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.42
20:c:509:CLA:H192	20:c:512:CLA:HMD1	2.01	0.42
36:d:408:LHG:H141	36:d:408:LHG:H111	1.82	0.42
22:j:102:BCR:H382	22:j:102:BCR:C23	2.50	0.42
2:B:80:ILE:HD12	2:B:80:ILE:HA	1.80	0.42
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.01	0.42
2:b:80:ILE:HD12	2:b:80:ILE:HA	1.94	0.42
2:B:422:ARG:O	2:B:425:ILE:HG12	2.20	0.42
20:C:501:CLA:H42	20:C:502:CLA:HMD3	2.01	0.42
34:B:627:LMT:H12	12:M:6:LEU:HD11	2.01	0.41
20:C:501:CLA:C4D	20:C:503:CLA:H2	2.49	0.41
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.19	0.41
13:O:69:LYS:HE2	41:O:480:HOH:O	2.19	0.41
20:b:604:CLA:H111	20:b:604:CLA:H151	1.94	0.41
3:c:397:THR:HA	28:c:536:DMS:H21	2.02	0.41
4:d:23:LYS:HD3	4:d:135:LEU:HD21	2.02	0.41
5:e:68:ASP:O	5:e:72:ALA:HB2	2.20	0.41
3:C:472:LEU:HD11	4:D:255:GLN:HG3	2.01	0.41
28:D:415:DMS:H22	13:O:182:LEU:HD11	2.03	0.41
35:H:102:DGD:HE5	41:H:238:HOH:O	2.19	0.41
28:V:205:DMS:H23	41:V:343:HOH:O	2.19	0.41
2:b:12:LEU:HB2	20:b:614:CLA:HMC2	2.02	0.41
2:b:445:THR:HA	41:b:709:HOH:O	2.18	0.41
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:446:SER:HB2	2:b:447:PRO:HD2	2.01	0.41
22:j:102:BCR:C23	22:j:102:BCR:C38	2.98	0.41
13:o:66:VAL:HB	13:o:67:PRO:HD2	2.01	0.41
16:v:79:PRO:HD3	16:v:94:SER:HB3	2.02	0.41
2:B:72:THR:HB	28:B:642:DMS:H11	2.02	0.41
20:B:607:CLA:H202	32:B:632:HTG:H61	2.01	0.41
5:E:63:ILE:HG23	5:E:64:PRO:HD2	2.02	0.41
8:I:33:LYS:HB3	8:I:34:ARG:H	1.70	0.41
2:b:467:ILE:HG12	4:d:126:MET:CE	2.50	0.41
20:b:608:CLA:H93	20:b:608:CLA:H111	1.92	0.41
22:k:101:BCR:H371	22:k:101:BCR:H24C	1.85	0.41
1:a:114:LEU:C	1:a:114:LEU:HD23	2.45	0.41
2:b:451:PHE:CD2	2:b:451:PHE:C	2.98	0.41
3:c:135[A]:ARG:NH2	34:z:102:LMT:H5B	2.35	0.41
2:B:81:THR:HG21	28:B:642:DMS:S	2.60	0.41
28:B:635:DMS:H13	41:B:763:HOH:O	2.21	0.41
22:K:101:BCR:C8	22:K:101:BCR:H311	2.50	0.41
16:v:118:HIS:HE1	41:v:395:HOH:O	2.03	0.41
1:A:153:SER:HB2	20:A:401:CLA:H43	2.03	0.41
3:C:406:SER:HA	3:C:420:VAL:HG23	2.02	0.41
22:D:405:BCR:HC21	35:D:406:DGD:HAT2	2.02	0.41
28:D:415:DMS:H13	41:M:205:HOH:O	2.20	0.41
2:b:420:TYR:CE1	32:b:625:HTG:H3'1	2.56	0.41
10:k:17:ILE:HG23	10:k:18:PHE:CD2	2.56	0.41
1:A:11:ALA:HB1	1:A:15:GLU:OE1	2.20	0.41
2:B:262:THR:C	2:B:264:PRO:HD3	2.45	0.41
22:B:619:BCR:H371	22:B:619:BCR:H24C	1.82	0.41
22:C:514:BCR:H15C	22:C:514:BCR:H351	1.92	0.41
2:b:113:TRP:CD1	20:b:618:CLA:HBA2	2.56	0.41
1:A:221:SER:HB2	4:D:139:ARG:O	2.21	0.41
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.50	0.41
2:B:498:LYS:HE3	4:D:20:ASP:HA	2.02	0.41
3:C:377:LEU:HB3	13:O:80:GLN:OE1	2.21	0.41
20:C:509:CLA:H91	20:C:509:CLA:H111	1.89	0.41
20:C:513:CLA:HBC2	32:C:534:HTG:H6'2	2.03	0.41
36:D:409:LHG:H362	36:D:409:LHG:H332	1.81	0.41
24:a:410:LMG:H401	24:a:410:LMG:H371	1.69	0.41
20:b:613:CLA:H112	20:b:613:CLA:H72	1.88	0.41
22:k:101:BCR:H20C	22:k:101:BCR:H361	1.96	0.41
23:l:101:SQD:H311	23:l:101:SQD:H341	1.67	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:472:ARG:HG2	28:D:414:DMS:H11	2.02	0.41
5:E:60:GLN:O	5:E:61:ARG:NE	2.54	0.41
20:a:403:CLA:CBD	20:d:403:CLA:HAC2	2.51	0.41
3:c:406:SER:O	3:c:418:ASN:HA	2.21	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.95	0.40
2:B:347[B]:ARG:HG2	2:B:353:GLU:HA	2.04	0.40
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.56	0.40
13:O:98:GLU:HG3	41:O:418:HOH:O	2.21	0.40
3:c:156:LYS:HE3	41:c:675:HOH:O	2.20	0.40
20:c:501:CLA:H42	20:c:502:CLA:HMD3	2.03	0.40
5:e:8:ARG:NH1	9:j:3:SER:O	2.55	0.40
5:e:27:ILE:HG12	37:e:102:HEM:HMC3	2.02	0.40
1:A:202:VAL:HG11	20:A:402:CLA:C3D	2.51	0.40
32:B:622:HTG:C7'	41:O:407:HOH:O	2.69	0.40
3:C:38:GLY:O	3:C:41:ARG:HB2	2.22	0.40
20:D:401:CLA:HBC3	20:D:401:CLA:HHD	2.04	0.40
15:U:17:LEU:CD2	28:U:903[B]:DMS:H12	2.50	0.40
2:b:419:SER:CB	32:b:625:HTG:H3'2	2.51	0.40
20:b:608:CLA:H193	26:b:642:UNL:C4	2.52	0.40
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.02	0.40
22:A:405:BCR:C23	22:A:405:BCR:C38	2.98	0.40
2:B:286:ARG:HG2	2:B:286:ARG:NH1	2.37	0.40
20:D:402:CLA:H162	20:D:402:CLA:H203	1.80	0.40
28:O:308:DMS:H11	41:O:648:HOH:O	2.21	0.40
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.56	0.40
3:c:142:GLU:H	3:c:142:GLU:CD	2.30	0.40
3:c:453:ALA:O	8:i:34[B]:ARG:HG2	2.22	0.40
20:c:506:CLA:HMB1	20:c:507:CLA:NB	2.36	0.40
1:A:15:GLU:O	1:A:19[A]:ASN:CG	2.64	0.40
1:A:265:PHE:HE2	27:A:411:PL9:C12	2.32	0.40
2:B:224[B]:ARG:HG2	7:H:24:GLY:C	2.46	0.40
28:B:641:DMS:C1	41:B:931:HOH:O	2.64	0.40
3:C:38:GLY:HA3	20:C:511:CLA:HMD2	2.03	0.40
35:D:406:DGD:C4D	5:E:45:ASP:HB3	2.47	0.40
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.93	0.40
20:b:604:CLA:H111	20:b:604:CLA:H91	1.89	0.40
3:c:135[A]:ARG:CZ	34:z:102:LMT:H5B	2.51	0.40
3:c:457:LYS:NZ	41:c:614:HOH:O	2.55	0.40
20:c:501:CLA:C4D	20:c:503:CLA:H2	2.51	0.40
20:c:513:CLA:HMD3	34:z:102:LMT:H5'	2.03	0.40
6:f:36:ALA:O	6:f:40:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:81:ILE:HA	13:o:100:GLY:HA3	2.03	0.40
13:o:93:LEU:O	13:o:128:SER:HA	2.21	0.40
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.04	0.40
2:B:341:LYS:HZ1	32:B:622:HTG:C2	2.30	0.40
20:B:612:CLA:HMB3	20:B:612:CLA:HBB1	2.04	0.40
20:C:507:CLA:H41	20:C:507:CLA:H61	1.84	0.40
22:K:102:BCR:H24C	22:K:102:BCR:H371	1.86	0.40
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.56	0.40
20:b:617:CLA:H2	20:b:618:CLA:CBB	2.50	0.40
22:k:102:BCR:H24C	22:k:102:BCR:H371	1.94	0.40
13:o:183:ALA:HB3	28:o:303:DMS:C2	2.52	0.40
22:t:101:BCR:H311	22:t:101:BCR:C8	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	36 25
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	36 25
2	B	514/505 (102%)	503 (98%)	11 (2%)	0	100 100
2	b	493/505 (98%)	485 (98%)	8 (2%)	0	100 100
3	C	450/455 (99%)	436 (97%)	13 (3%)	1 (0%)	43 31
3	c	454/455 (100%)	442 (97%)	11 (2%)	1 (0%)	43 31
4	D	341/342 (100%)	334 (98%)	6 (2%)	1 (0%)	36 25
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100 100
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100 100
5	e	78/83 (94%)	78 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	31/44 (70%)	31 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	247/244 (101%)	235 (95%)	11 (4%)	1 (0%)	30	17
13	o	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	10	2
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	138/137 (101%)	133 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	1
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	0
All	All	5201/5350 (97%)	5069 (98%)	120 (2%)	12 (0%)	43	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	60	ARG
19	z	32	ASP
3	C	416	SER
4	D	12	ARG
13	O	61	GLN
3	c	416	SER
19	z	31	GLN
19	Z	30	PRO
13	o	34	SER
13	o	61	GLN
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	269/279 (96%)	268 (100%)	1 (0%)	84 82
1	a	270/279 (97%)	269 (100%)	1 (0%)	84 82
2	B	405/403 (100%)	401 (99%)	4 (1%)	68 60
2	b	390/403 (97%)	385 (99%)	5 (1%)	61 51
3	C	351/356 (99%)	347 (99%)	4 (1%)	65 57
3	c	356/356 (100%)	353 (99%)	3 (1%)	73 67
4	D	277/277 (100%)	274 (99%)	3 (1%)	65 57
4	d	276/277 (100%)	274 (99%)	2 (1%)	76 70
5	E	68/72 (94%)	65 (96%)	3 (4%)	25 10
5	e	68/72 (94%)	64 (94%)	4 (6%)	18 5
6	F	27/38 (71%)	27 (100%)	0	100 100
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	53 (98%)	1 (2%)	50 38
7	h	54/54 (100%)	53 (98%)	1 (2%)	50 38
8	I	30/34 (88%)	30 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	i	32/34 (94%)	28 (88%)	4 (12%)	4 0
9	J	23/28 (82%)	21 (91%)	2 (9%)	9 2
9	j	24/28 (86%)	24 (100%)	0	100 100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33 18
10	k	28/30 (93%)	26 (93%)	2 (7%)	13 3
11	L	34/35 (97%)	34 (100%)	0	100 100
11	l	33/35 (94%)	33 (100%)	0	100 100
12	M	30/33 (91%)	29 (97%)	1 (3%)	33 18
12	m	30/33 (91%)	30 (100%)	0	100 100
13	O	207/207 (100%)	204 (99%)	3 (1%)	59 49
13	o	199/207 (96%)	199 (100%)	0	100 100
14	T	26/28 (93%)	23 (88%)	3 (12%)	5 1
14	t	26/28 (93%)	25 (96%)	1 (4%)	29 14
15	U	82/89 (92%)	82 (100%)	0	100 100
15	u	83/89 (93%)	82 (99%)	1 (1%)	63 55
16	V	120/117 (103%)	119 (99%)	1 (1%)	73 67
16	v	114/117 (97%)	113 (99%)	1 (1%)	70 64
17	Y	21/23 (91%)	19 (90%)	2 (10%)	8 1
17	y	21/23 (91%)	21 (100%)	0	100 100
18	X	29/33 (88%)	29 (100%)	0	100 100
18	x	27/33 (82%)	27 (100%)	0	100 100
19	Z	44/52 (85%)	43 (98%)	1 (2%)	44 30
19	z	39/52 (75%)	37 (95%)	2 (5%)	21 7
All	All	4223/4376 (96%)	4166 (99%)	57 (1%)	63 51

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
2	B	80	ILE
2	B	307[A]	GLU
2	B	307[B]	GLU
2	B	467	ILE
3	C	78	GLU

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Mol	Chain	Res	Type
3	C	255	THR
3	C	289	PHE
3	C	315	MET
4	D	90	LEU
4	D	136	VAL
4	D	149	PRO
5	E	4	THR
5	E	25	ILE
5	E	61	ARG
7	H	63	LYS
9	J	8	ILE
9	J	10	LEU
10	K	17	ILE
12	M	5	GLN
13	O	23	ASP
13	O	130[A]	GLN
13	O	130[B]	GLN
14	T	2	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
16	V	86	GLN
17	Y	27	MET
17	Y	30	ILE
19	Z	46	LEU
1	a	244	GLU
2	b	80	ILE
2	b	223	GLN
2	b	362	PHE
2	b	467	ILE
2	b	472	ARG
3	c	255	THR
3	c	289	PHE
3	c	355	THR
4	d	233	ARG
4	d	329	MET
5	e	60[A]	GLN
5	e	60[B]	GLN
5	e	71	GLU
5	e	81	GLU
7	h	63	LYS
8	i	33	LYS
8	i	34[A]	ARG

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Mol	Chain	Res	Type
8	i	34[B]	ARG
8	i	36	ASP
10	k	17	ILE
10	k	19	ASP
14	t	2	GLU
15	u	9	LEU
16	v	6	GLU
19	z	29	SER
19	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	315	ASN
2	B	53	ASN
2	B	179	GLN
2	B	409	GLN
3	C	44	ASN
4	D	186	GLN
4	D	255	GLN
7	H	59	ASN
12	M	5	GLN
13	O	82	GLN
16	V	34	GLN
1	a	165	GLN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
3	c	44	ASN
4	d	186	GLN
4	d	255	GLN
4	d	301	GLN
4	d	332	GLN
6	f	44	GLN
13	o	82	GLN
13	o	155	ASN
13	o	231	HIS
15	u	73	GLN
16	v	34	GLN

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Mol	Chain	Res	Type
16	v	118	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.68	0	8,9,11	1.06	0
8	FME	i	1	8	8,9,10	0.52	0	8,9,11	1.51	1 (12%)
14	FME	T	1	14	8,9,10	0.45	0	8,9,11	1.59	1 (12%)
14	FME	t	1	14	8,9,10	0.49	0	8,9,11	1.70	3 (37%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	C-CA-N	2.81	114.93	109.50
14	T	1	FME	O-C-CA	-2.50	118.34	124.77
14	t	1	FME	O-C-CA	-2.28	118.90	124.77
14	t	1	FME	C-CA-N	2.25	113.84	109.50
14	t	1	FME	CG-CB-CA	2.24	119.72	112.87

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 349 ligands modelled in this entry, 14 are monoatomic and 55 are unknown - leaving 280 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	$\#\|Z\|>2$
37	HEM	e	102	5,6	50,50,50	1.98	10 (20%)	67,82,82	1.41	8 (11%)
20	CLA	C	504	41	69,73,73	2.21	17 (24%)	82,113,113	2.19	25 (30%)
28	DMS	c	536	-	3,3,3	2.91	1 (33%)	3,3,3	1.24	0
24	LMG	j	101	39	45,45,55	1.01	3 (6%)	53,53,63	1.03	6 (11%)
28	DMS	V	205	-	3,3,3	2.77	1 (33%)	3,3,3	0.55	0
28	DMS	U	904	-	3,3,3	2.92	1 (33%)	3,3,3	0.71	0
20	CLA	B	613	-	69,73,73	2.12	18 (26%)	82,113,113	2.24	29 (35%)
20	CLA	C	509	-	69,73,73	2.22	17 (24%)	82,113,113	2.39	27 (32%)
22	BCR	b	621	-	41,41,41	0.82	1 (2%)	56,56,56	1.49	8 (14%)
28	DMS	B	634	-	3,3,3	1.98	1 (33%)	3,3,3	0.29	0
30	OEX	A	420	41,1,3	0,15,15	-	-	-		
28	DMS	c	531	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
23	SQD	b	622	-	52,54,54	1.05	2 (3%)	62,65,65	1.52	11 (17%)
28	DMS	B	638	-	3,3,3	2.82	1 (33%)	3,3,3	0.84	0
35	DGD	c	516	-	58,58,67	0.86	2 (3%)	72,72,81	1.12	6 (8%)
28	DMS	h	102	-	3,3,3	2.82	1 (33%)	3,3,3	0.58	0
20	CLA	c	509	-	69,73,73	2.22	19 (27%)	82,113,113	2.39	31 (37%)
28	DMS	c	530	-	3,3,3	2.86	1 (33%)	3,3,3	1.02	0
28	DMS	B	644	-	3,3,3	2.94	1 (33%)	3,3,3	1.30	0
27	PL9	d	412	-	55,55,55	1.08	4 (7%)	68,69,69	1.56	17 (25%)
28	DMS	b	635	-	3,3,3	2.75	1 (33%)	3,3,3	0.77	0
28	DMS	i	104	-	3,3,3	2.69	1 (33%)	3,3,3	0.34	0
22	BCR	K	101	-	41,41,41	0.83	1 (2%)	56,56,56	1.52	14 (25%)
20	CLA	d	404	-	69,73,73	1.98	18 (26%)	82,113,113	2.38	32 (39%)
20	CLA	D	401	-	69,73,73	1.92	19 (27%)	82,113,113	2.28	29 (35%)
22	BCR	b	619	-	41,41,41	0.95	0	56,56,56	1.79	10 (17%)
20	CLA	b	610	-	69,73,73	2.23	18 (26%)	82,113,113	2.15	24 (29%)
23	SQD	A	412	-	52,54,54	0.96	2 (3%)	62,65,65	1.68	10 (16%)
34	LMT	a	418	-	36,36,36	0.68	2 (5%)	47,47,47	1.56	6 (12%)
24	LMG	C	519	-	51,51,55	1.04	2 (3%)	59,59,63	1.23	8 (13%)
20	CLA	B	610	-	69,73,73	2.28	19 (27%)	82,113,113	2.15	26 (31%)
28	DMS	C	525[A]	-	3,3,3	2.86	1 (33%)	3,3,3	0.87	0
28	DMS	C	528	-	3,3,3	2.37	1 (33%)	3,3,3	0.60	0
20	CLA	B	611	41	69,73,73	2.25	18 (26%)	82,113,113	2.36	28 (34%)
28	DMS	V	206	-	3,3,3	2.74	1 (33%)	3,3,3	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	HTG	C	520	-	19,19,19	0.82	1 (5%)	23,24,24	1.29	1 (4%)
20	CLA	B	609	-	69,73,73	1.95	18 (26%)	82,113,113	2.27	28 (34%)
34	LMT	I	101	-	36,36,36	0.65	1 (2%)	47,47,47	1.31	6 (12%)
22	BCR	A	405	-	41,41,41	0.97	3 (7%)	56,56,56	1.27	8 (14%)
20	CLA	C	508	-	64,68,73	2.48	19 (29%)	76,107,113	2.34	28 (36%)
28	DMS	O	311	-	3,3,3	2.94	1 (33%)	3,3,3	0.94	0
28	DMS	B	640	-	3,3,3	2.61	1 (33%)	3,3,3	0.99	0
28	DMS	O	305	-	3,3,3	2.69	1 (33%)	3,3,3	0.80	0
28	DMS	o	305	-	3,3,3	2.79	1 (33%)	3,3,3	0.79	0
20	CLA	B	604	-	69,73,73	2.08	22 (31%)	82,113,113	2.38	29 (35%)
20	CLA	b	613	-	69,73,73	2.02	13 (18%)	82,113,113	2.18	28 (34%)
36	LHG	L	101	-	48,48,48	0.92	3 (6%)	51,54,54	0.92	1 (1%)
38	RRX	x	101	-	42,42,42	0.84	0	56,58,58	1.24	5 (8%)
30	OEX	a	419	41,1,3	0,15,15	-	-	-		
23	SQD	A	406	-	52,54,54	0.95	2 (3%)	62,65,65	1.72	14 (22%)
32	HTG	B	631	-	19,19,19	0.86	1 (5%)	23,24,24	1.93	5 (21%)
34	LMT	Z	101	-	36,36,36	0.69	1 (2%)	47,47,47	0.99	3 (6%)
24	LMG	c	518	-	51,51,55	1.11	3 (5%)	59,59,63	1.32	7 (11%)
36	LHG	D	409	-	48,48,48	0.96	2 (4%)	51,54,54	1.07	3 (5%)
28	DMS	v	204	-	3,3,3	2.71	1 (33%)	3,3,3	0.82	0
36	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	5 (9%)
28	DMS	b	638	-	3,3,3	2.85	1 (33%)	3,3,3	0.96	0
28	DMS	O	307	-	3,3,3	2.75	1 (33%)	3,3,3	0.44	0
28	DMS	v	203	-	3,3,3	2.65	1 (33%)	3,3,3	0.86	0
20	CLA	b	616	-	69,73,73	2.01	14 (20%)	82,113,113	2.51	35 (42%)
28	DMS	v	209	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
32	HTG	b	625	-	19,19,19	1.17	2 (10%)	23,24,24	1.33	4 (17%)
28	DMS	d	413	-	3,3,3	2.63	1 (33%)	3,3,3	0.92	0
20	CLA	C	506	-	69,73,73	2.37	23 (33%)	82,113,113	2.23	23 (28%)
28	DMS	c	532	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
34	LMT	E	101	-	24,24,36	0.63	1 (4%)	29,29,47	1.00	3 (10%)
20	CLA	b	611	-	69,73,73	2.64	21 (30%)	82,113,113	1.88	25 (30%)
28	DMS	U	903[A]	-	3,3,3	2.62	1 (33%)	3,3,3	0.77	0
28	DMS	C	525[B]	-	3,3,3	2.65	1 (33%)	3,3,3	0.81	0
28	DMS	c	529	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	v	202	-	3,3,3	2.55	1 (33%)	3,3,3	0.60	0
21	PHO	a	405	-	58,69,69	2.25	13 (22%)	55,99,99	2.80	14 (25%)
28	DMS	D	416	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
28	DMS	C	532	-	3,3,3	3.36	1 (33%)	3,3,3	1.32	1 (33%)
28	DMS	b	640	-	3,3,3	2.83	1 (33%)	3,3,3	1.39	1 (33%)
31	BCT	A	421	29	3,3,3	1.22	1 (33%)	2,3,3	1.20	0
20	CLA	b	604	-	69,73,73	2.11	19 (27%)	82,113,113	2.18	30 (36%)
40	HEC	v	201	16	46,50,50	2.01	9 (19%)	58,82,82	1.46	9 (15%)
22	BCR	a	408	-	41,41,41	1.21	3 (7%)	56,56,56	1.46	8 (14%)
32	HTG	v	210	-	14,14,19	0.57	0	18,19,24	2.11	4 (22%)
28	DMS	d	415	-	3,3,3	2.78	1 (33%)	3,3,3	0.55	0
28	DMS	C	531	-	3,3,3	2.72	1 (33%)	3,3,3	0.99	0
28	DMS	V	207	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
23	SQD	a	401	-	52,54,54	1.06	2 (3%)	62,65,65	1.39	6 (9%)
28	DMS	C	526	-	3,3,3	2.62	1 (33%)	3,3,3	0.82	0
21	PHO	a	406	-	58,69,69	2.56	12 (20%)	55,99,99	3.05	16 (29%)
22	BCR	T	101	-	41,41,41	0.83	0	56,56,56	1.53	12 (21%)
20	CLA	C	512	-	59,63,73	2.74	23 (38%)	70,101,113	2.39	27 (38%)
32	HTG	O	302	-	19,19,19	1.23	2 (10%)	23,24,24	1.16	2 (8%)
20	CLA	B	615	-	69,73,73	2.06	19 (27%)	82,113,113	2.52	30 (36%)
20	CLA	C	513	-	69,73,73	2.52	20 (28%)	82,113,113	2.17	23 (28%)
21	PHO	D	403	-	58,69,69	2.60	11 (18%)	55,99,99	3.07	17 (30%)
28	DMS	b	636	-	3,3,3	2.78	1 (33%)	3,3,3	0.76	0
28	DMS	B	635	-	3,3,3	2.69	1 (33%)	3,3,3	0.48	0
28	DMS	c	533	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
28	DMS	u	202	-	3,3,3	2.72	1 (33%)	3,3,3	1.32	0
28	DMS	v	207	-	3,3,3	2.82	1 (33%)	3,3,3	0.57	0
32	HTG	b	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.44	2 (8%)
20	CLA	c	503	-	69,73,73	2.48	22 (31%)	82,113,113	2.26	27 (32%)
28	DMS	F	102	-	3,3,3	2.70	1 (33%)	3,3,3	0.62	0
32	HTG	V	202	-	12,13,19	0.75	0	17,18,24	3.07	7 (41%)
28	DMS	B	641	-	3,3,3	2.72	1 (33%)	3,3,3	0.65	0
34	LMT	f	102	-	24,24,36	0.80	1 (4%)	29,29,47	0.97	2 (6%)
20	CLA	c	502	-	69,73,73	2.18	17 (24%)	82,113,113	2.39	29 (35%)
28	DMS	O	310	-	3,3,3	2.77	1 (33%)	3,3,3	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	D	404	-	69,73,73	2.09	20 (28%)	82,113,113	2.24	28 (34%)
32	HTG	c	520	-	19,19,19	0.82	2 (10%)	23,24,24	1.20	2 (8%)
34	LMT	B	627	-	15,15,36	0.48	0	14,14,47	0.70	1 (7%)
34	LMT	m	102	-	36,36,36	0.58	0	47,47,47	1.16	4 (8%)
28	DMS	U	903[B]	-	3,3,3	2.50	1 (33%)	3,3,3	0.17	0
20	CLA	d	403	41	69,73,73	2.01	17 (24%)	82,113,113	2.17	26 (31%)
36	LHG	d	407	-	48,48,48	0.74	2 (4%)	51,54,54	1.00	6 (11%)
20	CLA	a	403	-	69,73,73	1.84	15 (21%)	82,113,113	2.15	28 (34%)
20	CLA	B	606	-	69,73,73	1.92	16 (23%)	82,113,113	2.30	30 (36%)
32	HTG	b	601	-	19,19,19	0.96	2 (10%)	23,24,24	1.15	2 (8%)
28	DMS	o	308	-	3,3,3	2.92	1 (33%)	3,3,3	0.83	0
32	HTG	c	521	-	19,19,19	0.89	1 (5%)	23,24,24	1.86	3 (13%)
28	DMS	j	105	-	3,3,3	2.87	1 (33%)	3,3,3	0.87	0
35	DGD	d	416	-	51,51,67	1.11	3 (5%)	59,59,81	1.21	6 (10%)
34	LMT	B	625	-	24,24,36	0.54	0	29,29,47	1.25	4 (13%)
28	DMS	B	637	-	3,3,3	2.62	1 (33%)	3,3,3	0.74	0
20	CLA	c	507	41	69,73,73	2.27	16 (23%)	82,113,113	2.35	28 (34%)
20	CLA	A	404	-	69,73,73	1.99	19 (27%)	82,113,113	2.50	31 (37%)
24	LMG	J	101	39	45,45,55	1.01	2 (4%)	53,53,63	0.99	3 (5%)
31	BCT	a	413	29	3,3,3	1.37	1 (33%)	2,3,3	1.51	0
22	BCR	B	617	-	41,41,41	0.96	1 (2%)	56,56,56	1.64	11 (19%)
22	BCR	b	620	-	41,41,41	1.10	1 (2%)	56,56,56	1.26	5 (8%)
28	DMS	O	308	-	3,3,3	2.82	1 (33%)	3,3,3	0.80	0
28	DMS	v	208	-	3,3,3	2.69	1 (33%)	3,3,3	0.68	0
20	CLA	B	608	41	69,73,73	1.94	14 (20%)	82,113,113	2.08	23 (28%)
32	HTG	B	622	-	19,19,19	1.26	2 (10%)	23,24,24	1.83	6 (26%)
32	HTG	b	602	-	19,19,19	0.93	2 (10%)	23,24,24	1.03	1 (4%)
20	CLA	c	505	-	69,73,73	2.20	21 (30%)	82,113,113	2.04	25 (30%)
32	HTG	B	621	-	19,19,19	1.36	3 (15%)	23,24,24	1.73	6 (26%)
37	HEM	E	104	5,6	50,50,50	2.21	9 (18%)	67,82,82	1.56	11 (16%)
28	DMS	A	417	-	3,3,3	2.69	1 (33%)	3,3,3	0.46	0
20	CLA	B	603	-	69,73,73	2.17	21 (30%)	82,113,113	2.16	27 (32%)
20	CLA	B	616	-	69,73,73	2.14	17 (24%)	82,113,113	2.13	23 (28%)
20	CLA	b	618	-	69,73,73	2.17	21 (30%)	82,113,113	2.27	28 (34%)
22	BCR	d	405	-	41,41,41	0.94	0	56,56,56	1.88	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCR	c	514	-	41,41,41	0.84	1 (2%)	56,56,56	1.50	8 (14%)
22	BCR	j	102	-	41,41,41	0.85	0	56,56,56	1.40	10 (17%)
28	DMS	C	530	-	3,3,3	2.67	1 (33%)	3,3,3	1.01	0
28	DMS	B	643	-	3,3,3	2.84	1 (33%)	3,3,3	0.76	0
28	DMS	D	414	-	3,3,3	2.58	1 (33%)	3,3,3	0.26	0
32	HTG	B	632	-	19,19,19	0.94	1 (5%)	23,24,24	1.18	2 (8%)
34	LMT	z	102	-	36,36,36	0.77	1 (2%)	47,47,47	1.54	8 (17%)
28	DMS	B	639	-	3,3,3	2.79	1 (33%)	3,3,3	0.65	0
28	DMS	b	641	-	3,3,3	2.85	1 (33%)	3,3,3	1.14	0
34	LMT	b	627	-	33,33,36	0.88	1 (3%)	44,44,47	1.82	10 (22%)
28	DMS	v	206	-	3,3,3	2.72	1 (33%)	3,3,3	0.68	0
32	HTG	C	522	-	19,19,19	0.97	2 (10%)	23,24,24	1.36	1 (4%)
38	RRX	H	101	-	42,42,42	0.77	1 (2%)	56,58,58	1.53	9 (16%)
22	BCR	D	405	-	41,41,41	1.00	2 (4%)	56,56,56	1.77	14 (25%)
22	BCR	t	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.77	19 (33%)
20	CLA	c	510	-	69,73,73	1.98	20 (28%)	82,113,113	2.19	31 (37%)
20	CLA	a	407	-	51,55,73	2.36	18 (35%)	60,91,113	2.44	27 (45%)
34	LMT	M	101	-	36,36,36	0.63	0	47,47,47	0.94	2 (4%)
35	DGD	c	515	-	63,63,67	0.85	3 (4%)	77,77,81	1.17	7 (9%)
23	SQD	l	101	-	52,54,54	1.05	3 (5%)	62,65,65	1.62	8 (12%)
20	CLA	B	605	-	69,73,73	2.11	18 (26%)	82,113,113	2.00	26 (31%)
20	CLA	b	608	-	69,73,73	2.33	18 (26%)	82,113,113	2.15	26 (31%)
28	DMS	O	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.66	0
22	BCR	k	102	-	41,41,41	0.80	0	56,56,56	1.30	9 (16%)
35	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	4 (5%)
32	HTG	D	417	-	19,19,19	0.98	1 (5%)	23,24,24	1.38	3 (13%)
35	DGD	C	517	-	56,56,67	0.98	2 (3%)	70,70,81	0.91	4 (5%)
32	HTG	B	623	-	19,19,19	0.89	1 (5%)	23,24,24	1.39	1 (4%)
34	LMT	B	626	-	24,24,36	0.54	0	29,29,47	1.15	3 (10%)
20	CLA	A	402	41	63,67,73	1.85	18 (28%)	74,105,113	2.75	33 (44%)
28	DMS	B	642	-	3,3,3	2.86	1 (33%)	3,3,3	0.77	0
20	CLA	b	609	41	69,73,73	2.09	20 (28%)	82,113,113	2.04	28 (34%)
28	DMS	A	415	-	3,3,3	2.81	1 (33%)	3,3,3	1.04	0
32	HTG	C	534	-	19,19,19	1.00	1 (5%)	23,24,24	1.40	5 (21%)
20	CLA	d	402	-	69,73,73	1.88	20 (28%)	82,113,113	1.97	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	DGD	C	516	-	63,63,67	0.90	2 (3%)	77,77,81	1.19	7 (9%)
35	DGD	c	517	-	63,63,67	1.05	4 (6%)	77,77,81	1.19	7 (9%)
28	DMS	A	414	-	3,3,3	2.02	1 (33%)	3,3,3	0.55	0
28	DMS	o	306	-	3,3,3	2.85	1 (33%)	3,3,3	1.05	0
20	CLA	b	603	41	69,73,73	2.85	19 (27%)	82,113,113	2.32	24 (29%)
24	LMG	B	620	-	51,51,55	1.02	3 (5%)	59,59,63	1.32	5 (8%)
20	CLA	C	501	-	69,73,73	2.08	18 (26%)	82,113,113	2.16	23 (28%)
20	CLA	C	505	-	69,73,73	2.37	20 (28%)	82,113,113	2.02	25 (30%)
28	DMS	O	306	-	3,3,3	2.59	1 (33%)	3,3,3	0.66	0
34	LMT	T	102	-	24,24,36	0.45	0	29,29,47	1.15	2 (6%)
20	CLA	c	504	41	69,73,73	2.13	22 (31%)	82,113,113	2.61	31 (37%)
20	CLA	B	607	-	69,73,73	2.36	19 (27%)	82,113,113	2.41	30 (36%)
22	BCR	B	618	-	41,41,41	1.08	0	56,56,56	1.28	7 (12%)
20	CLA	A	401	-	69,73,73	1.92	18 (26%)	82,113,113	2.02	23 (28%)
28	DMS	u	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.80	0
36	LHG	d	406	-	48,48,48	0.95	2 (4%)	51,54,54	1.18	5 (9%)
28	DMS	b	639	-	3,3,3	2.88	1 (33%)	3,3,3	0.59	0
28	DMS	B	645	-	3,3,3	2.79	1 (33%)	3,3,3	0.96	0
28	DMS	d	414	-	3,3,3	2.56	1 (33%)	3,3,3	0.24	0
23	SQD	a	409	-	52,54,54	0.93	3 (5%)	62,65,65	2.05	11 (17%)
20	CLA	b	615	-	69,73,73	1.93	19 (27%)	82,113,113	2.31	27 (32%)
20	CLA	B	612	-	69,73,73	1.86	15 (21%)	82,113,113	2.25	30 (36%)
20	CLA	c	506	-	69,73,73	2.38	19 (27%)	82,113,113	2.21	25 (30%)
28	DMS	b	634	-	3,3,3	2.73	1 (33%)	3,3,3	0.70	0
28	DMS	C	529	-	3,3,3	2.75	1 (33%)	3,3,3	0.83	0
20	CLA	c	511	3	69,73,73	2.47	18 (26%)	82,113,113	2.25	24 (29%)
28	DMS	C	533	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
36	LHG	l	102	-	48,48,48	0.79	2 (4%)	51,54,54	1.01	2 (3%)
21	PHO	A	403	-	58,69,69	2.34	12 (20%)	55,99,99	3.23	12 (21%)
28	DMS	o	307	-	3,3,3	2.71	1 (33%)	3,3,3	0.87	0
20	CLA	b	607	-	69,73,73	2.07	19 (27%)	82,113,113	2.23	23 (28%)
24	LMG	b	623	-	49,49,55	0.96	2 (4%)	57,57,63	1.32	6 (10%)
20	CLA	C	502	-	69,73,73	2.22	18 (26%)	82,113,113	2.27	30 (36%)
22	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.61	10 (17%)
20	CLA	b	614	-	69,73,73	2.02	20 (28%)	82,113,113	2.26	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	b	606	-	69,73,73	2.01	19 (27%)	82,113,113	2.30	27 (32%)
32	HTG	u	201	-	7,7,19	0.37	0	6,6,24	0.75	0
34	LMT	b	628	-	25,25,36	0.56	0	30,30,47	1.21	3 (10%)
24	LMG	a	410	-	51,51,55	0.90	2 (3%)	59,59,63	1.09	2 (3%)
28	DMS	O	304	-	3,3,3	2.67	1 (33%)	3,3,3	0.61	0
28	DMS	c	527	-	3,3,3	2.36	1 (33%)	3,3,3	0.49	0
20	CLA	c	513	-	69,73,73	2.51	18 (26%)	82,113,113	2.18	26 (31%)
22	BCR	K	102	-	41,41,41	0.90	1 (2%)	56,56,56	1.49	5 (8%)
28	DMS	b	637	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
28	DMS	D	413	-	3,3,3	2.79	1 (33%)	3,3,3	0.67	0
28	DMS	o	302	-	3,3,3	2.82	1 (33%)	3,3,3	0.91	0
28	DMS	c	534	-	3,3,3	2.76	1 (33%)	3,3,3	0.77	0
32	HTG	C	521	-	19,19,19	0.93	2 (10%)	23,24,24	1.85	3 (13%)
34	LMT	c	523	-	36,36,36	0.82	1 (2%)	47,47,47	1.61	6 (12%)
28	DMS	o	303	-	3,3,3	2.74	1 (33%)	3,3,3	0.51	0
23	SQD	f	101	-	38,40,54	1.35	2 (5%)	48,51,65	3.36	12 (25%)
28	DMS	b	632	-	3,3,3	2.78	1 (33%)	3,3,3	0.57	0
28	DMS	U	902	-	3,3,3	2.72	1 (33%)	3,3,3	1.66	1 (33%)
20	CLA	D	402	41	69,73,73	1.93	20 (28%)	82,113,113	2.16	24 (29%)
28	DMS	V	204	-	3,3,3	2.71	1 (33%)	3,3,3	0.80	0
20	CLA	b	612	41	69,73,73	2.09	21 (30%)	82,113,113	2.18	27 (32%)
28	DMS	b	631	-	3,3,3	2.95	1 (33%)	3,3,3	1.26	0
20	CLA	a	404	41	64,68,73	1.90	17 (26%)	76,107,113	2.30	28 (36%)
35	DGD	D	406	-	51,51,67	1.11	2 (3%)	59,59,81	1.21	5 (8%)
27	PL9	D	412	-	55,55,55	1.09	3 (5%)	68,69,69	1.44	10 (14%)
28	DMS	V	209	-	3,3,3	2.67	1 (33%)	3,3,3	0.66	0
28	DMS	H	103	-	3,3,3	2.81	1 (33%)	3,3,3	0.65	0
32	HTG	d	401	-	19,19,19	1.01	1 (5%)	23,24,24	2.09	4 (17%)
36	LHG	D	407	-	48,48,48	0.87	1 (2%)	51,54,54	1.28	5 (9%)
34	LMT	J	103	-	24,24,36	0.65	1 (4%)	29,29,47	1.12	1 (3%)
35	DGD	h	101	-	63,63,67	0.99	3 (4%)	77,77,81	1.04	6 (7%)
20	CLA	c	501	-	69,73,73	2.13	17 (24%)	82,113,113	2.76	30 (36%)
28	DMS	b	633	-	3,3,3	2.61	1 (33%)	3,3,3	1.07	0
35	DGD	H	102	-	63,63,67	1.05	3 (4%)	77,77,81	1.27	8 (10%)
20	CLA	C	511	3	69,73,73	2.30	21 (30%)	82,113,113	2.40	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	LHG	D	408	-	48,48,48	0.83	2 (4%)	51,54,54	1.05	1 (1%)
24	LMG	A	407	-	51,51,55	0.96	2 (3%)	59,59,63	1.07	3 (5%)
40	HEC	V	201	16	46,50,50	1.98	9 (19%)	58,82,82	1.41	7 (12%)
36	LHG	E	103	-	46,46,48	1.04	2 (4%)	48,50,54	1.15	5 (10%)
23	SQD	F	101	-	33,35,54	0.95	1 (3%)	42,45,65	1.56	7 (16%)
22	BCR	k	101	-	41,41,41	0.95	0	56,56,56	1.13	6 (10%)
28	DMS	O	309	-	3,3,3	2.74	1 (33%)	3,3,3	1.17	0
20	CLA	c	508	-	64,68,73	2.31	17 (26%)	76,107,113	2.29	27 (35%)
28	DMS	c	535	-	3,3,3	2.84	1 (33%)	3,3,3	0.82	0
20	CLA	C	503	-	69,73,73	2.40	22 (31%)	82,113,113	2.03	27 (32%)
20	CLA	b	605	-	69,73,73	2.11	20 (28%)	82,113,113	2.24	32 (39%)
28	DMS	A	416	-	3,3,3	2.74	1 (33%)	3,3,3	0.80	0
24	LMG	c	519	-	51,51,55	1.01	3 (5%)	59,59,63	1.18	7 (11%)
24	LMG	C	524	-	45,45,55	1.10	3 (6%)	53,53,63	1.37	5 (9%)
28	DMS	V	208	-	3,3,3	2.71	1 (33%)	3,3,3	0.75	0
28	DMS	D	415	-	3,3,3	2.99	1 (33%)	3,3,3	0.75	0
20	CLA	c	512	-	69,73,73	2.36	22 (31%)	82,113,113	2.29	24 (29%)
28	DMS	u	204	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
28	DMS	v	205	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
34	LMT	m	101	-	36,36,36	0.61	1 (2%)	47,47,47	0.97	2 (4%)
27	PL9	a	415	-	55,55,55	0.81	3 (5%)	68,69,69	1.68	16 (23%)
20	CLA	C	510	-	69,73,73	2.20	19 (27%)	82,113,113	2.20	28 (34%)
28	DMS	A	418	-	3,3,3	2.86	1 (33%)	3,3,3	0.75	0
20	CLA	C	507	41	69,73,73	2.38	20 (28%)	82,113,113	2.33	26 (31%)
28	DMS	B	636	-	3,3,3	2.83	1 (33%)	3,3,3	0.80	0
22	BCR	C	515	-	41,41,41	0.97	0	56,56,56	1.21	5 (8%)
20	CLA	B	601	-	69,73,73	2.06	18 (26%)	82,113,113	2.16	29 (35%)
20	CLA	B	602	41	69,73,73	2.57	20 (28%)	82,113,113	2.49	29 (35%)
28	DMS	c	528	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
22	BCR	C	514	-	41,41,41	0.87	0	56,56,56	1.33	8 (14%)
20	CLA	B	614	-	69,73,73	1.90	16 (23%)	82,113,113	2.14	25 (30%)
28	DMS	o	304	-	3,3,3	2.70	1 (33%)	3,3,3	0.67	0
28	DMS	C	527	-	3,3,3	2.62	1 (33%)	3,3,3	0.51	0
20	CLA	b	617	-	69,73,73	2.13	19 (27%)	82,113,113	2.19	25 (30%)
27	PL9	A	411	-	55,55,55	0.82	4 (7%)	68,69,69	1.69	18 (26%)

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
37	HEM	e	102	5,6	-	4/14/54/54	-
20	CLA	C	504	41	-	11/39/115/115	-
24	LMG	j	101	39	-	15/40/60/70	0/1/1/1
20	CLA	B	613	-	1/1/15/20	1/39/115/115	-
20	CLA	C	509	-	1/1/15/20	9/39/115/115	-
22	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	SQD	b	622	-	-	23/49/69/69	0/1/1/1
35	DGD	c	516	-	-	12/46/86/95	0/2/2/2
20	CLA	c	509	-	1/1/15/20	9/39/115/115	-
27	PL9	d	412	-	-	1/53/73/73	0/1/1/1
22	BCR	K	101	-	-	4/29/63/63	0/2/2/2
20	CLA	d	404	-	-	8/39/115/115	-
20	CLA	D	401	-	1/1/15/20	6/39/115/115	-
22	BCR	b	619	-	-	1/29/63/63	0/2/2/2
20	CLA	b	610	-	-	1/39/115/115	-
23	SQD	A	412	-	-	24/49/69/69	0/1/1/1
34	LMT	a	418	-	-	11/21/61/61	0/2/2/2
24	LMG	C	519	-	-	19/46/66/70	0/1/1/1
20	CLA	B	610	-	1/1/15/20	2/39/115/115	-
20	CLA	B	611	41	1/1/15/20	3/39/115/115	-
32	HTG	C	520	-	-	4/10/30/30	0/1/1/1
20	CLA	B	609	-	-	1/39/115/115	-
34	LMT	I	101	-	-	9/21/61/61	0/2/2/2
22	BCR	A	405	-	-	0/29/63/63	0/2/2/2
20	CLA	C	508	-	1/1/14/20	4/33/109/115	-
20	CLA	B	604	-	1/1/15/20	2/39/115/115	-
20	CLA	b	613	-	-	5/39/115/115	-
36	LHG	L	101	-	-	17/53/53/53	-
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
32	HTG	B	631	-	-	5/10/30/30	0/1/1/1
23	SQD	A	406	-	-	21/49/69/69	0/1/1/1
34	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
24	LMG	c	518	-	-	8/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	D	409	-	-	13/53/53/53	-
36	LHG	d	408	-	-	14/53/53/53	-
20	CLA	b	616	-	1/1/15/20	15/39/115/115	-
32	HTG	b	625	-	-	4/10/30/30	0/1/1/1
20	CLA	C	506	-	1/1/15/20	11/39/115/115	-
34	LMT	E	101	-	-	8/15/35/61	0/1/1/2
20	CLA	b	611	-	-	1/39/115/115	-
21	PHO	a	405	-	-	3/37/103/103	0/5/6/6
40	HEC	v	201	16	-	6/14/54/54	-
20	CLA	b	604	-	1/1/15/20	6/39/115/115	-
22	BCR	a	408	-	-	0/29/63/63	0/2/2/2
32	HTG	v	210	-	-	3/5/25/30	0/1/1/1
23	SQD	a	401	-	-	21/49/69/69	0/1/1/1
21	PHO	a	406	-	-	2/37/103/103	0/5/6/6
22	BCR	T	101	-	-	1/29/63/63	0/2/2/2
20	CLA	C	512	-	1/1/13/20	3/27/103/115	-
32	HTG	O	302	-	-	5/10/30/30	0/1/1/1
20	CLA	B	615	-	1/1/15/20	7/39/115/115	-
20	CLA	C	513	-	-	10/39/115/115	-
21	PHO	D	403	-	-	2/37/103/103	0/5/6/6
32	HTG	b	624	-	-	0/10/30/30	0/1/1/1
20	CLA	c	503	-	-	2/39/115/115	-
32	HTG	V	202	-	-	1/4/24/30	0/1/1/1
34	LMT	f	102	-	-	8/15/35/61	0/1/1/2
20	CLA	c	502	-	-	4/39/115/115	-
34	LMT	B	627	-	-	7/13/13/61	-
20	CLA	D	404	-	1/1/15/20	12/39/115/115	-
32	HTG	c	520	-	-	5/10/30/30	0/1/1/1
34	LMT	m	102	-	-	3/21/61/61	0/2/2/2
36	LHG	d	407	-	-	10/53/53/53	-
20	CLA	d	403	41	-	3/39/115/115	-
20	CLA	a	403	-	1/1/15/20	3/39/115/115	-
20	CLA	B	606	-	1/1/15/20	3/39/115/115	-
32	HTG	b	601	-	-	2/10/30/30	0/1/1/1
32	HTG	c	521	-	-	5/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	d	416	-	-	30/46/66/95	0/1/1/2
34	LMT	B	625	-	-	4/15/35/61	0/1/1/2
20	CLA	c	507	41	1/1/15/20	6/39/115/115	-
20	CLA	A	404	-	-	10/39/115/115	-
24	LMG	J	101	39	-	8/40/60/70	0/1/1/1
22	BCR	B	617	-	-	2/29/63/63	0/2/2/2
22	BCR	b	620	-	-	0/29/63/63	0/2/2/2
32	HTG	B	622	-	-	5/10/30/30	0/1/1/1
32	HTG	b	602	-	-	3/10/30/30	0/1/1/1
20	CLA	B	608	41	1/1/15/20	1/39/115/115	-
20	CLA	c	505	-	1/1/15/20	0/39/115/115	-
32	HTG	B	621	-	-	5/10/30/30	0/1/1/1
37	HEM	E	104	5,6	-	7/14/54/54	-
20	CLA	B	603	-	1/1/15/20	0/39/115/115	-
20	CLA	B	616	-	1/1/15/20	5/39/115/115	-
20	CLA	b	618	-	1/1/15/20	17/39/115/115	-
22	BCR	d	405	-	-	4/29/63/63	0/2/2/2
22	BCR	c	514	-	-	0/29/63/63	0/2/2/2
22	BCR	j	102	-	-	2/29/63/63	0/2/2/2
32	HTG	B	632	-	-	2/10/30/30	0/1/1/1
34	LMT	z	102	-	-	13/21/61/61	0/2/2/2
34	LMT	b	627	-	-	10/18/58/61	0/2/2/2
32	HTG	C	522	-	-	3/10/30/30	0/1/1/1
38	RRX	H	101	-	-	1/29/65/65	0/2/2/2
22	BCR	D	405	-	-	4/29/63/63	0/2/2/2
22	BCR	t	101	-	-	3/29/63/63	0/2/2/2
20	CLA	c	510	-	1/1/15/20	3/39/115/115	-
20	CLA	a	407	-	-	0/18/94/115	-
34	LMT	M	101	-	-	1/21/61/61	0/2/2/2
23	SQD	l	101	-	-	27/49/69/69	0/1/1/1
20	CLA	B	605	-	1/1/15/20	6/39/115/115	-
20	CLA	b	608	-	1/1/15/20	7/39/115/115	-
22	BCR	k	102	-	-	0/29/63/63	0/2/2/2
35	DGD	C	518	-	-	12/51/91/95	0/2/2/2
32	HTG	D	417	-	-	4/10/30/30	0/1/1/1
35	DGD	C	517	-	-	11/44/84/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	B	623	-	-	6/10/30/30	0/1/1/1
34	LMT	B	626	-	-	7/15/35/61	0/1/1/2
20	CLA	A	402	41	-	1/32/108/115	-
20	CLA	b	609	41	1/1/15/20	2/39/115/115	-
32	HTG	C	534	-	-	4/10/30/30	0/1/1/1
35	DGD	C	516	-	-	17/51/91/95	0/2/2/2
20	CLA	d	402	-	1/1/15/20	5/39/115/115	-
35	DGD	c	517	-	-	13/51/91/95	0/2/2/2
35	DGD	c	515	-	-	17/51/91/95	0/2/2/2
20	CLA	b	603	41	1/1/15/20	16/39/115/115	-
24	LMG	B	620	-	-	19/46/66/70	0/1/1/1
20	CLA	C	505	-	1/1/15/20	1/39/115/115	-
20	CLA	C	501	-	1/1/15/20	3/39/115/115	-
34	LMT	T	102	-	-	11/15/35/61	0/1/1/2
20	CLA	c	504	41	1/1/15/20	4/39/115/115	-
20	CLA	B	607	-	1/1/15/20	9/39/115/115	-
22	BCR	B	618	-	-	0/29/63/63	0/2/2/2
20	CLA	A	401	-	1/1/15/20	4/39/115/115	-
36	LHG	d	406	-	-	11/53/53/53	-
23	SQD	a	409	-	-	19/49/69/69	0/1/1/1
20	CLA	b	615	-	1/1/15/20	6/39/115/115	-
20	CLA	B	612	-	1/1/15/20	3/39/115/115	-
20	CLA	c	506	-	1/1/15/20	9/39/115/115	-
20	CLA	c	511	3	1/1/15/20	0/39/115/115	-
36	LHG	l	102	-	-	18/53/53/53	-
21	PHO	A	403	-	-	0/37/103/103	0/5/6/6
20	CLA	b	607	-	1/1/15/20	3/39/115/115	-
24	LMG	b	623	-	-	14/44/64/70	0/1/1/1
20	CLA	C	502	-	-	5/39/115/115	-
22	BCR	B	619	-	-	0/29/63/63	0/2/2/2
20	CLA	b	614	-	1/1/15/20	5/39/115/115	-
20	CLA	b	606	-	1/1/15/20	1/39/115/115	-
32	HTG	u	201	-	-	1/5/5/30	-
34	LMT	b	628	-	-	9/17/37/61	0/1/1/2
24	LMG	a	410	-	-	18/46/66/70	0/1/1/1
20	CLA	c	513	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	K	102	-	-	2/29/63/63	0/2/2/2
34	LMT	c	523	-	-	8/21/61/61	0/2/2/2
32	HTG	C	521	-	-	6/10/30/30	0/1/1/1
23	SQD	f	101	-	-	17/34/54/69	0/1/1/1
35	DGD	D	406	-	-	26/46/66/95	0/1/1/2
20	CLA	D	402	41	-	3/39/115/115	-
20	CLA	b	612	41	1/1/15/20	5/39/115/115	-
20	CLA	a	404	41	-	6/33/109/115	-
27	PL9	D	412	-	-	3/53/73/73	0/1/1/1
32	HTG	d	401	-	-	8/10/30/30	0/1/1/1
36	LHG	D	407	-	-	9/53/53/53	-
34	LMT	J	103	-	-	7/15/35/61	0/1/1/2
35	DGD	h	101	-	-	15/51/91/95	0/2/2/2
20	CLA	c	501	-	1/1/15/20	2/39/115/115	-
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
20	CLA	C	511	3	-	0/39/115/115	-
36	LHG	D	408	-	-	9/53/53/53	-
24	LMG	A	407	-	-	28/46/66/70	0/1/1/1
40	HEC	V	201	16	-	6/14/54/54	-
36	LHG	E	103	-	-	26/45/45/53	-
23	SQD	F	101	-	-	17/28/48/69	0/1/1/1
22	BCR	k	101	-	-	3/29/63/63	0/2/2/2
20	CLA	c	508	-	-	0/33/109/115	-
20	CLA	C	503	-	-	3/39/115/115	-
20	CLA	b	605	-	1/1/15/20	1/39/115/115	-
24	LMG	c	519	-	-	26/46/66/70	0/1/1/1
24	LMG	C	524	-	-	22/40/60/70	0/1/1/1
20	CLA	c	512	-	1/1/15/20	8/39/115/115	-
34	LMT	m	101	-	-	15/21/61/61	0/2/2/2
27	PL9	a	415	-	-	11/53/73/73	0/1/1/1
20	CLA	C	510	-	1/1/15/20	2/39/115/115	-
20	CLA	C	507	41	1/1/15/20	11/39/115/115	-
22	BCR	C	515	-	-	0/29/63/63	0/2/2/2
20	CLA	B	601	-	1/1/15/20	18/39/115/115	-
20	CLA	B	602	41	1/1/15/20	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	C	514	-	-	5/29/63/63	0/2/2/2
20	CLA	B	614	-	1/1/15/20	5/39/115/115	-
20	CLA	b	617	-	1/1/15/20	8/39/115/115	-
27	PL9	A	411	-	-	11/53/73/73	0/1/1/1

All (1654) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	MG-NA	12.91	2.36	2.06
20	c	513	CLA	MG-NA	12.66	2.36	2.06
20	B	602	CLA	MG-NA	11.66	2.34	2.06
20	c	507	CLA	MG-NA	10.98	2.32	2.06
20	c	511	CLA	MG-NC	10.70	2.31	2.06
21	A	403	PHO	C1D-C2D	10.67	1.51	1.39
20	b	603	CLA	MG-NB	-10.46	1.85	2.05
20	C	502	CLA	MG-NA	10.10	2.30	2.06
20	C	506	CLA	MG-NA	10.02	2.30	2.06
20	b	608	CLA	MG-NA	9.93	2.29	2.06
20	c	502	CLA	MG-NA	9.90	2.29	2.06
20	C	511	CLA	MG-NA	9.62	2.29	2.06
20	C	508	CLA	MG-NA	9.57	2.29	2.06
20	B	605	CLA	MG-NA	9.52	2.28	2.06
20	c	503	CLA	MG-NA	9.50	2.28	2.06
20	b	603	CLA	MG-NC	9.40	2.28	2.06
21	a	406	PHO	C1B-C2B	9.32	1.49	1.39
20	b	617	CLA	MG-NA	9.30	2.28	2.06
20	B	613	CLA	MG-NA	9.26	2.28	2.06
21	D	403	PHO	C1B-C2B	9.25	1.49	1.39
20	c	509	CLA	MG-NA	9.07	2.27	2.06
21	a	406	PHO	C1D-C2D	9.06	1.49	1.39
20	C	509	CLA	MG-NA	9.01	2.27	2.06
20	C	503	CLA	MG-NA	8.95	2.27	2.06
21	D	403	PHO	C1D-C2D	8.93	1.49	1.39
20	b	613	CLA	MG-NA	8.84	2.27	2.06
20	b	603	CLA	MG-ND	8.72	2.23	2.05
20	c	508	CLA	MG-NA	8.69	2.26	2.06
20	d	403	CLA	MG-NA	8.65	2.26	2.06
20	c	506	CLA	MG-ND	-8.64	1.88	2.05
20	C	507	CLA	MG-NC	8.62	2.26	2.06
20	C	513	CLA	MG-NA	8.51	2.26	2.06
20	B	610	CLA	MG-NA	8.45	2.26	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	104	HEM	FE-NC	8.44	2.23	1.95
20	C	512	CLA	MG-NA	8.34	2.26	2.06
20	B	608	CLA	MG-NA	8.25	2.25	2.06
20	C	504	CLA	MG-NA	8.16	2.25	2.06
20	c	501	CLA	MG-NA	8.12	2.25	2.06
20	c	504	CLA	MG-NA	8.10	2.25	2.06
20	c	512	CLA	MG-NA	8.09	2.25	2.06
20	b	605	CLA	MG-NA	8.07	2.25	2.06
20	C	505	CLA	MG-NB	7.99	2.21	2.05
20	B	607	CLA	MG-NA	7.94	2.25	2.06
37	e	102	HEM	C3D-C2D	7.87	1.53	1.36
20	C	510	CLA	MG-NA	7.85	2.24	2.06
20	B	603	CLA	MG-NA	7.84	2.24	2.06
20	B	616	CLA	MG-NA	7.81	2.24	2.06
20	b	606	CLA	MG-NA	7.76	2.24	2.06
20	b	618	CLA	MG-NA	7.73	2.24	2.06
21	a	405	PHO	C1B-C2B	7.71	1.48	1.39
20	C	507	CLA	MG-NA	7.70	2.24	2.06
20	b	616	CLA	MG-NA	7.66	2.24	2.06
37	E	104	HEM	C3D-C2D	7.57	1.53	1.36
20	C	513	CLA	MG-NC	7.30	2.23	2.06
20	c	505	CLA	MG-NA	7.26	2.23	2.06
20	B	611	CLA	MG-NA	7.15	2.23	2.06
21	a	405	PHO	C1D-C2D	7.05	1.47	1.39
20	c	503	CLA	MG-NC	7.01	2.22	2.06
20	c	506	CLA	MG-NB	6.97	2.19	2.05
20	B	614	CLA	MG-NA	6.94	2.22	2.06
20	D	401	CLA	MG-NA	6.93	2.22	2.06
21	A	403	PHO	C1B-C2B	6.93	1.47	1.39
40	v	201	HEC	CAC-C3C	6.91	1.57	1.35
20	C	512	CLA	MG-NC	6.85	2.22	2.06
20	b	610	CLA	MG-NB	6.80	2.19	2.05
20	B	612	CLA	MG-NA	6.73	2.22	2.06
40	v	201	HEC	CAB-C3B	6.62	1.56	1.35
20	D	404	CLA	MG-NC	6.62	2.22	2.06
20	B	611	CLA	MG-NC	6.61	2.22	2.06
20	B	601	CLA	MG-NA	6.58	2.21	2.06
40	V	201	HEC	CAB-C3B	6.54	1.56	1.35
20	B	607	CLA	MG-NC	6.52	2.21	2.06
20	c	506	CLA	MG-NA	6.46	2.21	2.06
20	B	602	CLA	MG-ND	6.46	2.18	2.05
20	b	614	CLA	MG-NA	6.41	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	201	HEC	CAC-C3C	6.39	1.55	1.35
20	d	404	CLA	MG-NA	6.31	2.21	2.06
20	b	607	CLA	MG-NA	6.30	2.21	2.06
21	D	403	PHO	C3B-C2B	6.18	1.48	1.40
20	A	402	CLA	MG-NA	6.14	2.20	2.06
20	b	611	CLA	MG-NB	6.12	2.17	2.05
20	c	512	CLA	MG-NB	6.09	2.17	2.05
20	D	404	CLA	MG-NA	6.03	2.20	2.06
21	a	406	PHO	C3B-C4B	6.00	1.47	1.41
20	C	513	CLA	MG-ND	5.99	2.17	2.05
20	B	607	CLA	C3C-C2C	5.91	1.49	1.36
20	a	403	CLA	MG-NA	5.91	2.20	2.06
20	b	609	CLA	MG-NC	5.90	2.20	2.06
20	b	604	CLA	MG-NA	5.88	2.20	2.06
20	a	404	CLA	MG-NA	5.88	2.20	2.06
20	B	607	CLA	CHC-C1C	5.87	1.50	1.38
20	d	402	CLA	CHC-C1C	5.85	1.50	1.38
20	b	610	CLA	CHC-C1C	5.84	1.50	1.38
20	B	609	CLA	MG-NA	5.83	2.20	2.06
20	C	508	CLA	MG-ND	-5.81	1.94	2.05
20	b	609	CLA	MG-NA	5.81	2.20	2.06
20	a	407	CLA	CHC-C1C	5.77	1.50	1.38
20	b	607	CLA	MG-NB	5.72	2.17	2.05
20	C	512	CLA	C3C-C2C	5.72	1.49	1.36
20	b	605	CLA	CHC-C1C	5.72	1.49	1.38
20	c	503	CLA	MG-ND	5.71	2.17	2.05
28	C	532	DMS	O-S	5.70	1.87	1.50
20	b	610	CLA	C3C-C2C	5.67	1.49	1.36
20	C	503	CLA	CHC-C1C	5.66	1.49	1.38
20	c	503	CLA	C3C-C2C	5.65	1.49	1.36
20	b	608	CLA	MG-NC	5.65	2.19	2.06
20	C	513	CLA	C3C-C2C	5.59	1.48	1.36
20	b	615	CLA	CHC-C1C	5.59	1.49	1.38
21	D	403	PHO	C3D-C4D	-5.57	1.33	1.41
20	B	601	CLA	CHC-C1C	5.57	1.49	1.38
20	C	512	CLA	MG-NB	5.54	2.16	2.05
20	b	606	CLA	C3C-C2C	5.51	1.48	1.36
21	D	403	PHO	C4D-CHA	5.50	1.47	1.39
20	B	606	CLA	MG-NA	5.50	2.19	2.06
23	f	101	SQD	O47-C7	5.49	1.47	1.35
20	B	615	CLA	MG-NA	5.48	2.19	2.06
20	b	612	CLA	O2D-CGD	5.44	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	CHC-C1C	5.44	1.49	1.38
20	A	402	CLA	CHC-C1C	5.44	1.49	1.38
20	C	505	CLA	C3C-C2C	5.43	1.48	1.36
21	a	406	PHO	C4D-CHA	5.43	1.47	1.39
20	C	506	CLA	CHC-C1C	5.43	1.49	1.38
20	b	615	CLA	MG-NA	5.43	2.19	2.06
20	c	511	CLA	O2D-CGD	5.41	1.46	1.33
20	B	614	CLA	CHC-C1C	5.38	1.49	1.38
20	C	509	CLA	C3C-C2C	5.38	1.48	1.36
20	c	512	CLA	C3C-C2C	5.37	1.48	1.36
20	B	610	CLA	MG-NB	5.35	2.16	2.05
20	B	610	CLA	CHC-C1C	5.34	1.49	1.38
20	C	503	CLA	C3C-C2C	5.34	1.48	1.36
20	b	612	CLA	CHC-C1C	5.34	1.49	1.38
20	C	512	CLA	O2D-CGD	5.33	1.46	1.33
20	b	618	CLA	CHC-C1C	5.33	1.49	1.38
20	c	511	CLA	MG-NA	5.33	2.18	2.06
20	c	504	CLA	C3C-C2C	5.32	1.48	1.36
20	b	611	CLA	C3C-C2C	5.32	1.48	1.36
20	D	402	CLA	MG-NA	5.32	2.18	2.06
20	c	512	CLA	CHC-C1C	5.29	1.49	1.38
20	c	505	CLA	CHC-C1C	5.28	1.49	1.38
20	C	507	CLA	CHD-C1D	5.25	1.48	1.38
20	C	504	CLA	C3C-C2C	5.25	1.48	1.36
20	c	502	CLA	CHC-C1C	5.24	1.49	1.38
20	c	508	CLA	CHD-C1D	5.23	1.48	1.38
20	C	501	CLA	MG-NC	5.23	2.18	2.06
20	C	511	CLA	MG-NC	5.23	2.18	2.06
20	b	604	CLA	C3C-C2C	5.23	1.48	1.36
20	b	603	CLA	CHC-C1C	5.22	1.48	1.38
20	b	603	CLA	O2A-CGA	5.22	1.48	1.33
20	B	603	CLA	CHD-C1D	5.21	1.48	1.38
20	C	513	CLA	CHD-C1D	5.21	1.48	1.38
20	B	601	CLA	C3C-C2C	5.21	1.48	1.36
20	C	501	CLA	C3C-C2C	5.20	1.48	1.36
20	C	501	CLA	CHC-C1C	5.19	1.48	1.38
20	c	507	CLA	C3C-C2C	5.18	1.48	1.36
20	B	602	CLA	C3C-C2C	5.18	1.47	1.36
20	c	503	CLA	CHC-C1C	5.17	1.48	1.38
20	A	404	CLA	MG-NC	5.17	2.18	2.06
20	C	512	CLA	CHD-C1D	5.16	1.48	1.38
20	d	403	CLA	C3C-C2C	5.16	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	509	CLA	CHD-C1D	5.16	1.48	1.38
20	C	510	CLA	O2D-CGD	5.15	1.45	1.33
20	b	603	CLA	O2D-CGD	5.15	1.45	1.33
20	B	606	CLA	CHC-C1C	5.14	1.48	1.38
20	b	605	CLA	C3C-C2C	5.12	1.47	1.36
20	B	602	CLA	O2A-CGA	5.11	1.48	1.33
20	b	612	CLA	C1B-NB	-5.11	1.31	1.37
20	C	508	CLA	C3C-C2C	5.09	1.47	1.36
24	B	620	LMG	O8-C28	5.08	1.48	1.33
20	B	615	CLA	CHD-C1D	5.07	1.48	1.38
20	C	508	CLA	O2D-CGD	5.06	1.45	1.33
20	b	603	CLA	C3C-C2C	5.05	1.47	1.36
20	c	504	CLA	O2D-CGD	5.04	1.45	1.33
28	b	631	DMS	O-S	5.04	1.83	1.50
20	b	609	CLA	C3C-C2C	5.04	1.47	1.36
20	B	615	CLA	MG-NC	5.04	2.18	2.06
20	b	616	CLA	CHD-C1D	5.04	1.48	1.38
20	C	505	CLA	CHD-C1D	5.03	1.48	1.38
20	c	511	CLA	CHC-C1C	5.02	1.48	1.38
20	b	607	CLA	C3C-C2C	5.02	1.47	1.36
20	c	510	CLA	MG-ND	-5.02	1.95	2.05
28	D	415	DMS	O-S	5.01	1.83	1.50
20	c	508	CLA	C3C-C2C	5.00	1.47	1.36
20	b	604	CLA	MG-ND	5.00	2.15	2.05
20	C	513	CLA	O2D-CGD	5.00	1.45	1.33
20	c	506	CLA	O2D-CGD	4.99	1.45	1.33
20	C	502	CLA	O2D-CGD	4.98	1.45	1.33
20	c	513	CLA	O2D-CGD	4.98	1.45	1.33
21	A	403	PHO	C3B-C2B	4.98	1.47	1.40
20	D	404	CLA	C3C-C2C	4.98	1.47	1.36
20	c	501	CLA	OBD-CAD	4.96	1.31	1.22
20	a	403	CLA	CHC-C1C	4.96	1.48	1.38
20	c	513	CLA	C3C-C2C	4.96	1.47	1.36
20	C	511	CLA	O2D-CGD	4.95	1.45	1.33
40	v	201	HEC	C3D-C2D	4.94	1.51	1.38
20	C	506	CLA	O2D-CGD	4.94	1.45	1.33
20	b	607	CLA	CHC-C1C	4.94	1.48	1.38
20	C	505	CLA	CHC-C1C	4.93	1.48	1.38
20	C	504	CLA	O2D-CGD	4.93	1.45	1.33
21	A	403	PHO	C3B-C4B	4.93	1.46	1.41
28	c	536	DMS	O-S	4.93	1.82	1.50
20	C	507	CLA	C3C-C2C	4.93	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	604	CLA	C3C-C2C	4.92	1.47	1.36
20	a	403	CLA	C3C-C2C	4.92	1.47	1.36
20	c	505	CLA	C3C-C2C	4.92	1.47	1.36
20	C	506	CLA	C3C-C2C	4.91	1.47	1.36
20	b	614	CLA	C3C-C2C	4.91	1.47	1.36
28	B	644	DMS	O-S	4.91	1.82	1.50
20	B	604	CLA	MG-NB	-4.91	1.96	2.05
20	B	610	CLA	CHD-C1D	4.91	1.48	1.38
20	B	604	CLA	O2D-CGD	4.91	1.45	1.33
20	c	508	CLA	MG-NC	4.90	2.17	2.06
20	c	512	CLA	O2D-CGD	4.90	1.45	1.33
28	O	311	DMS	O-S	4.90	1.82	1.50
20	C	509	CLA	CHD-C1D	4.90	1.48	1.38
20	C	508	CLA	CHC-C1C	4.89	1.48	1.38
20	B	613	CLA	CHC-C1C	4.89	1.48	1.38
28	b	639	DMS	O-S	4.88	1.82	1.50
28	o	308	DMS	O-S	4.88	1.82	1.50
20	C	512	CLA	CHC-C1C	4.86	1.48	1.38
28	U	904	DMS	O-S	4.86	1.82	1.50
20	B	611	CLA	C3C-C2C	4.86	1.47	1.36
20	c	511	CLA	CHD-C1D	4.85	1.47	1.38
20	b	616	CLA	CHC-C1C	4.85	1.48	1.38
35	d	416	DGD	O2G-C1B	4.85	1.48	1.34
20	B	611	CLA	CHC-C1C	4.84	1.48	1.38
20	B	604	CLA	MG-NA	4.84	2.17	2.06
28	c	530	DMS	O-S	4.83	1.82	1.50
20	d	402	CLA	CHB-C1B	4.83	1.50	1.39
21	a	405	PHO	C4D-CHA	4.82	1.46	1.39
20	a	404	CLA	CHC-C1C	4.82	1.48	1.38
20	B	602	CLA	O2D-CGD	4.82	1.45	1.33
21	D	403	PHO	C3D-C2D	4.81	1.47	1.39
20	C	511	CLA	C3C-C2C	4.81	1.47	1.36
20	C	509	CLA	OBD-CAD	4.81	1.30	1.22
20	c	509	CLA	CHC-C1C	4.81	1.48	1.38
20	B	607	CLA	CHC-C4B	4.81	1.50	1.39
20	c	509	CLA	OBD-CAD	4.81	1.30	1.22
20	C	502	CLA	CHC-C1C	4.81	1.48	1.38
35	D	406	DGD	O2G-C1B	4.81	1.47	1.34
28	C	525[A]	DMS	O-S	4.80	1.81	1.50
20	a	407	CLA	MG-ND	4.79	2.15	2.05
35	D	406	DGD	O1G-C1A	4.79	1.47	1.33
28	o	302	DMS	O-S	4.79	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	506	CLA	CHC-C1C	4.79	1.48	1.38
28	B	642	DMS	O-S	4.79	1.81	1.50
28	B	643	DMS	O-S	4.79	1.81	1.50
28	A	418	DMS	O-S	4.79	1.81	1.50
20	B	606	CLA	C3C-C2C	4.79	1.47	1.36
20	B	616	CLA	O2D-CGD	4.78	1.45	1.33
20	c	505	CLA	CHD-C1D	4.78	1.47	1.38
28	j	105	DMS	O-S	4.78	1.81	1.50
20	b	618	CLA	C3C-C2C	4.77	1.47	1.36
28	b	638	DMS	O-S	4.77	1.81	1.50
20	B	610	CLA	C3C-C2C	4.77	1.47	1.36
20	b	616	CLA	C3C-C2C	4.77	1.47	1.36
37	E	104	HEM	FE-ND	4.77	2.09	1.94
20	b	613	CLA	CHD-C1D	4.76	1.47	1.38
20	b	611	CLA	O2D-CGD	4.76	1.44	1.33
20	b	607	CLA	C1D-ND	-4.76	1.31	1.37
20	b	615	CLA	O2D-CGD	4.75	1.44	1.33
20	B	615	CLA	CHC-C1C	4.75	1.48	1.38
28	o	306	DMS	O-S	4.75	1.81	1.50
21	a	406	PHO	C3B-C2B	4.75	1.46	1.40
20	b	612	CLA	C3C-C2C	4.75	1.47	1.36
20	A	404	CLA	C3C-C2C	4.75	1.47	1.36
28	A	415	DMS	O-S	4.75	1.81	1.50
20	b	617	CLA	C3C-C2C	4.74	1.47	1.36
24	c	518	LMG	O8-C28	4.74	1.47	1.33
28	O	308	DMS	O-S	4.73	1.81	1.50
24	C	519	LMG	O8-C28	4.73	1.47	1.33
28	b	641	DMS	O-S	4.73	1.81	1.50
28	B	638	DMS	O-S	4.72	1.81	1.50
20	A	404	CLA	CHC-C1C	4.72	1.47	1.38
24	C	524	LMG	O8-C28	4.72	1.47	1.33
20	C	502	CLA	CHB-C1B	4.72	1.50	1.39
20	b	606	CLA	CHC-C1C	4.72	1.47	1.38
35	d	416	DGD	O1G-C1A	4.72	1.47	1.33
28	B	636	DMS	O-S	4.71	1.81	1.50
20	B	603	CLA	C3C-C2C	4.71	1.46	1.36
28	v	207	DMS	O-S	4.71	1.81	1.50
24	J	101	LMG	O7-C10	4.71	1.47	1.34
20	c	501	CLA	MG-ND	-4.71	1.96	2.05
28	c	535	DMS	O-S	4.71	1.81	1.50
28	b	640	DMS	O-S	4.71	1.81	1.50
20	B	607	CLA	O2D-CGD	4.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	401	SQD	O48-C23	4.70	1.47	1.33
28	h	102	DMS	O-S	4.70	1.81	1.50
21	D	403	PHO	C3B-C4B	4.70	1.46	1.41
20	B	605	CLA	CHD-C1D	4.69	1.47	1.38
28	H	103	DMS	O-S	4.69	1.81	1.50
20	b	613	CLA	CHC-C1C	4.69	1.47	1.38
28	D	413	DMS	O-S	4.69	1.81	1.50
20	B	607	CLA	CHD-C1D	4.69	1.47	1.38
28	c	533	DMS	O-S	4.68	1.81	1.50
28	o	305	DMS	O-S	4.67	1.81	1.50
20	C	509	CLA	O2D-CGD	4.67	1.44	1.33
28	B	645	DMS	O-S	4.67	1.81	1.50
28	B	639	DMS	O-S	4.66	1.81	1.50
20	C	502	CLA	C3C-C2C	4.66	1.46	1.36
20	C	510	CLA	CHD-C1D	4.66	1.47	1.38
28	V	205	DMS	O-S	4.66	1.81	1.50
20	b	618	CLA	O2D-CGD	4.66	1.44	1.33
28	O	310	DMS	O-S	4.65	1.80	1.50
20	c	511	CLA	CHB-C1B	4.65	1.49	1.39
20	D	401	CLA	C3C-C2C	4.65	1.46	1.36
20	b	608	CLA	O2D-CGD	4.65	1.44	1.33
28	b	636	DMS	O-S	4.65	1.80	1.50
20	C	512	CLA	CHB-C1B	4.65	1.49	1.39
20	C	503	CLA	MG-NB	4.65	2.15	2.05
28	d	415	DMS	O-S	4.64	1.80	1.50
32	B	621	HTG	C1'-S1	-4.64	1.74	1.81
20	B	602	CLA	CHC-C1C	4.64	1.47	1.38
28	b	632	DMS	O-S	4.64	1.80	1.50
24	c	518	LMG	O7-C10	4.63	1.47	1.34
28	A	416	DMS	O-S	4.63	1.80	1.50
23	b	622	SQD	O47-C7	4.63	1.47	1.34
28	O	307	DMS	O-S	4.63	1.80	1.50
28	o	303	DMS	O-S	4.63	1.80	1.50
28	b	635	DMS	O-S	4.62	1.80	1.50
20	B	609	CLA	O2D-CGD	4.62	1.44	1.33
21	a	405	PHO	C3B-C4B	4.62	1.46	1.41
37	e	102	HEM	FE-ND	4.62	2.09	1.94
20	b	608	CLA	CHD-C1D	4.62	1.47	1.38
20	b	608	CLA	C3C-C2C	4.61	1.46	1.36
20	A	404	CLA	CHB-C1B	4.61	1.49	1.39
20	b	613	CLA	C3C-C2C	4.61	1.46	1.36
20	C	503	CLA	CHD-C4C	4.61	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	504	CLA	MG-ND	4.61	2.14	2.05
28	C	529	DMS	O-S	4.59	1.80	1.50
28	D	416	DMS	O-S	4.59	1.80	1.50
28	V	206	DMS	O-S	4.59	1.80	1.50
28	v	206	DMS	O-S	4.59	1.80	1.50
20	D	401	CLA	CHD-C1D	4.59	1.47	1.38
28	B	641	DMS	O-S	4.59	1.80	1.50
28	c	531	DMS	O-S	4.58	1.80	1.50
28	b	637	DMS	O-S	4.58	1.80	1.50
28	c	529	DMS	O-S	4.58	1.80	1.50
20	b	617	CLA	CHC-C1C	4.57	1.47	1.38
28	c	534	DMS	O-S	4.57	1.80	1.50
28	o	307	DMS	O-S	4.57	1.80	1.50
21	a	406	PHO	C3D-C2D	4.57	1.47	1.39
20	C	506	CLA	CHB-C1B	4.57	1.49	1.39
28	v	204	DMS	O-S	4.57	1.80	1.50
20	b	603	CLA	MG-NA	4.57	2.17	2.06
20	c	510	CLA	C3C-C2C	4.56	1.46	1.36
20	b	605	CLA	CHD-C1D	4.56	1.47	1.38
20	D	402	CLA	CHD-C4C	4.56	1.49	1.39
21	a	405	PHO	O2D-CGD	4.55	1.44	1.33
20	c	511	CLA	C3C-C2C	4.55	1.46	1.36
28	C	531	DMS	O-S	4.55	1.80	1.50
28	F	102	DMS	O-S	4.55	1.80	1.50
20	B	615	CLA	CHB-C1B	4.55	1.49	1.39
28	b	634	DMS	O-S	4.55	1.80	1.50
20	b	610	CLA	MG-NA	4.55	2.17	2.06
20	B	615	CLA	C3C-C2C	4.54	1.46	1.36
28	i	104	DMS	O-S	4.54	1.80	1.50
28	u	204	DMS	O-S	4.54	1.80	1.50
20	C	508	CLA	CHD-C1D	4.54	1.47	1.38
28	V	208	DMS	O-S	4.54	1.80	1.50
20	B	609	CLA	CHD-C1D	4.54	1.47	1.38
20	b	603	CLA	CHD-C1D	4.53	1.47	1.38
28	O	305	DMS	O-S	4.53	1.80	1.50
28	V	204	DMS	O-S	4.53	1.80	1.50
20	B	614	CLA	C3C-C2C	4.53	1.46	1.36
28	v	205	DMS	O-S	4.53	1.80	1.50
20	c	508	CLA	O2D-CGD	4.52	1.44	1.33
20	B	604	CLA	CHC-C1C	4.52	1.47	1.38
28	B	635	DMS	O-S	4.52	1.80	1.50
20	B	613	CLA	C3C-C2C	4.52	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	O	309	DMS	O-S	4.52	1.80	1.50
28	A	417	DMS	O-S	4.52	1.80	1.50
20	C	504	CLA	CHC-C1C	4.52	1.47	1.38
20	C	510	CLA	C3C-C2C	4.51	1.46	1.36
20	b	604	CLA	CHC-C1C	4.51	1.47	1.38
20	B	612	CLA	CHC-C1C	4.51	1.47	1.38
20	d	402	CLA	MG-NA	4.51	2.17	2.06
20	C	513	CLA	CHC-C1C	4.51	1.47	1.38
28	C	533	DMS	O-S	4.51	1.80	1.50
20	d	404	CLA	C3C-C2C	4.51	1.46	1.36
28	v	208	DMS	O-S	4.50	1.79	1.50
36	E	103	LHG	O8-C23	4.50	1.46	1.33
20	B	616	CLA	C3C-C2C	4.50	1.46	1.36
28	o	304	DMS	O-S	4.49	1.79	1.50
23	l	101	SQD	O47-C7	4.49	1.47	1.34
20	c	508	CLA	CHC-C1C	4.49	1.47	1.38
20	c	501	CLA	C3C-C2C	4.49	1.46	1.36
20	C	505	CLA	CHD-C4C	4.49	1.49	1.39
20	B	616	CLA	CHD-C1D	4.48	1.47	1.38
28	v	209	DMS	O-S	4.48	1.79	1.50
20	b	611	CLA	CHD-C1D	4.48	1.47	1.38
36	E	103	LHG	O7-C7	4.48	1.46	1.33
20	B	604	CLA	CHB-C1B	4.48	1.49	1.39
20	B	603	CLA	OBD-CAD	4.47	1.30	1.22
20	C	507	CLA	CHC-C1C	4.47	1.47	1.38
20	B	612	CLA	CHD-C1D	4.47	1.47	1.38
20	A	401	CLA	MG-ND	-4.47	1.96	2.05
21	a	405	PHO	C3D-C2D	4.46	1.47	1.39
20	C	505	CLA	MG-NA	4.46	2.16	2.06
20	b	608	CLA	CHC-C4B	4.45	1.49	1.39
23	b	622	SQD	O48-C23	4.45	1.46	1.33
37	E	104	HEM	FE-NA	4.45	2.09	1.95
20	C	513	CLA	CHB-C1B	4.45	1.49	1.39
28	c	532	DMS	O-S	4.45	1.79	1.50
28	O	303	DMS	O-S	4.45	1.79	1.50
28	V	209	DMS	O-S	4.45	1.79	1.50
20	B	611	CLA	CHD-C1D	4.44	1.47	1.38
28	C	525[B]	DMS	O-S	4.44	1.79	1.50
20	B	613	CLA	CHD-C1D	4.44	1.47	1.38
28	O	304	DMS	O-S	4.44	1.79	1.50
20	b	609	CLA	CHD-C1D	4.44	1.47	1.38
20	C	511	CLA	CHB-C1B	4.44	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	407	CLA	C3C-C2C	4.43	1.46	1.36
20	c	504	CLA	CHD-C1D	4.43	1.47	1.38
20	b	606	CLA	O2D-CGD	4.43	1.44	1.33
28	V	207	DMS	O-S	4.43	1.79	1.50
20	C	509	CLA	CHC-C1C	4.43	1.47	1.38
20	C	510	CLA	CHC-C1C	4.43	1.47	1.38
28	v	203	DMS	O-S	4.43	1.79	1.50
28	u	202	DMS	O-S	4.43	1.79	1.50
20	C	505	CLA	O2D-CGD	4.42	1.44	1.33
28	c	528	DMS	O-S	4.42	1.79	1.50
20	c	509	CLA	C3C-C2C	4.42	1.46	1.36
23	F	101	SQD	O48-C23	4.42	1.46	1.33
20	B	611	CLA	O2D-CGD	4.42	1.44	1.33
24	C	524	LMG	O7-C10	4.41	1.46	1.34
20	c	502	CLA	O2D-CGD	4.41	1.44	1.33
23	a	401	SQD	O47-C7	4.41	1.46	1.34
20	b	613	CLA	O2D-CGD	4.41	1.44	1.33
28	U	903[A]	DMS	O-S	4.40	1.79	1.50
20	c	506	CLA	C3C-C2C	4.40	1.46	1.36
20	B	603	CLA	O2D-CGD	4.40	1.44	1.33
20	c	510	CLA	O2D-CGD	4.40	1.44	1.33
20	B	602	CLA	CHD-C1D	4.40	1.47	1.38
28	C	526	DMS	O-S	4.40	1.79	1.50
28	C	527	DMS	O-S	4.40	1.79	1.50
28	D	414	DMS	O-S	4.39	1.79	1.50
20	c	509	CLA	O2D-CGD	4.39	1.44	1.33
20	b	612	CLA	CHD-C1D	4.39	1.47	1.38
20	c	503	CLA	CHB-C1B	4.39	1.49	1.39
21	a	406	PHO	O2D-CGD	4.38	1.44	1.33
20	c	511	CLA	OBD-CAD	4.38	1.30	1.22
20	b	614	CLA	C4B-NB	-4.38	1.32	1.37
28	b	633	DMS	O-S	4.37	1.79	1.50
28	U	902	DMS	O-S	4.37	1.79	1.50
28	d	413	DMS	O-S	4.36	1.79	1.50
20	C	506	CLA	O2A-CGA	4.36	1.46	1.33
28	C	530	DMS	O-S	4.36	1.79	1.50
20	C	505	CLA	MG-NC	4.36	2.16	2.06
20	C	505	CLA	C1B-NB	-4.36	1.32	1.37
24	A	407	LMG	O7-C10	4.36	1.46	1.34
23	f	101	SQD	O48-C23	4.35	1.46	1.33
20	a	407	CLA	O2D-CGD	4.35	1.43	1.33
28	B	637	DMS	O-S	4.35	1.78	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	513	CLA	CHC-C1C	4.35	1.47	1.38
28	d	414	DMS	O-S	4.35	1.78	1.50
20	a	407	CLA	CHB-C1B	4.35	1.49	1.39
20	B	606	CLA	O2D-CGD	4.34	1.43	1.33
20	a	404	CLA	CHD-C4C	4.34	1.49	1.39
20	A	401	CLA	CHD-C4C	4.34	1.49	1.39
20	c	513	CLA	CHD-C1D	4.33	1.46	1.38
20	b	618	CLA	CHD-C1D	4.33	1.46	1.38
20	a	407	CLA	C1D-ND	-4.33	1.32	1.37
20	C	503	CLA	MG-ND	4.33	2.14	2.05
20	c	512	CLA	CHD-C1D	4.33	1.46	1.38
20	c	509	CLA	CHB-C1B	4.33	1.49	1.39
20	C	501	CLA	MG-NB	4.33	2.14	2.05
20	c	505	CLA	CHB-C1B	4.33	1.49	1.39
20	C	503	CLA	O2D-CGD	4.33	1.43	1.33
20	b	608	CLA	CHB-C1B	4.32	1.49	1.39
20	B	605	CLA	CHC-C1C	4.32	1.47	1.38
23	A	412	SQD	O48-C23	4.32	1.45	1.33
28	u	203	DMS	O-S	4.32	1.78	1.50
23	l	101	SQD	O48-C23	4.32	1.45	1.33
20	c	501	CLA	CHC-C4B	4.31	1.49	1.39
37	e	102	HEM	FE-NB	4.31	2.08	1.94
28	O	306	DMS	O-S	4.30	1.78	1.50
20	B	616	CLA	C1B-NB	-4.30	1.32	1.37
20	d	403	CLA	CHC-C1C	4.29	1.47	1.38
20	c	507	CLA	CHC-C1C	4.29	1.47	1.38
20	C	507	CLA	CHD-C4C	4.29	1.49	1.39
36	D	407	LHG	O8-C23	4.28	1.45	1.33
20	C	506	CLA	CHC-C4B	4.28	1.49	1.39
20	C	506	CLA	CHD-C1D	4.28	1.46	1.38
20	a	407	CLA	O2A-CGA	4.28	1.45	1.33
20	B	603	CLA	CHC-C1C	4.28	1.47	1.38
20	c	513	CLA	MG-ND	4.27	2.14	2.05
20	C	501	CLA	CHD-C1D	4.27	1.46	1.38
24	c	519	LMG	O8-C28	4.27	1.45	1.33
28	v	202	DMS	O-S	4.26	1.78	1.50
20	c	501	CLA	CHC-C1C	4.26	1.47	1.38
24	b	623	LMG	O8-C28	4.26	1.45	1.33
20	B	608	CLA	CHD-C1D	4.24	1.46	1.38
20	c	510	CLA	CHC-C1C	4.24	1.47	1.38
20	c	506	CLA	CHD-C1D	4.24	1.46	1.38
20	b	605	CLA	O2D-CGD	4.23	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	504	CLA	CHD-C1D	4.23	1.46	1.38
20	b	613	CLA	CHB-C1B	4.23	1.48	1.39
20	b	614	CLA	CHC-C1C	4.23	1.47	1.38
20	C	512	CLA	O2A-CGA	4.23	1.45	1.33
23	A	406	SQD	O47-C7	4.23	1.46	1.34
28	U	903[B]	DMS	O-S	4.22	1.78	1.50
20	C	507	CLA	MG-ND	4.22	2.14	2.05
20	B	616	CLA	CHC-C1C	4.21	1.46	1.38
20	B	608	CLA	CHB-C1B	4.21	1.48	1.39
20	d	404	CLA	CHD-C1D	4.20	1.46	1.38
20	b	604	CLA	CHD-C4C	4.20	1.48	1.39
20	A	401	CLA	CHC-C1C	4.20	1.46	1.38
20	d	404	CLA	CHC-C1C	4.19	1.46	1.38
20	C	508	CLA	MG-NB	4.19	2.14	2.05
20	D	404	CLA	CHC-C1C	4.19	1.46	1.38
21	D	403	PHO	O2D-CGD	4.19	1.43	1.33
20	b	617	CLA	CHB-C1B	4.18	1.48	1.39
28	B	640	DMS	O-S	4.18	1.77	1.50
20	C	504	CLA	CHD-C4C	4.18	1.48	1.39
20	C	509	CLA	O2A-CGA	4.18	1.45	1.33
20	c	513	CLA	CHB-C1B	4.18	1.48	1.39
20	d	403	CLA	CHD-C1D	4.18	1.46	1.38
24	A	407	LMG	O8-C28	4.18	1.45	1.33
20	B	613	CLA	CHB-C1B	4.17	1.48	1.39
20	B	603	CLA	CHB-C1B	4.17	1.48	1.39
20	D	404	CLA	CHB-C1B	4.17	1.48	1.39
20	A	401	CLA	CHC-C4B	4.16	1.48	1.39
21	a	406	PHO	C3D-C4D	-4.16	1.35	1.41
20	b	610	CLA	OBD-CAD	4.15	1.29	1.22
20	c	501	CLA	CHD-C1D	4.15	1.46	1.38
20	c	512	CLA	CHD-C4C	4.15	1.48	1.39
24	j	101	LMG	O8-C28	4.15	1.45	1.33
20	A	404	CLA	CHC-C4B	4.14	1.48	1.39
20	b	610	CLA	CHB-C1B	4.14	1.48	1.39
20	c	502	CLA	CHD-C1D	4.14	1.46	1.38
21	A	403	PHO	C4D-CHA	4.13	1.45	1.39
24	b	623	LMG	O7-C10	4.13	1.45	1.34
20	B	608	CLA	CHC-C1C	4.13	1.46	1.38
24	a	410	LMG	O7-C10	4.13	1.45	1.34
20	c	512	CLA	CHC-C4B	4.13	1.48	1.39
36	D	409	LHG	O8-C23	4.12	1.45	1.33
35	c	517	DGD	O1G-C1A	4.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	519	LMG	O7-C10	4.12	1.45	1.34
20	A	401	CLA	OBD-CAD	4.12	1.29	1.22
20	c	507	CLA	O2D-CGD	4.12	1.43	1.33
20	c	507	CLA	CHD-C1D	4.12	1.46	1.38
20	C	513	CLA	CHD-C4C	4.12	1.48	1.39
20	D	402	CLA	MG-NC	4.11	2.16	2.06
20	b	610	CLA	CHD-C4C	4.11	1.48	1.39
20	B	611	CLA	C4C-C3C	4.11	1.52	1.45
20	C	507	CLA	CHB-C1B	4.11	1.48	1.39
20	d	404	CLA	CHC-C4B	4.11	1.48	1.39
20	B	608	CLA	C3C-C2C	4.10	1.45	1.36
20	b	617	CLA	O2D-CGD	4.10	1.43	1.33
20	C	510	CLA	CHB-C1B	4.10	1.48	1.39
23	A	412	SQD	O47-C7	4.10	1.45	1.34
20	B	613	CLA	O2D-CGD	4.09	1.43	1.33
20	B	608	CLA	CHC-C4B	4.09	1.48	1.39
20	c	506	CLA	O2A-CGA	4.09	1.45	1.33
20	b	617	CLA	CHD-C4C	4.09	1.48	1.39
20	b	609	CLA	CHC-C1C	4.09	1.46	1.38
20	B	606	CLA	CHD-C1D	4.08	1.46	1.38
20	b	614	CLA	MG-NB	4.07	2.13	2.05
20	B	604	CLA	CHD-C1D	4.07	1.46	1.38
20	b	610	CLA	C4B-NB	-4.07	1.32	1.37
20	c	513	CLA	O2A-CGA	4.07	1.45	1.33
20	C	511	CLA	CHC-C1C	4.07	1.46	1.38
20	c	507	CLA	CHB-C1B	4.06	1.48	1.39
24	a	410	LMG	O8-C28	4.05	1.45	1.33
20	B	601	CLA	O2D-CGD	4.05	1.43	1.33
20	c	510	CLA	CHD-C1D	4.05	1.46	1.38
20	b	618	CLA	CHB-C1B	4.05	1.48	1.39
20	b	611	CLA	O2A-CGA	4.04	1.45	1.33
20	c	504	CLA	CHC-C1C	4.04	1.46	1.38
21	D	403	PHO	OBD-CAD	4.04	1.27	1.22
20	b	604	CLA	C1B-NB	-4.04	1.32	1.37
20	b	610	CLA	C1D-ND	-4.04	1.32	1.37
20	b	603	CLA	CHC-C4B	4.04	1.48	1.39
20	C	511	CLA	CHD-C1D	4.04	1.46	1.38
20	C	505	CLA	CHC-C4B	4.04	1.48	1.39
20	c	505	CLA	CHD-C4C	4.04	1.48	1.39
35	h	101	DGD	O2G-C1B	4.03	1.45	1.34
20	C	512	CLA	CHD-C4C	4.03	1.48	1.39
20	C	501	CLA	CHC-C4B	4.03	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	503	CLA	CHC-C4B	4.03	1.48	1.39
20	b	618	CLA	O2A-CGA	4.03	1.45	1.33
20	b	615	CLA	C3C-C2C	4.03	1.45	1.36
20	c	505	CLA	C1B-NB	-4.03	1.32	1.37
35	H	102	DGD	O2G-C1B	4.02	1.45	1.34
20	C	510	CLA	MG-NB	4.02	2.13	2.05
20	d	404	CLA	CHB-C1B	4.01	1.48	1.39
20	C	508	CLA	CHB-C1B	4.01	1.48	1.39
24	C	519	LMG	O7-C10	4.00	1.45	1.34
20	b	612	CLA	MG-NC	4.00	2.15	2.06
20	b	604	CLA	C1D-ND	-4.00	1.32	1.37
20	b	606	CLA	CHD-C1D	4.00	1.46	1.38
20	C	505	CLA	O2A-CGA	4.00	1.45	1.33
20	B	609	CLA	CHD-C4C	4.00	1.48	1.39
36	d	406	LHG	O8-C23	3.99	1.45	1.33
20	c	507	CLA	O2A-CGA	3.99	1.45	1.33
20	c	503	CLA	CHD-C1D	3.99	1.46	1.38
20	D	402	CLA	C3C-C2C	3.98	1.45	1.36
23	a	409	SQD	O48-C23	3.98	1.45	1.33
20	c	510	CLA	CHB-C1B	3.98	1.48	1.39
20	d	402	CLA	C3C-C2C	3.97	1.45	1.36
20	a	407	CLA	CHD-C1D	3.97	1.46	1.38
20	B	610	CLA	CHB-C1B	3.97	1.48	1.39
21	a	405	PHO	OBD-CAD	3.97	1.27	1.22
20	C	513	CLA	O2A-CGA	3.97	1.44	1.33
20	B	606	CLA	CHD-C4C	3.97	1.48	1.39
20	C	503	CLA	CHD-C1D	3.97	1.46	1.38
28	c	527	DMS	O-S	3.96	1.76	1.50
20	C	502	CLA	CHD-C1D	3.96	1.46	1.38
20	B	602	CLA	CHC-C4B	3.96	1.48	1.39
20	B	601	CLA	C1D-ND	-3.96	1.32	1.37
20	A	404	CLA	CHD-C1D	3.96	1.46	1.38
20	B	610	CLA	C1B-NB	-3.96	1.32	1.37
20	B	612	CLA	CHC-C4B	3.96	1.48	1.39
20	b	607	CLA	O2D-CGD	3.95	1.42	1.33
20	b	608	CLA	CHC-C1C	3.95	1.46	1.38
20	b	604	CLA	CHD-C1D	3.95	1.46	1.38
20	a	403	CLA	CHB-C1B	3.95	1.48	1.39
20	C	507	CLA	O2D-CGD	3.95	1.42	1.33
20	C	505	CLA	C1D-ND	-3.94	1.32	1.37
20	c	503	CLA	O2D-CGD	3.94	1.42	1.33
20	B	614	CLA	O2A-CGA	3.94	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	508	CLA	O2A-CGA	3.94	1.44	1.33
20	C	501	CLA	O2D-CGD	3.93	1.42	1.33
20	B	616	CLA	MG-NC	3.92	2.15	2.06
20	A	401	CLA	O2D-CGD	3.92	1.42	1.33
20	c	513	CLA	CHD-C4C	3.92	1.48	1.39
35	C	516	DGD	O2G-C1B	3.92	1.45	1.34
20	b	615	CLA	CHD-C4C	3.92	1.48	1.39
20	a	407	CLA	OBD-CAD	3.92	1.29	1.22
20	C	501	CLA	MG-NA	3.91	2.15	2.06
20	B	604	CLA	CHD-C4C	3.91	1.48	1.39
20	D	402	CLA	CHC-C4B	3.91	1.48	1.39
20	c	501	CLA	O2D-CGD	3.91	1.42	1.33
20	c	512	CLA	O2A-CGA	3.91	1.44	1.33
20	d	404	CLA	C4C-C3C	3.90	1.51	1.45
20	D	401	CLA	CHD-C4C	3.90	1.48	1.39
20	B	602	CLA	CHB-C1B	3.90	1.48	1.39
20	b	611	CLA	CHB-C1B	3.90	1.48	1.39
20	c	507	CLA	CHC-C4B	3.88	1.48	1.39
21	A	403	PHO	C3D-C4D	-3.88	1.36	1.41
20	b	611	CLA	CHC-C4B	3.88	1.48	1.39
35	C	517	DGD	O1G-C1A	3.88	1.44	1.33
35	c	517	DGD	O2G-C1B	3.88	1.45	1.34
20	B	606	CLA	CHB-C1B	3.88	1.48	1.39
20	C	503	CLA	O2A-CGA	3.87	1.44	1.33
28	C	528	DMS	O-S	3.87	1.75	1.50
20	c	502	CLA	CHB-C1B	3.87	1.48	1.39
20	b	610	CLA	O2D-CGD	3.86	1.42	1.33
20	B	609	CLA	C3C-C2C	3.86	1.45	1.36
20	C	506	CLA	CHD-C4C	3.85	1.48	1.39
20	d	404	CLA	O2A-CGA	3.85	1.44	1.33
20	b	603	CLA	CHB-C1B	3.85	1.48	1.39
20	C	503	CLA	MG-NC	3.84	2.15	2.06
20	a	403	CLA	O2D-CGD	3.84	1.42	1.33
20	C	508	CLA	CHC-C4B	3.84	1.48	1.39
20	B	611	CLA	CHC-C4B	3.84	1.48	1.39
20	a	403	CLA	CHD-C4C	3.83	1.47	1.39
35	C	518	DGD	O1G-C1A	3.83	1.44	1.33
20	C	513	CLA	C3D-C2D	3.83	1.49	1.39
20	b	609	CLA	O2D-CGD	3.82	1.42	1.33
21	a	406	PHO	C3A-C2A	-3.82	1.51	1.54
20	C	501	CLA	CHD-C4C	3.82	1.47	1.39
20	C	513	CLA	CHC-C4B	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	508	CLA	OBD-CAD	3.82	1.29	1.22
20	B	614	CLA	CHB-C1B	3.82	1.48	1.39
21	D	403	PHO	C3A-C2A	-3.82	1.51	1.54
20	C	509	CLA	C3D-C2D	3.81	1.49	1.39
20	b	612	CLA	CHC-C4B	3.81	1.48	1.39
20	B	601	CLA	MG-NC	3.80	2.15	2.06
20	A	401	CLA	C4C-C3C	3.80	1.51	1.45
20	A	404	CLA	MG-NA	3.79	2.15	2.06
20	b	613	CLA	O2A-CGA	3.79	1.44	1.33
20	B	605	CLA	C3C-C2C	3.79	1.44	1.36
20	B	612	CLA	OBD-CAD	3.79	1.29	1.22
20	C	504	CLA	MG-NC	3.79	2.15	2.06
20	C	502	CLA	O2A-CGA	3.78	1.44	1.33
20	B	605	CLA	O2D-CGD	3.78	1.42	1.33
20	b	617	CLA	CHD-C1D	3.78	1.45	1.38
20	B	603	CLA	C4C-C3C	3.77	1.51	1.45
20	b	603	CLA	OBD-CAD	3.77	1.29	1.22
20	B	616	CLA	CHD-C4C	3.77	1.47	1.39
20	B	602	CLA	OBD-CAD	3.77	1.29	1.22
20	c	508	CLA	C3D-C2D	3.77	1.49	1.39
20	c	511	CLA	CHC-C4B	3.77	1.47	1.39
20	b	617	CLA	OBD-CAD	3.76	1.29	1.22
20	B	601	CLA	CHC-C4B	3.76	1.47	1.39
20	a	404	CLA	CHB-C1B	3.76	1.47	1.39
20	b	605	CLA	CHD-C4C	3.75	1.47	1.39
20	B	602	CLA	CHD-C4C	3.75	1.47	1.39
20	b	614	CLA	O2D-CGD	3.75	1.42	1.33
23	a	409	SQD	O47-C7	3.75	1.44	1.34
35	h	101	DGD	O5D-C1E	3.74	1.46	1.40
24	j	101	LMG	O7-C10	3.74	1.44	1.34
20	c	512	CLA	CHB-C1B	3.74	1.47	1.39
20	b	616	CLA	CHC-C4B	3.74	1.47	1.39
20	b	608	CLA	C3D-C2D	3.73	1.49	1.39
20	c	512	CLA	OBD-CAD	3.73	1.28	1.22
24	J	101	LMG	O8-C28	3.73	1.44	1.33
20	c	508	CLA	CHC-C4B	3.73	1.47	1.39
21	D	403	PHO	O2A-CGA	3.72	1.44	1.33
20	D	404	CLA	CHC-C4B	3.71	1.47	1.39
20	a	403	CLA	CHD-C1D	3.71	1.45	1.38
20	B	612	CLA	C3C-C2C	3.71	1.44	1.36
20	B	605	CLA	CHD-C4C	3.71	1.47	1.39
20	c	504	CLA	O2A-CGA	3.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	508	CLA	CHB-C1B	3.71	1.47	1.39
20	b	611	CLA	OBD-CAD	3.71	1.28	1.22
20	b	616	CLA	O2D-CGD	3.71	1.42	1.33
20	D	402	CLA	C4B-NB	-3.70	1.33	1.37
20	c	511	CLA	C3D-C2D	3.70	1.49	1.39
21	a	405	PHO	C3B-C2B	3.70	1.45	1.40
20	B	605	CLA	MG-ND	3.70	2.13	2.05
20	c	504	CLA	OBD-CAD	3.70	1.28	1.22
20	A	404	CLA	OBD-CAD	3.70	1.28	1.22
20	b	609	CLA	C3D-C2D	3.70	1.49	1.39
20	b	611	CLA	C3D-C2D	3.69	1.49	1.39
20	c	510	CLA	O2A-CGA	3.69	1.44	1.33
20	D	404	CLA	O2D-CGD	3.69	1.42	1.33
20	C	510	CLA	OBD-CAD	3.69	1.28	1.22
35	c	516	DGD	O1G-C1A	3.69	1.44	1.33
20	c	501	CLA	CHB-C1B	3.69	1.47	1.39
20	b	615	CLA	O2A-CGA	3.68	1.44	1.33
20	c	503	CLA	CHD-C4C	3.68	1.47	1.39
20	C	501	CLA	CHB-C1B	3.68	1.47	1.39
20	B	605	CLA	CHB-C1B	3.67	1.47	1.39
20	c	501	CLA	O2A-CGA	3.67	1.44	1.33
20	C	512	CLA	CHC-C4B	3.67	1.47	1.39
20	c	506	CLA	CHD-C4C	3.67	1.47	1.39
20	b	606	CLA	CHB-C1B	3.67	1.47	1.39
20	b	611	CLA	CHD-C4C	3.67	1.47	1.39
20	b	604	CLA	CHB-C1B	3.66	1.47	1.39
37	e	102	HEM	FE-NC	3.66	2.07	1.95
20	b	604	CLA	C1B-C2B	3.66	1.51	1.43
20	b	609	CLA	CHD-C4C	3.66	1.47	1.39
20	b	612	CLA	MG-NA	3.66	2.15	2.06
20	B	608	CLA	CHD-C4C	3.66	1.47	1.39
21	A	403	PHO	O2A-CGA	3.66	1.44	1.33
20	b	610	CLA	CHD-C1D	3.65	1.45	1.38
20	B	609	CLA	CHB-C1B	3.65	1.47	1.39
20	c	509	CLA	CHD-C4C	3.64	1.47	1.39
20	B	607	CLA	O2A-CGA	3.64	1.44	1.33
20	B	611	CLA	CHD-C4C	3.64	1.47	1.39
20	c	510	CLA	MG-NA	3.64	2.14	2.06
20	c	511	CLA	CHD-C4C	3.64	1.47	1.39
20	B	612	CLA	O2D-CGD	3.63	1.42	1.33
20	d	403	CLA	CHD-C4C	3.63	1.47	1.39
20	b	614	CLA	C1B-NB	-3.63	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	502	CLA	CHD-C4C	3.62	1.47	1.39
20	b	605	CLA	C1D-ND	-3.62	1.33	1.37
34	c	523	LMT	O1'-C1'	3.62	1.46	1.40
20	B	611	CLA	CHB-C1B	3.62	1.47	1.39
20	B	616	CLA	CHB-C1B	3.61	1.47	1.39
23	A	406	SQD	O48-C23	3.61	1.43	1.33
20	D	404	CLA	CHD-C4C	3.61	1.47	1.39
20	B	603	CLA	CHD-C4C	3.60	1.47	1.39
20	B	601	CLA	O2A-CGA	3.60	1.43	1.33
20	c	513	CLA	CHC-C4B	3.60	1.47	1.39
20	A	401	CLA	MG-NC	3.60	2.14	2.06
20	B	616	CLA	O2A-CGA	3.59	1.43	1.33
20	c	505	CLA	O2A-CGA	3.59	1.43	1.33
20	b	616	CLA	OBD-CAD	3.59	1.28	1.22
20	B	606	CLA	OBD-CAD	3.59	1.28	1.22
20	a	407	CLA	MG-NA	3.58	2.14	2.06
20	b	614	CLA	CHD-C1D	3.58	1.45	1.38
20	C	504	CLA	O2A-CGA	3.58	1.43	1.33
20	D	404	CLA	O2A-CGA	3.58	1.43	1.33
20	b	614	CLA	CHD-C4C	3.58	1.47	1.39
20	A	404	CLA	O2A-CGA	3.58	1.43	1.33
35	c	515	DGD	O1G-C1A	3.58	1.43	1.33
20	b	616	CLA	O2A-CGA	3.57	1.43	1.33
20	c	512	CLA	C4C-C3C	3.57	1.51	1.45
20	C	510	CLA	C3D-C2D	3.56	1.48	1.39
35	C	518	DGD	O2G-C1B	3.56	1.44	1.34
20	b	618	CLA	CHC-C4B	3.56	1.47	1.39
20	B	607	CLA	OBD-CAD	3.55	1.28	1.22
20	C	511	CLA	CHD-C4C	3.55	1.47	1.39
20	c	509	CLA	O2A-CGA	3.55	1.43	1.33
20	B	615	CLA	O2A-CGA	3.55	1.43	1.33
35	H	102	DGD	O5D-C1E	3.54	1.46	1.40
20	c	503	CLA	CHC-C4B	3.54	1.47	1.39
20	B	603	CLA	MG-NC	3.54	2.14	2.06
20	b	605	CLA	CHB-C1B	3.54	1.47	1.39
20	b	603	CLA	CHD-C4C	3.54	1.47	1.39
20	C	505	CLA	CHB-C1B	3.54	1.47	1.39
20	d	402	CLA	CHD-C1D	3.54	1.45	1.38
20	C	506	CLA	MG-NC	3.53	2.14	2.06
20	B	614	CLA	CHD-C4C	3.53	1.47	1.39
20	d	402	CLA	OBD-CAD	3.53	1.28	1.22
20	B	610	CLA	O2D-CGD	3.52	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	612	CLA	CHD-C4C	3.52	1.47	1.39
20	c	507	CLA	OBD-CAD	3.52	1.28	1.22
20	D	402	CLA	CHC-C1C	3.51	1.45	1.38
35	H	102	DGD	O1G-C1A	3.51	1.43	1.33
24	B	620	LMG	O7-C10	3.51	1.44	1.34
22	b	620	BCR	C5-C6	3.51	1.40	1.34
20	C	510	CLA	MG-ND	-3.51	1.98	2.05
20	C	507	CLA	O2A-CGA	3.50	1.43	1.33
20	b	607	CLA	C3B-C4B	3.50	1.52	1.42
20	c	503	CLA	C1D-ND	-3.50	1.33	1.37
20	c	507	CLA	CHD-C4C	3.50	1.47	1.39
21	a	406	PHO	O2A-CGA	3.50	1.43	1.33
20	C	504	CLA	C3D-C2D	3.50	1.48	1.39
20	C	511	CLA	OBD-CAD	3.49	1.28	1.22
32	B	622	HTG	C1'-S1	-3.49	1.76	1.81
20	B	615	CLA	CHC-C4B	3.48	1.47	1.39
20	C	509	CLA	CHB-C1B	3.48	1.47	1.39
20	b	604	CLA	O2A-CGA	3.48	1.43	1.33
20	b	616	CLA	CHD-C4C	3.47	1.47	1.39
20	C	501	CLA	O2A-CGA	3.47	1.43	1.33
20	b	616	CLA	CHB-C1B	3.47	1.47	1.39
20	a	404	CLA	C4B-NB	-3.46	1.33	1.37
20	C	511	CLA	CHC-C4B	3.46	1.47	1.39
20	B	614	CLA	C4C-C3C	3.46	1.50	1.45
20	b	612	CLA	C4C-C3C	3.46	1.50	1.45
20	C	507	CLA	CHC-C4B	3.46	1.47	1.39
20	B	613	CLA	C1D-ND	-3.46	1.33	1.37
20	b	607	CLA	C4B-NB	-3.46	1.33	1.37
20	b	608	CLA	C4D-CHA	3.46	1.50	1.38
40	V	201	HEC	CBC-CAC	-3.46	1.36	1.49
20	a	404	CLA	C3C-C2C	3.45	1.44	1.36
20	B	607	CLA	C1C-C2C	3.45	1.51	1.44
20	C	510	CLA	CHD-C4C	3.45	1.47	1.39
20	B	609	CLA	CHC-C1C	3.45	1.45	1.38
20	c	506	CLA	CHC-C4B	3.45	1.47	1.39
20	B	613	CLA	CHD-C4C	3.45	1.47	1.39
32	D	417	HTG	C1'-S1	-3.44	1.76	1.81
20	D	401	CLA	O2A-CGA	3.44	1.43	1.33
36	d	408	LHG	O8-C23	3.44	1.43	1.33
20	B	610	CLA	CHC-C4B	3.44	1.47	1.39
20	C	508	CLA	C3D-C2D	3.44	1.48	1.39
20	B	609	CLA	CHC-C4B	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	618	CLA	C3D-C2D	3.43	1.48	1.39
20	C	502	CLA	C4D-CHA	3.43	1.50	1.38
20	c	508	CLA	O2A-CGA	3.43	1.43	1.33
20	c	508	CLA	C1C-NC	-3.43	1.32	1.37
20	b	606	CLA	CHD-C4C	3.43	1.47	1.39
20	C	501	CLA	C3D-C2D	3.42	1.48	1.39
20	c	510	CLA	CHD-C4C	3.42	1.47	1.39
40	V	201	HEC	C3D-C2D	3.42	1.47	1.38
20	D	402	CLA	O2D-CGD	3.42	1.41	1.33
20	C	510	CLA	O2A-CGA	3.42	1.43	1.33
20	B	604	CLA	MG-NC	3.41	2.14	2.06
32	b	624	HTG	C1'-S1	-3.41	1.76	1.81
20	C	506	CLA	C4D-CHA	3.41	1.50	1.38
20	B	610	CLA	O2A-CGA	3.41	1.43	1.33
20	b	609	CLA	CHB-C1B	3.41	1.47	1.39
20	D	404	CLA	CHD-C1D	3.40	1.45	1.38
20	D	402	CLA	CHD-C1D	3.40	1.45	1.38
35	C	516	DGD	O1G-C1A	3.40	1.43	1.33
20	c	502	CLA	C3C-C2C	3.40	1.44	1.36
20	c	502	CLA	C1D-ND	-3.40	1.33	1.37
32	O	302	HTG	C1'-S1	-3.40	1.76	1.81
20	C	508	CLA	CHD-C4C	3.40	1.46	1.39
20	A	402	CLA	C3C-C2C	3.40	1.44	1.36
20	C	504	CLA	CHB-C1B	3.40	1.47	1.39
20	B	602	CLA	C4D-CHA	3.40	1.50	1.38
20	b	608	CLA	CHD-C4C	3.40	1.46	1.39
20	c	511	CLA	O2A-CGA	3.40	1.43	1.33
20	A	404	CLA	O2D-CGD	3.39	1.41	1.33
20	C	504	CLA	C4D-CHA	3.39	1.50	1.38
20	B	607	CLA	CHB-C1B	3.39	1.47	1.39
20	c	502	CLA	OBD-CAD	3.39	1.28	1.22
20	a	404	CLA	O2A-CGA	3.39	1.43	1.33
34	b	627	LMT	O1'-C1'	3.38	1.45	1.40
20	c	502	CLA	O2A-CGA	3.38	1.43	1.33
20	C	507	CLA	OBD-CAD	3.37	1.28	1.22
20	B	607	CLA	CHD-C4C	3.37	1.46	1.39
20	B	608	CLA	C3D-C2D	3.37	1.48	1.39
20	C	503	CLA	C1D-ND	-3.36	1.33	1.37
20	c	501	CLA	CHD-C4C	3.36	1.46	1.39
20	C	502	CLA	CHD-C4C	3.36	1.46	1.39
21	a	406	PHO	OBD-CAD	3.35	1.26	1.22
36	L	101	LHG	O7-C7	3.35	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	408	LHG	O8-C23	3.35	1.43	1.33
20	b	618	CLA	MG-NC	3.35	2.14	2.06
20	B	614	CLA	CHD-C1D	3.35	1.44	1.38
20	c	505	CLA	CHC-C4B	3.35	1.46	1.39
20	B	609	CLA	MG-NB	-3.35	1.99	2.05
20	b	610	CLA	C4D-CHA	3.34	1.49	1.38
20	b	605	CLA	C1B-NB	-3.34	1.33	1.37
20	B	613	CLA	C4B-NB	-3.34	1.33	1.37
20	B	601	CLA	CHB-C1B	3.34	1.46	1.39
20	d	404	CLA	OBD-CAD	3.34	1.28	1.22
32	C	534	HTG	C1'-S1	-3.34	1.76	1.81
20	C	511	CLA	C3D-C2D	3.34	1.48	1.39
20	B	615	CLA	O2D-CGD	3.34	1.41	1.33
32	d	401	HTG	C1'-S1	-3.33	1.76	1.81
20	C	512	CLA	C4C-C3C	3.33	1.50	1.45
36	L	101	LHG	O8-C23	3.33	1.43	1.33
20	B	611	CLA	C3D-C2D	3.33	1.48	1.39
20	d	404	CLA	MG-NC	3.32	2.14	2.06
21	a	405	PHO	CBD-CGD	-3.32	1.48	1.52
20	B	611	CLA	O2A-CGA	3.32	1.43	1.33
20	B	601	CLA	CHD-C1D	3.32	1.44	1.38
20	d	402	CLA	O2A-CGA	3.32	1.43	1.33
20	b	605	CLA	OBD-CAD	3.32	1.28	1.22
20	C	507	CLA	C3D-C2D	3.31	1.48	1.39
20	c	509	CLA	CHC-C4B	3.31	1.46	1.39
20	C	509	CLA	CHC-C4B	3.31	1.46	1.39
20	b	617	CLA	C1D-ND	-3.31	1.33	1.37
20	C	511	CLA	O2A-CGA	3.31	1.43	1.33
20	c	513	CLA	OBD-CAD	3.31	1.28	1.22
20	B	603	CLA	CHC-C4B	3.30	1.46	1.39
28	A	414	DMS	O-S	3.30	1.72	1.50
20	b	604	CLA	C4C-C3C	3.30	1.50	1.45
37	e	102	HEM	FE-NA	3.30	2.06	1.95
20	b	618	CLA	C4D-CHA	3.30	1.49	1.38
20	B	616	CLA	OBD-CAD	3.30	1.28	1.22
20	a	407	CLA	CHD-C4C	3.30	1.46	1.39
20	c	504	CLA	CHC-C4B	3.30	1.46	1.39
20	C	507	CLA	C4D-CHA	3.29	1.49	1.38
20	b	615	CLA	MG-NB	3.29	2.12	2.05
20	c	507	CLA	C4D-CHA	3.29	1.49	1.38
20	c	513	CLA	C1D-ND	-3.28	1.33	1.37
20	B	612	CLA	CHB-C1B	3.28	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	502	CLA	CHC-C4B	3.28	1.46	1.39
20	a	404	CLA	OBD-CAD	3.28	1.28	1.22
20	c	510	CLA	C1D-ND	-3.28	1.33	1.37
20	c	505	CLA	OBD-CAD	3.28	1.28	1.22
20	B	610	CLA	MG-NC	3.27	2.14	2.06
20	B	610	CLA	C3D-C2D	3.27	1.47	1.39
20	a	404	CLA	O2D-CGD	3.27	1.41	1.33
20	C	502	CLA	C3D-C2D	3.26	1.47	1.39
36	l	102	LHG	O8-C23	3.26	1.42	1.33
20	a	404	CLA	CHD-C1D	3.26	1.44	1.38
21	A	403	PHO	O2D-CGD	3.25	1.41	1.33
20	c	503	CLA	O2A-CGA	3.25	1.42	1.33
20	c	510	CLA	CHC-C4B	3.25	1.46	1.39
20	b	615	CLA	CHB-C1B	3.25	1.46	1.39
20	C	513	CLA	C4D-CHA	3.25	1.49	1.38
20	C	505	CLA	C3D-C2D	3.25	1.47	1.39
40	v	201	HEC	CBC-CAC	-3.24	1.37	1.49
20	B	615	CLA	OBD-CAD	3.24	1.28	1.22
20	c	502	CLA	C3D-C2D	3.24	1.47	1.39
20	C	512	CLA	C3D-C2D	3.24	1.47	1.39
20	B	610	CLA	C1D-ND	-3.24	1.33	1.37
20	B	609	CLA	O2A-CGA	3.24	1.42	1.33
20	c	508	CLA	CHD-C4C	3.24	1.46	1.39
20	C	510	CLA	CHC-C4B	3.24	1.46	1.39
35	C	517	DGD	O2G-C1B	3.24	1.43	1.34
20	B	601	CLA	CHD-C4C	3.23	1.46	1.39
20	b	618	CLA	CHD-C4C	3.23	1.46	1.39
20	c	505	CLA	C4D-CHA	3.23	1.49	1.38
20	d	402	CLA	CHD-C4C	3.23	1.46	1.39
20	B	611	CLA	C4D-CHA	3.23	1.49	1.38
20	C	503	CLA	C3D-C2D	3.23	1.47	1.39
20	b	603	CLA	C4D-CHA	3.22	1.49	1.38
20	c	508	CLA	C4C-C3C	3.22	1.50	1.45
20	a	407	CLA	C3D-C2D	3.22	1.47	1.39
20	c	506	CLA	CHB-C1B	3.22	1.46	1.39
20	c	503	CLA	C4D-CHA	3.22	1.49	1.38
20	A	402	CLA	MG-NB	-3.21	1.99	2.05
20	C	509	CLA	CHD-C4C	3.21	1.46	1.39
20	b	603	CLA	C3D-C2D	3.21	1.47	1.39
40	V	201	HEC	CMD-C2D	3.21	1.57	1.50
20	B	603	CLA	C3D-C2D	3.20	1.47	1.39
32	C	522	HTG	C1'-S1	-3.20	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	604	CLA	O2A-CGA	3.20	1.42	1.33
20	D	401	CLA	C4D-CHA	3.19	1.49	1.38
20	c	512	CLA	C3D-C2D	3.19	1.47	1.39
20	B	601	CLA	C3D-C2D	3.19	1.47	1.39
20	A	402	CLA	CHB-C1B	3.19	1.46	1.39
20	C	512	CLA	C4D-CHA	3.18	1.49	1.38
20	B	603	CLA	C1D-ND	-3.18	1.33	1.37
20	c	510	CLA	OBD-CAD	3.18	1.28	1.22
20	C	503	CLA	CHB-C1B	3.18	1.46	1.39
36	D	408	LHG	O7-C7	3.18	1.43	1.34
20	C	512	CLA	C1D-ND	-3.18	1.33	1.37
20	b	615	CLA	CHD-C1D	3.17	1.44	1.38
20	c	509	CLA	C3D-C2D	3.17	1.47	1.39
20	d	403	CLA	C1B-C2B	3.17	1.50	1.43
20	B	607	CLA	C4D-CHA	3.17	1.49	1.38
20	b	607	CLA	CHD-C1D	3.17	1.44	1.38
20	C	513	CLA	C4C-C3C	3.17	1.50	1.45
36	d	406	LHG	O7-C7	3.17	1.43	1.34
20	b	614	CLA	MG-ND	-3.16	1.99	2.05
20	D	401	CLA	CHB-C1B	3.16	1.46	1.39
20	b	614	CLA	CHC-C4B	3.16	1.46	1.39
20	b	609	CLA	CHC-C4B	3.16	1.46	1.39
32	B	632	HTG	C1'-S1	-3.16	1.77	1.81
20	d	404	CLA	CHD-C4C	3.16	1.46	1.39
20	D	401	CLA	O2D-CGD	3.15	1.41	1.33
20	c	505	CLA	C3D-C2D	3.15	1.47	1.39
20	B	610	CLA	OBD-CAD	3.15	1.27	1.22
20	c	508	CLA	OBD-CAD	3.14	1.27	1.22
20	B	615	CLA	C1C-NC	-3.14	1.32	1.37
20	b	614	CLA	C1B-C2B	3.14	1.50	1.43
20	b	608	CLA	MG-ND	3.13	2.12	2.05
20	C	505	CLA	OBD-CAD	3.13	1.27	1.22
20	b	613	CLA	CHC-C4B	3.12	1.46	1.39
20	A	404	CLA	MG-ND	-3.12	1.99	2.05
20	b	606	CLA	C3D-C2D	3.12	1.47	1.39
20	B	616	CLA	C1B-C2B	3.12	1.50	1.43
20	B	612	CLA	C1D-ND	-3.12	1.33	1.37
37	E	104	HEM	CAB-C3B	3.11	1.55	1.47
20	B	605	CLA	CHC-C4B	3.11	1.46	1.39
20	b	617	CLA	C4D-CHA	3.11	1.49	1.38
20	c	503	CLA	C3D-C2D	3.11	1.47	1.39
20	B	615	CLA	C1B-NB	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	606	CLA	O2A-CGA	3.11	1.42	1.33
22	a	408	BCR	C26-C25	3.11	1.39	1.34
20	b	609	CLA	C4D-CHA	3.10	1.49	1.38
20	D	404	CLA	C3D-C2D	3.09	1.47	1.39
20	D	401	CLA	CHC-C1C	3.09	1.44	1.38
20	c	504	CLA	C3D-C2D	3.09	1.47	1.39
20	C	510	CLA	C4D-CHA	3.09	1.49	1.38
20	b	618	CLA	C1D-ND	-3.09	1.33	1.37
20	b	610	CLA	C1B-NB	-3.09	1.33	1.37
20	c	510	CLA	C1B-NB	-3.09	1.33	1.37
20	B	616	CLA	CHC-C4B	3.09	1.46	1.39
20	B	605	CLA	O2A-CGA	3.09	1.42	1.33
20	b	604	CLA	C3B-C4B	3.09	1.51	1.42
37	E	104	HEM	CAC-C3C	3.08	1.55	1.47
20	c	504	CLA	CHB-C1B	3.08	1.46	1.39
20	c	505	CLA	C4B-NB	-3.08	1.33	1.37
20	C	511	CLA	C4D-CHA	3.08	1.48	1.38
36	D	409	LHG	O7-C7	3.08	1.43	1.34
20	B	601	CLA	C4D-CHA	3.08	1.48	1.38
20	C	511	CLA	C4C-C3C	3.08	1.50	1.45
28	B	634	DMS	O-S	3.07	1.70	1.50
20	b	614	CLA	O2A-CGA	3.07	1.42	1.33
20	C	503	CLA	C3B-C4B	3.07	1.51	1.42
20	d	404	CLA	O2D-CGD	3.07	1.40	1.33
35	c	516	DGD	O2G-C1B	3.07	1.42	1.34
20	b	612	CLA	CHB-C1B	3.07	1.46	1.39
20	d	402	CLA	C1D-ND	-3.06	1.33	1.37
20	B	606	CLA	C1B-C2B	3.06	1.50	1.43
20	c	506	CLA	OBD-CAD	3.05	1.27	1.22
20	c	513	CLA	C3D-C2D	3.05	1.47	1.39
20	C	501	CLA	C3B-C4B	3.05	1.51	1.42
20	c	506	CLA	C4D-CHA	3.04	1.48	1.38
32	B	631	HTG	C1'-S1	-3.04	1.77	1.81
20	C	506	CLA	OBD-CAD	3.04	1.27	1.22
20	B	616	CLA	C4D-CHA	3.03	1.48	1.38
20	b	613	CLA	C3D-C2D	3.03	1.47	1.39
20	c	511	CLA	MG-ND	3.03	2.11	2.05
20	B	613	CLA	O2A-CGA	3.03	1.42	1.33
20	b	604	CLA	O2D-CGD	3.02	1.40	1.33
36	d	408	LHG	O7-C7	3.02	1.42	1.34
20	C	506	CLA	C3D-C2D	3.01	1.47	1.39
20	B	614	CLA	O2D-CGD	3.01	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	508	CLA	C4C-C3C	3.01	1.50	1.45
20	b	607	CLA	CHB-C1B	3.01	1.46	1.39
20	B	615	CLA	C4C-C3C	3.01	1.50	1.45
35	h	101	DGD	O1G-C1A	3.01	1.42	1.33
20	b	614	CLA	CHB-C1B	3.00	1.46	1.39
32	b	601	HTG	C1'-S1	-3.00	1.77	1.81
20	c	501	CLA	C4D-CHA	3.00	1.48	1.38
20	B	612	CLA	CHD-C4C	2.99	1.46	1.39
20	b	608	CLA	O2A-CGA	2.99	1.42	1.33
20	d	404	CLA	C3D-C2D	2.99	1.47	1.39
20	c	505	CLA	MG-NB	2.99	2.11	2.05
20	A	401	CLA	C4D-CHA	2.99	1.48	1.38
20	C	513	CLA	OBD-CAD	2.98	1.27	1.22
20	c	511	CLA	C4C-C3C	2.98	1.50	1.45
37	e	102	HEM	CAB-C3B	2.98	1.55	1.47
20	a	403	CLA	O2A-C1	-2.98	1.38	1.46
20	b	612	CLA	C4D-CHA	2.98	1.48	1.38
20	b	605	CLA	C3D-C2D	2.98	1.47	1.39
20	a	403	CLA	C4D-CHA	2.98	1.48	1.38
20	b	613	CLA	C4D-CHA	2.97	1.48	1.38
20	c	507	CLA	C4B-NB	-2.97	1.34	1.37
20	a	403	CLA	O2A-CGA	2.97	1.42	1.33
37	e	102	HEM	CAC-C3C	2.97	1.55	1.47
20	D	402	CLA	C1B-C2B	2.97	1.50	1.43
20	b	609	CLA	C1B-C2B	2.96	1.50	1.43
20	b	603	CLA	C3B-C4B	2.95	1.51	1.42
20	b	612	CLA	C1D-ND	-2.95	1.34	1.37
20	A	402	CLA	C1B-C2B	2.95	1.50	1.43
20	A	401	CLA	C3C-C2C	2.95	1.43	1.36
20	B	610	CLA	C1B-C2B	2.95	1.50	1.43
34	Z	101	LMT	O1'-C1'	2.95	1.45	1.40
20	A	404	CLA	CHD-C4C	2.95	1.45	1.39
20	C	505	CLA	C4D-CHA	2.94	1.48	1.38
20	C	512	CLA	C1B-C2B	2.94	1.50	1.43
20	B	613	CLA	CHC-C4B	2.93	1.46	1.39
20	c	504	CLA	C4C-C3C	2.93	1.50	1.45
20	B	607	CLA	C3D-C2D	2.93	1.47	1.39
20	c	505	CLA	C1B-C2B	2.93	1.50	1.43
20	D	402	CLA	CHB-C1B	2.93	1.46	1.39
20	b	610	CLA	C3D-C2D	2.93	1.47	1.39
20	b	609	CLA	C1B-NB	-2.93	1.34	1.37
20	A	404	CLA	C4D-CHA	2.93	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	d	402	CLA	CHC-C4B	2.92	1.46	1.39
20	b	615	CLA	C3B-C4B	2.92	1.51	1.42
20	c	503	CLA	C1B-NB	-2.92	1.34	1.37
20	B	612	CLA	C4D-CHA	2.92	1.48	1.38
20	C	501	CLA	C4D-CHA	2.92	1.48	1.38
20	C	512	CLA	OBD-CAD	2.92	1.27	1.22
20	c	502	CLA	CHC-C4B	2.91	1.46	1.39
20	c	512	CLA	MG-NC	2.91	2.13	2.06
20	c	507	CLA	C3D-C2D	2.91	1.46	1.39
27	D	412	PL9	C6-C5	2.91	1.49	1.35
20	b	610	CLA	CHC-C4B	2.91	1.45	1.39
20	D	402	CLA	C3B-C4B	2.91	1.51	1.42
20	b	616	CLA	C3D-C2D	2.91	1.46	1.39
20	A	401	CLA	CHD-C1D	2.90	1.44	1.38
20	b	611	CLA	C4D-CHA	2.90	1.48	1.38
20	c	504	CLA	MG-NC	2.90	2.13	2.06
20	c	505	CLA	C1D-ND	-2.90	1.34	1.37
20	c	512	CLA	C4D-CHA	2.90	1.48	1.38
20	C	505	CLA	C4C-C3C	2.90	1.50	1.45
20	b	611	CLA	C3B-C4B	2.89	1.51	1.42
20	b	604	CLA	CHC-C4B	2.89	1.45	1.39
20	A	401	CLA	CHB-C1B	2.89	1.45	1.39
20	d	403	CLA	MG-ND	-2.89	2.00	2.05
20	c	501	CLA	C3D-C2D	2.89	1.46	1.39
20	b	614	CLA	C3D-C2D	2.89	1.46	1.39
20	C	513	CLA	C3B-C4B	2.89	1.51	1.42
20	a	404	CLA	C4D-CHA	2.89	1.48	1.38
20	D	404	CLA	C4C-C3C	2.89	1.49	1.45
20	C	507	CLA	C4C-C3C	2.89	1.49	1.45
20	B	609	CLA	OBD-CAD	2.89	1.27	1.22
20	C	505	CLA	C1B-C2B	2.88	1.49	1.43
20	c	506	CLA	C3D-C2D	2.88	1.46	1.39
20	B	602	CLA	C1D-ND	-2.88	1.34	1.37
20	C	501	CLA	OBD-CAD	2.88	1.27	1.22
20	D	402	CLA	C4D-CHA	2.88	1.48	1.38
20	D	404	CLA	OBD-CAD	2.88	1.27	1.22
20	B	615	CLA	CHD-C4C	2.88	1.45	1.39
20	C	503	CLA	C4D-CHA	2.88	1.48	1.38
20	b	615	CLA	CHC-C4B	2.87	1.45	1.39
20	b	607	CLA	CHD-C4C	2.87	1.45	1.39
21	a	406	PHO	CBD-CGD	-2.87	1.48	1.52
20	C	503	CLA	C1B-NB	-2.87	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	612	CLA	C1B-C2B	2.87	1.49	1.43
20	d	404	CLA	C4D-CHA	2.87	1.48	1.38
20	b	616	CLA	C4C-C3C	2.86	1.49	1.45
20	B	606	CLA	C1B-NB	-2.86	1.34	1.37
32	b	602	HTG	C1'-S1	-2.86	1.77	1.81
20	B	610	CLA	C3B-C4B	2.86	1.51	1.42
20	b	614	CLA	OBD-CAD	2.85	1.27	1.22
20	c	513	CLA	C4D-CHA	2.85	1.48	1.38
20	A	402	CLA	CHD-C1D	2.85	1.44	1.38
20	C	509	CLA	MG-NB	-2.84	2.00	2.05
20	B	609	CLA	MG-NC	2.84	2.13	2.06
20	B	611	CLA	C3B-C4B	2.84	1.51	1.42
20	a	404	CLA	C3D-C2D	2.84	1.46	1.39
20	c	511	CLA	C3B-C4B	2.83	1.51	1.42
20	c	511	CLA	C4D-CHA	2.83	1.48	1.38
20	B	610	CLA	C4D-CHA	2.83	1.48	1.38
20	d	403	CLA	OBD-CAD	2.83	1.27	1.22
20	c	505	CLA	C3B-C4B	2.83	1.51	1.42
20	c	505	CLA	O2D-CGD	2.83	1.40	1.33
20	D	404	CLA	C4D-CHA	2.83	1.48	1.38
20	b	606	CLA	C4B-NB	-2.82	1.34	1.37
32	b	625	HTG	C1-S1	2.82	1.85	1.80
20	b	609	CLA	O2A-CGA	2.81	1.41	1.33
20	B	615	CLA	C1B-C2B	2.81	1.49	1.43
20	B	608	CLA	C3B-C4B	2.81	1.50	1.42
32	B	623	HTG	C1'-S1	-2.81	1.77	1.81
20	C	512	CLA	C3B-C4B	2.81	1.50	1.42
20	B	604	CLA	C1D-ND	-2.80	1.34	1.37
21	A	403	PHO	C4B-NB	-2.80	1.33	1.38
20	C	509	CLA	C4D-CHA	2.80	1.48	1.38
20	b	617	CLA	O2A-CGA	2.79	1.41	1.33
40	v	201	HEC	CBB-CAB	-2.79	1.39	1.49
20	a	403	CLA	C4B-NB	-2.79	1.34	1.37
20	b	606	CLA	O2A-CGA	2.79	1.41	1.33
27	a	415	PL9	C6-C5	2.78	1.48	1.35
20	A	402	CLA	C3D-C2D	2.78	1.46	1.39
40	v	201	HEC	CMC-C2C	2.78	1.56	1.50
20	c	504	CLA	CHD-C4C	2.78	1.45	1.39
20	b	617	CLA	MG-NC	2.78	2.12	2.06
20	C	503	CLA	OBD-CAD	2.77	1.27	1.22
20	c	502	CLA	C4D-CHA	2.77	1.47	1.38
20	C	510	CLA	C4C-C3C	2.77	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	405	PHO	C3D-C4D	-2.77	1.37	1.41
27	A	411	PL9	C6-C5	2.77	1.48	1.35
20	b	610	CLA	C3B-C4B	2.77	1.50	1.42
20	B	612	CLA	C3D-C2D	2.77	1.46	1.39
32	c	521	HTG	C1'-S1	-2.77	1.77	1.81
20	B	611	CLA	OBD-CAD	2.77	1.27	1.22
20	c	505	CLA	MG-ND	2.76	2.11	2.05
20	B	609	CLA	C3D-C2D	2.76	1.46	1.39
20	B	614	CLA	C4D-CHA	2.76	1.47	1.38
20	c	510	CLA	C4D-CHA	2.76	1.47	1.38
40	V	201	HEC	CMC-C2C	2.75	1.56	1.50
20	B	602	CLA	C3B-C4B	2.75	1.50	1.42
27	a	415	PL9	C2-C3	2.75	1.41	1.34
20	c	509	CLA	C4D-CHA	2.75	1.47	1.38
20	B	607	CLA	C4C-C3C	2.75	1.49	1.45
20	b	612	CLA	O2A-CGA	2.75	1.41	1.33
20	B	609	CLA	C1D-ND	-2.74	1.34	1.37
20	C	504	CLA	C1D-ND	-2.74	1.34	1.37
20	B	608	CLA	O2A-CGA	2.74	1.41	1.33
20	A	402	CLA	C1C-NC	-2.74	1.33	1.37
20	B	615	CLA	C3B-C4B	2.74	1.50	1.42
21	a	405	PHO	C4B-NB	-2.74	1.33	1.38
20	C	504	CLA	C3B-C4B	2.74	1.50	1.42
20	D	401	CLA	C3B-C4B	2.74	1.50	1.42
20	C	510	CLA	C1C-NC	-2.74	1.33	1.37
20	B	601	CLA	OBD-CAD	2.74	1.27	1.22
20	b	617	CLA	CHC-C4B	2.74	1.45	1.39
20	D	404	CLA	MG-ND	-2.74	2.00	2.05
20	b	609	CLA	MG-ND	2.73	2.11	2.05
40	V	201	HEC	CMA-C3A	2.73	1.56	1.50
20	c	509	CLA	C4C-C3C	2.73	1.49	1.45
20	B	603	CLA	C1B-NB	-2.72	1.34	1.37
20	B	616	CLA	C3D-C2D	2.72	1.46	1.39
20	B	613	CLA	C3D-C2D	2.72	1.46	1.39
20	b	605	CLA	C4D-CHA	2.72	1.47	1.38
20	b	617	CLA	C1B-C2B	2.71	1.49	1.43
20	b	607	CLA	O2A-CGA	2.71	1.41	1.33
20	B	604	CLA	C3D-C2D	2.71	1.46	1.39
20	B	605	CLA	C4D-CHA	2.71	1.47	1.38
20	B	606	CLA	C1D-ND	-2.70	1.34	1.37
20	b	606	CLA	C1B-C2B	2.70	1.49	1.43
20	b	612	CLA	C3B-C4B	2.70	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	401	CLA	MG-NB	2.70	2.11	2.05
20	a	407	CLA	C4D-CHA	2.70	1.47	1.38
20	b	613	CLA	CHD-C4C	2.69	1.45	1.39
40	V	201	HEC	CMB-C2B	2.69	1.56	1.50
20	b	607	CLA	OBD-CAD	2.69	1.27	1.22
20	b	615	CLA	OBD-CAD	2.69	1.27	1.22
32	C	520	HTG	C1'-S1	-2.69	1.77	1.81
20	C	506	CLA	C4C-C3C	2.69	1.49	1.45
20	c	508	CLA	C1D-ND	-2.69	1.34	1.37
20	a	407	CLA	C1B-NB	-2.69	1.34	1.37
20	B	615	CLA	C4D-CHA	2.69	1.47	1.38
20	B	604	CLA	C1B-C2B	2.69	1.49	1.43
20	b	612	CLA	C3D-C4D	-2.68	1.38	1.44
20	b	616	CLA	C4D-CHA	2.68	1.47	1.38
27	d	412	PL9	C6-C5	2.68	1.48	1.35
20	C	506	CLA	C1D-ND	-2.68	1.34	1.37
20	B	602	CLA	C3D-C2D	2.68	1.46	1.39
20	b	605	CLA	C1B-C2B	2.68	1.49	1.43
20	B	602	CLA	C1B-C2B	2.67	1.49	1.43
20	C	502	CLA	OBD-CAD	2.67	1.27	1.22
40	V	201	HEC	CBB-CAB	-2.67	1.39	1.49
32	C	521	HTG	C1'-S1	-2.67	1.77	1.81
20	b	617	CLA	C3D-C2D	2.67	1.46	1.39
20	b	615	CLA	C1C-NC	-2.67	1.33	1.37
32	B	622	HTG	O5-C1	2.66	1.46	1.42
27	d	412	PL9	C7-C3	2.66	1.54	1.51
35	c	515	DGD	O2G-C1B	2.66	1.41	1.34
20	c	512	CLA	C1B-NB	-2.66	1.34	1.37
37	e	102	HEM	CMC-C2C	2.66	1.56	1.50
20	B	610	CLA	C4B-NB	-2.66	1.34	1.37
37	E	104	HEM	CMD-C2D	2.66	1.56	1.50
20	A	402	CLA	O2D-CGD	2.66	1.39	1.33
20	c	504	CLA	C1B-NB	-2.66	1.34	1.37
20	B	614	CLA	CHC-C4B	2.65	1.45	1.39
20	C	504	CLA	C4B-NB	-2.65	1.34	1.37
20	D	402	CLA	C4C-C3C	2.65	1.49	1.45
32	b	624	HTG	C1-S1	-2.65	1.76	1.80
20	b	610	CLA	O2A-CGA	2.65	1.41	1.33
20	D	402	CLA	O2A-CGA	2.65	1.41	1.33
20	d	402	CLA	C3B-C4B	2.65	1.50	1.42
21	A	403	PHO	CBD-CGD	-2.64	1.49	1.52
20	b	615	CLA	MG-NC	2.64	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	604	CLA	OBD-CAD	2.64	1.27	1.22
20	b	606	CLA	C4D-CHA	2.64	1.47	1.38
22	a	408	BCR	C40-C30	2.63	1.58	1.53
20	c	503	CLA	C4C-C3C	2.63	1.49	1.45
20	D	401	CLA	CHC-C4B	2.62	1.45	1.39
36	l	102	LHG	O7-C7	2.62	1.41	1.34
20	a	407	CLA	C1B-C2B	2.62	1.49	1.43
20	B	616	CLA	C4C-C3C	2.62	1.49	1.45
20	B	613	CLA	C1B-NB	-2.62	1.34	1.37
20	a	407	CLA	CHC-C4B	2.62	1.45	1.39
20	A	404	CLA	C4C-C3C	2.62	1.49	1.45
20	B	609	CLA	C4D-CHA	2.61	1.47	1.38
24	c	519	LMG	O1-C1	2.61	1.44	1.40
20	C	510	CLA	C1D-ND	-2.61	1.34	1.37
20	c	510	CLA	MG-NC	2.60	2.12	2.06
20	B	609	CLA	MG-ND	2.60	2.10	2.05
20	A	401	CLA	C3D-C2D	2.60	1.46	1.39
20	B	601	CLA	MG-NB	-2.60	2.00	2.05
20	b	613	CLA	C3B-C4B	2.60	1.50	1.42
34	f	102	LMT	O1'-C1'	2.60	1.44	1.40
20	B	607	CLA	MG-ND	2.60	2.10	2.05
20	A	404	CLA	C3D-C2D	2.59	1.46	1.39
20	D	401	CLA	MG-NB	-2.59	2.00	2.05
20	a	403	CLA	C3D-C2D	2.59	1.46	1.39
20	C	506	CLA	C3B-C4B	2.59	1.50	1.42
20	b	606	CLA	C3B-C4B	2.59	1.50	1.42
20	B	603	CLA	C1B-C2B	2.58	1.49	1.43
20	c	512	CLA	C1D-ND	-2.58	1.34	1.37
20	b	604	CLA	C3D-C2D	2.58	1.46	1.39
34	z	102	LMT	O1'-C1'	2.58	1.44	1.40
20	c	509	CLA	C1B-C2B	2.58	1.49	1.43
20	C	507	CLA	C1B-C2B	2.58	1.49	1.43
20	C	511	CLA	C1B-C2B	2.58	1.49	1.43
20	b	604	CLA	OBD-CAD	2.58	1.26	1.22
20	B	613	CLA	C1B-C2B	2.57	1.49	1.43
20	b	609	CLA	C1D-ND	-2.57	1.34	1.37
20	b	607	CLA	C4D-CHA	2.57	1.47	1.38
27	A	411	PL9	C2-C3	2.57	1.41	1.34
20	B	602	CLA	MG-NC	2.56	2.12	2.06
20	B	605	CLA	C1B-C2B	2.56	1.49	1.43
20	A	402	CLA	C1B-NB	-2.56	1.34	1.37
20	D	402	CLA	C1C-NC	-2.56	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	608	CLA	C4C-C3C	2.56	1.49	1.45
20	D	402	CLA	C1D-ND	-2.56	1.34	1.37
20	C	501	CLA	C1B-NB	-2.56	1.34	1.37
20	C	508	CLA	C3B-C4B	2.56	1.50	1.42
20	B	613	CLA	OBD-CAD	2.56	1.26	1.22
27	D	412	PL9	C2-C3	2.55	1.41	1.34
20	C	511	CLA	C1D-ND	-2.55	1.34	1.37
20	b	603	CLA	C1C-NC	-2.55	1.33	1.37
20	A	402	CLA	C4D-CHA	2.55	1.47	1.38
20	c	508	CLA	C4D-CHA	2.55	1.47	1.38
20	c	504	CLA	C4D-CHA	2.54	1.47	1.38
20	b	605	CLA	O2A-CGA	2.54	1.40	1.33
35	c	515	DGD	O5D-C1E	2.54	1.44	1.40
20	B	609	CLA	CBD-CAD	-2.54	1.45	1.56
20	b	609	CLA	C3B-C4B	2.54	1.50	1.42
20	c	512	CLA	C3B-C4B	2.54	1.50	1.42
20	c	511	CLA	C1B-C2B	2.53	1.49	1.43
20	c	513	CLA	C1C-C2C	2.53	1.49	1.44
20	D	401	CLA	C1D-ND	-2.53	1.34	1.37
20	C	511	CLA	C3B-C4B	2.53	1.50	1.42
21	a	405	PHO	O2A-CGA	2.53	1.40	1.33
20	A	402	CLA	C3B-C4B	2.53	1.50	1.42
20	c	505	CLA	C4C-C3C	2.53	1.49	1.45
32	O	302	HTG	O5-C1	2.53	1.46	1.42
20	b	607	CLA	CHC-C4B	2.52	1.45	1.39
20	B	608	CLA	C4C-C3C	2.52	1.49	1.45
20	C	503	CLA	C1B-C2B	2.52	1.49	1.43
20	d	402	CLA	C4C-C3C	2.52	1.49	1.45
20	A	401	CLA	O2A-CGA	2.52	1.40	1.33
20	D	401	CLA	C4B-NB	-2.52	1.34	1.37
20	a	403	CLA	CHC-C4B	2.52	1.45	1.39
20	c	513	CLA	C4B-NB	-2.52	1.34	1.37
20	b	617	CLA	C4C-C3C	2.52	1.49	1.45
20	B	603	CLA	C4D-CHA	2.51	1.47	1.38
20	B	604	CLA	C3B-C4B	2.51	1.50	1.42
20	A	402	CLA	CHD-C4C	2.51	1.44	1.39
23	l	101	SQD	O6-C1	2.51	1.44	1.40
20	D	404	CLA	C3B-C4B	2.51	1.50	1.42
20	B	615	CLA	C3D-C2D	2.51	1.45	1.39
40	v	201	HEC	CMB-C2B	2.51	1.55	1.50
20	b	618	CLA	C1C-C2C	2.50	1.49	1.44
20	b	611	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	612	CLA	C3D-C2D	2.50	1.45	1.39
20	C	510	CLA	C3D-C4D	-2.50	1.38	1.44
20	B	604	CLA	C4C-C3C	2.50	1.49	1.45
20	c	509	CLA	C1D-ND	-2.50	1.34	1.37
20	B	616	CLA	CBD-CAD	-2.50	1.45	1.56
20	c	509	CLA	MG-NC	2.49	2.12	2.06
20	C	513	CLA	C1B-C2B	2.49	1.49	1.43
20	A	401	CLA	C1D-C2D	2.49	1.50	1.45
20	C	509	CLA	C4C-C3C	2.49	1.49	1.45
20	B	606	CLA	C4D-CHA	2.49	1.46	1.38
24	c	518	LMG	O1-C1	2.49	1.44	1.40
22	D	405	BCR	C12-C13	2.49	1.51	1.46
36	d	407	LHG	O8-C23	2.48	1.40	1.33
20	d	403	CLA	C3D-C2D	2.48	1.45	1.39
40	v	201	HEC	CMD-C2D	2.48	1.55	1.50
20	B	605	CLA	C3D-C2D	2.48	1.45	1.39
20	C	502	CLA	C3B-C4B	2.48	1.49	1.42
20	B	611	CLA	C1C-C2C	2.48	1.49	1.44
20	b	615	CLA	C1B-NB	-2.47	1.34	1.37
24	C	524	LMG	O1-C1	2.47	1.44	1.40
20	b	618	CLA	OBD-CAD	2.47	1.26	1.22
37	e	102	HEM	CMA-C3A	2.47	1.55	1.50
20	c	504	CLA	C1C-NC	-2.47	1.34	1.37
20	b	606	CLA	C1B-NB	-2.47	1.34	1.37
20	c	512	CLA	C1B-C2B	2.46	1.48	1.43
20	B	605	CLA	OBD-CAD	2.46	1.26	1.22
20	c	502	CLA	MG-NB	-2.46	2.00	2.05
20	D	404	CLA	C1B-C2B	2.46	1.48	1.43
20	A	402	CLA	OBD-CAD	2.46	1.26	1.22
20	b	612	CLA	C4B-NB	-2.46	1.34	1.37
35	d	416	DGD	O3G-C1D	2.46	1.44	1.40
20	C	508	CLA	C4D-CHA	2.46	1.46	1.38
20	b	614	CLA	C4D-CHA	2.46	1.46	1.38
20	A	402	CLA	CHC-C4B	2.46	1.44	1.39
37	E	104	HEM	CMB-C2B	2.46	1.55	1.50
20	b	606	CLA	C1D-ND	-2.45	1.34	1.37
20	C	503	CLA	C1C-C2C	2.45	1.49	1.44
20	B	605	CLA	C1D-ND	-2.45	1.34	1.37
20	B	604	CLA	C1C-NC	-2.44	1.34	1.37
20	c	510	CLA	MG-NB	2.44	2.10	2.05
37	E	104	HEM	CMC-C2C	2.44	1.55	1.50
32	c	520	HTG	C1'-S1	-2.44	1.78	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	504	CLA	C3B-C4B	2.44	1.49	1.42
20	C	509	CLA	C1B-C2B	2.44	1.48	1.43
20	b	607	CLA	C1B-C2B	2.44	1.48	1.43
20	b	607	CLA	C1B-NB	-2.44	1.34	1.37
20	B	603	CLA	CBD-CAD	-2.43	1.45	1.56
34	E	101	LMT	O1'-C1'	2.43	1.44	1.40
20	B	606	CLA	C3B-C4B	2.43	1.49	1.42
32	B	621	HTG	C1-C2	2.43	1.57	1.53
20	d	403	CLA	O2A-CGA	2.43	1.40	1.33
20	C	504	CLA	CHC-C4B	2.43	1.44	1.39
36	L	101	LHG	O7-C5	-2.42	1.40	1.46
20	A	401	CLA	C1B-C2B	2.42	1.48	1.43
20	b	618	CLA	C3B-C4B	2.42	1.49	1.42
20	c	501	CLA	C4C-C3C	2.42	1.49	1.45
20	c	510	CLA	C3D-C2D	2.42	1.45	1.39
20	A	402	CLA	C3D-C4D	-2.42	1.38	1.44
20	B	604	CLA	C4D-CHA	2.42	1.46	1.38
20	c	506	CLA	C1B-C2B	2.42	1.48	1.43
20	c	501	CLA	C4B-NB	-2.42	1.34	1.37
20	c	507	CLA	C3B-C4B	2.41	1.49	1.42
20	a	404	CLA	CHC-C4B	2.41	1.44	1.39
20	c	502	CLA	C3D-C4D	-2.41	1.38	1.44
20	b	608	CLA	OBD-CAD	2.41	1.26	1.22
20	B	614	CLA	C3D-C2D	2.41	1.45	1.39
20	C	507	CLA	C3B-C4B	2.41	1.49	1.42
20	C	510	CLA	C4B-NB	-2.40	1.34	1.37
20	b	605	CLA	CHC-C4B	2.40	1.44	1.39
20	B	605	CLA	C4C-C3C	2.40	1.49	1.45
20	B	606	CLA	C3D-C2D	2.40	1.45	1.39
20	d	404	CLA	C1B-NB	-2.40	1.34	1.37
20	c	507	CLA	C1C-C2C	2.40	1.49	1.44
20	b	615	CLA	C3D-C2D	2.39	1.45	1.39
20	d	403	CLA	CHB-C1B	2.39	1.44	1.39
20	d	403	CLA	CHC-C4B	2.39	1.44	1.39
20	c	510	CLA	C3D-C4D	-2.39	1.38	1.44
35	c	517	DGD	O2G-C2G	-2.39	1.41	1.46
20	B	607	CLA	C1D-ND	-2.39	1.34	1.37
27	d	412	PL9	C43-C44	2.39	1.38	1.33
20	c	506	CLA	C1C-NC	-2.39	1.34	1.37
21	a	405	PHO	C1B-NB	-2.39	1.34	1.38
20	b	611	CLA	C1D-ND	-2.39	1.34	1.37
20	d	402	CLA	MG-NC	2.39	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	d	403	CLA	MG-NC	-2.38	2.00	2.06
20	d	403	CLA	O2D-CGD	2.38	1.39	1.33
20	b	611	CLA	C4C-C3C	2.38	1.49	1.45
20	c	511	CLA	C1C-C2C	2.38	1.49	1.44
20	c	504	CLA	C1D-ND	-2.38	1.34	1.37
20	c	501	CLA	C1B-C2B	2.38	1.48	1.43
20	b	606	CLA	C4C-C3C	2.37	1.49	1.45
20	c	502	CLA	C4C-C3C	2.37	1.49	1.45
20	d	404	CLA	C3D-C4D	-2.37	1.38	1.44
20	D	404	CLA	C1C-NC	-2.37	1.34	1.37
20	B	602	CLA	C1C-C2C	2.37	1.49	1.44
20	b	608	CLA	C3B-C2B	2.36	1.49	1.41
20	A	404	CLA	C3D-C4D	-2.36	1.38	1.44
20	b	604	CLA	C4D-CHA	2.36	1.46	1.38
20	B	608	CLA	OBD-CAD	2.36	1.26	1.22
20	B	612	CLA	CBD-CAD	-2.36	1.46	1.56
32	b	625	HTG	O5-C1	2.36	1.46	1.42
20	B	612	CLA	O2A-CGA	2.36	1.40	1.33
20	C	512	CLA	C1C-C2C	2.36	1.49	1.44
20	B	601	CLA	C3B-C4B	2.36	1.49	1.42
20	c	504	CLA	MG-NB	2.36	2.10	2.05
20	A	404	CLA	C3B-C4B	2.35	1.49	1.42
32	b	601	HTG	C1-S1	-2.35	1.76	1.80
35	c	517	DGD	O5D-C1E	2.34	1.44	1.40
20	B	601	CLA	MG-ND	2.34	2.10	2.05
20	C	502	CLA	C1B-C2B	2.34	1.48	1.43
20	b	607	CLA	C3D-C2D	2.34	1.45	1.39
20	C	506	CLA	C1C-C2C	2.34	1.49	1.44
20	b	608	CLA	C1C-C2C	2.33	1.49	1.44
20	c	503	CLA	C1B-C2B	2.33	1.48	1.43
20	B	614	CLA	OBD-CAD	2.32	1.26	1.22
20	c	506	CLA	C3B-C4B	2.32	1.49	1.42
20	C	509	CLA	C4B-NB	-2.32	1.34	1.37
20	C	511	CLA	C1C-NC	-2.32	1.34	1.37
20	C	507	CLA	C3B-C2B	2.32	1.49	1.41
20	B	604	CLA	CHC-C4B	2.32	1.44	1.39
20	d	402	CLA	C3D-C2D	2.32	1.45	1.39
20	C	505	CLA	C3B-C4B	2.31	1.49	1.42
34	J	103	LMT	O1'-C1'	2.31	1.44	1.40
20	d	402	CLA	C1B-C2B	2.31	1.48	1.43
20	d	403	CLA	C1B-NB	-2.31	1.34	1.37
20	b	610	CLA	MG-NC	2.31	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	415	PL9	C7-C3	2.30	1.54	1.51
20	b	612	CLA	OBD-CAD	2.30	1.26	1.22
20	c	505	CLA	C1D-C2D	2.30	1.49	1.45
20	b	605	CLA	C3B-C4B	2.30	1.49	1.42
20	b	616	CLA	MG-NC	2.30	2.11	2.06
20	a	407	CLA	C3B-C4B	2.30	1.49	1.42
20	B	601	CLA	C4C-C3C	2.30	1.48	1.45
20	b	606	CLA	MG-NB	2.30	2.10	2.05
36	d	407	LHG	O7-C7	2.29	1.40	1.34
40	v	201	HEC	CMA-C3A	2.29	1.55	1.50
20	b	605	CLA	C4C-C3C	2.29	1.48	1.45
20	b	603	CLA	C4C-C3C	2.29	1.48	1.45
20	c	502	CLA	C3B-C4B	2.29	1.49	1.42
20	b	618	CLA	MG-ND	2.29	2.10	2.05
20	B	606	CLA	CHC-C4B	2.29	1.44	1.39
20	c	509	CLA	C1C-NC	-2.28	1.34	1.37
20	d	404	CLA	C1C-C2C	2.28	1.49	1.44
20	D	402	CLA	C1B-NB	-2.28	1.34	1.37
20	b	609	CLA	OBD-CAD	2.28	1.26	1.22
20	B	608	CLA	C4D-CHA	2.27	1.46	1.38
20	C	505	CLA	C4B-NB	-2.27	1.34	1.37
20	B	610	CLA	CHD-C4C	2.27	1.44	1.39
20	b	615	CLA	C4D-CHA	2.27	1.46	1.38
20	B	603	CLA	C3B-C4B	2.27	1.49	1.42
20	B	607	CLA	C1B-C2B	2.27	1.48	1.43
20	C	506	CLA	C1B-C2B	2.27	1.48	1.43
24	j	101	LMG	O7-C8	-2.27	1.41	1.46
20	a	407	CLA	CBD-CAD	-2.27	1.46	1.56
20	b	615	CLA	C1D-ND	-2.27	1.34	1.37
20	A	402	CLA	O2A-CGA	2.27	1.40	1.33
20	D	401	CLA	C3D-C2D	2.26	1.45	1.39
20	b	605	CLA	C4B-NB	-2.26	1.34	1.37
20	c	512	CLA	C1C-C2C	2.26	1.49	1.44
20	D	401	CLA	MG-ND	2.26	2.10	2.05
20	A	401	CLA	MG-NA	2.25	2.11	2.06
20	B	605	CLA	C3B-C4B	2.25	1.49	1.42
20	d	402	CLA	C4D-CHA	2.25	1.46	1.38
22	b	621	BCR	C26-C25	2.25	1.38	1.34
20	a	404	CLA	C1D-ND	-2.25	1.34	1.37
21	A	403	PHO	C3D-C2D	2.24	1.43	1.39
20	b	618	CLA	C1B-C2B	2.24	1.48	1.43
20	c	513	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	604	CLA	CBD-CAD	-2.24	1.46	1.56
20	C	501	CLA	C1B-C2B	2.24	1.48	1.43
20	D	402	CLA	MG-NB	2.24	2.10	2.05
20	C	508	CLA	MG-NC	2.24	2.11	2.06
20	C	503	CLA	CBD-CAD	-2.23	1.46	1.56
37	e	102	HEM	CMB-C2B	2.23	1.55	1.50
20	B	602	CLA	C4C-C3C	2.22	1.48	1.45
20	C	502	CLA	C4B-NB	-2.22	1.34	1.37
20	b	605	CLA	MG-NB	2.22	2.10	2.05
20	b	611	CLA	C4B-NB	-2.22	1.34	1.37
20	d	403	CLA	C4D-CHA	2.22	1.46	1.38
20	c	512	CLA	C3B-C2B	2.22	1.48	1.41
20	C	507	CLA	C1A-CHA	2.22	1.52	1.43
20	C	506	CLA	MG-NB	2.22	2.10	2.05
22	A	405	BCR	C19-C18	2.22	1.50	1.46
20	c	503	CLA	C3D-C4D	-2.22	1.39	1.44
20	C	504	CLA	C1B-NB	-2.22	1.35	1.37
20	b	614	CLA	C4C-C3C	2.21	1.48	1.45
20	c	507	CLA	C1D-ND	-2.21	1.35	1.37
20	B	605	CLA	C4B-NB	-2.21	1.35	1.37
31	a	413	BCT	O1-C	2.21	1.33	1.25
20	B	613	CLA	C3B-C4B	2.20	1.49	1.42
23	a	409	SQD	O47-C45	-2.20	1.41	1.46
34	I	101	LMT	O1'-C1'	2.20	1.43	1.40
20	C	512	CLA	C3B-C2B	2.20	1.48	1.41
20	C	513	CLA	C3B-C2B	2.20	1.48	1.41
20	c	503	CLA	OBD-CAD	2.20	1.26	1.22
20	C	506	CLA	C4B-NB	-2.20	1.35	1.37
20	C	513	CLA	C1D-ND	-2.20	1.35	1.37
20	C	511	CLA	MG-NB	-2.20	2.01	2.05
20	b	611	CLA	C1C-C2C	2.20	1.49	1.44
20	C	506	CLA	C1B-NB	-2.19	1.35	1.37
20	a	404	CLA	C3B-C4B	2.19	1.49	1.42
20	B	614	CLA	C1C-C2C	2.19	1.49	1.44
20	C	502	CLA	CAA-C2A	2.19	1.58	1.54
20	C	502	CLA	MG-NC	2.19	2.11	2.06
20	C	512	CLA	C1B-NB	-2.18	1.35	1.37
20	c	504	CLA	C4B-NB	-2.18	1.35	1.37
20	b	617	CLA	C3B-C2B	2.18	1.48	1.41
20	b	608	CLA	C3B-C4B	2.18	1.49	1.42
20	b	614	CLA	C3B-C4B	2.18	1.49	1.42
32	C	522	HTG	C1-S1	-2.17	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	C1B-NB	-2.17	1.35	1.37
20	C	512	CLA	MG-ND	2.17	2.10	2.05
20	C	508	CLA	C1C-NC	-2.17	1.34	1.37
20	D	401	CLA	C4C-C3C	2.17	1.48	1.45
20	B	614	CLA	C1B-NB	-2.17	1.35	1.37
20	a	404	CLA	C3D-C4D	-2.17	1.39	1.44
20	d	402	CLA	C1B-NB	-2.17	1.35	1.37
20	B	614	CLA	C1-C2	2.17	1.55	1.49
20	B	611	CLA	C1B-C2B	2.17	1.48	1.43
20	b	606	CLA	MG-NC	2.17	2.11	2.06
34	a	418	LMT	O5B-C1B	2.17	1.47	1.41
32	B	621	HTG	O5-C1	2.17	1.45	1.42
20	B	611	CLA	C1C-NC	-2.16	1.34	1.37
20	C	513	CLA	C1C-C2C	2.16	1.48	1.44
20	B	609	CLA	C3D-C4D	-2.16	1.39	1.44
20	c	504	CLA	C3D-C4D	-2.16	1.39	1.44
20	b	606	CLA	CHC-C4B	2.16	1.44	1.39
20	B	602	CLA	C1C-NC	-2.15	1.34	1.37
20	c	503	CLA	C3B-C4B	2.15	1.49	1.42
20	A	404	CLA	C1C-NC	-2.15	1.34	1.37
20	C	501	CLA	C4C-C3C	2.15	1.48	1.45
20	c	508	CLA	C3B-C4B	2.15	1.49	1.42
20	c	504	CLA	C1B-C2B	2.15	1.48	1.43
27	A	411	PL9	C7-C3	2.14	1.54	1.51
20	d	403	CLA	C1D-ND	-2.14	1.35	1.37
20	c	501	CLA	C1C-C2C	2.14	1.48	1.44
20	b	615	CLA	C4B-NB	-2.14	1.35	1.37
20	B	613	CLA	MG-NB	2.14	2.10	2.05
20	b	607	CLA	MG-ND	-2.14	2.01	2.05
22	t	101	BCR	C20-C21	2.14	1.49	1.43
20	a	403	CLA	C4C-C3C	2.14	1.48	1.45
20	A	404	CLA	CBD-CAD	-2.14	1.46	1.56
20	d	402	CLA	O2D-CGD	2.13	1.38	1.33
20	b	613	CLA	C1B-NB	-2.13	1.35	1.37
20	c	510	CLA	CBD-CAD	-2.13	1.46	1.56
22	D	405	BCR	C20-C21	2.13	1.49	1.43
20	c	506	CLA	MG-NC	2.12	2.11	2.06
34	a	418	LMT	O1'-C1'	2.12	1.43	1.40
20	b	617	CLA	C3B-C4B	2.12	1.48	1.42
24	B	620	LMG	O7-C8	-2.12	1.41	1.46
20	d	402	CLA	C1D-C2D	2.12	1.49	1.45
20	C	507	CLA	C1C-C2C	2.12	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	402	CLA	C3D-C2D	2.12	1.44	1.39
22	B	619	BCR	C20-C21	2.12	1.49	1.43
20	c	503	CLA	C1C-NC	-2.11	1.34	1.37
20	B	607	CLA	C3D-C4D	-2.11	1.39	1.44
20	d	404	CLA	C4B-NB	-2.11	1.35	1.37
20	b	609	CLA	C4C-C3C	2.11	1.48	1.45
20	C	506	CLA	CBD-CAD	-2.11	1.47	1.56
27	D	412	PL9	C28-C29	2.10	1.37	1.33
22	K	101	BCR	C12-C13	2.10	1.50	1.46
20	C	511	CLA	C3D-C4D	-2.10	1.39	1.44
20	c	506	CLA	C1C-C2C	2.10	1.48	1.44
20	b	618	CLA	C3D-C4D	-2.09	1.39	1.44
20	b	609	CLA	C1C-NC	-2.09	1.34	1.37
20	C	503	CLA	C4C-C3C	2.09	1.48	1.45
22	A	405	BCR	C15-C14	2.09	1.49	1.43
22	A	405	BCR	C8-C9	2.09	1.50	1.46
20	b	604	CLA	CAB-C3B	2.09	1.53	1.47
22	t	101	BCR	C23-C22	2.09	1.50	1.46
20	D	404	CLA	C1D-ND	-2.09	1.35	1.37
20	C	511	CLA	CBD-CAD	-2.09	1.47	1.56
20	b	614	CLA	C1D-ND	-2.08	1.35	1.37
20	D	404	CLA	C4B-NB	-2.07	1.35	1.37
20	c	510	CLA	C5-C3	2.07	1.55	1.51
20	B	613	CLA	C4C-C3C	2.07	1.48	1.45
27	A	411	PL9	C6-C1	2.07	1.52	1.48
20	b	611	CLA	C1A-CHA	2.07	1.51	1.43
32	C	521	HTG	O5-C1	2.07	1.45	1.42
20	c	509	CLA	C3B-C2B	2.06	1.48	1.41
20	B	615	CLA	C4B-NB	-2.06	1.35	1.37
20	B	603	CLA	O2A-CGA	2.05	1.39	1.33
20	b	603	CLA	C1C-C2C	2.05	1.48	1.44
20	c	503	CLA	C1C-C2C	2.05	1.48	1.44
34	m	101	LMT	O1'-C1'	2.05	1.43	1.40
32	c	520	HTG	C1-S1	-2.05	1.77	1.80
22	c	514	BCR	C12-C13	2.04	1.50	1.46
20	a	403	CLA	C3B-C4B	2.04	1.48	1.42
20	d	402	CLA	C3B-C2B	2.04	1.48	1.41
21	A	403	PHO	OBD-CAD	2.04	1.25	1.22
20	c	513	CLA	MG-NC	2.04	2.11	2.06
20	C	508	CLA	C3B-C2B	2.04	1.48	1.41
20	B	612	CLA	C3B-C4B	2.04	1.48	1.42
20	b	605	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	602	HTG	C1-S1	-2.03	1.77	1.80
20	C	512	CLA	C3D-C4D	-2.03	1.39	1.44
20	b	618	CLA	C4B-NB	-2.03	1.35	1.37
20	B	603	CLA	MG-ND	2.03	2.09	2.05
22	B	617	BCR	C24-C25	2.03	1.52	1.45
20	D	401	CLA	C1B-NB	-2.03	1.35	1.37
38	H	101	RRX	C5-C6	2.03	1.37	1.34
31	A	421	BCT	O1-C	2.03	1.32	1.25
20	D	401	CLA	C1B-C2B	2.03	1.47	1.43
20	C	502	CLA	C1C-C2C	2.03	1.48	1.44
20	C	509	CLA	C3B-C4B	2.03	1.48	1.42
20	B	608	CLA	C3D-C4D	-2.02	1.39	1.44
20	c	512	CLA	C3D-C4D	-2.02	1.39	1.44
27	d	412	PL9	C52-C5	2.02	1.54	1.50
20	b	618	CLA	C1C-NC	-2.02	1.34	1.37
20	c	509	CLA	C3B-C4B	2.02	1.48	1.42
20	B	604	CLA	CAA-C2A	2.02	1.57	1.54
20	a	404	CLA	CBD-CAD	-2.01	1.47	1.56
22	K	102	BCR	C23-C22	2.01	1.50	1.46
20	b	617	CLA	CBD-CAD	-2.01	1.47	1.56
20	B	603	CLA	C3D-C4D	-2.01	1.39	1.44
20	C	506	CLA	C1A-CHA	2.01	1.51	1.43
20	b	612	CLA	CBD-CAD	-2.01	1.47	1.56
22	a	408	BCR	C20-C21	2.01	1.49	1.43
20	B	604	CLA	MG-ND	2.01	2.09	2.05

All (2627) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	504	CLA	C4A-NA-C1A	12.07	112.19	106.68
20	C	511	CLA	C4A-NA-C1A	11.64	111.99	106.68
20	c	501	CLA	C4A-NA-C1A	11.31	111.84	106.68
23	f	101	SQD	O9-S-C6	-11.06	90.24	106.76
20	c	509	CLA	C4A-NA-C1A	10.68	111.55	106.68
21	A	403	PHO	C2D-C1D-ND	10.66	117.13	109.43
21	a	405	PHO	C3B-C4B-NB	10.66	114.41	107.46
20	C	507	CLA	C4A-NA-C1A	10.38	111.42	106.68
23	f	101	SQD	O8-S-O9	-10.32	85.57	111.40
20	c	503	CLA	C4A-NA-C1A	10.30	111.38	106.68
20	c	502	CLA	C4A-NA-C1A	10.11	111.29	106.68
23	f	101	SQD	O9-S-O7	-10.06	81.11	113.82
21	a	406	PHO	C3B-C4B-NB	9.84	113.88	107.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	403	PHO	C3B-C4B-NB	9.81	113.86	107.46
21	a	405	PHO	C2D-C1D-ND	9.77	116.49	109.43
20	B	611	CLA	C4A-NA-C1A	9.57	111.05	106.68
20	C	506	CLA	C4A-NA-C1A	9.55	111.04	106.68
23	a	409	SQD	O6-C1-C2	9.55	122.78	108.27
21	D	403	PHO	C2D-C1D-ND	9.44	116.25	109.43
20	C	512	CLA	C4A-NA-C1A	9.41	110.97	106.68
20	c	511	CLA	C4A-NA-C1A	9.39	110.96	106.68
21	D	403	PHO	C3B-C4B-NB	9.30	113.53	107.46
21	A	403	PHO	C2B-C1B-NB	9.14	116.04	109.43
20	b	606	CLA	C4A-NA-C1A	9.10	110.83	106.68
21	D	403	PHO	C2B-C1B-NB	8.98	115.92	109.43
21	a	406	PHO	C2D-C1D-ND	8.81	115.80	109.43
20	B	602	CLA	C4A-NA-C1A	8.71	110.65	106.68
20	b	616	CLA	C4A-NA-C1A	8.64	110.62	106.68
20	b	615	CLA	C4A-NA-C1A	8.54	110.58	106.68
32	d	401	HTG	C1'-S1-C1	8.43	118.65	100.45
20	A	404	CLA	C1D-ND-C4D	-8.42	100.40	106.31
21	a	406	PHO	C2B-C1B-NB	8.40	115.50	109.43
20	A	402	CLA	C4A-NA-C1A	8.35	110.49	106.68
20	B	615	CLA	C4A-NA-C1A	8.26	110.45	106.68
23	f	101	SQD	O7-S-C6	8.22	119.03	106.76
32	V	202	HTG	C2-C1-S1	8.21	123.67	111.30
21	A	403	PHO	C4D-ND-C1D	-8.08	99.19	108.87
20	C	502	CLA	C4A-NA-C1A	8.03	110.34	106.68
20	C	509	CLA	C4A-NA-C1A	7.81	110.24	106.68
20	c	508	CLA	C4A-NA-C1A	7.80	110.24	106.68
21	a	405	PHO	C2B-C1B-NB	7.74	115.03	109.43
20	C	508	CLA	C4A-NA-C1A	7.72	110.20	106.68
20	B	603	CLA	C4A-NA-C1A	7.63	110.16	106.68
20	c	512	CLA	C4A-NA-C1A	7.58	110.14	106.68
20	B	607	CLA	C4A-NA-C1A	7.48	110.09	106.68
21	A	403	PHO	C3D-C4D-ND	7.44	117.25	107.71
20	C	513	CLA	C4A-NA-C1A	7.28	110.00	106.68
20	c	507	CLA	C4A-NA-C1A	7.23	109.98	106.68
21	D	403	PHO	C3D-C4D-ND	7.17	116.90	107.71
20	D	401	CLA	C4A-NA-C1A	7.17	109.95	106.68
20	b	617	CLA	C4A-NA-C1A	7.15	109.94	106.68
21	D	403	PHO	C4D-ND-C1D	-7.09	100.38	108.87
20	D	404	CLA	C4A-NA-C1A	7.09	109.91	106.68
20	b	603	CLA	C4A-NA-C1A	7.04	109.89	106.68
20	c	513	CLA	C4A-NA-C1A	6.97	109.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	404	CLA	C4A-NA-C1A	6.97	109.86	106.68
20	B	615	CLA	C4D-CHA-C1A	-6.97	112.93	121.24
22	d	405	BCR	C24-C23-C22	-6.94	115.96	126.23
20	A	404	CLA	C2D-C1D-ND	6.90	116.95	110.13
20	B	602	CLA	O2D-CGD-CBD	6.87	123.25	111.23
20	b	618	CLA	O2D-CGD-CBD	6.87	123.24	111.23
20	b	618	CLA	C4A-NA-C1A	6.80	109.78	106.68
20	B	612	CLA	CHD-C4C-C3C	-6.78	114.89	124.77
20	B	613	CLA	C4A-NA-C1A	6.74	109.75	106.68
20	b	605	CLA	C2C-C1C-NC	6.70	117.02	109.98
20	B	606	CLA	CHD-C4C-C3C	-6.69	115.02	124.77
20	B	604	CLA	C2C-C1C-NC	6.69	117.00	109.98
20	C	501	CLA	O2D-CGD-CBD	6.63	122.82	111.23
20	d	403	CLA	C2C-C1C-NC	6.56	116.87	109.98
21	A	403	PHO	O2D-CGD-CBD	6.55	118.15	110.95
20	C	505	CLA	C4A-NA-C1A	6.55	109.67	106.68
21	a	406	PHO	C4D-ND-C1D	-6.54	101.03	108.87
20	b	613	CLA	C4A-NA-C1A	6.50	109.65	106.68
20	B	616	CLA	C4A-NA-C1A	6.46	109.62	106.68
20	B	609	CLA	C4A-NA-C1A	6.44	109.62	106.68
20	b	608	CLA	C4A-NA-C1A	6.44	109.62	106.68
21	a	406	PHO	O2D-CGD-CBD	6.41	117.99	110.95
20	B	615	CLA	O2D-CGD-O1D	-6.41	111.37	123.85
23	f	101	SQD	O47-C7-C8	6.38	122.47	111.09
20	B	610	CLA	C4A-NA-C1A	6.36	109.58	106.68
20	B	613	CLA	CAC-C3C-C4C	6.34	133.04	124.79
20	b	614	CLA	C2C-C1C-NC	6.28	116.58	109.98
20	b	607	CLA	C2C-C1C-NC	6.27	116.57	109.98
23	a	409	SQD	O9-S-C6	6.25	116.09	106.76
20	A	402	CLA	CAC-C3C-C4C	6.25	132.92	124.79
21	a	406	PHO	C3D-C4D-ND	6.23	115.69	107.71
32	c	521	HTG	C1'-S1-C1	6.21	113.87	100.45
20	c	501	CLA	C1D-ND-C4D	-6.15	102.00	106.31
20	b	603	CLA	O2D-CGD-CBD	6.11	121.91	111.23
20	C	508	CLA	C1D-ND-C4D	-6.10	102.03	106.31
20	C	510	CLA	C4A-NA-C1A	6.09	109.46	106.68
20	a	404	CLA	C2C-C1C-NC	6.06	116.34	109.98
20	c	501	CLA	C2D-C1D-ND	6.00	116.07	110.13
20	B	607	CLA	CHD-C4C-C3C	-6.00	116.02	124.77
20	c	505	CLA	C4A-NA-C1A	5.99	109.41	106.68
22	b	619	BCR	C7-C8-C9	-5.90	117.50	126.23
20	C	510	CLA	CHD-C4C-C3C	-5.90	116.17	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	403	CLA	C4A-NA-C1A	5.89	109.37	106.68
20	b	616	CLA	C4D-CHA-C1A	-5.88	114.23	121.24
20	D	401	CLA	C2C-C1C-NC	5.85	116.12	109.98
20	C	510	CLA	C2C-C1C-NC	5.83	116.11	109.98
20	c	504	CLA	C2D-C1D-ND	5.83	115.90	110.13
20	C	504	CLA	C4A-NA-C1A	5.83	109.34	106.68
20	b	606	CLA	C2C-C1C-NC	5.82	116.09	109.98
20	b	618	CLA	CHD-C4C-C3C	-5.81	116.30	124.77
20	B	615	CLA	C1D-ND-C4D	-5.81	102.23	106.31
20	B	608	CLA	C2C-C1C-NC	5.80	116.08	109.98
20	c	501	CLA	C3B-C2B-C1B	-5.80	100.33	107.17
20	c	510	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
20	B	615	CLA	C2D-C1D-ND	5.78	115.85	110.13
32	B	631	HTG	C1'-S1-C1	5.78	112.92	100.45
20	B	605	CLA	C2C-C1C-NC	5.77	116.04	109.98
20	b	605	CLA	C1C-C2C-C3C	-5.76	100.92	106.98
20	c	501	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
20	a	404	CLA	C1C-C2C-C3C	-5.75	100.93	106.98
20	b	614	CLA	C4A-NA-C1A	5.73	109.30	106.68
20	C	504	CLA	C2C-C1C-NC	5.72	115.98	109.98
20	b	612	CLA	C2B-C1B-NB	5.71	116.25	110.33
20	B	604	CLA	C1C-C2C-C3C	-5.71	100.97	106.98
20	B	602	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
32	C	522	HTG	C1'-S1-C1	5.67	112.70	100.45
21	A	403	PHO	CBC-CAC-C3C	-5.67	104.76	112.87
23	l	101	SQD	O6-C1-C2	5.66	116.86	108.27
20	A	402	CLA	C2B-C1B-NB	5.64	116.17	110.33
38	H	101	RRX	C24-C23-C22	-5.61	117.93	126.23
20	b	605	CLA	O2D-CGD-O1D	-5.61	112.93	123.85
20	C	507	CLA	O2D-CGD-CBD	5.61	121.04	111.23
20	B	606	CLA	C2D-C1D-ND	5.61	115.68	110.13
20	B	609	CLA	C2D-C1D-ND	5.61	115.68	110.13
32	C	521	HTG	C1-O5-C5	5.57	122.56	112.56
23	A	406	SQD	O6-C1-C2	5.57	116.73	108.27
20	c	513	CLA	CHD-C4C-C3C	-5.56	116.66	124.77
20	A	404	CLA	C2B-C1B-NB	5.56	116.09	110.33
32	V	202	HTG	O5-C1-C2	-5.56	102.65	110.32
20	C	509	CLA	C2C-C1C-NC	5.55	115.81	109.98
23	a	409	SQD	C1-O5-C5	-5.55	102.88	113.72
34	c	523	LMT	C1'-O5'-C5'	5.55	124.55	113.72
20	b	614	CLA	CHD-C4C-C3C	-5.55	116.69	124.77
20	A	402	CLA	C2D-C1D-ND	5.54	115.61	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	614	CLA	C2C-C1C-NC	5.53	115.79	109.98
20	D	402	CLA	C2C-C1C-NC	5.52	115.78	109.98
20	d	403	CLA	C4A-NA-C1A	5.49	109.18	106.68
20	b	607	CLA	CAC-C3C-C4C	5.48	131.91	124.79
20	C	504	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
20	B	611	CLA	CHD-C4C-C3C	-5.46	116.82	124.77
21	a	405	PHO	C4D-ND-C1D	-5.45	102.34	108.87
20	a	407	CLA	O2D-CGD-CBD	5.44	120.74	111.23
20	B	612	CLA	C4A-NA-C1A	5.44	109.16	106.68
20	b	612	CLA	O2D-CGD-CBD	5.44	120.73	111.23
20	A	404	CLA	C4D-CHA-C1A	-5.43	114.76	121.24
20	C	508	CLA	C2D-C1D-ND	5.43	115.50	110.13
20	d	404	CLA	C2D-C1D-ND	5.43	115.50	110.13
20	B	604	CLA	CHD-C4C-C3C	-5.42	116.87	124.77
20	b	603	CLA	C2B-C1B-NB	5.41	115.93	110.33
20	c	506	CLA	C4A-NA-C1A	5.40	109.14	106.68
20	b	614	CLA	CAC-C3C-C4C	5.39	131.81	124.79
32	v	210	HTG	C1'-S1-C1	5.39	110.47	100.16
20	D	402	CLA	C4A-NA-C1A	5.37	109.13	106.68
23	A	412	SQD	O6-C1-C2	5.35	116.40	108.27
24	C	524	LMG	O7-C10-C11	5.34	123.04	111.48
35	D	406	DGD	O2G-C1B-C2B	5.34	123.04	111.48
22	D	405	BCR	C24-C23-C22	-5.33	118.35	126.23
34	I	101	LMT	O1B-C4'-C3'	5.32	120.75	107.23
20	B	603	CLA	C2C-C1C-NC	5.31	115.56	109.98
20	C	506	CLA	O2D-CGD-CBD	5.30	120.50	111.23
20	c	504	CLA	C2B-C1B-NB	5.30	115.82	110.33
20	C	502	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
20	B	604	CLA	C2B-C1B-NB	5.29	115.81	110.33
20	c	507	CLA	O2D-CGD-CBD	5.28	120.47	111.23
20	d	404	CLA	C1D-ND-C4D	-5.28	102.61	106.31
20	c	502	CLA	C2D-C1D-ND	5.28	115.35	110.13
22	B	617	BCR	C7-C8-C9	-5.27	118.44	126.23
22	D	405	BCR	C7-C8-C9	-5.27	118.44	126.23
20	A	402	CLA	C3B-C4B-NB	5.26	115.23	110.53
20	a	407	CLA	CAC-C3C-C4C	5.26	131.63	124.79
32	C	521	HTG	C1'-S1-C1	5.26	111.80	100.45
20	c	501	CLA	C2B-C1B-NB	5.25	115.78	110.33
20	B	613	CLA	C2C-C1C-NC	5.25	115.50	109.98
20	c	508	CLA	C2B-C1B-NB	5.25	115.77	110.33
20	A	402	CLA	C2C-C1C-NC	5.24	115.48	109.98
20	C	501	CLA	O2D-CGD-O1D	-5.24	113.66	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	616	CLA	C2D-C1D-ND	5.23	115.31	110.13
20	B	609	CLA	CHD-C4C-C3C	-5.22	117.16	124.77
20	c	512	CLA	O2D-CGD-CBD	5.22	120.35	111.23
40	v	201	HEC	CBB-CAB-C3B	-5.22	117.01	127.43
20	b	615	CLA	C1-C2-C3	-5.22	117.65	126.20
20	c	507	CLA	C2C-C1C-NC	5.21	115.46	109.98
20	B	607	CLA	CMB-C2B-C1B	5.21	133.35	125.42
20	c	505	CLA	CHD-C4C-C3C	-5.19	117.20	124.77
20	c	502	CLA	CAC-C3C-C4C	5.19	131.54	124.79
20	b	606	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
20	c	507	CLA	CHD-C4C-C3C	-5.17	117.23	124.77
20	b	614	CLA	C4D-CHA-C1A	-5.17	115.08	121.24
20	d	402	CLA	C2C-C1C-NC	5.17	115.41	109.98
34	c	523	LMT	C1B-O5B-C5B	5.16	123.80	113.72
20	B	614	CLA	C4D-CHA-C1A	-5.16	115.09	121.24
34	b	627	LMT	C3B-C4B-C5B	5.15	119.58	110.23
20	C	509	CLA	C4D-CHA-C1A	-5.15	115.10	121.24
20	D	402	CLA	CAC-C3C-C4C	5.15	131.49	124.79
20	B	616	CLA	C2D-C1D-ND	5.14	115.22	110.13
20	d	404	CLA	C2B-C1B-NB	5.14	115.66	110.33
20	C	505	CLA	CHD-C4C-C3C	-5.14	117.28	124.77
20	a	407	CLA	C2C-C1C-NC	5.14	115.38	109.98
20	b	615	CLA	C2C-C1C-NC	5.14	115.38	109.98
20	a	403	CLA	CHD-C4C-C3C	-5.14	117.28	124.77
20	d	404	CLA	C4A-NA-C1A	5.13	109.02	106.68
20	B	610	CLA	CHD-C4C-C3C	-5.13	117.29	124.77
20	b	610	CLA	CAC-C3C-C4C	5.13	131.46	124.79
20	b	612	CLA	C2D-C1D-ND	5.11	115.19	110.13
20	d	404	CLA	CHD-C4C-C3C	-5.11	117.32	124.77
20	C	508	CLA	C4D-CHA-C1A	-5.11	115.15	121.24
32	B	623	HTG	C1'-S1-C1	5.10	111.47	100.45
20	C	509	CLA	C2B-C1B-NB	5.10	115.61	110.33
20	b	610	CLA	C2C-C1C-NC	5.10	115.34	109.98
20	b	613	CLA	C2D-C1D-ND	5.10	115.17	110.13
20	C	511	CLA	C2C-C1C-NC	5.09	115.33	109.98
20	C	505	CLA	C2C-C1C-NC	5.08	115.32	109.98
23	f	101	SQD	O8-S-O7	5.07	124.09	111.40
34	a	418	LMT	C3'-C4'-C5'	-5.06	99.72	110.93
20	B	609	CLA	C2C-C1C-NC	5.06	115.29	109.98
32	C	520	HTG	C1'-S1-C1	5.05	111.36	100.45
20	B	616	CLA	C2C-C1C-NC	5.05	115.29	109.98
20	B	610	CLA	C2C-C1C-NC	5.05	115.28	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	506	CLA	CHD-C4C-C3C	-5.04	117.42	124.77
20	b	607	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
20	d	404	CLA	C2C-C1C-NC	5.03	115.26	109.98
20	B	604	CLA	O2D-CGD-CBD	5.02	120.01	111.23
20	C	502	CLA	C2D-C1D-ND	5.00	115.08	110.13
20	b	607	CLA	C4D-CHA-C1A	-5.00	115.28	121.24
20	c	507	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
20	C	509	CLA	C1C-C2C-C3C	-5.00	101.73	106.98
20	B	612	CLA	C2D-C1D-ND	4.99	115.06	110.13
34	z	102	LMT	O1B-C4'-C3'	4.98	119.89	107.23
20	b	607	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
20	b	603	CLA	C2D-C1D-ND	4.98	115.06	110.13
20	c	501	CLA	O2D-CGD-CBD	4.98	119.93	111.23
20	d	404	CLA	C4D-CHA-C1A	-4.97	115.31	121.24
20	D	404	CLA	C2D-C1D-ND	4.97	115.04	110.13
23	l	101	SQD	O7-S-C6	4.97	114.17	106.76
20	D	402	CLA	CHD-C4C-C3C	-4.96	117.55	124.77
20	B	607	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
20	B	609	CLA	CHD-C1D-ND	-4.95	117.83	124.80
20	B	607	CLA	O2D-CGD-O1D	-4.95	114.22	123.85
20	b	609	CLA	C2C-C1C-NC	4.93	115.16	109.98
20	B	616	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
20	B	604	CLA	C2D-C1D-ND	4.92	115.00	110.13
20	C	509	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
20	a	407	CLA	CHD-C4C-C3C	-4.91	117.61	124.77
20	B	614	CLA	CHD-C4C-C3C	-4.90	117.63	124.77
20	b	611	CLA	C2C-C1C-NC	4.90	115.12	109.98
21	D	403	PHO	O2D-CGD-CBD	4.88	116.31	110.95
20	B	611	CLA	O2D-CGD-CBD	4.88	119.76	111.23
20	C	511	CLA	C2D-C1D-ND	4.88	114.95	110.13
20	c	501	CLA	C2C-C1C-NC	4.87	115.10	109.98
20	c	501	CLA	C4D-CHA-C1A	-4.86	115.44	121.24
20	b	608	CLA	CHD-C4C-C3C	-4.86	117.69	124.77
20	c	510	CLA	C4D-CHA-C1A	-4.86	115.45	121.24
20	B	605	CLA	C4A-NA-C1A	4.85	108.89	106.68
20	B	615	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
22	b	619	BCR	C24-C23-C22	-4.84	119.07	126.23
20	c	502	CLA	C2B-C1B-NB	4.84	115.34	110.33
20	B	608	CLA	C2B-C1B-NB	4.83	115.33	110.33
20	A	401	CLA	C1D-CHD-C4C	-4.83	115.75	126.02
20	b	615	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
20	A	401	CLA	C2B-C1B-NB	4.82	115.33	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	d	403	CLA	CHD-C4C-C3C	-4.81	117.75	124.77
21	a	406	PHO	CMA-C3A-C4A	-4.81	104.24	114.61
20	b	610	CLA	CHD-C4C-C3C	-4.81	117.76	124.77
20	b	605	CLA	CHD-C4C-C3C	-4.81	117.77	124.77
20	a	404	CLA	O2D-CGD-CBD	4.80	119.62	111.23
23	A	406	SQD	C1-C2-C3	-4.80	99.91	110.01
22	c	514	BCR	C24-C23-C22	-4.80	119.14	126.23
20	b	616	CLA	CMB-C2B-C1B	4.79	132.71	125.42
20	b	616	CLA	C1-C2-C3	-4.79	118.36	126.20
20	B	614	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
20	b	612	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
20	D	402	CLA	C1C-C2C-C3C	-4.78	101.95	106.98
20	c	504	CLA	C1D-ND-C4D	-4.77	102.96	106.31
20	B	606	CLA	C2B-C1B-NB	4.77	115.27	110.33
20	B	608	CLA	C1C-C2C-C3C	-4.77	101.96	106.98
20	C	506	CLA	CHD-C4C-C3C	-4.76	117.83	124.77
36	D	407	LHG	O8-C23-O10	-4.76	111.72	123.63
20	C	503	CLA	C1C-C2C-C3C	-4.76	101.97	106.98
20	b	608	CLA	C2C-C1C-NC	4.76	114.98	109.98
20	A	402	CLA	O2D-CGD-CBD	4.76	119.55	111.23
20	B	601	CLA	C2D-C1D-ND	4.75	114.83	110.13
20	B	614	CLA	C4A-NA-C1A	4.75	108.85	106.68
20	B	615	CLA	C2B-C1B-NB	4.75	115.25	110.33
32	b	624	HTG	C1'-S1-C1	4.75	110.71	100.45
20	b	616	CLA	C2B-C1B-NB	4.75	115.25	110.33
20	c	513	CLA	C2D-C1D-ND	4.74	114.82	110.13
20	D	404	CLA	C2B-C1B-NB	4.74	115.24	110.33
20	C	513	CLA	C2B-C1B-NB	4.74	115.24	110.33
20	b	613	CLA	C2C-C1C-NC	4.73	114.95	109.98
20	c	512	CLA	CHD-C4C-C3C	-4.73	117.88	124.77
20	b	610	CLA	C1C-C2C-C3C	-4.73	102.01	106.98
20	c	503	CLA	C2C-C1C-NC	4.73	114.94	109.98
20	C	507	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
20	D	404	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
20	C	501	CLA	CHD-C4C-C3C	-4.72	117.90	124.77
20	B	604	CLA	C3B-C4B-NB	4.71	114.73	110.53
27	D	412	PL9	C40-C39-C41	4.70	123.39	115.23
20	c	513	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	f	101	SQD	O8-S-C6	4.70	115.04	105.97
20	b	613	CLA	CHD-C4C-C3C	-4.70	117.93	124.77
36	D	407	LHG	O8-C23-C24	4.70	126.15	111.83
20	c	512	CLA	C3B-C2B-C1B	-4.69	101.64	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	513	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
20	c	501	CLA	O2D-CGD-O1D	-4.68	114.73	123.85
20	B	604	CLA	C4A-NA-C1A	4.68	108.81	106.68
20	c	503	CLA	CHD-C4C-C3C	-4.68	117.95	124.77
20	B	606	CLA	C4D-CHA-C1A	-4.68	115.66	121.24
37	E	104	HEM	CBD-CAD-C3D	-4.67	99.61	112.53
20	b	616	CLA	C1D-ND-C4D	-4.67	103.03	106.31
20	b	615	CLA	CHD-C4C-C3C	-4.67	117.96	124.77
20	B	609	CLA	C2B-C1B-NB	4.67	115.17	110.33
20	c	508	CLA	C4D-CHA-C1A	-4.66	115.68	121.24
20	b	608	CLA	O2D-CGD-CBD	4.65	119.35	111.23
20	C	509	CLA	CMB-C2B-C1B	4.64	132.49	125.42
20	c	501	CLA	C1C-C2C-C3C	-4.64	102.10	106.98
20	b	603	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
20	a	407	CLA	C2D-C1D-ND	4.64	114.72	110.13
20	c	510	CLA	C2D-C1D-ND	4.64	114.72	110.13
20	B	606	CLA	C2C-C1C-NC	4.64	114.85	109.98
20	C	512	CLA	O2D-CGD-CBD	4.63	119.33	111.23
23	A	412	SQD	O9-S-C6	4.63	113.67	106.76
20	B	607	CLA	C2B-C1B-NB	4.63	115.13	110.33
20	B	602	CLA	CHD-C1D-ND	-4.63	118.29	124.80
23	A	406	SQD	O47-C7-C8	4.63	121.49	111.48
22	b	621	BCR	C24-C23-C22	-4.62	119.40	126.23
20	c	511	CLA	O2D-CGD-CBD	4.62	119.30	111.23
20	b	617	CLA	C2D-C1D-ND	4.61	114.69	110.13
21	a	405	PHO	C3D-C4D-ND	4.59	113.59	107.71
20	A	402	CLA	C1D-ND-C4D	-4.59	103.09	106.31
20	C	503	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
22	B	619	BCR	C38-C26-C25	-4.59	119.48	124.48
20	C	513	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
20	B	611	CLA	C2C-C1C-NC	4.59	114.80	109.98
20	c	509	CLA	C2D-C1D-ND	4.58	114.66	110.13
20	B	611	CLA	C2D-C1D-ND	4.58	114.66	110.13
20	c	508	CLA	C2D-C1D-ND	4.58	114.66	110.13
21	a	406	PHO	C1-C2-C3	-4.58	118.69	126.20
20	c	511	CLA	CHD-C4C-C3C	-4.57	118.11	124.77
20	c	510	CLA	C2B-C1B-NB	4.57	115.07	110.33
20	c	503	CLA	C1C-C2C-C3C	-4.57	102.17	106.98
20	a	403	CLA	C1D-CHD-C4C	-4.57	116.31	126.02
20	B	602	CLA	CHD-C4C-NC	4.57	131.31	124.23
20	C	510	CLA	O2D-CGD-CBD	4.56	119.21	111.23
20	b	617	CLA	CHD-C4C-C3C	-4.56	118.12	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	401	CLA	C1C-C2C-C3C	-4.56	102.19	106.98
20	b	606	CLA	C2D-C1D-ND	4.56	114.64	110.13
20	C	501	CLA	C2C-C1C-NC	4.56	114.77	109.98
32	v	210	HTG	O5-C1-C2	-4.56	104.03	110.32
20	B	601	CLA	CHC-C4B-NB	4.55	130.88	124.05
20	A	402	CLA	CMD-C2D-C1D	4.55	132.74	124.73
20	B	608	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
20	B	601	CLA	C2C-C1C-NC	4.55	114.76	109.98
20	B	611	CLA	C2B-C1B-NB	4.54	115.04	110.33
20	b	615	CLA	C2D-C1D-ND	4.54	114.62	110.13
20	b	610	CLA	C2D-C1D-ND	4.54	114.62	110.13
20	b	604	CLA	C2C-C1C-NC	4.54	114.75	109.98
20	c	506	CLA	C2D-C1D-ND	4.54	114.62	110.13
20	c	512	CLA	C1-C2-C3	-4.54	118.77	126.20
20	d	403	CLA	C1C-C2C-C3C	-4.53	102.21	106.98
20	C	511	CLA	C2B-C1B-NB	4.53	115.03	110.33
20	a	404	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
20	a	403	CLA	CHD-C4C-NC	4.53	131.26	124.23
20	C	504	CLA	CHD-C4C-C3C	-4.53	118.17	124.77
20	c	504	CLA	C4D-CHA-C1A	-4.51	115.86	121.24
23	a	409	SQD	C1-C2-C3	-4.51	100.52	110.01
20	B	613	CLA	C4D-CHA-C1A	-4.51	115.86	121.24
20	a	404	CLA	CAC-C3C-C4C	4.51	130.66	124.79
20	d	404	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
20	c	509	CLA	CHD-C4C-C3C	-4.50	118.21	124.77
20	C	510	CLA	CHD-C4C-NC	4.50	131.21	124.23
20	b	603	CLA	C1C-C2C-C3C	-4.50	102.25	106.98
20	c	509	CLA	C2B-C1B-NB	4.50	114.99	110.33
20	c	502	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
20	b	613	CLA	C4D-CHA-C1A	-4.49	115.88	121.24
20	B	601	CLA	C2B-C1B-NB	4.49	114.98	110.33
20	B	601	CLA	CAC-C3C-C4C	4.48	130.62	124.79
24	c	518	LMG	O7-C10-C11	4.48	121.18	111.48
20	b	606	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
20	B	607	CLA	O2D-CGD-CBD	4.47	119.05	111.23
20	B	613	CLA	CHD-C4C-C3C	-4.47	118.25	124.77
20	b	603	CLA	CHD-C4C-C3C	-4.47	118.26	124.77
32	B	622	HTG	C1'-S1-C1	4.46	110.09	100.45
20	C	505	CLA	C1C-C2C-C3C	-4.46	102.29	106.98
20	D	401	CLA	C2B-C1B-NB	4.46	114.95	110.33
20	c	505	CLA	C2C-C1C-NC	4.46	114.67	109.98
20	D	404	CLA	C1C-C2C-C3C	-4.45	102.30	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	606	CLA	C3B-C2B-C1B	-4.45	101.93	107.17
20	C	502	CLA	C4D-CHA-C1A	-4.44	115.94	121.24
20	c	511	CLA	C1C-C2C-C3C	-4.44	102.31	106.98
20	b	610	CLA	C2B-C1B-NB	4.44	114.93	110.33
20	b	616	CLA	O2D-CGD-CBD	4.43	118.98	111.23
20	b	610	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
20	d	404	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
20	C	512	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
20	B	612	CLA	C2B-C1B-NB	4.42	114.91	110.33
20	B	614	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
20	b	606	CLA	O2D-CGD-CBD	4.42	118.96	111.23
20	A	404	CLA	C4-C3-C5	4.42	122.90	115.23
20	c	507	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
20	B	616	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	A	412	SQD	C1-O5-C5	-4.41	105.10	113.72
20	b	607	CLA	C2D-C1D-ND	4.41	114.49	110.13
35	d	416	DGD	O2G-C1B-C2B	4.41	121.02	111.48
20	C	503	CLA	O2D-CGD-CBD	4.41	118.93	111.23
20	c	504	CLA	CHD-C4C-C3C	-4.40	118.35	124.77
20	C	512	CLA	C1-O2A-CGA	4.40	127.31	116.65
20	A	404	CLA	C3B-C2B-C1B	-4.40	101.99	107.17
20	A	402	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
22	K	101	BCR	C33-C5-C6	-4.40	119.69	124.48
20	B	602	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
20	C	503	CLA	CHD-C4C-C3C	-4.39	118.37	124.77
20	C	513	CLA	C2C-C1C-NC	4.39	114.59	109.98
22	B	617	BCR	C15-C14-C13	-4.39	121.12	127.28
34	z	102	LMT	C1B-O1B-C4'	4.39	128.38	117.98
20	B	613	CLA	CHD-C1D-ND	-4.39	118.62	124.80
20	c	507	CLA	C2D-C1D-ND	4.38	114.47	110.13
37	e	102	HEM	C4D-ND-C1D	4.38	110.40	105.21
20	B	607	CLA	CHC-C4B-NB	4.38	130.62	124.05
20	d	404	CLA	CMB-C2B-C1B	4.38	132.09	125.42
20	C	501	CLA	C4A-NA-C1A	4.38	108.68	106.68
20	b	609	CLA	CHD-C4C-C3C	-4.38	118.39	124.77
20	c	510	CLA	C1C-C2C-C3C	-4.38	102.38	106.98
32	c	521	HTG	C1-O5-C5	4.38	120.41	112.56
20	C	508	CLA	C2B-C1B-NB	4.38	114.86	110.33
20	B	612	CLA	C1D-CHD-C4C	-4.37	116.72	126.02
20	C	504	CLA	O2D-CGD-CBD	4.37	118.87	111.23
21	a	405	PHO	O2D-CGD-CBD	4.37	115.75	110.95
20	b	609	CLA	C4-C3-C5	4.37	122.81	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	615	CLA	CMD-C2D-C1D	4.37	132.42	124.73
20	C	511	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
20	a	403	CLA	CAC-C3C-C4C	4.36	130.46	124.79
20	b	612	CLA	C4A-NA-C1A	4.35	108.66	106.68
20	d	403	CLA	C2D-C1D-ND	4.35	114.43	110.13
20	B	608	CLA	CHD-C4C-C3C	-4.35	118.44	124.77
20	B	614	CLA	C2D-C1D-ND	4.34	114.42	110.13
20	c	502	CLA	C2C-C1C-NC	4.34	114.54	109.98
20	C	508	CLA	CAC-C3C-C4C	4.34	130.43	124.79
32	V	202	HTG	C1-O5-C5	-4.33	104.78	112.56
23	b	622	SQD	O47-C7-C8	4.33	120.86	111.48
20	B	616	CLA	C2B-C1B-NB	4.33	114.81	110.33
20	b	613	CLA	O2D-CGD-CBD	4.33	118.80	111.23
20	b	604	CLA	C1C-C2C-C3C	-4.33	102.43	106.98
20	c	506	CLA	C2B-C1B-NB	4.33	114.81	110.33
20	B	603	CLA	C1C-C2C-C3C	-4.33	102.43	106.98
20	a	404	CLA	CMD-C2D-C1D	4.32	132.34	124.73
20	A	401	CLA	CAC-C3C-C4C	4.32	130.41	124.79
20	b	617	CLA	CAC-C3C-C4C	4.32	130.41	124.79
20	c	506	CLA	C2C-C1C-NC	4.31	114.51	109.98
20	D	401	CLA	C4D-CHA-C1A	-4.31	116.11	121.24
20	C	501	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
20	B	612	CLA	CHD-C4C-NC	4.31	130.91	124.23
20	d	402	CLA	C4A-NA-C1A	4.30	108.64	106.68
20	D	401	CLA	CHD-C4C-C3C	-4.30	118.50	124.77
20	c	508	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
20	C	503	CLA	C4A-NA-C1A	4.30	108.64	106.68
20	c	506	CLA	C1C-C2C-C3C	-4.30	102.46	106.98
20	C	504	CLA	CHD-C1D-ND	-4.29	118.76	124.80
20	b	618	CLA	C2B-C1B-NB	4.29	114.78	110.33
20	B	601	CLA	CHD-C4C-C3C	-4.29	118.52	124.77
20	D	401	CLA	C3C-C4C-NC	4.29	115.92	110.43
20	b	604	CLA	C1-C2-C3	-4.29	119.17	126.20
20	C	509	CLA	O2D-CGD-CBD	4.29	118.72	111.23
22	t	101	BCR	C29-C28-C27	-4.28	101.86	111.28
20	b	615	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
32	V	202	HTG	C1-C2-C3	-4.27	102.19	110.55
20	b	614	CLA	C2D-C1D-ND	4.27	114.35	110.13
20	A	402	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
20	C	506	CLA	CHA-C4D-ND	4.27	141.36	132.55
20	b	604	CLA	C2D-C1D-ND	4.27	114.35	110.13
20	B	605	CLA	C1C-C2C-C3C	-4.26	102.50	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	620	LMG	O7-C10-C11	4.26	120.70	111.48
20	D	402	CLA	C2D-C1D-ND	4.26	114.34	110.13
20	B	615	CLA	O2D-CGD-CBD	4.26	118.68	111.23
34	b	627	LMT	O5'-C5'-C4'	4.26	118.53	109.72
20	d	402	CLA	C4-C3-C5	4.26	122.62	115.23
20	B	602	CLA	O2A-CGA-CBA	4.25	124.81	111.83
27	A	411	PL9	C53-C6-C1	4.25	123.98	115.28
20	C	512	CLA	C4D-CHA-C1A	-4.25	116.17	121.24
23	A	412	SQD	O47-C7-C8	4.25	120.68	111.48
22	K	102	BCR	C7-C8-C9	-4.24	119.96	126.23
20	b	612	CLA	C2C-C1C-NC	4.23	114.42	109.98
20	C	507	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
23	F	101	SQD	O6-C1-C2	4.22	114.68	108.27
20	b	617	CLA	C2C-C1C-NC	4.21	114.41	109.98
20	b	603	CLA	C4D-CHA-C1A	-4.21	116.22	121.24
20	c	506	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
20	b	608	CLA	C1C-C2C-C3C	-4.21	102.56	106.98
20	B	606	CLA	C1D-CHD-C4C	-4.20	117.10	126.02
20	b	617	CLA	C1D-CHD-C4C	-4.19	117.11	126.02
20	c	508	CLA	CHD-C4C-C3C	-4.19	118.66	124.77
20	b	612	CLA	CHD-C4C-C3C	-4.19	118.66	124.77
22	B	619	BCR	C24-C23-C22	-4.19	120.03	126.23
20	C	501	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
35	H	102	DGD	O1G-C1A-O1A	-4.19	113.15	123.63
20	c	502	CLA	O2D-CGD-CBD	4.19	118.55	111.23
22	d	405	BCR	C11-C10-C9	-4.19	121.41	127.28
20	C	503	CLA	C2C-C1C-NC	4.18	114.38	109.98
20	A	401	CLA	C3B-C4B-NB	4.18	114.26	110.53
22	D	405	BCR	C29-C30-C25	4.17	116.50	110.44
20	B	605	CLA	CHD-C4C-C3C	-4.17	118.69	124.77
20	c	504	CLA	C3B-C4B-NB	4.17	114.25	110.53
20	c	504	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
20	b	604	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
20	b	617	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
20	C	512	CLA	CHD-C4C-C3C	-4.16	118.70	124.77
20	c	513	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
37	e	102	HEM	CBA-CAA-C2A	-4.16	101.04	112.53
20	c	508	CLA	C2C-C1C-NC	4.16	114.35	109.98
20	B	608	CLA	C2D-C1D-ND	4.16	114.24	110.13
20	C	506	CLA	C2D-C1D-ND	4.16	114.24	110.13
20	c	503	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
20	b	611	CLA	C1C-C2C-C3C	-4.15	102.61	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	616	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
20	B	614	CLA	CMD-C2D-C1D	4.15	132.03	124.73
37	E	104	HEM	CHC-C4B-NB	4.15	128.88	124.42
20	B	609	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
20	C	510	CLA	C2B-C1B-NB	4.14	114.62	110.33
20	c	512	CLA	C2B-C1B-NB	4.14	114.62	110.33
20	A	402	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
20	d	402	CLA	C4B-C3B-C2B	-4.14	102.16	107.30
20	b	609	CLA	C4D-CHA-C1A	-4.13	116.31	121.24
20	B	610	CLA	C4D-CHA-C1A	-4.13	116.32	121.24
20	D	402	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
20	b	607	CLA	CMC-C2C-C1C	4.13	131.48	125.03
20	A	402	CLA	C4D-CHA-C1A	-4.12	116.33	121.24
20	b	608	CLA	C2D-C1D-ND	4.12	114.20	110.13
20	B	606	CLA	CAC-C3C-C4C	4.12	130.15	124.79
20	b	612	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
35	C	516	DGD	O3G-C3G-C2G	-4.11	100.82	110.82
20	B	602	CLA	C2D-C1D-ND	4.11	114.19	110.13
20	B	616	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
20	A	402	CLA	CHD-C1D-ND	-4.11	119.02	124.80
20	A	401	CLA	C4-C3-C5	4.11	122.36	115.23
20	d	403	CLA	C4D-CHA-C1A	-4.11	116.34	121.24
20	b	611	CLA	CAC-C3C-C4C	4.11	130.13	124.79
37	E	104	HEM	C4D-ND-C1D	4.11	110.07	105.21
20	B	610	CLA	CAC-C3C-C4C	4.11	130.13	124.79
20	c	504	CLA	CHD-C1D-ND	-4.10	119.03	124.80
20	B	610	CLA	C1-C2-C3	-4.10	119.48	126.20
20	B	612	CLA	C1-C2-C3	-4.10	119.48	126.20
20	B	603	CLA	CHC-C4B-NB	4.10	130.20	124.05
20	c	507	CLA	C2B-C1B-NB	4.10	114.58	110.33
32	D	417	HTG	C1'-S1-C1	4.10	109.30	100.45
23	a	401	SQD	O47-C7-C8	4.09	120.34	111.48
20	B	610	CLA	CHA-C4D-ND	4.09	141.00	132.55
20	B	607	CLA	CMD-C2D-C1D	4.09	131.94	124.73
20	C	509	CLA	C2D-C1D-ND	4.09	114.17	110.13
24	b	623	LMG	O7-C10-C11	4.09	120.33	111.48
36	D	409	LHG	O4-P-O5	4.09	131.46	112.44
20	C	506	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
20	b	605	CLA	O2D-CGD-CBD	4.09	118.37	111.23
20	D	401	CLA	CMC-C2C-C1C	4.09	131.42	125.03
20	B	611	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
20	c	506	CLA	C3D-C2D-C1D	-4.08	100.26	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	516	DGD	O2G-C1B-C2B	4.08	120.31	111.48
20	D	402	CLA	O2D-CGD-CBD	4.08	118.36	111.23
20	c	509	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
20	c	504	CLA	C2C-C1C-NC	4.07	114.26	109.98
20	B	608	CLA	O2D-CGD-O1D	-4.07	115.92	123.85
20	B	601	CLA	C3B-C2B-C1B	-4.07	102.38	107.17
20	b	614	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
20	A	402	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
20	b	609	CLA	CHC-C4B-NB	4.06	130.15	124.05
20	A	401	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
20	C	508	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
20	c	511	CLA	O2D-CGD-O1D	-4.06	115.95	123.85
20	B	606	CLA	CHD-C4C-NC	4.06	130.52	124.23
20	A	402	CLA	O2D-CGD-O1D	-4.05	115.95	123.85
20	C	508	CLA	C2C-C1C-NC	4.05	114.24	109.98
20	b	607	CLA	C2B-C1B-NB	4.05	114.53	110.33
20	C	513	CLA	O2A-CGA-CBA	4.05	124.18	111.83
20	c	511	CLA	C2C-C1C-NC	4.04	114.23	109.98
34	a	418	LMT	O5B-C5B-C6B	4.04	116.46	106.44
20	b	604	CLA	C2B-C1B-NB	4.04	114.52	110.33
20	b	604	CLA	CHD-C1D-ND	-4.04	119.11	124.80
34	b	627	LMT	C1'-O5'-C5'	4.04	121.61	113.72
20	d	404	CLA	CHD-C4C-NC	4.04	130.49	124.23
20	d	403	CLA	C1D-CHD-C4C	-4.03	117.45	126.02
20	C	503	CLA	CHA-C4D-ND	4.03	140.87	132.55
20	a	404	CLA	CHD-C4C-C3C	-4.03	118.90	124.77
20	C	504	CLA	C2B-C1B-NB	4.03	114.50	110.33
20	b	608	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
20	C	508	CLA	C3B-C2B-C1B	-4.02	102.43	107.17
20	C	511	CLA	C3B-C2B-C1B	-4.01	102.44	107.17
20	b	614	CLA	C3C-C4C-NC	4.01	115.57	110.43
23	a	401	SQD	C1-O5-C5	-4.01	105.89	113.72
20	c	506	CLA	CHD-C1D-ND	-4.01	119.16	124.80
20	B	609	CLA	C1C-C2C-C3C	-4.01	102.77	106.98
20	b	614	CLA	CHC-C4B-NB	4.01	130.06	124.05
24	b	623	LMG	C9-C8-C7	-4.00	102.45	111.78
23	a	401	SQD	O6-C1-C2	4.00	114.35	108.27
20	C	507	CLA	CHD-C4C-C3C	-4.00	118.94	124.77
20	c	501	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
34	b	628	LMT	O5'-C5'-C4'	4.00	117.99	109.72
20	A	404	CLA	CMB-C2B-C1B	4.00	131.50	125.42
20	c	503	CLA	C2D-C1D-ND	4.00	114.08	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	l	101	SQD	O48-C23-C24	3.99	124.01	111.83
20	b	609	CLA	CAC-C3C-C4C	3.99	129.99	124.79
20	b	607	CLA	O2D-CGD-CBD	3.99	118.21	111.23
20	C	501	CLA	C2D-C1D-ND	3.99	114.08	110.13
20	c	506	CLA	CHC-C4B-NB	3.99	130.03	124.05
20	b	616	CLA	C1C-C2C-C3C	-3.99	102.79	106.98
20	c	505	CLA	C3B-C2B-C1B	-3.98	102.47	107.17
20	b	610	CLA	O2A-CGA-O1A	-3.97	113.69	123.63
20	B	616	CLA	CHD-C4C-C3C	-3.97	118.98	124.77
20	c	504	CLA	C3B-C2B-C1B	-3.97	102.49	107.17
20	b	606	CLA	O2D-CGD-O1D	-3.97	116.13	123.85
20	c	509	CLA	C4D-CHA-C1A	-3.96	116.52	121.24
20	c	504	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
20	B	610	CLA	CHC-C4B-NB	3.96	129.99	124.05
35	H	102	DGD	O1G-C1A-C2A	3.96	123.91	111.83
20	c	504	CLA	CMD-C2D-C1D	3.96	131.70	124.73
20	D	404	CLA	C4D-CHA-C1A	-3.96	116.52	121.24
20	b	616	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
20	b	617	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
20	a	404	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
20	B	602	CLA	CHC-C4B-NB	3.95	129.97	124.05
20	B	614	CLA	C4B-C3B-C2B	-3.95	102.39	107.30
34	c	523	LMT	O5B-C5B-C4B	3.95	116.81	109.70
20	b	604	CLA	CHA-C4D-ND	3.94	140.69	132.55
40	V	201	HEC	CBB-CAB-C3B	-3.94	119.55	127.43
20	C	509	CLA	CHC-C4B-NB	3.94	129.96	124.05
20	C	513	CLA	CHD-C4C-C3C	-3.94	119.03	124.77
20	B	607	CLA	CHD-C4C-NC	3.94	130.34	124.23
20	C	509	CLA	CHD-C4C-C3C	-3.94	119.03	124.77
20	c	511	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
20	b	607	CLA	C4-C3-C5	3.94	122.06	115.23
20	a	403	CLA	C2D-C1D-ND	3.93	114.02	110.13
20	C	510	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
20	C	504	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
20	C	503	CLA	CHC-C4B-NB	3.93	129.94	124.05
20	c	513	CLA	C2C-C1C-NC	3.93	114.11	109.98
20	a	407	CLA	CHC-C4B-NB	3.92	129.94	124.05
20	c	507	CLA	CMB-C2B-C1B	3.92	131.39	125.42
20	c	507	CLA	C4D-CHA-C1A	-3.92	116.56	121.24
20	c	510	CLA	C3B-C2B-C1B	-3.92	102.55	107.17
20	c	503	CLA	CHC-C4B-NB	3.92	129.93	124.05
20	c	512	CLA	CHD-C1D-ND	-3.92	119.29	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	604	CLA	CHD-C1D-ND	-3.92	119.29	124.80
20	B	612	CLA	C3D-C2D-C1D	-3.92	100.49	105.83
20	b	618	CLA	C4-C3-C5	3.91	122.02	115.23
20	b	617	CLA	O2D-CGD-CBD	3.91	118.07	111.23
20	A	404	CLA	CHD-C4C-C3C	-3.91	119.07	124.77
20	C	503	CLA	C2B-C1B-NB	3.91	114.38	110.33
20	B	616	CLA	CHA-C4D-ND	3.91	140.61	132.55
20	B	605	CLA	C4D-CHA-C1A	-3.91	116.59	121.24
20	b	613	CLA	C2B-C1B-NB	3.90	114.38	110.33
20	c	505	CLA	O2D-CGD-CBD	3.90	118.05	111.23
20	a	407	CLA	C3B-C2B-C1B	-3.90	102.57	107.17
20	C	505	CLA	O2D-CGD-CBD	3.90	118.05	111.23
20	B	607	CLA	C2D-C1D-ND	3.90	113.99	110.13
20	B	611	CLA	CMD-C2D-C1D	3.90	131.59	124.73
20	b	610	CLA	O2D-CGD-CBD	3.90	118.04	111.23
20	C	502	CLA	C2C-C1C-NC	3.89	114.07	109.98
20	C	507	CLA	C2C-C1C-NC	3.89	114.07	109.98
20	b	616	CLA	CHB-C4A-NA	3.89	130.02	124.40
20	C	513	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
20	c	512	CLA	CHD-C4C-NC	3.89	130.26	124.23
20	c	513	CLA	C2B-C1B-NB	3.89	114.36	110.33
20	c	506	CLA	O2D-CGD-CBD	3.89	118.03	111.23
20	C	501	CLA	CHD-C1D-ND	-3.88	119.33	124.80
20	b	604	CLA	C3D-C2D-C1D	-3.88	100.53	105.83
20	C	509	CLA	C1-C2-C3	-3.88	119.84	126.20
20	C	506	CLA	C1-C2-C3	-3.88	119.84	126.20
20	b	606	CLA	C4D-CHA-C1A	-3.88	116.62	121.24
20	B	614	CLA	C3B-C4B-NB	3.88	113.99	110.53
20	c	511	CLA	C2D-C1D-ND	3.88	113.96	110.13
20	b	616	CLA	CHD-C4C-C3C	-3.87	119.12	124.77
20	b	610	CLA	C3B-C2B-C1B	-3.87	102.61	107.17
20	B	610	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
20	b	611	CLA	CHC-C4B-NB	3.87	129.85	124.05
20	D	401	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
20	b	613	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
20	c	512	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
20	c	510	CLA	CHD-C4C-NC	3.86	130.22	124.23
20	b	605	CLA	C3B-C2B-C1B	-3.86	102.62	107.17
20	c	507	CLA	CHD-C1D-ND	-3.84	119.39	124.80
20	b	607	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
20	b	609	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
32	B	622	HTG	C1-C2-C3	3.84	118.06	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	615	CLA	CHD-C1D-ND	-3.84	119.40	124.80
23	A	406	SQD	C1-O5-C5	-3.84	106.23	113.72
20	b	606	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
20	B	613	CLA	C2D-C1D-ND	3.83	113.92	110.13
20	c	511	CLA	C2B-C1B-NB	3.83	114.30	110.33
20	C	512	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
20	C	501	CLA	C4D-CHA-C1A	-3.82	116.68	121.24
20	a	403	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
21	D	403	PHO	C1-C2-C3	-3.82	119.94	126.20
20	B	601	CLA	O2D-CGD-CBD	3.82	117.91	111.23
20	B	601	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
20	c	502	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
20	B	605	CLA	O2D-CGD-CBD	3.82	117.90	111.23
27	A	411	PL9	C20-C19-C21	3.81	121.84	115.23
20	b	611	CLA	CHD-C4C-C3C	-3.81	119.22	124.77
20	c	510	CLA	O2D-CGD-CBD	3.81	117.89	111.23
20	c	509	CLA	C2C-C1C-NC	3.81	113.98	109.98
20	c	507	CLA	C3D-C2D-C1D	-3.80	100.64	105.83
20	B	603	CLA	O2D-CGD-CBD	3.80	117.87	111.23
34	c	523	LMT	O5'-C5'-C4'	3.80	117.58	109.72
20	b	616	CLA	C2C-C1C-NC	3.80	113.97	109.98
32	B	631	HTG	C3-C4-C5	3.80	117.11	110.23
20	a	404	CLA	C2B-C1B-NB	3.79	114.26	110.33
20	B	615	CLA	CHD-C4C-C3C	-3.79	119.24	124.77
20	C	513	CLA	C4D-CHA-C1A	-3.79	116.72	121.24
20	a	404	CLA	C4D-CHA-C1A	-3.79	116.72	121.24
20	c	506	CLA	CMD-C2D-C1D	3.79	131.40	124.73
27	a	415	PL9	O1-C4-C3	-3.79	116.73	120.73
20	b	607	CLA	C3B-C2B-C1B	-3.79	102.70	107.17
20	c	510	CLA	C2C-C1C-NC	3.79	113.96	109.98
24	a	410	LMG	O7-C10-C11	3.79	119.67	111.48
20	B	603	CLA	CHD-C4C-C3C	-3.78	119.26	124.77
21	D	403	PHO	CED-O2D-CGD	3.78	124.49	115.92
20	D	404	CLA	C2C-C1C-NC	3.77	113.95	109.98
20	B	602	CLA	CMD-C2D-C1D	3.77	131.37	124.73
20	B	612	CLA	O2D-CGD-CBD	3.77	117.83	111.23
20	b	610	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
20	B	607	CLA	CHD-C1D-ND	-3.77	119.50	124.80
20	B	601	CLA	CHA-C4D-ND	3.77	140.32	132.55
20	C	502	CLA	C4B-C3B-C2B	-3.77	102.62	107.30
20	C	504	CLA	C2D-C1D-ND	3.77	113.85	110.13
20	c	512	CLA	C2C-C1C-NC	3.76	113.94	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	501	CLA	CHD-C4C-NC	3.76	130.07	124.23
20	D	401	CLA	C2D-C1D-ND	3.76	113.85	110.13
27	d	412	PL9	C40-C39-C41	3.76	121.75	115.23
20	c	507	CLA	CHC-C4B-NB	3.76	129.69	124.05
20	b	618	CLA	C3B-C4B-NB	3.76	113.88	110.53
20	b	611	CLA	C3B-C2B-C1B	-3.76	102.74	107.17
20	b	618	CLA	C2D-C1D-ND	3.75	113.84	110.13
20	B	612	CLA	C2C-C1C-NC	3.75	113.92	109.98
20	b	605	CLA	C2B-C1B-NB	3.75	114.22	110.33
20	c	504	CLA	O2D-CGD-CBD	3.75	117.79	111.23
20	b	603	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
20	c	512	CLA	C2D-C1D-ND	3.75	113.83	110.13
22	b	620	BCR	C29-C30-C25	3.75	115.88	110.44
20	A	401	CLA	C7-C6-C5	-3.74	103.28	113.26
20	a	403	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
22	d	405	BCR	C39-C30-C25	-3.74	104.38	110.24
20	b	617	CLA	CHA-C4D-ND	3.74	140.26	132.55
20	A	404	CLA	C2C-C1C-NC	3.74	113.91	109.98
20	C	506	CLA	C2C-C1C-NC	3.74	113.91	109.98
20	C	506	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
20	C	502	CLA	C1C-C2C-C3C	-3.73	103.05	106.98
20	b	606	CLA	C3C-C4C-NC	3.73	115.21	110.43
20	c	501	CLA	C3B-C4B-NB	3.73	113.86	110.53
20	c	510	CLA	C1D-CHD-C4C	-3.72	118.10	126.02
20	B	606	CLA	C1-C2-C3	-3.72	120.09	126.20
37	e	102	HEM	CBD-CAD-C3D	-3.72	102.25	112.53
20	B	602	CLA	O1D-CGD-CBD	-3.72	117.19	124.52
22	t	101	BCR	C33-C5-C6	-3.71	120.43	124.48
20	C	507	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
32	B	621	HTG	C1-O5-C5	3.71	119.22	112.56
21	D	403	PHO	OBD-CAD-C3D	-3.71	122.11	127.89
22	B	617	BCR	C24-C23-C22	-3.70	120.76	126.23
20	b	609	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
20	A	404	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
23	l	101	SQD	O47-C7-C8	3.70	119.48	111.48
20	d	402	CLA	C3B-C4B-NB	3.70	113.83	110.53
20	C	505	CLA	C3B-C2B-C1B	-3.70	102.81	107.17
20	C	513	CLA	O2D-CGD-CBD	3.70	117.69	111.23
24	c	519	LMG	O7-C10-C11	3.70	119.48	111.48
20	d	404	CLA	CHD-C1D-ND	-3.70	119.60	124.80
20	c	506	CLA	CHA-C4D-ND	3.69	140.17	132.55
23	A	412	SQD	O48-C23-C24	3.69	123.08	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	604	CLA	C1D-ND-C4D	-3.69	103.72	106.31
27	a	415	PL9	C30-C29-C31	3.69	121.63	115.23
20	c	510	CLA	CHA-C4D-ND	3.69	140.15	132.55
20	b	603	CLA	CHA-C4D-ND	3.68	140.15	132.55
20	D	402	CLA	C3B-C2B-C1B	-3.68	102.83	107.17
20	C	511	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
20	b	607	CLA	CHA-C4D-ND	3.68	140.15	132.55
20	C	513	CLA	CHC-C4B-NB	3.68	129.56	124.05
20	B	611	CLA	C3B-C2B-C1B	-3.67	102.84	107.17
20	a	407	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
20	b	613	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	B	620	LMG	O8-C28-C29	3.67	123.02	111.83
20	B	608	CLA	CBC-CAC-C3C	-3.66	102.49	112.42
27	a	415	PL9	C53-C6-C1	3.66	122.78	115.28
20	A	401	CLA	CHD-C4C-C3C	-3.66	119.44	124.77
20	c	513	CLA	CHD-C1D-ND	-3.66	119.65	124.80
20	B	607	CLA	C4D-CHA-C1A	-3.66	116.88	121.24
21	a	405	PHO	O2D-CGD-O1D	-3.66	116.72	123.85
32	b	602	HTG	C1'-S1-C1	3.66	108.35	100.45
32	b	601	HTG	C1'-S1-C1	3.66	108.35	100.45
20	d	404	CLA	C3D-C2D-C1D	-3.66	100.84	105.83
20	C	502	CLA	C3D-C2D-C1D	-3.66	100.84	105.83
22	b	619	BCR	C33-C5-C6	-3.65	120.50	124.48
20	b	606	CLA	CHA-C4D-ND	3.65	140.09	132.55
22	d	405	BCR	C29-C30-C25	3.65	115.75	110.44
20	d	404	CLA	C3B-C4B-NB	3.65	113.79	110.53
20	d	402	CLA	C2A-C1A-CHA	-3.65	117.54	123.87
20	b	604	CLA	C1-O2A-CGA	3.64	125.47	116.65
20	D	402	CLA	CHD-C4C-NC	3.64	129.88	124.23
20	b	615	CLA	CAC-C3C-C4C	3.64	129.52	124.79
20	B	610	CLA	CED-O2D-CGD	3.64	124.17	115.92
20	c	508	CLA	CMB-C2B-C1B	3.64	130.96	125.42
20	a	404	CLA	C2D-C1D-ND	3.64	113.72	110.13
20	C	512	CLA	C2B-C1B-NB	3.63	114.09	110.33
20	C	502	CLA	CMD-C2D-C1D	3.63	131.13	124.73
22	B	618	BCR	C29-C30-C25	3.63	115.72	110.44
20	C	512	CLA	C2D-C1D-ND	3.63	113.72	110.13
20	b	603	CLA	C2C-C1C-NC	3.63	113.80	109.98
20	C	502	CLA	CMB-C2B-C1B	3.62	130.94	125.42
21	D	403	PHO	C4B-NB-C1B	-3.62	103.54	108.82
20	C	501	CLA	C2B-C1B-NB	3.62	114.08	110.33
35	c	515	DGD	O2G-C1B-C2B	3.62	119.31	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	h	101	DGD	O2G-C1B-C2B	3.62	119.31	111.48
20	B	603	CLA	C3B-C2B-C1B	-3.62	102.91	107.17
20	C	507	CLA	C2B-C1B-NB	3.62	114.08	110.33
20	c	508	CLA	C3D-C2D-C1D	-3.62	100.90	105.83
20	c	511	CLA	C4D-CHA-C1A	-3.62	116.93	121.24
20	b	618	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
20	B	601	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
20	c	501	CLA	CMB-C2B-C1B	3.61	130.92	125.42
20	B	607	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
35	c	517	DGD	O1G-C1A-O1A	-3.61	114.60	123.63
20	b	613	CLA	CHC-C4B-NB	3.61	129.46	124.05
20	B	603	CLA	CHA-C4D-ND	3.61	139.99	132.55
20	C	512	CLA	CHA-C4D-ND	3.60	139.99	132.55
20	B	613	CLA	C3B-C2B-C1B	-3.60	102.92	107.17
23	b	622	SQD	C3-C4-C5	3.60	116.77	110.23
20	C	507	CLA	CHA-C4D-ND	3.60	139.98	132.55
20	B	602	CLA	C3D-C2D-C1D	-3.60	100.92	105.83
20	B	604	CLA	C3B-C2B-C1B	-3.60	102.93	107.17
20	c	505	CLA	CHD-C1D-ND	-3.60	119.74	124.80
20	A	401	CLA	CMD-C2D-C3D	3.60	135.94	127.69
20	a	403	CLA	C2C-C1C-NC	3.60	113.76	109.98
20	b	603	CLA	CMB-C2B-C1B	3.60	130.89	125.42
20	b	617	CLA	CHC-C4B-NB	3.59	129.44	124.05
36	d	406	LHG	O8-C23-C24	3.59	122.79	111.83
20	b	614	CLA	CMC-C2C-C1C	3.59	130.65	125.03
20	a	404	CLA	C4A-NA-C1A	3.59	108.32	106.68
20	B	603	CLA	C2B-C1B-NB	3.59	114.05	110.33
21	A	403	PHO	O2D-CGD-O1D	-3.59	116.86	123.85
20	B	610	CLA	C3C-C4C-NC	3.59	115.03	110.43
20	c	509	CLA	CAC-C3C-C4C	3.59	129.46	124.79
20	b	617	CLA	CHD-C4C-NC	3.59	129.79	124.23
20	A	401	CLA	C2D-C1D-ND	3.58	113.67	110.13
32	c	520	HTG	C1'-S1-C1	3.58	108.19	100.45
20	b	608	CLA	C1-O2A-CGA	3.58	125.32	116.65
20	c	503	CLA	C3B-C2B-C1B	-3.58	102.95	107.17
20	D	404	CLA	O2D-CGD-CBD	3.58	117.48	111.23
20	C	513	CLA	CHA-C4D-ND	3.57	139.92	132.55
20	b	609	CLA	C3B-C2B-C1B	-3.57	102.96	107.17
20	b	614	CLA	C3B-C2B-C1B	-3.57	102.96	107.17
22	C	514	BCR	C38-C26-C25	-3.57	120.59	124.48
20	B	611	CLA	C1D-CHD-C4C	-3.57	118.43	126.02
20	b	607	CLA	C3C-C4C-NC	3.57	115.00	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	511	CLA	CHD-C4C-C3C	-3.57	119.57	124.77
20	b	613	CLA	CMD-C2D-C1D	3.57	131.01	124.73
20	c	503	CLA	CHA-C4D-ND	3.57	139.91	132.55
36	E	103	LHG	O7-C7-C8	3.56	122.69	111.83
20	c	510	CLA	C4-C3-C5	3.56	121.41	115.23
22	k	101	BCR	C7-C8-C9	-3.56	120.97	126.23
20	B	608	CLA	C4D-CHA-C1A	-3.56	117.00	121.24
23	b	622	SQD	O6-C1-C2	3.55	113.67	108.27
23	b	622	SQD	O5-C1-C2	-3.55	103.07	110.37
20	c	508	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
20	d	402	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
20	B	604	CLA	C3D-C2D-C1D	-3.55	100.98	105.83
20	b	618	CLA	CBC-CAC-C3C	-3.55	102.79	112.42
38	H	101	RRX	C7-C8-C9	-3.55	120.98	126.23
20	b	617	CLA	CMC-C2C-C1C	3.55	130.58	125.03
20	B	605	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
20	B	601	CLA	C4A-NA-C1A	3.54	108.30	106.68
36	d	406	LHG	O8-C23-O10	-3.54	114.77	123.63
20	b	607	CLA	CHD-C1D-ND	-3.54	119.82	124.80
20	B	615	CLA	C2C-C1C-NC	3.54	113.70	109.98
24	B	620	LMG	O7-C10-O9	-3.54	115.43	123.70
20	b	612	CLA	C1D-CHD-C4C	-3.54	118.51	126.02
20	B	606	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
20	C	512	CLA	C2C-C1C-NC	3.53	113.69	109.98
20	b	603	CLA	C3D-C2D-C1D	-3.53	101.01	105.83
20	b	618	CLA	C3B-C2B-C1B	-3.53	103.01	107.17
20	b	608	CLA	C4D-CHA-C1A	-3.53	117.04	121.24
20	D	404	CLA	CAC-C3C-C4C	3.52	129.38	124.79
20	c	503	CLA	C4-C3-C5	3.52	121.34	115.23
20	B	615	CLA	C3D-C2D-C1D	-3.52	101.03	105.83
20	B	610	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
20	C	507	CLA	CHD-C4C-NC	3.52	129.68	124.23
20	c	512	CLA	C3D-C2D-C1D	-3.51	101.04	105.83
20	b	618	CLA	CAC-C3C-C4C	3.51	129.36	124.79
20	d	402	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
20	B	613	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
20	b	610	CLA	CHA-C4D-ND	3.50	139.78	132.55
20	b	605	CLA	C4-C3-C5	3.50	121.31	115.23
20	C	506	CLA	C3D-C2D-C1D	-3.50	101.06	105.83
22	b	620	BCR	C38-C26-C25	-3.50	120.67	124.48
21	a	406	PHO	C4B-NB-C1B	-3.49	103.72	108.82
22	B	619	BCR	C2-C1-C6	3.49	115.51	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	401	CLA	C3B-C2B-C1B	-3.49	103.05	107.17
21	A	403	PHO	C4B-NB-C1B	-3.49	103.73	108.82
20	c	512	CLA	C4D-CHA-C1A	-3.49	117.08	121.24
20	b	617	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
20	C	507	CLA	CHC-C4B-NB	3.49	129.28	124.05
20	B	602	CLA	CMB-C2B-C1B	3.49	130.73	125.42
20	B	602	CLA	C2B-C1B-NB	3.49	113.94	110.33
24	C	519	LMG	O8-C28-C29	3.48	122.46	111.83
20	B	615	CLA	C2A-C1A-CHA	-3.48	117.82	123.87
20	B	606	CLA	CHA-C4D-ND	3.48	139.74	132.55
20	B	607	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
20	B	608	CLA	C2A-C1A-CHA	-3.48	117.83	123.87
20	A	404	CLA	CHD-C1D-ND	-3.48	119.91	124.80
20	B	611	CLA	C4C-C3C-C2C	-3.48	101.83	106.89
20	b	616	CLA	C3B-C4B-NB	3.48	113.64	110.53
20	d	404	CLA	C4-C3-C5	3.48	121.26	115.23
20	C	510	CLA	C3B-C2B-C1B	-3.48	103.07	107.17
40	V	201	HEC	CBD-CAD-C3D	-3.47	102.93	112.53
20	B	606	CLA	C1D-ND-C4D	-3.47	103.88	106.31
20	b	610	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
20	b	616	CLA	CHC-C4B-NB	3.47	129.26	124.05
20	b	618	CLA	C2C-C1C-NC	3.47	113.63	109.98
20	a	403	CLA	C4D-CHA-C1A	-3.47	117.11	121.24
20	a	404	CLA	CHC-C4B-NB	3.47	129.25	124.05
20	c	513	CLA	CHC-C4B-NB	3.47	129.25	124.05
20	c	506	CLA	CHD-C4C-NC	3.47	129.61	124.23
20	c	511	CLA	CHC-C4B-NB	3.47	129.25	124.05
38	H	101	RRX	C10-C11-C12	-3.47	113.16	123.20
20	d	403	CLA	CBC-CAC-C3C	-3.46	103.03	112.42
23	l	101	SQD	C1-O5-C5	-3.46	106.96	113.72
20	C	508	CLA	C3D-C4D-ND	3.46	115.62	109.99
20	B	605	CLA	CHA-C4D-ND	3.46	139.69	132.55
20	D	404	CLA	CHD-C1D-ND	-3.46	119.94	124.80
20	C	504	CLA	C3B-C2B-C1B	-3.45	103.10	107.17
20	c	505	CLA	CAC-C3C-C4C	3.45	129.28	124.79
20	B	609	CLA	O2D-CGD-CBD	3.45	117.27	111.23
20	b	608	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
20	c	502	CLA	C1D-CHD-C4C	-3.45	118.68	126.02
20	B	610	CLA	O2D-CGD-CBD	3.45	117.26	111.23
20	c	509	CLA	CHC-C4B-NB	3.45	129.22	124.05
20	d	402	CLA	C4D-CHA-C1A	-3.45	117.13	121.24
20	B	614	CLA	C2B-C1B-NB	3.44	113.90	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	f	101	SQD	O48-C23-C24	3.44	122.33	111.83
20	C	510	CLA	CHD-C1D-ND	-3.44	119.96	124.80
20	c	502	CLA	CHC-C4B-NB	3.44	129.21	124.05
20	B	606	CLA	C3D-C2D-C1D	-3.44	101.14	105.83
20	C	510	CLA	C4D-CHA-C1A	-3.43	117.15	121.24
20	a	407	CLA	CHD-C1D-ND	-3.43	119.97	124.80
40	v	201	HEC	C2A-C1A-NA	-3.43	107.01	110.32
20	c	513	CLA	O2D-CGD-CBD	3.43	117.23	111.23
20	c	502	CLA	CHD-C4C-C3C	-3.43	119.77	124.77
20	C	502	CLA	C3B-C4B-NB	3.43	113.59	110.53
20	B	604	CLA	CHC-C1C-NC	-3.43	119.15	124.31
20	c	502	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
20	b	605	CLA	CHD-C1D-ND	-3.42	119.98	124.80
20	b	611	CLA	C4A-NA-C1A	3.42	108.24	106.68
20	a	407	CLA	C4D-CHA-C1A	-3.42	117.17	121.24
34	b	627	LMT	O5B-C5B-C6B	3.41	114.90	106.44
23	b	622	SQD	O7-S-C6	3.41	111.85	106.76
20	D	401	CLA	CHA-C4D-ND	3.41	139.59	132.55
20	B	603	CLA	C3D-C2D-C1D	-3.41	101.18	105.83
20	B	601	CLA	CMB-C2B-C1B	3.41	130.61	125.42
34	J	103	LMT	C3'-C4'-C5'	-3.41	104.05	110.23
20	c	510	CLA	C4A-NA-C1A	3.41	108.23	106.68
20	c	505	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
22	b	619	BCR	C23-C22-C21	-3.40	113.66	119.01
20	C	506	CLA	C1D-CHD-C4C	-3.40	118.79	126.02
24	c	519	LMG	O8-C28-C29	3.40	122.20	111.83
20	C	504	CLA	CHD-C4C-NC	3.40	129.50	124.23
20	c	511	CLA	CMC-C2C-C1C	3.40	130.35	125.03
20	C	501	CLA	C3B-C2B-C1B	-3.40	103.16	107.17
20	c	509	CLA	C1C-C2C-C3C	-3.40	103.41	106.98
22	a	408	BCR	C29-C30-C25	3.39	115.37	110.44
20	b	618	CLA	CHD-C4C-NC	3.39	129.49	124.23
22	b	621	BCR	C38-C26-C25	-3.39	120.78	124.48
20	c	509	CLA	C1-C2-C3	-3.39	120.64	126.20
20	b	605	CLA	CHA-C4D-ND	3.39	139.54	132.55
20	c	513	CLA	CHD-C4C-NC	3.39	129.49	124.23
20	C	511	CLA	CHC-C4B-NB	3.39	129.13	124.05
22	T	101	BCR	C35-C13-C12	3.38	123.26	118.09
23	F	101	SQD	O9-S-C6	3.38	111.81	106.76
20	c	509	CLA	CHD-C4C-NC	3.38	129.48	124.23
20	b	611	CLA	CHA-C4D-ND	3.38	139.52	132.55
20	d	403	CLA	C3D-C2D-C1D	-3.38	101.22	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	505	CLA	CHD-C4C-NC	3.38	129.47	124.23
24	C	519	LMG	O7-C10-C11	3.38	118.79	111.48
20	d	403	CLA	CHC-C4B-NB	3.37	129.11	124.05
40	V	201	HEC	CBC-CAC-C3C	-3.37	120.69	127.43
20	A	404	CLA	CHB-C4A-NA	3.37	129.27	124.40
24	b	623	LMG	O8-C28-C29	3.37	122.12	111.83
20	a	404	CLA	CMC-C2C-C1C	3.37	130.30	125.03
20	B	613	CLA	CHC-C4B-NB	3.37	129.10	124.05
20	C	505	CLA	CHA-C4D-ND	3.37	139.50	132.55
20	b	605	CLA	CMC-C2C-C1C	3.37	130.30	125.03
20	C	512	CLA	C3D-C2D-C1D	-3.37	101.23	105.83
20	D	404	CLA	C3D-C2D-C1D	-3.37	101.23	105.83
20	B	609	CLA	C3B-C4B-NB	3.37	113.54	110.53
22	K	102	BCR	C24-C23-C22	-3.37	121.26	126.23
23	F	101	SQD	C1-C2-C3	-3.37	102.93	110.01
20	c	511	CLA	C1-O2A-CGA	3.36	124.80	116.65
20	B	608	CLA	CAC-C3C-C4C	3.36	129.16	124.79
20	B	604	CLA	C4D-CHA-C1A	-3.36	117.23	121.24
20	b	603	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
20	B	611	CLA	CHA-C4D-ND	3.36	139.48	132.55
22	K	102	BCR	C38-C26-C25	-3.36	120.82	124.48
20	B	609	CLA	C3B-C2B-C1B	-3.36	103.21	107.17
32	B	631	HTG	O5-C5-C4	3.36	115.75	109.70
20	b	612	CLA	CHA-C4D-ND	3.36	139.47	132.55
22	c	514	BCR	C32-C1-C6	-3.36	104.98	110.24
20	d	404	CLA	CMD-C2D-C1D	3.35	130.64	124.73
20	C	505	CLA	C4D-CHA-C1A	-3.35	117.24	121.24
20	C	502	CLA	O2D-CGD-CBD	3.35	117.09	111.23
20	b	617	CLA	C3B-C2B-C1B	-3.35	103.22	107.17
22	C	515	BCR	C7-C8-C9	-3.35	121.28	126.23
23	A	406	SQD	O9-S-C6	3.35	111.75	106.76
20	a	404	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
20	c	506	CLA	C4D-CHA-C1A	-3.35	117.25	121.24
38	H	101	RRX	C16-C15-C14	-3.35	116.67	123.52
20	C	503	CLA	CHD-C1D-ND	-3.34	120.11	124.80
20	B	602	CLA	C2C-C1C-NC	3.34	113.49	109.98
20	b	608	CLA	C2B-C1B-NB	3.34	113.78	110.33
20	D	404	CLA	CHA-C4D-ND	3.33	139.43	132.55
20	c	506	CLA	C1D-CHD-C4C	-3.33	118.93	126.02
20	B	604	CLA	C2A-C1A-CHA	-3.33	118.09	123.87
20	C	502	CLA	C1D-ND-C4D	-3.33	103.98	106.31
34	B	625	LMT	O5'-C5'-C4'	3.33	115.70	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	504	CLA	CHD-C4C-NC	3.33	129.39	124.23
20	B	602	CLA	C3B-C2B-C1B	-3.33	103.25	107.17
20	B	604	CLA	CHD-C4C-NC	3.32	129.38	124.23
20	C	506	CLA	CHD-C1D-ND	-3.32	120.13	124.80
20	c	509	CLA	C3B-C4B-NB	3.32	113.49	110.53
20	c	505	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
20	c	512	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
20	a	407	CLA	C3D-C2D-C1D	-3.31	101.31	105.83
20	a	407	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
20	b	609	CLA	C2B-C1B-NB	3.31	113.76	110.33
20	c	505	CLA	C2B-C1B-NB	3.31	113.76	110.33
20	c	508	CLA	O2D-CGD-CBD	3.31	117.01	111.23
20	c	509	CLA	CHD-C1D-ND	-3.31	120.15	124.80
20	C	511	CLA	CMB-C2B-C1B	3.31	130.45	125.42
20	c	504	CLA	C4B-C3B-C2B	-3.31	103.19	107.30
24	c	518	LMG	C4-C3-C2	3.30	116.63	110.83
20	d	403	CLA	O2D-CGD-CBD	3.30	117.00	111.23
27	A	411	PL9	C30-C29-C31	3.30	120.96	115.23
20	b	616	CLA	CHD-C4C-NC	3.30	129.35	124.23
20	B	614	CLA	C2A-C1A-CHA	-3.30	118.14	123.87
22	T	101	BCR	C38-C26-C25	-3.30	120.89	124.48
20	c	503	CLA	CHD-C1D-ND	-3.30	120.16	124.80
23	b	622	SQD	O48-C23-C24	3.30	121.88	111.83
20	b	605	CLA	CHC-C4B-NB	3.30	128.99	124.05
27	d	412	PL9	O1-C4-C3	-3.29	117.26	120.73
20	B	614	CLA	O2A-CGA-CBA	3.29	121.87	111.83
20	b	611	CLA	CMB-C2B-C1B	3.29	130.43	125.42
20	c	507	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
21	D	403	PHO	C4D-CHA-CBD	3.29	110.03	108.45
20	b	606	CLA	C3B-C2B-C1B	-3.29	103.29	107.17
20	c	501	CLA	CHD-C1D-ND	-3.28	120.18	124.80
20	C	509	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
20	b	604	CLA	C16-C17-C18	-3.28	101.28	115.94
20	D	404	CLA	CMD-C2D-C1D	3.28	130.51	124.73
20	b	615	CLA	C2B-C1B-NB	3.28	113.73	110.33
20	C	513	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
40	V	201	HEC	C4D-ND-C1D	3.28	111.17	105.82
20	b	614	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
20	B	602	CLA	CHA-C4D-ND	3.28	139.31	132.55
20	c	504	CLA	CAC-C3C-C4C	3.28	129.05	124.79
20	c	506	CLA	CMB-C2B-C1B	3.28	130.41	125.42
20	C	507	CLA	C4-C3-C5	3.28	120.92	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	512	CLA	CMD-C2D-C1D	3.28	130.50	124.73
20	c	513	CLA	C3D-C2D-C1D	-3.27	101.36	105.83
20	b	604	CLA	C1D-CHD-C4C	-3.27	119.06	126.02
27	a	415	PL9	C3-C4-C5	3.27	122.65	118.57
20	D	404	CLA	C1D-ND-C4D	-3.27	104.02	106.31
20	c	501	CLA	CMD-C2D-C1D	3.27	130.49	124.73
20	a	407	CLA	C2B-C1B-NB	3.27	113.72	110.33
20	C	501	CLA	CHD-C4C-NC	3.27	129.30	124.23
20	b	616	CLA	C3D-C2D-C1D	-3.27	101.38	105.83
20	B	613	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
20	C	503	CLA	C3D-C2D-C1D	-3.26	101.38	105.83
35	c	517	DGD	O1G-C1A-C2A	3.26	121.79	111.83
20	c	507	CLA	CHA-C4D-ND	3.26	139.28	132.55
20	b	611	CLA	C4D-CHA-C1A	-3.26	117.35	121.24
20	c	505	CLA	C3D-C2D-C1D	-3.26	101.38	105.83
20	c	511	CLA	C3D-C2D-C1D	-3.26	101.38	105.83
20	B	605	CLA	CHC-C4B-NB	3.26	128.94	124.05
22	a	408	BCR	C15-C16-C17	-3.26	116.85	123.52
20	C	508	CLA	CHD-C4C-C3C	-3.26	120.02	124.77
20	C	507	CLA	CBC-CAC-C3C	-3.26	103.59	112.42
20	a	403	CLA	CHA-C4D-ND	3.26	139.27	132.55
20	A	402	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
35	C	517	DGD	O2G-C1B-C2B	3.26	118.52	111.48
20	D	401	CLA	C2A-C1A-CHA	-3.25	118.22	123.87
20	b	612	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
40	v	201	HEC	CBD-CAD-C3D	-3.25	103.54	112.53
20	B	615	CLA	CHB-C4A-NA	3.25	129.09	124.40
20	C	504	CLA	C4D-CHA-C1A	-3.25	117.37	121.24
20	B	615	CLA	CAC-C3C-C4C	3.25	129.01	124.79
20	B	611	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
20	c	511	CLA	CHA-C4D-ND	3.25	139.25	132.55
27	d	412	PL9	C3-C4-C5	3.25	122.62	118.57
22	B	617	BCR	C33-C5-C6	-3.24	120.95	124.48
20	A	404	CLA	C3D-C2D-C1D	-3.24	101.41	105.83
20	D	401	CLA	C1D-CHD-C4C	-3.24	119.14	126.02
27	a	415	PL9	C25-C24-C26	3.24	120.84	115.23
20	b	604	CLA	CMC-C2C-C1C	3.24	130.09	125.03
20	B	610	CLA	C2D-C1D-ND	3.24	113.33	110.13
35	c	516	DGD	O2G-C1B-C2B	3.23	118.48	111.48
20	C	504	CLA	C4B-C3B-C2B	-3.23	103.28	107.30
20	C	502	CLA	CHD-C4C-NC	3.23	129.25	124.23
22	B	619	BCR	C23-C24-C25	-3.23	118.36	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	T	101	BCR	C23-C24-C25	-3.23	118.36	127.00
20	B	615	CLA	CMB-C2B-C1B	3.23	130.34	125.42
20	b	603	CLA	C1-O2A-CGA	3.23	124.48	116.65
20	b	604	CLA	CMB-C2B-C3B	3.23	134.15	126.55
20	c	503	CLA	CHD-C4C-NC	3.23	129.24	124.23
32	B	621	HTG	C1'-S1-C1	3.23	107.43	100.45
20	b	615	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
34	m	101	LMT	C1'-O5'-C5'	3.23	120.03	113.72
22	K	102	BCR	C34-C9-C8	3.22	123.01	118.09
22	D	405	BCR	C38-C26-C25	-3.22	120.97	124.48
20	b	610	CLA	CED-O2D-CGD	3.22	123.22	115.92
22	b	620	BCR	C8-C7-C6	-3.22	118.39	127.00
35	c	515	DGD	O5D-C6D-C5D	-3.21	102.18	109.42
20	C	509	CLA	C4-C3-C5	3.21	120.80	115.23
20	b	606	CLA	C2B-C1B-NB	3.21	113.65	110.33
20	B	609	CLA	CHD-C4C-NC	3.21	129.20	124.23
20	B	603	CLA	O2A-CGA-O1A	-3.20	115.61	123.63
20	C	501	CLA	C2A-C1A-CHA	-3.20	118.31	123.87
20	b	618	CLA	O1D-CGD-CBD	-3.20	118.20	124.52
20	C	504	CLA	CHA-C4D-ND	3.20	139.15	132.55
20	b	608	CLA	CHD-C1D-ND	-3.20	120.30	124.80
20	B	601	CLA	C4D-CHA-C1A	-3.20	117.43	121.24
37	E	104	HEM	CMD-C2D-C1D	3.20	130.03	125.03
20	d	403	CLA	C2B-C1B-NB	3.20	113.64	110.33
20	B	615	CLA	CMD-C2D-C1D	3.20	130.36	124.73
20	c	505	CLA	CMC-C2C-C1C	3.20	130.03	125.03
20	B	613	CLA	C3D-C2D-C1D	-3.19	101.47	105.83
27	D	412	PL9	C10-C9-C11	3.19	120.77	115.23
20	b	609	CLA	CHA-C4D-ND	3.19	139.14	132.55
32	b	625	HTG	C1-O5-C5	3.19	118.29	112.56
20	b	605	CLA	C4D-CHA-C1A	-3.19	117.44	121.24
20	c	510	CLA	C1D-ND-C4D	-3.19	104.07	106.31
20	D	402	CLA	CHD-C1D-ND	-3.19	120.31	124.80
20	b	612	CLA	CHB-C1B-NB	-3.19	119.26	124.05
20	C	502	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
20	B	606	CLA	C3B-C4B-NB	3.19	113.38	110.53
20	C	504	CLA	CAC-C3C-C4C	3.19	128.94	124.79
23	A	412	SQD	C1-C2-C3	-3.19	103.31	110.01
36	L	101	LHG	O4-P-O5	3.18	127.26	112.44
20	b	608	CLA	CHC-C4B-NB	3.18	128.83	124.05
22	B	619	BCR	C33-C5-C6	-3.18	121.01	124.48
20	C	511	CLA	O2D-CGD-CBD	3.18	116.79	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	401	CLA	C3D-C2D-C1D	-3.18	101.49	105.83
20	b	617	CLA	C1-O2A-CGA	3.18	124.34	116.65
20	C	505	CLA	CHC-C4B-NB	3.18	128.81	124.05
20	b	618	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
20	C	502	CLA	CHA-C4D-ND	3.17	139.09	132.55
20	B	611	CLA	C3C-C4C-NC	3.17	114.49	110.43
34	b	627	LMT	C3'-C4'-C5'	3.17	117.96	110.93
20	D	401	CLA	C3D-C2D-C1D	-3.17	101.50	105.83
20	C	507	CLA	C1-O2A-CGA	3.17	124.31	116.65
20	b	616	CLA	O2A-CGA-O1A	-3.17	115.71	123.63
20	A	401	CLA	C2C-C1C-NC	3.17	113.31	109.98
24	C	519	LMG	O1-C7-C8	-3.17	103.12	110.82
20	D	402	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
32	B	632	HTG	C1'-S1-C1	3.16	107.28	100.45
20	C	508	CLA	C4-C3-C5	3.16	120.72	115.23
20	B	601	CLA	C1-O2A-CGA	3.16	124.31	116.65
24	c	518	LMG	O1-C1-C2	3.16	113.08	108.27
20	c	510	CLA	CHD-C1D-ND	-3.16	120.35	124.80
32	v	210	HTG	C1-C2-C3	-3.16	104.37	110.55
20	b	603	CLA	CHD-C4C-NC	3.16	129.13	124.23
20	d	402	CLA	C2B-C1B-NB	3.16	113.60	110.33
20	B	609	CLA	C1D-ND-C4D	-3.16	104.10	106.31
20	C	505	CLA	C3D-C2D-C1D	-3.15	101.53	105.83
20	b	618	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
20	B	608	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
20	c	511	CLA	CHD-C4C-NC	3.15	129.11	124.23
20	d	402	CLA	C2D-C1D-ND	3.15	113.24	110.13
20	D	401	CLA	CMD-C2D-C1D	3.14	130.26	124.73
20	D	402	CLA	C2B-C1B-NB	3.14	113.59	110.33
22	T	101	BCR	C7-C8-C9	-3.14	121.59	126.23
20	C	503	CLA	CMC-C2C-C1C	3.14	129.94	125.03
20	B	606	CLA	C3C-C4C-NC	3.14	114.45	110.43
20	D	401	CLA	C3B-C4B-NB	3.14	113.33	110.53
24	j	101	LMG	O2-C2-C1	-3.14	102.60	110.08
20	B	609	CLA	CAC-C3C-C4C	3.14	128.87	124.79
20	d	403	CLA	C3C-C4C-NC	3.13	114.45	110.43
20	c	507	CLA	O2A-CGA-CBA	3.13	121.39	111.83
20	B	612	CLA	CAC-C3C-C4C	3.13	128.87	124.79
20	c	502	CLA	C1-C2-C3	-3.13	121.06	126.20
20	c	512	CLA	CBC-CAC-C3C	-3.13	103.93	112.42
20	C	513	CLA	C2D-C1D-ND	3.13	113.22	110.13
20	c	513	CLA	CMC-C2C-C1C	3.13	129.92	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	402	CLA	CBC-CAC-C3C	-3.13	103.95	112.42
20	c	509	CLA	CMC-C2C-C1C	3.12	129.91	125.03
20	B	608	CLA	C3B-C2B-C1B	-3.12	103.49	107.17
22	C	514	BCR	C15-C14-C13	-3.12	122.90	127.28
20	b	605	CLA	C3D-C2D-C1D	-3.12	101.57	105.83
20	B	612	CLA	C3B-C2B-C1B	-3.12	103.49	107.17
36	d	408	LHG	O7-C7-O9	-3.12	116.41	123.70
20	c	510	CLA	C3D-C2D-C1D	-3.12	101.58	105.83
22	b	621	BCR	C33-C5-C6	-3.12	121.08	124.48
20	C	509	CLA	C3B-C4B-NB	3.12	113.31	110.53
20	c	505	CLA	CHD-C4C-NC	3.11	129.06	124.23
21	a	406	PHO	O2D-CGD-O1D	-3.11	117.79	123.85
34	b	627	LMT	C4B-C3B-C2B	3.11	116.30	110.83
38	x	101	RRX	C16-C17-C18	-3.11	122.91	127.28
20	D	402	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
27	d	412	PL9	C7-C8-C9	-3.11	121.47	126.83
20	b	616	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
22	B	617	BCR	C20-C21-C22	-3.11	122.92	127.28
20	B	613	CLA	C2A-C1A-CHA	-3.10	118.48	123.87
22	C	515	BCR	C23-C24-C25	-3.10	118.71	127.00
22	t	101	BCR	C12-C13-C14	-3.10	114.13	119.01
20	C	502	CLA	CAC-C3C-C4C	3.10	128.82	124.79
22	d	405	BCR	C38-C26-C25	-3.10	121.10	124.48
20	c	505	CLA	CHC-C4B-NB	3.10	128.69	124.05
24	B	620	LMG	C9-C8-C7	-3.10	104.57	111.78
20	C	507	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
20	C	512	CLA	C4-C3-C5	3.09	120.60	115.23
21	D	403	PHO	O2D-CGD-O1D	-3.09	117.83	123.85
20	c	511	CLA	C4-C3-C5	3.09	120.60	115.23
35	d	416	DGD	O1G-C1A-C2A	3.09	121.26	111.83
20	B	605	CLA	C2D-C1D-ND	3.09	113.18	110.13
36	E	103	LHG	O8-C23-C24	3.09	121.25	111.83
20	C	509	CLA	O2A-CGA-CBA	3.09	121.24	111.83
27	A	411	PL9	C3-C4-C5	3.08	122.42	118.57
20	D	404	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
20	b	612	CLA	CAC-C3C-C4C	3.08	128.80	124.79
20	b	612	CLA	C3B-C4B-NB	3.08	113.28	110.53
20	b	604	CLA	C2A-C1A-CHA	-3.08	118.52	123.87
20	B	609	CLA	CHA-C4D-ND	3.08	138.91	132.55
20	b	607	CLA	C1-C2-C3	-3.08	121.15	126.20
20	B	611	CLA	CAA-CBA-CGA	-3.08	104.47	113.21
20	c	507	CLA	CMD-C2D-C1D	3.08	130.14	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	606	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
20	B	603	CLA	CHD-C1D-ND	-3.07	120.48	124.80
27	D	412	PL9	C22-C23-C24	-3.07	120.59	127.62
20	d	403	CLA	C3B-C2B-C1B	-3.07	103.55	107.17
20	c	513	CLA	CHA-C4D-ND	3.07	138.88	132.55
22	t	101	BCR	C15-C16-C17	-3.07	117.24	123.52
20	C	504	CLA	C1-C2-C3	-3.07	121.17	126.20
20	C	511	CLA	CHA-C4D-ND	3.07	138.88	132.55
20	b	615	CLA	CHD-C4C-NC	3.07	128.98	124.23
20	b	606	CLA	C3B-C4B-NB	3.06	113.27	110.53
20	B	611	CLA	CMB-C2B-C1B	3.06	130.08	125.42
20	C	510	CLA	CHC-C4B-NB	3.06	128.64	124.05
20	b	604	CLA	CHC-C4B-NB	3.06	128.64	124.05
35	c	517	DGD	O2G-C1B-C2B	3.06	118.10	111.48
20	a	403	CLA	C4-C3-C5	3.06	120.53	115.23
22	a	408	BCR	C7-C8-C9	-3.06	121.71	126.23
32	b	624	HTG	O5-C1-C2	-3.05	106.11	110.32
20	B	613	CLA	O2D-CGD-CBD	3.05	116.56	111.23
20	C	511	CLA	C4D-CHA-C1A	-3.05	117.61	121.24
20	B	603	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
20	c	507	CLA	CHD-C4C-NC	3.05	128.96	124.23
22	A	405	BCR	C38-C26-C25	-3.05	121.16	124.48
20	C	506	CLA	CHC-C4B-NB	3.05	128.62	124.05
20	C	506	CLA	CAC-C3C-C4C	3.05	128.76	124.79
20	b	614	CLA	O2D-CGD-CBD	3.05	116.56	111.23
20	B	604	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
34	m	102	LMT	C3'-C4'-C5'	-3.05	104.18	110.93
20	B	601	CLA	CHD-C1D-ND	-3.05	120.52	124.80
20	d	402	CLA	C1D-CHD-C4C	-3.04	119.55	126.02
20	B	604	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
20	b	608	CLA	C3B-C2B-C1B	-3.04	103.58	107.17
22	b	619	BCR	C11-C10-C9	-3.04	123.01	127.28
20	c	502	CLA	C1D-ND-C4D	-3.04	104.18	106.31
22	b	621	BCR	C7-C8-C9	-3.04	121.74	126.23
35	c	515	DGD	O2G-C1B-O1B	-3.04	116.60	123.70
20	C	512	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
20	b	614	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
34	a	418	LMT	O1'-C1'-C2'	3.04	112.88	108.27
20	B	615	CLA	CHC-C4B-NB	3.04	128.60	124.05
20	b	613	CLA	C3B-C2B-C1B	-3.03	103.59	107.17
20	C	510	CLA	C3B-C4B-NB	3.03	113.24	110.53
20	D	402	CLA	C3B-C4B-NB	3.03	113.24	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	604	CLA	C4-C3-C5	3.03	120.49	115.23
20	b	613	CLA	CBC-CAC-C3C	-3.03	104.20	112.42
34	T	102	LMT	C1'-C2'-C3'	3.03	116.38	110.01
22	K	101	BCR	C38-C26-C25	-3.03	121.18	124.48
20	a	403	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
32	C	521	HTG	O5-C5-C4	3.03	115.16	109.70
20	b	606	CLA	CAC-C3C-C4C	3.03	128.73	124.79
24	b	623	LMG	O8-C28-O10	-3.03	116.06	123.63
20	b	612	CLA	CMB-C2B-C1B	3.02	130.02	125.42
20	a	404	CLA	C1-C2-C3	-3.02	121.25	126.20
20	B	601	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
20	B	602	CLA	C2A-C1A-CHA	-3.02	118.62	123.87
24	A	407	LMG	O7-C10-C11	3.02	118.01	111.48
20	B	605	CLA	CMD-C2D-C1D	3.02	130.04	124.73
20	C	510	CLA	C3D-C2D-C1D	-3.02	101.71	105.83
20	B	606	CLA	O2D-CGD-CBD	3.02	116.51	111.23
20	b	611	CLA	C2B-C1B-NB	3.02	113.45	110.33
24	C	524	LMG	O8-C28-C29	3.02	121.03	111.83
22	c	514	BCR	C21-C20-C19	-3.01	114.47	123.20
20	B	615	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
20	B	601	CLA	C3C-C4C-NC	3.01	114.28	110.43
20	C	508	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
22	B	619	BCR	C21-C20-C19	-3.01	114.49	123.20
20	b	609	CLA	CHD-C1D-ND	-3.00	120.58	124.80
20	b	617	CLA	CHD-C1D-ND	-3.00	120.58	124.80
21	a	405	PHO	C4B-NB-C1B	-3.00	104.44	108.82
20	c	512	CLA	CHC-C4B-NB	3.00	128.55	124.05
20	c	510	CLA	C2A-C1A-CHA	-3.00	118.66	123.87
20	D	404	CLA	CMA-C3A-C4A	-3.00	103.72	111.77
20	c	513	CLA	C1D-CHD-C4C	-3.00	119.65	126.02
20	d	402	CLA	CAC-C3C-C4C	3.00	128.69	124.79
20	C	507	CLA	CHD-C1D-ND	-3.00	120.59	124.80
23	a	401	SQD	O48-C23-C24	3.00	120.97	111.83
20	C	506	CLA	C2B-C1B-NB	3.00	113.43	110.33
20	B	613	CLA	CMD-C2D-C1D	2.99	130.00	124.73
20	D	401	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
20	b	608	CLA	CHD-C4C-NC	2.99	128.87	124.23
20	C	503	CLA	C1D-CHD-C4C	-2.99	119.67	126.02
20	c	505	CLA	C2D-C1D-ND	2.99	113.08	110.13
20	C	510	CLA	C2D-C1D-ND	2.99	113.08	110.13
20	c	509	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
20	B	605	CLA	C3C-C4C-NC	2.98	114.25	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	412	SQD	O6-C44-C45	-2.98	103.56	110.82
20	B	603	CLA	C2D-C1D-ND	2.98	113.08	110.13
20	b	618	CLA	CHA-C4D-ND	2.98	138.70	132.55
20	b	610	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
27	A	411	PL9	C17-C18-C19	-2.98	120.81	127.62
20	C	510	CLA	C4-C3-C5	2.98	120.40	115.23
32	B	631	HTG	C1-O5-C5	2.98	117.90	112.56
20	B	607	CLA	CHA-C4D-ND	2.98	138.69	132.55
23	a	409	SQD	O47-C7-C8	2.98	117.92	111.48
20	B	601	CLA	CBC-CAC-C3C	-2.97	104.36	112.42
20	c	513	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	B	606	CLA	CHC-C4B-NB	2.97	128.51	124.05
20	c	508	CLA	C2A-C1A-CHA	-2.97	118.71	123.87
20	B	605	CLA	C3D-C2D-C1D	-2.97	101.78	105.83
20	c	508	CLA	CHD-C1D-ND	-2.97	120.62	124.80
20	C	501	CLA	CHA-C4D-ND	2.97	138.67	132.55
20	A	401	CLA	C4D-CHA-C1A	-2.97	117.70	121.24
20	B	613	CLA	C4B-CHC-C1C	-2.97	119.27	126.25
20	B	615	CLA	CHD-C4C-NC	2.97	128.83	124.23
20	C	503	CLA	CHD-C4C-NC	2.96	128.83	124.23
20	b	603	CLA	C1D-ND-C4D	-2.96	104.23	106.31
20	b	616	CLA	CAC-C3C-C4C	2.96	128.64	124.79
22	t	101	BCR	C21-C20-C19	-2.96	114.62	123.20
34	a	418	LMT	C1B-O5B-C5B	2.96	119.50	113.72
20	b	604	CLA	O2D-CGD-CBD	2.96	116.40	111.23
20	b	611	CLA	CBC-CAC-C3C	-2.96	104.40	112.42
20	b	617	CLA	C2B-C1B-NB	2.96	113.39	110.33
32	B	621	HTG	O5-C5-C6	2.96	113.77	106.44
20	c	512	CLA	C1-O2A-CGA	2.96	123.81	116.65
20	A	401	CLA	CHA-C4D-ND	2.96	138.65	132.55
20	d	403	CLA	C3B-C4B-NB	2.96	113.17	110.53
20	b	610	CLA	CHD-C4C-NC	2.95	128.81	124.23
20	B	601	CLA	C1C-C2C-C3C	-2.95	103.87	106.98
20	A	404	CLA	C3B-C4B-NB	2.95	113.17	110.53
20	C	509	CLA	CMD-C2D-C1D	2.95	129.93	124.73
21	a	405	PHO	CMB-C2B-C3B	2.95	130.58	124.68
20	A	404	CLA	CHB-C1B-NB	-2.95	119.62	124.05
20	C	510	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
20	c	503	CLA	C1-C2-C3	-2.95	121.36	126.20
37	E	104	HEM	C3B-C2B-C1B	2.95	108.62	106.41
20	C	502	CLA	C16-C17-C18	-2.95	102.78	115.94
20	b	618	CLA	C3C-C4C-NC	2.95	114.21	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	508	CLA	CHB-C4A-NA	2.95	128.65	124.40
20	B	609	CLA	CMC-C2C-C1C	2.95	129.64	125.03
22	B	619	BCR	C32-C1-C6	-2.95	105.62	110.24
20	B	602	CLA	C1D-CHD-C4C	-2.94	119.76	126.02
20	C	506	CLA	C4-C3-C5	2.94	120.34	115.23
20	B	612	CLA	C3C-C4C-NC	2.94	114.20	110.43
20	c	501	CLA	CHC-C4B-NB	2.94	128.46	124.05
20	b	611	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
20	C	511	CLA	C1-O2A-CGA	2.94	123.76	116.65
20	b	607	CLA	CMD-C2D-C1D	2.93	129.90	124.73
20	b	612	CLA	C4B-C3B-C2B	-2.93	103.65	107.30
20	B	611	CLA	C1C-C2C-C3C	-2.93	103.89	106.98
20	A	404	CLA	C3D-C4D-ND	2.93	114.75	109.99
20	c	507	CLA	O2A-CGA-O1A	-2.93	116.29	123.63
20	B	609	CLA	C4D-CHA-C1A	-2.93	117.75	121.24
20	C	506	CLA	CMC-C2C-C1C	2.93	129.61	125.03
22	T	101	BCR	C15-C16-C17	-2.93	117.52	123.52
20	b	608	CLA	C1-C2-C3	-2.93	121.40	126.20
34	B	625	LMT	C1-O1'-C1'	-2.93	108.68	113.68
20	c	508	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
20	c	508	CLA	C1-C2-C3	-2.93	121.40	126.20
20	B	603	CLA	C1-O2A-CGA	2.93	123.73	116.65
20	b	612	CLA	C4D-CHA-C1A	-2.93	117.75	121.24
23	f	101	SQD	C1-O5-C5	2.92	119.43	113.72
38	x	101	RRX	C33-C5-C6	-2.92	121.30	124.48
32	O	302	HTG	C1-O5-C5	2.92	117.80	112.56
35	d	416	DGD	C3D-C4D-C5D	2.92	115.53	110.23
34	b	628	LMT	C1'-O5'-C5'	2.92	119.42	113.72
20	b	618	CLA	CHD-C1D-ND	-2.92	120.69	124.80
20	D	401	CLA	CHC-C4B-NB	2.92	128.43	124.05
32	C	534	HTG	C1'-S1-C1	2.92	106.75	100.45
20	C	505	CLA	CHD-C1D-ND	-2.92	120.69	124.80
22	B	617	BCR	C21-C20-C19	-2.92	114.75	123.20
20	c	509	CLA	C3D-C2D-C1D	-2.92	101.85	105.83
22	k	102	BCR	C33-C5-C6	-2.91	121.30	124.48
20	B	610	CLA	OBD-CAD-C3D	-2.91	121.61	128.42
32	D	417	HTG	O5-C5-C6	2.91	113.66	106.44
22	D	405	BCR	C36-C18-C19	2.91	122.54	118.09
20	B	610	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
20	d	402	CLA	CHA-C4D-ND	2.91	138.55	132.55
20	B	613	CLA	C4-C3-C5	2.91	120.28	115.23
20	B	610	CLA	C3B-C2B-C1B	-2.91	103.74	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	502	CLA	CHA-C4D-ND	2.91	138.54	132.55
20	B	609	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
34	B	626	LMT	O1'-C1'-C2'	2.90	112.68	108.27
22	B	618	BCR	C11-C10-C9	-2.90	123.21	127.28
20	D	404	CLA	CHC-C4B-NB	2.90	128.40	124.05
20	C	510	CLA	C4B-CHC-C1C	-2.90	119.43	126.25
20	c	512	CLA	CHA-C4D-ND	2.90	138.53	132.55
20	b	604	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
27	a	415	PL9	C7-C8-C9	-2.90	121.84	126.83
20	b	613	CLA	CHA-C4D-ND	2.90	138.53	132.55
20	b	605	CLA	CAC-C3C-C4C	2.90	128.56	124.79
22	b	619	BCR	C15-C16-C17	-2.89	117.60	123.52
20	B	605	CLA	C6-C5-C3	-2.89	106.42	113.47
27	a	415	PL9	C42-C43-C44	-2.89	121.00	127.62
20	c	507	CLA	CBC-CAC-C3C	-2.89	104.58	112.42
20	b	615	CLA	CHC-C4B-NB	2.89	128.39	124.05
20	b	608	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
20	A	401	CLA	CMB-C2B-C1B	2.89	129.82	125.42
20	a	407	CLA	CMC-C2C-C1C	2.89	129.55	125.03
20	B	607	CLA	O2A-CGA-O1A	-2.89	116.41	123.63
20	B	612	CLA	CHA-C4D-ND	2.89	138.51	132.55
20	B	615	CLA	CHA-C4D-ND	2.89	138.51	132.55
34	z	102	LMT	O5'-C1'-C2'	-2.88	104.44	110.37
40	V	201	HEC	C4B-NB-C1B	2.88	110.52	105.82
20	a	403	CLA	CMB-C2B-C1B	2.88	129.81	125.42
35	c	516	DGD	O6E-C5E-C6E	2.88	113.58	106.44
20	c	504	CLA	C4-C3-C5	2.88	120.23	115.23
20	b	618	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
20	c	502	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
20	b	606	CLA	C1D-CHD-C4C	-2.88	119.90	126.02
20	b	614	CLA	C1D-ND-C4D	-2.88	104.29	106.31
22	t	101	BCR	C28-C27-C26	-2.88	108.92	114.06
20	a	407	CLA	CED-O2D-CGD	2.88	122.44	115.92
20	c	511	CLA	CBC-CAC-C3C	-2.88	104.62	112.42
20	d	403	CLA	C1D-ND-C4D	-2.87	104.30	106.31
20	b	604	CLA	CBB-CAB-C3B	-2.87	113.20	127.53
20	b	613	CLA	C3C-C4C-NC	2.87	114.10	110.43
20	C	501	CLA	CMD-C2D-C1D	2.87	129.78	124.73
34	b	627	LMT	O2'-C2'-C3'	-2.87	103.62	110.38
22	t	101	BCR	C34-C9-C8	2.86	122.46	118.09
20	C	501	CLA	C1-O2A-CGA	2.86	123.58	116.65
20	b	615	CLA	C4D-CHA-C1A	-2.86	117.83	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	625	HTG	C1-C2-C3	2.86	116.15	110.55
20	a	403	CLA	C3B-C2B-C1B	-2.86	103.80	107.17
20	b	604	CLA	C4D-CHA-C1A	-2.86	117.83	121.24
22	t	101	BCR	C11-C10-C9	-2.86	123.27	127.28
34	Z	101	LMT	C1'-O5'-C5'	2.86	119.31	113.72
20	a	403	CLA	CHC-C4B-NB	2.86	128.34	124.05
20	c	509	CLA	CHB-C4A-NA	2.86	128.53	124.40
20	c	508	CLA	CHC-C4B-NB	2.86	128.34	124.05
20	D	404	CLA	CHD-C4C-C3C	-2.86	120.61	124.77
20	b	613	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	A	411	PL9	C45-C44-C46	2.86	120.19	115.23
20	d	402	CLA	C3D-C2D-C1D	-2.86	101.93	105.83
20	B	612	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
34	E	101	LMT	C1'-C2'-C3'	2.86	116.02	110.01
20	b	605	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
35	c	515	DGD	O3G-C3G-C2G	-2.85	103.88	110.82
20	B	611	CLA	C4D-CHA-C1A	-2.85	117.84	121.24
20	B	602	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	C	519	LMG	O8-C28-O10	-2.84	116.51	123.63
23	F	101	SQD	O48-C23-C24	2.84	120.50	111.83
34	B	625	LMT	C1'-O5'-C5'	2.84	119.27	113.72
20	a	407	CLA	CHA-C4D-ND	2.84	138.41	132.55
20	B	606	CLA	CMC-C2C-C1C	2.84	129.47	125.03
23	A	406	SQD	O48-C23-O10	-2.84	116.53	123.63
35	c	516	DGD	O1G-C1A-O1A	-2.84	116.53	123.63
20	b	603	CLA	O2A-CGA-CBA	2.84	120.48	111.83
20	B	613	CLA	CHA-C4D-ND	2.84	138.40	132.55
27	D	412	PL9	C40-C39-C38	-2.84	116.34	123.63
20	b	609	CLA	CHD-C4C-NC	2.84	128.63	124.23
20	c	504	CLA	CHB-C4A-NA	2.84	128.49	124.40
20	B	607	CLA	C2C-C1C-NC	2.83	112.96	109.98
20	b	606	CLA	C6-C5-C3	-2.83	106.57	113.47
32	B	632	HTG	C1-O5-C5	2.83	117.64	112.56
20	D	404	CLA	C6-C7-C8	-2.83	106.56	115.97
20	C	504	CLA	C1-O2A-CGA	2.83	123.50	116.65
32	C	534	HTG	O5-C5-C4	2.83	114.80	109.70
20	c	513	CLA	O2A-CGA-CBA	2.83	120.45	111.83
20	C	511	CLA	C3B-C4B-NB	2.83	113.05	110.53
35	c	517	DGD	O3G-C3G-C2G	-2.83	103.94	110.82
20	C	507	CLA	CMC-C2C-C1C	2.82	129.45	125.03
20	C	510	CLA	CAC-C3C-C4C	2.82	128.47	124.79
38	H	101	RRX	C34-C9-C8	2.82	122.40	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	D	406	DGD	O1G-C1A-C2A	2.82	120.44	111.83
20	b	608	CLA	CAC-C3C-C4C	2.82	128.46	124.79
20	b	613	CLA	C2A-C1A-CHA	-2.82	118.97	123.87
20	B	611	CLA	CHD-C4C-NC	2.82	128.60	124.23
22	K	101	BCR	C7-C8-C9	-2.82	122.07	126.23
20	c	501	CLA	C3D-C4D-ND	2.82	114.57	109.99
20	A	404	CLA	C2A-C1A-CHA	-2.82	118.98	123.87
20	b	604	CLA	OBD-CAD-C3D	-2.82	121.83	128.42
21	a	406	PHO	C4-C3-C5	2.82	120.11	115.23
20	c	503	CLA	C2B-C1B-NB	2.81	113.24	110.33
20	C	513	CLA	CHD-C4C-NC	2.81	128.59	124.23
22	k	101	BCR	C3-C4-C5	-2.81	109.05	114.06
20	C	508	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
20	A	401	CLA	C3C-C4C-NC	2.80	114.02	110.43
34	c	523	LMT	O1'-C1'-C2'	2.80	112.53	108.27
20	b	613	CLA	C1D-ND-C4D	-2.80	104.34	106.31
20	C	512	CLA	CED-O2D-CGD	2.80	122.27	115.92
38	x	101	RRX	C38-C26-C25	-2.80	121.43	124.48
20	C	510	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
35	c	517	DGD	O6D-C1D-O3G	-2.80	103.43	110.04
20	C	509	CLA	CHD-C1D-ND	-2.80	120.86	124.80
20	B	606	CLA	C4-C3-C5	2.80	120.09	115.23
38	H	101	RRX	C16-C17-C18	-2.80	123.35	127.28
38	x	101	RRX	C24-C23-C22	-2.80	122.10	126.23
20	A	404	CLA	C1D-CHD-C4C	-2.80	120.08	126.02
20	D	402	CLA	C4-C3-C5	2.80	120.08	115.23
20	A	402	CLA	CHC-C4B-NB	2.80	128.24	124.05
23	a	409	SQD	O5-C1-C2	-2.79	104.63	110.37
20	a	407	CLA	C3C-C4C-NC	2.79	114.00	110.43
20	b	608	CLA	CHA-C4D-ND	2.79	138.31	132.55
20	C	507	CLA	C4D-CHA-C1A	-2.79	117.92	121.24
20	c	504	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
20	c	509	CLA	C1D-ND-C4D	-2.79	104.36	106.31
20	c	504	CLA	CMB-C2B-C1B	2.79	129.66	125.42
27	a	415	PL9	C2-C1-C6	2.79	122.31	119.00
20	a	403	CLA	C4B-CHC-C1C	-2.78	119.70	126.25
20	B	606	CLA	C2A-C1A-CHA	-2.78	119.04	123.87
20	B	605	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
20	C	506	CLA	CHD-C4C-NC	2.78	128.54	124.23
20	b	609	CLA	O2D-CGD-CBD	2.78	116.09	111.23
20	c	509	CLA	CHA-C4D-ND	2.78	138.28	132.55
24	C	524	LMG	O1-C1-C2	2.78	112.49	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406	SQD	C44-O6-C1	-2.77	107.85	113.80
22	t	101	BCR	C35-C13-C12	2.77	122.33	118.09
20	c	512	CLA	O2A-CGA-CBA	2.77	120.29	111.83
20	B	616	CLA	C4D-CHA-C1A	-2.77	117.94	121.24
24	C	519	LMG	C8-O7-C10	-2.77	111.17	117.80
22	k	102	BCR	C11-C10-C9	-2.77	123.40	127.28
20	A	404	CLA	CHD-C4C-NC	2.77	128.52	124.23
20	B	611	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
20	B	604	CLA	C1D-CHD-C4C	-2.76	120.14	126.02
24	c	518	LMG	C3-C4-C5	2.76	115.25	110.23
20	B	612	CLA	C1D-ND-C4D	-2.76	104.37	106.31
20	C	507	CLA	C1D-CHD-C4C	-2.76	120.15	126.02
20	C	512	CLA	CMB-C2B-C1B	2.76	129.62	125.42
20	B	604	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
22	c	514	BCR	C38-C26-C25	-2.76	121.47	124.48
20	c	505	CLA	C4D-CHA-C1A	-2.76	117.95	121.24
20	b	616	CLA	CMD-C2D-C1D	2.76	129.59	124.73
20	d	403	CLA	CHA-C4D-ND	2.76	138.24	132.55
20	b	612	CLA	CMC-C2C-C1C	2.76	129.34	125.03
20	c	506	CLA	CED-O2D-CGD	2.76	122.17	115.92
20	b	618	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
20	B	612	CLA	C3B-C4B-NB	2.76	112.99	110.53
20	B	605	CLA	CAC-C3C-C4C	2.76	128.38	124.79
20	B	616	CLA	CHD-C1D-ND	-2.75	120.93	124.80
20	D	404	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
20	C	510	CLA	CMB-C2B-C1B	2.75	129.61	125.42
23	b	622	SQD	O9-S-C6	2.75	110.86	106.76
20	c	510	CLA	CMB-C2B-C1B	2.74	129.60	125.42
20	a	404	CLA	C3C-C4C-NC	2.74	113.94	110.43
36	d	406	LHG	C6-O8-C23	2.74	127.14	117.12
22	d	405	BCR	C10-C11-C12	-2.74	115.25	123.20
20	D	401	CLA	CAC-C3C-C4C	2.74	128.36	124.79
20	b	608	CLA	CMB-C2B-C1B	2.74	129.59	125.42
20	B	606	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
20	c	508	CLA	CMA-C3A-C4A	-2.74	104.41	111.77
20	C	504	CLA	C3B-C4B-NB	2.74	112.98	110.53
20	D	404	CLA	CBC-CAC-C3C	-2.74	105.00	112.42
27	a	415	PL9	C37-C38-C39	-2.74	121.36	127.62
20	A	402	CLA	CHB-C1B-NB	-2.74	119.94	124.05
20	b	609	CLA	C2D-C1D-ND	2.74	112.83	110.13
34	f	102	LMT	O5'-C5'-C6'	2.74	113.22	106.44
20	B	614	CLA	CHA-C4D-ND	2.74	138.19	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	t	101	BCR	C23-C24-C25	-2.73	119.69	127.00
20	b	605	CLA	C3C-C4C-NC	2.73	113.93	110.43
20	a	404	CLA	CHD-C1D-ND	-2.73	120.95	124.80
20	B	607	CLA	C1-O2A-CGA	2.73	123.27	116.65
20	B	610	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
20	C	509	CLA	CHA-C4D-ND	2.73	138.18	132.55
20	B	602	CLA	CMC-C2C-C1C	2.73	129.30	125.03
34	B	626	LMT	O5'-C5'-C6'	2.73	113.20	106.44
22	D	405	BCR	C10-C11-C12	-2.73	115.29	123.20
20	c	508	CLA	CHD-C4C-NC	2.73	128.46	124.23
20	c	502	CLA	C4D-CHA-C1A	-2.73	117.99	121.24
20	B	614	CLA	CHD-C4C-NC	2.73	128.46	124.23
27	d	412	PL9	C2-C1-C6	2.73	122.24	119.00
22	B	618	BCR	C24-C23-C22	-2.73	122.20	126.23
20	C	504	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
20	C	513	CLA	O2A-CGA-O1A	-2.72	116.81	123.63
20	A	401	CLA	C4C-C3C-C2C	-2.72	102.93	106.89
20	B	612	CLA	CMB-C2B-C1B	2.72	129.57	125.42
22	t	101	BCR	C7-C6-C5	-2.72	115.29	121.56
20	C	513	CLA	CHD-C1D-ND	-2.72	120.97	124.80
20	b	604	CLA	CHD-C4C-C3C	-2.72	120.81	124.77
20	B	614	CLA	C3C-C4C-NC	2.72	113.91	110.43
23	b	622	SQD	C4-C3-C2	2.71	115.59	110.83
35	C	516	DGD	C3D-C4D-C5D	-2.71	105.31	110.23
20	B	606	CLA	CHD-C1D-ND	-2.71	120.99	124.80
20	d	404	CLA	C2A-C1A-CHA	-2.71	119.17	123.87
20	b	616	CLA	CHD-C1D-ND	-2.71	120.99	124.80
20	B	602	CLA	O2A-C1-C2	2.71	118.53	108.11
20	b	617	CLA	C2A-C1A-CHA	-2.71	119.17	123.87
22	K	102	BCR	C20-C21-C22	-2.71	123.48	127.28
22	A	405	BCR	C15-C16-C17	-2.71	117.98	123.52
20	b	612	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
27	a	415	PL9	C40-C39-C41	2.71	119.93	115.23
20	C	507	CLA	CMD-C2D-C1D	2.71	129.49	124.73
20	C	512	CLA	CHD-C4C-NC	2.70	128.43	124.23
22	a	408	BCR	C35-C13-C12	2.70	122.22	118.09
23	b	622	SQD	O47-C7-O49	-2.70	117.39	123.70
20	B	603	CLA	CMA-C3A-C4A	-2.70	104.52	111.77
32	c	521	HTG	O5-C5-C4	2.70	114.56	109.70
24	c	518	LMG	O8-C28-C29	2.70	120.06	111.83
35	h	101	DGD	O1G-C1A-O1A	-2.69	116.89	123.63
22	t	101	BCR	C38-C26-C25	-2.69	121.54	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	504	CLA	CHC-C4B-NB	2.69	128.09	124.05
20	C	511	CLA	C1D-ND-C4D	-2.69	104.42	106.31
27	d	412	PL9	C15-C14-C16	2.69	119.90	115.23
23	A	406	SQD	O8-S-C6	2.69	111.17	105.97
20	b	610	CLA	C6-C5-C3	-2.69	106.91	113.47
35	C	517	DGD	O2G-C1B-O1B	-2.69	117.41	123.70
20	b	618	CLA	O2A-CGA-CBA	2.69	120.04	111.83
20	b	614	CLA	C2A-C1A-CHA	-2.69	119.20	123.87
20	d	403	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
20	B	605	CLA	C3B-C2B-C1B	-2.69	104.00	107.17
20	b	611	CLA	C3C-C4C-NC	2.68	113.87	110.43
20	C	508	CLA	CMD-C2D-C1D	2.68	129.45	124.73
20	C	505	CLA	C2B-C1B-NB	2.68	113.11	110.33
20	C	503	CLA	C2D-C1D-ND	2.68	112.78	110.13
20	b	612	CLA	CHD-C4C-NC	2.68	128.38	124.23
37	E	104	HEM	C4C-NC-C1C	2.68	110.19	105.82
36	D	407	LHG	C11-C10-C9	-2.68	100.83	114.37
20	a	407	CLA	CHD-C4C-NC	2.68	128.38	124.23
20	C	505	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
20	C	510	CLA	C1-C2-C3	-2.67	121.82	126.20
35	H	102	DGD	C2G-O2G-C1B	-2.67	111.40	117.80
20	b	605	CLA	CHC-C1C-NC	-2.67	120.28	124.31
22	d	405	BCR	C2-C1-C6	2.67	114.32	110.44
20	B	609	CLA	C1-O2A-CGA	2.67	123.11	116.65
20	B	610	CLA	CMC-C2C-C1C	2.67	129.20	125.03
20	c	503	CLA	C4D-CHA-C1A	-2.67	118.06	121.24
20	a	407	CLA	CMD-C2D-C3D	2.67	133.81	127.69
20	a	403	CLA	C1-C2-C3	-2.67	121.83	126.20
20	b	605	CLA	C4A-NA-C1A	2.66	107.89	106.68
20	B	608	CLA	C3B-C4B-NB	2.66	112.91	110.53
20	c	512	CLA	CBA-CAA-C2A	-2.66	105.87	113.79
37	e	102	HEM	C3B-C4B-NB	-2.66	107.56	109.47
20	C	503	CLA	CAC-C3C-C4C	2.66	128.25	124.79
20	b	616	CLA	C4-C3-C5	2.66	119.84	115.23
20	c	513	CLA	C3C-C4C-NC	2.66	113.84	110.43
21	D	403	PHO	CMB-C2B-C3B	2.66	129.99	124.68
20	b	609	CLA	C2A-C1A-CHA	-2.66	119.26	123.87
20	b	617	CLA	C4-C3-C5	2.66	119.84	115.23
20	b	613	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
20	B	612	CLA	CHC-C4B-NB	2.66	128.03	124.05
20	d	402	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
20	A	404	CLA	O2D-CGD-CBD	2.65	115.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	402	CLA	CHD-C4C-NC	2.65	128.34	124.23
20	C	508	CLA	CHD-C1D-ND	-2.65	121.07	124.80
32	C	534	HTG	C1-O5-C5	2.65	117.32	112.56
20	a	403	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
20	c	505	CLA	CHA-C4D-ND	2.65	138.02	132.55
20	C	508	CLA	C5-C3-C2	-2.65	115.22	121.17
20	A	402	CLA	CMB-C2B-C1B	2.65	129.45	125.42
21	D	403	PHO	CMA-C3A-C4A	-2.65	108.90	114.61
20	b	611	CLA	C1-O2A-CGA	2.65	123.06	116.65
20	b	606	CLA	C4-C3-C5	2.65	119.82	115.23
20	B	609	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
23	a	409	SQD	C44-O6-C1	-2.65	108.12	113.80
20	C	508	CLA	O2D-CGD-CBD	2.65	115.86	111.23
20	b	615	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
20	D	401	CLA	CAA-CBA-CGA	-2.65	105.69	113.21
20	B	612	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
22	t	101	BCR	C1-C6-C7	2.64	122.82	115.65
27	d	412	PL9	C36-C34-C33	-2.64	115.24	121.17
20	C	505	CLA	C7-C6-C5	-2.64	106.22	113.26
22	A	405	BCR	C24-C23-C22	-2.64	122.33	126.23
20	C	510	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
37	E	104	HEM	C2A-C1A-NA	-2.64	107.22	110.15
20	b	609	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
20	B	602	CLA	C4-C3-C2	-2.64	116.85	123.63
20	B	607	CLA	O2A-CGA-CBA	2.64	119.88	111.83
24	C	524	LMG	O7-C10-O9	-2.64	117.54	123.70
20	d	404	CLA	O2D-CGD-CBD	2.64	115.84	111.23
20	a	403	CLA	C5-C3-C2	-2.64	115.25	121.17
20	a	403	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
20	A	404	CLA	CHC-C4B-NB	2.64	128.00	124.05
20	b	613	CLA	C1-C2-C3	-2.64	121.88	126.20
20	c	502	CLA	C16-C17-C18	-2.63	104.18	115.94
20	a	404	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
20	b	616	CLA	C4-C3-C2	-2.63	116.87	123.63
20	B	611	CLA	CHC-C4B-NB	2.63	128.00	124.05
20	a	403	CLA	O2A-CGA-CBA	2.63	119.86	111.83
22	j	102	BCR	C33-C5-C6	-2.63	121.62	124.48
20	b	614	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
36	D	408	LHG	C13-C12-C11	-2.63	101.10	114.37
34	I	101	LMT	C3'-C4'-C5'	-2.62	105.11	110.93
21	a	406	PHO	CED-O2D-CGD	2.62	121.87	115.92
20	c	512	CLA	CMC-C2C-C1C	2.62	129.13	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	j	102	BCR	C16-C17-C18	-2.62	123.60	127.28
20	B	608	CLA	CHD-C1D-ND	-2.62	121.11	124.80
20	B	605	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
20	b	615	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
35	H	102	DGD	O3G-C3G-C2G	-2.62	104.44	110.82
20	B	611	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
20	c	509	CLA	O2D-CGD-CBD	2.62	115.81	111.23
20	c	507	CLA	C3C-C4C-NC	2.62	113.78	110.43
24	c	519	LMG	O5-C6-C5	-2.62	102.42	111.33
20	c	511	CLA	CMB-C2B-C1B	2.62	129.40	125.42
36	D	407	LHG	O4-P-O5	2.62	124.62	112.44
20	b	605	CLA	CHD-C4C-NC	2.62	128.29	124.23
20	c	508	CLA	C7-C6-C5	-2.61	106.30	113.26
20	B	616	CLA	C1D-ND-C4D	-2.61	104.48	106.31
20	D	404	CLA	C4-C3-C5	2.61	119.77	115.23
24	A	407	LMG	O1-C1-C2	2.61	112.24	108.27
20	B	613	CLA	CHD-C4C-NC	2.61	128.28	124.23
20	A	401	CLA	CHC-C1C-C2C	-2.61	119.53	126.95
34	Z	101	LMT	O1B-C4'-C3'	2.61	113.86	107.23
20	d	402	CLA	O2A-CGA-CBA	2.61	119.79	111.83
20	b	612	CLA	C1D-ND-C4D	-2.61	104.48	106.31
20	D	404	CLA	C3B-C4B-NB	2.61	112.86	110.53
20	A	402	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
20	C	513	CLA	C1D-CHD-C4C	-2.61	120.48	126.02
32	B	622	HTG	O2-C2-C3	-2.60	104.24	110.38
27	A	411	PL9	C25-C24-C26	2.60	119.75	115.23
20	c	506	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
20	b	603	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
20	D	401	CLA	O2D-CGD-CBD	2.60	115.78	111.23
20	C	510	CLA	O1D-CGD-CBD	-2.60	119.38	124.52
20	B	614	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
23	F	101	SQD	O6-C44-C45	2.60	113.73	108.81
20	C	507	CLA	C7-C6-C5	-2.60	106.33	113.26
20	c	513	CLA	C4D-CHA-C1A	-2.60	118.14	121.24
20	B	607	CLA	C1-C2-C3	-2.60	121.94	126.20
20	A	402	CLA	C4-C3-C5	2.60	119.74	115.23
20	d	403	CLA	CAC-C3C-C4C	2.60	128.17	124.79
20	b	613	CLA	CHD-C1D-ND	-2.60	121.15	124.80
20	b	618	CLA	C4D-CHA-C1A	-2.60	118.15	121.24
20	a	404	CLA	C3B-C4B-NB	2.60	112.85	110.53
22	k	101	BCR	C20-C21-C22	-2.60	123.64	127.28
20	b	609	CLA	C1D-ND-C4D	2.59	108.13	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	513	CLA	C1D-ND-C4D	-2.59	104.49	106.31
34	z	102	LMT	O1B-C1B-C2B	2.59	114.47	108.09
20	C	504	CLA	CMC-C2C-C1C	2.59	129.08	125.03
20	b	606	CLA	C4C-C3C-C2C	-2.59	103.12	106.89
20	B	612	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
20	C	508	CLA	CHC-C4B-NB	2.59	127.93	124.05
20	d	403	CLA	C4B-C3B-C2B	-2.59	104.09	107.30
20	C	513	CLA	C4-C3-C5	2.59	119.72	115.23
20	B	614	CLA	CHD-C1D-ND	-2.59	121.16	124.80
20	b	607	CLA	C2A-C1A-CHA	-2.58	119.38	123.87
20	B	605	CLA	C1D-CHD-C4C	-2.58	120.53	126.02
20	B	605	CLA	CGD-CBD-CAD	-2.58	102.48	110.85
20	B	604	CLA	C3C-C4C-NC	2.58	113.74	110.43
21	D	403	PHO	C4-C3-C5	2.58	119.71	115.23
22	C	515	BCR	C33-C5-C6	-2.58	121.67	124.48
20	b	612	CLA	CHD-C1D-ND	-2.58	121.17	124.80
27	a	415	PL9	C10-C9-C11	2.58	119.71	115.23
20	b	607	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
20	b	607	CLA	CHC-C1C-NC	-2.58	120.42	124.31
20	c	503	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
20	c	505	CLA	C3C-C4C-NC	2.58	113.73	110.43
20	C	506	CLA	CMD-C2D-C1D	2.58	129.27	124.73
20	b	615	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
20	C	511	CLA	CHD-C1D-ND	-2.57	121.18	124.80
35	d	416	DGD	O6D-C5D-C4D	2.57	114.34	109.70
20	b	614	CLA	CHD-C1D-ND	-2.57	121.18	124.80
20	B	611	CLA	C3B-C4B-NB	2.57	112.83	110.53
20	D	401	CLA	C4-C3-C5	2.57	119.69	115.23
20	A	404	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
20	b	615	CLA	O2D-CGD-CBD	2.57	115.72	111.23
23	A	412	SQD	O48-C46-C45	2.57	115.80	108.40
20	b	608	CLA	O2A-CGA-CBA	2.57	119.67	111.83
20	b	605	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
34	T	102	LMT	O1'-C1'-C2'	-2.57	104.38	108.27
20	B	613	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
20	d	404	CLA	CHC-C4B-NB	2.56	127.90	124.05
20	c	508	CLA	CHA-C4D-ND	2.56	137.84	132.55
20	B	614	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
20	c	504	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
35	C	518	DGD	O2G-C1B-C2B	2.56	117.02	111.48
20	B	609	CLA	C6-C5-C3	-2.56	107.23	113.47
20	B	607	CLA	CAC-C3C-C2C	2.56	132.26	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	511	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
23	a	409	SQD	C45-O47-C7	-2.56	111.67	117.80
20	d	404	CLA	C3D-C4D-ND	2.56	114.14	109.99
20	B	604	CLA	CMC-C2C-C1C	2.56	129.03	125.03
40	v	201	HEC	C4D-ND-C1D	2.56	109.99	105.82
20	B	612	CLA	C4D-CHA-C1A	-2.56	118.19	121.24
20	a	404	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
27	A	411	PL9	C2-C1-C6	2.56	122.03	119.00
22	j	102	BCR	C37-C22-C23	2.55	121.99	118.09
23	A	406	SQD	O3-C3-C4	2.55	116.40	110.38
20	A	402	CLA	C1-O2A-CGA	2.55	122.83	116.65
22	j	102	BCR	C38-C26-C25	-2.55	121.70	124.48
20	b	603	CLA	CHD-C1D-ND	-2.55	121.21	124.80
20	c	509	CLA	CMD-C2D-C1D	2.55	129.22	124.73
27	d	412	PL9	C21-C19-C18	-2.55	115.44	121.17
22	K	101	BCR	C37-C22-C23	2.55	121.99	118.09
20	b	615	CLA	O2A-CGA-CBA	2.55	119.61	111.83
24	c	518	LMG	C8-O7-C10	-2.55	111.69	117.80
20	B	603	CLA	CHD-C4C-NC	2.55	128.19	124.23
20	B	616	CLA	O2D-CGD-CBD	2.55	115.69	111.23
20	B	606	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
37	E	104	HEM	C4A-NA-C1A	2.55	109.97	105.82
34	E	101	LMT	C4'-C3'-C2'	2.55	115.30	110.83
20	A	404	CLA	CAC-C3C-C4C	2.54	128.10	124.79
20	C	503	CLA	C5-C3-C2	-2.54	115.46	121.17
20	C	509	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
24	a	410	LMG	O8-C28-C29	2.54	119.59	111.83
20	B	608	CLA	C4A-NA-C1A	2.54	107.84	106.68
20	b	610	CLA	CHD-C1D-ND	-2.54	121.23	124.80
20	b	613	CLA	C1D-CHD-C4C	-2.54	120.62	126.02
32	V	202	HTG	O5-C1-S1	2.54	117.24	110.30
20	C	509	CLA	CAC-C3C-C4C	2.54	128.10	124.79
24	B	620	LMG	O6-C5-C6	2.54	112.73	106.44
20	C	502	CLA	CED-O2D-CGD	2.54	121.67	115.92
22	c	514	BCR	C11-C10-C9	-2.54	123.72	127.28
20	B	607	CLA	C4-C3-C5	2.54	119.63	115.23
23	A	406	SQD	C45-O47-C7	-2.53	111.73	117.80
20	c	501	CLA	C2A-C1A-CHA	-2.53	119.48	123.87
20	D	404	CLA	CED-O2D-CGD	2.53	121.65	115.92
20	B	614	CLA	C16-C15-C13	-2.53	107.56	115.97
20	c	512	CLA	CAC-C3C-C4C	2.53	128.08	124.79
24	J	101	LMG	O8-C28-O10	-2.53	117.31	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	101	LMT	O3'-C3'-C4'	2.53	116.41	109.94
20	a	404	CLA	O2A-CGA-CBA	2.52	119.53	111.83
27	A	411	PL9	C32-C33-C34	-2.52	121.85	127.62
20	B	610	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
20	C	505	CLA	O2A-CGA-CBA	2.52	119.52	111.83
20	C	505	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
20	c	505	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
20	d	404	CLA	CHB-C4A-NA	2.52	128.03	124.40
23	A	412	SQD	O5-C1-C2	-2.52	105.20	110.37
20	b	614	CLA	C4C-C3C-C2C	-2.52	103.23	106.89
23	F	101	SQD	C1-O5-C5	-2.52	108.81	113.72
20	C	511	CLA	C1D-CHD-C4C	-2.52	120.67	126.02
20	A	402	CLA	CAC-C3C-C2C	-2.51	122.94	127.56
20	D	402	CLA	CHC-C4B-NB	2.51	127.82	124.05
22	K	101	BCR	C24-C23-C22	-2.51	122.52	126.23
20	a	407	CLA	C1D-CHD-C4C	-2.51	120.68	126.02
20	C	509	CLA	C3C-C4C-NC	2.51	113.64	110.43
23	A	406	SQD	O48-C23-C24	2.51	119.49	111.83
20	c	503	CLA	CMC-C2C-C1C	2.51	128.96	125.03
20	B	613	CLA	C2B-C1B-NB	2.51	112.93	110.33
34	m	102	LMT	C1'-O5'-C5'	-2.51	108.82	113.72
20	c	511	CLA	O2A-CGA-CBA	2.51	119.48	111.83
20	c	510	CLA	CHC-C4B-NB	2.51	127.81	124.05
20	B	607	CLA	C3C-C4C-NC	2.51	113.64	110.43
22	T	101	BCR	C33-C5-C6	-2.51	121.75	124.48
20	c	508	CLA	C3B-C4B-NB	2.50	112.77	110.53
20	c	510	CLA	CMC-C2C-C1C	2.50	128.95	125.03
40	v	201	HEC	CMD-C2D-C1D	2.50	129.23	125.42
20	C	505	CLA	C1D-ND-C4D	2.50	108.07	106.31
20	A	402	CLA	CHC-C4B-C3B	-2.50	116.52	127.37
20	c	511	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
20	C	512	CLA	CAC-C3C-C4C	2.50	128.04	124.79
20	c	510	CLA	CMD-C2D-C1D	2.50	129.12	124.73
20	c	512	CLA	CMB-C2B-C1B	2.50	129.22	125.42
20	C	502	CLA	C3C-C4C-NC	2.50	113.63	110.43
35	D	406	DGD	O2G-C1B-O1B	-2.50	117.87	123.70
20	B	602	CLA	CHB-C1B-NB	-2.49	120.31	124.05
20	b	614	CLA	C4-C3-C5	2.49	119.56	115.23
20	B	614	CLA	C7-C6-C5	-2.49	106.62	113.26
20	d	403	CLA	CMD-C2D-C1D	2.49	129.12	124.73
20	C	506	CLA	C3C-C4C-NC	2.49	113.62	110.43
20	C	507	CLA	C2D-C1D-ND	2.49	112.59	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	603	CLA	O2A-CGA-CBA	2.49	119.42	111.83
35	c	516	DGD	O1G-C1A-C2A	2.49	119.42	111.83
20	C	508	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
36	E	103	LHG	O7-C7-O9	-2.49	117.40	123.63
23	A	406	SQD	O9-S-O7	-2.49	105.73	113.82
20	b	603	CLA	CHC-C4B-NB	2.49	127.78	124.05
20	B	609	CLA	C3C-C4C-NC	2.49	113.62	110.43
20	c	505	CLA	C4C-C3C-C2C	-2.49	103.27	106.89
20	B	608	CLA	C1D-CHD-C4C	-2.49	120.74	126.02
20	B	608	CLA	CHD-C4C-NC	2.49	128.09	124.23
21	a	405	PHO	CMC-C2C-C1C	2.48	129.20	124.73
20	B	615	CLA	CMA-C3A-C4A	-2.48	105.11	111.77
20	b	617	CLA	C6-C5-C3	-2.48	107.43	113.47
20	b	609	CLA	O2A-CGA-CBA	2.48	119.39	111.83
20	C	502	CLA	C1D-CHD-C4C	-2.48	120.75	126.02
27	D	412	PL9	C36-C34-C33	-2.48	115.60	121.17
20	C	501	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
20	B	602	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
20	b	615	CLA	C3B-C2B-C1B	-2.48	104.25	107.17
20	B	608	CLA	CHA-C4D-ND	2.48	137.66	132.55
32	C	534	HTG	C1-C2-C3	-2.48	105.71	110.55
20	B	607	CLA	C4C-C3C-C2C	-2.48	103.29	106.89
20	c	509	CLA	C4B-C3B-C2B	-2.47	104.22	107.30
20	B	616	CLA	C1-O2A-CGA	2.47	122.64	116.65
20	B	608	CLA	CMD-C2D-C1D	2.47	129.08	124.73
22	k	101	BCR	C38-C26-C25	-2.47	121.78	124.48
20	b	614	CLA	CHC-C1C-NC	-2.47	120.59	124.31
20	b	609	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
22	B	617	BCR	C8-C7-C6	-2.47	120.40	127.00
21	D	403	PHO	C3D-CAD-CBD	2.47	110.86	107.61
20	D	402	CLA	CMC-C2C-C1C	2.47	128.89	125.03
20	B	604	CLA	C4-C3-C5	2.47	119.52	115.23
20	A	402	CLA	C4B-CHC-C1C	-2.47	120.44	126.25
22	d	405	BCR	C2-C3-C4	2.47	116.70	111.28
22	C	515	BCR	C38-C26-C25	-2.47	121.79	124.48
20	a	407	CLA	C4C-C3C-C2C	-2.47	103.30	106.89
20	B	607	CLA	C4B-CHC-C1C	-2.46	120.45	126.25
20	C	505	CLA	CAC-C3C-C4C	2.46	128.00	124.79
20	a	407	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
20	b	605	CLA	C3B-C4B-NB	2.46	112.73	110.53
20	A	401	CLA	OBD-CAD-C3D	-2.46	122.66	128.42
20	a	404	CLA	CHC-C1C-C2C	-2.46	119.95	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	d	402	CLA	C3B-C2B-C1B	-2.46	104.27	107.17
20	c	504	CLA	C1D-CHD-C4C	-2.46	120.79	126.02
20	B	609	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
27	A	411	PL9	C15-C14-C16	2.46	119.50	115.23
20	b	614	CLA	C3B-C4B-NB	2.46	112.73	110.53
20	b	609	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
20	B	603	CLA	CMB-C2B-C3B	2.46	132.33	126.55
20	c	509	CLA	O2A-CGA-CBA	2.46	119.33	111.83
20	c	505	CLA	C4B-C3B-C2B	-2.46	104.25	107.30
32	d	401	HTG	C1-C2-C3	2.46	115.35	110.55
20	B	616	CLA	C1-C2-C3	-2.46	122.17	126.20
32	b	601	HTG	C2'-C1'-S1	-2.46	104.09	112.36
20	C	506	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
20	B	615	CLA	C4C-C3C-C2C	-2.45	103.32	106.89
20	C	509	CLA	CHC-C4B-C3B	-2.45	116.72	127.37
34	Z	101	LMT	O1B-C4'-C5'	2.45	115.91	109.48
20	B	603	CLA	C4D-CHA-C1A	-2.45	118.32	121.24
27	d	412	PL9	C42-C41-C39	-2.45	105.06	113.19
20	c	508	CLA	C4-C3-C5	2.45	119.49	115.23
20	d	404	CLA	C4B-C3B-C2B	-2.45	104.25	107.30
20	d	404	CLA	CAC-C3C-C4C	2.45	127.98	124.79
20	b	604	CLA	CAC-C3C-C4C	2.45	127.98	124.79
22	b	621	BCR	C16-C15-C14	-2.45	118.50	123.52
23	F	101	SQD	C3-C4-C5	2.45	114.67	110.23
38	H	101	RRX	C38-C26-C25	-2.45	121.81	124.48
20	B	607	CLA	CHB-C1B-NB	-2.45	120.38	124.05
24	c	519	LMG	O7-C10-O9	-2.45	117.99	123.70
20	B	616	CLA	CHD-C4C-NC	2.45	128.02	124.23
20	B	613	CLA	CAC-C3C-C2C	-2.45	123.06	127.56
20	C	502	CLA	O2A-CGA-CBA	2.44	119.29	111.83
20	D	402	CLA	CMD-C2D-C3D	2.44	133.29	127.69
20	c	506	CLA	CAC-C3C-C4C	2.44	127.97	124.79
20	C	501	CLA	CMB-C2B-C1B	2.44	129.14	125.42
23	a	409	SQD	O9-S-O7	-2.44	105.89	113.82
20	B	601	CLA	CHC-C4B-C3B	-2.44	116.78	127.37
20	c	501	CLA	C3C-C4C-NC	2.44	113.55	110.43
20	c	502	CLA	C2A-C1A-CHA	-2.44	119.64	123.87
20	c	510	CLA	C4D-C3D-CAD	2.44	110.75	108.11
20	c	504	CLA	CHB-C1B-NB	-2.44	120.39	124.05
27	A	411	PL9	O1-C4-C3	-2.43	118.16	120.73
20	b	612	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
20	b	617	CLA	C4B-C3B-C2B	-2.43	104.28	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	602	CLA	C1-O2A-CGA	2.43	122.54	116.65
20	c	504	CLA	C3D-C4D-ND	2.43	113.94	109.99
23	l	101	SQD	O48-C23-O10	-2.43	117.55	123.63
20	c	507	CLA	C4-C3-C5	2.43	119.45	115.23
20	D	404	CLA	O2A-CGA-CBA	2.43	119.25	111.83
20	b	618	CLA	C4-C3-C2	-2.43	117.39	123.63
20	b	615	CLA	C7-C6-C5	-2.43	106.79	113.26
20	b	605	CLA	O2A-CGA-CBA	2.43	119.24	111.83
22	K	101	BCR	C8-C9-C10	-2.43	115.19	119.01
20	c	513	CLA	C4-C3-C5	2.43	119.44	115.23
22	D	405	BCR	C15-C14-C13	-2.43	123.87	127.28
20	b	609	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
36	d	408	LHG	O8-C23-C24	2.43	119.24	111.83
35	H	102	DGD	C6D-C5D-C4D	2.43	117.16	112.07
24	j	101	LMG	C9-C8-C7	-2.43	106.13	111.78
22	B	617	BCR	C16-C15-C14	-2.43	118.56	123.52
20	d	402	CLA	O1D-CGD-CBD	2.42	129.30	124.52
20	b	611	CLA	O2D-CGD-CBD	2.42	115.47	111.23
22	d	405	BCR	C7-C8-C9	-2.42	122.65	126.23
27	A	411	PL9	O2-C1-C2	-2.42	116.32	121.83
20	b	610	CLA	CMD-C2D-C3D	2.42	133.24	127.69
20	D	402	CLA	C1D-CHD-C4C	-2.42	120.87	126.02
23	A	412	SQD	O48-C23-O10	-2.42	117.57	123.63
20	B	615	CLA	CHD-C1D-ND	-2.42	121.40	124.80
20	c	504	CLA	CHA-C4D-ND	2.42	137.54	132.55
27	D	412	PL9	C27-C28-C29	-2.42	122.09	127.62
27	a	415	PL9	C45-C44-C46	2.42	119.43	115.23
20	B	616	CLA	C11-C10-C8	-2.41	107.94	115.97
32	v	210	HTG	O5-C1-S1	2.41	116.57	109.94
20	b	611	CLA	CMD-C2D-C1D	2.41	128.98	124.73
20	b	617	CLA	C11-C10-C8	-2.41	107.94	115.97
20	c	511	CLA	C1D-CHD-C4C	-2.41	120.89	126.02
20	B	616	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
20	B	612	CLA	CBC-CAC-C3C	-2.41	105.89	112.42
20	b	608	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
20	B	604	CLA	CHC-C4B-NB	2.41	127.66	124.05
40	v	201	HEC	CHA-C1A-NA	2.41	127.08	124.45
20	b	605	CLA	C2D-C1D-ND	2.41	112.51	110.13
20	C	513	CLA	C2A-C1A-CHA	-2.41	119.69	123.87
35	h	101	DGD	C6D-C5D-C4D	2.41	117.12	112.07
20	c	510	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
35	C	518	DGD	O3G-C3G-C2G	-2.40	104.98	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	618	CLA	C1D-CHD-C4C	-2.40	120.92	126.02
20	B	616	CLA	CHC-C4B-NB	2.40	127.65	124.05
20	C	502	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
32	V	202	HTG	O2-C2-C1	2.40	114.56	110.30
32	c	520	HTG	C3-C4-C5	2.40	114.58	110.23
22	B	619	BCR	C23-C22-C21	-2.40	115.24	119.01
20	a	403	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
20	B	603	CLA	C1D-CHD-C4C	-2.40	120.92	126.02
27	d	412	PL9	C25-C24-C26	2.40	119.39	115.23
22	B	618	BCR	C30-C25-C26	-2.40	119.36	122.64
20	c	513	CLA	C2A-C1A-CHA	-2.40	119.71	123.87
20	b	613	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
20	A	401	CLA	C1D-ND-C4D	-2.40	104.63	106.31
22	a	408	BCR	C8-C7-C6	-2.40	120.60	127.00
20	B	601	CLA	C4-C3-C5	2.40	119.39	115.23
20	D	401	CLA	CMB-C2B-C3B	2.40	132.18	126.55
20	B	612	CLA	C4C-C3C-C2C	-2.40	103.41	106.89
28	b	640	DMS	C2-S-C1	2.39	110.69	98.42
20	b	606	CLA	CHC-C4B-NB	2.39	127.64	124.05
35	D	406	DGD	C3D-C4D-C5D	2.39	114.57	110.23
20	b	616	CLA	CMC-C2C-C1C	2.39	128.77	125.03
20	B	607	CLA	CHC-C4B-C3B	-2.39	117.00	127.37
20	d	403	CLA	CHC-C1C-C2C	-2.39	120.16	126.95
20	a	404	CLA	CHA-C4D-ND	2.39	137.48	132.55
20	C	502	CLA	C2B-C1B-NB	2.39	112.80	110.33
20	C	508	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
20	B	615	CLA	C1D-CHD-C4C	-2.39	120.94	126.02
22	B	618	BCR	C28-C27-C26	-2.39	109.80	114.06
22	C	514	BCR	C29-C30-C25	2.39	113.91	110.44
20	b	611	CLA	CHC-C1C-NC	-2.39	120.72	124.31
20	B	615	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
20	b	611	CLA	CED-O2D-CGD	2.38	121.32	115.92
20	b	605	CLA	C2A-C1A-CHA	-2.38	119.73	123.87
36	E	103	LHG	O4-P-O5	2.38	120.11	110.83
21	A	403	PHO	CMB-C2B-C3B	2.38	129.44	124.68
20	C	501	CLA	CHC-C4B-NB	2.38	127.62	124.05
22	K	101	BCR	C10-C11-C12	-2.38	116.31	123.20
20	b	611	CLA	C2D-C1D-ND	2.38	112.48	110.13
20	C	506	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
20	b	617	CLA	CMD-C2D-C3D	2.38	133.15	127.69
23	A	406	SQD	O47-C7-O49	-2.38	118.14	123.70
40	v	201	HEC	CBC-CAC-C3C	-2.38	122.68	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	411	PL9	C7-C3-C4	2.38	118.87	116.91
35	d	416	DGD	O3G-C1D-C2D	2.38	111.88	108.27
40	v	201	HEC	CMB-C2B-C1B	-2.38	121.80	125.42
34	M	101	LMT	C3'-C4'-C5'	-2.38	105.66	110.93
20	b	612	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
20	B	615	CLA	C3D-C4D-ND	2.38	113.85	109.99
27	D	412	PL9	C35-C34-C36	2.38	119.35	115.23
20	b	605	CLA	C1-O2A-CGA	2.38	122.40	116.65
34	a	418	LMT	O1B-C4'-C5'	2.37	115.71	109.48
36	d	408	LHG	O8-C23-O10	-2.37	117.69	123.63
20	b	611	CLA	CHD-C1D-ND	-2.37	121.46	124.80
20	c	506	CLA	CBC-CAC-C3C	-2.37	105.99	112.42
22	T	101	BCR	C12-C13-C14	-2.37	115.28	119.01
20	b	616	CLA	CHC-C4B-C3B	-2.37	117.08	127.37
34	b	627	LMT	C2'-C3'-C4'	2.37	115.06	109.68
22	B	618	BCR	C33-C5-C6	-2.37	121.90	124.48
20	c	513	CLA	CHC-C1C-NC	-2.37	120.74	124.31
20	c	509	CLA	C1-O2A-CGA	2.37	122.39	116.65
20	b	611	CLA	C4C-C3C-C2C	-2.37	103.44	106.89
20	B	608	CLA	C3C-C4C-NC	2.37	113.46	110.43
20	B	613	CLA	C3C-C4C-NC	2.37	113.46	110.43
34	m	102	LMT	O1'-C1'-C2'	2.37	111.87	108.27
20	c	503	CLA	CBC-CAC-C3C	-2.37	106.01	112.42
22	K	101	BCR	C7-C6-C5	-2.36	116.11	121.56
20	c	510	CLA	C3C-C4C-NC	2.36	113.46	110.43
22	C	514	BCR	C23-C24-C25	-2.36	120.69	127.00
20	D	404	CLA	C6-C5-C3	-2.36	107.72	113.47
20	b	616	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
37	e	102	HEM	C1B-NB-C4B	2.36	108.00	105.21
24	c	519	LMG	O3-C3-C4	-2.36	104.81	110.38
20	c	509	CLA	C4D-C3D-CAD	2.36	110.67	108.11
20	c	506	CLA	C1-C2-C3	-2.36	122.33	126.20
22	K	101	BCR	C21-C20-C19	-2.36	116.37	123.20
35	H	102	DGD	O4D-C4D-C3D	-2.36	104.82	110.38
20	C	505	CLA	C2D-C1D-ND	2.36	112.46	110.13
27	d	412	PL9	C20-C19-C21	2.36	119.32	115.23
20	B	601	CLA	C4B-CHC-C1C	-2.36	120.71	126.25
20	A	401	CLA	C2A-C1A-CHA	-2.36	119.78	123.87
20	c	503	CLA	C1D-CHD-C4C	-2.36	121.01	126.02
20	B	609	CLA	C1D-CHD-C4C	-2.35	121.02	126.02
20	B	601	CLA	O2A-CGA-CBA	2.35	119.00	111.83
20	b	608	CLA	C3C-C4C-NC	2.35	113.44	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	k	102	BCR	C37-C22-C23	2.35	121.68	118.09
20	c	507	CLA	C4B-CHC-C1C	-2.35	120.72	126.25
20	B	606	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
20	C	501	CLA	CAC-C3C-C4C	2.35	127.84	124.79
20	B	615	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
20	c	502	CLA	C6-C5-C3	-2.35	107.75	113.47
24	A	407	LMG	O8-C28-C29	2.35	118.99	111.83
20	C	503	CLA	CHC-C1C-NC	-2.34	120.78	124.31
20	c	511	CLA	CHC-C1C-NC	-2.34	120.78	124.31
20	b	614	CLA	CHC-C4B-C3B	-2.34	117.20	127.37
20	b	610	CLA	O2A-CGA-CBA	2.34	118.98	111.83
27	a	415	PL9	C20-C19-C21	2.34	119.29	115.23
20	b	614	CLA	O2A-CGA-CBA	2.34	118.98	111.83
20	B	611	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	t	101	BCR	C2-C1-C6	2.34	113.84	110.44
27	A	411	PL9	C37-C38-C39	-2.34	122.26	127.62
20	B	611	CLA	O2A-CGA-CBA	2.34	118.97	111.83
20	c	502	CLA	OBD-CAD-C3D	-2.34	122.94	128.42
22	K	101	BCR	C1-C6-C7	2.34	122.00	115.65
20	b	613	CLA	CHD-C4C-NC	2.34	127.86	124.23
35	c	517	DGD	C3A-C2A-C1A	2.34	122.27	113.69
20	c	501	CLA	C1D-CHD-C4C	-2.34	121.05	126.02
32	B	622	HTG	C1-O5-C5	2.34	116.75	112.56
22	D	405	BCR	C28-C27-C26	-2.34	109.89	114.06
21	a	405	PHO	C4D-CHA-CBD	-2.34	107.33	108.45
32	C	534	HTG	C3-C4-C5	2.34	114.47	110.23
27	a	415	PL9	C15-C14-C16	2.33	119.28	115.23
20	a	403	CLA	CHC-C1C-NC	2.33	127.83	124.31
20	b	607	CLA	C4B-C3B-C2B	-2.33	104.40	107.30
20	b	605	CLA	C7-C6-C5	-2.33	107.04	113.26
20	C	502	CLA	C1-C2-C3	-2.33	122.38	126.20
20	C	511	CLA	CHB-C4A-NA	2.33	127.76	124.40
20	B	601	CLA	C1D-CHD-C4C	-2.33	121.06	126.02
20	B	613	CLA	CBC-CAC-C3C	-2.33	106.10	112.42
38	x	101	RRX	C16-C15-C14	-2.33	118.75	123.52
20	B	614	CLA	CAC-C3C-C4C	2.33	127.82	124.79
20	C	503	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
22	k	101	BCR	C8-C7-C6	-2.33	120.77	127.00
20	b	604	CLA	CMA-C3A-C4A	-2.33	105.52	111.77
20	C	511	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
22	c	514	BCR	C29-C30-C25	2.33	113.82	110.44
20	a	403	CLA	CHD-C1D-ND	-2.33	121.53	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	610	CLA	C3C-C4C-NC	2.32	113.41	110.43
20	c	509	CLA	CHC-C4B-C3B	-2.32	117.29	127.37
20	d	404	CLA	C1-C2-C3	-2.32	122.39	126.20
20	C	502	CLA	C3B-C2B-C1B	-2.32	104.43	107.17
20	C	505	CLA	CMC-C2C-C1C	2.32	128.66	125.03
36	d	408	LHG	O7-C7-C8	2.32	116.50	111.48
20	C	503	CLA	C1D-ND-C4D	2.32	107.94	106.31
20	C	503	CLA	CBC-CAC-C3C	-2.32	106.13	112.42
22	b	619	BCR	C21-C20-C19	-2.32	116.48	123.20
20	A	404	CLA	CMD-C2D-C1D	2.32	128.81	124.73
20	d	404	CLA	C1D-CHD-C4C	-2.32	121.10	126.02
20	b	615	CLA	CHA-C4D-ND	2.32	137.33	132.55
36	d	406	LHG	O4-P-O5	2.32	123.22	112.44
36	d	407	LHG	O7-C7-O9	-2.31	118.29	123.70
20	c	503	CLA	CMB-C2B-C1B	2.31	128.94	125.42
20	b	603	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
20	b	605	CLA	C1D-CHD-C4C	-2.31	121.10	126.02
20	C	508	CLA	CHD-C4C-NC	2.31	127.82	124.23
35	H	102	DGD	O2G-C1B-C2B	2.31	116.48	111.48
20	C	512	CLA	CHC-C4B-NB	2.31	127.52	124.05
20	C	503	CLA	C4-C3-C5	2.31	119.24	115.23
20	b	610	CLA	C4A-NA-C1A	2.31	107.73	106.68
35	C	517	DGD	O5D-C6D-C5D	2.31	114.63	109.42
24	J	101	LMG	O7-C10-C11	2.31	116.48	111.48
20	D	401	CLA	C4C-C3C-C2C	-2.31	103.53	106.89
21	a	406	PHO	CMB-C2B-C3B	2.31	129.30	124.68
20	b	604	CLA	CHC-C1C-NC	-2.31	120.83	124.31
20	b	603	CLA	CED-O2D-CGD	2.31	121.16	115.92
20	C	508	CLA	CMB-C2B-C1B	2.31	128.94	125.42
20	c	501	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
20	B	609	CLA	CBB-CAB-C3B	-2.31	116.00	127.53
22	b	621	BCR	C24-C25-C26	-2.31	116.24	121.56
22	D	405	BCR	C40-C30-C25	-2.31	106.62	110.24
20	B	604	CLA	CHA-C4D-ND	2.31	137.31	132.55
20	b	609	CLA	C4C-C3C-C2C	-2.30	103.54	106.89
24	C	519	LMG	C9-C8-C7	-2.30	106.41	111.78
22	t	101	BCR	C7-C8-C9	-2.30	122.83	126.23
20	b	614	CLA	C3D-C4D-ND	2.30	113.73	109.99
32	V	202	HTG	O5-C5-C6	2.30	112.14	106.44
20	b	611	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
20	b	609	CLA	CHC-C4B-C3B	-2.30	117.39	127.37
20	d	403	CLA	CHC-C4B-C3B	-2.30	117.39	127.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	405	BCR	C30-C25-C24	2.30	121.88	115.65
20	b	616	CLA	CHA-C4D-ND	2.30	137.29	132.55
20	B	612	CLA	CMC-C2C-C1C	2.30	128.62	125.03
36	d	407	LHG	O8-C23-O10	-2.30	117.88	123.63
20	C	511	CLA	C4-C3-C5	2.30	119.21	115.23
20	b	606	CLA	CMC-C2C-C1C	2.30	128.62	125.03
20	b	616	CLA	C3D-C4D-ND	2.29	113.72	109.99
20	c	503	CLA	CMD-C2D-C1D	2.29	128.77	124.73
20	b	605	CLA	C5-C3-C2	-2.29	116.02	121.17
36	l	102	LHG	O4-P-O5	2.29	123.10	112.44
20	B	602	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
20	B	610	CLA	C1D-ND-C4D	2.29	107.92	106.31
20	d	402	CLA	CMB-C2B-C1B	2.29	128.90	125.42
20	D	402	CLA	CHA-C4D-ND	2.29	137.27	132.55
24	c	519	LMG	O8-C28-O10	-2.29	117.91	123.63
22	C	515	BCR	C24-C23-C22	-2.29	122.85	126.23
24	c	519	LMG	O1-C7-C8	-2.29	105.26	110.82
20	C	506	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
20	C	503	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
20	C	509	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
20	B	615	CLA	C4-C3-C5	2.28	119.19	115.23
20	b	616	CLA	C2A-C1A-CHA	-2.28	119.90	123.87
20	c	502	CLA	CMD-C2D-C3D	2.28	132.93	127.69
24	C	519	LMG	O6-C5-C6	2.28	112.10	106.44
20	c	510	CLA	CHB-C1B-NB	-2.28	120.62	124.05
22	b	620	BCR	C33-C5-C6	2.28	126.97	124.48
35	C	516	DGD	O1G-C1A-O1A	-2.28	117.92	123.63
35	c	515	DGD	O1G-C1G-C2G	-2.28	101.83	108.40
40	v	201	HEC	CHB-C1B-NB	2.28	127.99	123.86
20	a	407	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
20	c	503	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
24	c	518	LMG	O7-C10-O9	-2.28	118.38	123.70
20	c	508	CLA	C1-O2A-CGA	2.28	122.16	116.65
20	c	503	CLA	CAC-C3C-C4C	2.28	127.75	124.79
20	d	403	CLA	CHD-C4C-NC	2.28	127.76	124.23
34	z	102	LMT	O1'-C1'-C2'	2.28	111.73	108.27
20	B	606	CLA	OBD-CAD-C3D	-2.27	123.10	128.42
20	B	610	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
20	A	404	CLA	CHA-C4D-ND	2.27	137.24	132.55
20	C	511	CLA	CBC-CAC-C3C	-2.27	106.27	112.42
36	d	408	LHG	O4-P-O5	2.27	123.00	112.44
36	D	409	LHG	O8-C23-O10	-2.27	117.95	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	606	CLA	C4C-C3C-C2C	-2.27	103.59	106.89
20	B	602	CLA	C4D-CHA-C1A	-2.27	118.54	121.24
23	l	101	SQD	O5-C5-C4	-2.27	105.61	109.70
20	C	504	CLA	CMD-C2D-C1D	2.27	128.72	124.73
20	C	504	CLA	C4-C3-C5	2.27	119.17	115.23
20	D	404	CLA	CHD-C4C-NC	2.27	127.75	124.23
21	a	405	PHO	CMD-C2D-C3D	2.27	129.21	124.68
27	D	412	PL9	C53-C6-C1	2.27	119.92	115.28
20	A	402	CLA	C3D-C4D-ND	2.26	113.67	109.99
20	B	603	CLA	CHB-C4A-NA	2.26	127.67	124.40
27	a	415	PL9	C35-C34-C36	2.26	119.16	115.23
32	D	417	HTG	C1-C2-C3	2.26	114.97	110.55
20	c	510	CLA	C3B-C4B-NB	2.26	112.55	110.53
20	d	404	CLA	C6-C7-C8	-2.26	108.45	115.97
27	A	411	PL9	C40-C39-C41	2.26	119.15	115.23
22	T	101	BCR	C21-C20-C19	-2.26	116.65	123.20
35	C	517	DGD	O1G-C1A-O1A	-2.26	117.98	123.63
20	C	510	CLA	CMC-C2C-C3C	2.26	132.26	126.15
20	a	403	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
20	c	506	CLA	O2A-CGA-CBA	2.26	118.72	111.83
20	b	618	CLA	C1-O2A-CGA	2.26	122.11	116.65
20	b	616	CLA	C1D-CHD-C4C	-2.26	121.22	126.02
20	b	612	CLA	CMD-C2D-C1D	2.25	128.70	124.73
22	j	102	BCR	C10-C11-C12	-2.25	116.67	123.20
20	B	603	CLA	C4B-C3B-C2B	-2.25	104.50	107.30
20	c	501	CLA	CHC-C4B-C3B	-2.25	117.60	127.37
20	B	604	CLA	CHC-C4B-C3B	-2.25	117.60	127.37
22	k	102	BCR	C24-C23-C22	-2.25	122.91	126.23
34	z	102	LMT	O2'-C2'-C3'	2.25	115.68	110.38
20	c	503	CLA	CHC-C1C-NC	-2.25	120.92	124.31
34	b	627	LMT	O2'-C2'-C1'	2.25	115.44	110.08
20	C	512	CLA	OBD-CAD-C3D	-2.25	123.16	128.42
20	b	604	CLA	O2A-CGA-CBA	2.25	118.68	111.83
22	j	102	BCR	C8-C9-C10	-2.25	115.48	119.01
22	T	101	BCR	C7-C6-C5	-2.25	116.38	121.56
20	c	502	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
22	A	405	BCR	C39-C30-C25	-2.24	106.72	110.24
20	d	402	CLA	CMC-C2C-C1C	2.24	128.54	125.03
20	b	609	CLA	CGD-CBD-CAD	-2.24	103.59	110.85
20	D	401	CLA	CHB-C1B-C2B	-2.24	120.92	127.43
20	C	502	CLA	C4B-CHC-C1C	-2.24	120.98	126.25
20	C	501	CLA	O2A-CGA-O1A	-2.24	118.03	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	T	101	BCR	C20-C21-C22	-2.24	124.14	127.28
20	C	510	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
21	A	403	PHO	C7-C6-C5	-2.24	107.30	113.26
20	c	511	CLA	CHD-C1D-ND	-2.24	121.66	124.80
20	C	511	CLA	C4C-C3C-C2C	-2.24	103.64	106.89
20	b	614	CLA	CHD-C4C-NC	2.24	127.70	124.23
20	c	509	CLA	C4-C3-C5	2.24	119.11	115.23
20	b	610	CLA	C3B-C4B-NB	2.23	112.53	110.53
20	c	501	CLA	O2A-CGA-CBA	2.23	118.64	111.83
22	k	102	BCR	C20-C21-C22	-2.23	124.15	127.28
20	B	610	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
20	D	402	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
20	B	603	CLA	C4-C3-C5	2.23	119.10	115.23
20	B	601	CLA	CMC-C2C-C3C	2.23	132.18	126.15
20	c	502	CLA	CMB-C2B-C1B	2.23	128.81	125.42
20	d	404	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
20	c	510	CLA	C4-C3-C2	-2.23	117.91	123.63
23	f	101	SQD	O48-C23-O10	-2.23	118.06	123.63
20	C	509	CLA	CHC-C1C-NC	-2.23	120.96	124.31
20	c	510	CLA	C4B-C3B-C2B	-2.23	104.53	107.30
20	c	503	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
36	E	103	LHG	O7-C5-C6	2.22	115.12	108.61
20	B	610	CLA	CHD-C4C-NC	2.22	127.68	124.23
27	d	412	PL9	C22-C23-C24	-2.22	122.54	127.62
20	C	512	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
37	e	102	HEM	CHD-C4C-NC	2.22	126.87	124.45
20	C	505	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
20	c	504	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
22	k	101	BCR	C24-C23-C22	-2.22	122.95	126.23
20	B	610	CLA	C7-C6-C5	-2.22	107.35	113.26
24	j	101	LMG	O7-C10-C11	2.22	116.28	111.48
20	B	605	CLA	C3B-C4B-NB	2.22	112.51	110.53
20	C	510	CLA	CHA-C4D-ND	2.22	137.12	132.55
20	b	611	CLA	CMC-C2C-C1C	2.22	128.50	125.03
20	c	502	CLA	CHD-C1D-ND	-2.21	121.69	124.80
21	a	406	PHO	C4D-CHA-CBD	2.21	109.52	108.45
20	c	508	CLA	CHB-C4A-NA	2.21	127.59	124.40
20	c	506	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
20	B	606	CLA	CMD-C2D-C3D	2.21	132.76	127.69
23	a	409	SQD	O8-S-C6	2.21	110.24	105.97
20	b	603	CLA	C1-C2-C3	-2.21	122.57	126.20
20	B	611	CLA	CAC-C3C-C2C	2.21	131.62	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	506	CLA	CHC-C4B-C3B	-2.21	117.79	127.37
24	b	623	LMG	C13-C12-C11	2.21	121.24	113.13
22	b	621	BCR	C23-C24-C25	-2.21	121.10	127.00
23	f	101	SQD	O47-C7-O49	-2.21	118.73	122.99
20	c	510	CLA	O2A-CGA-CBA	2.21	118.56	111.83
22	T	101	BCR	C29-C30-C25	2.21	113.64	110.44
20	b	613	CLA	C6-C5-C3	2.21	118.84	113.47
20	C	511	CLA	CHC-C4B-C3B	-2.20	117.80	127.37
20	C	512	CLA	C1D-CHD-C4C	-2.20	121.34	126.02
20	a	404	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
20	B	615	CLA	C4D-C3D-CAD	2.20	110.50	108.11
20	B	601	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
20	c	513	CLA	CBB-CAB-C3B	-2.20	116.53	127.53
20	C	505	CLA	C3C-C4C-NC	2.20	113.25	110.43
20	B	613	CLA	O2A-CGA-CBA	2.20	118.54	111.83
20	C	508	CLA	O2A-CGA-CBA	2.20	118.54	111.83
20	A	402	CLA	CHA-C4D-ND	2.20	137.08	132.55
20	c	507	CLA	CHC-C4B-C3B	-2.20	117.83	127.37
20	b	606	CLA	CGD-CBD-CAD	-2.20	103.74	110.85
20	b	612	CLA	C4-C3-C5	2.20	119.04	115.23
24	J	101	LMG	O7-C10-O9	-2.20	118.57	123.70
35	D	406	DGD	O6D-C5D-C4D	2.19	113.65	109.70
20	b	605	CLA	CMD-C2D-C1D	2.19	128.59	124.73
34	z	102	LMT	C1B-O5B-C5B	2.19	118.00	113.72
20	B	616	CLA	CBB-CAB-C3B	-2.19	116.57	127.53
20	c	501	CLA	CMC-C2C-C1C	2.19	128.46	125.03
27	D	412	PL9	C2-C3-C4	2.19	121.72	118.78
20	d	402	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
20	B	608	CLA	CHB-C1B-C2B	-2.19	121.07	127.43
20	B	604	CLA	C3D-C4D-ND	2.19	113.55	109.99
20	b	608	CLA	CMD-C2D-C1D	2.19	128.58	124.73
32	d	401	HTG	C2'-C1'-S1	-2.19	104.99	112.36
28	U	902	DMS	O-S-C1	2.19	117.44	106.49
36	D	409	LHG	O8-C23-C24	2.19	118.50	111.83
32	B	621	HTG	O4-C4-C3	-2.19	105.22	110.38
20	C	507	CLA	CED-O2D-CGD	2.19	120.88	115.92
22	j	102	BCR	C1-C6-C7	2.19	121.58	115.65
20	b	606	CLA	CMD-C2D-C1D	2.19	128.58	124.73
32	b	625	HTG	C4-C3-C2	2.19	114.67	110.83
20	c	501	CLA	CHB-C1B-NB	-2.19	120.77	124.05
20	B	612	CLA	CMD-C2D-C1D	2.19	128.58	124.73
20	D	404	CLA	C2A-C1A-CHA	-2.19	120.08	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	402	CLA	C3C-C4C-NC	2.18	113.23	110.43
24	b	623	LMG	O7-C10-O9	-2.18	118.60	123.70
35	c	516	DGD	O2G-C1B-O1B	-2.18	118.60	123.70
27	a	415	PL9	C17-C18-C19	-2.18	122.62	127.62
20	a	404	CLA	CHC-C4B-C3B	-2.18	117.89	127.37
22	j	102	BCR	C21-C20-C19	-2.18	116.87	123.20
20	d	404	CLA	CHA-C4D-ND	2.18	137.05	132.55
20	C	505	CLA	C1D-CHD-C4C	-2.18	121.38	126.02
34	a	418	LMT	O3'-C3'-C2'	2.18	115.52	110.38
20	B	608	CLA	CMC-C2C-C3C	2.18	132.05	126.15
20	c	507	CLA	C3B-C4B-NB	2.18	112.48	110.53
20	b	609	CLA	CMD-C2D-C1D	2.18	128.57	124.73
32	B	621	HTG	O3-C3-C4	-2.18	105.24	110.38
35	c	517	DGD	C3E-C4E-C5E	-2.18	106.28	110.23
22	B	617	BCR	C40-C30-C25	-2.18	106.83	110.24
20	B	612	CLA	C4B-C3B-C2B	-2.18	104.59	107.30
20	C	512	CLA	CHD-C1D-ND	-2.18	121.74	124.80
20	B	605	CLA	O2A-CGA-CBA	2.18	118.47	111.83
20	a	407	CLA	O2A-CGA-CBA	2.18	118.47	111.83
24	j	101	LMG	O8-C28-C29	2.18	118.47	111.83
20	C	508	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
20	B	603	CLA	CHC-C4B-C3B	-2.17	117.94	127.37
35	C	518	DGD	O1G-C1A-C2A	2.17	118.46	111.83
22	D	405	BCR	C29-C28-C27	-2.17	106.50	111.28
20	A	404	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
22	k	102	BCR	C16-C17-C18	-2.17	124.24	127.28
23	b	622	SQD	O48-C23-O10	-2.17	118.21	123.63
21	a	406	PHO	CBC-CAC-C3C	2.16	115.97	112.87
20	A	402	CLA	CBC-CAC-C3C	-2.16	106.55	112.42
20	B	603	CLA	CBC-CAC-C3C	-2.16	106.56	112.42
20	c	509	CLA	C4C-C3C-C2C	-2.16	103.74	106.89
22	k	102	BCR	C35-C13-C12	2.16	121.39	118.09
20	b	610	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
20	b	613	CLA	CAC-C3C-C4C	2.16	127.60	124.79
22	B	617	BCR	C34-C9-C10	-2.16	119.32	122.82
22	D	405	BCR	C32-C1-C6	2.16	113.63	110.24
24	j	101	LMG	O8-C28-O10	-2.16	118.23	123.63
20	C	503	CLA	CHB-C1B-NB	-2.16	120.81	124.05
35	d	416	DGD	C4D-C3D-C2D	2.16	114.62	110.83
24	C	524	LMG	O6-C5-C6	2.15	111.78	106.44
20	a	407	CLA	CHC-C4B-C3B	-2.15	118.03	127.37
20	c	513	CLA	C1-O2A-CGA	2.15	121.85	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	609	CLA	O2A-CGA-CBA	2.15	118.39	111.83
35	C	516	DGD	C4A-C3A-C2A	-2.15	105.23	113.13
36	l	102	LHG	O7-C7-C8	2.15	116.13	111.48
20	a	403	CLA	CMD-C2D-C1D	2.15	128.51	124.73
20	B	611	CLA	C1D-ND-C4D	-2.15	104.81	106.31
27	d	412	PL9	C11-C9-C8	-2.15	116.35	121.17
35	H	102	DGD	O5E-C6E-C5E	-2.14	104.03	111.33
22	A	405	BCR	C3-C4-C5	-2.14	110.23	114.06
27	A	411	PL9	C16-C14-C13	-2.14	116.36	121.17
23	b	622	SQD	O9-S-O7	-2.14	106.86	113.82
20	D	401	CLA	C14-C13-C15	-2.14	103.64	111.27
20	b	614	CLA	CMD-C2D-C1D	2.14	128.50	124.73
22	a	408	BCR	C38-C26-C25	-2.14	122.15	124.48
20	B	605	CLA	C4-C3-C5	2.14	118.94	115.23
20	C	508	CLA	C3B-C4B-NB	2.14	112.44	110.53
20	b	616	CLA	C4B-C3B-C2B	-2.14	104.64	107.30
20	b	609	CLA	C3B-C4B-NB	2.14	112.44	110.53
22	a	408	BCR	C33-C5-C6	-2.14	122.15	124.48
20	A	401	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
23	a	409	SQD	O48-C23-C24	2.14	118.35	111.83
20	B	606	CLA	CHC-C4B-C3B	-2.14	118.09	127.37
20	B	607	CLA	C7-C6-C5	-2.14	107.57	113.26
20	c	510	CLA	CED-O2D-CGD	2.14	120.76	115.92
20	b	615	CLA	CBC-CAC-C3C	-2.14	106.63	112.42
27	A	411	PL9	C10-C9-C11	2.14	118.93	115.23
20	d	404	CLA	C6-C5-C3	-2.13	108.27	113.47
20	C	510	CLA	CHC-C4B-C3B	-2.13	118.11	127.37
20	C	502	CLA	CHD-C1D-ND	-2.13	121.80	124.80
20	c	505	CLA	C2A-C1A-CHA	-2.13	120.17	123.87
20	d	404	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
20	C	511	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
27	A	411	PL9	C51-C49-C50	2.13	119.49	114.59
34	B	625	LMT	C3'-C4'-C5'	2.13	114.09	110.23
22	K	101	BCR	C15-C16-C17	-2.13	119.16	123.52
20	B	605	CLA	CHD-C1D-ND	-2.13	121.81	124.80
22	t	101	BCR	C8-C9-C10	-2.13	115.66	119.01
20	c	504	CLA	CHC-C4B-NB	2.13	127.24	124.05
32	b	625	HTG	C3-C4-C5	-2.13	106.37	110.23
20	b	611	CLA	C4-C3-C5	2.13	118.92	115.23
20	b	606	CLA	CHD-C4C-NC	2.13	127.53	124.23
20	B	615	CLA	O2A-CGA-CBA	2.13	118.33	111.83
20	B	613	CLA	C3B-C4B-NB	2.13	112.43	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	406	PHO	C1A-C2A-C3A	-2.13	100.81	102.84
20	C	509	CLA	C1-O2A-CGA	2.13	121.80	116.65
34	I	101	LMT	O1B-C4'-C5'	2.13	115.05	109.48
20	c	509	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
32	B	622	HTG	C3-C4-C5	-2.12	106.38	110.23
20	D	401	CLA	CHC-C4B-C3B	-2.12	118.16	127.37
20	c	505	CLA	C7-C6-C5	-2.12	107.61	113.26
20	a	407	CLA	C2A-C1A-CHA	-2.12	120.18	123.87
40	V	201	HEC	O2D-CGD-CBD	2.12	120.70	114.00
20	a	403	CLA	C2B-C1B-NB	2.12	112.52	110.33
22	B	618	BCR	C8-C7-C6	-2.12	121.34	127.00
22	d	405	BCR	C30-C25-C24	2.12	121.40	115.65
34	I	101	LMT	C1B-O1B-C4'	2.12	123.00	117.98
22	a	408	BCR	C2-C1-C6	2.12	113.52	110.44
34	c	523	LMT	O5B-C1B-C2B	2.12	114.72	110.37
35	c	515	DGD	O2D-C2D-C1D	-2.12	105.03	110.08
20	c	505	CLA	CMD-C2D-C1D	2.12	128.45	124.73
20	b	616	CLA	OBD-CAD-C3D	-2.12	123.47	128.42
20	a	404	CLA	C4-C3-C5	2.11	118.90	115.23
32	d	401	HTG	C1-O5-C5	2.11	116.35	112.56
20	C	502	CLA	C4C-C3C-C2C	-2.11	103.81	106.89
20	b	617	CLA	CHC-C4B-C3B	-2.11	118.20	127.37
20	b	614	CLA	C4B-CHC-C1C	-2.11	121.28	126.25
22	T	101	BCR	C1-C6-C7	2.11	121.38	115.65
23	a	401	SQD	C1-C2-C3	-2.11	105.57	110.01
20	b	616	CLA	O2A-CGA-CBA	2.11	118.27	111.83
32	B	621	HTG	O3-C3-C2	2.11	115.35	110.38
20	c	513	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
20	B	601	CLA	C4-C3-C2	-2.11	118.21	123.63
37	e	102	HEM	C4C-NC-C1C	2.11	109.26	105.82
20	C	511	CLA	CHD-C4C-NC	2.11	127.50	124.23
36	D	407	LHG	O7-C7-O9	-2.11	118.78	123.70
20	C	501	CLA	CHC-C1C-NC	-2.11	121.14	124.31
20	C	512	CLA	CHB-C4A-NA	2.11	127.44	124.40
34	E	101	LMT	O5'-C5'-C6'	2.11	111.66	106.44
24	C	519	LMG	O7-C10-O9	-2.11	118.78	123.70
20	d	404	CLA	CHC-C4B-C3B	-2.11	118.23	127.37
20	A	404	CLA	C5-C3-C2	-2.10	116.44	121.17
38	H	101	RRX	C21-C20-C19	-2.10	117.10	123.20
22	b	619	BCR	C35-C13-C12	2.10	121.30	118.09
20	B	612	CLA	C16-C15-C13	2.10	122.95	115.97
20	C	513	CLA	C4B-C3B-C2B	-2.10	104.69	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	d	403	CLA	C6-C5-C3	-2.10	108.35	113.47
20	c	507	CLA	CMC-C2C-C3C	2.10	131.83	126.15
22	j	102	BCR	C7-C6-C5	-2.10	116.72	121.56
21	a	405	PHO	CAC-C3C-C4C	2.10	129.43	124.03
34	B	627	LMT	O5'-C1'-O1'	-2.10	108.91	112.83
20	B	605	CLA	C4C-C3C-C2C	-2.10	103.84	106.89
20	b	613	CLA	C4C-C3C-C2C	-2.10	103.84	106.89
20	b	605	CLA	CHC-C4B-C3B	-2.10	118.27	127.37
20	c	502	CLA	C3B-C4B-NB	2.10	112.40	110.53
28	C	532	DMS	O-S-C2	2.10	116.98	106.49
20	c	504	CLA	C4C-C3C-C2C	-2.10	103.84	106.89
20	C	504	CLA	C7-C6-C5	-2.09	107.68	113.26
20	b	608	CLA	C7-C6-C5	-2.09	107.68	113.26
20	B	613	CLA	CBB-CAB-C3B	-2.09	117.07	127.53
34	I	101	LMT	C2'-C3'-C4'	-2.09	104.93	109.68
22	t	101	BCR	C33-C5-C4	2.09	118.06	113.60
20	C	503	CLA	CMB-C2B-C1B	2.09	128.60	125.42
20	b	604	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
20	B	614	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
22	B	619	BCR	C37-C22-C21	2.09	126.20	122.82
20	B	609	CLA	C2A-C3A-C4A	-2.09	98.49	101.87
20	C	511	CLA	CHB-C1B-NB	-2.09	120.92	124.05
21	D	403	PHO	C1A-C2A-C3A	-2.09	100.85	102.84
20	b	618	CLA	CED-O2D-CGD	2.09	120.65	115.92
22	t	101	BCR	C40-C30-C25	-2.09	106.97	110.24
35	c	515	DGD	CDB-CCB-CBB	-2.09	103.82	114.37
22	b	619	BCR	C15-C14-C13	-2.09	124.35	127.28
20	C	509	CLA	CED-O2D-CGD	2.09	120.65	115.92
22	d	405	BCR	C34-C9-C10	-2.09	119.44	122.82
22	D	405	BCR	C30-C25-C26	-2.09	119.79	122.64
34	b	628	LMT	C6'-C5'-C4'	-2.09	107.52	113.38
20	b	604	CLA	C4B-CHC-C1C	2.09	131.15	126.25
22	B	617	BCR	C16-C17-C18	-2.08	124.35	127.28
20	C	504	CLA	OBD-CAD-C3D	-2.08	123.54	128.42
20	c	507	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
20	B	605	CLA	CHC-C4B-C3B	-2.08	118.33	127.37
20	b	607	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
20	C	512	CLA	CHB-C1B-NB	-2.08	120.92	124.05
20	A	402	CLA	C1-C2-C3	-2.08	122.78	126.20
22	d	405	BCR	C34-C9-C8	2.08	121.27	118.09
20	C	508	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
21	a	405	PHO	OBD-CAD-C3D	-2.08	124.64	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	607	CLA	CHD-C4C-NC	2.08	127.46	124.23
20	C	503	CLA	CBB-CAB-C3B	-2.08	117.12	127.53
35	c	516	DGD	C6D-O5D-C1E	2.08	118.26	113.80
27	d	412	PL9	C35-C34-C36	2.08	118.84	115.23
22	C	514	BCR	C11-C10-C9	-2.08	124.36	127.28
27	d	412	PL9	C37-C36-C34	-2.08	106.29	113.19
20	C	502	CLA	CHC-C4B-NB	2.08	127.17	124.05
34	m	102	LMT	O5B-C5B-C6B	2.08	111.59	106.44
22	b	619	BCR	C23-C24-C25	-2.08	121.44	127.00
34	M	101	LMT	O5B-C5B-C6B	2.08	111.59	106.44
20	b	616	CLA	CHB-C1B-NB	-2.08	120.93	124.05
23	A	406	SQD	O5-C1-C2	-2.07	106.11	110.37
37	E	104	HEM	C1B-NB-C4B	2.07	107.66	105.21
20	c	502	CLA	CHC-C4B-C3B	-2.07	118.37	127.37
27	d	412	PL9	C36-C37-C38	-2.07	101.77	112.02
36	d	407	LHG	O7-C7-C8	2.07	115.96	111.48
22	C	514	BCR	C33-C5-C6	-2.07	122.23	124.48
20	b	608	CLA	C4B-CHC-C1C	-2.07	121.38	126.25
20	B	609	CLA	C11-C10-C8	-2.07	109.09	115.97
20	B	604	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
20	A	404	CLA	C1-C2-C3	-2.07	122.81	126.20
37	E	104	HEM	CAD-C3D-C4D	2.07	128.30	124.70
22	K	101	BCR	C20-C21-C22	-2.07	124.38	127.28
23	f	101	SQD	O5-C5-C4	2.07	113.42	109.70
22	A	405	BCR	C37-C22-C21	2.07	126.16	122.82
20	a	407	CLA	C1-O2A-CGA	2.07	122.54	116.67
20	b	615	CLA	C12-C11-C10	-2.07	104.02	113.28
20	c	504	CLA	C4D-C3D-CAD	2.07	110.35	108.11
20	B	613	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
20	D	401	CLA	CHC-C1C-C2C	-2.06	121.08	126.95
20	b	609	CLA	C4B-CHC-C1C	-2.06	121.39	126.25
20	b	613	CLA	C7-C6-C5	-2.06	107.76	113.26
22	k	102	BCR	C7-C8-C9	-2.06	123.19	126.23
20	d	403	CLA	C2A-C1A-CHA	-2.06	120.29	123.87
20	b	618	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
20	C	513	CLA	CHC-C4B-C3B	-2.06	118.43	127.37
22	A	405	BCR	C8-C7-C6	-2.06	121.50	127.00
20	C	507	CLA	CMB-C2B-C1B	2.06	128.55	125.42
20	C	512	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
20	C	511	CLA	CAC-C3C-C4C	2.06	127.47	124.79
20	B	610	CLA	C1D-CHD-C4C	-2.06	121.65	126.02
20	b	612	CLA	O1D-CGD-CBD	-2.06	120.46	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	h	101	DGD	O3G-C3G-C2G	-2.06	105.82	110.82
20	c	508	CLA	CMD-C2D-C1D	2.06	128.35	124.73
20	C	510	CLA	C4C-C3C-C2C	-2.05	103.90	106.89
20	B	614	CLA	C1-C2-C3	-2.05	122.83	126.20
34	b	627	LMT	C1-O1'-C1'	2.05	117.19	113.68
20	B	613	CLA	CHC-C4B-C3B	-2.05	118.46	127.37
20	C	507	CLA	CHB-C1B-NB	-2.05	120.97	124.05
20	C	507	CLA	C4B-C3B-C2B	-2.05	104.75	107.30
35	C	516	DGD	O1G-C1G-C2G	-2.05	102.48	108.40
20	c	508	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
27	d	412	PL9	C32-C33-C34	-2.05	122.93	127.62
20	A	404	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
22	k	102	BCR	C15-C14-C13	-2.05	124.40	127.28
22	C	514	BCR	C20-C21-C22	-2.05	124.41	127.28
22	b	620	BCR	C15-C16-C17	-2.05	119.33	123.52
34	f	102	LMT	O1B-C4'-C5'	2.05	114.37	109.32
20	b	604	CLA	CAA-CBA-CGA	-2.05	107.40	113.21
40	V	201	HEC	CHD-C4C-NC	2.05	126.68	124.45
20	a	404	CLA	C7-C6-C5	-2.05	107.81	113.26
20	b	605	CLA	C2A-C3A-C4A	-2.04	98.57	101.87
20	c	504	CLA	CHC-C4B-C3B	-2.04	118.51	127.37
20	c	508	CLA	CHC-C1C-NC	-2.04	121.23	124.31
20	B	612	CLA	C4B-CHC-C1C	-2.04	121.45	126.25
20	b	615	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
20	c	509	CLA	CMB-C2B-C1B	2.04	128.53	125.42
37	e	102	HEM	C4C-C3C-C2C	2.04	108.58	106.81
20	d	402	CLA	CHD-C4C-C3C	-2.04	121.80	124.77
20	c	501	CLA	CBB-CAB-C3B	-2.04	117.35	127.53
22	c	514	BCR	C32-C1-C31	2.04	114.47	108.63
36	d	407	LHG	O2-C2-C3	-2.04	102.66	109.70
32	B	631	HTG	O5-C1-C2	-2.04	107.51	110.32
20	B	606	CLA	CMB-C2B-C3B	2.04	131.34	126.55
20	c	501	CLA	C4-C3-C5	2.03	118.76	115.23
20	B	604	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
20	b	606	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
22	K	101	BCR	C34-C9-C8	2.03	121.19	118.09
35	h	101	DGD	O2G-C1B-O1B	-2.03	118.96	123.70
22	c	514	BCR	C34-C9-C8	2.03	121.19	118.09
34	m	101	LMT	C1B-O1B-C4'	-2.03	113.17	117.98
34	z	102	LMT	O2B-C2B-C3B	2.03	115.16	110.38
38	H	101	RRX	C20-C19-C18	-2.03	120.80	126.36
20	c	505	CLA	CHC-C1C-NC	-2.03	121.26	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	E	104	HEM	C3B-C4B-NB	-2.03	108.01	109.47
20	c	503	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
20	d	404	CLA	CBC-CAC-C3C	-2.02	106.93	112.42
22	b	621	BCR	C23-C22-C21	-2.02	115.83	119.01
32	B	622	HTG	O4-C4-C5	2.02	114.31	109.32
32	O	302	HTG	C4-C3-C2	2.02	114.38	110.83
20	b	615	CLA	C3C-C4C-NC	2.02	113.02	110.43
20	C	505	CLA	C1-O2A-CGA	2.02	121.54	116.65
21	A	403	PHO	C1A-C2A-C3A	-2.02	100.92	102.84
27	D	412	PL9	C11-C9-C8	-2.02	116.63	121.17
36	d	407	LHG	O8-C23-C24	2.02	117.99	111.83
20	A	402	CLA	CHB-C4A-NA	2.02	127.31	124.40
20	A	401	CLA	CHD-C1D-ND	-2.02	121.96	124.80
22	B	619	BCR	C16-C15-C14	-2.02	119.39	123.52
36	d	407	LHG	C13-C12-C11	-2.02	104.17	114.37
20	B	614	CLA	CBB-CAB-C3B	-2.02	117.44	127.53
20	B	612	CLA	CHD-C1D-ND	-2.02	121.97	124.80
22	D	405	BCR	C2-C1-C6	2.02	113.37	110.44
20	A	404	CLA	C4C-C3C-C2C	-2.02	103.96	106.89
35	C	518	DGD	C3G-C2G-C1G	-2.02	107.09	111.78
20	C	513	CLA	CHC-C1C-NC	-2.02	121.28	124.31
20	B	602	CLA	CED-O2D-CGD	2.01	120.49	115.92
23	a	401	SQD	O9-S-C6	2.01	109.76	106.76
20	C	512	CLA	CMD-C2D-C3D	2.01	132.31	127.69
20	c	501	CLA	C1-O2A-CGA	2.01	121.53	116.65
24	j	101	LMG	O1-C7-C8	-2.01	105.92	110.82
20	c	502	CLA	CBB-CAB-C3B	-2.01	117.47	127.53
22	A	405	BCR	C7-C8-C9	-2.01	123.26	126.23
20	B	601	CLA	C3B-C4B-NB	2.01	112.32	110.53
20	B	616	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
34	B	626	LMT	O3'-C3'-C4'	-2.01	105.64	110.38
20	c	502	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
35	h	101	DGD	O5D-C1E-C2E	2.01	111.32	108.27
20	b	614	CLA	C2B-C1B-NB	2.01	112.41	110.33
36	d	406	LHG	C11-C10-C9	-2.01	104.22	114.37
20	b	606	CLA	CHB-C4A-NA	2.01	127.30	124.40
22	t	101	BCR	C3-C4-C5	-2.01	110.48	114.06
22	j	102	BCR	C16-C15-C14	-2.01	119.42	123.52
20	B	607	CLA	C3B-C4B-NB	2.01	112.32	110.53
20	B	611	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
23	l	101	SQD	C25-C24-C23	-2.00	106.35	113.69
20	C	503	CLA	C7-C6-C5	-2.00	107.92	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	101	BCR	C23-C22-C21	-2.00	115.86	119.01
20	c	507	CLA	CED-O2D-CGD	2.00	120.46	115.92
20	B	603	CLA	C1-C2-C3	-2.00	122.91	126.20
22	C	514	BCR	C37-C22-C23	2.00	121.15	118.09
20	D	402	CLA	CAC-C3C-C2C	-2.00	123.88	127.56
20	b	614	CLA	CHA-C4D-ND	2.00	136.68	132.55
20	c	510	CLA	CHB-C4A-NA	2.00	127.29	124.40
20	B	616	CLA	C4C-C3C-C2C	-2.00	103.98	106.89
35	C	516	DGD	C1E-O6E-C5E	2.00	117.63	113.72
20	c	503	CLA	CHC-C4B-C3B	-2.00	118.69	127.37

All (50) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	401	CLA	ND
20	B	601	CLA	ND
20	B	602	CLA	ND
20	B	603	CLA	ND
20	B	604	CLA	ND
20	B	605	CLA	ND
20	B	606	CLA	ND
20	B	607	CLA	ND
20	B	608	CLA	ND
20	B	610	CLA	ND
20	B	611	CLA	ND
20	B	612	CLA	ND
20	B	613	CLA	ND
20	B	614	CLA	ND
20	B	615	CLA	ND
20	B	616	CLA	ND
20	C	501	CLA	ND
20	C	505	CLA	ND
20	C	506	CLA	ND
20	C	507	CLA	ND
20	C	508	CLA	ND
20	C	509	CLA	ND
20	C	510	CLA	ND
20	C	512	CLA	ND
20	D	401	CLA	ND
20	D	404	CLA	ND
20	a	403	CLA	ND
20	b	603	CLA	ND

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Mol	Chain	Res	Type	Atom
20	b	604	CLA	ND
20	b	605	CLA	ND
20	b	606	CLA	ND
20	b	607	CLA	ND
20	b	608	CLA	ND
20	b	609	CLA	ND
20	b	612	CLA	ND
20	b	614	CLA	ND
20	b	615	CLA	ND
20	b	616	CLA	ND
20	b	617	CLA	ND
20	b	618	CLA	ND
20	c	501	CLA	ND
20	c	504	CLA	ND
20	c	505	CLA	ND
20	c	506	CLA	ND
20	c	507	CLA	ND
20	c	509	CLA	ND
20	c	510	CLA	ND
20	c	511	CLA	ND
20	c	512	CLA	ND
20	d	402	CLA	ND

All (1332) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	B	601	CLA	C11-C10-C8-C9
20	B	602	CLA	CBA-CGA-O2A-C1
20	B	602	CLA	O1A-CGA-O2A-C1
20	B	602	CLA	CAD-CBD-CGD-O2D
20	B	607	CLA	C11-C12-C13-C14
20	B	608	CLA	CAD-CBD-CGD-O2D
20	B	615	CLA	CAD-CBD-CGD-O1D
20	B	615	CLA	CAD-CBD-CGD-O2D
20	C	502	CLA	CAD-CBD-CGD-O1D
20	C	507	CLA	CHA-CBD-CGD-O1D
20	C	507	CLA	CHA-CBD-CGD-O2D
20	C	509	CLA	C11-C10-C8-C9
20	b	603	CLA	CAD-CBD-CGD-O2D
20	b	603	CLA	C11-C10-C8-C9
20	b	608	CLA	C6-C7-C8-C10
20	b	616	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	b	616	CLA	CAD-CBD-CGD-O2D
20	b	618	CLA	CHA-CBD-CGD-O1D
20	c	502	CLA	CAD-CBD-CGD-O2D
20	c	507	CLA	CHA-CBD-CGD-O1D
20	c	507	CLA	CHA-CBD-CGD-O2D
20	c	509	CLA	CHA-CBD-CGD-O1D
22	D	405	BCR	C21-C22-C23-C24
22	D	405	BCR	C37-C22-C23-C24
22	d	405	BCR	C37-C22-C23-C24
22	k	101	BCR	C7-C8-C9-C10
22	t	101	BCR	C11-C12-C13-C14
22	t	101	BCR	C11-C12-C13-C35
23	F	101	SQD	C44-C45-C46-O48
23	a	401	SQD	C2-C1-O6-C44
23	a	401	SQD	O6-C44-C45-O47
23	b	622	SQD	O5-C1-O6-C44
23	b	622	SQD	C46-C45-O47-C7
23	b	622	SQD	O49-C7-O47-C45
23	b	622	SQD	C8-C7-O47-C45
23	f	101	SQD	C8-C7-O47-C45
23	f	101	SQD	C5-C6-S-O8
23	l	101	SQD	C8-C7-O47-C45
23	l	101	SQD	O10-C23-O48-C46
23	l	101	SQD	C24-C23-O48-C46
23	l	101	SQD	O5-C5-C6-S
24	C	524	LMG	C11-C10-O7-C8
27	a	415	PL9	C9-C11-C12-C13
27	a	415	PL9	C25-C24-C26-C27
32	B	622	HTG	C2'-C1'-S1-C1
32	B	623	HTG	O5-C1-S1-C1'
32	C	522	HTG	O5-C1-S1-C1'
32	V	202	HTG	C2-C1-S1-C1'
32	c	520	HTG	O5-C1-S1-C1'
32	c	521	HTG	C2'-C1'-S1-C1
32	d	401	HTG	C2-C1-S1-C1'
32	d	401	HTG	O5-C1-S1-C1'
34	B	627	LMT	C2-C1-O1'-C1'
34	m	101	LMT	O5'-C1'-O1'-C1
35	D	406	DGD	C2B-C1B-O2G-C2G
35	D	406	DGD	C2D-C1D-O3G-C3G
35	D	406	DGD	O6D-C1D-O3G-C3G
36	D	408	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
36	D	408	LHG	C4-O6-P-O4
36	E	103	LHG	O1-C1-C2-C3
36	E	103	LHG	C6-C5-O7-C7
36	L	101	LHG	C4-O6-P-O3
36	L	101	LHG	C4-O6-P-O4
36	L	101	LHG	C4-O6-P-O5
36	d	407	LHG	O1-C1-C2-C3
36	d	407	LHG	C3-O3-P-O5
36	l	102	LHG	C4-O6-P-O3
36	l	102	LHG	C4-O6-P-O4
36	l	102	LHG	C4-O6-P-O5
40	V	201	HEC	C2B-C3B-CAB-CBB
40	V	201	HEC	C4B-C3B-CAB-CBB
40	V	201	HEC	C2C-C3C-CAC-CBC
40	V	201	HEC	C4C-C3C-CAC-CBC
40	v	201	HEC	C2B-C3B-CAB-CBB
40	v	201	HEC	C4B-C3B-CAB-CBB
40	v	201	HEC	C2C-C3C-CAC-CBC
40	v	201	HEC	C4C-C3C-CAC-CBC
23	f	101	SQD	O49-C7-O47-C45
34	z	102	LMT	O5B-C1B-O1B-C4'
23	F	101	SQD	O10-C23-O48-C46
36	E	103	LHG	O10-C23-O8-C6
20	B	611	CLA	C15-C16-C17-C18
36	E	103	LHG	C8-C7-O7-C5
36	E	103	LHG	C24-C23-O8-C6
35	d	416	DGD	O1A-C1A-O1G-C1G
36	E	103	LHG	O9-C7-O7-C5
34	b	627	LMT	C2B-C1B-O1B-C4'
20	b	617	CLA	C13-C15-C16-C17
34	I	101	LMT	C3'-C4'-O1B-C1B
23	l	101	SQD	O49-C7-O47-C45
24	C	524	LMG	O9-C10-O7-C8
20	B	601	CLA	C3-C5-C6-C7
20	B	602	CLA	C3-C5-C6-C7
20	b	603	CLA	C3-C5-C6-C7
23	F	101	SQD	C24-C23-O48-C46
20	B	606	CLA	C4-C3-C5-C6
20	b	616	CLA	C4-C3-C5-C6
20	b	618	CLA	C4-C3-C5-C6
20	A	404	CLA	C2-C3-C5-C6
20	B	606	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	b	618	CLA	C2-C3-C5-C6
27	a	415	PL9	C23-C24-C26-C27
20	B	615	CLA	C3-C5-C6-C7
23	b	622	SQD	C24-C23-O48-C46
35	d	416	DGD	C2A-C1A-O1G-C1G
32	v	210	HTG	O5-C5-C6-O6
34	Z	101	LMT	O5B-C5B-C6B-O6B
35	D	406	DGD	O1B-C1B-O2G-C2G
20	B	605	CLA	C3-C5-C6-C7
32	C	534	HTG	O5-C5-C6-O6
32	c	521	HTG	O5-C5-C6-O6
34	m	101	LMT	O5'-C5'-C6'-O6'
34	z	102	LMT	C4'-C5'-C6'-O6'
34	z	102	LMT	C3'-C4'-O1B-C1B
34	c	523	LMT	O5'-C5'-C6'-O6'
20	C	513	CLA	CBD-CGD-O2D-CED
32	c	520	HTG	C4-C5-C6-O6
32	C	520	HTG	S1-C1'-C2'-C3'
32	D	417	HTG	S1-C1'-C2'-C3'
34	B	627	LMT	O1'-C1'-O5'-C5'
20	A	404	CLA	C4-C3-C5-C6
20	B	601	CLA	C4-C3-C5-C6
27	a	415	PL9	C30-C29-C31-C32
20	B	601	CLA	C2-C3-C5-C6
20	b	607	CLA	C2-C3-C5-C6
20	b	616	CLA	C2-C3-C5-C6
27	a	415	PL9	C28-C29-C31-C32
23	b	622	SQD	O10-C23-O48-C46
34	a	418	LMT	O5'-C5'-C6'-O6'
34	b	627	LMT	O5'-C5'-C6'-O6'
35	d	416	DGD	O6D-C5D-C6D-O5D
27	A	411	PL9	C9-C11-C12-C13
27	A	411	PL9	C24-C26-C27-C28
27	a	415	PL9	C14-C16-C17-C18
32	v	210	HTG	C4-C5-C6-O6
34	b	627	LMT	C4B-C5B-C6B-O6B
32	D	417	HTG	O5-C5-C6-O6
24	A	407	LMG	O10-C28-O8-C9
23	A	412	SQD	O5-C1-O6-C44
34	a	418	LMT	O5'-C1'-O1'-C1
34	f	102	LMT	O5'-C1'-O1'-C1
34	z	102	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
32	B	623	HTG	O5-C5-C6-O6
32	c	520	HTG	O5-C5-C6-O6
34	J	103	LMT	O5'-C5'-C6'-O6'
34	z	102	LMT	O5'-C5'-C6'-O6'
34	Z	101	LMT	C4B-C5B-C6B-O6B
20	C	513	CLA	CBA-CGA-O2A-C1
24	A	407	LMG	C29-C28-O8-C9
36	D	409	LHG	C31-C32-C33-C34
32	B	631	HTG	O5-C5-C6-O6
34	T	102	LMT	O5'-C5'-C6'-O6'
34	f	102	LMT	O5'-C5'-C6'-O6'
34	f	102	LMT	C4'-C5'-C6'-O6'
24	a	410	LMG	C37-C38-C39-C40
34	T	102	LMT	C4'-C5'-C6'-O6'
20	C	513	CLA	O1A-CGA-O2A-C1
24	c	519	LMG	O10-C28-O8-C9
23	f	101	SQD	C24-C23-O48-C46
24	c	519	LMG	C29-C28-O8-C9
32	B	622	HTG	C3'-C4'-C5'-C6'
35	c	515	DGD	C2A-C3A-C4A-C5A
20	b	618	CLA	CBD-CGD-O2D-CED
23	l	101	SQD	C31-C32-C33-C34
24	b	623	LMG	C10-C11-C12-C13
23	b	622	SQD	C31-C32-C33-C34
32	B	631	HTG	C4-C5-C6-O6
34	b	627	LMT	C4'-C5'-C6'-O6'
20	B	602	CLA	C11-C10-C8-C9
20	C	504	CLA	C11-C12-C13-C14
20	b	603	CLA	C14-C13-C15-C16
20	c	506	CLA	C6-C7-C8-C9
20	c	513	CLA	C11-C10-C8-C9
20	c	513	CLA	C14-C13-C15-C16
32	D	417	HTG	C4-C5-C6-O6
23	A	412	SQD	C2-C1-O6-C44
34	a	418	LMT	C2'-C1'-O1'-C1
34	f	102	LMT	C2'-C1'-O1'-C1
24	j	101	LMG	C10-C11-C12-C13
35	c	516	DGD	C1A-C2A-C3A-C4A
36	d	407	LHG	O2-C2-C3-O3
34	J	103	LMT	C4'-C5'-C6'-O6'
22	K	101	BCR	C36-C18-C19-C20
22	k	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
32	C	521	HTG	S1-C1'-C2'-C3'
22	d	405	BCR	C21-C22-C23-C24
23	F	101	SQD	O47-C45-C46-O48
23	f	101	SQD	O10-C23-O48-C46
32	B	623	HTG	C4-C5-C6-O6
32	c	521	HTG	C4-C5-C6-O6
23	A	412	SQD	O6-C44-C45-O47
24	A	407	LMG	C15-C16-C17-C18
20	B	602	CLA	C10-C11-C12-C13
20	b	618	CLA	C8-C10-C11-C12
20	A	404	CLA	C12-C13-C15-C16
20	D	401	CLA	C12-C13-C15-C16
20	b	615	CLA	C11-C12-C13-C15
36	d	408	LHG	C11-C12-C13-C14
32	B	621	HTG	C4-C5-C6-O6
22	T	101	BCR	C13-C14-C15-C16
22	t	101	BCR	C13-C14-C15-C16
34	m	101	LMT	O1'-C1-C2-C3
27	A	411	PL9	C19-C21-C22-C23
20	A	404	CLA	C15-C16-C17-C18
20	C	506	CLA	C10-C11-C12-C13
20	b	616	CLA	C10-C11-C12-C13
23	A	412	SQD	C23-C24-C25-C26
23	a	409	SQD	C7-C8-C9-C10
23	b	622	SQD	C23-C24-C25-C26
35	C	517	DGD	C1B-C2B-C3B-C4B
20	A	404	CLA	C13-C15-C16-C17
34	a	418	LMT	C4'-C5'-C6'-O6'
20	B	612	CLA	C15-C16-C17-C18
20	b	616	CLA	C8-C10-C11-C12
20	c	513	CLA	C8-C10-C11-C12
23	a	401	SQD	C23-C24-C25-C26
24	a	410	LMG	C10-C11-C12-C13
24	c	519	LMG	C10-C11-C12-C13
23	a	401	SQD	O5-C1-O6-C44
24	a	410	LMG	O6-C1-O1-C7
34	B	626	LMT	O5'-C1'-O1'-C1
23	a	409	SQD	C9-C10-C11-C12
35	D	406	DGD	C7B-C8B-C9B-CAB
20	B	601	CLA	C10-C11-C12-C13
20	B	615	CLA	C5-C6-C7-C8
20	D	404	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	b	618	CLA	C15-C16-C17-C18
20	c	509	CLA	C13-C15-C16-C17
36	D	408	LHG	O2-C2-C3-O3
24	B	620	LMG	C37-C38-C39-C40
35	d	416	DGD	C4D-C5D-C6D-O5D
32	C	534	HTG	C4-C5-C6-O6
20	A	404	CLA	C3-C5-C6-C7
20	B	615	CLA	C8-C10-C11-C12
20	c	506	CLA	C10-C11-C12-C13
34	T	102	LMT	O1'-C1-C2-C3
24	c	519	LMG	C28-C29-C30-C31
20	B	602	CLA	O1D-CGD-O2D-CED
35	D	406	DGD	C2A-C1A-O1G-C1G
32	b	625	HTG	S1-C1'-C2'-C3'
32	B	621	HTG	O5-C5-C6-O6
20	b	614	CLA	C13-C15-C16-C17
34	Z	101	LMT	C5'-C4'-O1B-C1B
20	C	507	CLA	C5-C6-C7-C8
24	A	407	LMG	C10-C11-C12-C13
36	D	408	LHG	C1-C2-C3-O3
36	d	407	LHG	C1-C2-C3-O3
20	B	607	CLA	C2A-CAA-CBA-CGA
20	B	601	CLA	C13-C15-C16-C17
20	c	513	CLA	C10-C11-C12-C13
20	c	513	CLA	C13-C15-C16-C17
20	C	503	CLA	O1D-CGD-O2D-CED
20	a	404	CLA	C8-C10-C11-C12
32	B	622	HTG	S1-C1'-C2'-C3'
20	b	606	CLA	C15-C16-C17-C18
20	b	608	CLA	C15-C16-C17-C18
20	b	604	CLA	C14-C13-C15-C16
24	C	524	LMG	O6-C5-C6-O5
23	b	622	SQD	C2-C1-O6-C44
24	A	407	LMG	C2-C1-O1-C7
34	B	626	LMT	C2'-C1'-O1'-C1
20	B	616	CLA	C10-C11-C12-C13
20	b	605	CLA	C5-C6-C7-C8
20	b	608	CLA	C16-C17-C18-C20
20	c	506	CLA	C15-C16-C17-C18
34	b	627	LMT	O5B-C5B-C6B-O6B
24	J	101	LMG	O6-C5-C6-O5
36	d	406	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
35	c	517	DGD	C1A-C2A-C3A-C4A
36	d	406	LHG	C23-C24-C25-C26
20	C	503	CLA	CBD-CGD-O2D-CED
23	l	101	SQD	C46-C45-O47-C7
24	C	524	LMG	C9-C8-O7-C10
20	C	502	CLA	C16-C17-C18-C20
20	b	618	CLA	C16-C17-C18-C20
20	c	502	CLA	C16-C17-C18-C19
34	I	101	LMT	O1'-C1-C2-C3
24	A	407	LMG	O9-C10-O7-C8
24	A	407	LMG	O6-C1-O1-C7
24	C	524	LMG	C34-C35-C36-C37
24	A	407	LMG	C11-C10-O7-C8
24	c	519	LMG	C11-C10-O7-C8
32	B	622	HTG	C1'-C2'-C3'-C4'
36	E	103	LHG	C11-C10-C9-C8
34	b	627	LMT	C1-C2-C3-C4
20	B	602	CLA	C13-C15-C16-C17
20	d	404	CLA	C13-C15-C16-C17
20	C	509	CLA	C2-C1-O2A-CGA
20	C	506	CLA	C16-C17-C18-C20
20	C	507	CLA	C16-C17-C18-C20
20	b	608	CLA	C16-C17-C18-C19
20	b	615	CLA	C16-C17-C18-C19
20	c	509	CLA	C16-C17-C18-C19
35	D	406	DGD	O1A-C1A-O1G-C1G
34	z	102	LMT	C5'-C4'-O1B-C1B
24	c	519	LMG	C39-C40-C41-C42
35	d	416	DGD	C2A-C3A-C4A-C5A
24	A	407	LMG	C11-C12-C13-C14
24	B	620	LMG	C32-C33-C34-C35
24	a	410	LMG	C34-C35-C36-C37
24	c	519	LMG	C16-C17-C18-C19
24	c	519	LMG	C32-C33-C34-C35
34	m	101	LMT	C7-C8-C9-C10
35	D	406	DGD	C5A-C6A-C7A-C8A
35	c	515	DGD	C5A-C6A-C7A-C8A
36	d	406	LHG	C29-C30-C31-C32
20	c	501	CLA	O1D-CGD-O2D-CED
23	F	101	SQD	C28-C29-C30-C31
23	a	401	SQD	C15-C16-C17-C18
24	A	407	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
24	B	620	LMG	C31-C32-C33-C34
35	d	416	DGD	C7A-C8A-C9A-CAA
36	L	101	LHG	C27-C28-C29-C30
23	A	406	SQD	C11-C12-C13-C14
23	A	412	SQD	C27-C28-C29-C30
23	A	412	SQD	C28-C29-C30-C31
23	l	101	SQD	C15-C16-C17-C18
24	a	410	LMG	C35-C36-C37-C38
34	b	628	LMT	C5-C6-C7-C8
35	C	518	DGD	CBB-CCB-CDB-CEB
35	D	406	DGD	C2A-C3A-C4A-C5A
35	d	416	DGD	C3B-C4B-C5B-C6B
36	d	408	LHG	C10-C11-C12-C13
34	m	101	LMT	C2-C1-O1'-C1'
36	E	103	LHG	O1-C1-C2-O2
35	D	406	DGD	C6A-C7A-C8A-C9A
36	d	408	LHG	C28-C29-C30-C31
20	B	607	CLA	O1D-CGD-O2D-CED
20	B	610	CLA	C4B-C3B-CAB-CBB
24	C	519	LMG	C10-C11-C12-C13
35	C	517	DGD	C1A-C2A-C3A-C4A
36	D	407	LHG	C23-C24-C25-C26
23	a	401	SQD	C29-C30-C31-C32
34	z	102	LMT	C5-C6-C7-C8
35	C	517	DGD	C8B-C9B-CAB-CBB
35	d	416	DGD	C7B-C8B-C9B-CAB
36	E	103	LHG	C28-C29-C30-C31
20	B	605	CLA	C16-C17-C18-C20
20	C	506	CLA	C16-C17-C18-C19
20	C	507	CLA	C16-C17-C18-C19
20	b	617	CLA	C16-C17-C18-C19
20	b	617	CLA	C16-C17-C18-C20
35	D	406	DGD	C8B-C9B-CAB-CBB
36	D	407	LHG	C27-C28-C29-C30
20	b	617	CLA	C10-C11-C12-C13
23	A	406	SQD	C18-C19-C20-C21
35	h	101	DGD	C6B-C7B-C8B-C9B
20	D	402	CLA	O1D-CGD-O2D-CED
20	b	616	CLA	C11-C10-C8-C7
23	b	622	SQD	C24-C25-C26-C27
24	A	407	LMG	C21-C22-C23-C24
24	A	407	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
36	l	102	LHG	C27-C28-C29-C30
23	F	101	SQD	C23-C24-C25-C26
24	J	101	LMG	C10-C11-C12-C13
24	c	518	LMG	C10-C11-C12-C13
20	b	603	CLA	C10-C11-C12-C13
23	A	412	SQD	C26-C27-C28-C29
23	F	101	SQD	C32-C33-C34-C35
24	A	407	LMG	C17-C18-C19-C20
35	C	516	DGD	C7A-C8A-C9A-CAA
35	C	517	DGD	C3A-C4A-C5A-C6A
35	c	515	DGD	C7A-C8A-C9A-CAA
36	D	409	LHG	C15-C16-C17-C18
23	l	101	SQD	C29-C30-C31-C32
34	B	627	LMT	C11-C10-C9-C8
35	h	101	DGD	C6A-C7A-C8A-C9A
36	D	409	LHG	C28-C29-C30-C31
24	B	620	LMG	C15-C16-C17-C18
24	a	410	LMG	C17-C18-C19-C20
23	l	101	SQD	C11-C12-C13-C14
35	c	517	DGD	C8A-C9A-CAA-CBA
20	B	605	CLA	C16-C17-C18-C19
20	b	618	CLA	C16-C17-C18-C19
20	c	509	CLA	C16-C17-C18-C20
35	c	515	DGD	O6D-C5D-C6D-O5D
34	J	103	LMT	C1-C2-C3-C4
20	a	403	CLA	C2C-C3C-CAC-CBC
34	B	627	LMT	O5'-C1'-O1'-C1
24	C	519	LMG	C14-C15-C16-C17
24	C	519	LMG	C17-C18-C19-C20
24	C	519	LMG	C20-C21-C22-C23
24	a	410	LMG	C16-C17-C18-C19
20	C	512	CLA	O1D-CGD-O2D-CED
24	C	519	LMG	C34-C35-C36-C37
24	C	524	LMG	C33-C34-C35-C36
32	C	522	HTG	C1'-C2'-C3'-C4'
24	A	407	LMG	C13-C14-C15-C16
24	B	620	LMG	C34-C35-C36-C37
24	B	620	LMG	C35-C36-C37-C38
24	C	519	LMG	C33-C34-C35-C36
24	j	101	LMG	C18-C19-C20-C21
35	d	416	DGD	CAB-CBB-CCB-CDB
35	C	518	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
20	A	402	CLA	C10-C11-C12-C13
32	C	521	HTG	O5-C5-C6-O6
20	B	616	CLA	C5-C6-C7-C8
23	A	406	SQD	C34-C35-C36-C37
23	f	101	SQD	C25-C26-C27-C28
24	c	519	LMG	C35-C36-C37-C38
32	B	621	HTG	C3'-C4'-C5'-C6'
34	c	523	LMT	C5-C6-C7-C8
36	D	407	LHG	C28-C29-C30-C31
36	D	408	LHG	C11-C10-C9-C8
20	B	610	CLA	C2B-C3B-CAB-CBB
22	B	617	BCR	C1-C6-C7-C8
22	C	514	BCR	C23-C24-C25-C30
22	d	405	BCR	C23-C24-C25-C26
22	d	405	BCR	C23-C24-C25-C30
23	A	412	SQD	C10-C11-C12-C13
23	a	409	SQD	C11-C10-C9-C8
23	a	409	SQD	C27-C28-C29-C30
34	b	628	LMT	C2-C3-C4-C5
35	C	516	DGD	C8B-C9B-CAB-CBB
20	C	510	CLA	O1D-CGD-O2D-CED
24	a	410	LMG	C30-C31-C32-C33
34	I	101	LMT	C4-C5-C6-C7
35	D	406	DGD	C9B-CAB-CBB-CCB
35	c	515	DGD	C8A-C9A-CAA-CBA
35	c	516	DGD	C3A-C4A-C5A-C6A
23	A	406	SQD	C31-C32-C33-C34
23	A	412	SQD	C9-C10-C11-C12
24	c	519	LMG	O9-C10-O7-C8
20	b	607	CLA	C4-C3-C5-C6
24	C	519	LMG	C39-C40-C41-C42
34	f	102	LMT	C3-C4-C5-C6
35	D	406	DGD	CCB-CDB-CEB-CFB
35	c	515	DGD	C4B-C5B-C6B-C7B
35	c	517	DGD	C8B-C9B-CAB-CBB
36	E	103	LHG	C29-C30-C31-C32
36	d	408	LHG	C17-C18-C19-C20
20	C	507	CLA	C2-C3-C5-C6
23	a	401	SQD	C24-C25-C26-C27
23	f	101	SQD	C24-C25-C26-C27
24	A	407	LMG	C29-C30-C31-C32
24	B	620	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	C	524	LMG	C19-C20-C21-C22
35	C	516	DGD	C3B-C4B-C5B-C6B
35	H	102	DGD	C9B-CAB-CBB-CCB
20	d	403	CLA	C2C-C3C-CAC-CBC
34	b	627	LMT	C6-C7-C8-C9
23	F	101	SQD	C27-C28-C29-C30
23	a	409	SQD	C18-C19-C20-C21
32	D	417	HTG	C2'-C3'-C4'-C5'
35	D	406	DGD	C6B-C7B-C8B-C9B
20	B	601	CLA	C15-C16-C17-C18
23	A	412	SQD	C31-C32-C33-C34
23	a	409	SQD	C26-C27-C28-C29
23	l	101	SQD	C14-C15-C16-C17
24	A	407	LMG	C20-C21-C22-C23
24	b	623	LMG	C14-C15-C16-C17
32	B	632	HTG	C3'-C4'-C5'-C6'
23	a	409	SQD	C30-C31-C32-C33
24	b	623	LMG	C32-C33-C34-C35
32	B	623	HTG	C3'-C4'-C5'-C6'
35	C	517	DGD	C4B-C5B-C6B-C7B
35	d	416	DGD	CCB-CDB-CEB-CFB
20	B	607	CLA	C15-C16-C17-C18
20	b	608	CLA	C10-C11-C12-C13
23	A	412	SQD	C25-C26-C27-C28
23	a	401	SQD	C25-C26-C27-C28
34	B	625	LMT	C7-C8-C9-C10
36	E	103	LHG	C26-C27-C28-C29
34	E	101	LMT	C1-C2-C3-C4
23	a	401	SQD	C27-C28-C29-C30
24	C	524	LMG	C18-C19-C20-C21
34	I	101	LMT	C5-C6-C7-C8
36	D	407	LHG	C25-C26-C27-C28
23	A	406	SQD	C30-C31-C32-C33
23	a	409	SQD	C17-C18-C19-C20
23	b	622	SQD	C27-C28-C29-C30
34	b	628	LMT	O1'-C1-C2-C3
32	C	520	HTG	C3'-C4'-C5'-C6'
35	d	416	DGD	C2B-C1B-O2G-C2G
23	b	622	SQD	C7-C8-C9-C10
35	d	416	DGD	O1B-C1B-O2G-C2G
32	c	521	HTG	C1'-C2'-C3'-C4'
20	b	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
35	c	517	DGD	C7B-C8B-C9B-CAB
36	L	101	LHG	C31-C32-C33-C34
35	C	516	DGD	C1B-C2B-C3B-C4B
24	a	410	LMG	C18-C19-C20-C21
35	C	517	DGD	C5D-C6D-O5D-C1E
34	f	102	LMT	C4-C5-C6-C7
35	d	416	DGD	C6A-C7A-C8A-C9A
20	C	502	CLA	C16-C17-C18-C19
20	b	615	CLA	C16-C17-C18-C20
20	b	616	CLA	C16-C17-C18-C19
24	b	623	LMG	C35-C36-C37-C38
24	c	519	LMG	C18-C19-C20-C21
34	J	103	LMT	C5-C6-C7-C8
34	b	628	LMT	C7-C8-C9-C10
35	C	518	DGD	C2A-C3A-C4A-C5A
35	C	518	DGD	C9A-CAA-CBA-CCA
35	D	406	DGD	CBB-CCB-CDB-CEB
36	E	103	LHG	C34-C35-C36-C37
20	C	507	CLA	C4-C3-C5-C6
34	T	102	LMT	C1-C2-C3-C4
34	a	418	LMT	C1-C2-C3-C4
34	B	627	LMT	C1-C2-C3-C4
23	a	401	SQD	C28-C29-C30-C31
23	b	622	SQD	C33-C34-C35-C36
23	l	101	SQD	C12-C13-C14-C15
24	b	623	LMG	C33-C34-C35-C36
34	E	101	LMT	C2-C3-C4-C5
34	z	102	LMT	C6-C7-C8-C9
35	H	102	DGD	C8A-C9A-CAA-CBA
20	b	609	CLA	C3-C5-C6-C7
24	c	519	LMG	C12-C13-C14-C15
34	f	102	LMT	C1-C2-C3-C4
24	j	101	LMG	C32-C33-C34-C35
32	B	623	HTG	C2'-C3'-C4'-C5'
35	C	518	DGD	CAA-CBA-CCA-CDA
35	C	518	DGD	C9B-CAB-CBB-CCB
20	C	504	CLA	C13-C15-C16-C17
32	v	210	HTG	C2'-C1'-S1-C1
24	c	519	LMG	C15-C16-C17-C18
32	B	631	HTG	C2'-C3'-C4'-C5'
36	d	408	LHG	C30-C31-C32-C33
23	a	409	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
36	d	408	LHG	C32-C33-C34-C35
34	m	101	LMT	C4'-C5'-C6'-O6'
20	B	607	CLA	C13-C15-C16-C17
20	C	510	CLA	C8-C10-C11-C12
20	c	509	CLA	C15-C16-C17-C18
23	b	622	SQD	C29-C30-C31-C32
32	b	601	HTG	C3'-C4'-C5'-C6'
20	b	618	CLA	C3-C5-C6-C7
23	A	406	SQD	O6-C44-C45-O47
23	A	412	SQD	C11-C10-C9-C8
23	l	101	SQD	C17-C18-C19-C20
34	T	102	LMT	C6-C7-C8-C9
36	d	406	LHG	C27-C28-C29-C30
32	d	401	HTG	C3'-C4'-C5'-C6'
35	c	515	DGD	C2B-C3B-C4B-C5B
20	B	607	CLA	C8-C10-C11-C12
23	b	622	SQD	C18-C19-C20-C21
32	O	302	HTG	C3'-C4'-C5'-C6'
32	b	625	HTG	C3'-C4'-C5'-C6'
34	I	101	LMT	C11-C10-C9-C8
34	m	101	LMT	C6-C7-C8-C9
23	l	101	SQD	C28-C29-C30-C31
24	c	519	LMG	C29-C30-C31-C32
32	C	520	HTG	C2'-C3'-C4'-C5'
23	f	101	SQD	C26-C27-C28-C29
24	c	519	LMG	C34-C35-C36-C37
36	l	102	LHG	C28-C29-C30-C31
20	b	608	CLA	C2A-CAA-CBA-CGA
34	z	102	LMT	C2B-C1B-O1B-C4'
24	B	620	LMG	C33-C34-C35-C36
34	z	102	LMT	C2-C3-C4-C5
35	h	101	DGD	CBB-CCB-CDB-CEB
20	b	615	CLA	C8-C10-C11-C12
34	T	102	LMT	C9-C10-C11-C12
24	j	101	LMG	O6-C5-C6-O5
36	d	406	LHG	O1-C1-C2-O2
23	l	101	SQD	C11-C10-C9-C8
35	C	518	DGD	C7B-C8B-C9B-CAB
36	l	102	LHG	C11-C10-C9-C8
24	B	620	LMG	C12-C13-C14-C15
20	C	506	CLA	C1A-C2A-CAA-CBA
24	B	620	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	c	504	CLA	C13-C15-C16-C17
23	a	401	SQD	C18-C19-C20-C21
23	f	101	SQD	C27-C28-C29-C30
24	c	518	LMG	C39-C40-C41-C42
24	C	519	LMG	C19-C20-C21-C22
35	C	517	DGD	C6B-C7B-C8B-C9B
35	c	517	DGD	CAA-CBA-CCA-CDA
35	d	416	DGD	C3A-C4A-C5A-C6A
34	B	625	LMT	C11-C10-C9-C8
35	c	516	DGD	C5A-C6A-C7A-C8A
20	A	404	CLA	C6-C7-C8-C10
20	B	601	CLA	C11-C10-C8-C7
20	B	602	CLA	C11-C12-C13-C15
20	B	607	CLA	C11-C12-C13-C15
20	C	506	CLA	C11-C12-C13-C15
20	C	507	CLA	C11-C10-C8-C7
20	C	508	CLA	C11-C10-C8-C7
20	C	513	CLA	C11-C10-C8-C7
20	b	603	CLA	C12-C13-C15-C16
20	c	513	CLA	C11-C10-C8-C7
35	C	517	DGD	C5B-C6B-C7B-C8B
20	b	604	CLA	C16-C17-C18-C19
32	d	401	HTG	C2'-C3'-C4'-C5'
35	c	516	DGD	CBB-CCB-CDB-CEB
23	A	406	SQD	C14-C15-C16-C17
36	E	103	LHG	C23-C24-C25-C26
23	a	401	SQD	C33-C34-C35-C36
35	c	517	DGD	CCA-CDA-CEA-CFA
24	j	101	LMG	C34-C35-C36-C37
23	l	101	SQD	C27-C28-C29-C30
20	D	404	CLA	C13-C15-C16-C17
20	b	615	CLA	C11-C12-C13-C14
24	a	410	LMG	C19-C20-C21-C22
24	c	519	LMG	C20-C21-C22-C23
24	j	101	LMG	C13-C14-C15-C16
34	B	627	LMT	C4-C5-C6-C7
35	C	516	DGD	C6B-C7B-C8B-C9B
34	B	626	LMT	C7-C8-C9-C10
20	b	603	CLA	CBA-CGA-O2A-C1
35	D	406	DGD	CCA-CDA-CEA-CFA
23	A	412	SQD	C16-C17-C18-C19
34	b	627	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
34	b	628	LMT	C1-C2-C3-C4
23	A	412	SQD	O6-C44-C45-C46
23	a	409	SQD	O6-C44-C45-C46
24	c	519	LMG	C7-C8-C9-O8
35	c	517	DGD	C7A-C8A-C9A-CAA
34	Z	101	LMT	C3'-C4'-O1B-C1B
34	c	523	LMT	C7-C8-C9-C10
24	c	518	LMG	C38-C39-C40-C41
35	D	406	DGD	O6D-C5D-C6D-O5D
35	c	515	DGD	O6E-C5E-C6E-O5E
20	c	513	CLA	C16-C17-C18-C19
21	D	403	PHO	C2C-C3C-CAC-CBC
23	a	409	SQD	C14-C15-C16-C17
34	I	101	LMT	C6-C7-C8-C9
34	T	102	LMT	C2-C3-C4-C5
20	B	615	CLA	O1D-CGD-O2D-CED
24	C	524	LMG	C20-C21-C22-C23
35	h	101	DGD	C7A-C8A-C9A-CAA
34	J	103	LMT	C7-C8-C9-C10
21	a	405	PHO	C8-C10-C11-C12
24	J	101	LMG	C12-C13-C14-C15
24	b	623	LMG	C29-C30-C31-C32
20	B	602	CLA	C16-C17-C18-C20
23	l	101	SQD	C26-C27-C28-C29
32	B	632	HTG	O5-C5-C6-O6
36	E	103	LHG	C3-O3-P-O5
34	I	101	LMT	O5B-C5B-C6B-O6B
35	C	516	DGD	O6E-C5E-C6E-O5E
24	a	410	LMG	C36-C37-C38-C39
34	T	102	LMT	C3-C4-C5-C6
35	h	101	DGD	C8A-C9A-CAA-CBA
23	F	101	SQD	O6-C44-C45-O47
24	c	519	LMG	C33-C34-C35-C36
36	d	407	LHG	C34-C35-C36-C37
35	C	516	DGD	CBA-CCA-CDA-CEA
23	a	409	SQD	C33-C34-C35-C36
23	b	622	SQD	C30-C31-C32-C33
24	B	620	LMG	C18-C19-C20-C21
24	j	101	LMG	C12-C13-C14-C15
23	A	406	SQD	C28-C29-C30-C31
36	D	407	LHG	C34-C35-C36-C37
23	b	622	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
34	m	101	LMT	C9-C10-C11-C12
32	B	631	HTG	C1'-C2'-C3'-C4'
23	b	622	SQD	C11-C10-C9-C8
24	C	519	LMG	C21-C22-C23-C24
36	D	408	LHG	C32-C33-C34-C35
36	D	409	LHG	C17-C18-C19-C20
36	d	408	LHG	C16-C17-C18-C19
23	f	101	SQD	C35-C36-C37-C38
23	a	401	SQD	C31-C32-C33-C34
20	d	404	CLA	C16-C17-C18-C20
36	d	406	LHG	C31-C32-C33-C34
36	l	102	LHG	C32-C33-C34-C35
23	a	401	SQD	C19-C20-C21-C22
23	a	409	SQD	C35-C36-C37-C38
21	a	406	PHO	C2C-C3C-CAC-CBC
23	l	101	SQD	C10-C11-C12-C13
32	O	302	HTG	C2'-C3'-C4'-C5'
35	C	516	DGD	C5B-C6B-C7B-C8B
23	a	409	SQD	O6-C44-C45-O47
32	b	601	HTG	C4'-C5'-C6'-C7'
34	B	625	LMT	C4'-C5'-C6'-O6'
34	E	101	LMT	C6-C7-C8-C9
34	a	418	LMT	C9-C10-C11-C12
23	F	101	SQD	C30-C31-C32-C33
24	A	407	LMG	C32-C33-C34-C35
35	D	406	DGD	C4B-C5B-C6B-C7B
35	c	517	DGD	C9A-CAA-CBA-CCA
24	c	519	LMG	C22-C23-C24-C25
23	a	401	SQD	C26-C27-C28-C29
23	l	101	SQD	C16-C17-C18-C19
35	H	102	DGD	CDA-CEA-CFA-CGA
24	C	519	LMG	C22-C23-C24-C25
35	C	518	DGD	CAB-CBB-CCB-CDB
35	D	406	DGD	C4A-C5A-C6A-C7A
35	d	416	DGD	CBB-CCB-CDB-CEB
23	a	409	SQD	C31-C32-C33-C34
36	L	101	LHG	C33-C34-C35-C36
20	c	513	CLA	CBA-CGA-O2A-C1
24	C	519	LMG	C29-C28-O8-C9
23	A	406	SQD	C15-C16-C17-C18
36	E	103	LHG	C9-C10-C11-C12
24	A	407	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	CDB-CEB-CFB-CGB
35	h	101	DGD	CDB-CEB-CFB-CGB
24	c	519	LMG	C40-C41-C42-C43
20	C	506	CLA	C5-C6-C7-C8
20	b	616	CLA	C16-C17-C18-C20
23	F	101	SQD	C33-C34-C35-C36
36	d	408	LHG	C35-C36-C37-C38
23	a	401	SQD	C16-C17-C18-C19
32	b	625	HTG	C2'-C3'-C4'-C5'
34	c	523	LMT	C4'-C5'-C6'-O6'
34	M	101	LMT	O5'-C5'-C6'-O6'
24	C	524	LMG	C17-C18-C19-C20
35	H	102	DGD	CAA-CBA-CCA-CDA
34	z	102	LMT	C2-C1-O1'-C1'
20	A	404	CLA	C6-C7-C8-C9
20	B	602	CLA	C11-C12-C13-C14
20	B	602	CLA	C14-C13-C15-C16
20	B	605	CLA	C6-C7-C8-C9
20	B	607	CLA	C11-C10-C8-C9
20	B	614	CLA	C14-C13-C15-C16
20	C	506	CLA	C11-C12-C13-C14
20	C	507	CLA	C11-C10-C8-C9
20	C	513	CLA	C11-C10-C8-C9
20	D	401	CLA	C14-C13-C15-C16
20	b	618	CLA	C11-C10-C8-C9
20	C	509	CLA	C15-C16-C17-C18
20	c	512	CLA	C4B-C3B-CAB-CBB
24	b	623	LMG	C12-C13-C14-C15
35	h	101	DGD	O2G-C1B-C2B-C3B
23	A	406	SQD	C9-C10-C11-C12
36	d	407	LHG	C11-C10-C9-C8
20	B	605	CLA	C13-C15-C16-C17
20	c	502	CLA	C16-C17-C18-C20
32	B	631	HTG	C4'-C5'-C6'-C7'
24	A	407	LMG	C12-C13-C14-C15
24	A	407	LMG	C22-C23-C24-C25
36	D	409	LHG	C35-C36-C37-C38
36	d	408	LHG	C19-C20-C21-C22
20	B	605	CLA	C6-C7-C8-C10
20	B	607	CLA	C11-C10-C8-C7
20	B	614	CLA	C12-C13-C15-C16
20	C	504	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	C	509	CLA	C11-C10-C8-C7
20	D	404	CLA	C6-C7-C8-C10
20	b	603	CLA	C11-C12-C13-C15
20	b	618	CLA	C11-C10-C8-C7
20	c	507	CLA	C11-C10-C8-C7
20	c	512	CLA	C11-C10-C8-C7
20	d	404	CLA	C6-C7-C8-C10
20	B	615	CLA	C10-C11-C12-C13
35	C	518	DGD	CDB-CEB-CFB-CGB
23	a	401	SQD	C35-C36-C37-C38
34	I	101	LMT	C9-C10-C11-C12
24	B	620	LMG	C19-C20-C21-C22
34	B	625	LMT	C6-C7-C8-C9
23	A	406	SQD	C27-C28-C29-C30
35	d	416	DGD	C4A-C5A-C6A-C7A
35	c	515	DGD	C4D-C5D-C6D-O5D
20	b	603	CLA	O1A-CGA-O2A-C1
24	J	101	LMG	C36-C37-C38-C39
20	B	602	CLA	C4-C3-C5-C6
35	c	515	DGD	C4A-C5A-C6A-C7A
35	C	517	DGD	C5A-C6A-C7A-C8A
36	d	407	LHG	C32-C33-C34-C35
32	d	401	HTG	C4-C5-C6-O6
35	C	516	DGD	C8A-C9A-CAA-CBA
23	a	401	SQD	C34-C35-C36-C37
35	d	416	DGD	C8A-C9A-CAA-CBA
34	a	418	LMT	C4-C5-C6-C7
23	A	406	SQD	O6-C44-C45-C46
23	f	101	SQD	C44-C45-C46-O48
24	A	407	LMG	O1-C7-C8-C9
24	A	407	LMG	C7-C8-C9-O8
35	d	416	DGD	O1G-C1G-C2G-C3G
20	a	404	CLA	C11-C12-C13-C15
20	B	601	CLA	C8-C10-C11-C12
20	b	618	CLA	C13-C15-C16-C17
24	c	519	LMG	C21-C22-C23-C24
35	c	515	DGD	CAA-CBA-CCA-CDA
35	c	516	DGD	C6A-C7A-C8A-C9A
20	d	404	CLA	C8-C10-C11-C12
23	A	406	SQD	C26-C27-C28-C29
34	m	101	LMT	C5-C6-C7-C8
36	d	406	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
36	l	102	LHG	C31-C32-C33-C34
20	a	403	CLA	C4C-C3C-CAC-CBC
24	C	524	LMG	C31-C32-C33-C34
34	T	102	LMT	C7-C8-C9-C10
24	J	101	LMG	C35-C36-C37-C38
23	a	409	SQD	C13-C14-C15-C16
20	b	604	CLA	C16-C17-C18-C20
20	c	513	CLA	C16-C17-C18-C20
34	c	523	LMT	C4B-C5B-C6B-O6B
34	m	101	LMT	C1-C2-C3-C4
20	d	402	CLA	C2C-C3C-CAC-CBC
22	D	405	BCR	C23-C24-C25-C30
24	j	101	LMG	C36-C37-C38-C39
36	E	103	LHG	C13-C14-C15-C16
24	c	519	LMG	C14-C15-C16-C17
23	A	406	SQD	C32-C33-C34-C35
24	C	519	LMG	C30-C31-C32-C33
35	d	416	DGD	C4B-C5B-C6B-C7B
20	B	602	CLA	C16-C17-C18-C19
20	D	404	CLA	C16-C17-C18-C19
20	b	617	CLA	C5-C6-C7-C8
20	c	510	CLA	C8-C10-C11-C12
23	b	622	SQD	O47-C45-C46-O48
23	l	101	SQD	O6-C44-C45-O47
24	C	524	LMG	O7-C8-C9-O8
24	c	519	LMG	O7-C8-C9-O8
35	D	406	DGD	O2G-C2G-C3G-O3G
35	d	416	DGD	O1G-C1G-C2G-O2G
27	A	411	PL9	C4-C3-C7-C8
27	a	415	PL9	C4-C3-C7-C8
34	Z	101	LMT	C2-C3-C4-C5
24	B	620	LMG	C11-C12-C13-C14
23	A	406	SQD	C12-C13-C14-C15
35	H	102	DGD	C3B-C4B-C5B-C6B
34	E	101	LMT	O1'-C1-C2-C3
20	d	404	CLA	C16-C17-C18-C19
24	C	524	LMG	C21-C22-C23-C24
34	B	626	LMT	C11-C10-C9-C8
32	b	602	HTG	C4-C5-C6-O6
23	A	412	SQD	C7-C8-C9-C10
20	C	513	CLA	C3-C5-C6-C7
20	B	601	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	C	504	CLA	C11-C10-C8-C9
20	b	612	CLA	C11-C12-C13-C14
20	c	506	CLA	C14-C13-C15-C16
20	c	512	CLA	C11-C10-C8-C9
23	F	101	SQD	O6-C44-C45-C46
24	j	101	LMG	C31-C32-C33-C34
35	H	102	DGD	CBB-CCB-CDB-CEB
35	d	416	DGD	C9A-CAA-CBA-CCA
34	b	628	LMT	C2'-C1'-O1'-C1
34	B	626	LMT	C6-C7-C8-C9
35	C	516	DGD	O6D-C5D-C6D-O5D
32	O	302	HTG	C1'-C2'-C3'-C4'
24	b	623	LMG	C31-C32-C33-C34
20	b	618	CLA	C10-C11-C12-C13
34	T	102	LMT	C5-C6-C7-C8
36	L	101	LHG	C7-C8-C9-C10
36	l	102	LHG	O6-C4-C5-C6
22	C	514	BCR	C37-C22-C23-C24
20	B	601	CLA	C11-C12-C13-C15
20	C	504	CLA	C12-C13-C15-C16
20	b	603	CLA	C11-C10-C8-C7
20	b	617	CLA	C12-C13-C15-C16
20	c	513	CLA	C11-C12-C13-C15
20	c	513	CLA	C12-C13-C15-C16
32	d	401	HTG	S1-C1'-C2'-C3'
23	A	406	SQD	C35-C36-C37-C38
24	a	410	LMG	C29-C30-C31-C32
20	b	613	CLA	C13-C15-C16-C17
22	C	514	BCR	C21-C22-C23-C24
36	d	407	LHG	C26-C27-C28-C29
23	F	101	SQD	C45-C44-O6-C1
24	C	524	LMG	C8-C7-O1-C1
24	c	518	LMG	C8-C7-O1-C1
35	C	517	DGD	C2G-C3G-O3G-C1D
35	c	516	DGD	C2G-C3G-O3G-C1D
35	c	516	DGD	C5D-C6D-O5D-C1E
20	c	512	CLA	C15-C16-C17-C18
23	b	622	SQD	C28-C29-C30-C31
20	c	513	CLA	O1A-CGA-O2A-C1
37	E	104	HEM	C2C-C3C-CAC-CBC
24	C	519	LMG	O10-C28-O8-C9
24	j	101	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	b	613	CLA	C16-C17-C18-C20
35	c	515	DGD	CCA-CDA-CEA-CFA
36	L	101	LHG	O6-C4-C5-O7
36	l	102	LHG	O6-C4-C5-O7
23	a	409	SQD	C28-C29-C30-C31
35	d	416	DGD	C5B-C6B-C7B-C8B
23	a	401	SQD	O6-C44-C45-C46
20	B	612	CLA	C16-C17-C18-C20
34	m	102	LMT	O5'-C5'-C6'-O6'
32	B	621	HTG	C4'-C5'-C6'-C7'
23	A	412	SQD	C17-C18-C19-C20
32	B	623	HTG	C2-C1-S1-C1'
32	C	521	HTG	C2-C1-S1-C1'
32	c	520	HTG	C2-C1-S1-C1'
23	A	412	SQD	C15-C16-C17-C18
23	a	409	SQD	C12-C13-C14-C15
23	f	101	SQD	O47-C45-C46-O48
23	l	101	SQD	O47-C45-C46-O48
24	A	407	LMG	O1-C7-C8-O7
24	A	407	LMG	O7-C8-C9-O8
35	d	416	DGD	O2G-C2G-C3G-O3G
20	B	614	CLA	C10-C11-C12-C13
20	C	508	CLA	C11-C10-C8-C9
20	d	404	CLA	C6-C7-C8-C9
35	c	516	DGD	C2B-C3B-C4B-C5B
24	j	101	LMG	C17-C18-C19-C20
34	m	101	LMT	C2-C3-C4-C5
35	C	516	DGD	C9A-CAA-CBA-CCA
35	c	517	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	CCB-CDB-CEB-CFB
20	B	611	CLA	C8-C10-C11-C12
20	c	506	CLA	C5-C6-C7-C8
20	c	506	CLA	C13-C15-C16-C17
24	B	620	LMG	C30-C31-C32-C33
24	j	101	LMG	C14-C15-C16-C17
34	c	523	LMT	C4-C5-C6-C7
20	B	601	CLA	C2-C1-O2A-CGA
20	c	509	CLA	C2-C1-O2A-CGA
20	a	404	CLA	C11-C12-C13-C14
20	c	507	CLA	C5-C6-C7-C8
23	l	101	SQD	C35-C36-C37-C38
35	c	515	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
27	a	415	PL9	C15-C14-C16-C17
20	D	401	CLA	C2C-C3C-CAC-CBC
24	C	524	LMG	C29-C28-O8-C9
20	C	509	CLA	C13-C15-C16-C17
24	C	524	LMG	O10-C28-O8-C9
24	A	407	LMG	C39-C40-C41-C42
20	B	602	CLA	C4B-C3B-CAB-CBB
20	C	501	CLA	C4B-C3B-CAB-CBB
23	b	622	SQD	C11-C12-C13-C14
20	D	404	CLA	C10-C11-C12-C13
35	H	102	DGD	O2G-C1B-C2B-C3B
34	m	101	LMT	C4-C5-C6-C7
36	l	102	LHG	C30-C31-C32-C33
24	a	410	LMG	C20-C21-C22-C23
35	C	516	DGD	CBB-CCB-CDB-CEB
34	E	101	LMT	C7-C8-C9-C10
20	B	601	CLA	C6-C7-C8-C10
20	C	509	CLA	C6-C7-C8-C10
20	D	404	CLA	C11-C12-C13-C15
20	c	506	CLA	C12-C13-C15-C16
20	d	404	CLA	C11-C12-C13-C15
34	m	101	LMT	O5B-C5B-C6B-O6B
34	c	523	LMT	C11-C10-C9-C8
35	H	102	DGD	C6A-C7A-C8A-C9A
36	d	408	LHG	C2-C3-O3-P
35	C	516	DGD	CDA-CEA-CFA-CGA
21	a	405	PHO	C4-C3-C5-C6
20	C	502	CLA	C14-C13-C15-C16
20	b	603	CLA	C11-C12-C13-C14
20	c	507	CLA	C11-C10-C8-C9
20	c	513	CLA	C11-C12-C13-C14
34	Z	101	LMT	O5'-C5'-C6'-O6'
20	b	603	CLA	C16-C17-C18-C19
36	D	409	LHG	C34-C35-C36-C37
35	D	406	DGD	CAB-CBB-CCB-CDB
32	C	534	HTG	C4'-C5'-C6'-C7'
35	c	515	DGD	CBA-CCA-CDA-CEA
36	l	102	LHG	C10-C11-C12-C13
24	a	410	LMG	O7-C8-C9-O8
24	a	410	LMG	C7-C8-C9-O8
35	d	416	DGD	C1G-C2G-C3G-O3G
35	c	515	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
34	m	101	LMT	C4B-C5B-C6B-O6B
20	C	502	CLA	CAD-CBD-CGD-O2D
20	b	609	CLA	CAD-CBD-CGD-O2D
20	b	611	CLA	CAD-CBD-CGD-O2D
34	b	628	LMT	O5'-C1'-O1'-C1
35	d	416	DGD	O6D-C1D-O3G-C3G
20	B	609	CLA	C13-C15-C16-C17
20	C	508	CLA	C11-C12-C13-C14
23	l	101	SQD	C25-C26-C27-C28
36	D	409	LHG	C12-C13-C14-C15
36	L	101	LHG	C30-C31-C32-C33
20	B	601	CLA	CHA-CBD-CGD-O1D
20	B	602	CLA	CAD-CBD-CGD-O1D
20	B	606	CLA	CAD-CBD-CGD-O1D
20	C	504	CLA	CAD-CBD-CGD-O1D
20	C	506	CLA	CAD-CBD-CGD-O1D
20	C	509	CLA	CHA-CBD-CGD-O1D
20	b	603	CLA	CAD-CBD-CGD-O1D
20	b	607	CLA	CAD-CBD-CGD-O1D
20	b	618	CLA	CHA-CBD-CGD-O2D
20	c	501	CLA	CAD-CBD-CGD-O1D
20	c	502	CLA	CAD-CBD-CGD-O1D
20	c	504	CLA	CAD-CBD-CGD-O1D
21	D	403	PHO	CHA-CBD-CGD-O1D
36	D	408	LHG	C3-O3-P-O5
36	D	408	LHG	C4-O6-P-O5
36	D	409	LHG	C10-C11-C12-C13
34	m	102	LMT	C5-C6-C7-C8
20	B	602	CLA	C2B-C3B-CAB-CBB
35	h	101	DGD	C7B-C8B-C9B-CAB
27	a	415	PL9	C13-C14-C16-C17
20	C	503	CLA	C8-C10-C11-C12
36	D	409	LHG	C2-C3-O3-P
32	O	302	HTG	C4'-C5'-C6'-C7'
36	E	103	LHG	C7-C8-C9-C10
36	L	101	LHG	C28-C29-C30-C31
32	C	521	HTG	C2'-C3'-C4'-C5'
24	B	620	LMG	C14-C15-C16-C17
24	J	101	LMG	C34-C35-C36-C37
32	B	622	HTG	C4'-C5'-C6'-C7'
35	d	416	DGD	CAA-CBA-CCA-CDA
36	d	406	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
35	d	416	DGD	CDB-CEB-CFB-CGB
20	B	602	CLA	C2-C3-C5-C6
23	b	622	SQD	C9-C10-C11-C12
23	A	406	SQD	C11-C10-C9-C8
20	D	404	CLA	C16-C17-C18-C20
36	D	408	LHG	C14-C15-C16-C17
20	b	618	CLA	CBA-CGA-O2A-C1
20	A	404	CLA	C14-C13-C15-C16
20	B	601	CLA	C14-C13-C15-C16
20	C	504	CLA	C14-C13-C15-C16
20	d	404	CLA	C11-C12-C13-C14
20	B	601	CLA	C12-C13-C15-C16
20	C	504	CLA	C11-C12-C13-C15
20	c	509	CLA	C12-C13-C15-C16
35	h	101	DGD	C9B-CAB-CBB-CCB
36	d	408	LHG	C33-C34-C35-C36
20	b	618	CLA	O1A-CGA-O2A-C1
24	b	623	LMG	C13-C14-C15-C16
27	D	412	PL9	C30-C29-C31-C32
34	B	626	LMT	C4-C5-C6-C7
24	c	519	LMG	O1-C7-C8-O7
24	B	620	LMG	O8-C28-C29-C30
35	D	406	DGD	C8A-C9A-CAA-CBA
23	l	101	SQD	C7-C8-C9-C10
23	A	412	SQD	C24-C25-C26-C27
35	D	406	DGD	CBA-CCA-CDA-CEA
24	C	524	LMG	C32-C33-C34-C35
36	L	101	LHG	C11-C12-C13-C14
20	b	613	CLA	C16-C17-C18-C19
24	C	519	LMG	C12-C13-C14-C15
23	b	622	SQD	C44-C45-C46-O48
24	C	524	LMG	C7-C8-C9-O8
35	D	406	DGD	C1G-C2G-C3G-O3G
35	C	518	DGD	O6D-C5D-C6D-O5D
34	a	418	LMT	C11-C10-C9-C8
36	l	102	LHG	C5-C6-O8-C23
23	A	412	SQD	C24-C23-O48-C46
35	c	515	DGD	C5D-C6D-O5D-C1E
22	k	101	BCR	C19-C20-C21-C22
38	x	101	RRX	C9-C10-C11-C12
24	C	519	LMG	C28-C29-C30-C31
32	u	201	HTG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
35	C	516	DGD	C5A-C6A-C7A-C8A
24	C	519	LMG	C11-C12-C13-C14
34	J	103	LMT	C2-C3-C4-C5
34	T	102	LMT	C2-C1-O1'-C1'
34	m	102	LMT	C2-C1-O1'-C1'
36	d	407	LHG	O1-C1-C2-O2
36	D	407	LHG	C35-C36-C37-C38
34	c	523	LMT	O1'-C1-C2-C3
20	D	404	CLA	C6-C7-C8-C9
20	D	404	CLA	C11-C12-C13-C14
20	b	617	CLA	C14-C13-C15-C16
35	h	101	DGD	C5B-C6B-C7B-C8B
34	b	627	LMT	C3-C4-C5-C6
36	L	101	LHG	C17-C18-C19-C20
24	c	518	LMG	C11-C12-C13-C14
23	F	101	SQD	C24-C25-C26-C27
24	b	623	LMG	C30-C31-C32-C33
24	A	407	LMG	C37-C38-C39-C40
20	D	401	CLA	C15-C16-C17-C18
20	C	513	CLA	C4-C3-C5-C6
27	A	411	PL9	C15-C14-C16-C17
35	c	517	DGD	O6D-C5D-C6D-O5D
36	L	101	LHG	O6-C4-C5-C6
20	d	403	CLA	C4C-C3C-CAC-CBC
34	E	101	LMT	C11-C10-C9-C8
32	d	401	HTG	O5-C5-C6-O6
24	C	524	LMG	C29-C30-C31-C32
35	c	517	DGD	CBB-CCB-CDB-CEB
20	B	602	CLA	C11-C10-C8-C7
20	b	614	CLA	C10-C11-C12-C13
20	b	616	CLA	C15-C16-C17-C18
32	c	521	HTG	C2'-C3'-C4'-C5'
35	H	102	DGD	C5B-C6B-C7B-C8B
23	A	406	SQD	C10-C11-C12-C13
32	b	602	HTG	C3'-C4'-C5'-C6'
23	f	101	SQD	C31-C32-C33-C34
35	d	416	DGD	C6B-C7B-C8B-C9B
24	C	524	LMG	O1-C7-C8-O7
36	d	406	LHG	C11-C10-C9-C8
24	B	620	LMG	C28-C29-C30-C31
23	l	101	SQD	C32-C33-C34-C35
34	a	418	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	J	101	LMG	C30-C31-C32-C33
20	C	513	CLA	C8-C10-C11-C12
20	b	617	CLA	C8-C10-C11-C12
20	C	504	CLA	C5-C6-C7-C8
20	b	616	CLA	C2-C1-O2A-CGA
36	D	409	LHG	C29-C30-C31-C32
24	c	519	LMG	C31-C32-C33-C34
20	b	603	CLA	C13-C15-C16-C17
20	c	506	CLA	C8-C10-C11-C12
35	h	101	DGD	CCB-CDB-CEB-CFB
36	D	409	LHG	C11-C12-C13-C14
36	E	103	LHG	O2-C2-C3-O3
32	C	521	HTG	C4-C5-C6-O6
27	A	411	PL9	C14-C16-C17-C18
27	D	412	PL9	C39-C41-C42-C43
32	B	621	HTG	S1-C1'-C2'-C3'
20	c	503	CLA	C10-C11-C12-C13
20	c	504	CLA	C11-C12-C13-C14
20	c	509	CLA	C14-C13-C15-C16
24	a	410	LMG	C31-C32-C33-C34
34	b	627	LMT	C2-C3-C4-C5
36	E	103	LHG	C32-C33-C34-C35
20	A	401	CLA	C2C-C3C-CAC-CBC
34	Z	101	LMT	C3-C4-C5-C6
36	l	102	LHG	C17-C18-C19-C20
24	C	524	LMG	C11-C12-C13-C14
20	C	508	CLA	CBD-CGD-O2D-CED
35	C	518	DGD	CCA-CDA-CEA-CFA
23	a	409	SQD	C11-C12-C13-C14
20	C	501	CLA	C2B-C3B-CAB-CBB
20	d	402	CLA	C2B-C3B-CAB-CBB
22	B	617	BCR	C5-C6-C7-C8
22	C	514	BCR	C23-C24-C25-C26
22	D	405	BCR	C23-C24-C25-C26
38	x	101	RRX	C23-C24-C25-C30
37	E	104	HEM	CAD-CBD-CGD-O2D
23	A	412	SQD	O10-C23-O48-C46
36	d	406	LHG	C7-C8-C9-C10
27	A	411	PL9	C13-C14-C16-C17
34	f	102	LMT	C5-C6-C7-C8
37	E	104	HEM	C2A-CAA-CBA-CGA
40	V	201	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	C	506	CLA	C6-C7-C8-C10
20	C	507	CLA	C11-C12-C13-C15
20	D	402	CLA	C2C-C3C-CAC-CBC
35	H	102	DGD	O1G-C1G-C2G-O2G
32	C	521	HTG	O5-C1-S1-C1'
20	b	615	CLA	C15-C16-C17-C18
24	b	623	LMG	C36-C37-C38-C39
36	D	409	LHG	C14-C15-C16-C17
36	E	103	LHG	C5-C6-O8-C23
36	E	103	LHG	C1-C2-C3-O3
20	C	513	CLA	C2-C3-C5-C6
21	a	405	PHO	C2-C3-C5-C6
32	O	302	HTG	O5-C5-C6-O6
34	z	102	LMT	O5B-C5B-C6B-O6B
27	a	415	PL9	C2-C3-C7-C8
34	E	101	LMT	C5-C6-C7-C8
20	A	404	CLA	C8-C10-C11-C12
37	E	104	HEM	CAD-CBD-CGD-O1D
20	a	404	CLA	C6-C7-C8-C9
35	d	416	DGD	C5A-C6A-C7A-C8A
36	l	102	LHG	C29-C30-C31-C32
24	a	410	LMG	C39-C40-C41-C42
36	d	408	LHG	C13-C14-C15-C16
20	B	614	CLA	C15-C16-C17-C18
27	A	411	PL9	C20-C19-C21-C22
36	D	407	LHG	C29-C30-C31-C32
34	a	418	LMT	C6-C7-C8-C9
35	D	406	DGD	CDA-CEA-CFA-CGA
23	F	101	SQD	C25-C26-C27-C28
23	l	101	SQD	O6-C44-C45-C46
20	b	616	CLA	O1D-CGD-O2D-CED
34	B	626	LMT	C4'-C5'-C6'-O6'
35	C	516	DGD	C4D-C5D-C6D-O5D
35	h	101	DGD	O1B-C1B-C2B-C3B
23	A	412	SQD	C11-C12-C13-C14
20	B	616	CLA	C13-C15-C16-C17
20	b	612	CLA	C16-C17-C18-C20
20	c	503	CLA	C8-C10-C11-C12
36	E	103	LHG	C30-C31-C32-C33
36	d	408	LHG	C14-C15-C16-C17
20	d	402	CLA	C4C-C3C-CAC-CBC
20	b	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	b	623	LMG	C38-C39-C40-C41
32	c	520	HTG	C2'-C3'-C4'-C5'
20	d	402	CLA	C4B-C3B-CAB-CBB
35	D	406	DGD	C5B-C6B-C7B-C8B
20	a	403	CLA	O1D-CGD-O2D-CED
24	a	410	LMG	C11-C12-C13-C14
20	C	504	CLA	C15-C16-C17-C18
36	l	102	LHG	C11-C12-C13-C14
34	J	103	LMT	C6-C7-C8-C9
36	D	407	LHG	C17-C18-C19-C20
24	J	101	LMG	C32-C33-C34-C35
36	E	103	LHG	C2-C3-O3-P
24	C	519	LMG	C32-C33-C34-C35
34	E	101	LMT	C3-C4-C5-C6
24	B	620	LMG	C20-C21-C22-C23
40	v	201	HEC	CAD-CBD-CGD-O2D
20	B	604	CLA	C6-C7-C8-C9
20	C	509	CLA	C6-C7-C8-C9
20	D	404	CLA	C11-C10-C8-C9
20	b	608	CLA	C6-C7-C8-C9
36	D	409	LHG	C33-C34-C35-C36
23	a	401	SQD	C45-C44-O6-C1
23	f	101	SQD	C30-C31-C32-C33
40	V	201	HEC	CAD-CBD-CGD-O1D
24	c	518	LMG	C14-C15-C16-C17
20	C	506	CLA	C15-C16-C17-C18
20	B	612	CLA	C16-C17-C18-C19
32	b	602	HTG	O5-C5-C6-O6
20	c	510	CLA	C16-C17-C18-C19
35	c	517	DGD	C6A-C7A-C8A-C9A
40	v	201	HEC	CAD-CBD-CGD-O1D
20	C	513	CLA	C10-C11-C12-C13
34	Z	101	LMT	C11-C10-C9-C8
23	l	101	SQD	C44-C45-C46-O48
24	c	519	LMG	O1-C7-C8-C9
27	A	411	PL9	C39-C41-C42-C43
20	d	403	CLA	C13-C15-C16-C17
37	E	104	HEM	C4C-C3C-CAC-CBC
20	B	601	CLA	C16-C17-C18-C19
24	A	407	LMG	C38-C39-C40-C41
36	d	408	LHG	C31-C32-C33-C34
24	j	101	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
23	A	412	SQD	C14-C15-C16-C17
24	C	524	LMG	C4-C5-C6-O5
38	H	101	RRX	C9-C10-C11-C12
36	L	101	LHG	C32-C33-C34-C35
20	b	614	CLA	C8-C10-C11-C12
24	C	519	LMG	C15-C16-C17-C18
35	d	416	DGD	CCA-CDA-CEA-CFA
20	b	612	CLA	C14-C13-C15-C16
20	b	616	CLA	C11-C10-C8-C9
32	b	625	HTG	C4'-C5'-C6'-C7'
36	d	407	LHG	C31-C32-C33-C34
20	B	616	CLA	C12-C13-C15-C16
20	D	404	CLA	C12-C13-C15-C16
20	b	618	CLA	C12-C13-C15-C16
20	c	509	CLA	O1D-CGD-O2D-CED
20	a	404	CLA	C2B-C3B-CAB-CBB
20	c	512	CLA	C2B-C3B-CAB-CBB
20	c	513	CLA	C2B-C3B-CAB-CBB
22	K	101	BCR	C1-C6-C7-C8
22	K	101	BCR	C5-C6-C7-C8
22	b	619	BCR	C1-C6-C7-C8
22	j	102	BCR	C1-C6-C7-C8
22	j	102	BCR	C5-C6-C7-C8
38	x	101	RRX	C23-C24-C25-C26
23	A	406	SQD	O47-C7-C8-C9
36	l	102	LHG	C9-C10-C11-C12
22	C	514	BCR	C9-C10-C11-C12
34	b	628	LMT	C6-C7-C8-C9
20	b	614	CLA	C3-C5-C6-C7
27	a	415	PL9	C39-C41-C42-C43
23	F	101	SQD	O48-C23-C24-C25
35	c	516	DGD	O6E-C1E-O5D-C6D
27	D	412	PL9	C28-C29-C31-C32
27	d	412	PL9	C43-C44-C46-C47
20	B	611	CLA	C4C-C3C-CAC-CBC
32	C	520	HTG	C2'-C1'-S1-C1
32	C	534	HTG	C2'-C1'-S1-C1
36	E	103	LHG	O7-C5-C6-O8
32	d	401	HTG	C4'-C5'-C6'-C7'
36	L	101	LHG	C25-C26-C27-C28
20	A	401	CLA	C4C-C3C-CAC-CBC
20	C	512	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	b	623	LMG	C17-C18-C19-C20
35	H	102	DGD	C6B-C7B-C8B-C9B
20	b	604	CLA	C8-C10-C11-C12
34	b	628	LMT	C11-C10-C9-C8
34	a	418	LMT	O1'-C1-C2-C3
35	c	516	DGD	C4E-C5E-C6E-O5E
20	B	601	CLA	C6-C7-C8-C9
20	B	616	CLA	C14-C13-C15-C16
20	C	507	CLA	C11-C12-C13-C14
36	E	103	LHG	O8-C23-C24-C25
20	c	512	CLA	C1A-C2A-CAA-CBA
23	A	412	SQD	C33-C34-C35-C36
36	L	101	LHG	C13-C14-C15-C16
20	c	512	CLA	CAA-CBA-CGA-O2A
23	f	101	SQD	O48-C23-C24-C25
24	j	101	LMG	O7-C10-C11-C12
37	E	104	HEM	CAA-CBA-CGA-O1A
37	E	104	HEM	CAA-CBA-CGA-O2A
37	e	102	HEM	CAA-CBA-CGA-O1A
37	e	102	HEM	CAA-CBA-CGA-O2A
37	e	102	HEM	CAD-CBD-CGD-O2D
23	a	401	SQD	C30-C31-C32-C33
20	b	616	CLA	C2A-CAA-CBA-CGA
37	e	102	HEM	CAD-CBD-CGD-O1D
23	f	101	SQD	C5-C6-S-O9
20	B	604	CLA	C5-C6-C7-C8
20	b	613	CLA	C8-C10-C11-C12
35	h	101	DGD	CDA-CEA-CFA-CGA
20	d	402	CLA	C2-C1-O2A-CGA
35	C	516	DGD	C7B-C8B-C9B-CAB
20	b	604	CLA	C12-C13-C15-C16
20	b	612	CLA	C12-C13-C15-C16
20	b	613	CLA	C12-C13-C15-C16
20	c	504	CLA	C12-C13-C15-C16
20	c	506	CLA	C11-C10-C8-C7
20	c	507	CLA	C11-C12-C13-C15
20	A	401	CLA	C15-C16-C17-C18
36	l	102	LHG	C26-C27-C28-C29
35	C	517	DGD	C4A-C5A-C6A-C7A
35	C	518	DGD	C4B-C5B-C6B-C7B
22	K	102	BCR	C19-C20-C21-C22
20	C	501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	b	604	CLA	C2A-CAA-CBA-CGA
35	H	102	DGD	CCA-CDA-CEA-CFA
20	D	401	CLA	C4C-C3C-CAC-CBC
36	E	103	LHG	O10-C23-C24-C25
27	A	411	PL9	C18-C19-C21-C22
24	A	407	LMG	C19-C20-C21-C22
35	C	516	DGD	C2A-C3A-C4A-C5A
35	H	102	DGD	CCB-CDB-CEB-CFB
35	h	101	DGD	C9A-CAA-CBA-CCA
35	H	102	DGD	O1B-C1B-C2B-C3B
35	h	101	DGD	CAA-CBA-CCA-CDA
32	C	522	HTG	C4-C5-C6-O6
23	A	412	SQD	C13-C14-C15-C16
20	c	510	CLA	C16-C17-C18-C20
20	B	614	CLA	C13-C15-C16-C17
20	c	512	CLA	CAA-CBA-CGA-O1A
23	F	101	SQD	O10-C23-C24-C25
23	A	406	SQD	O49-C7-C8-C9
36	d	406	LHG	C32-C33-C34-C35
24	b	623	LMG	O8-C28-C29-C30
22	K	101	BCR	C17-C18-C19-C20
22	K	102	BCR	C7-C8-C9-C10
24	C	519	LMG	C16-C17-C18-C19
24	c	518	LMG	C32-C33-C34-C35
35	c	516	DGD	C7A-C8A-C9A-CAA
24	c	518	LMG	O6-C5-C6-O5
34	z	102	LMT	C4-C5-C6-C7
24	B	620	LMG	C36-C37-C38-C39
34	B	627	LMT	C2-C3-C4-C5
20	C	512	CLA	CAA-CBA-CGA-O1A
35	c	515	DGD	C6A-C7A-C8A-C9A
20	B	602	CLA	C5-C6-C7-C8
20	D	402	CLA	C15-C16-C17-C18
24	j	101	LMG	O9-C10-C11-C12
20	b	612	CLA	C16-C17-C18-C19
20	A	401	CLA	CAD-CBD-CGD-O2D
20	B	613	CLA	CAD-CBD-CGD-O2D
20	C	504	CLA	CAD-CBD-CGD-O2D
20	C	506	CLA	CAD-CBD-CGD-O2D
20	C	509	CLA	CAD-CBD-CGD-O2D
20	D	404	CLA	CAD-CBD-CGD-O2D
20	b	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	a	406	PHO	CAD-CBD-CGD-O2D
20	b	603	CLA	C8-C10-C11-C12
34	m	101	LMT	C11-C10-C9-C8
35	c	516	DGD	C4A-C5A-C6A-C7A
20	D	401	CLA	C2-C1-O2A-CGA
34	I	101	LMT	C5'-C4'-O1B-C1B
23	A	406	SQD	C33-C34-C35-C36
20	a	404	CLA	C6-C7-C8-C10
20	b	616	CLA	C6-C7-C8-C10
27	A	411	PL9	C2-C3-C7-C8
36	L	101	LHG	C26-C27-C28-C29
20	C	505	CLA	CAA-CBA-CGA-O2A
23	f	101	SQD	O10-C23-C24-C25
36	D	407	LHG	C11-C10-C9-C8

There are no ring outliers.

186 monomers are involved in 488 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	e	102	HEM	3	0
20	C	504	CLA	3	0
28	c	536	DMS	8	0
28	V	205	DMS	1	0
28	U	904	DMS	3	0
20	C	509	CLA	5	0
22	b	621	BCR	4	0
23	b	622	SQD	3	0
35	c	516	DGD	2	0
20	c	509	CLA	2	0
28	c	530	DMS	7	0
28	B	644	DMS	5	0
28	b	635	DMS	1	0
28	i	104	DMS	4	0
22	K	101	BCR	2	0
20	d	404	CLA	2	0
20	D	401	CLA	1	0
20	b	610	CLA	1	0
23	A	412	SQD	2	0
34	a	418	LMT	10	0
24	C	519	LMG	3	0
20	B	611	CLA	4	0
28	V	206	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	C	520	HTG	1	0
34	I	101	LMT	2	0
22	A	405	BCR	5	0
20	C	508	CLA	3	0
28	O	305	DMS	1	0
20	B	604	CLA	2	0
20	b	613	CLA	1	0
38	x	101	RRX	3	0
23	A	406	SQD	3	0
32	B	631	HTG	1	0
36	D	409	LHG	19	0
36	d	408	LHG	20	0
28	b	638	DMS	3	0
28	O	307	DMS	2	0
20	b	616	CLA	1	0
32	b	625	HTG	6	0
28	d	413	DMS	3	0
20	C	506	CLA	2	0
20	b	611	CLA	2	0
28	U	903[A]	DMS	2	0
21	a	405	PHO	1	0
28	C	532	DMS	6	0
28	b	640	DMS	3	0
31	A	421	BCT	5	0
20	b	604	CLA	3	0
22	a	408	BCR	1	0
32	v	210	HTG	1	0
28	C	531	DMS	5	0
23	a	401	SQD	4	0
21	a	406	PHO	1	0
22	T	101	BCR	4	0
20	C	513	CLA	2	0
21	D	403	PHO	1	0
28	B	635	DMS	4	0
28	c	533	DMS	1	0
28	u	202	DMS	2	0
20	c	503	CLA	2	0
28	F	102	DMS	3	0
28	B	641	DMS	3	0
20	c	502	CLA	3	0
28	O	310	DMS	2	0
32	c	520	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	627	LMT	1	0
34	m	102	LMT	1	0
28	U	903[B]	DMS	10	0
20	d	403	CLA	2	0
20	a	403	CLA	4	0
20	B	606	CLA	6	0
28	o	308	DMS	1	0
35	d	416	DGD	2	0
34	B	625	LMT	1	0
28	B	637	DMS	1	0
20	c	507	CLA	3	0
22	b	620	BCR	1	0
28	O	308	DMS	1	0
32	B	622	HTG	8	0
20	c	505	CLA	1	0
32	B	621	HTG	6	0
37	E	104	HEM	1	0
28	A	417	DMS	1	0
20	B	603	CLA	1	0
20	B	616	CLA	2	0
20	b	618	CLA	5	0
22	d	405	BCR	3	0
22	c	514	BCR	1	0
22	j	102	BCR	5	0
28	C	530	DMS	1	0
28	B	643	DMS	1	0
28	D	414	DMS	8	0
32	B	632	HTG	2	0
34	z	102	LMT	5	0
28	b	641	DMS	2	0
34	b	627	LMT	2	0
28	v	206	DMS	4	0
22	D	405	BCR	3	0
22	t	101	BCR	4	0
20	c	510	CLA	2	0
23	l	101	SQD	2	0
20	B	605	CLA	2	0
20	b	608	CLA	4	0
22	k	102	BCR	3	0
32	D	417	HTG	3	0
34	B	626	LMT	2	0
20	A	402	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	642	DMS	8	0
20	b	609	CLA	2	0
28	A	415	DMS	2	0
32	C	534	HTG	1	0
35	c	517	DGD	2	0
28	o	306	DMS	5	0
20	b	603	CLA	1	0
20	C	501	CLA	3	0
28	O	306	DMS	1	0
20	c	504	CLA	3	0
20	B	607	CLA	1	0
22	B	618	BCR	3	0
20	A	401	CLA	6	0
28	u	203	DMS	1	0
36	d	406	LHG	2	0
28	b	639	DMS	9	0
28	B	645	DMS	2	0
28	d	414	DMS	5	0
23	a	409	SQD	5	0
20	b	615	CLA	2	0
20	B	612	CLA	1	0
20	c	506	CLA	4	0
28	b	634	DMS	2	0
20	c	511	CLA	1	0
36	l	102	LHG	1	0
21	A	403	PHO	1	0
28	o	307	DMS	3	0
20	b	607	CLA	4	0
24	b	623	LMG	2	0
20	C	502	CLA	2	0
22	B	619	BCR	3	0
20	b	614	CLA	1	0
20	b	606	CLA	3	0
34	b	628	LMT	1	0
24	a	410	LMG	4	0
20	c	513	CLA	3	0
22	K	102	BCR	1	0
28	D	413	DMS	2	0
28	o	302	DMS	9	0
34	c	523	LMT	2	0
28	o	303	DMS	4	0
23	f	101	SQD	2	0

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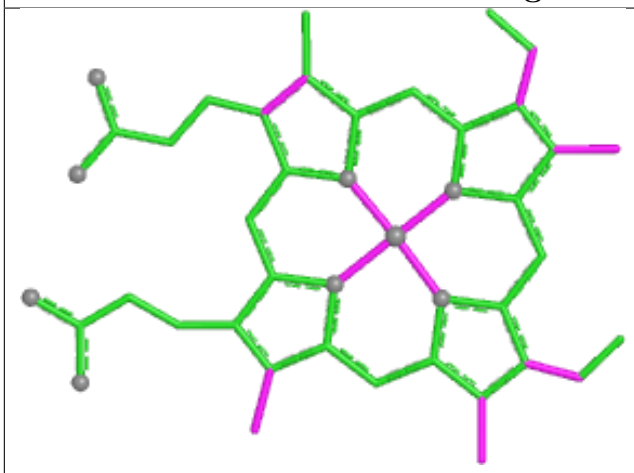
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	632	DMS	2	0
28	U	902	DMS	1	0
20	D	402	CLA	3	0
28	V	204	DMS	1	0
20	b	612	CLA	3	0
28	b	631	DMS	6	0
20	a	404	CLA	1	0
35	D	406	DGD	5	0
34	J	103	LMT	1	0
35	h	101	DGD	1	0
20	c	501	CLA	3	0
35	H	102	DGD	2	0
20	C	511	CLA	1	0
24	A	407	LMG	4	0
36	E	103	LHG	6	0
23	F	101	SQD	1	0
22	k	101	BCR	3	0
20	c	508	CLA	6	0
20	C	503	CLA	2	0
20	b	605	CLA	2	0
28	A	416	DMS	3	0
24	C	524	LMG	2	0
28	V	208	DMS	1	0
28	D	415	DMS	2	0
20	c	512	CLA	3	0
27	a	415	PL9	10	0
20	C	510	CLA	3	0
28	A	418	DMS	3	0
20	C	507	CLA	2	0
22	C	515	BCR	1	0
20	B	601	CLA	4	0
20	B	602	CLA	2	0
22	C	514	BCR	2	0
20	B	614	CLA	1	0
28	C	527	DMS	3	0
20	b	617	CLA	2	0
27	A	411	PL9	11	0

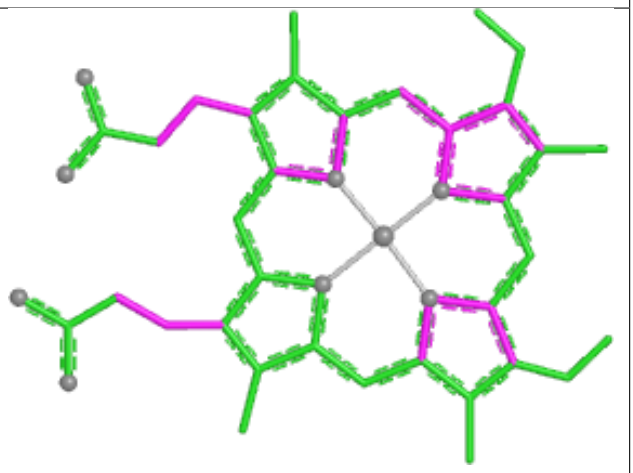
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

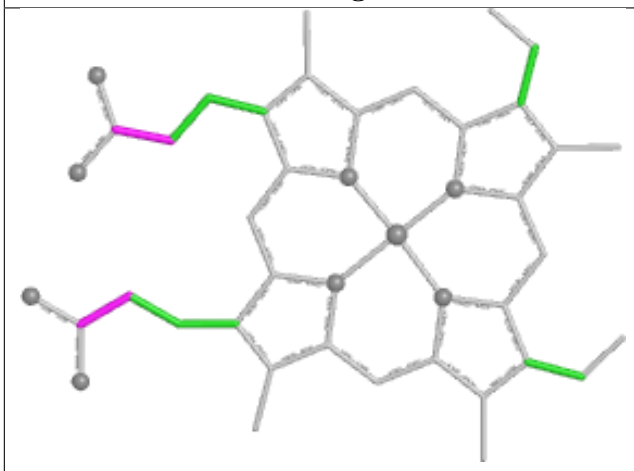
Ligand HEM e 102



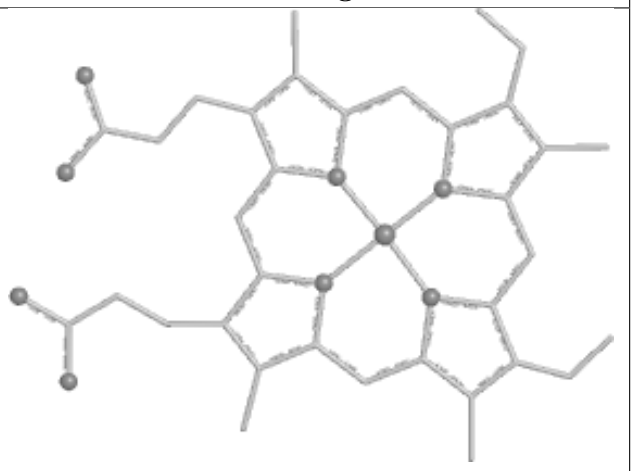
Bond lengths



Bond angles

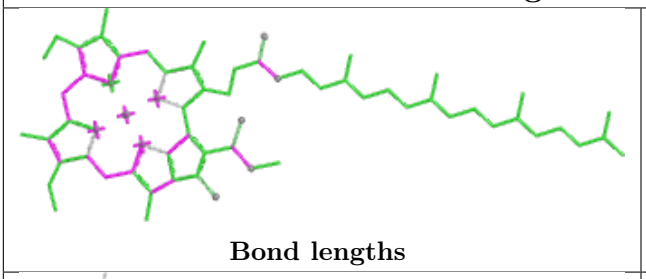


Torsions

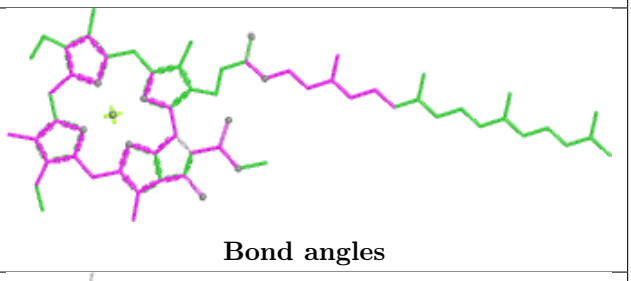


Rings

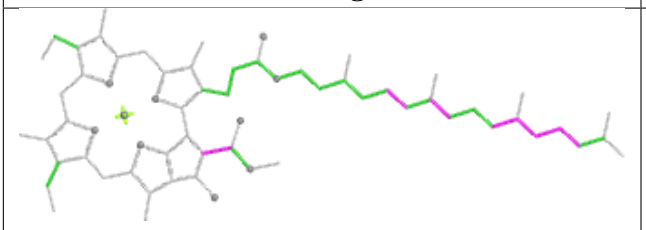
Ligand CLA C 504



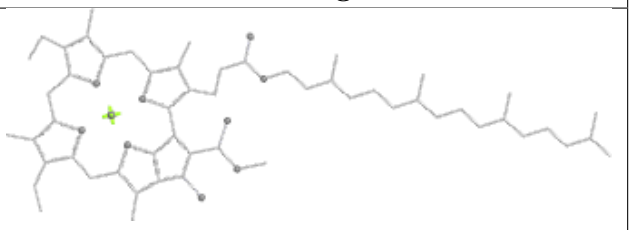
Bond lengths



Bond angles

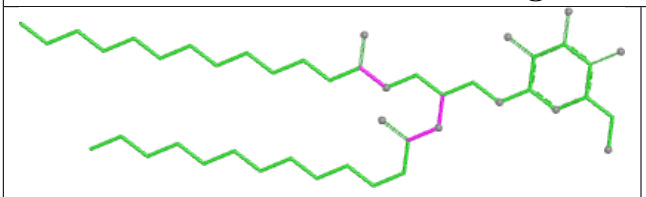


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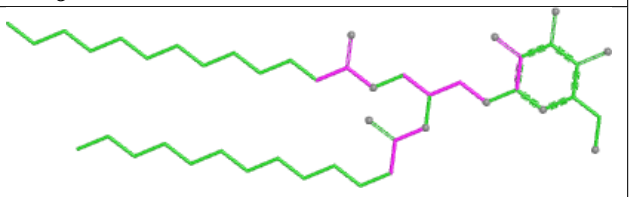


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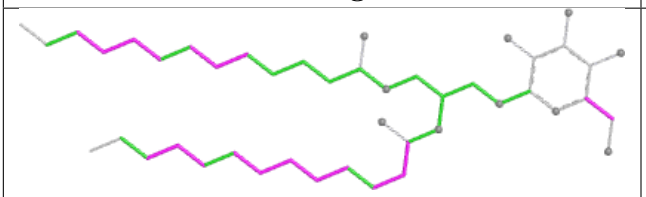
Ligand LMG j 101



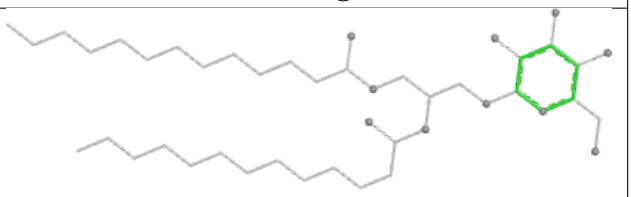
Bond lengths



Bond angles

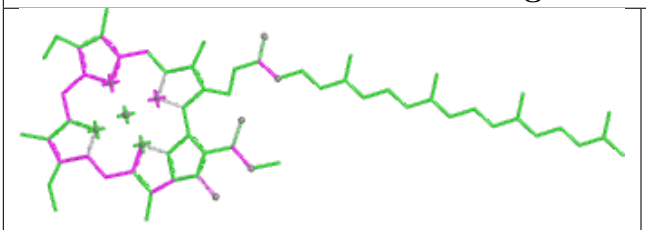


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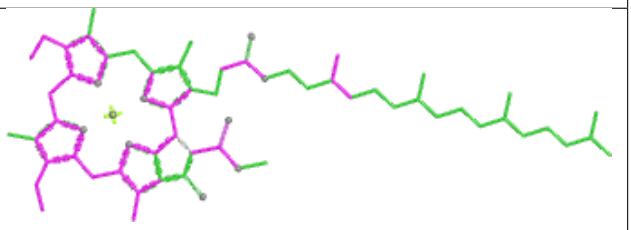


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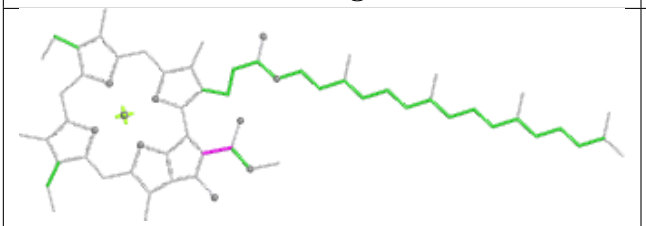
Ligand CLA B 613



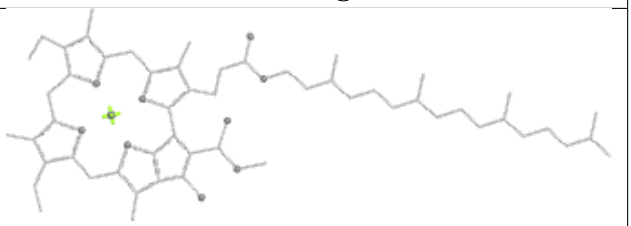
Bond lengths



Bond angles

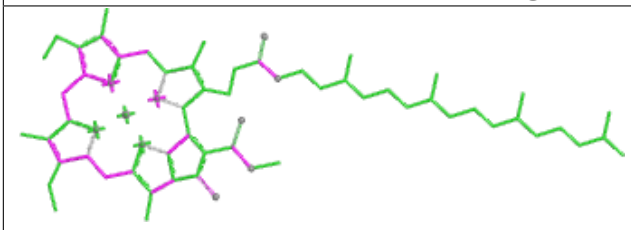


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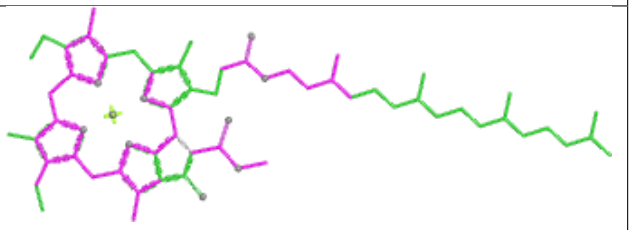


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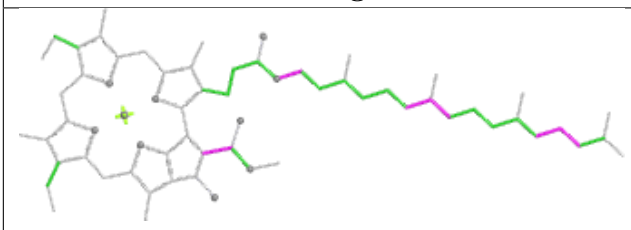
Ligand CLA C 509



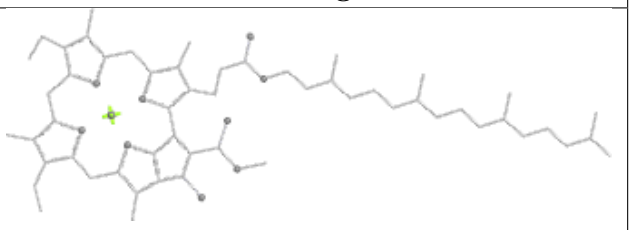
Bond lengths



Bond angles



Torsions

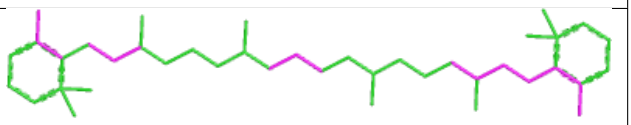


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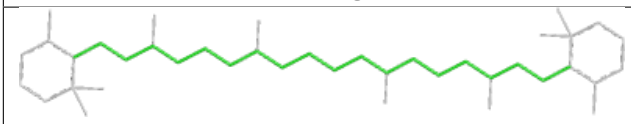
Ligand BCR b 621



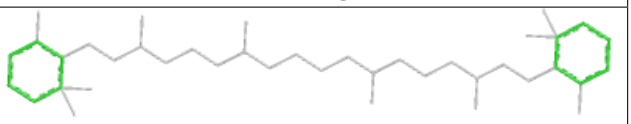
Bond lengths



Bond angles

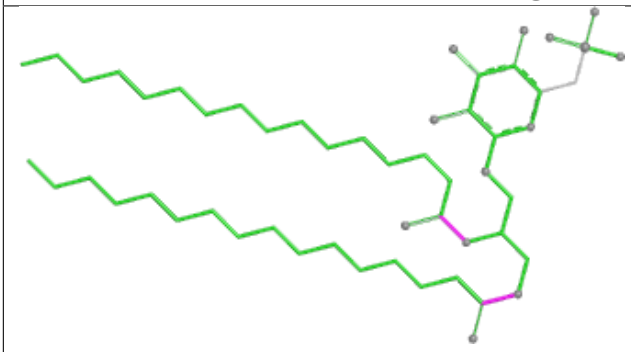


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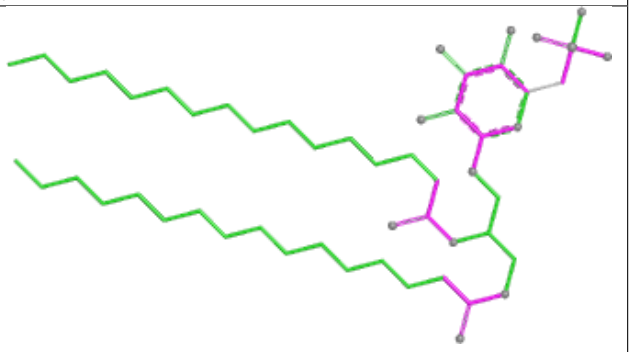


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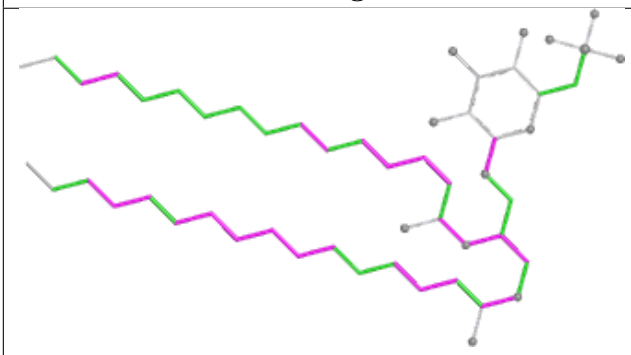
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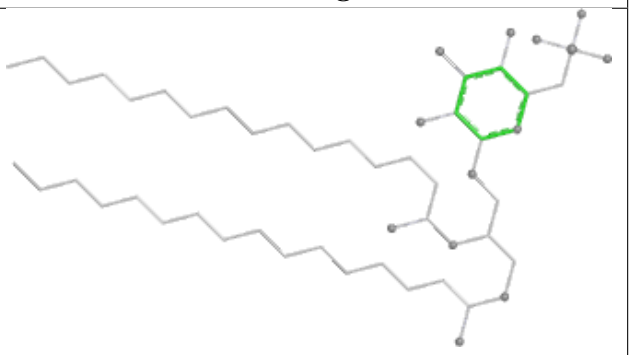
Bond lengths



Bond angles

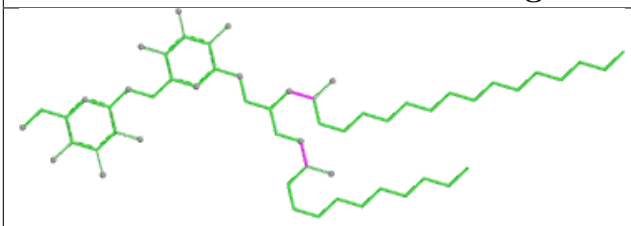


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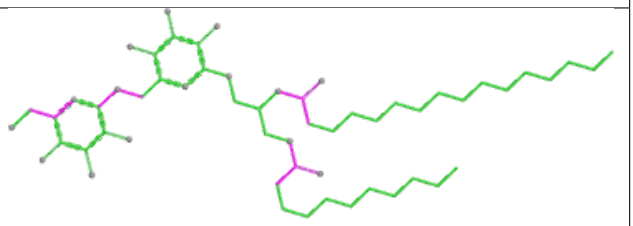


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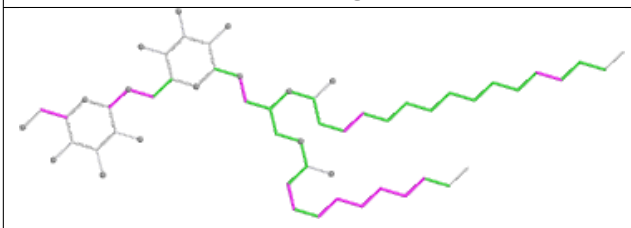
Ligand DGD c 516



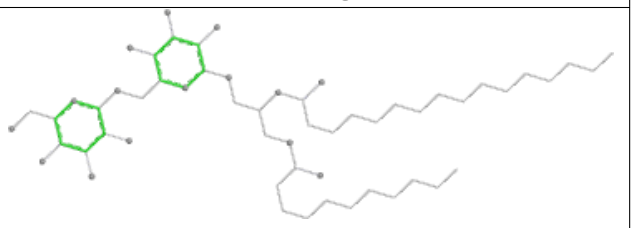
Bond lengths



Bond angles

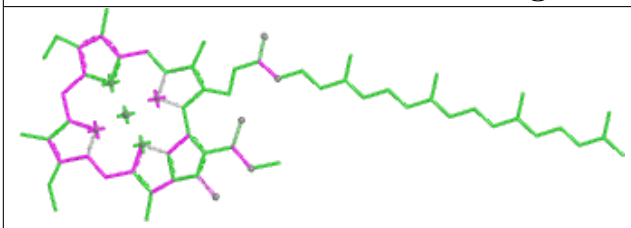


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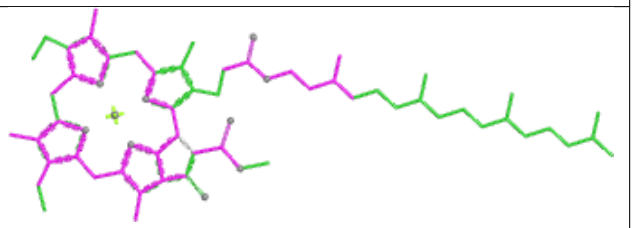


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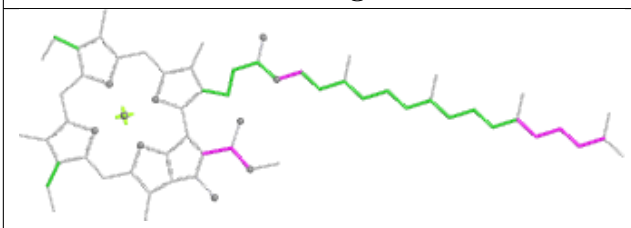
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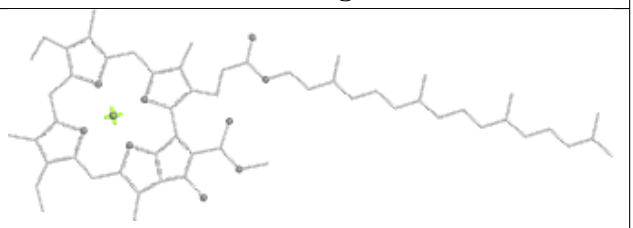
Bond lengths



Bond angles



Torsions

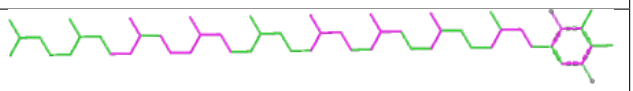


Rings

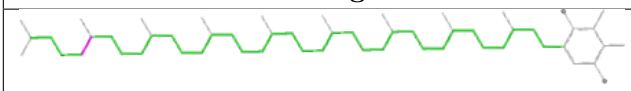
Ligand PL9 d 412



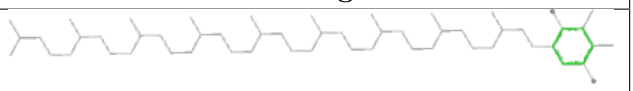
Bond lengths



Bond angles



Torsions

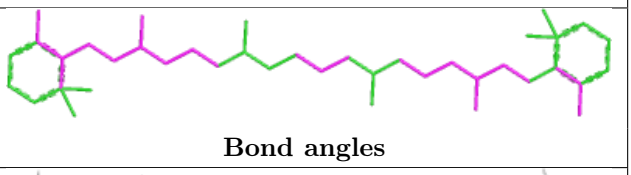


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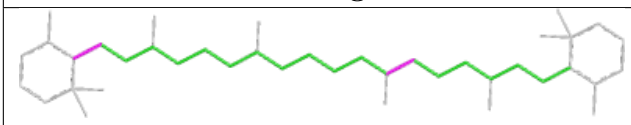
Ligand BCR K 101



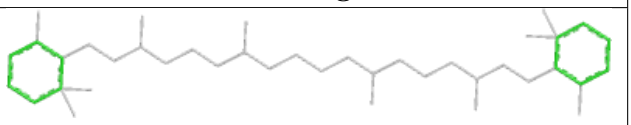
Bond lengths



Bond angles

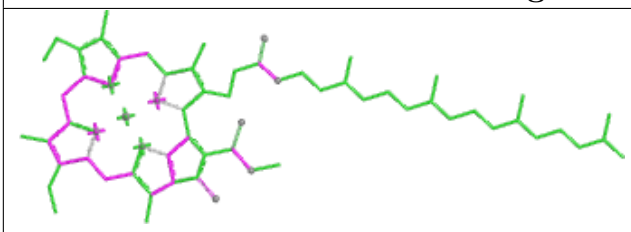


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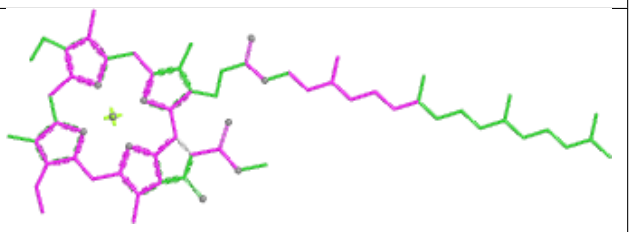


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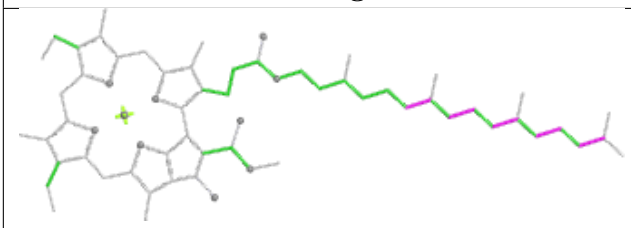
Ligand CLA d 404



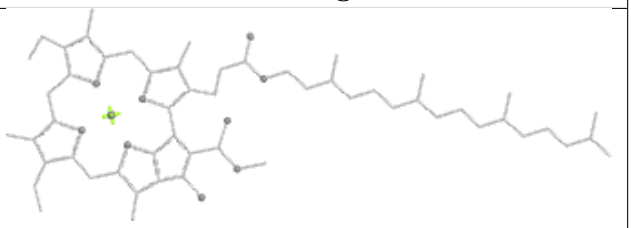
Bond lengths



Bond angles

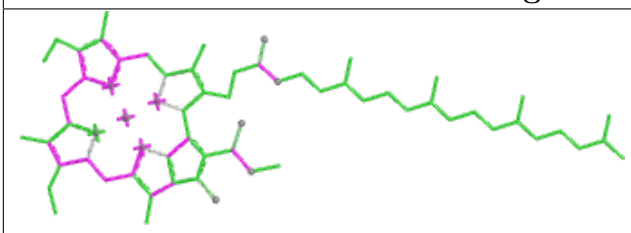


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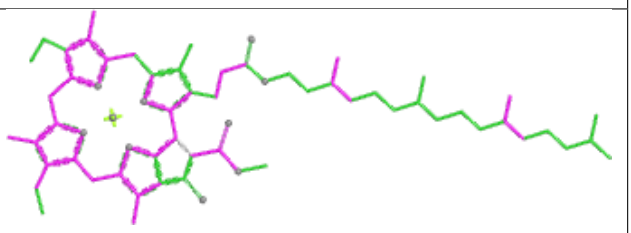


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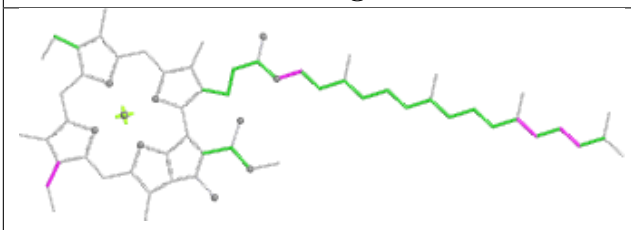
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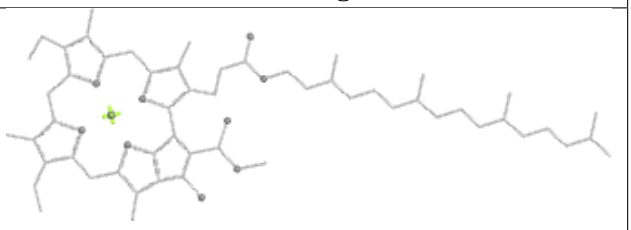
Bond lengths



Bond angles

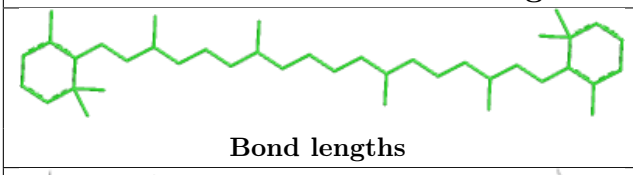


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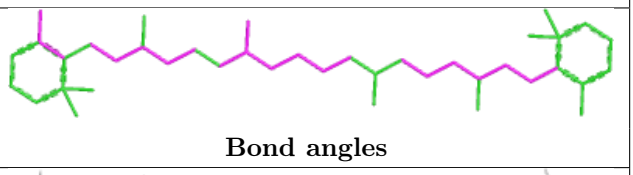


Rings

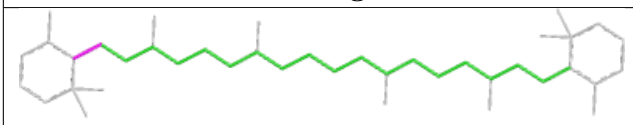
Ligand BCR b 619



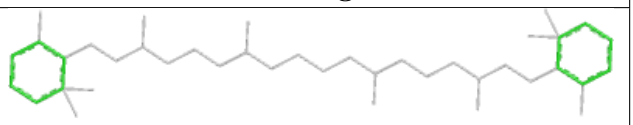
Bond lengths



Bond angles

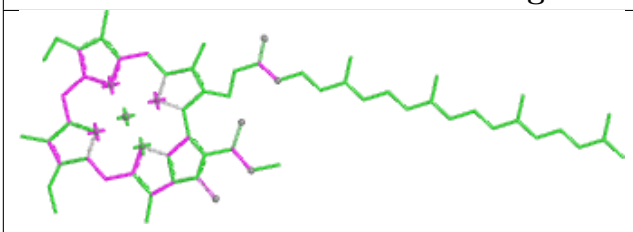


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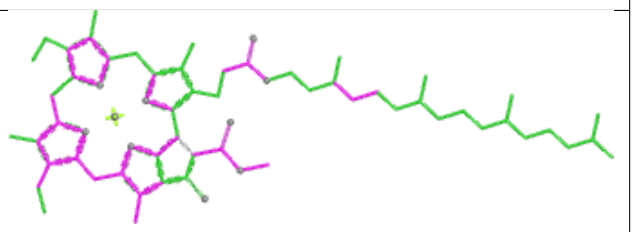


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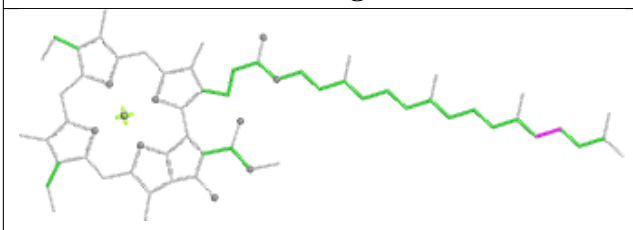
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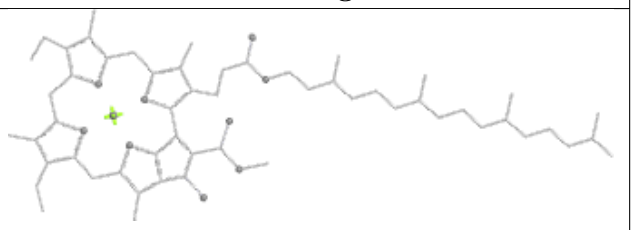
Bond lengths



Bond angles

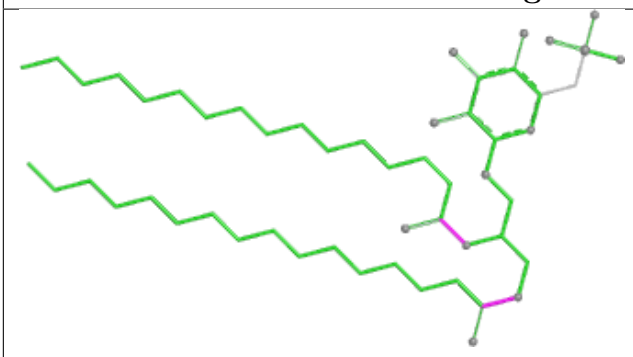


Torsions

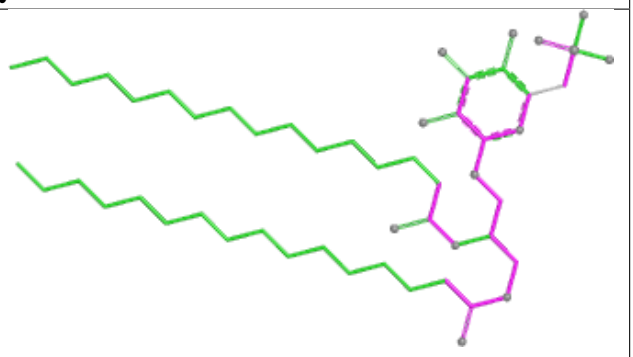


Rings

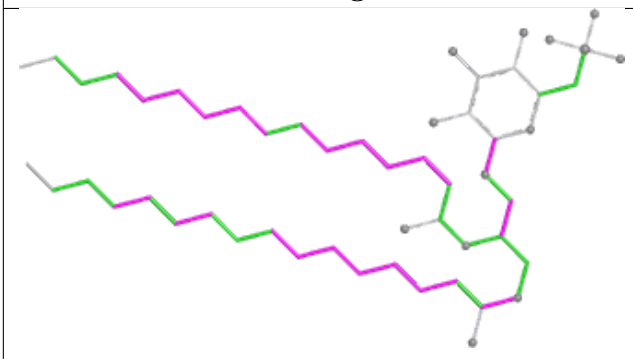
Ligand SQD A 412



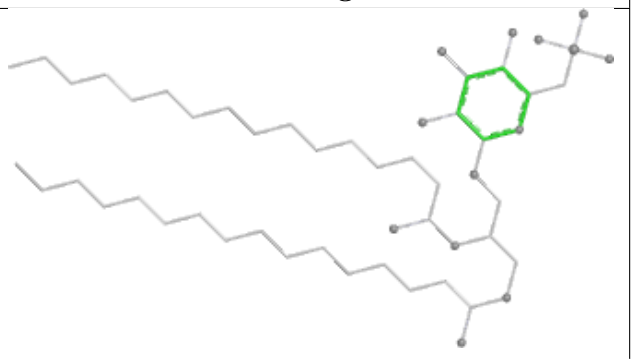
Bond lengths



Bond angles

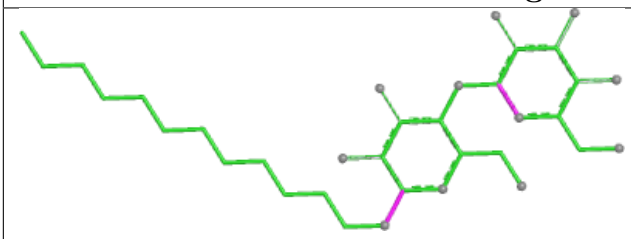


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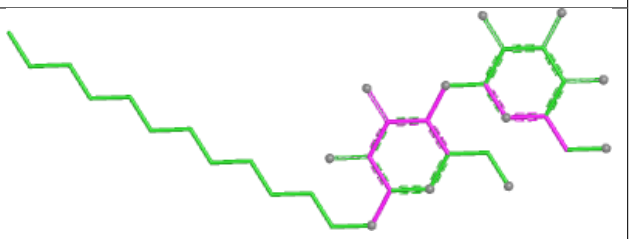


Rings

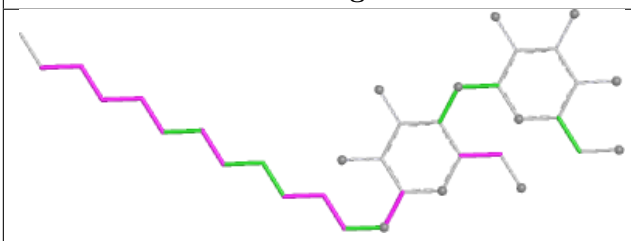
Ligand LMT a 418



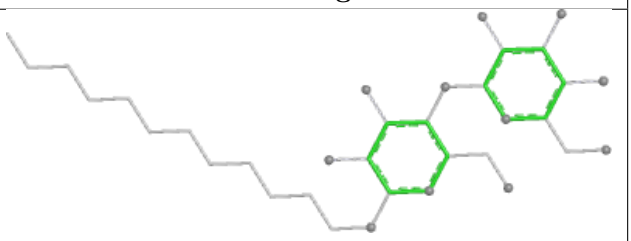
Bond lengths



Bond angles

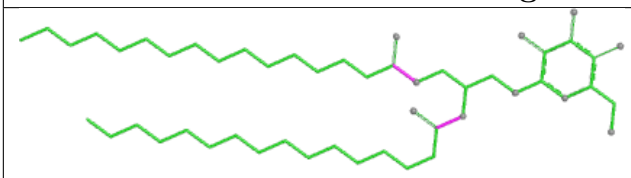


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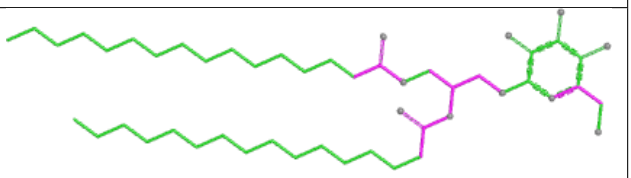


Rings

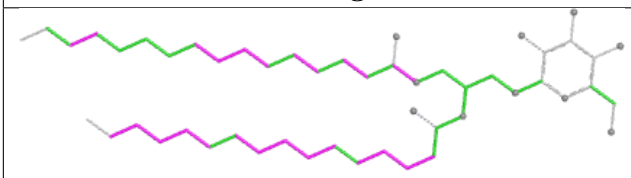
Ligand LMG C 519



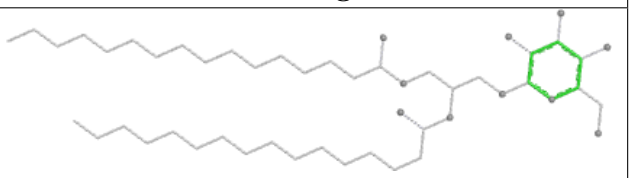
Bond lengths



Bond angles

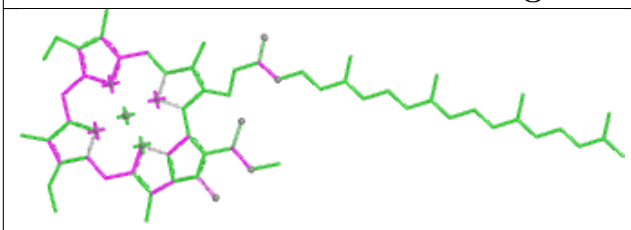


Torsions

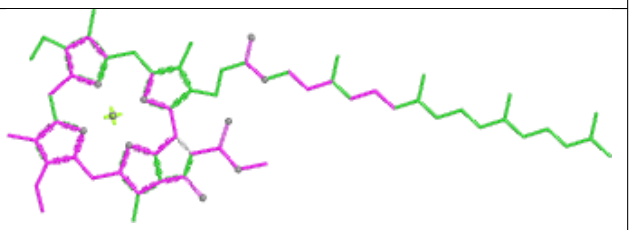


Rings

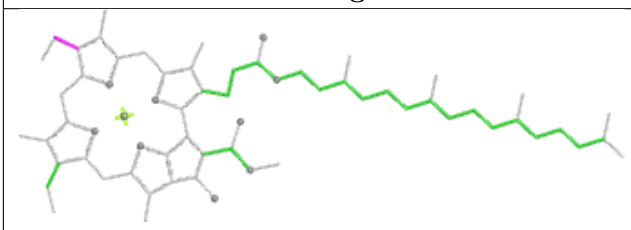
Ligand CLA B 610



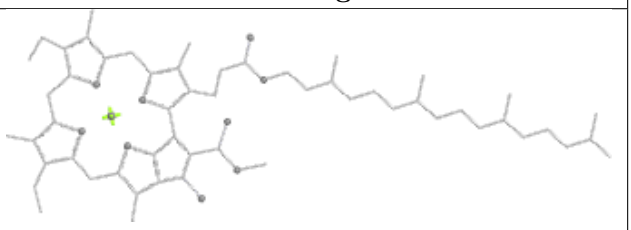
Bond lengths



Bond angles

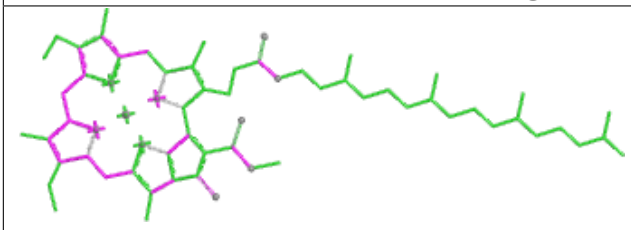


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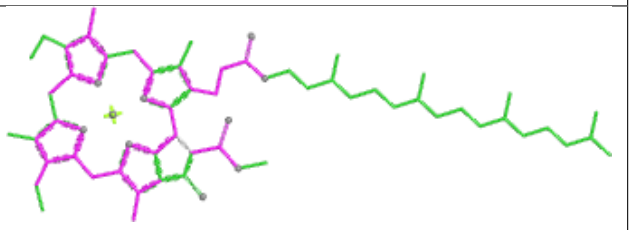


Rings

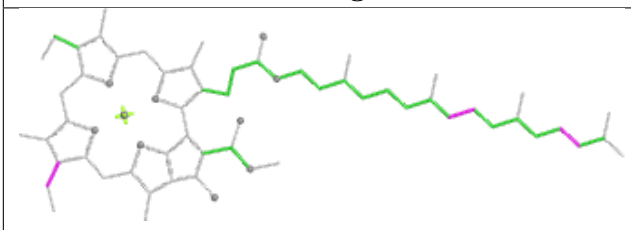
Ligand CLA B 611



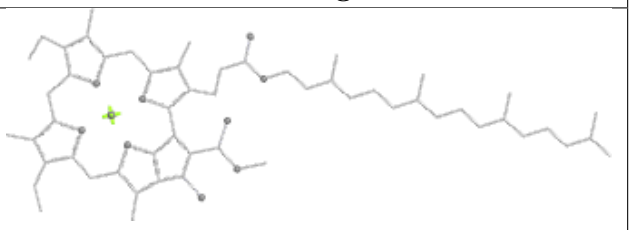
Bond lengths



Bond angles

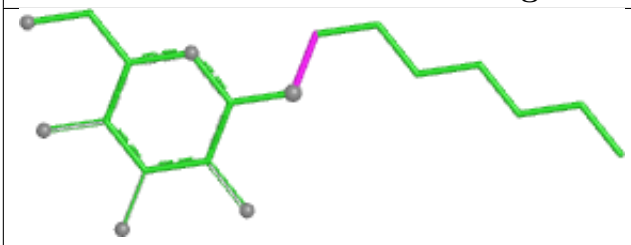


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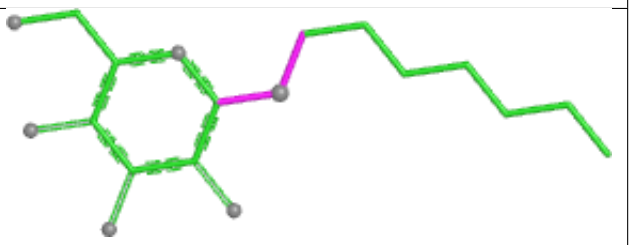


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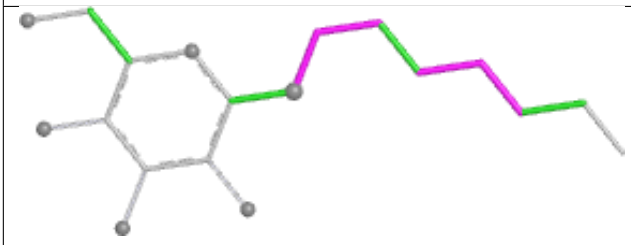
Ligand HTG C 520



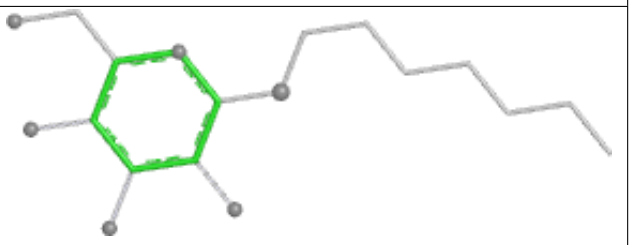
Bond lengths



Bond angles

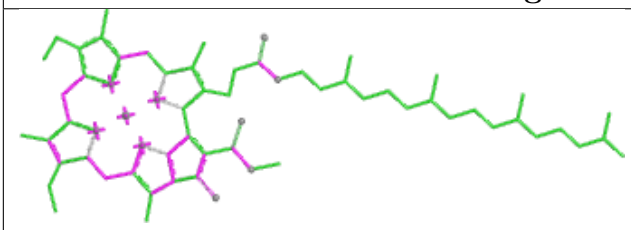


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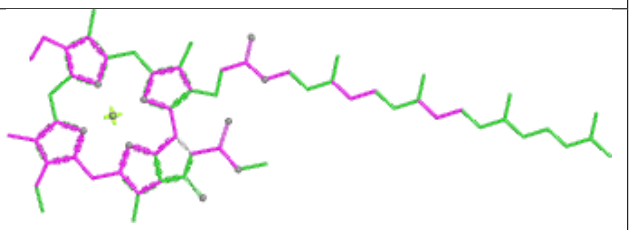


Rings

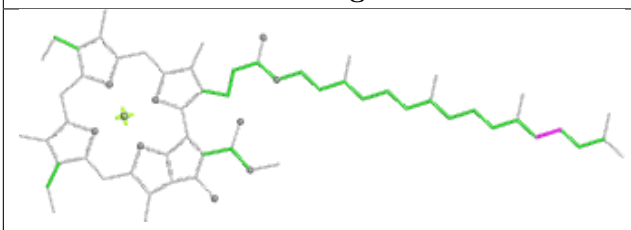
Ligand CLA B 609



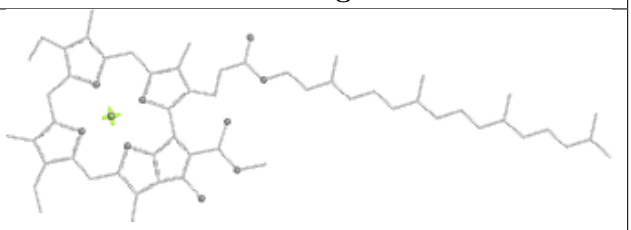
Bond lengths



Bond angles

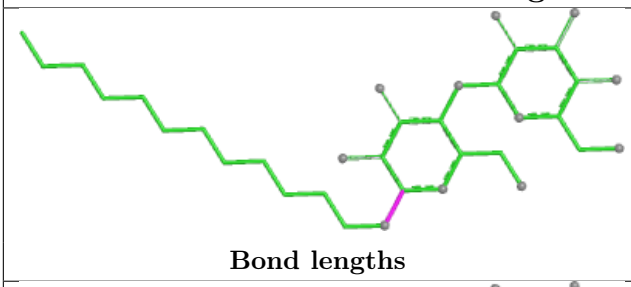


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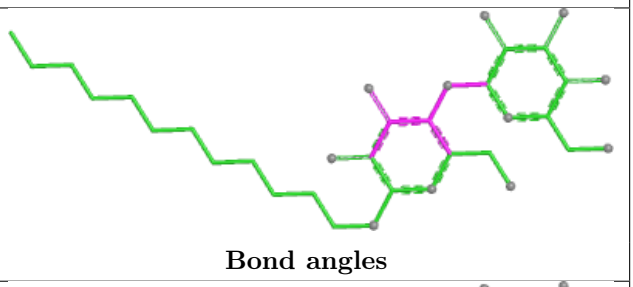


Rings

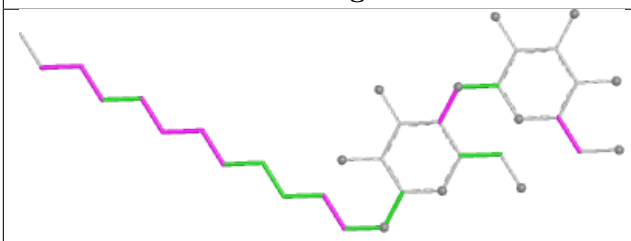
Ligand LMT I 101



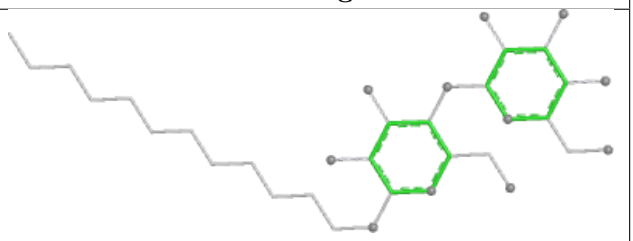
Bond lengths



Bond angles

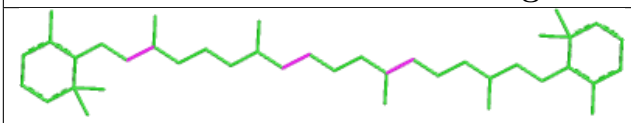


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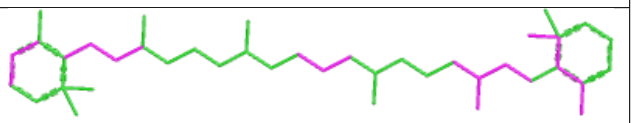


Rings

Ligand BCR A 405



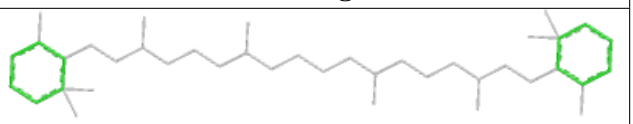
Bond lengths



Bond angles

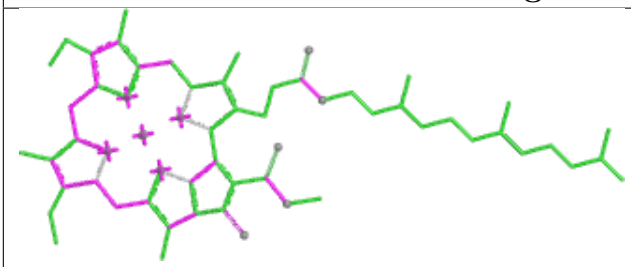


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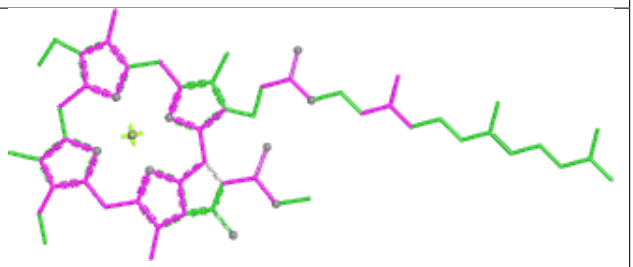


Rings

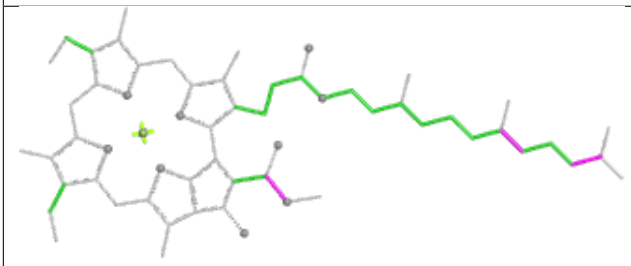
Ligand CLA C 508



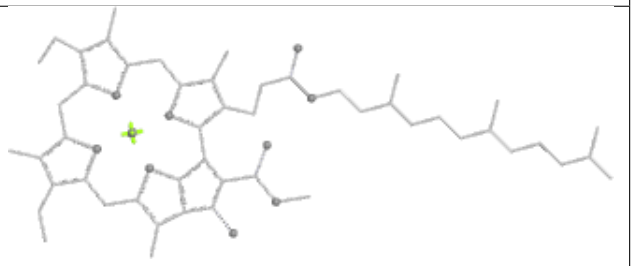
Bond lengths



Bond angles

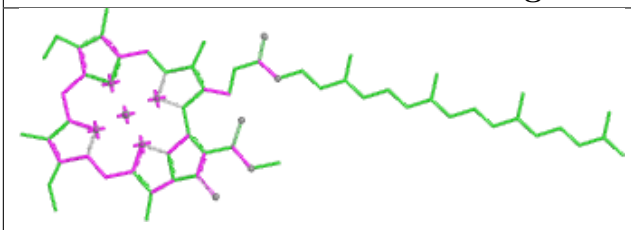


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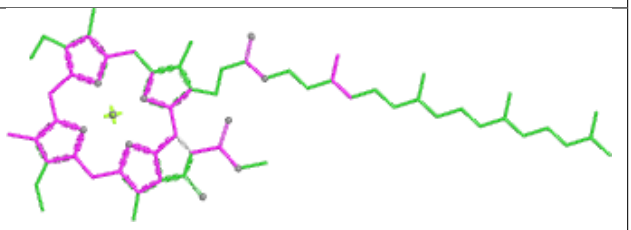


Rings

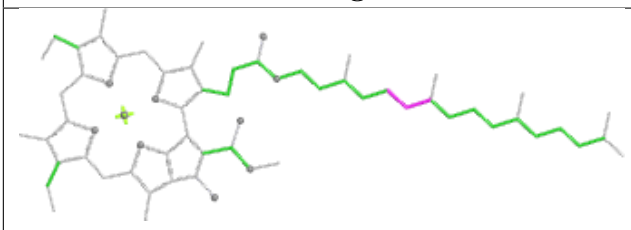
Ligand CLA B 604



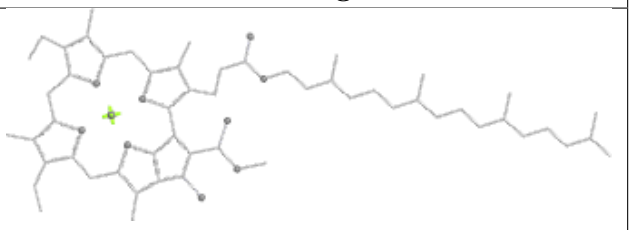
Bond lengths



Bond angles

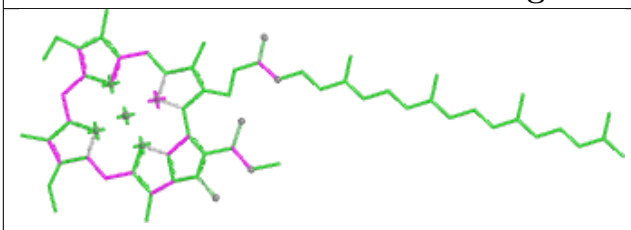


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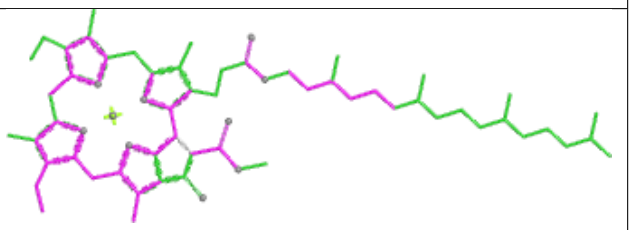


Rings

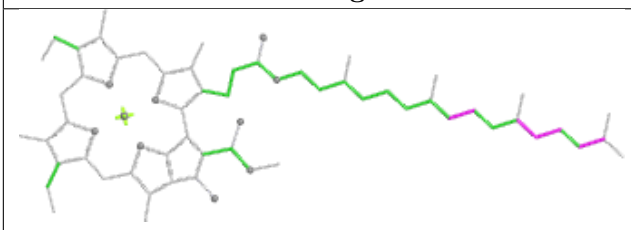
Ligand CLA b 613



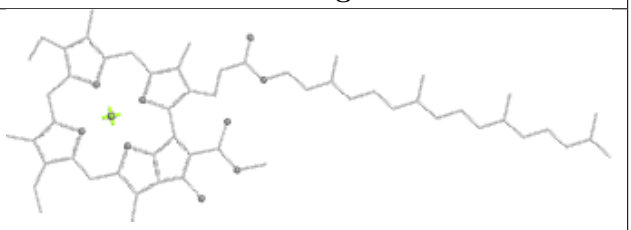
Bond lengths



Bond angles

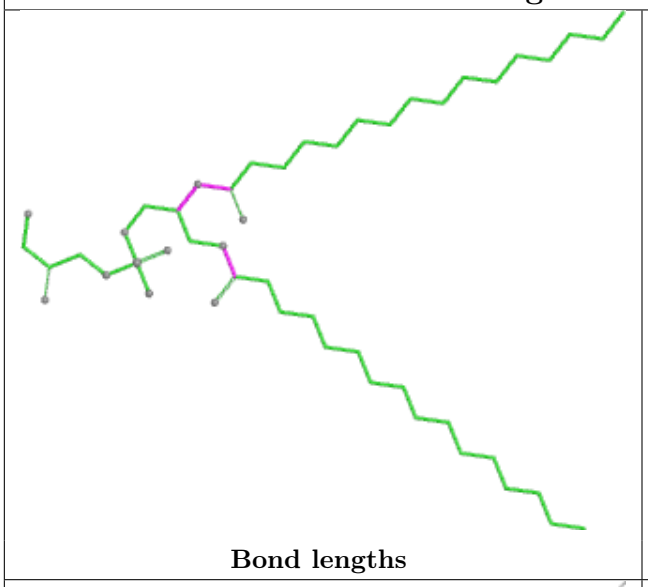


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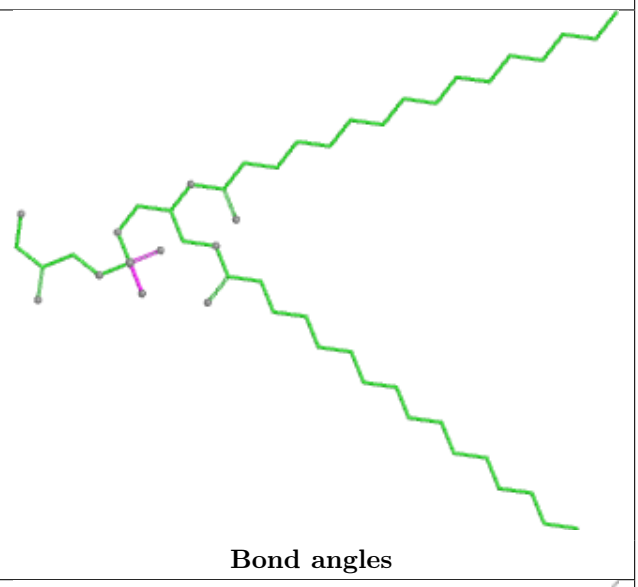


Rings

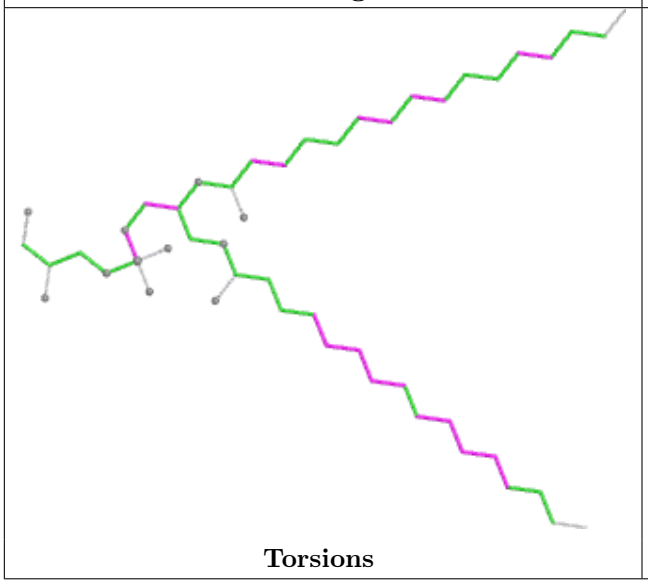
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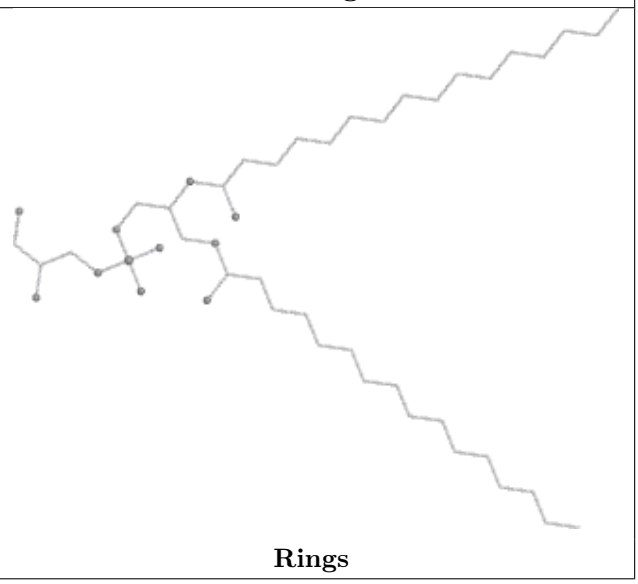
Bond lengths



Bond angles



Torsions

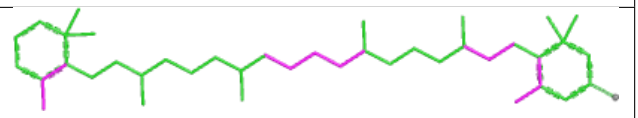


Rings

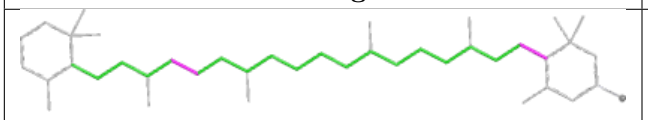
Ligand RRX x 101



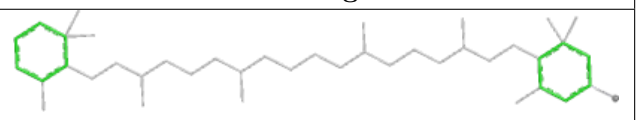
Bond lengths



Bond angles

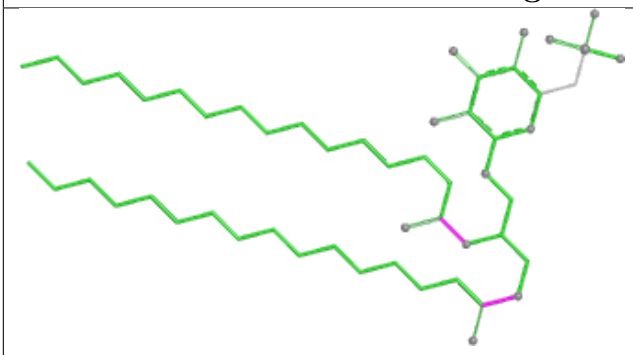


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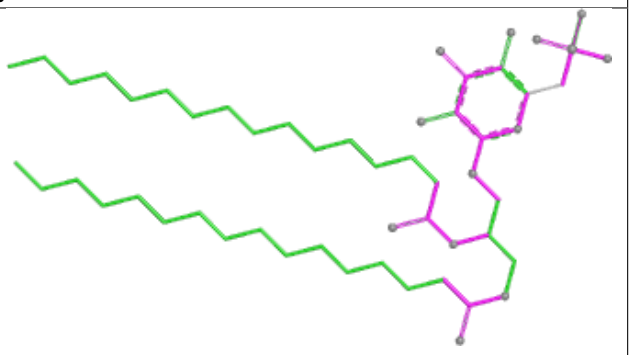


Rings

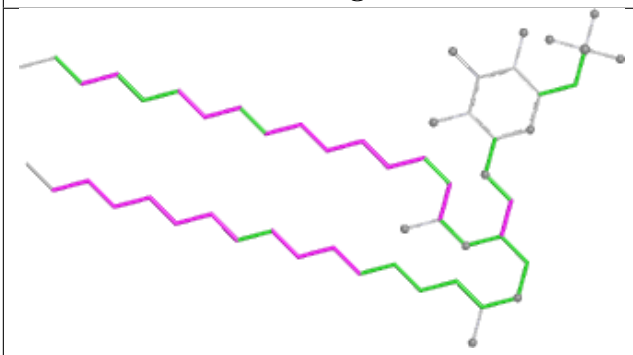
Ligand SQD A 406



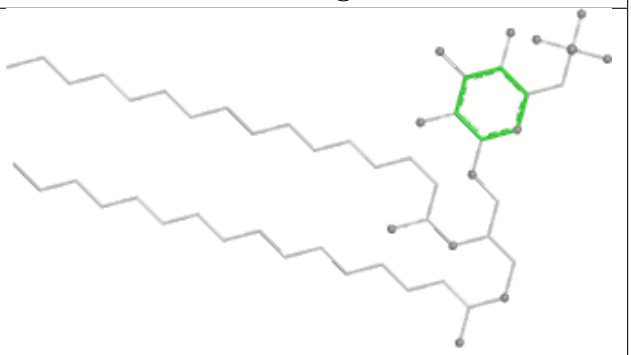
Bond lengths



Bond angles

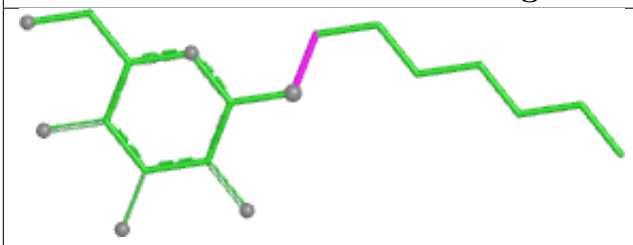


Torsions

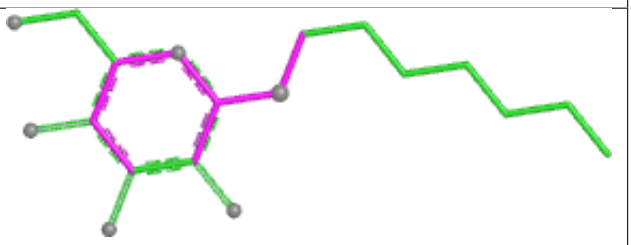


Rings

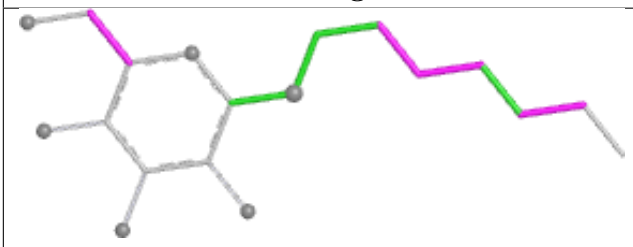
Ligand HTG B 631



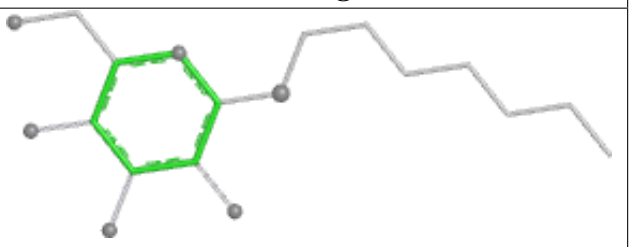
Bond lengths



Bond angles

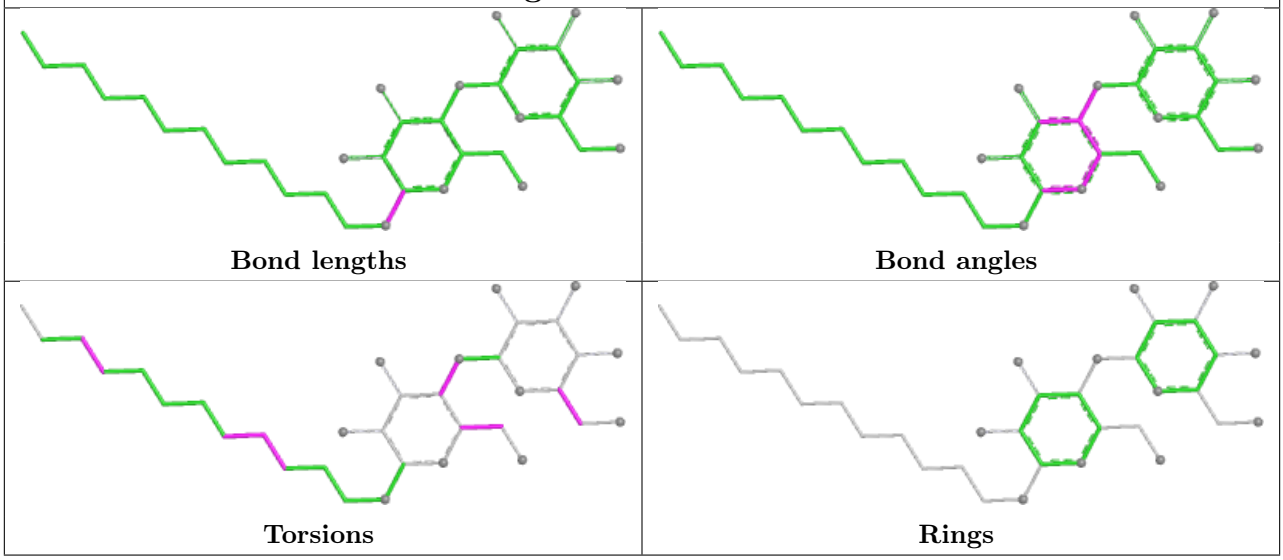


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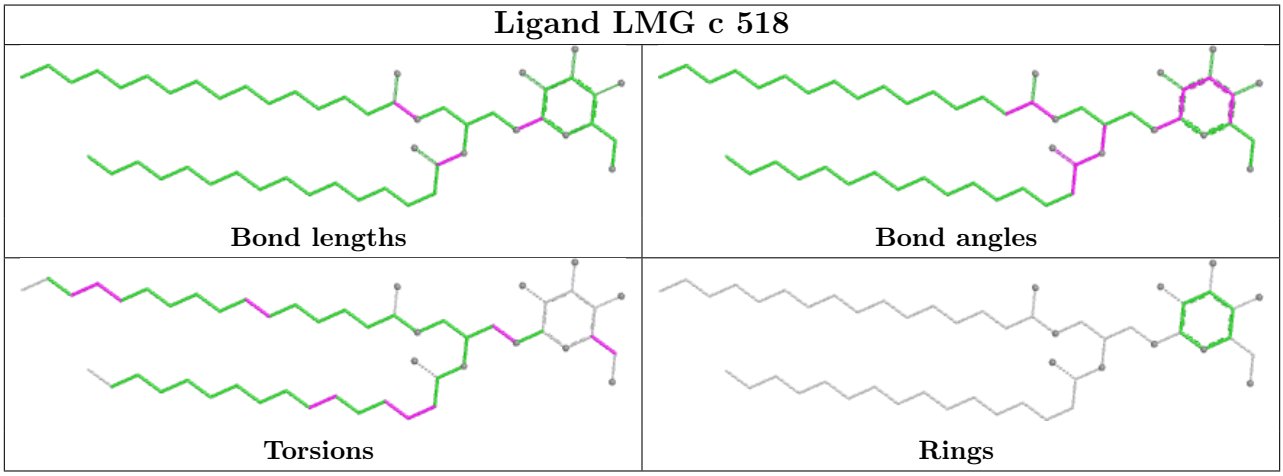


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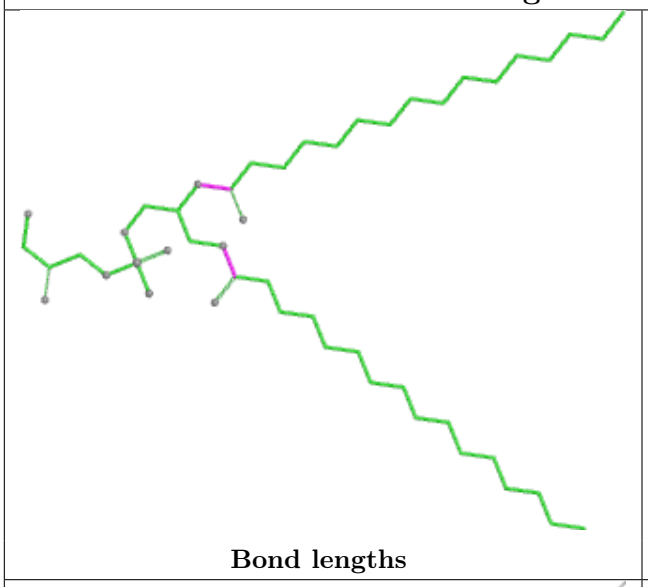
Ligand LMT Z 101



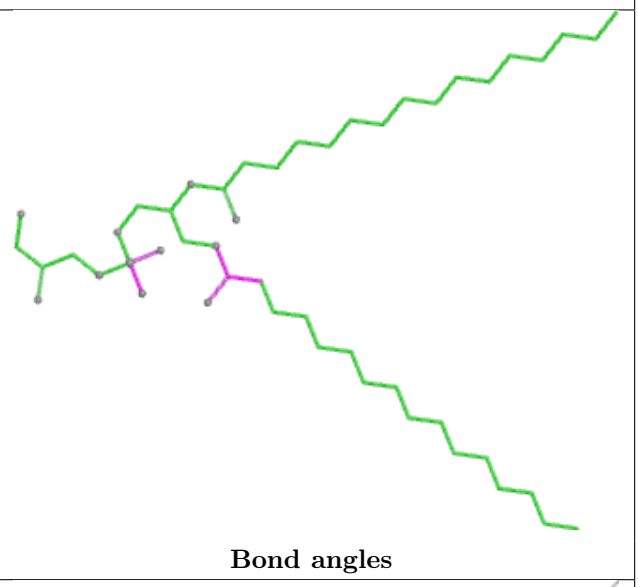
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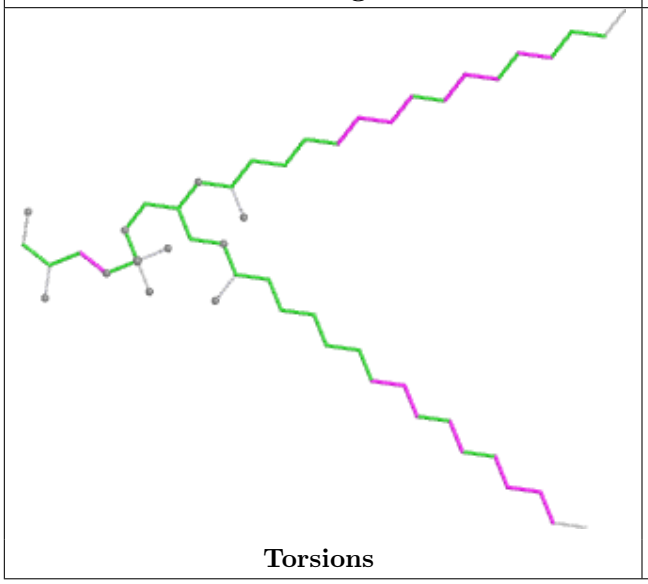
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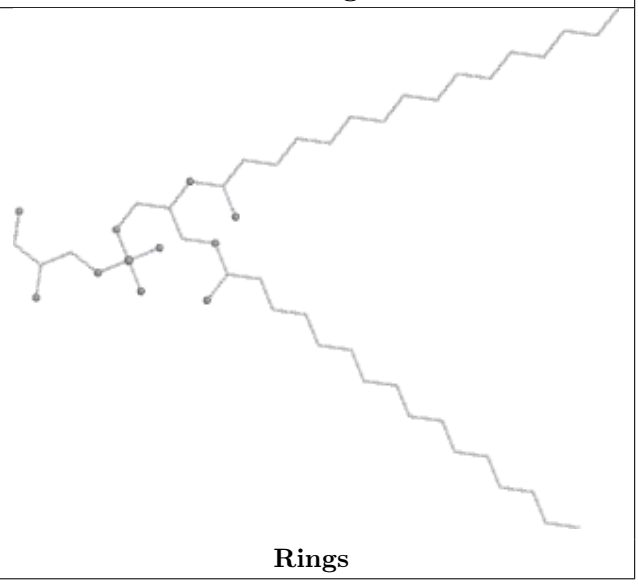
Bond lengths



Bond angles

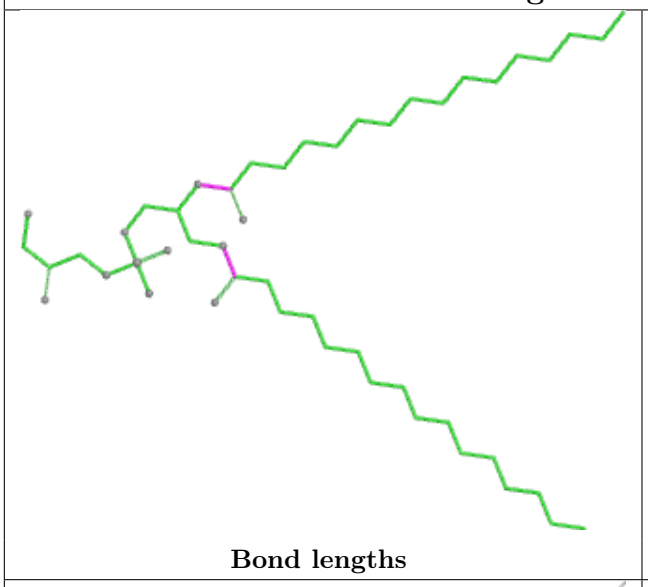


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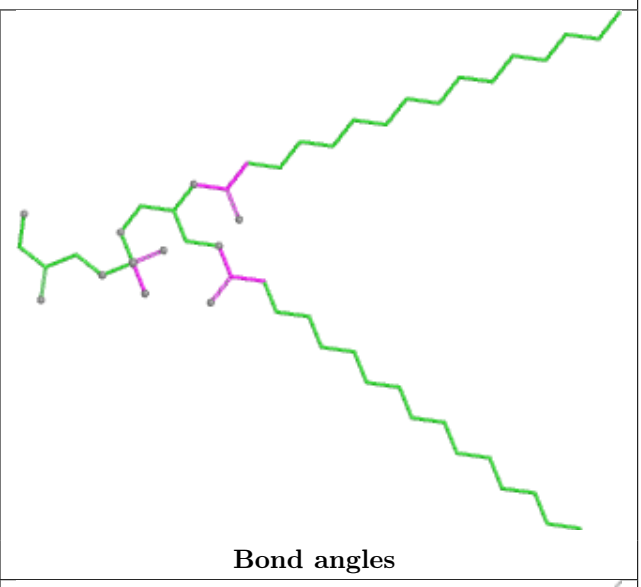


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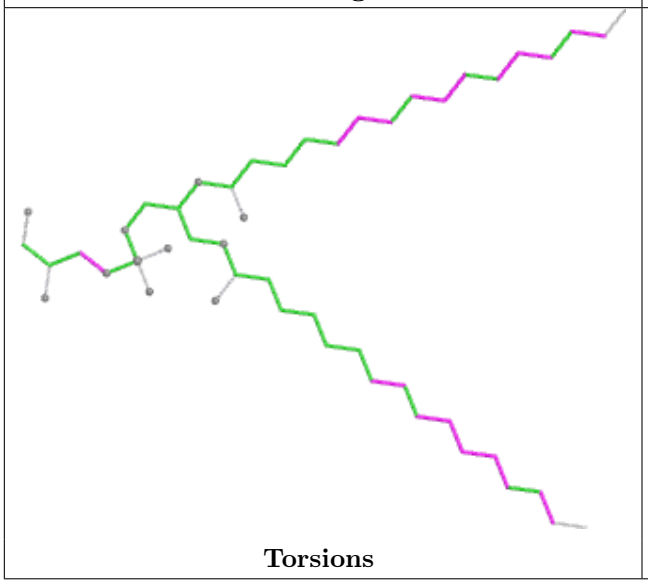
Ligand LHG d 408



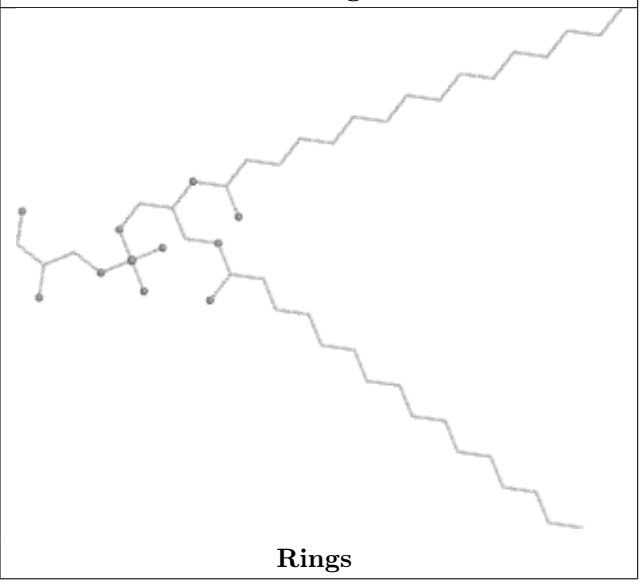
Bond lengths



Bond angles

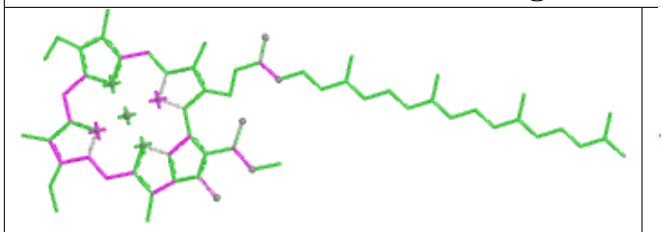


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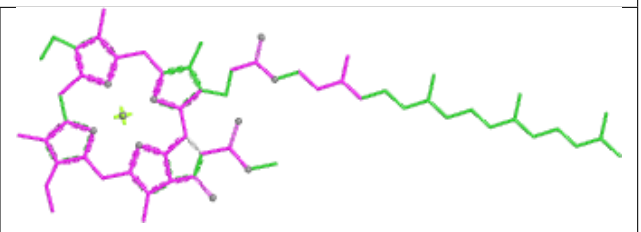


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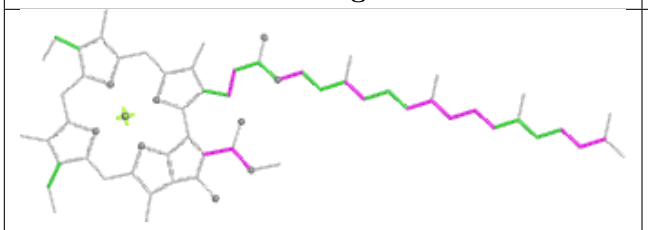
Ligand CLA b 616



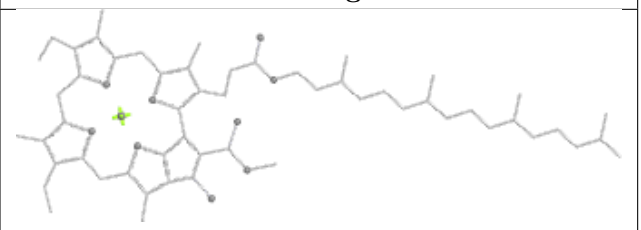
Bond lengths



Bond angles

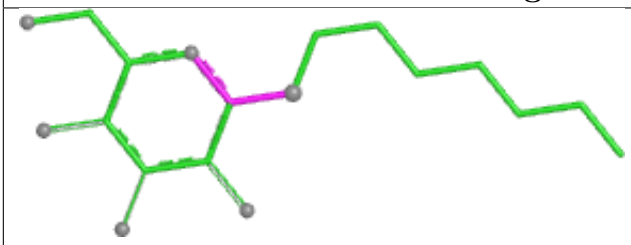


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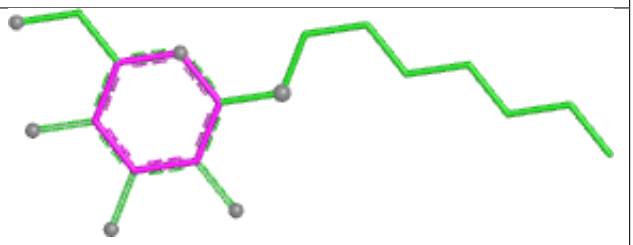


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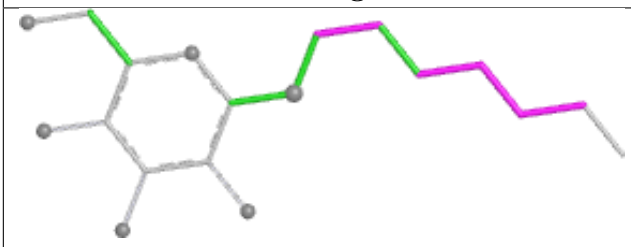
Ligand HTG b 625



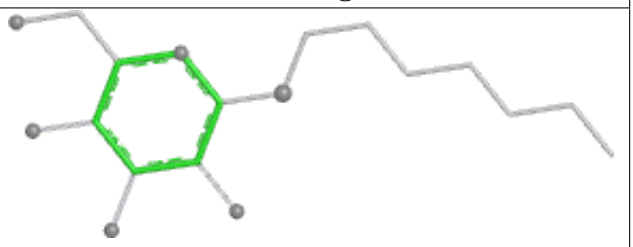
Bond lengths



Bond angles

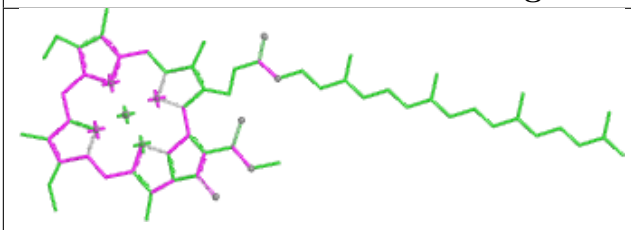


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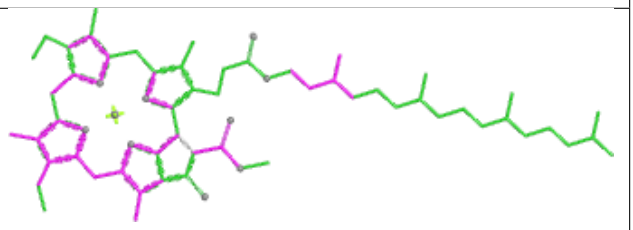


Rings

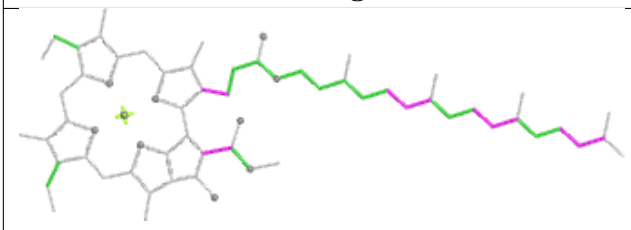
Ligand CLA C 506



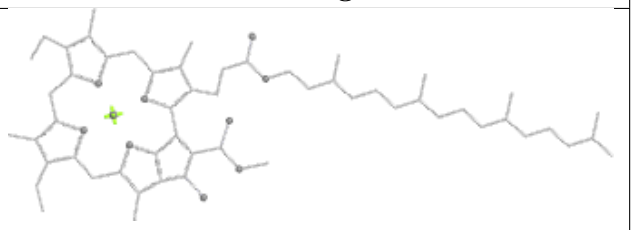
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Bond angles

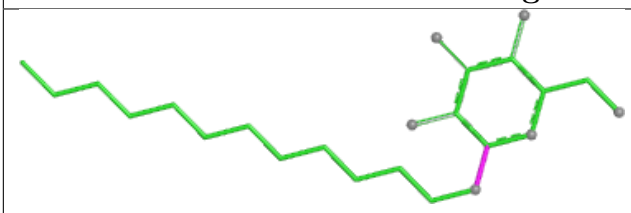


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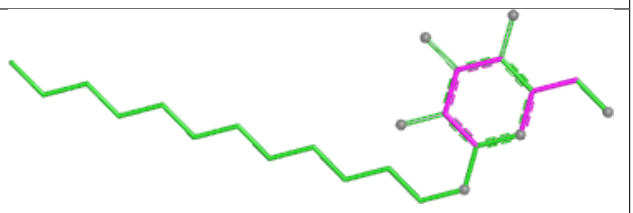


Rings

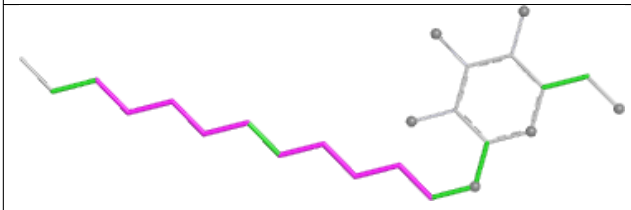
Ligand LMT E 101



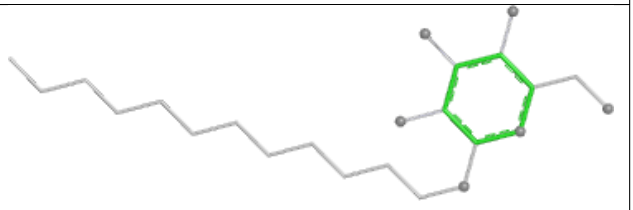
Bond lengths



Bond angles

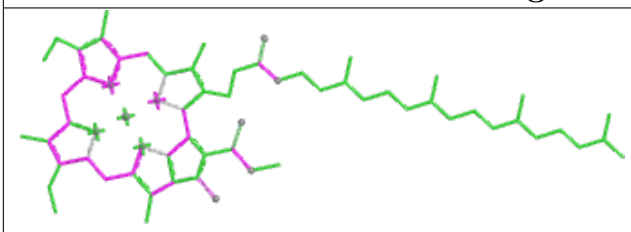


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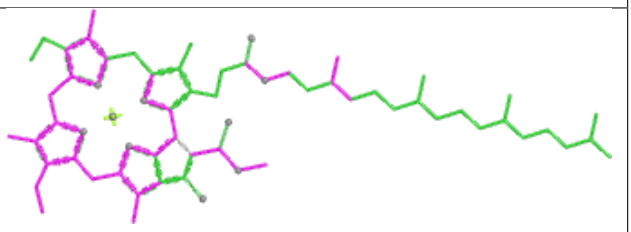


Rings

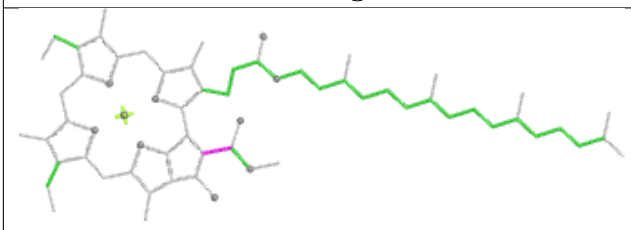
Ligand CLA b 611



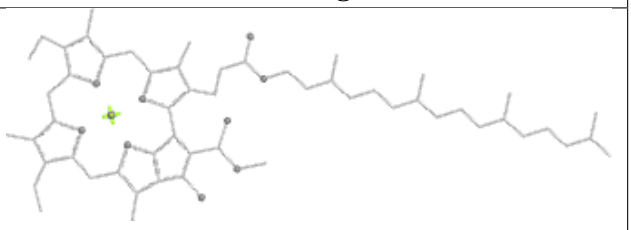
Bond lengths



Bond angles



Torsions



Rings

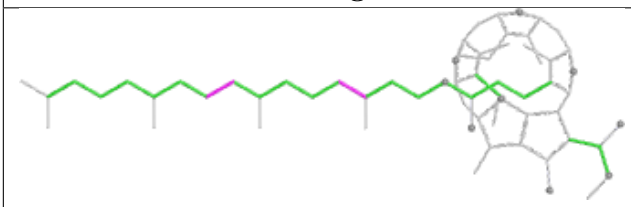
Ligand PHO a 405



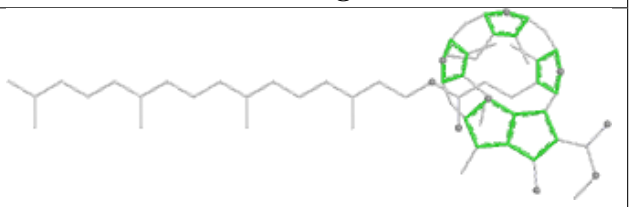
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Bond angles

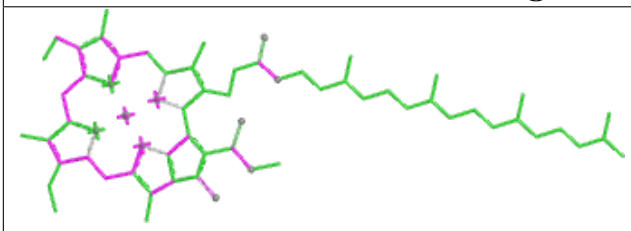


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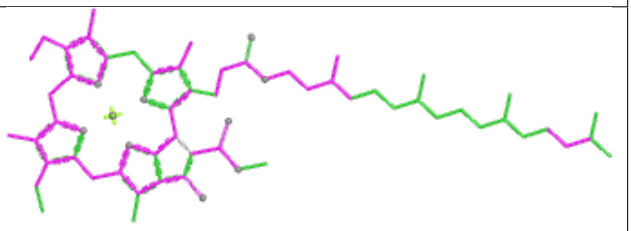


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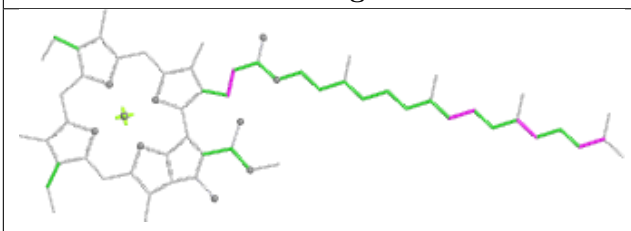
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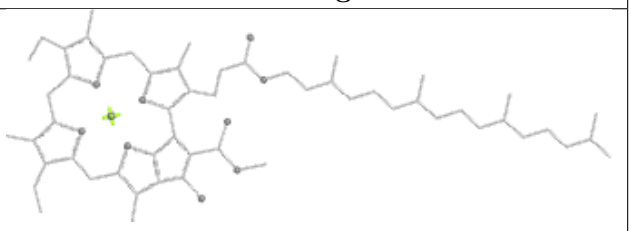
Bond lengths



Bond angles

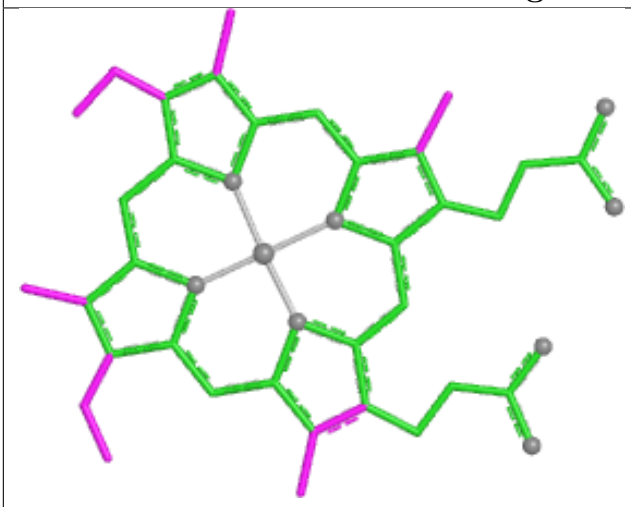


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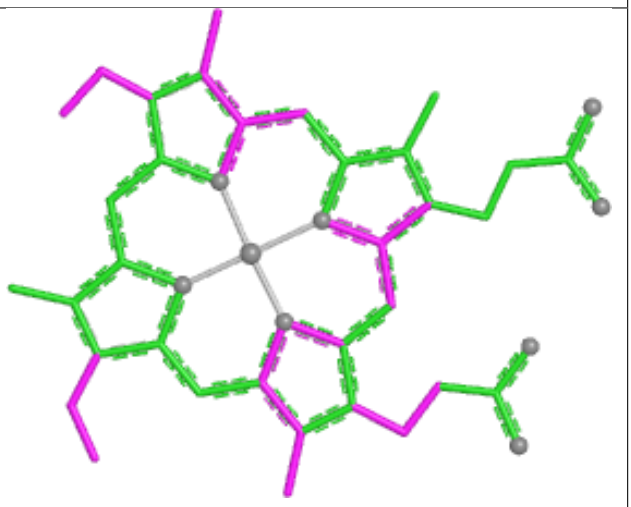


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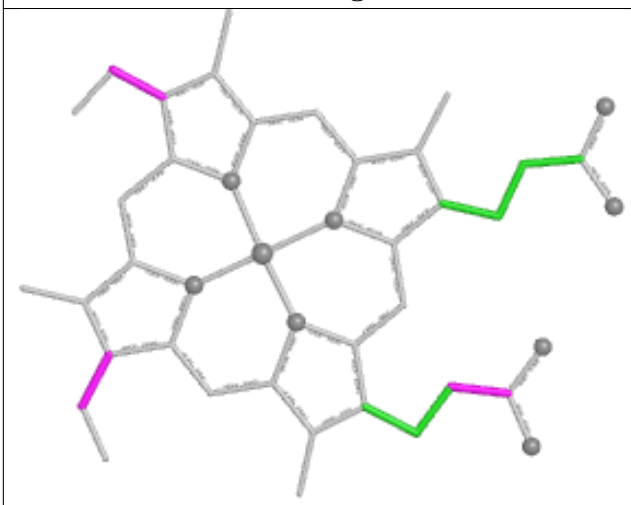
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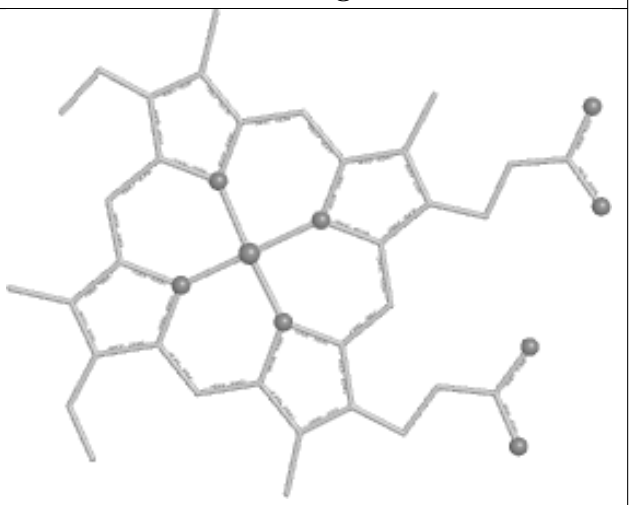
Bond lengths



Bond angles



Torsions

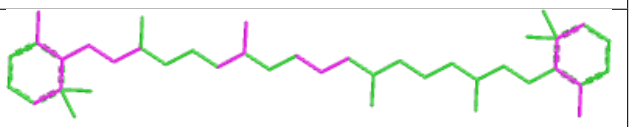


Rings

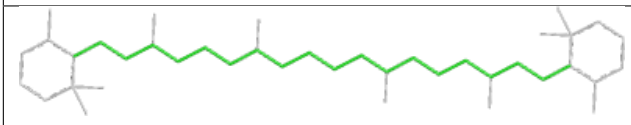
Ligand BCR a 408



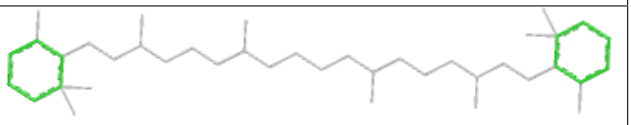
Bond lengths



Bond angles

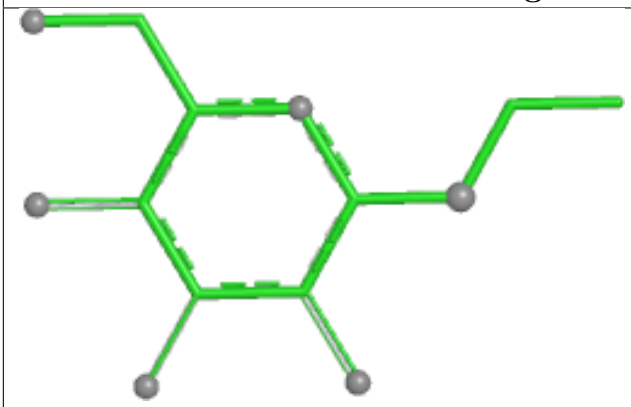


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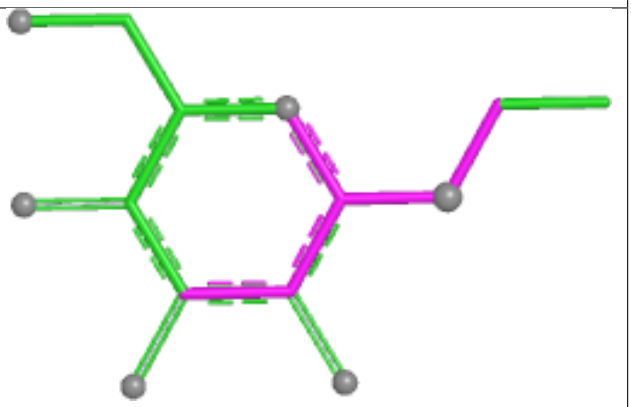


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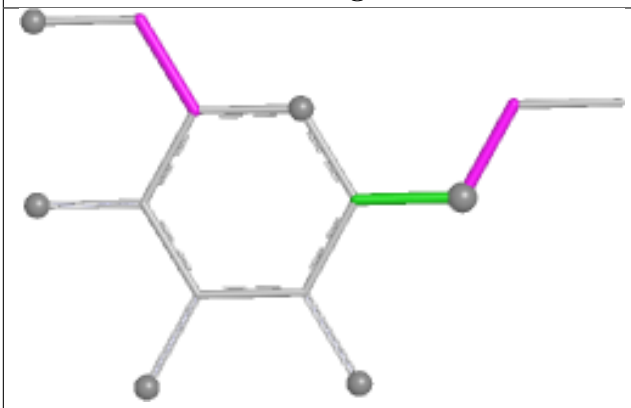
Ligand HTG v 210



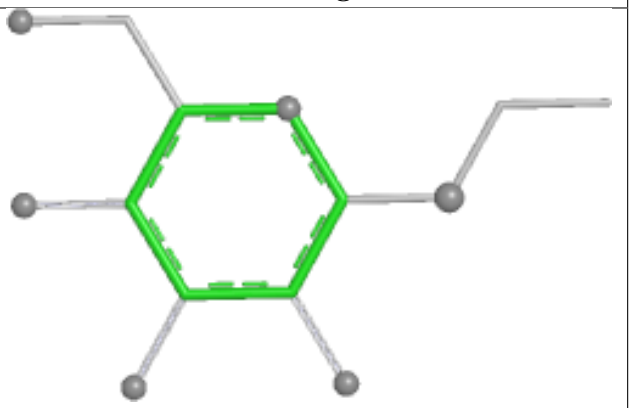
Bond lengths



Bond angles

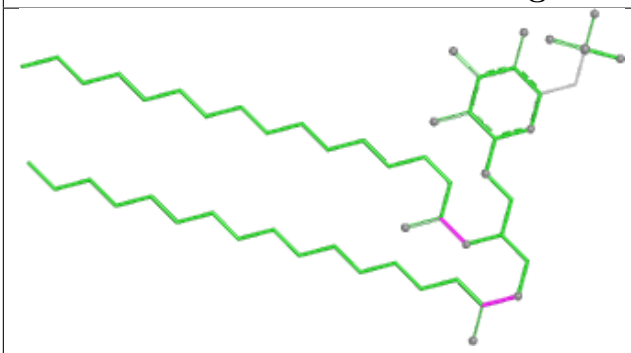


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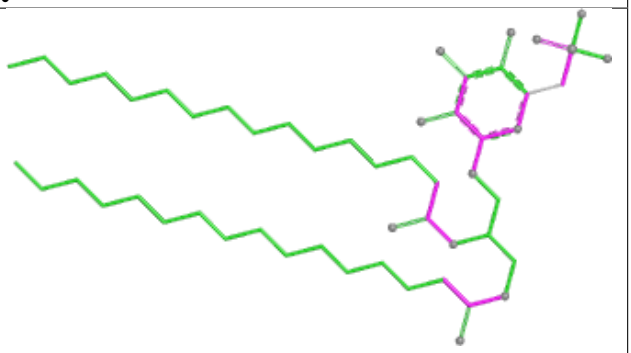


Rings

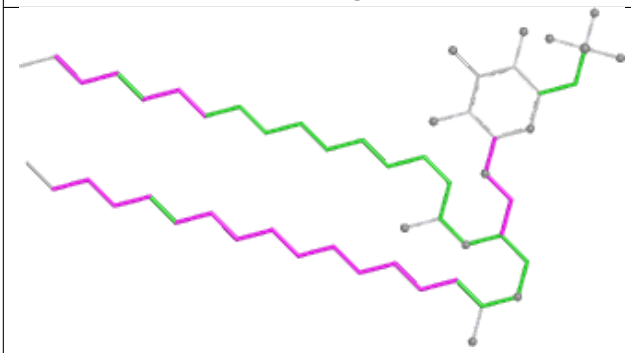
Ligand SQD a 401



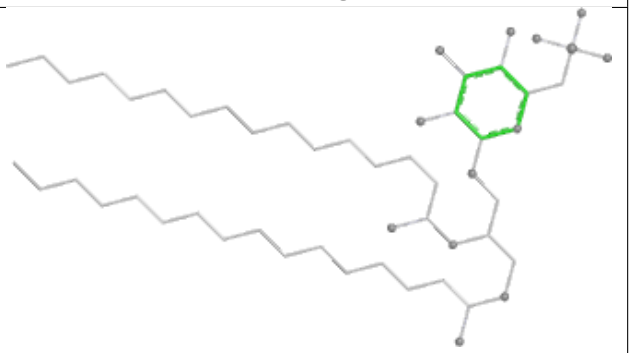
Bond lengths



Bond angles

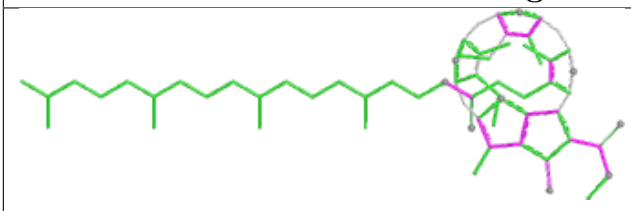


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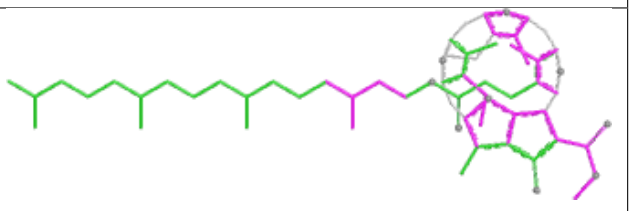


Rings

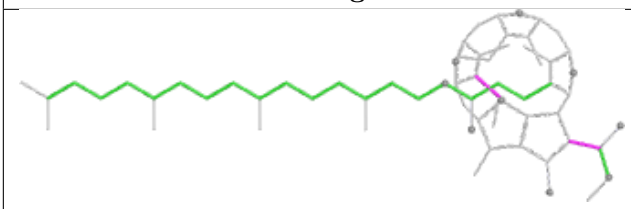
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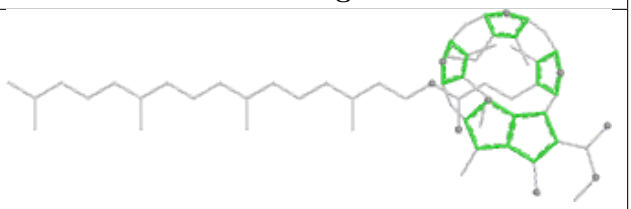
Bond lengths



Bond angles



Torsions

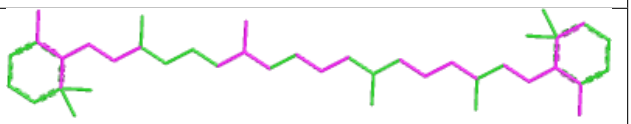


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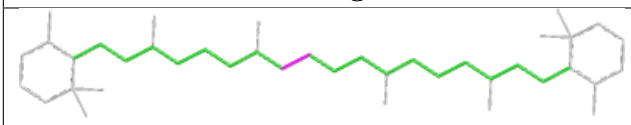
Ligand BCR T 101



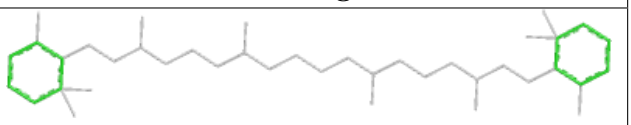
Bond lengths



Bond angles

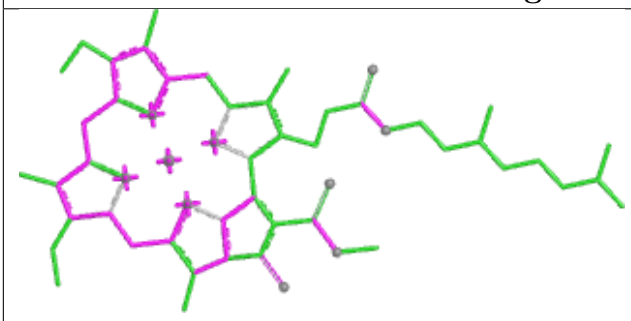


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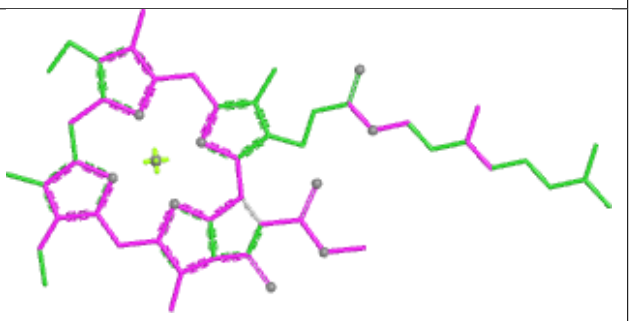


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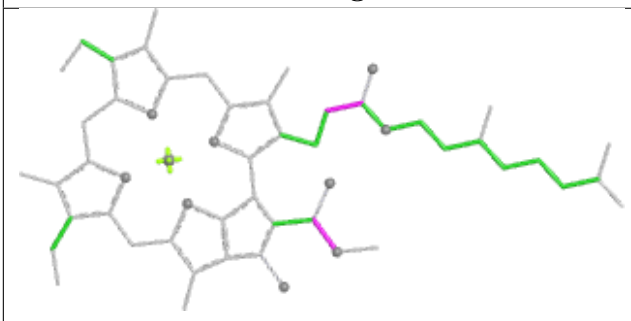
Ligand CLA C 512



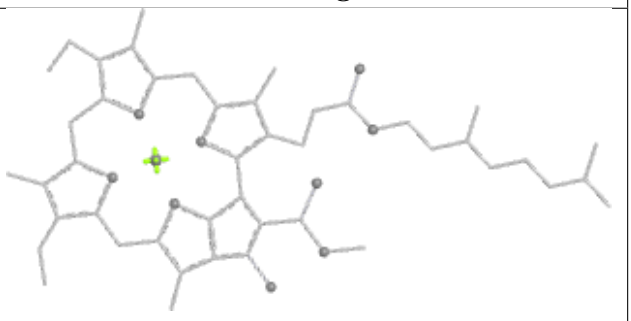
Bond lengths



Bond angles

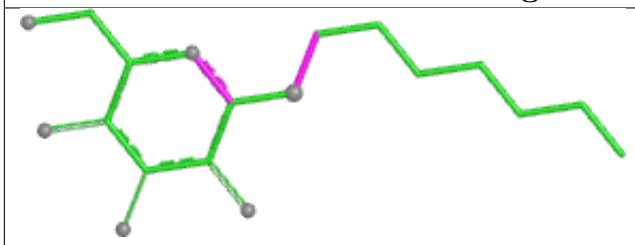


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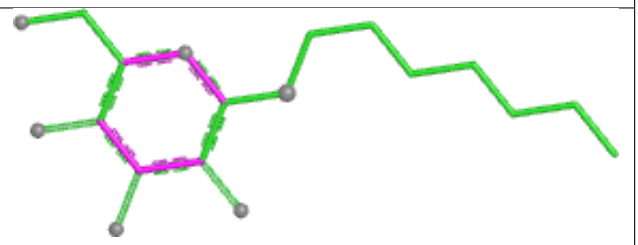


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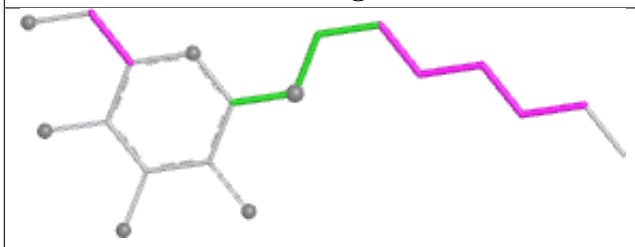
Ligand HTG O 302



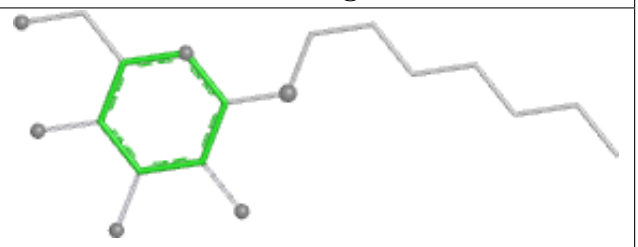
Bond lengths



Bond angles

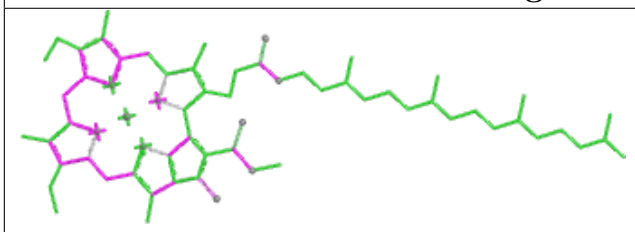


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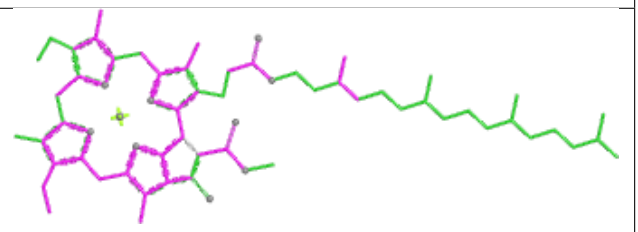


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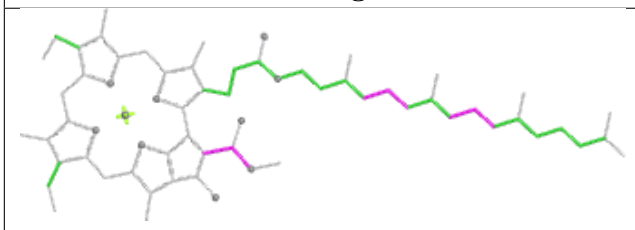
Ligand CLA B 615



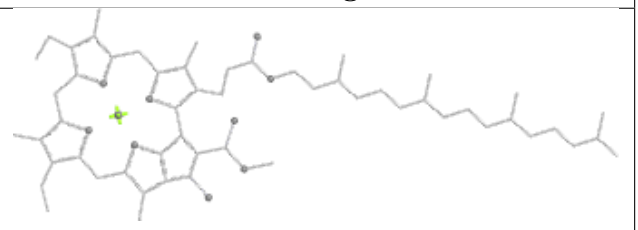
Bond lengths



Bond angles

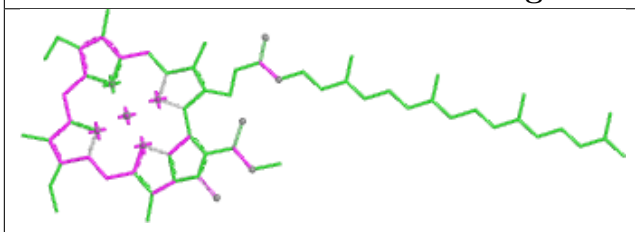


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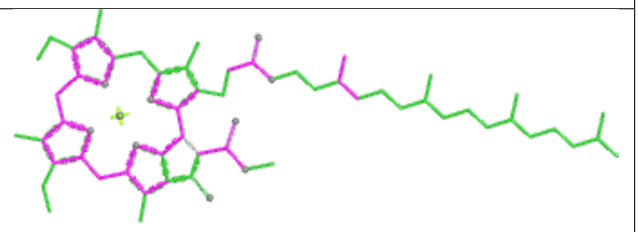


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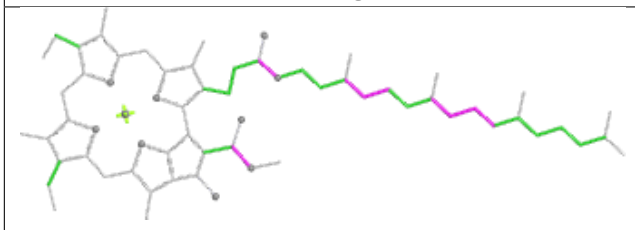
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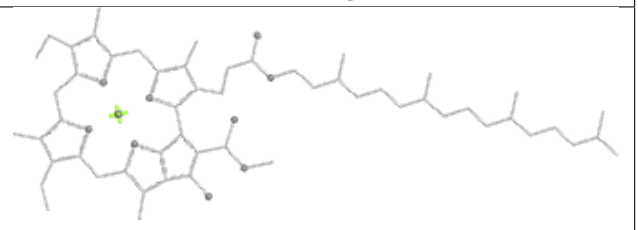
Bond lengths



Bond angles

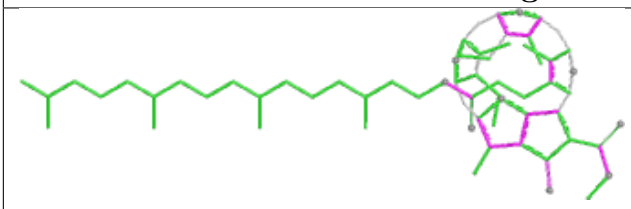


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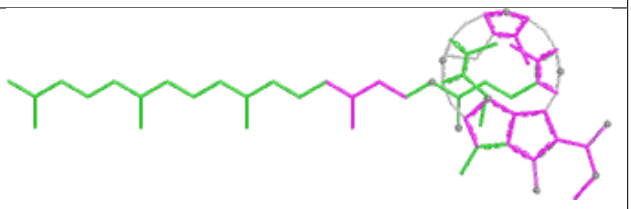


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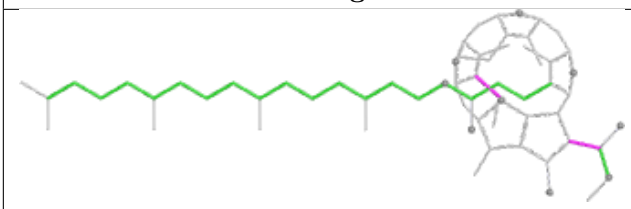
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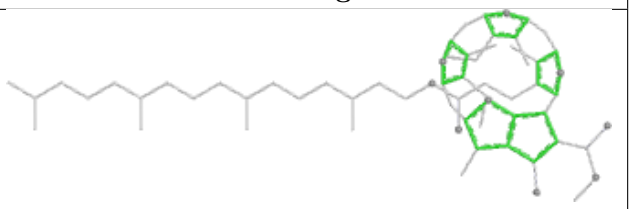
Bond lengths



Bond angles

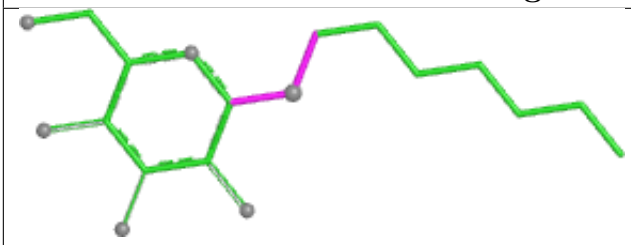


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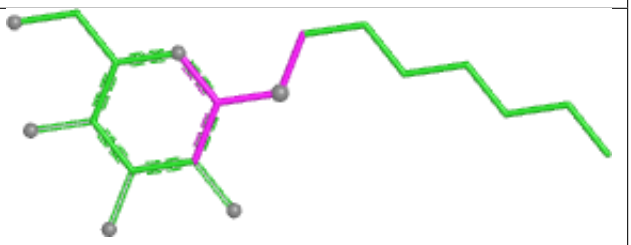


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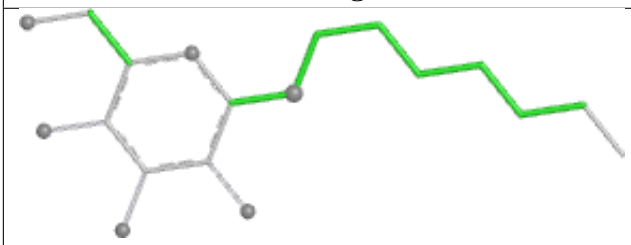
Ligand HTG b 624



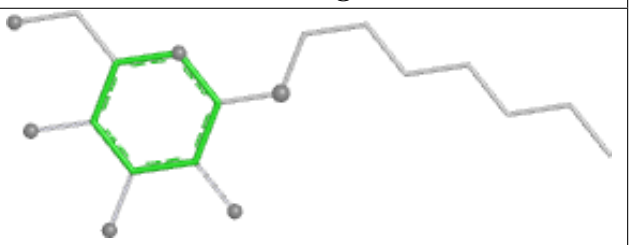
Bond lengths



Bond angles

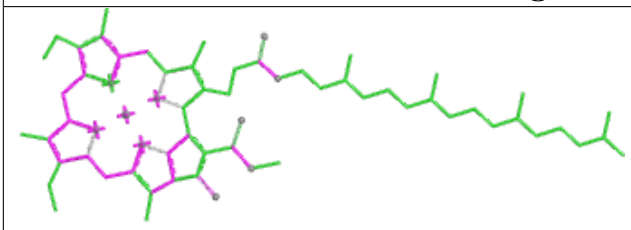


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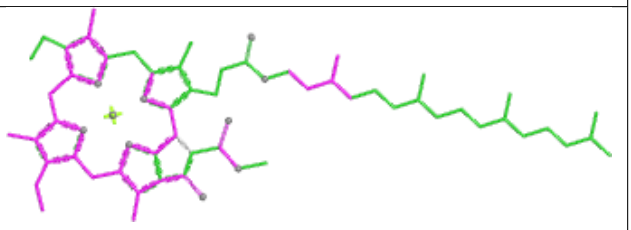


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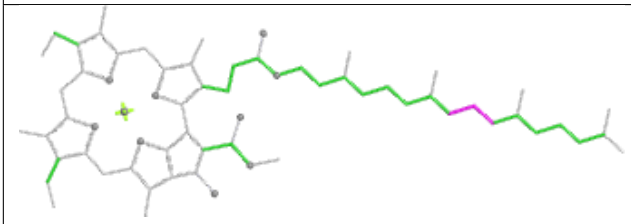
Ligand CLA c 503



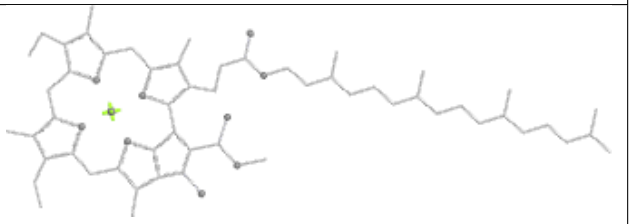
Bond lengths



Bond angles

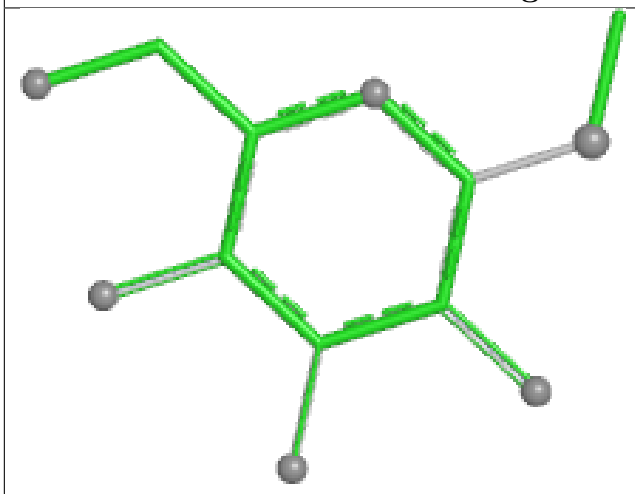


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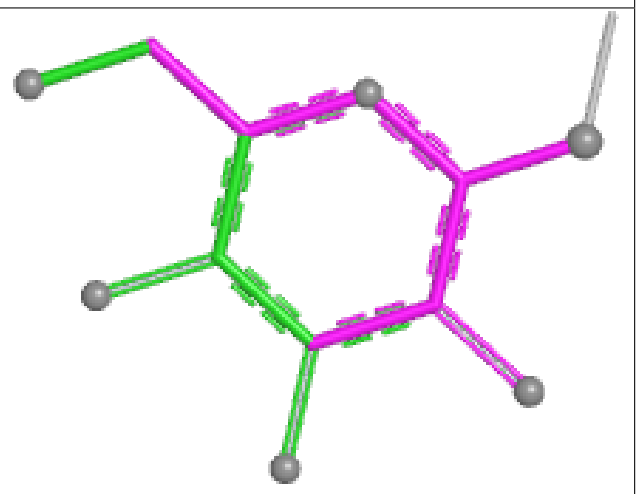


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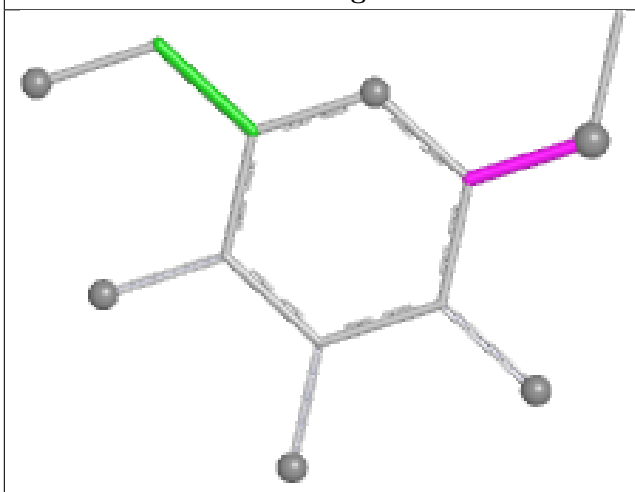
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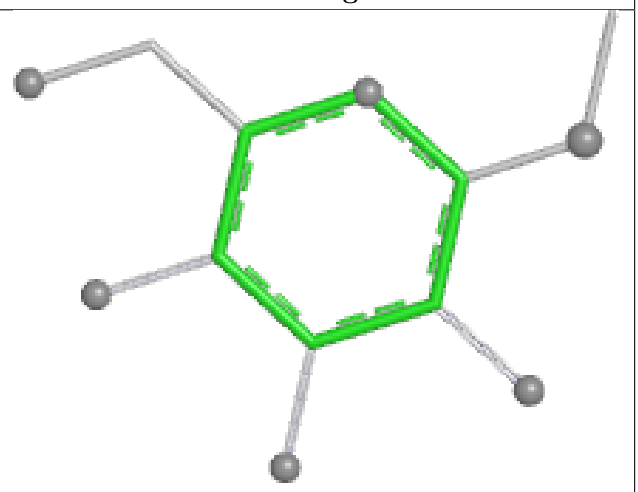
Bond lengths



Bond angles



Torsions



Rings

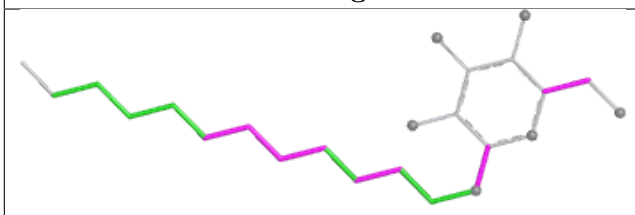
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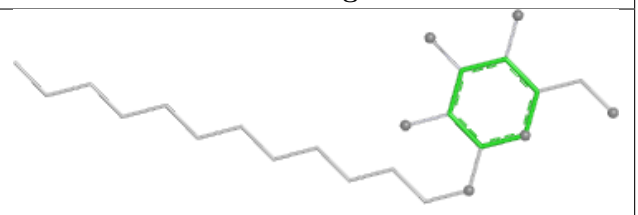
Bond lengths



Bond angles

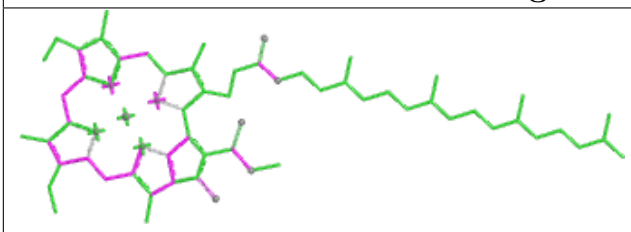


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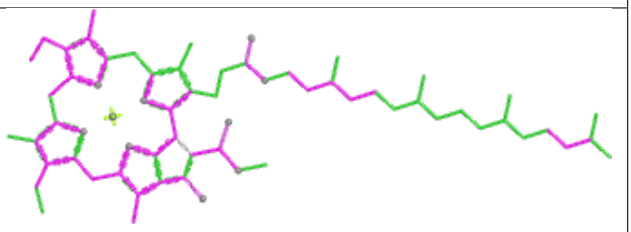


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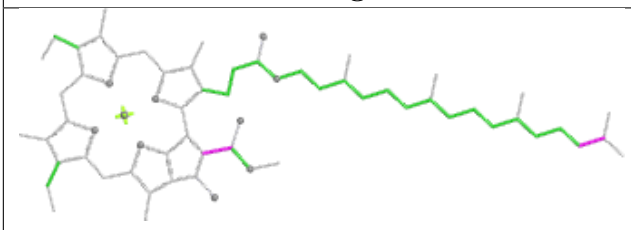
Ligand CLA c 502



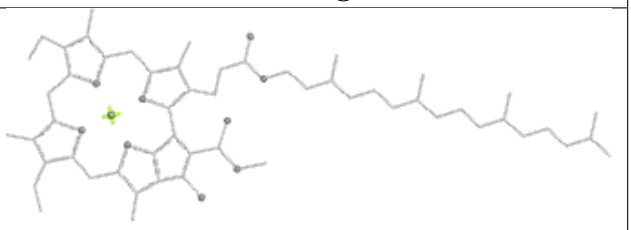
Bond lengths



Bond angles

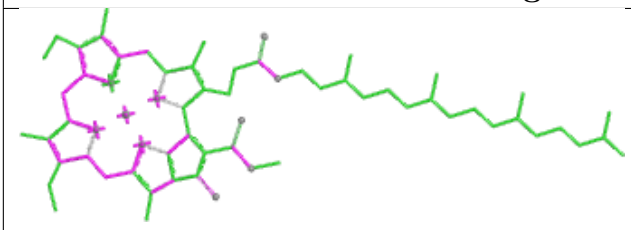


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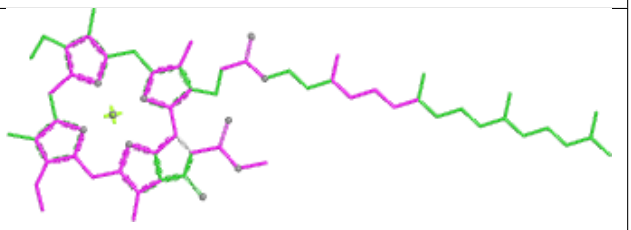


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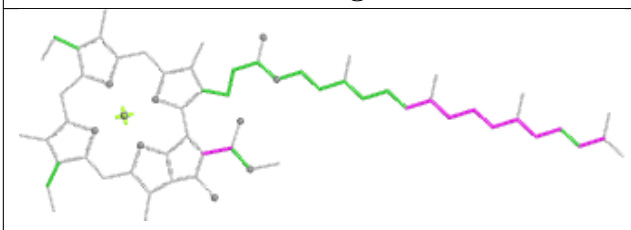
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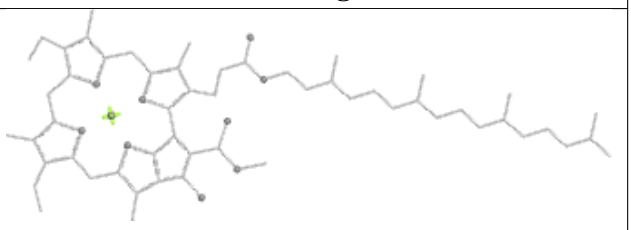
Bond lengths



Bond angles

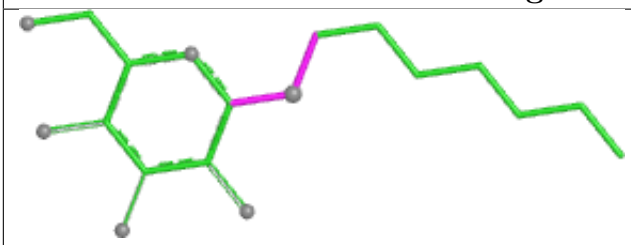


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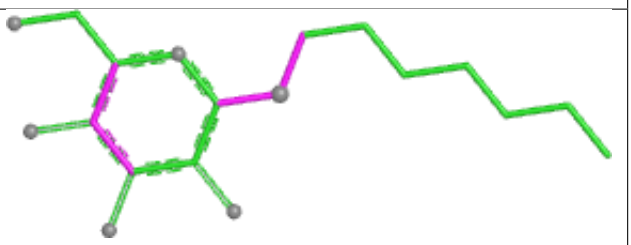


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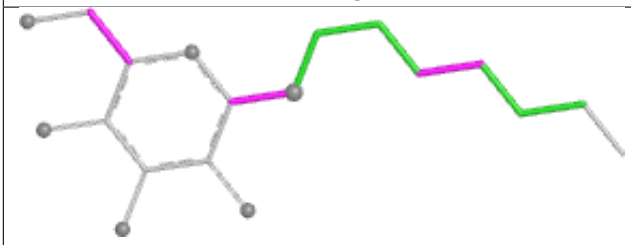
Ligand HTG c 520



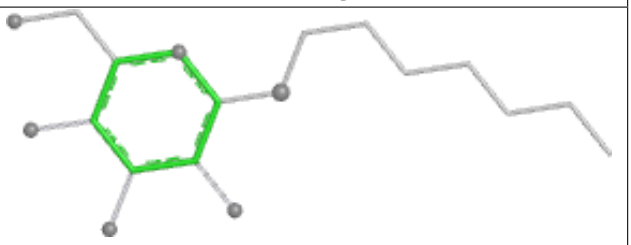
Bond lengths



Bond angles

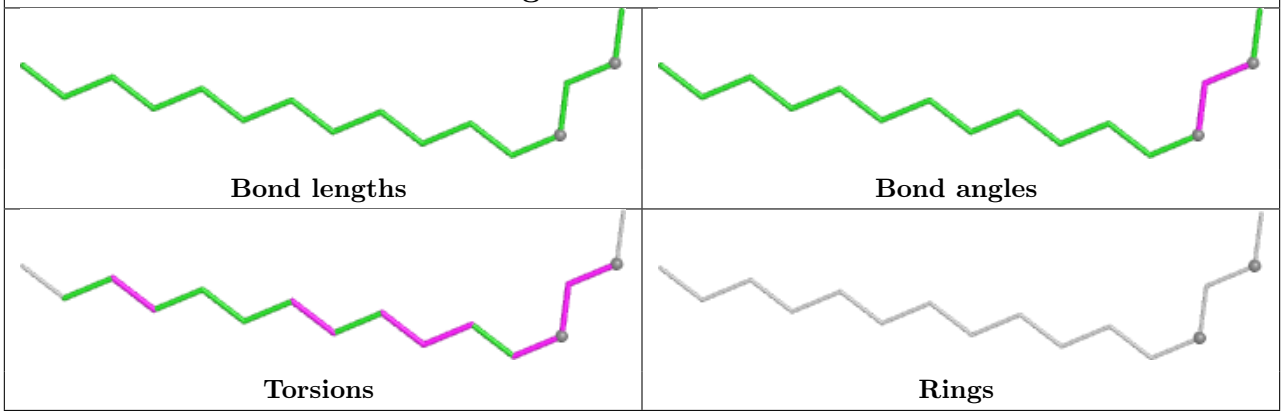


Torsions

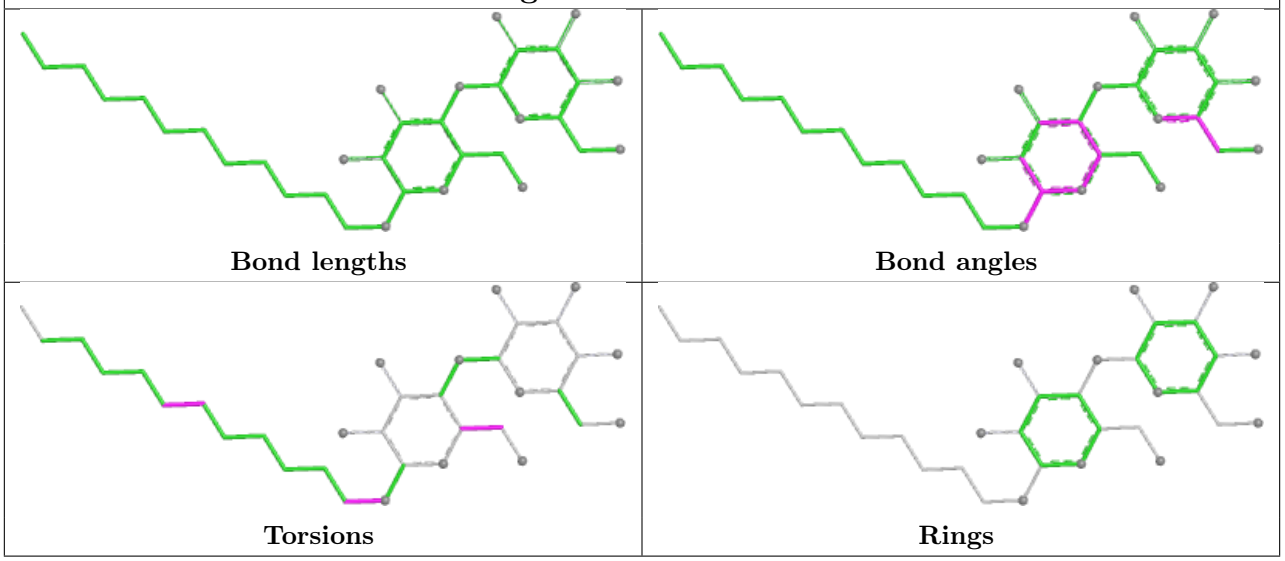


Rings

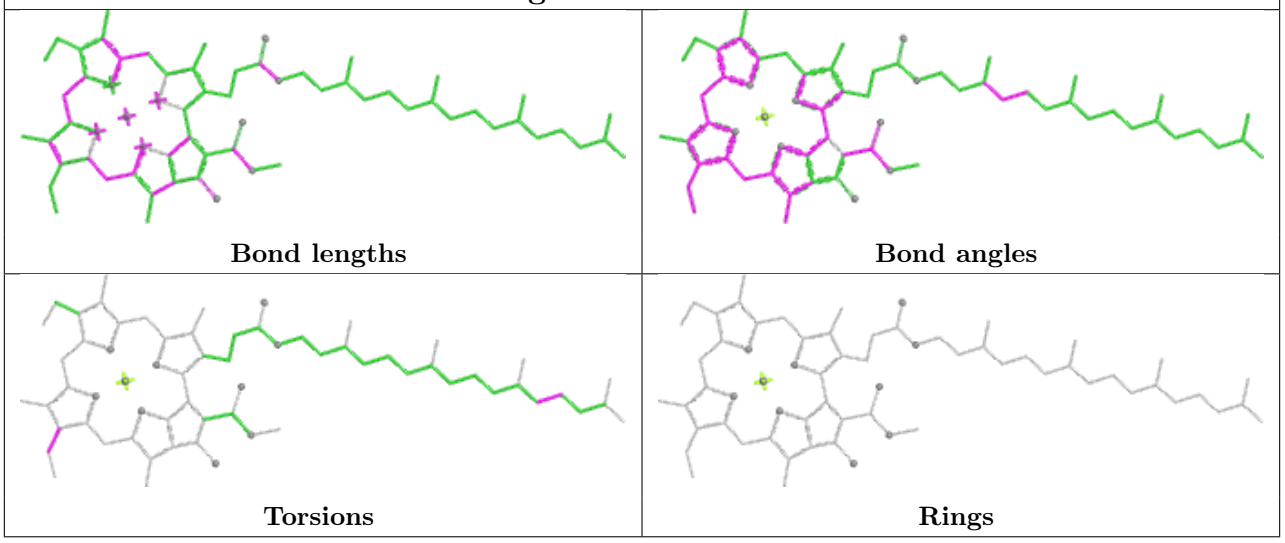
Ligand LMT B 627



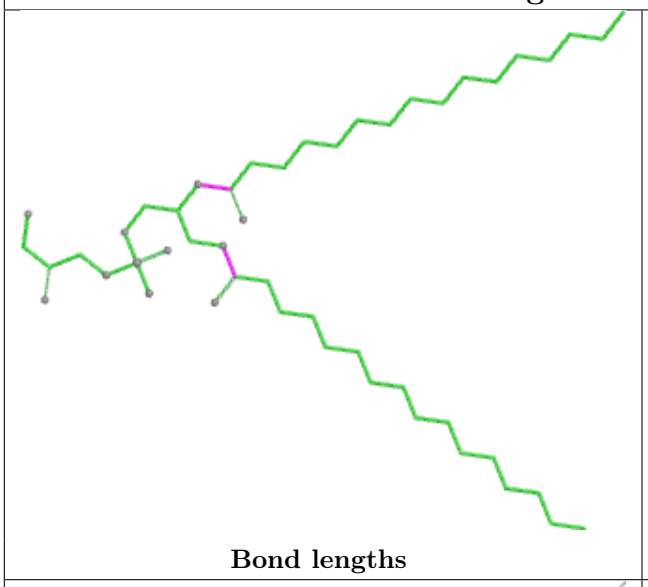
Ligand LMT m 102



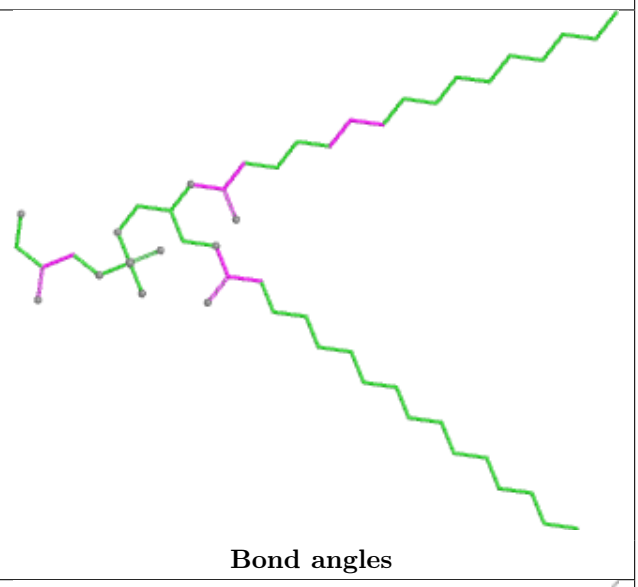
Ligand CLA d 403



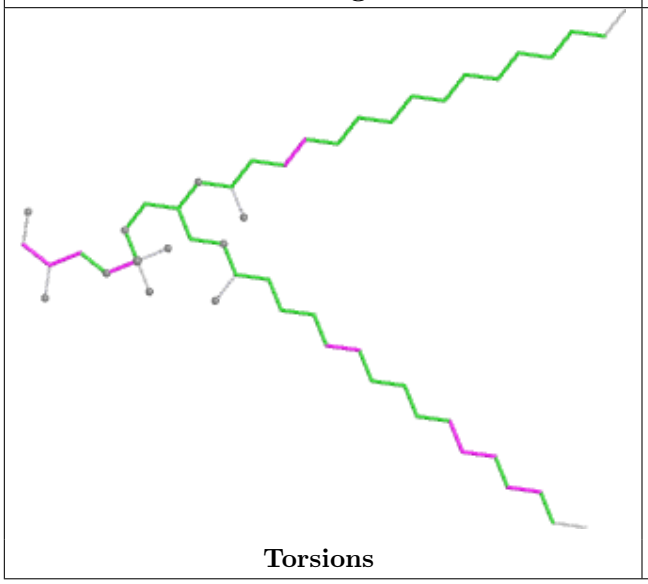
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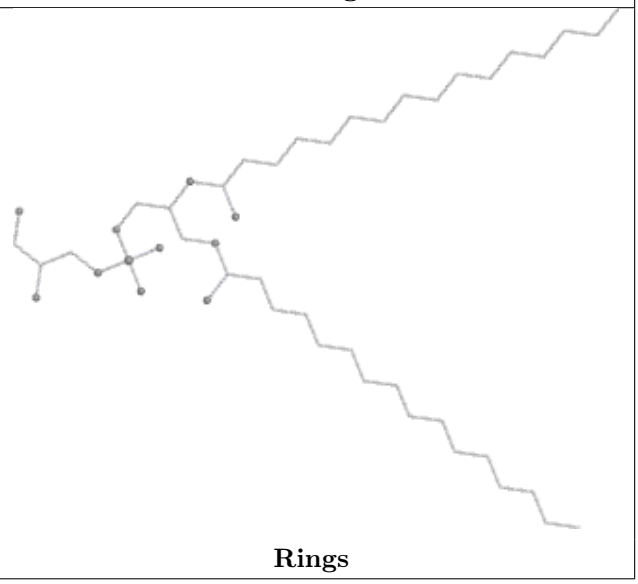
Bond lengths



Bond angles

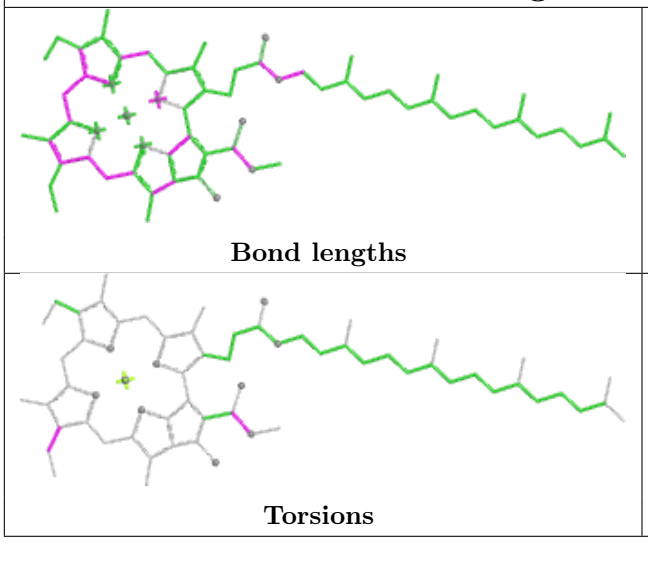


Torsions

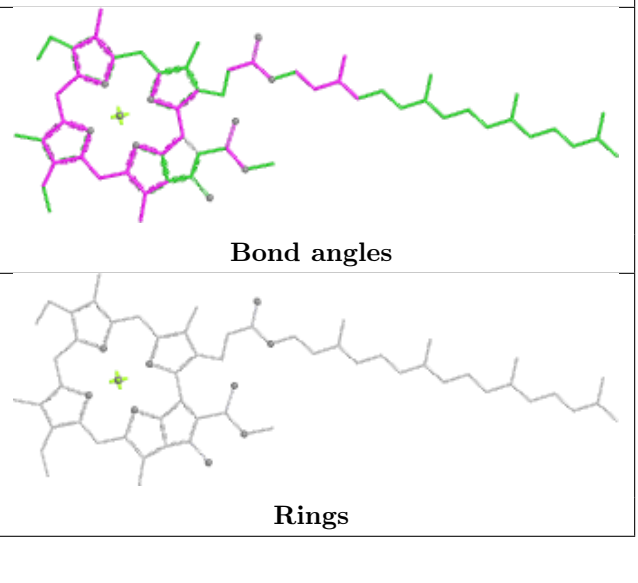


Rings

Ligand CLA a 403



Bond lengths

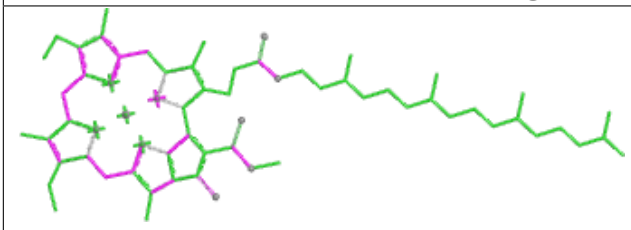


Bond angles

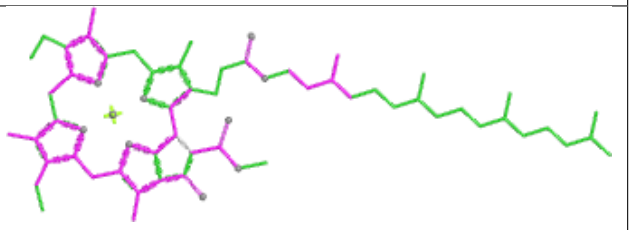
Torsions

Rings

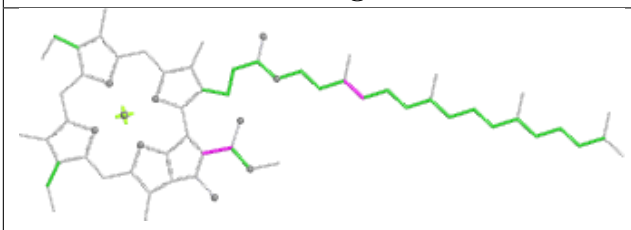
Ligand CLA B 606



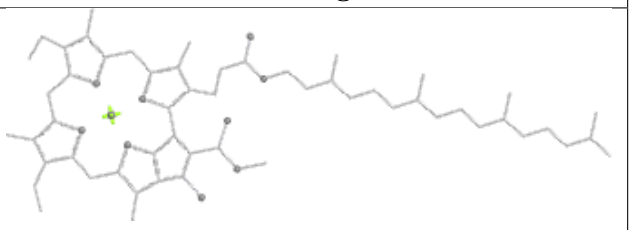
Bond lengths



Bond angles

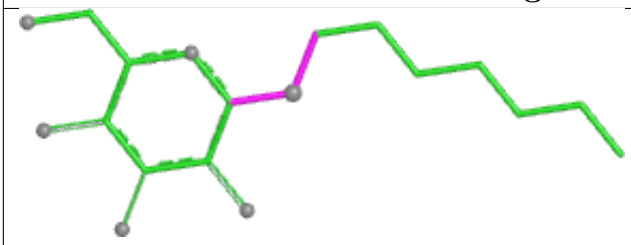


Torsions

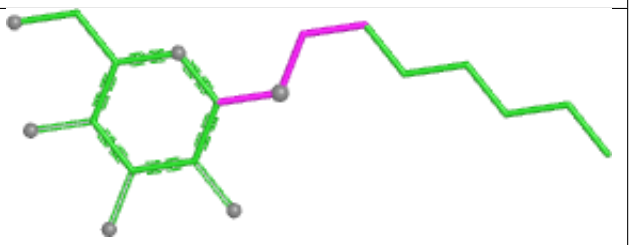


Rings

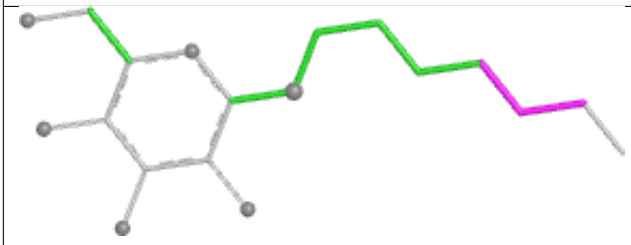
Ligand HTG b 601



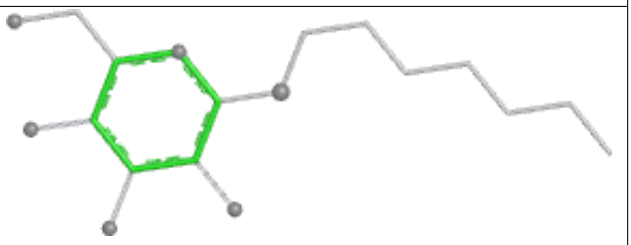
Bond lengths



Bond angles

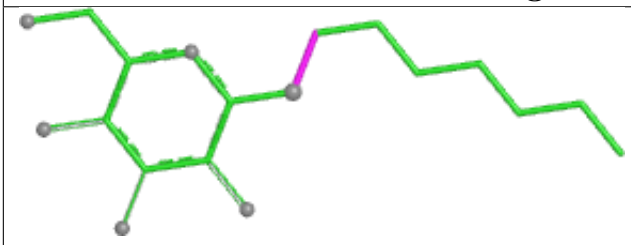


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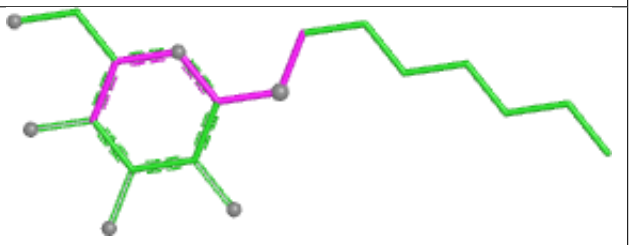


Rings

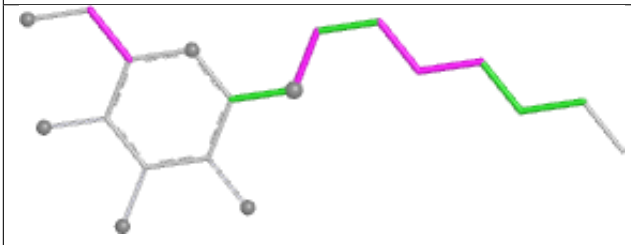
Ligand HTG c 521



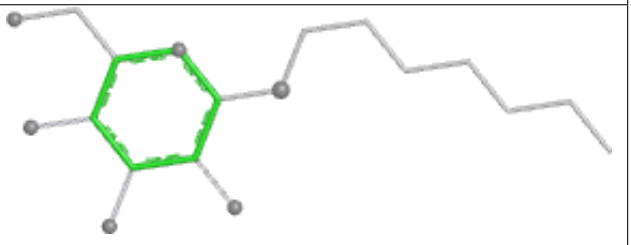
Bond lengths



Bond angles

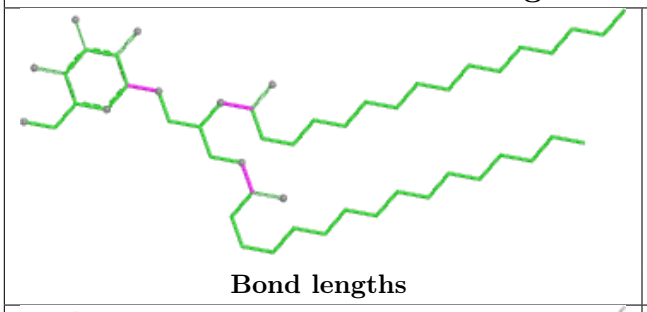


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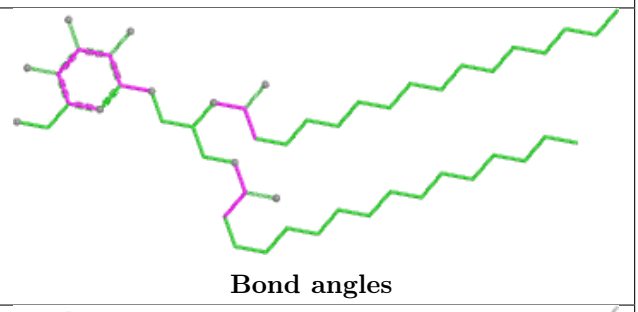


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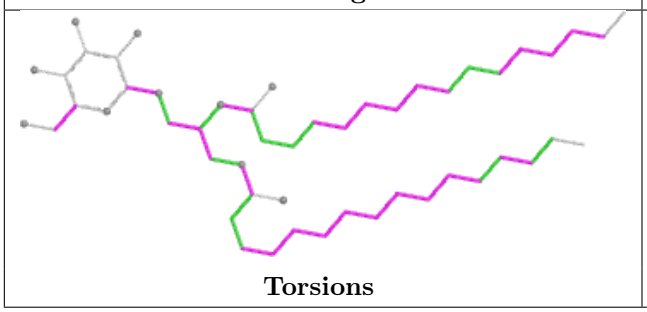
Ligand DGD d 416



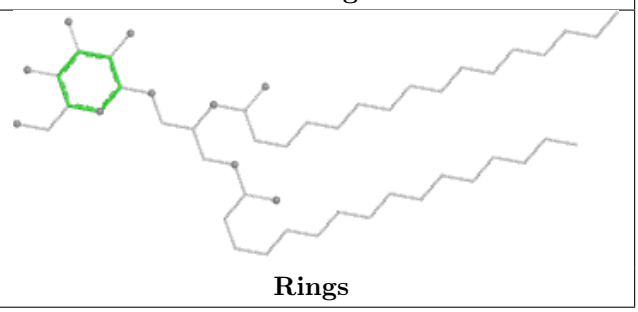
Bond lengths



Bond angles

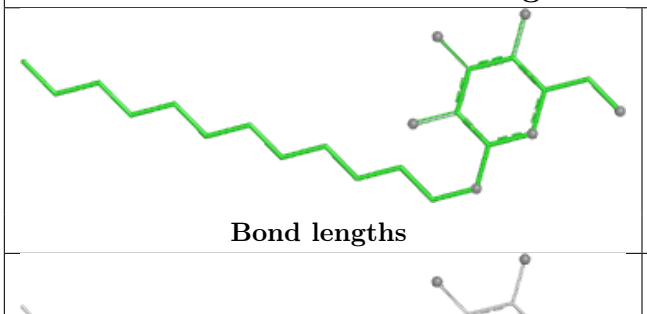


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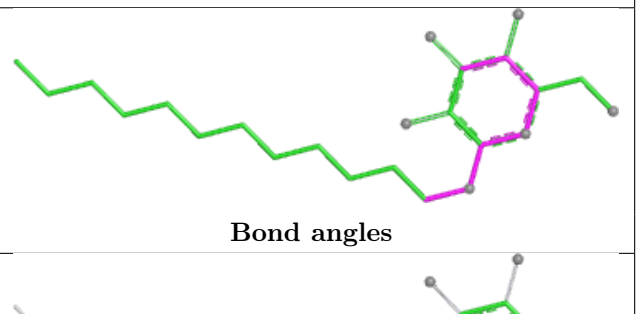


Rings

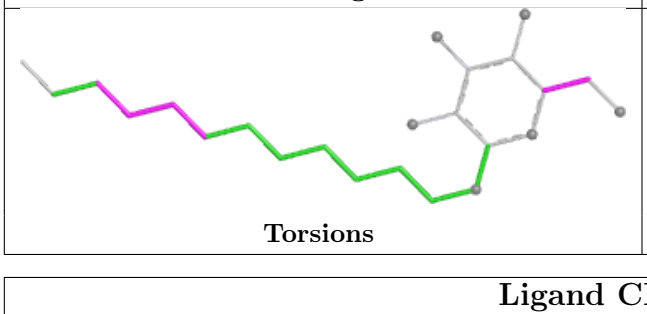
Ligand LMT B 625



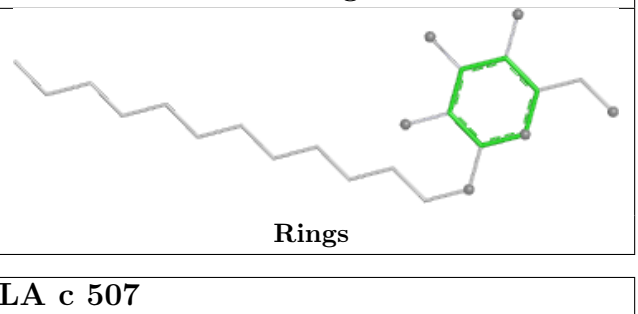
Bond lengths



Bond angles

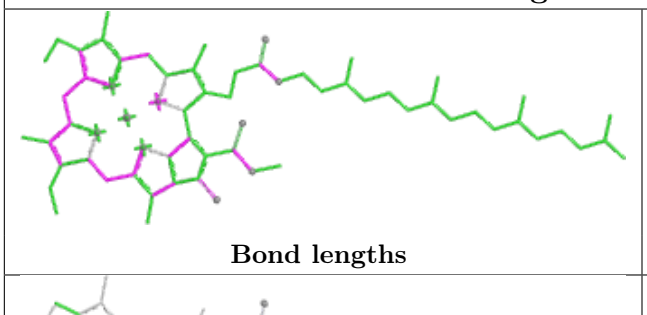


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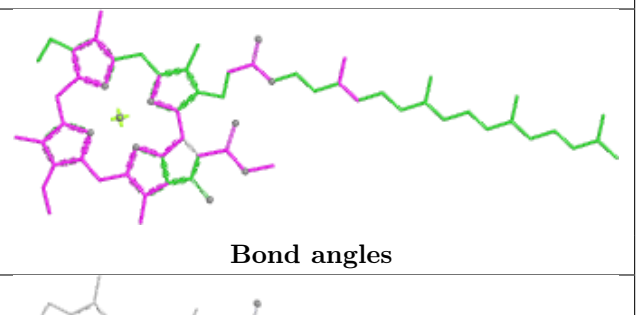


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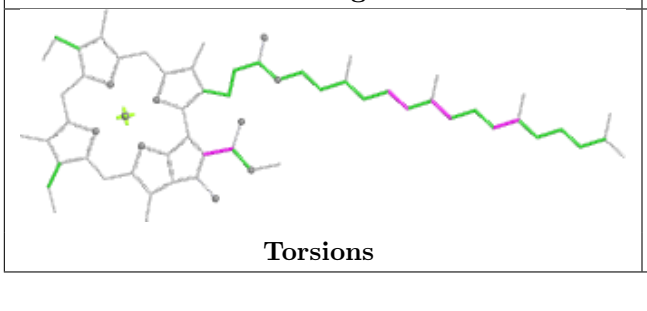
Ligand CLA c 507



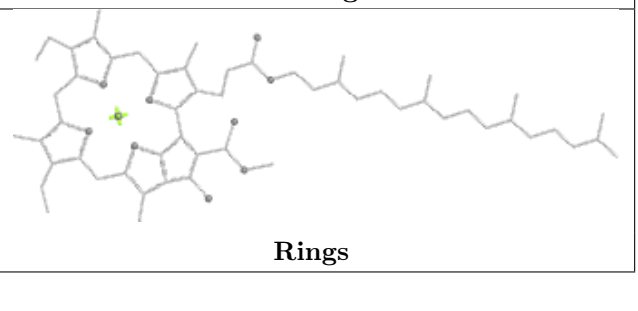
Bond lengths



Bond angles

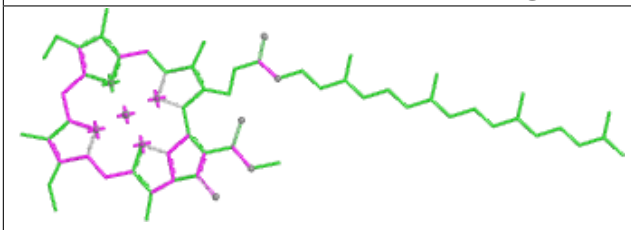


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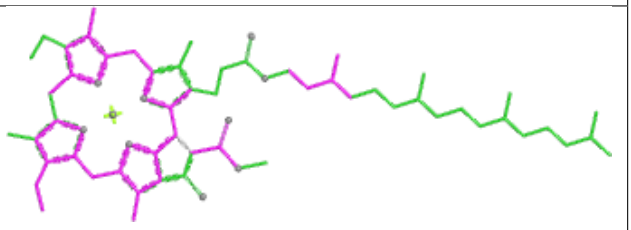


Rings

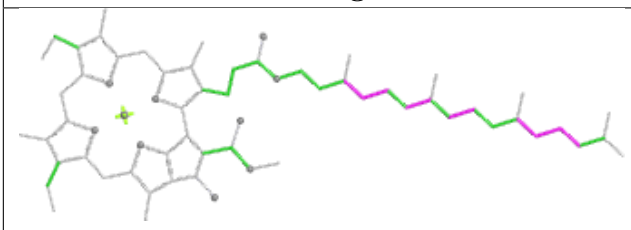
Ligand CLA A 404



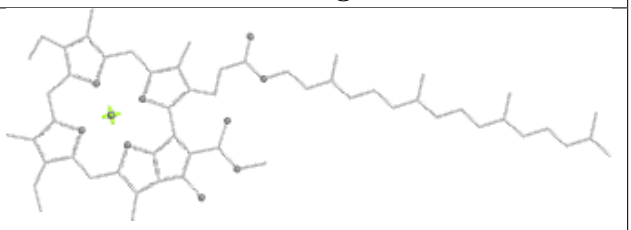
Bond lengths



Bond angles

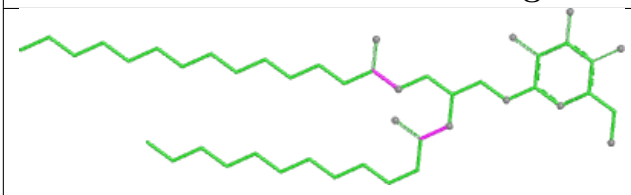


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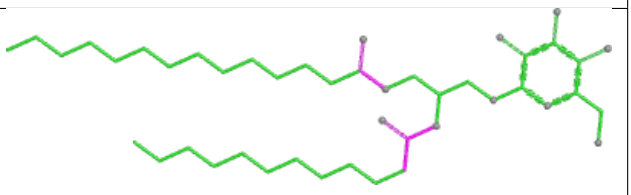


Rings

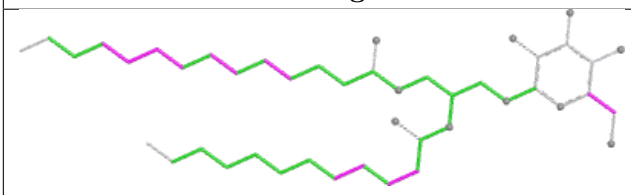
Ligand LMG J 101



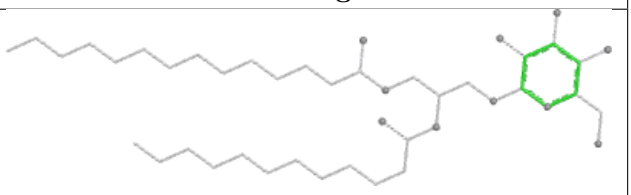
Bond lengths



Bond angles

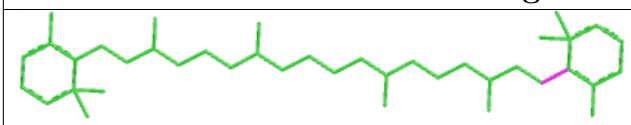


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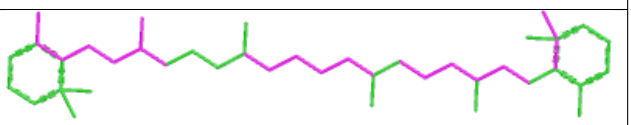


Rings

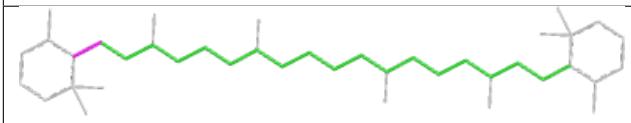
Ligand BCR B 617



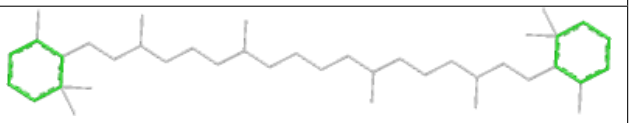
Bond lengths



Bond angles

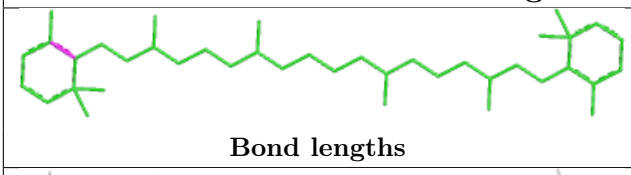


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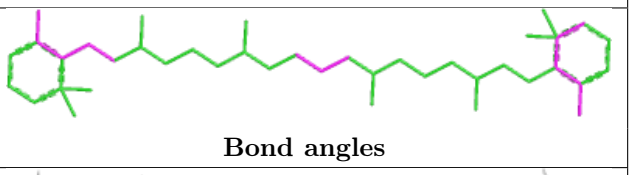


Rings

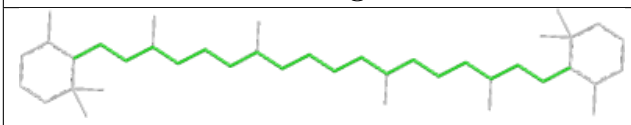
Ligand BCR b 620



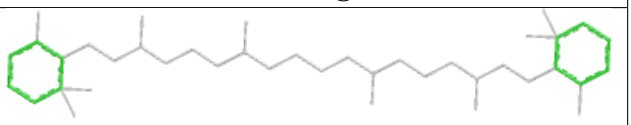
Bond lengths



Bond angles

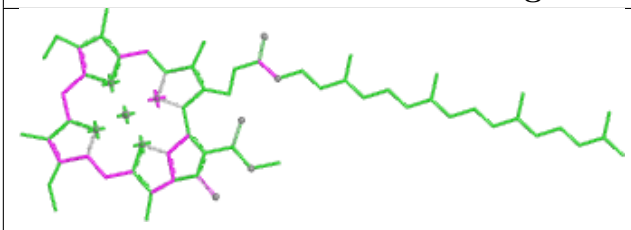


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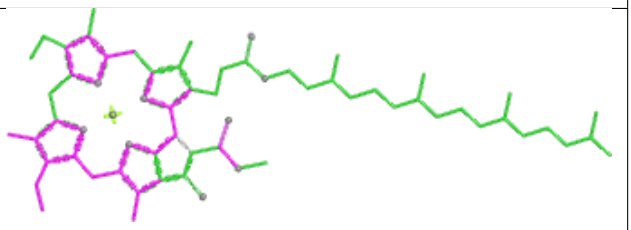


Rings

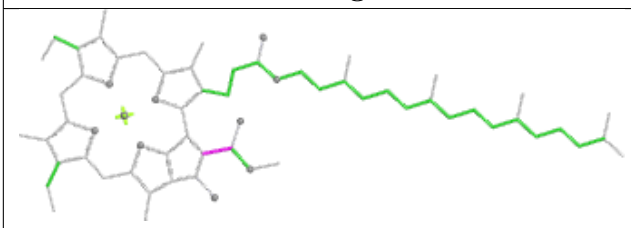
Ligand CLA B 608



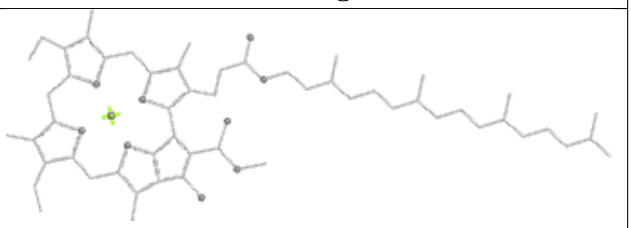
Bond lengths



Bond angles

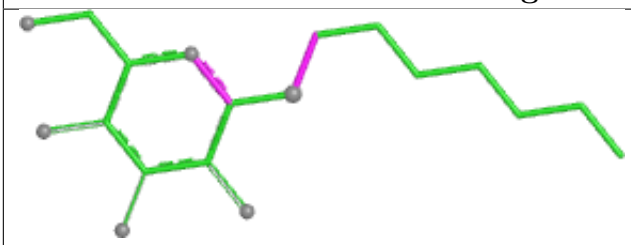


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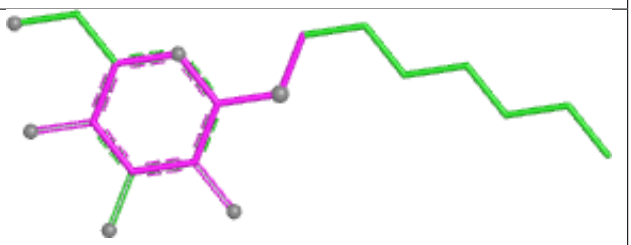


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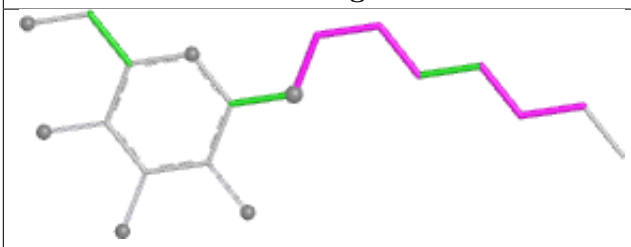
Ligand HTG B 622



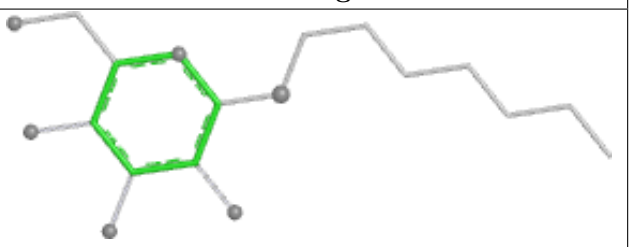
Bond lengths



Bond angles

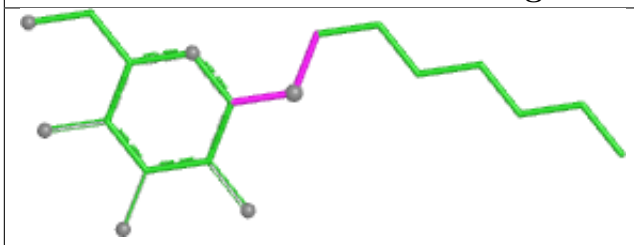


Torsions

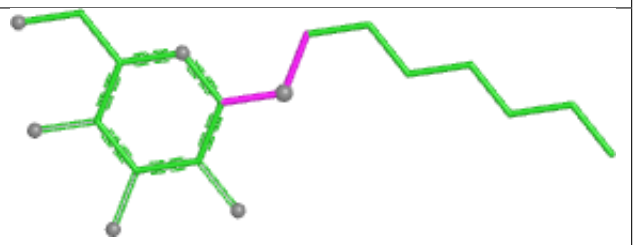


Rings

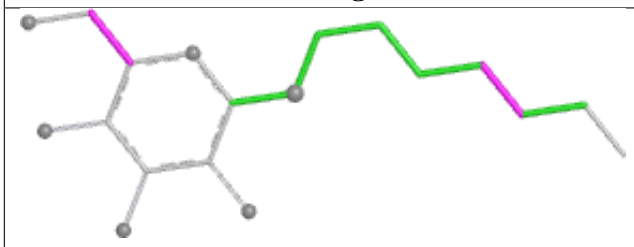
Ligand HTG b 602



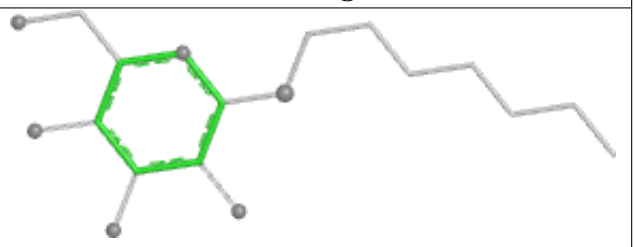
Bond lengths



Bond angles

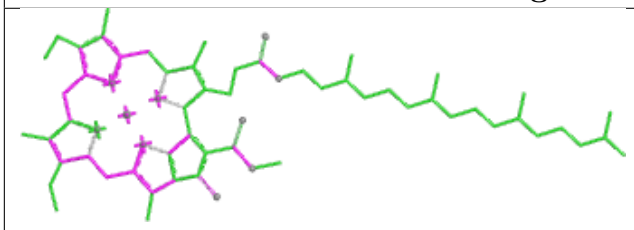


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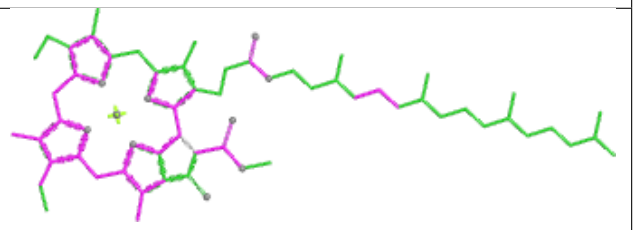


Rings

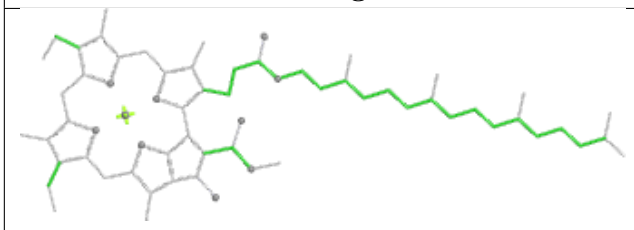
Ligand CLA c 505



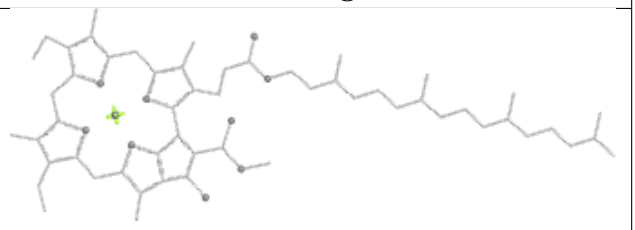
Bond lengths



Bond angles

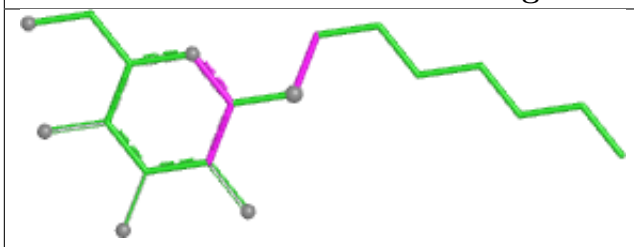


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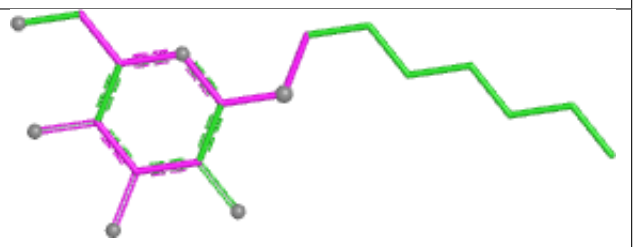


Rings

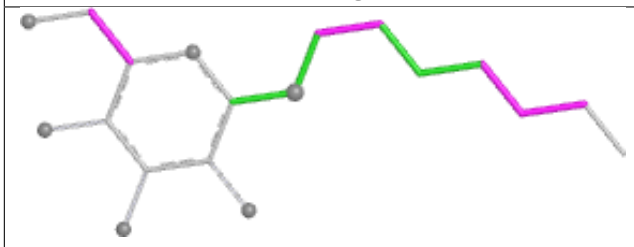
Ligand HTG B 621



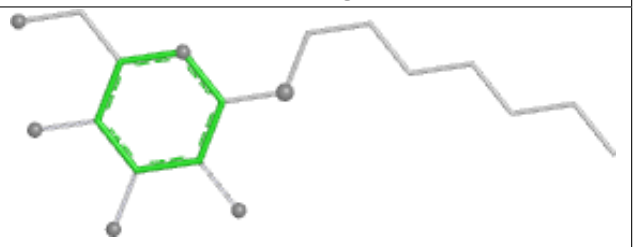
Bond lengths



Bond angles

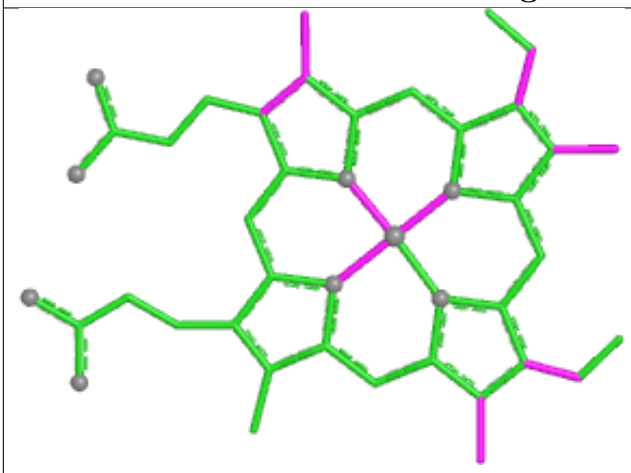


Torsions

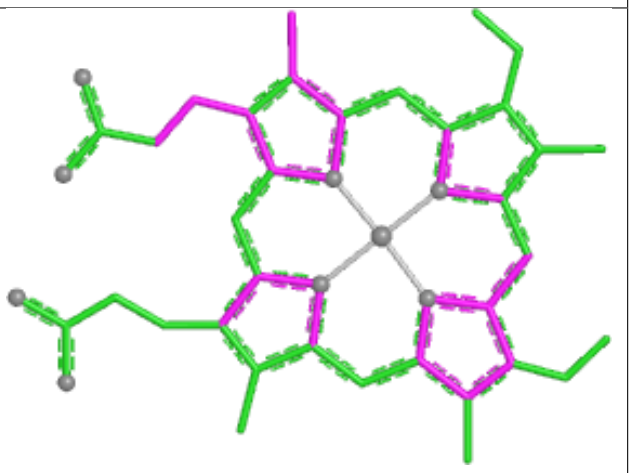


Rings

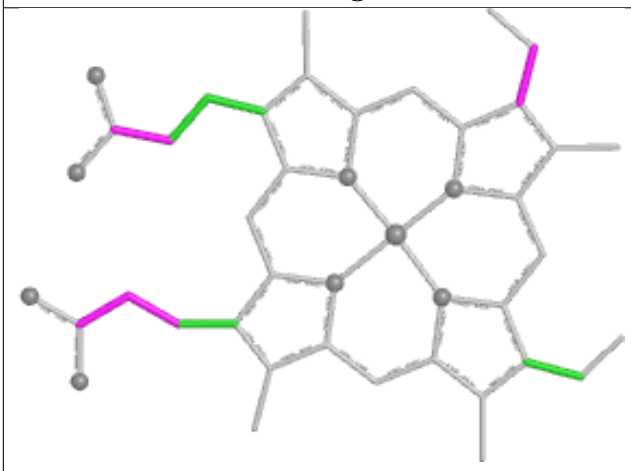
Ligand HEM E 104



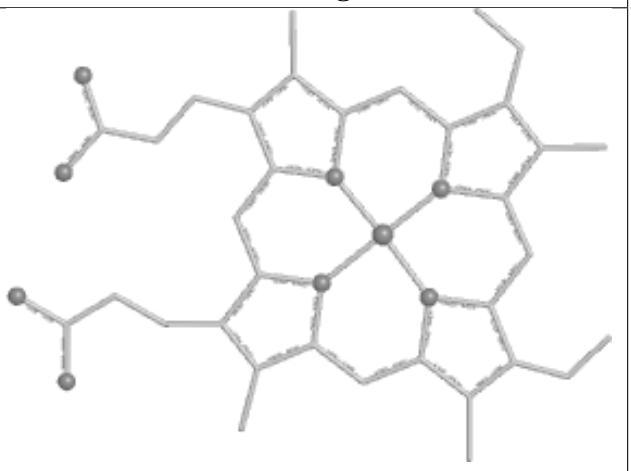
Bond lengths



Bond angles

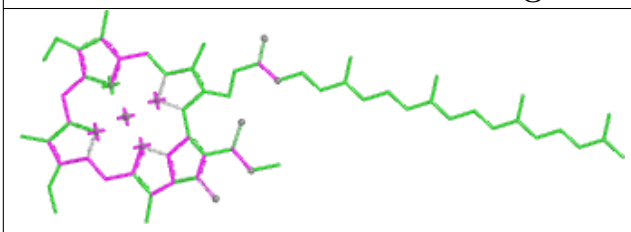


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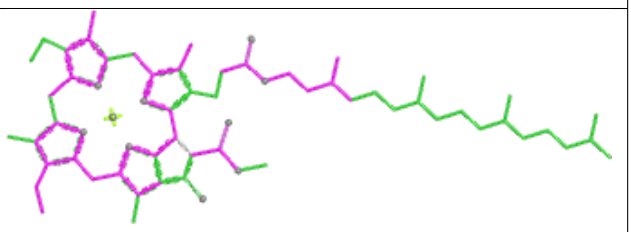


Rings

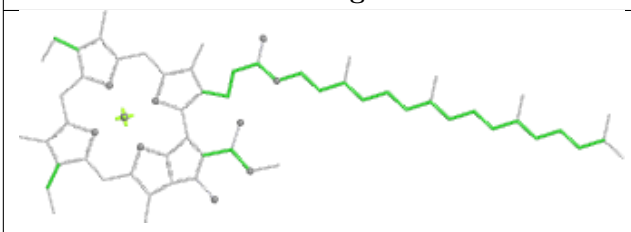
Ligand CLA B 603



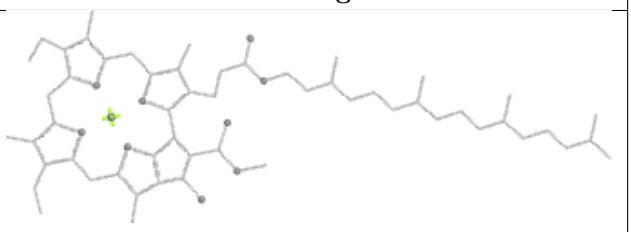
Bond lengths



Bond angles

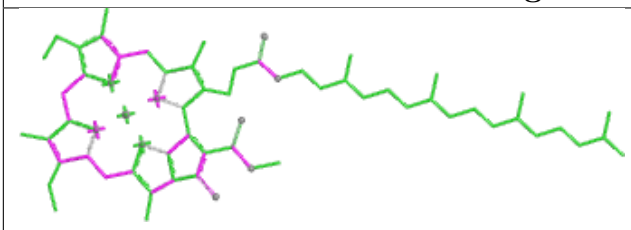


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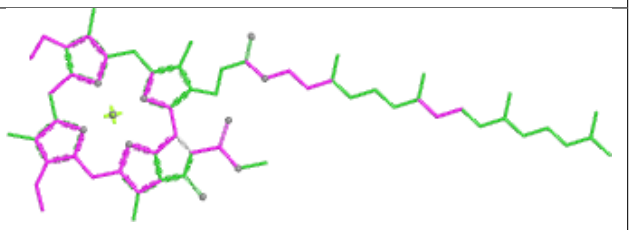


Rings

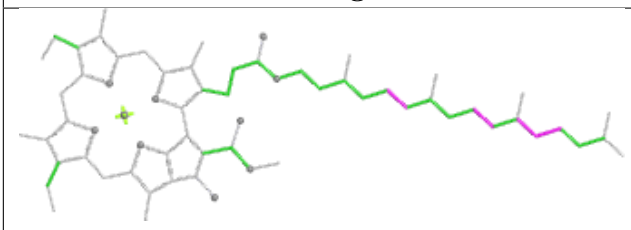
Ligand CLA B 616



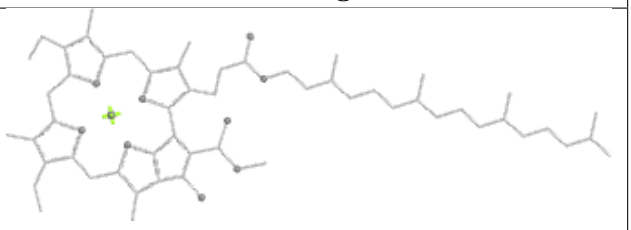
Bond lengths



Bond angles

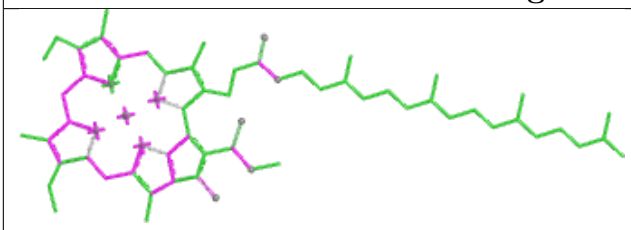


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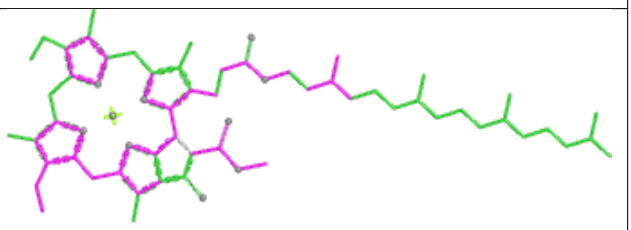


Rings

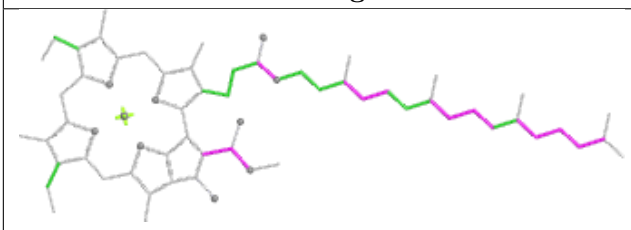
Ligand CLA b 618



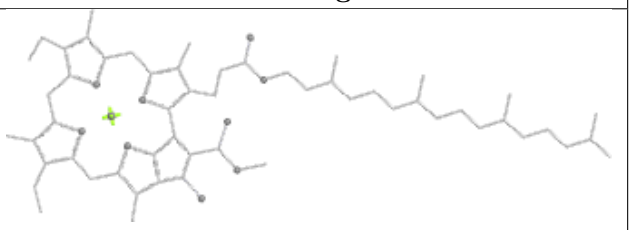
Bond lengths



Bond angles



Torsions



Rings

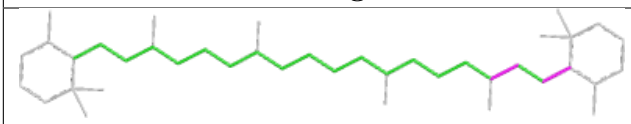
Ligand BCR d 405



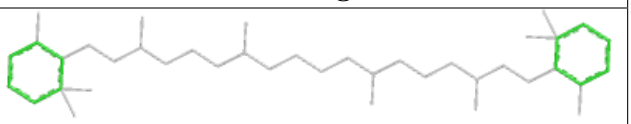
Bond lengths



Bond angles

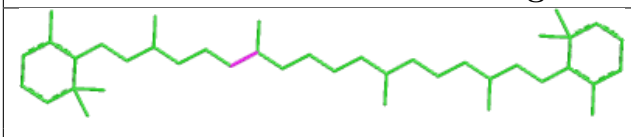


Torsions

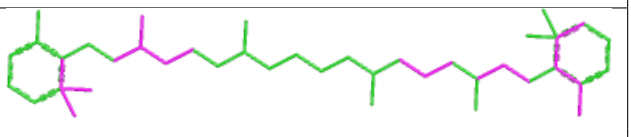


Rings

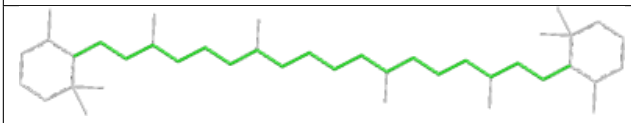
Ligand BCR c 514



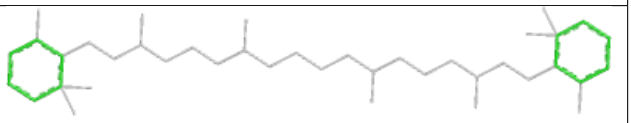
Bond lengths



Bond angles



Torsions

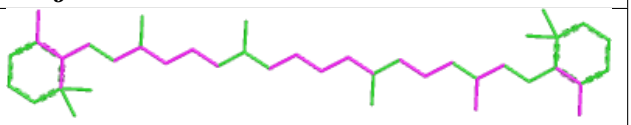


Rings

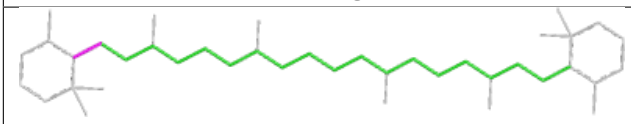
Ligand BCR j 102



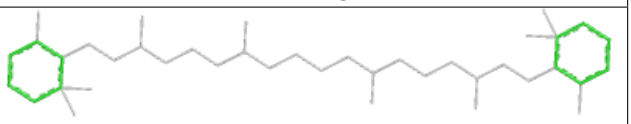
Bond lengths



Bond angles

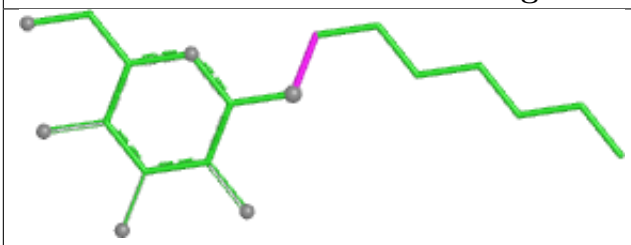


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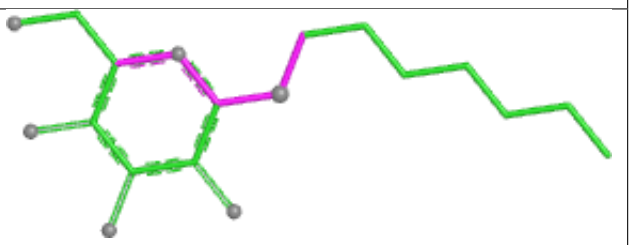


Rings

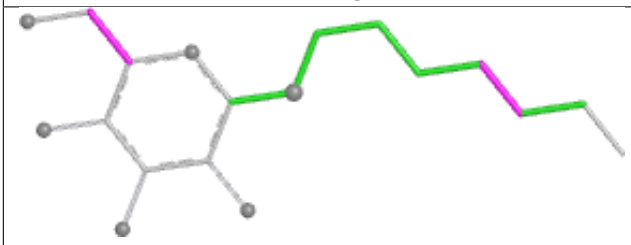
Ligand HTG B 632



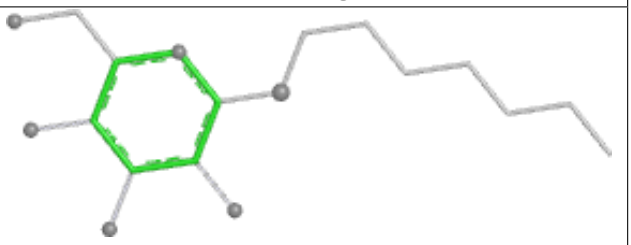
Bond lengths



Bond angles

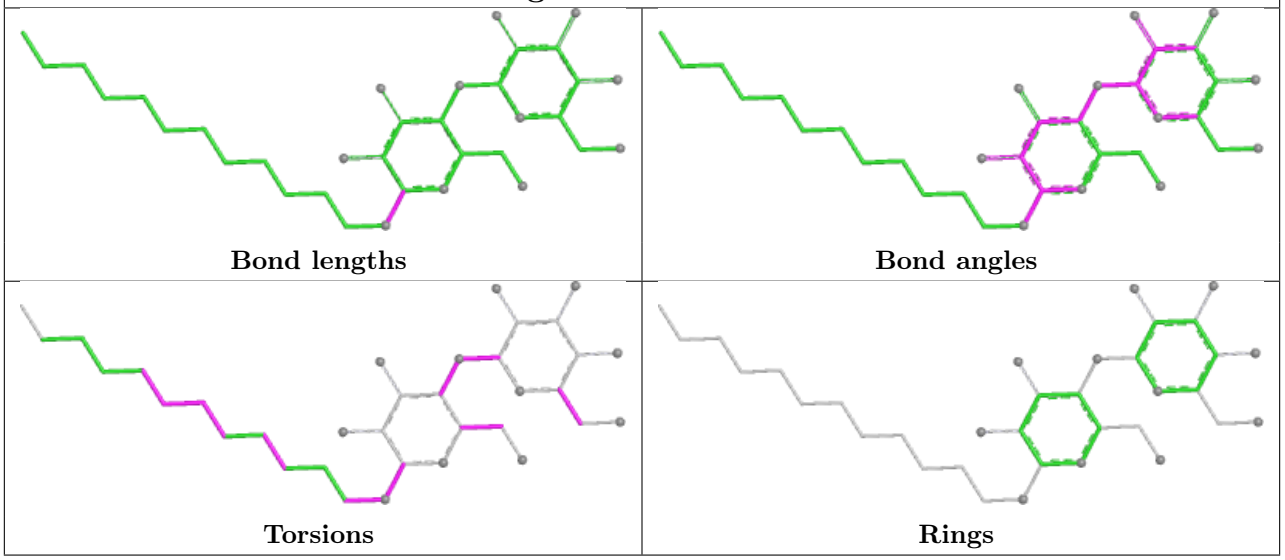


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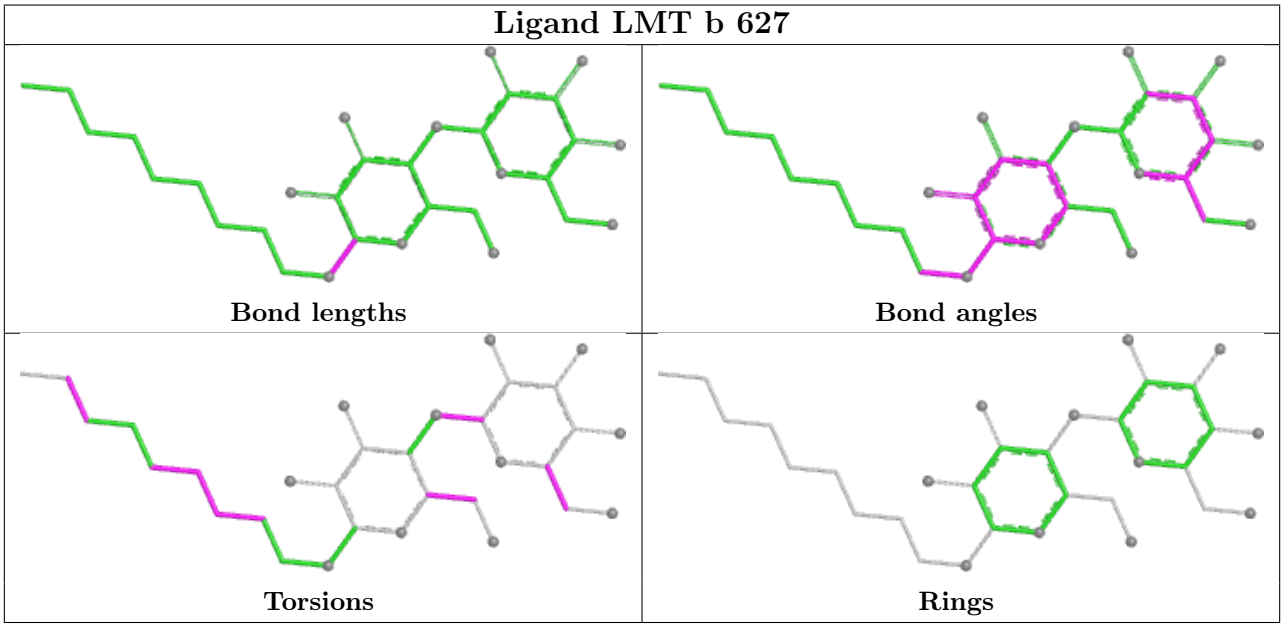


Rings

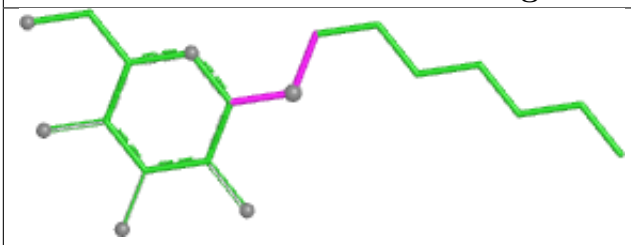
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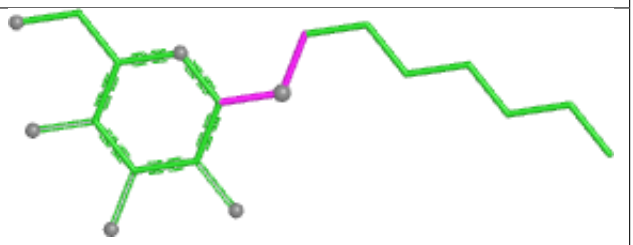
Ligand LMT b 627



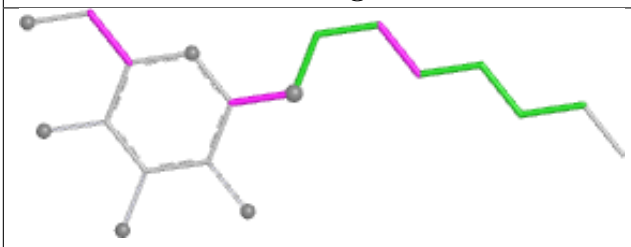
Ligand HTG C 522



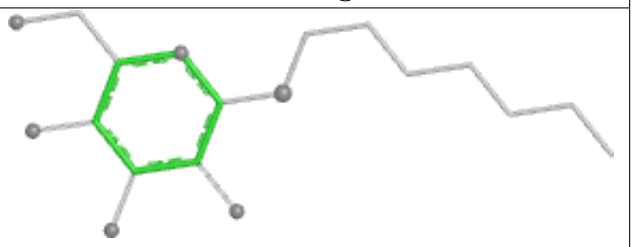
Bond lengths



Bond angles

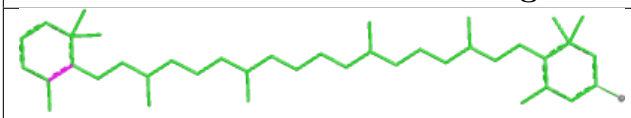


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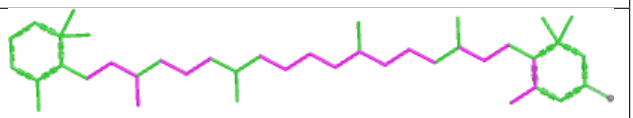


Rings

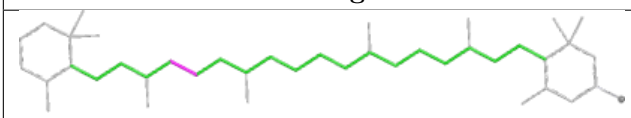
Ligand RRX H 101



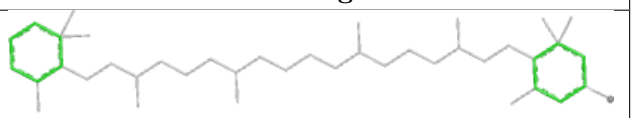
Bond lengths



Bond angles



Torsions



Rings

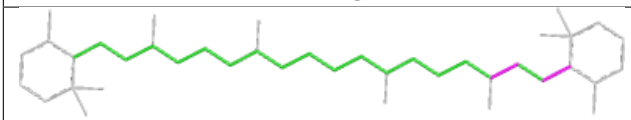
Ligand BCR D 405



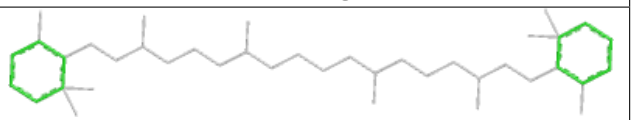
Bond lengths



Bond angles

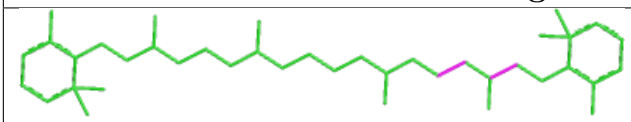


Torsions

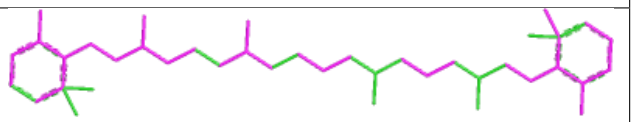


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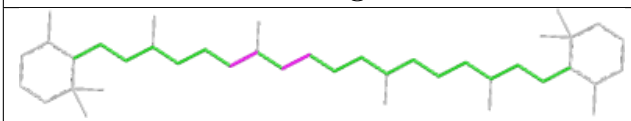
Ligand BCR t 101



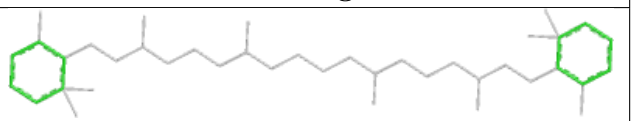
Bond lengths



Bond angles

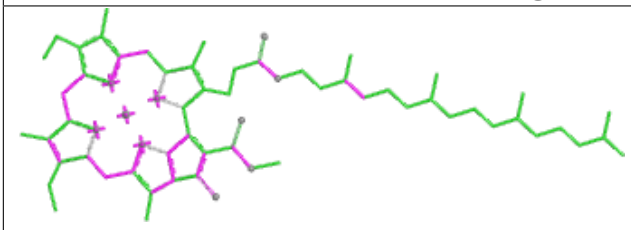


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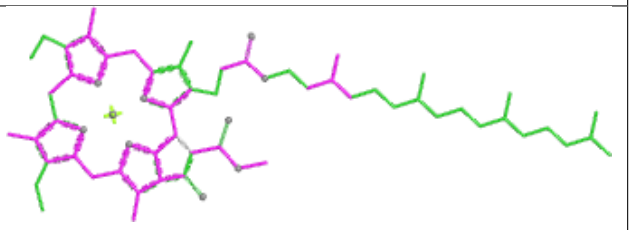


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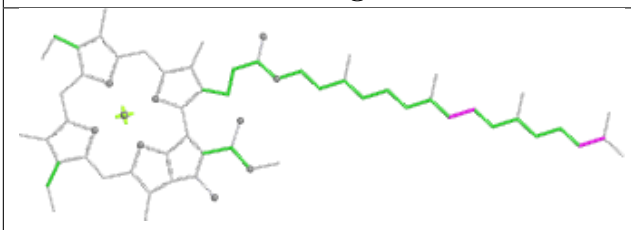
Ligand CLA c 510



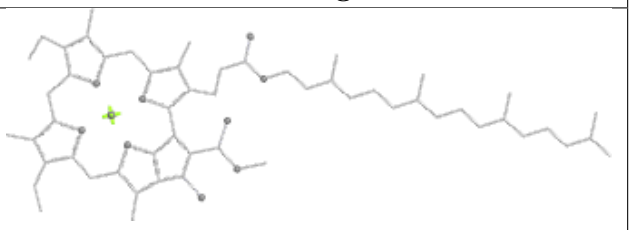
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Bond angles

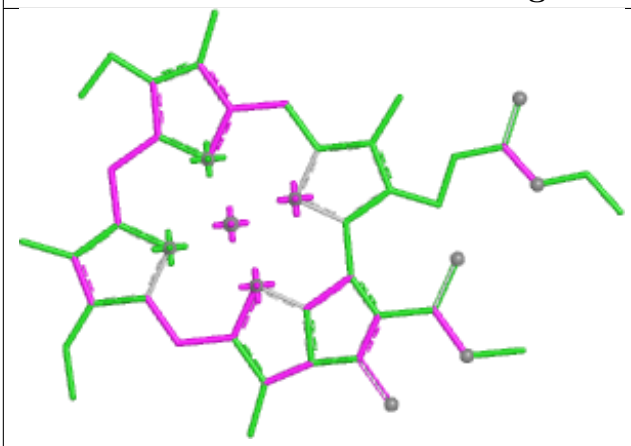


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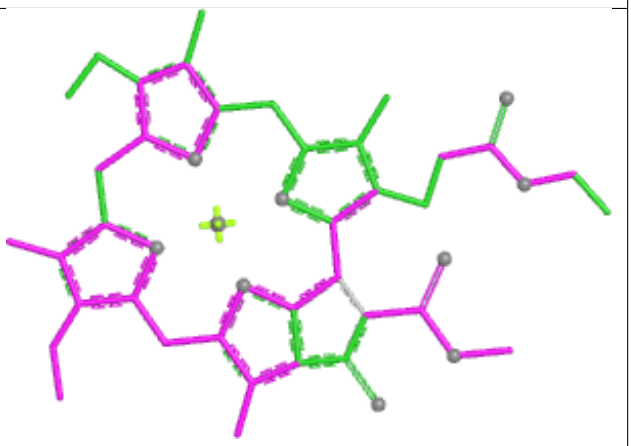


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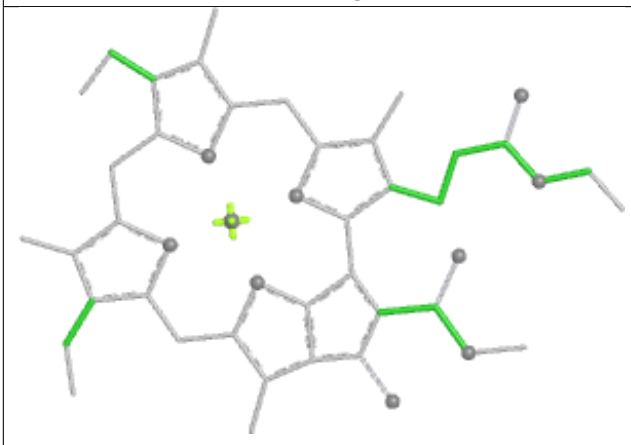
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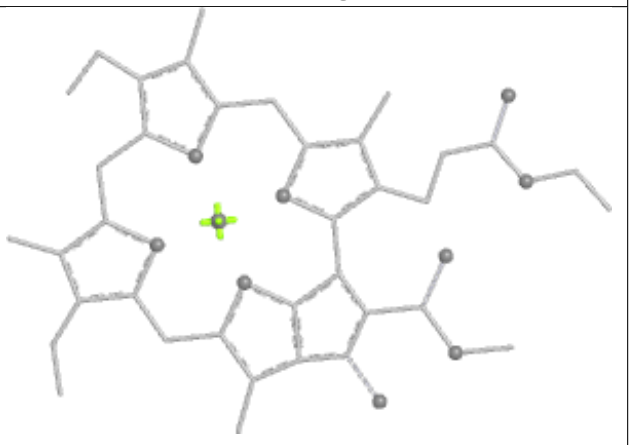
Bond lengths



Bond angles

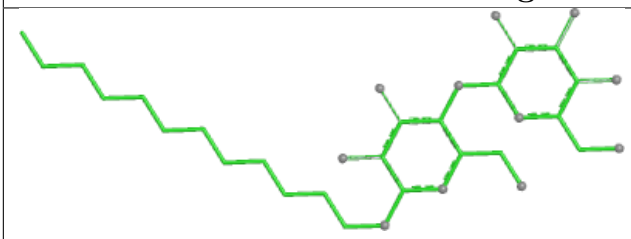


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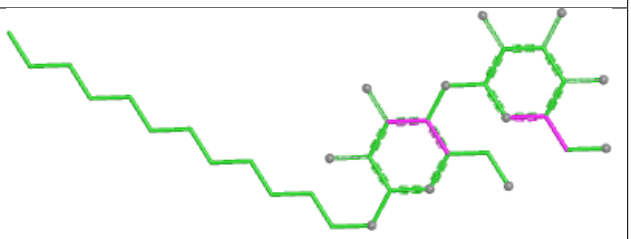


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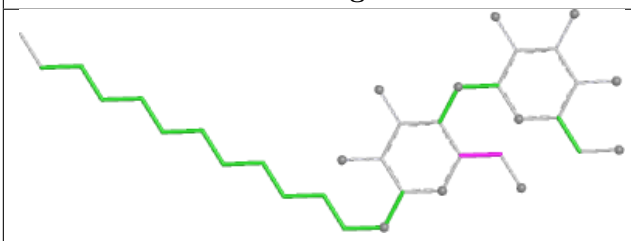
Ligand LMT M 101



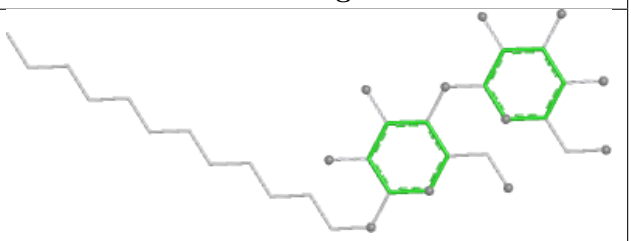
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Bond angles

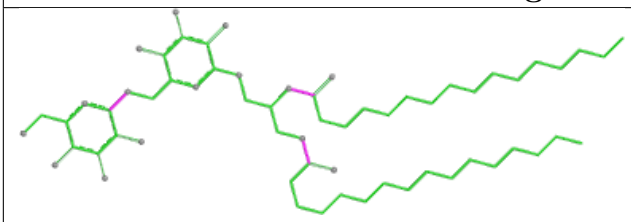


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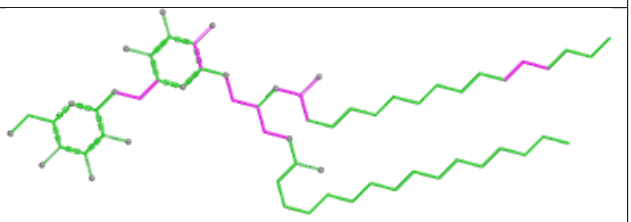


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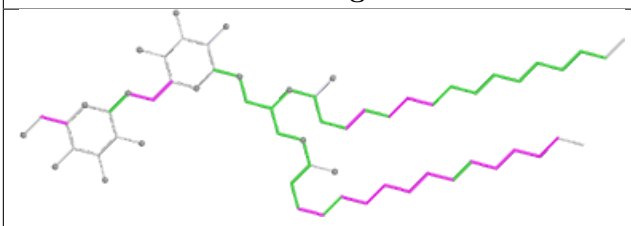
Ligand DGD c 515



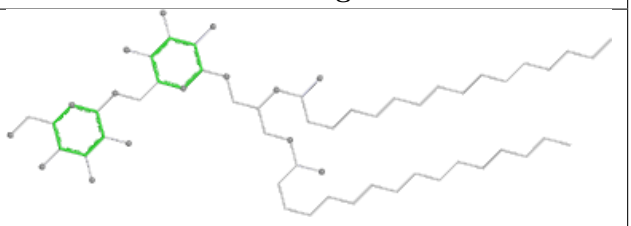
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Bond angles

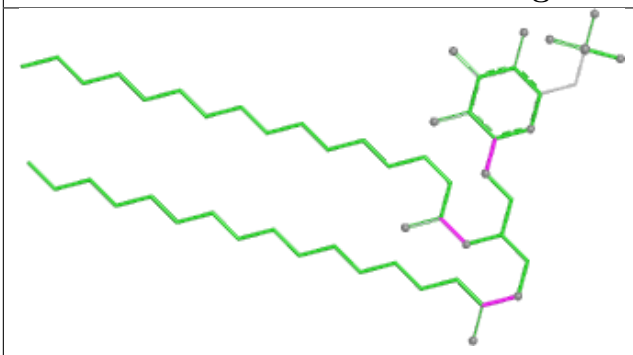


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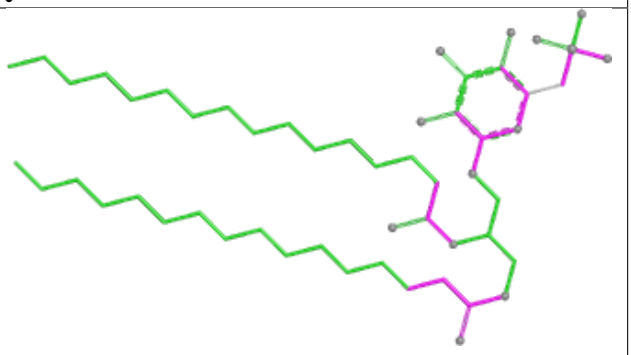


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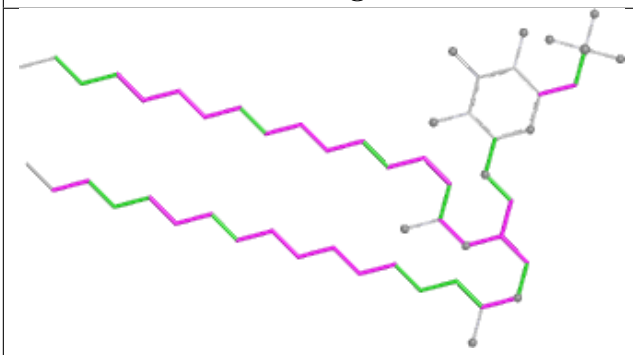
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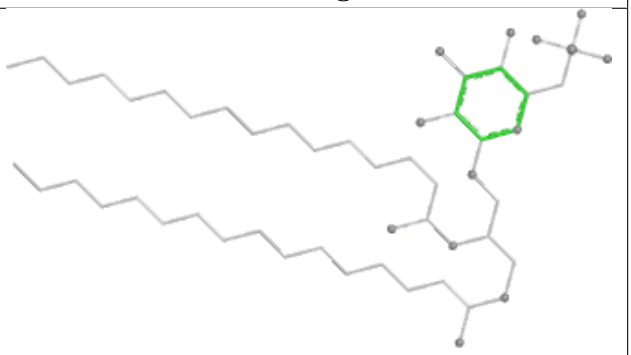
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Bond angles

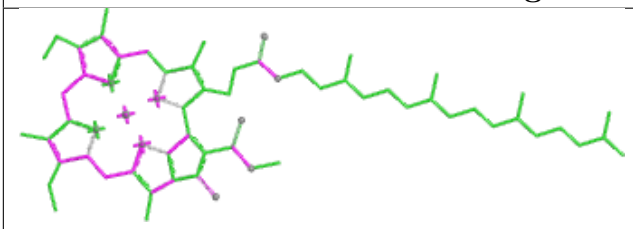


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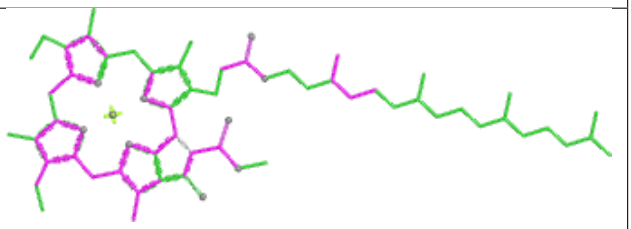


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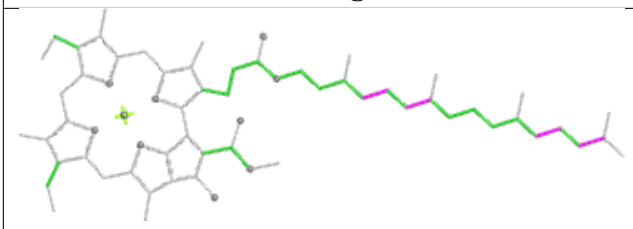
Ligand CLA B 605



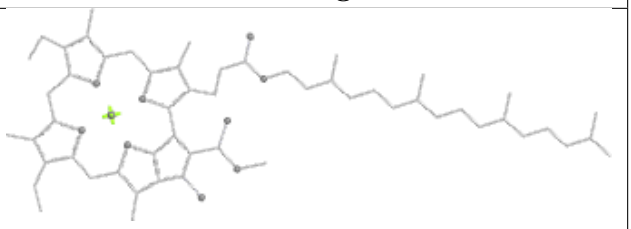
Bond lengths



Bond angles

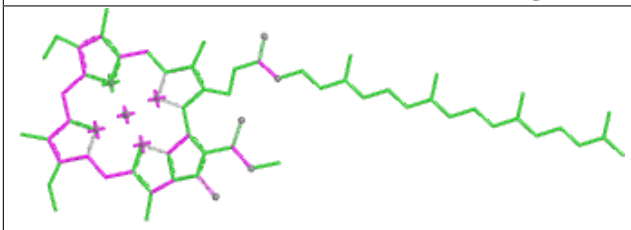


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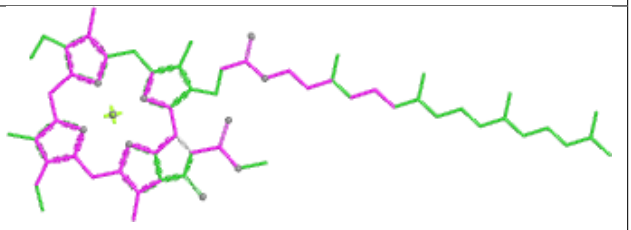


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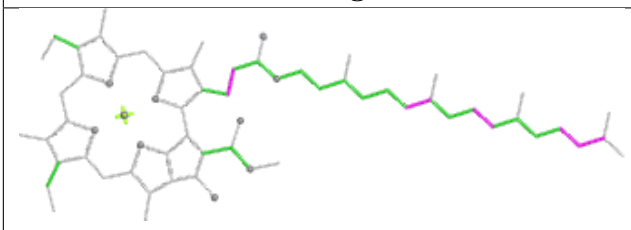
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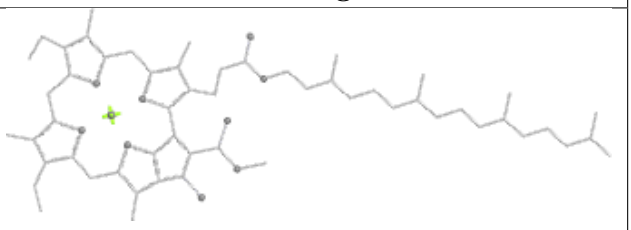
Bond lengths



Bond angles



Torsions

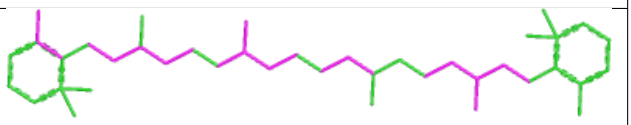


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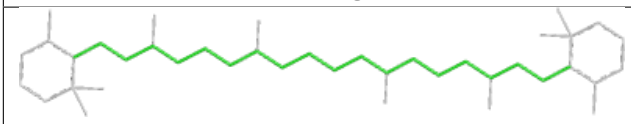
Ligand BCR k 102



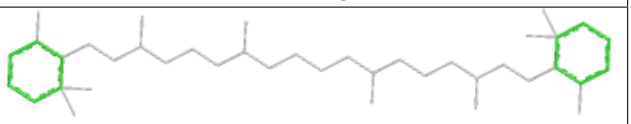
Bond lengths



Bond angles

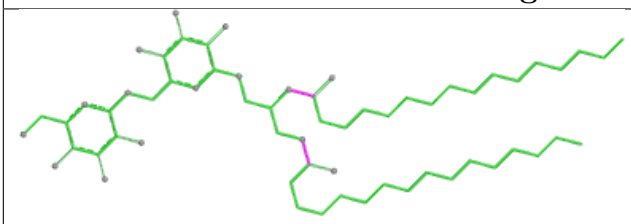


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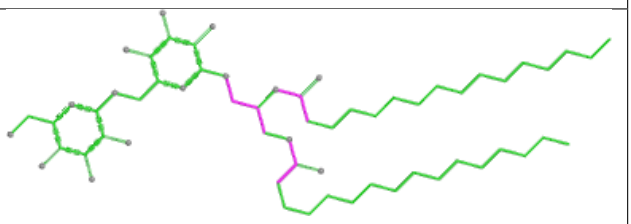


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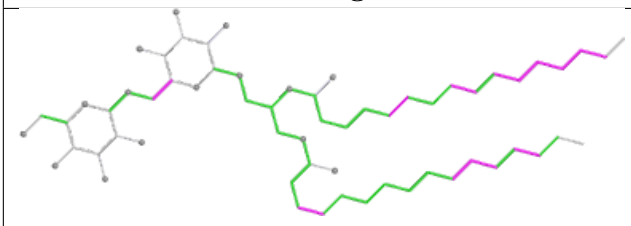
Ligand DGD C 518



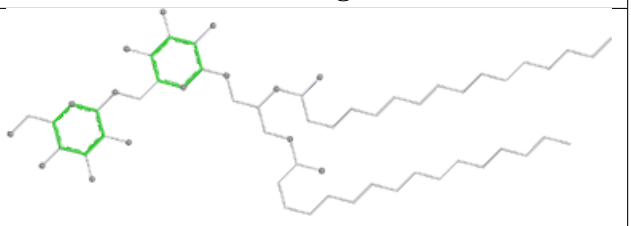
Bond lengths



Bond angles

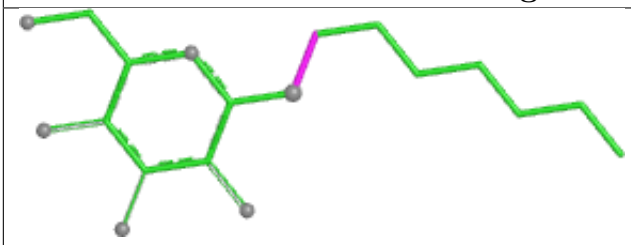


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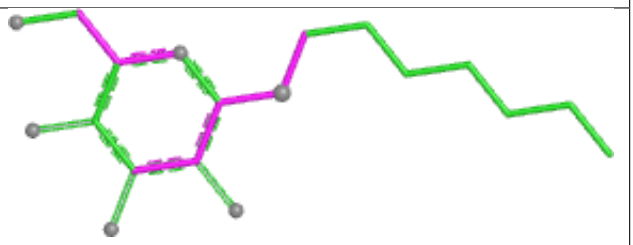


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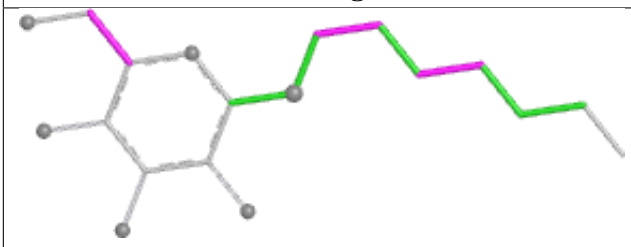
Ligand HTG D 417



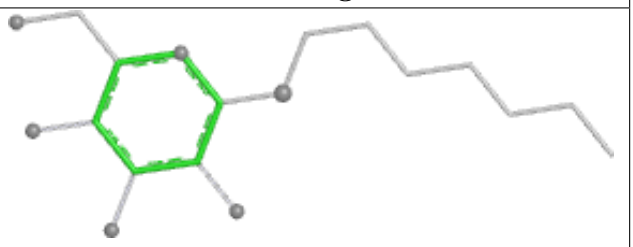
Bond lengths



Bond angles

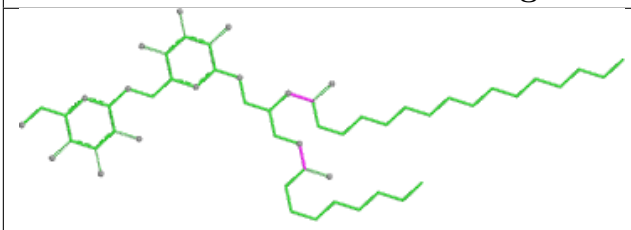


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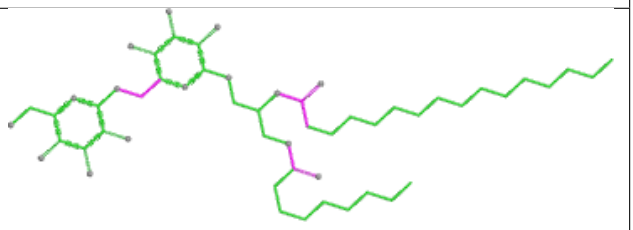


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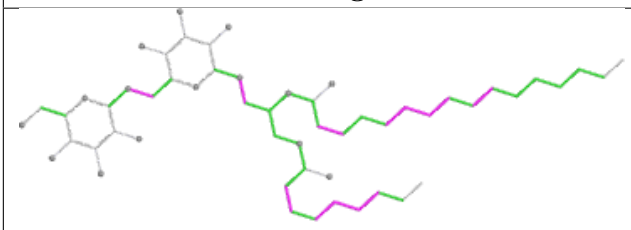
Ligand DGD C 517



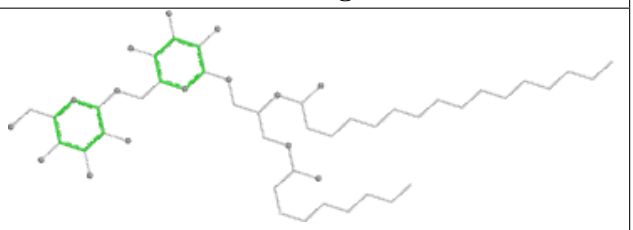
Bond lengths



Bond angles

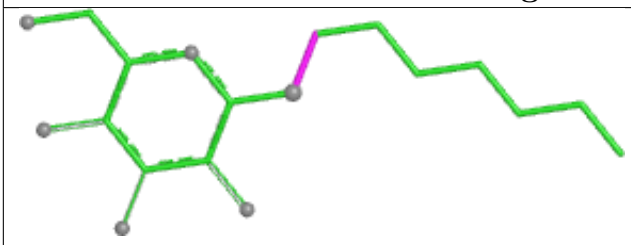


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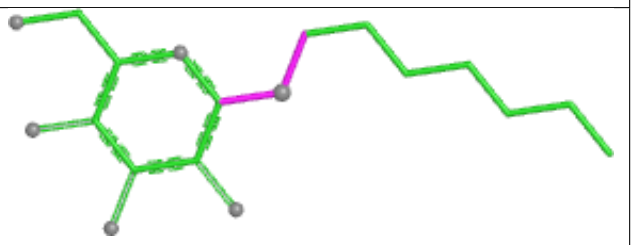


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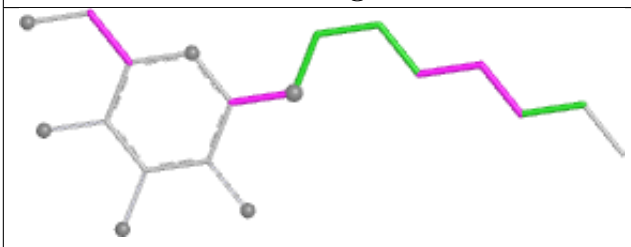
Ligand HTG B 623



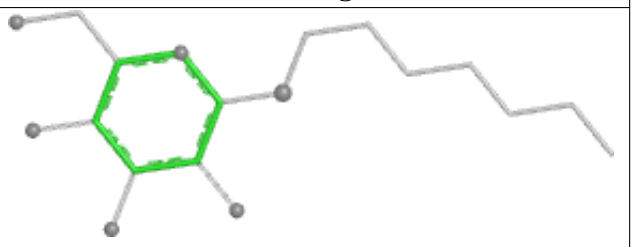
Bond lengths



Bond angles

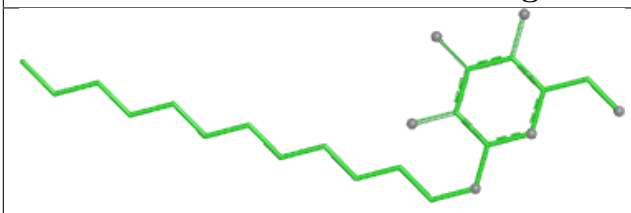


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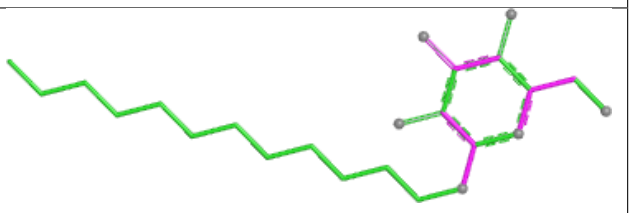


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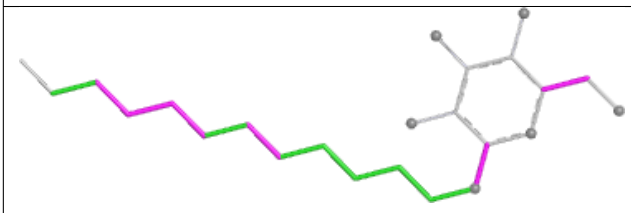
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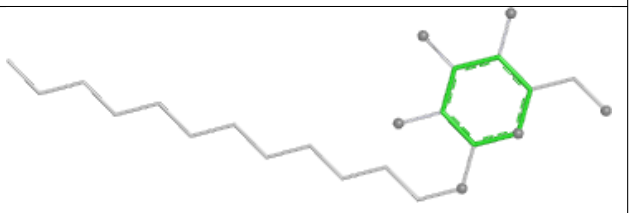
Bond lengths



Bond angles

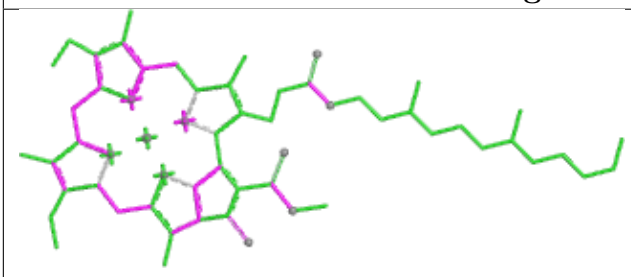


Torsions

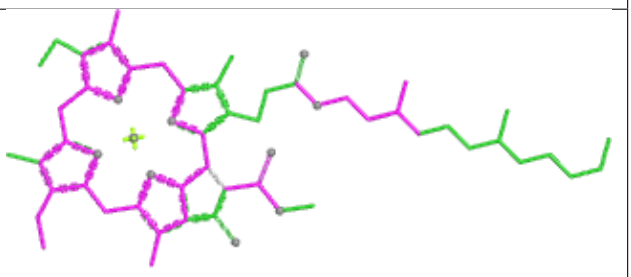


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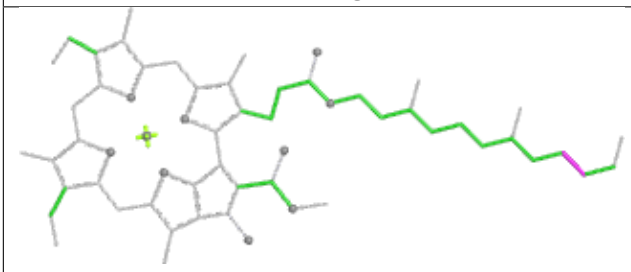
Ligand CLA A 402



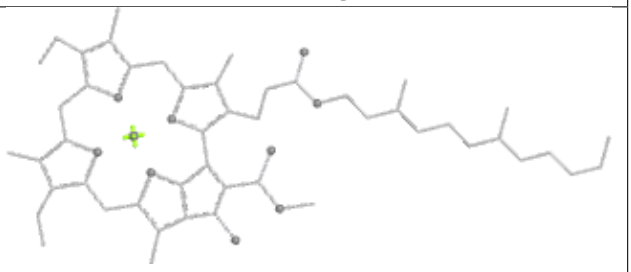
Bond lengths



Bond angles

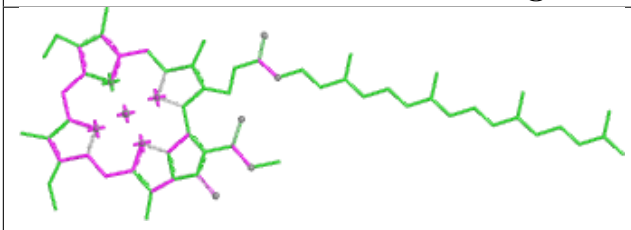


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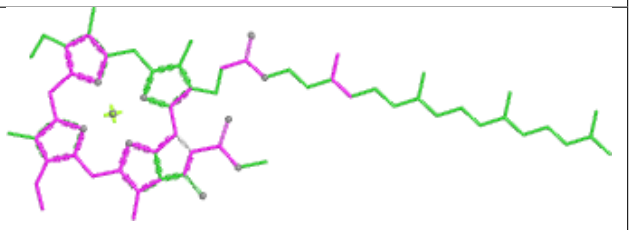


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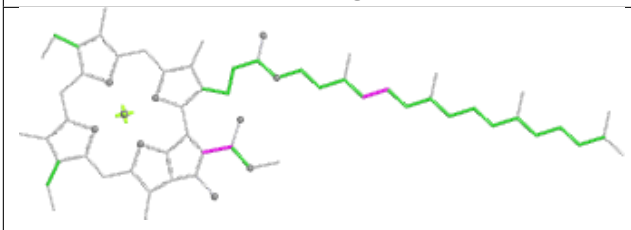
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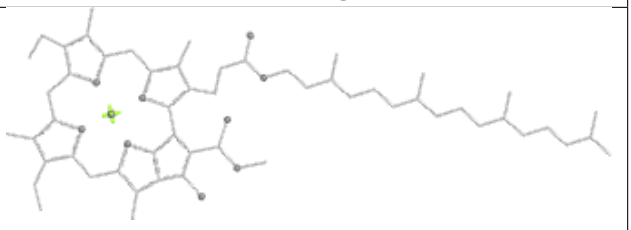
Bond lengths



Bond angles

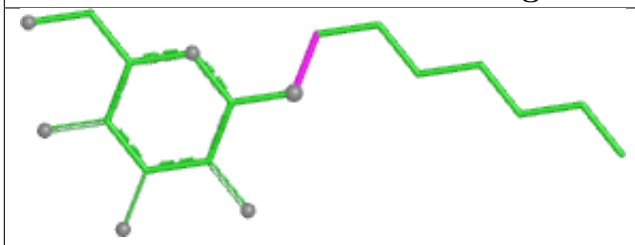


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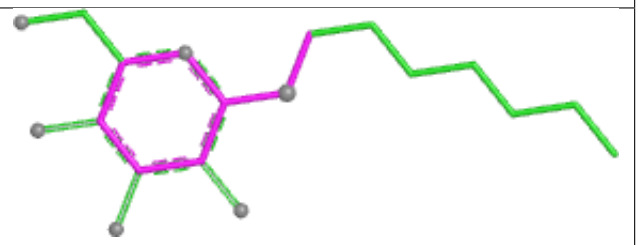


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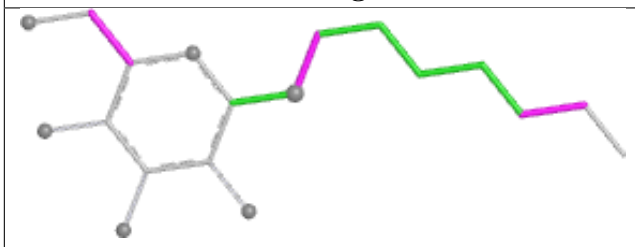
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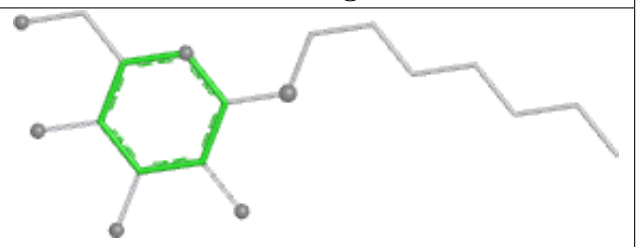
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Bond angles

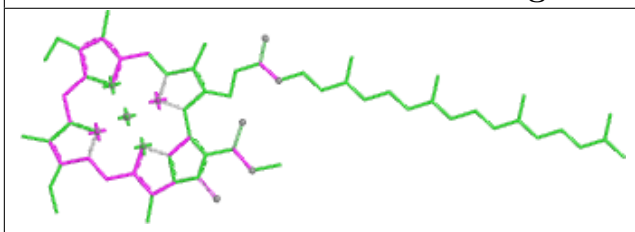


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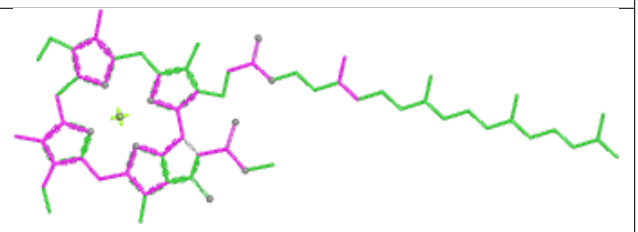


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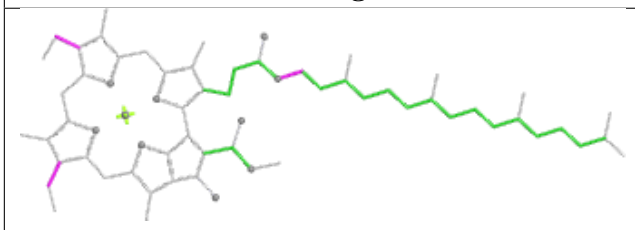
Ligand CLA d 402



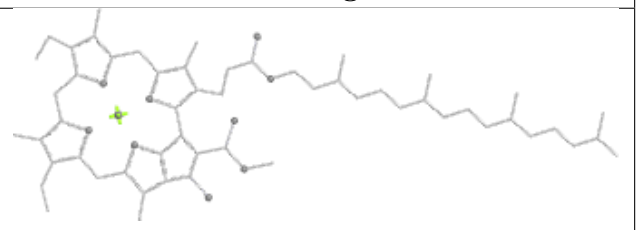
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Bond angles

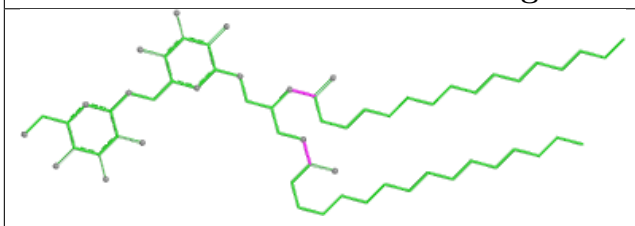


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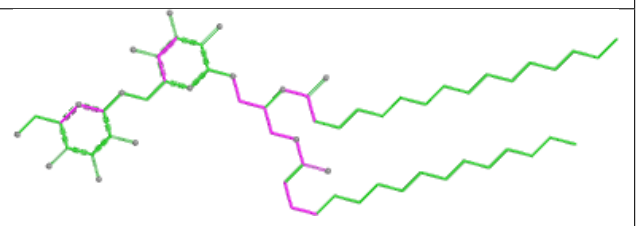


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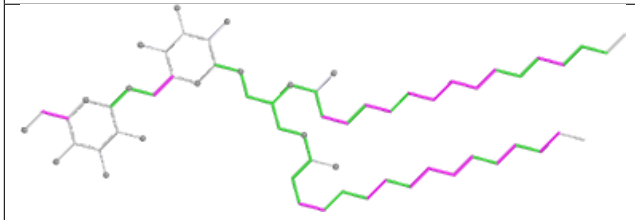
Ligand DGD C 516



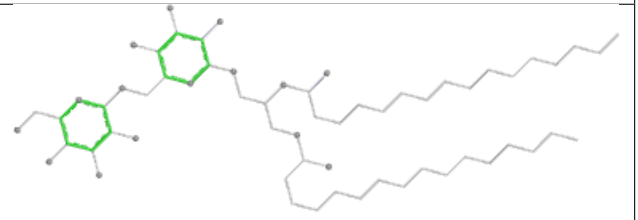
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Bond angles

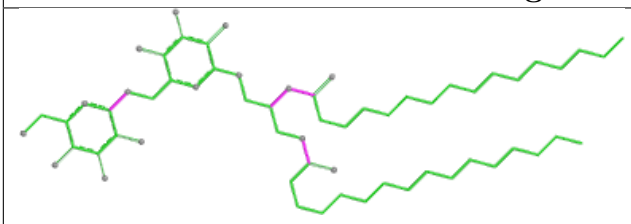


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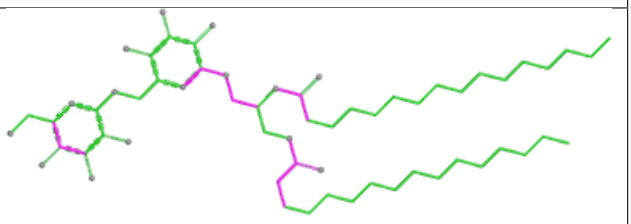


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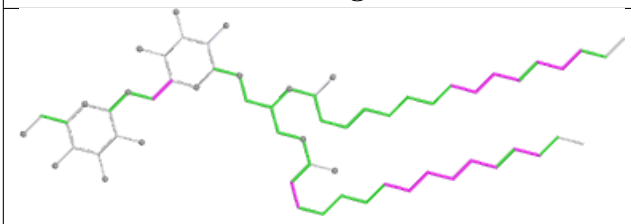
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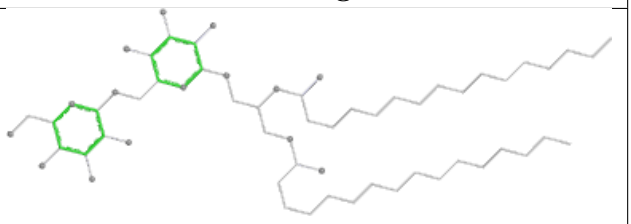
Bond lengths



Bond angles

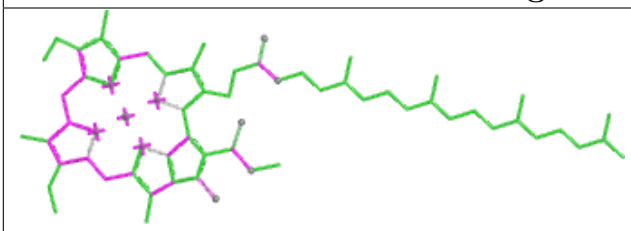


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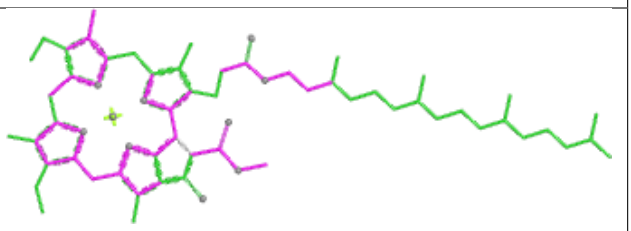


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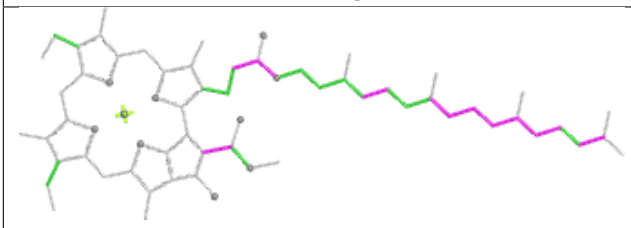
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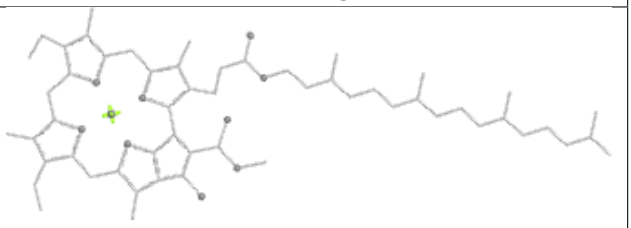
Bond lengths



Bond angles



Torsions

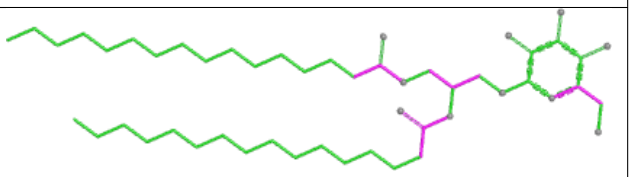


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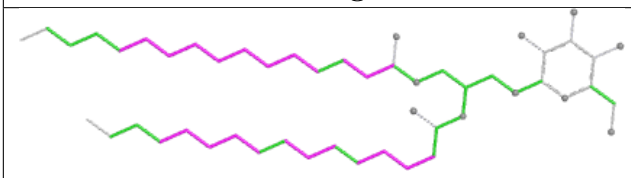
Ligand LMG B 620



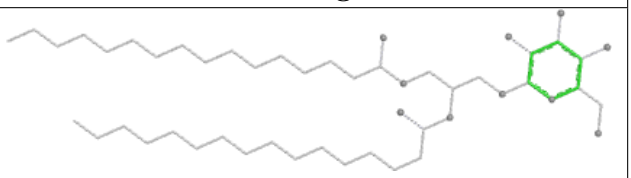
Bond lengths



Bond angles

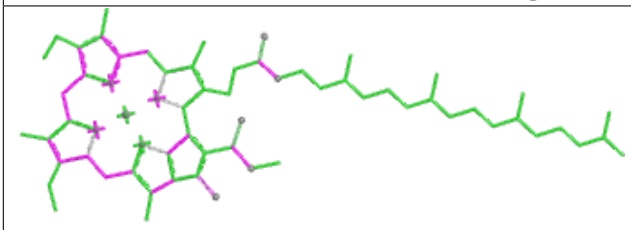


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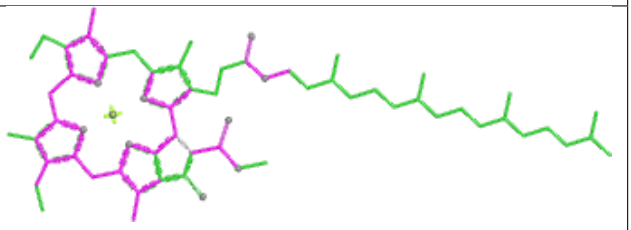


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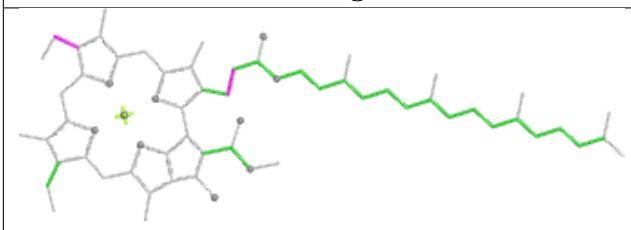
Ligand CLA C 501



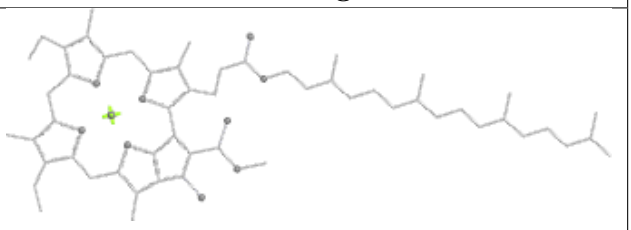
Bond lengths



Bond angles

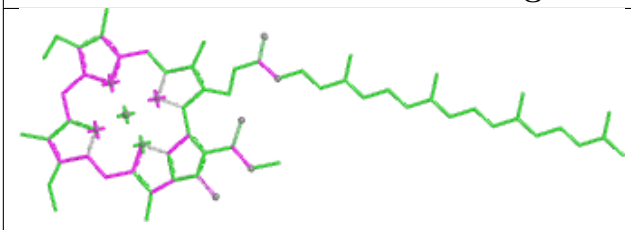


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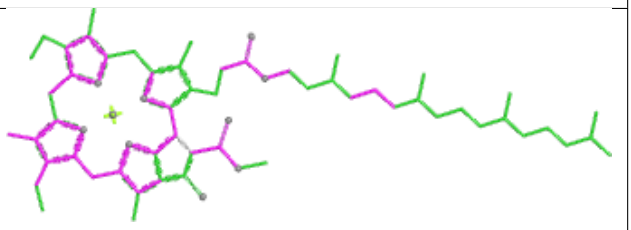


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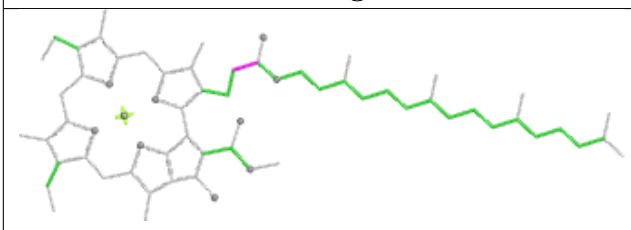
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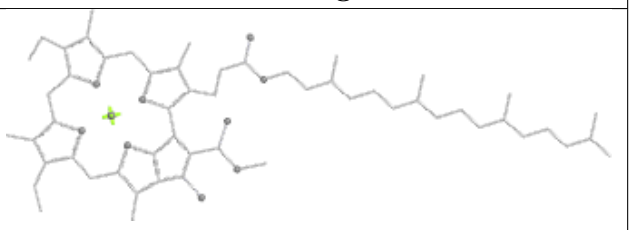
Bond lengths



Bond angles



Torsions

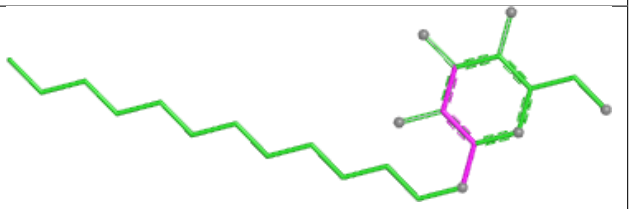


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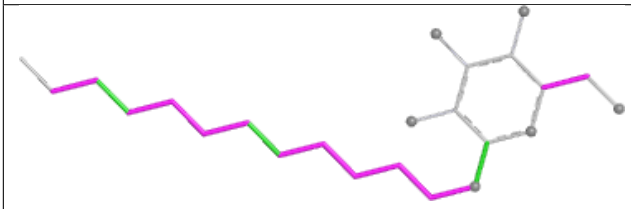
Ligand LMT T 102



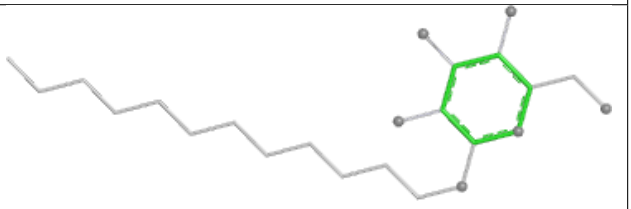
Bond lengths



Bond angles

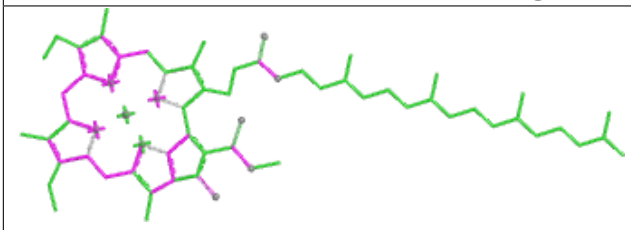


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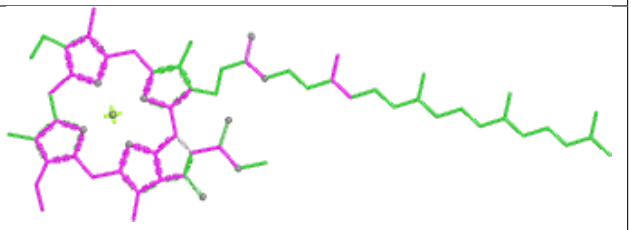


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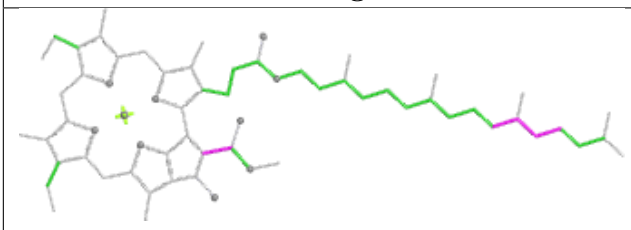
Ligand CLA c 504



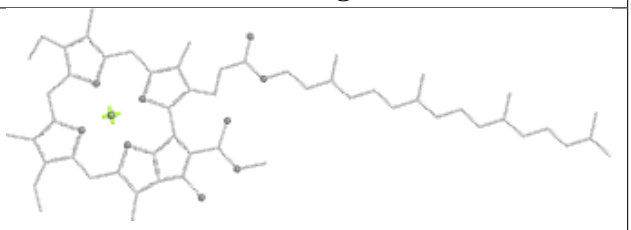
Bond lengths



Bond angles

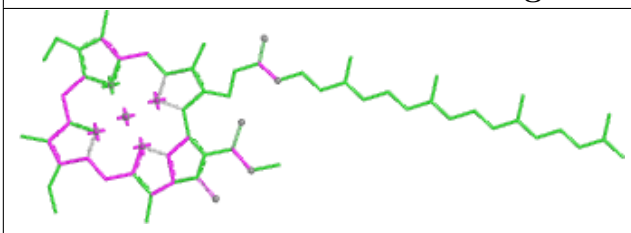


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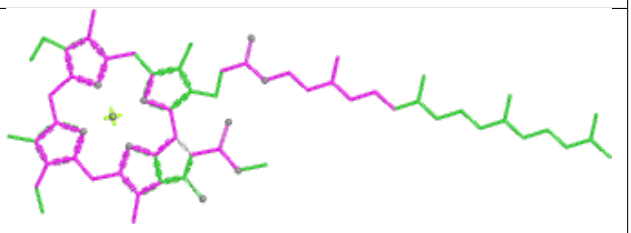


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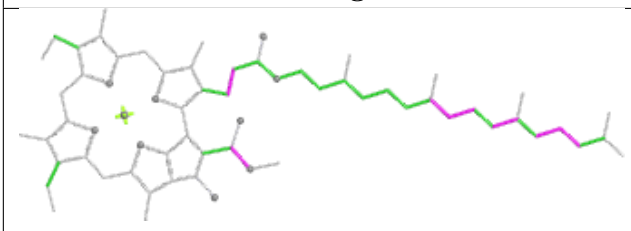
Ligand CLA B 607



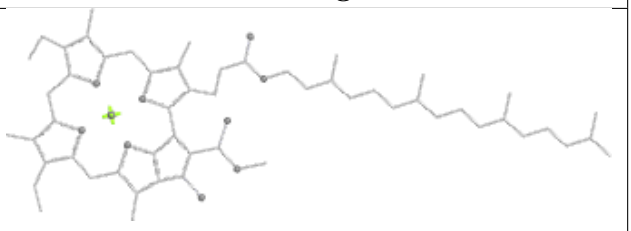
Bond lengths



Bond angles

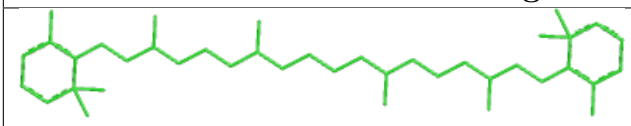


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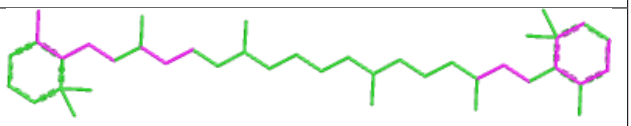


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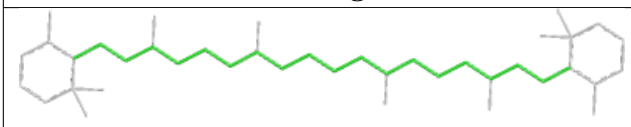
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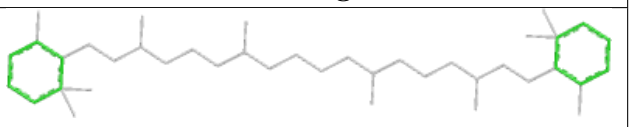
Bond lengths



Bond angles

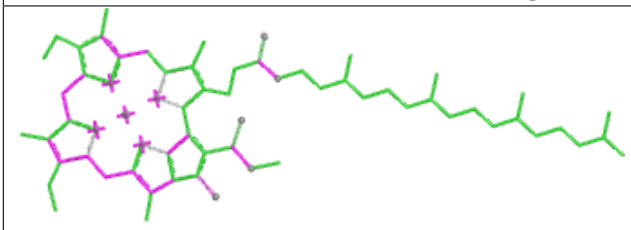


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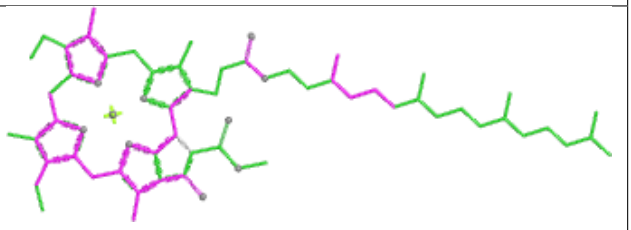


Rings

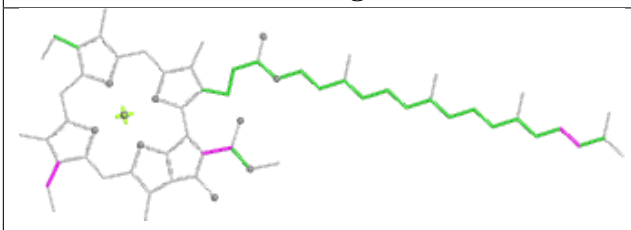
Ligand CLA A 401



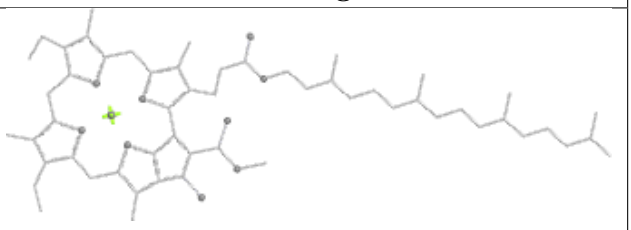
Bond lengths



Bond angles

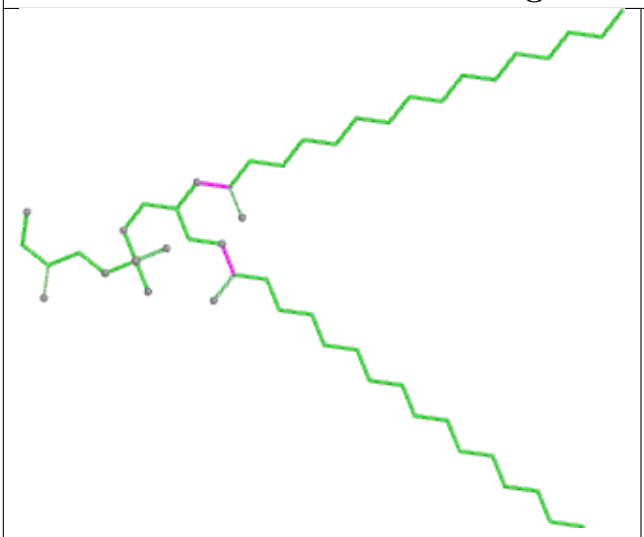


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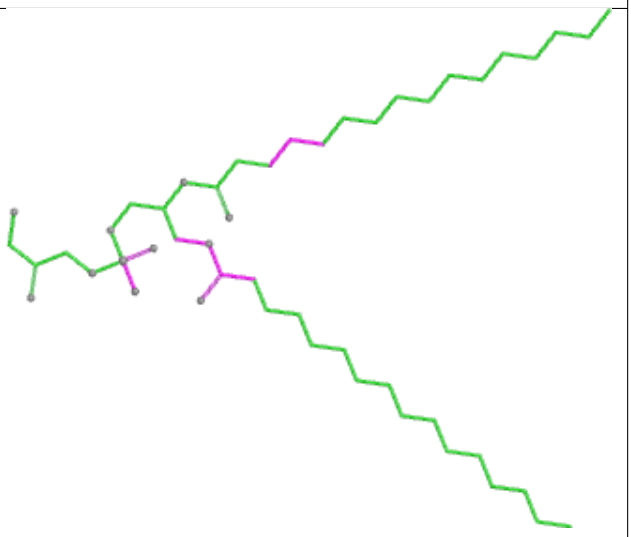


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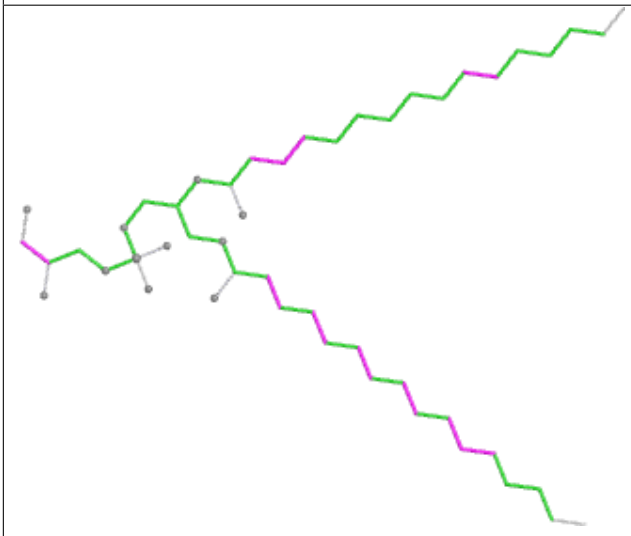
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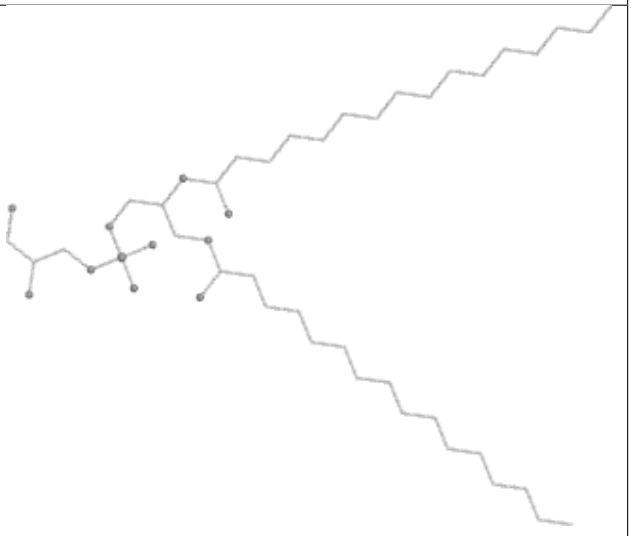
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Bond angles

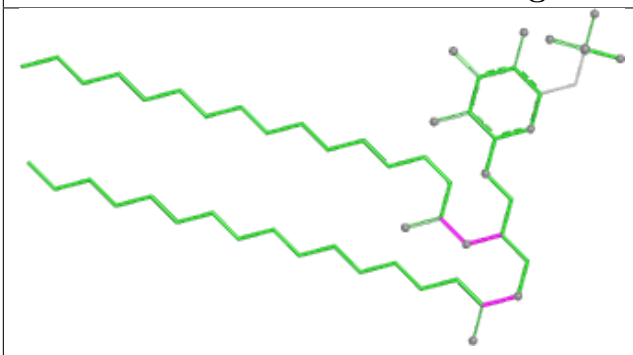


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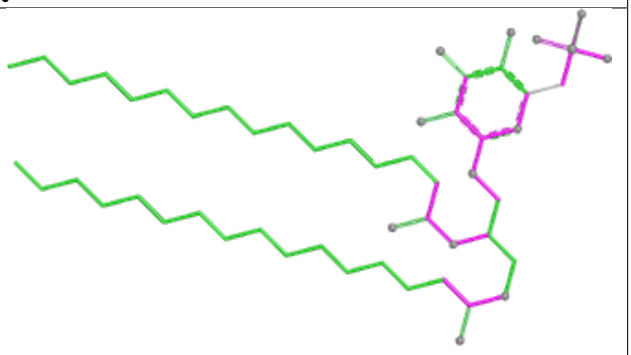


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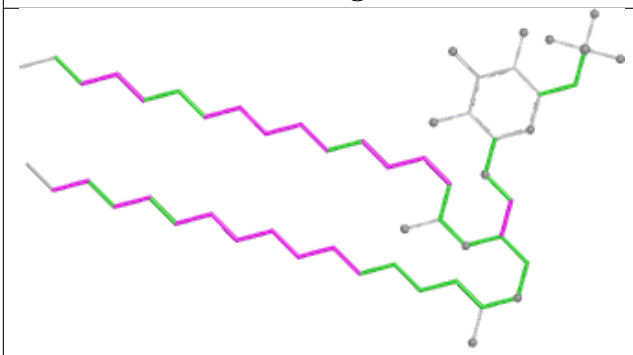
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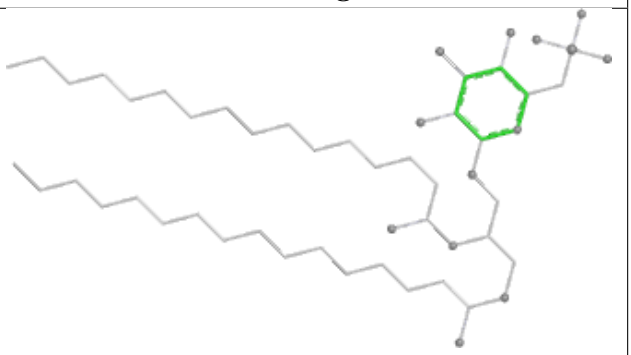
Bond lengths



Bond angles

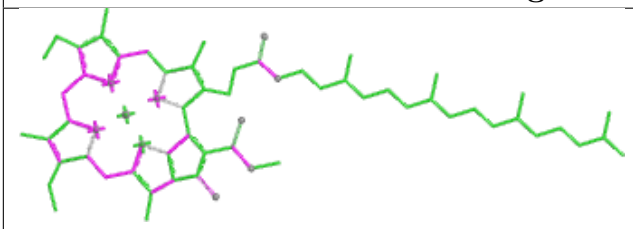


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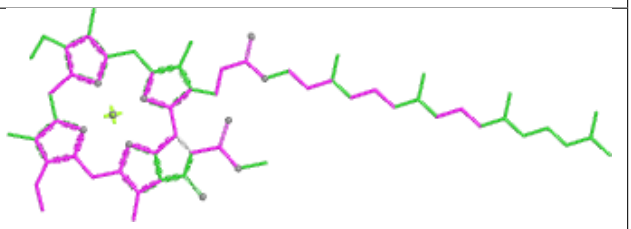


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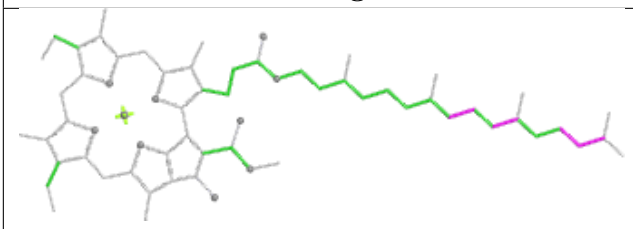
Ligand CLA b 615



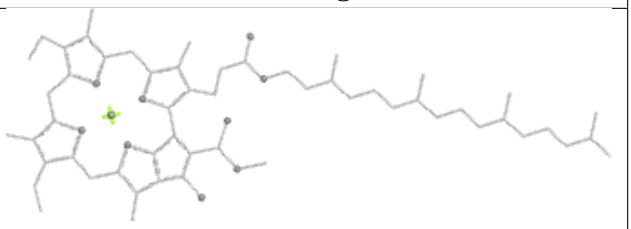
Bond lengths



Bond angles

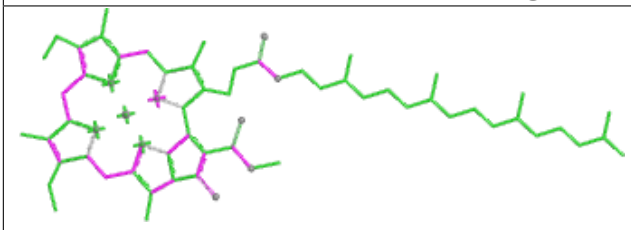


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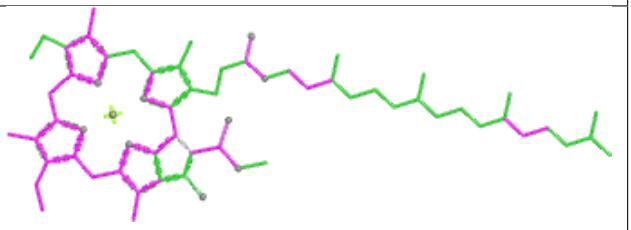


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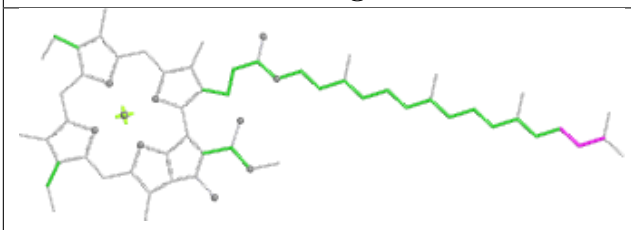
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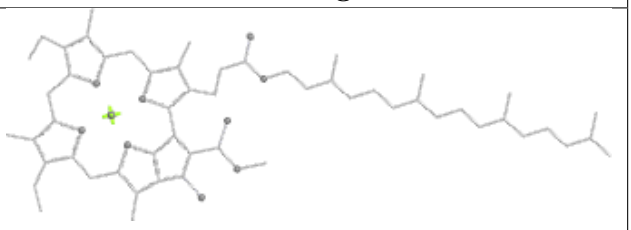
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Bond angles

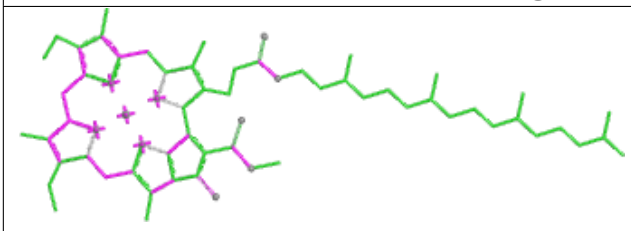


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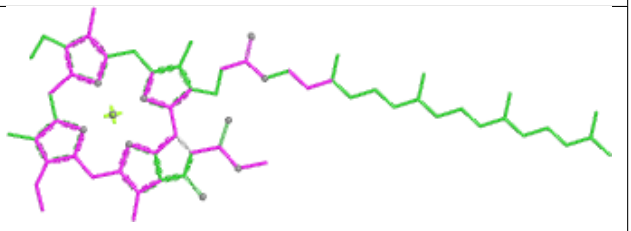


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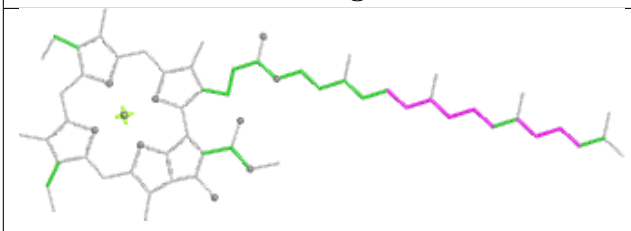
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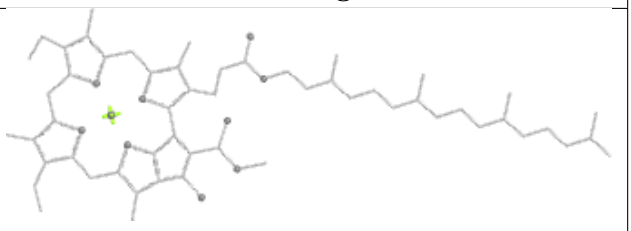
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Bond angles

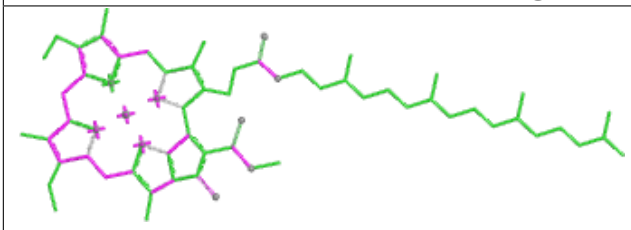


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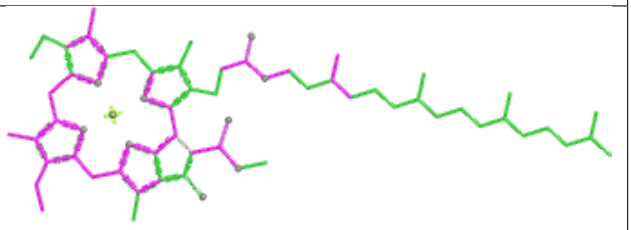


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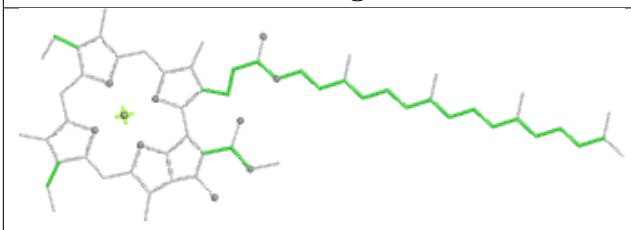
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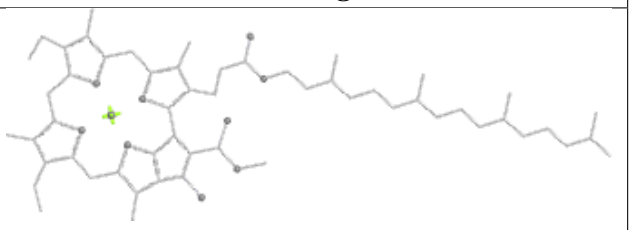
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Bond angles

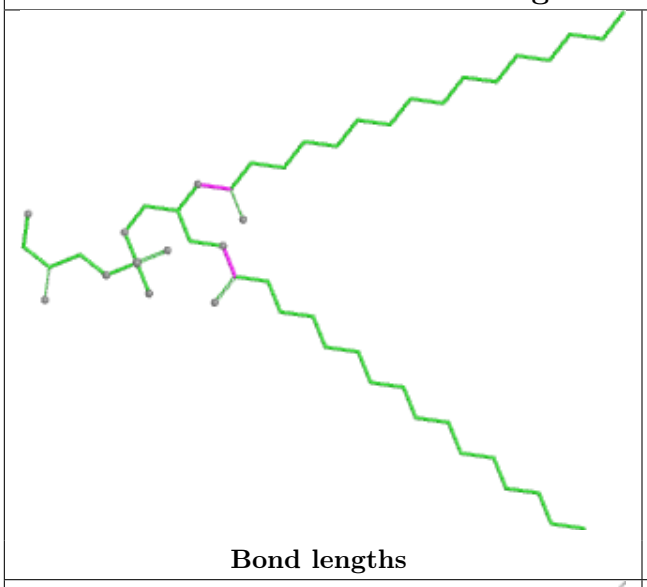


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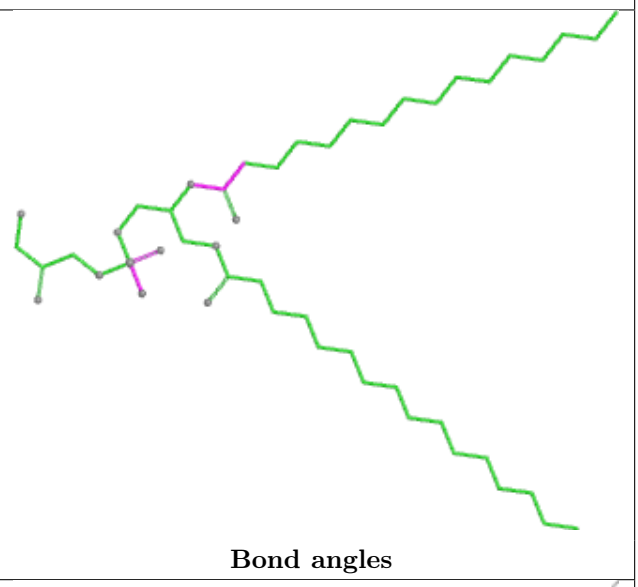


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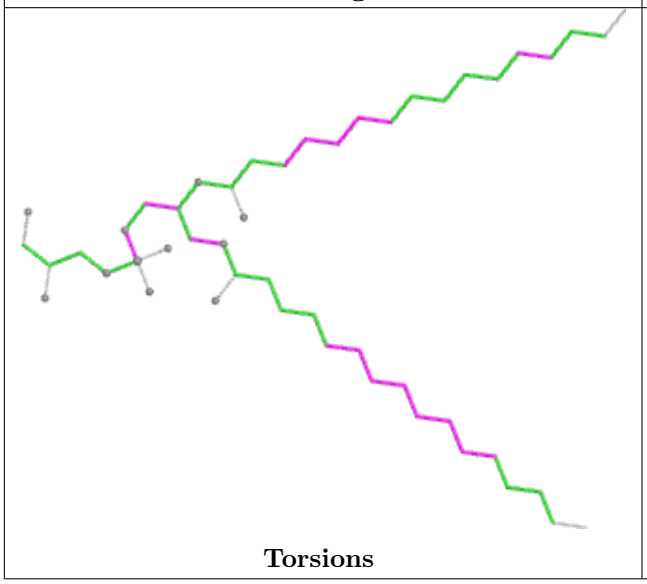
Ligand LHG l 102



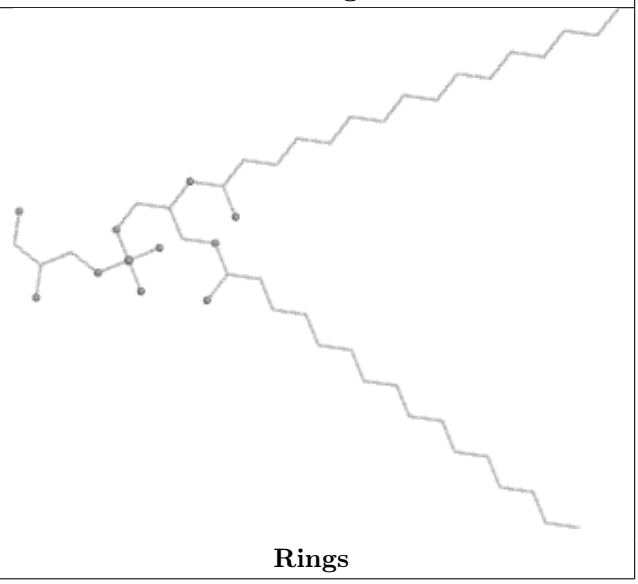
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Bond angles



Torsions

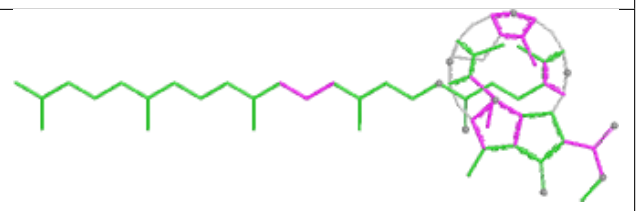


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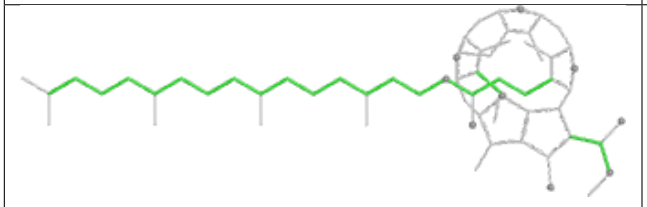
Ligand PHO A 403



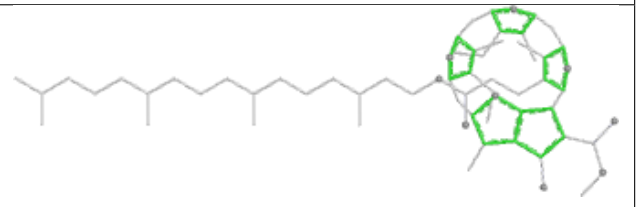
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Bond angles

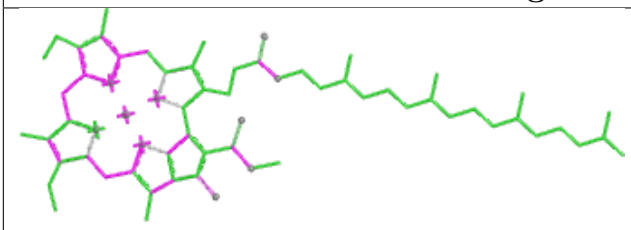


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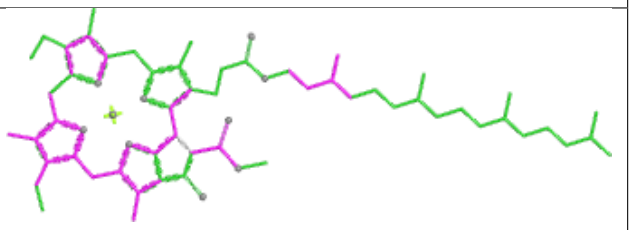


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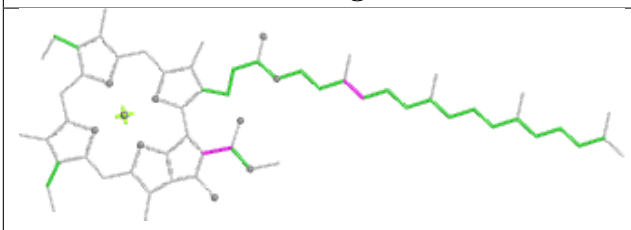
Ligand CLA b 607



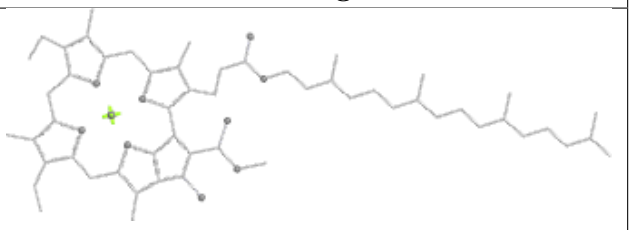
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Bond angles

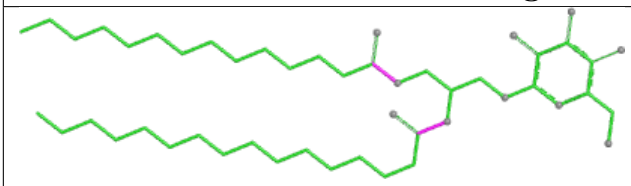


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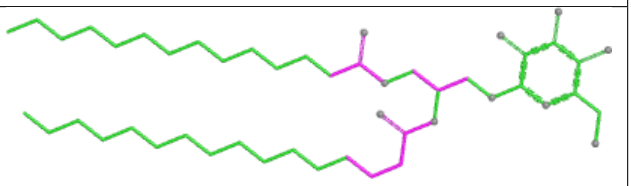


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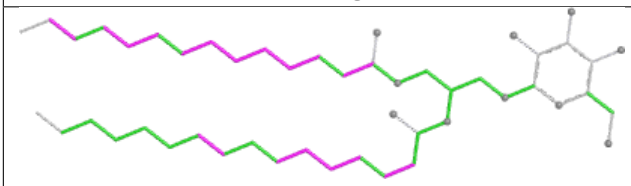
Ligand LMG b 623



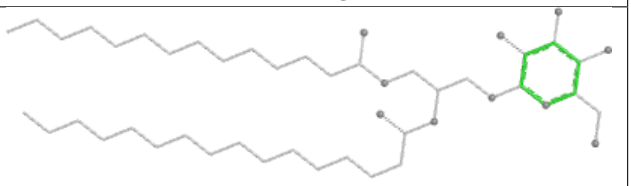
Bond lengths



Bond angles

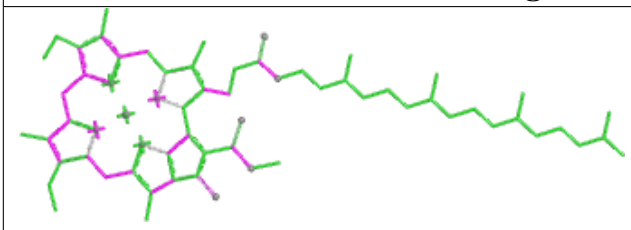


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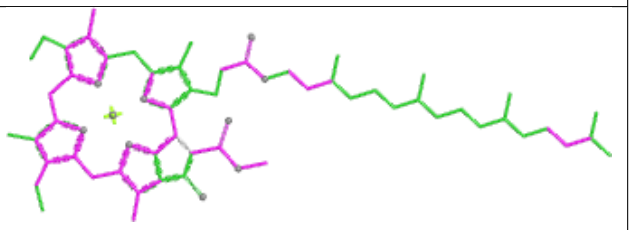


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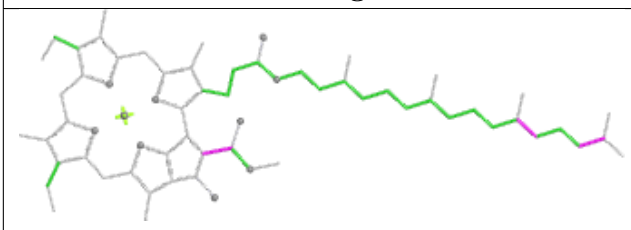
Ligand CLA C 502



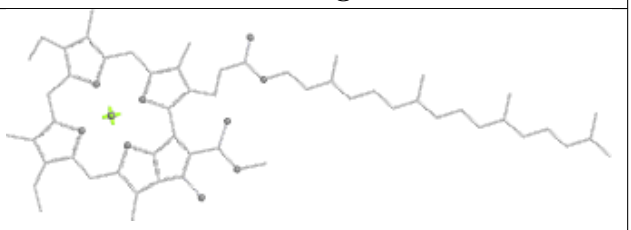
Bond lengths



Bond angles

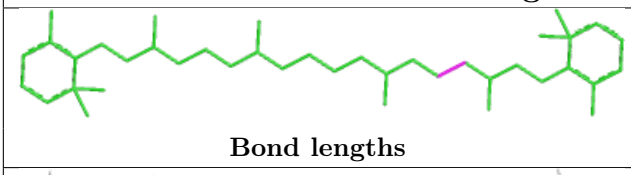


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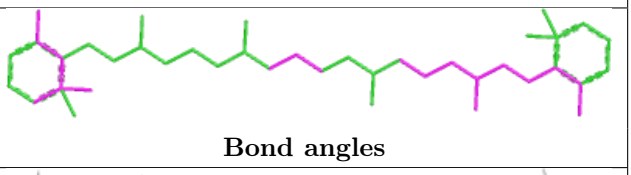


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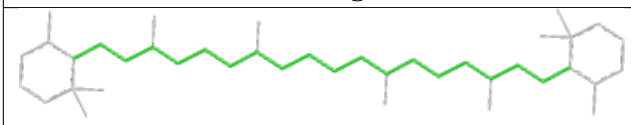
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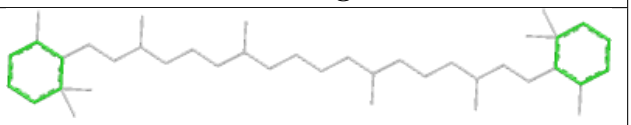
Bond lengths



Bond angles

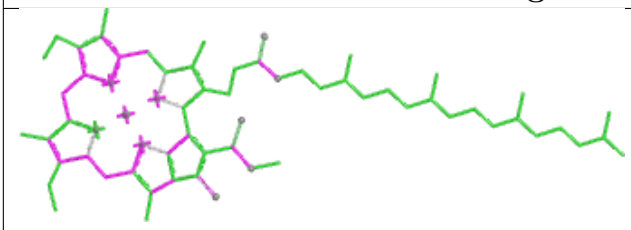


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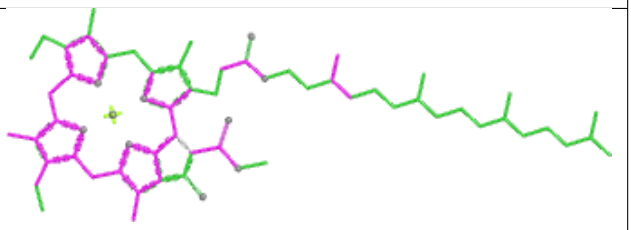


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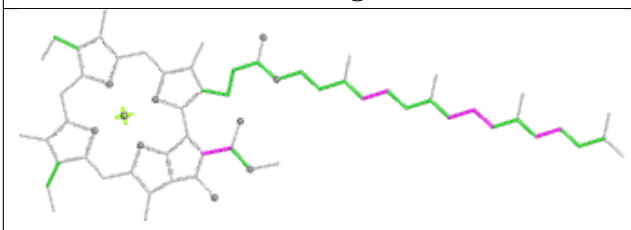
Ligand CLA b 614



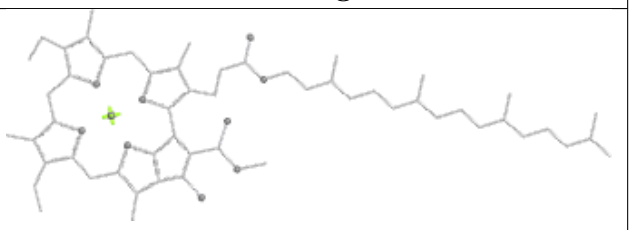
Bond lengths



Bond angles

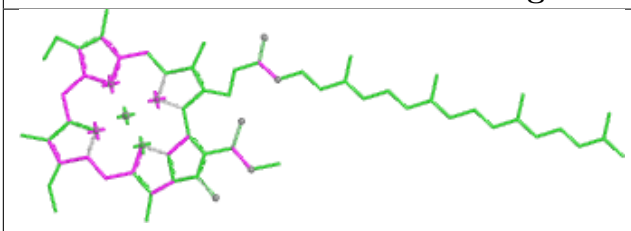


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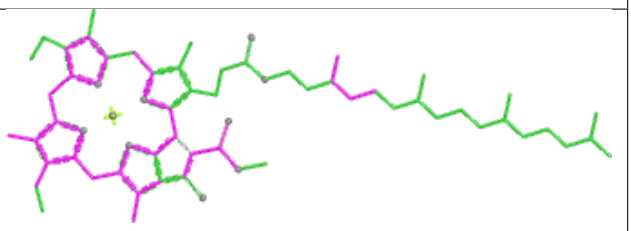


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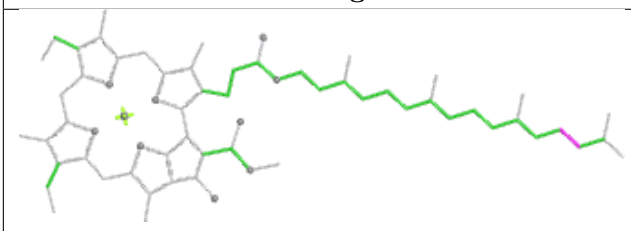
Ligand CLA b 606



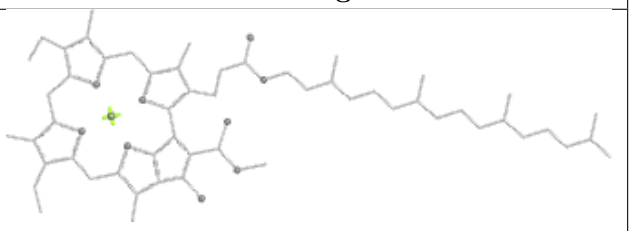
Bond lengths



Bond angles

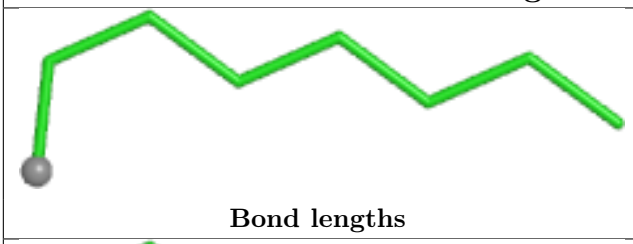


Torsions

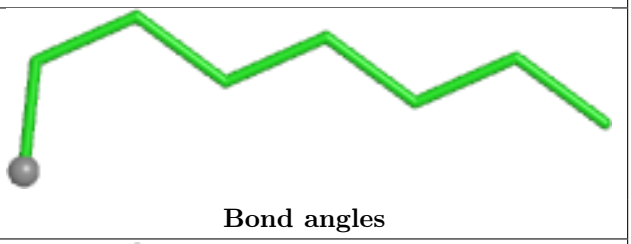


Rings

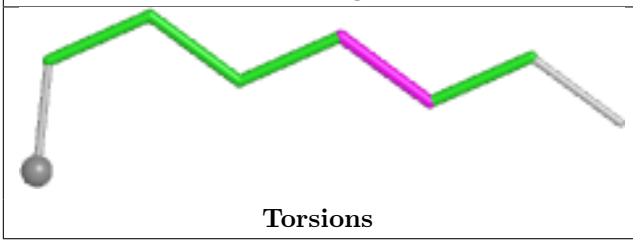
Ligand HTG u 201



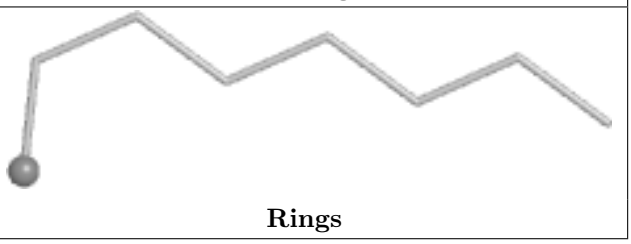
Bond lengths



Bond angles



Torsions

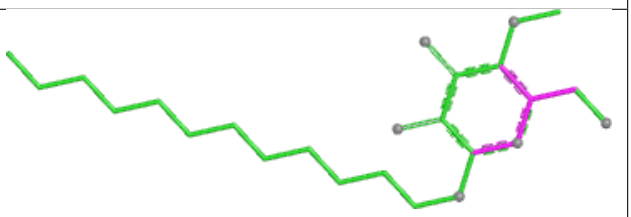


Rings

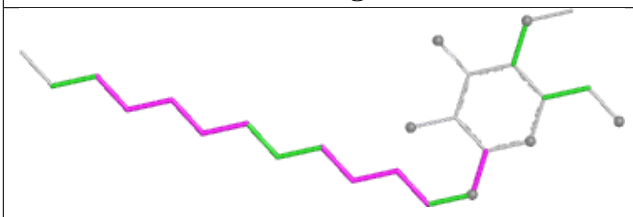
Ligand LMT b 628



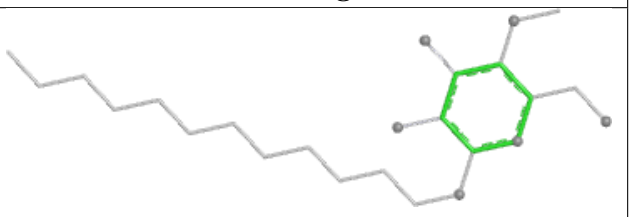
Bond lengths



Bond angles

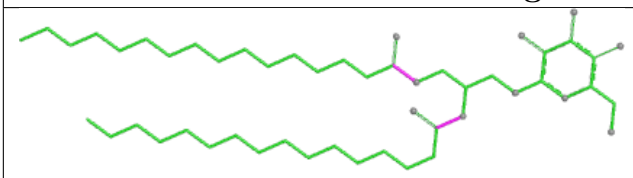


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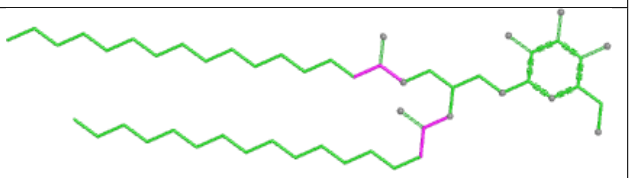


Rings

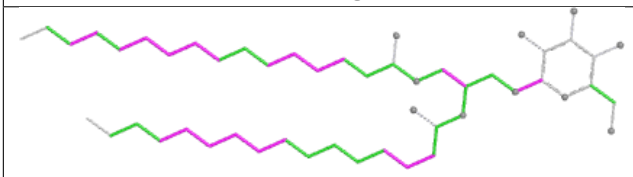
Ligand LMG a 410



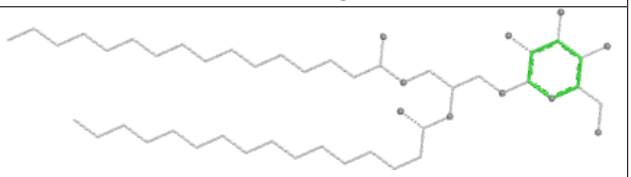
Bond lengths



Bond angles

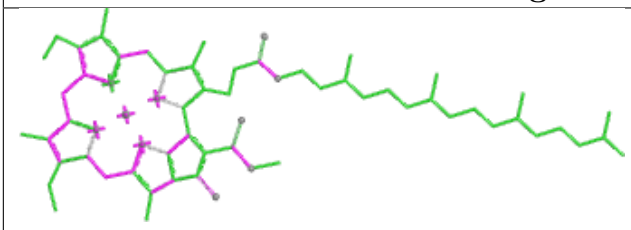


Torsions

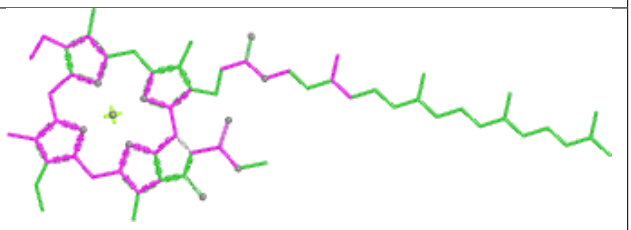


Rings

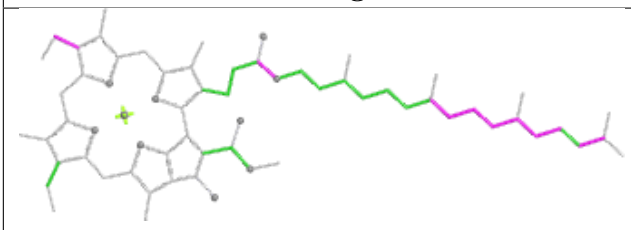
Ligand CLA c 513



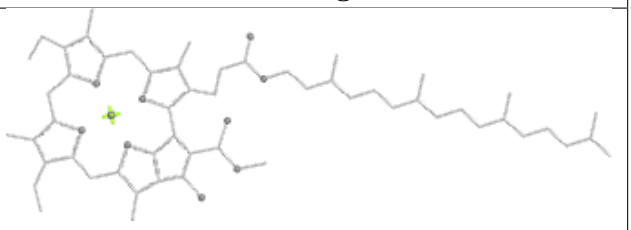
Bond lengths



Bond angles

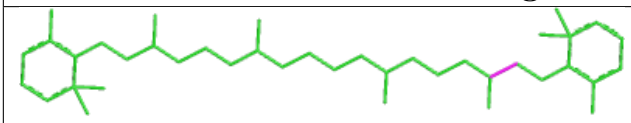


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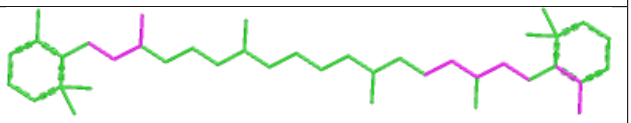


Rings

Ligand BCR K 102



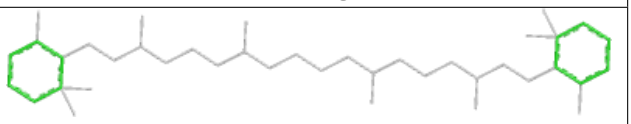
Bond lengths



Bond angles

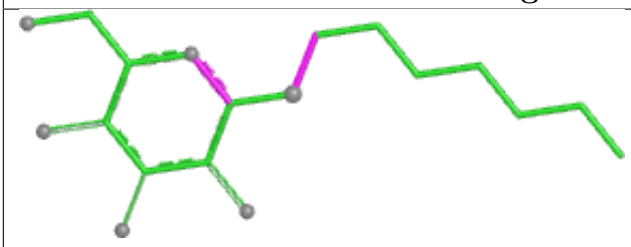


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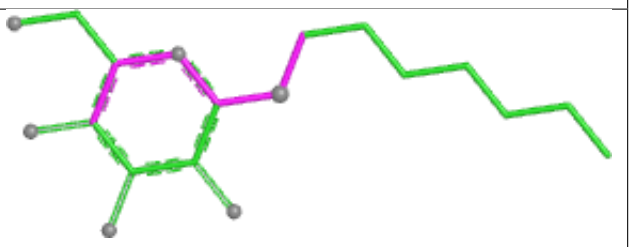


Rings

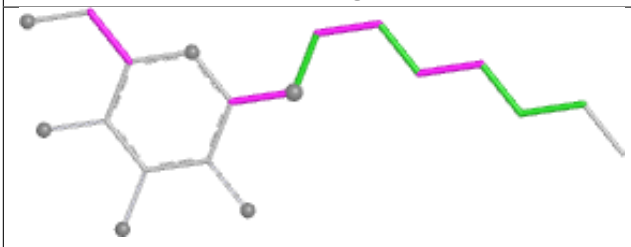
Ligand HTG C 521



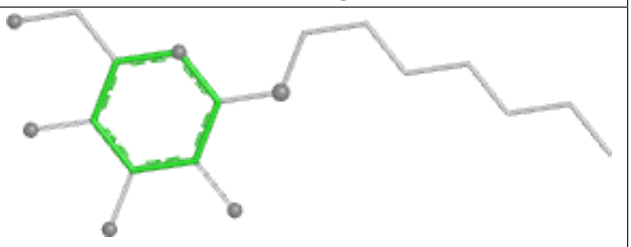
Bond lengths



Bond angles

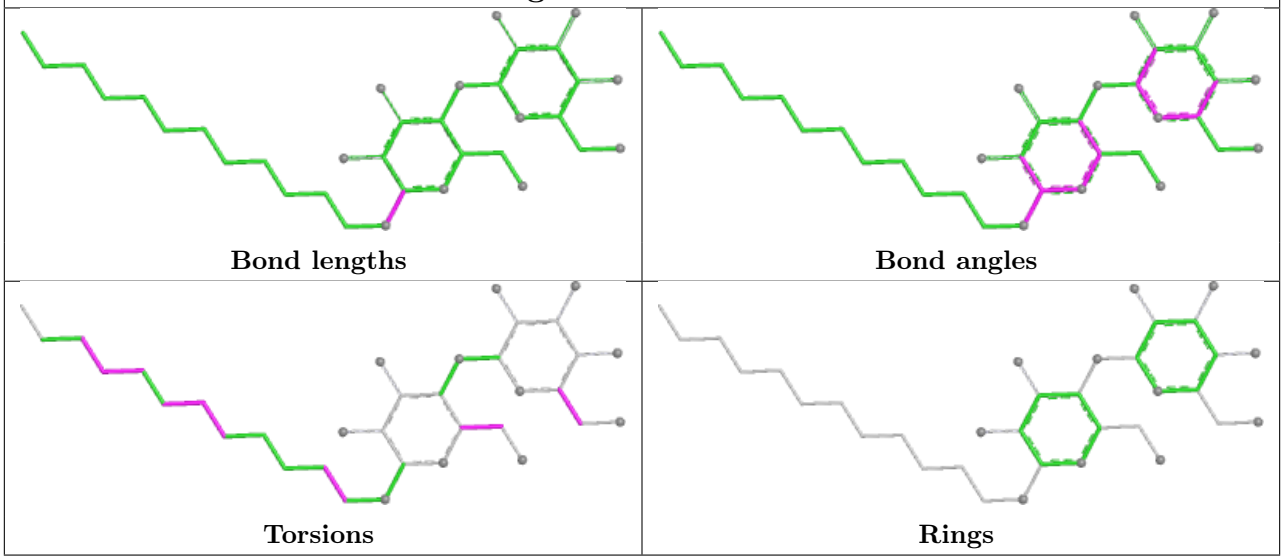


Torsions

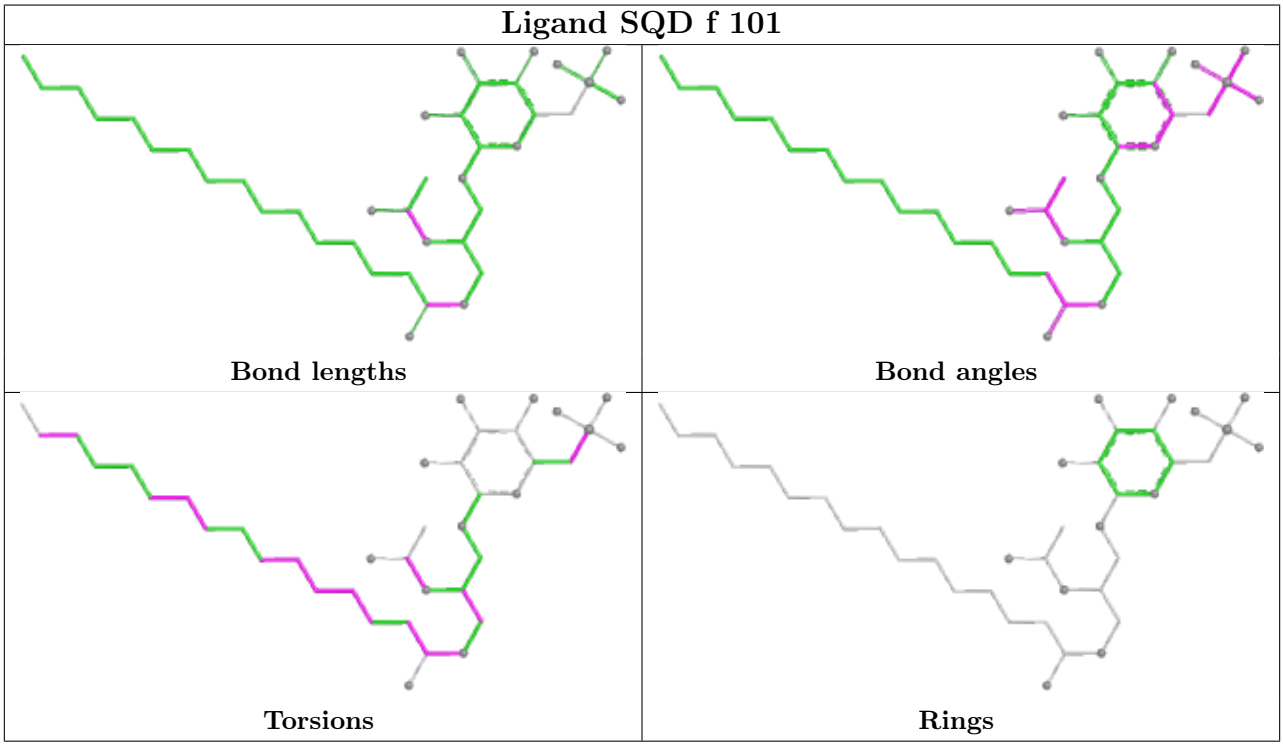


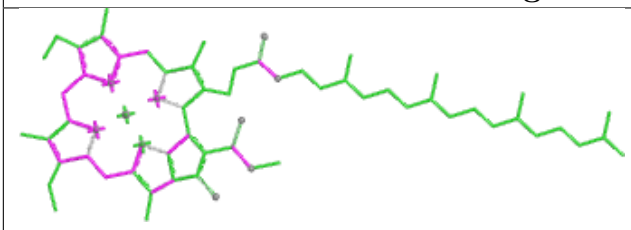
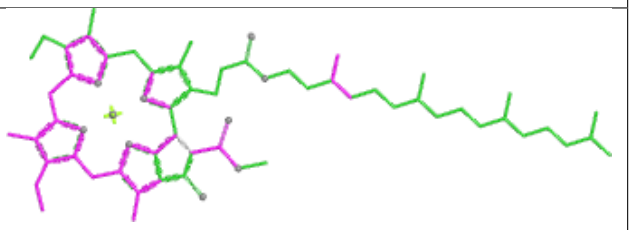
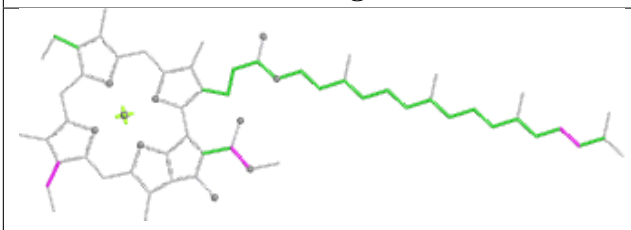
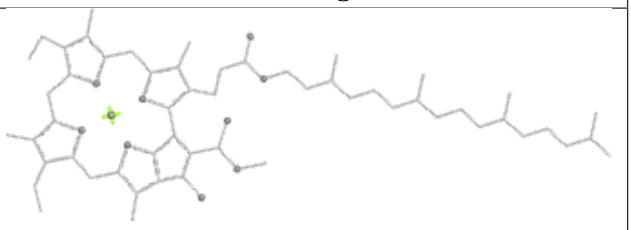
Rings

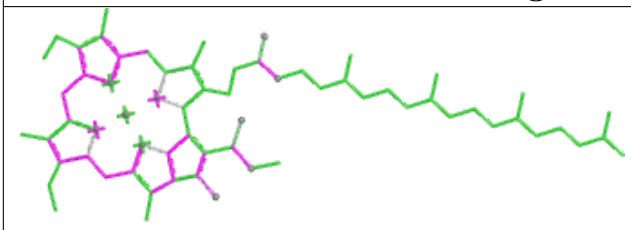
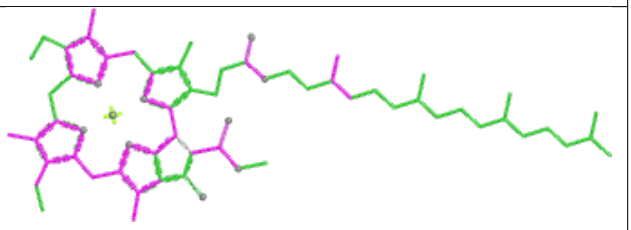
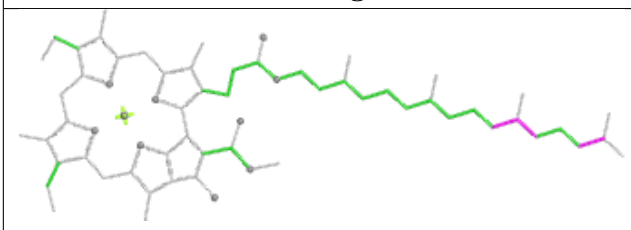
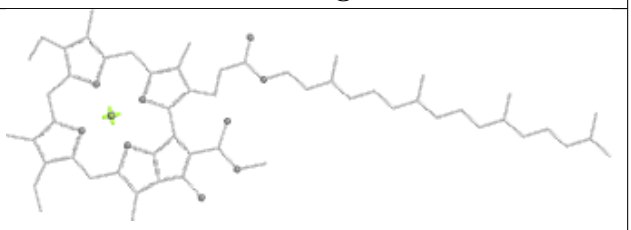
Ligand LMT c 523



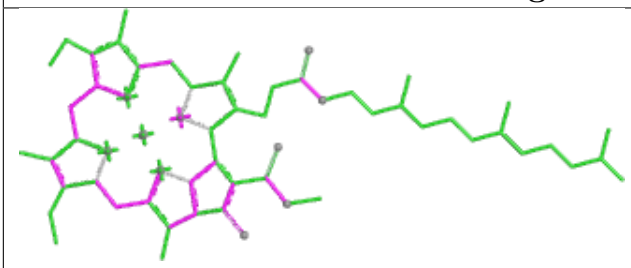
Ligand SQD f 101



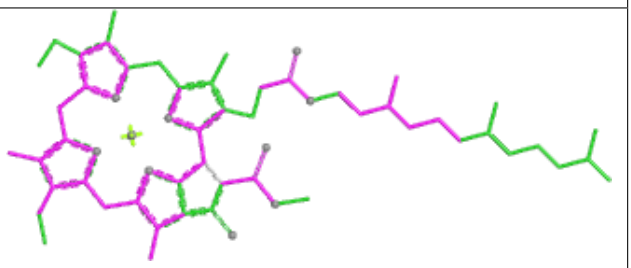
Ligand CLA D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

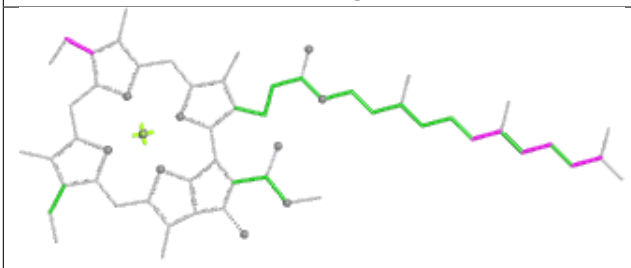
Ligand CLA a 404



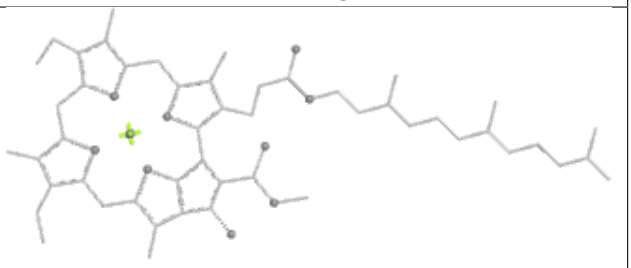
Bond lengths



Bond angles

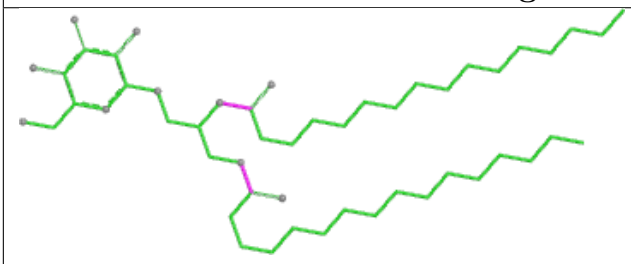


Torsions

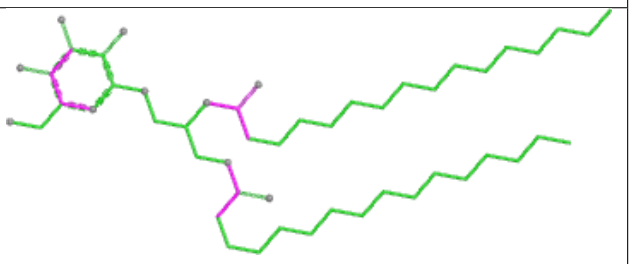


Rings

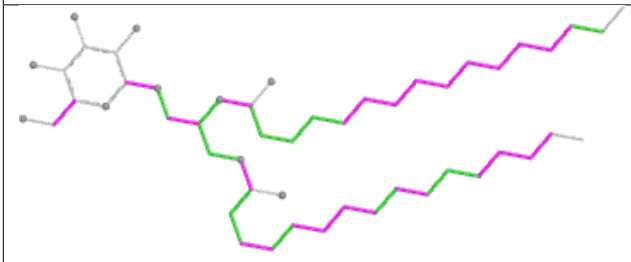
Ligand DGD D 406



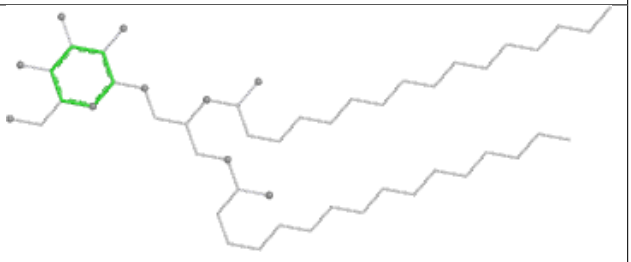
Bond lengths



Bond angles

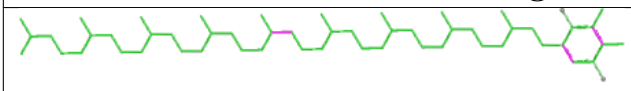


Torsions

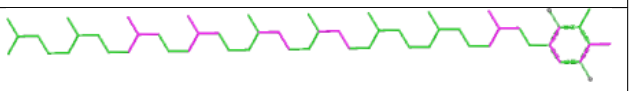


Rings

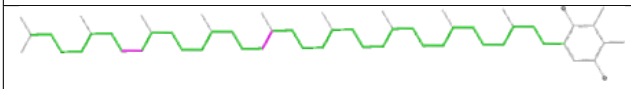
Ligand PL9 D 412



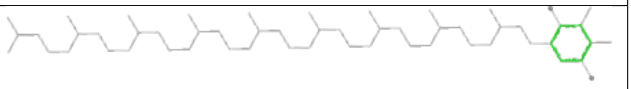
Bond lengths



Bond angles

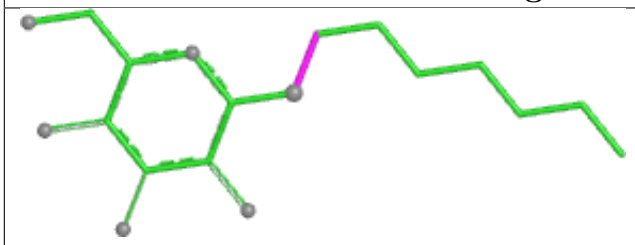


Torsions

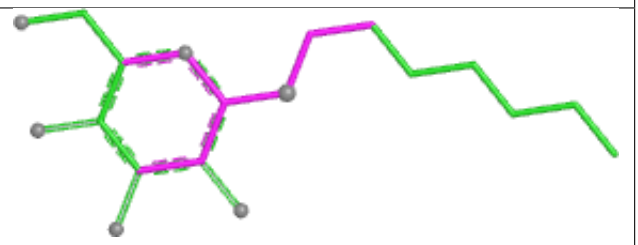


Rings

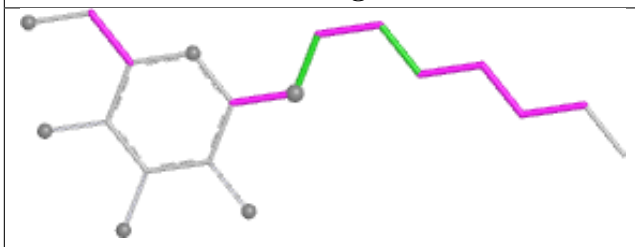
Ligand HTG d 401



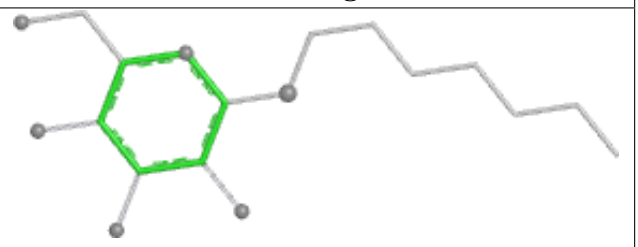
Bond lengths



Bond angles

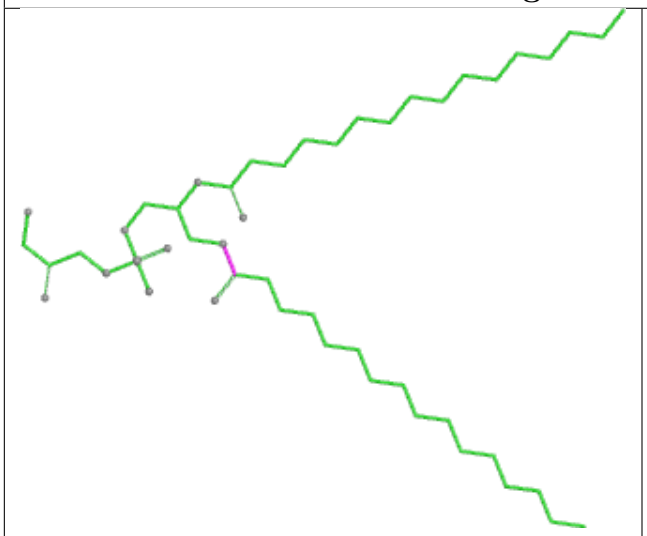


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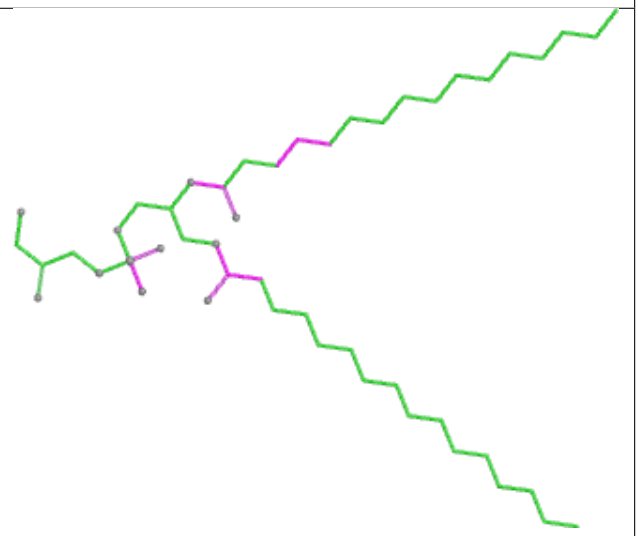


Rings

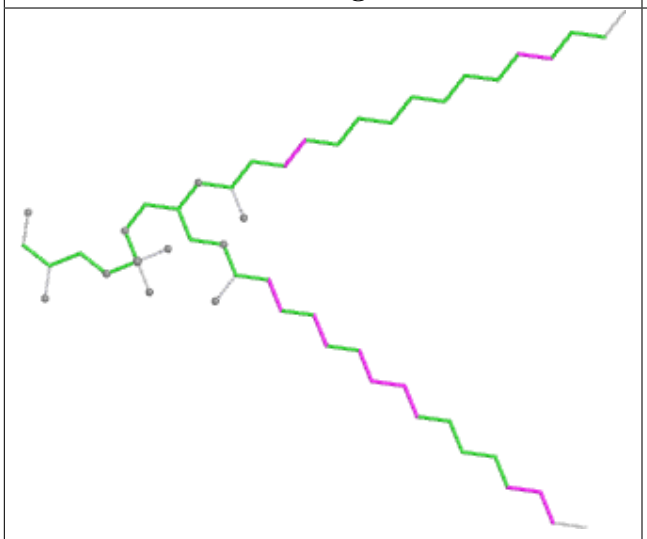
Ligand LHG D 407



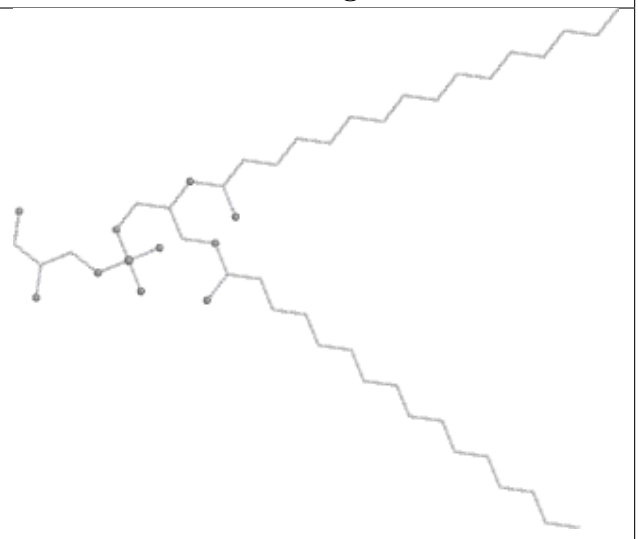
Bond lengths



Bond angles

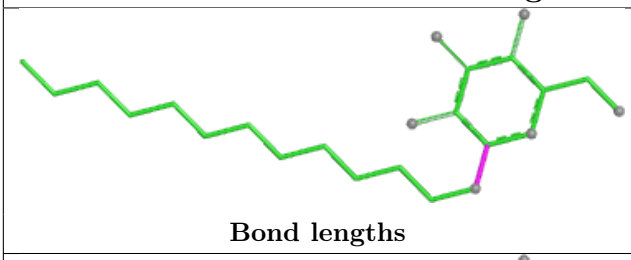


Torsions

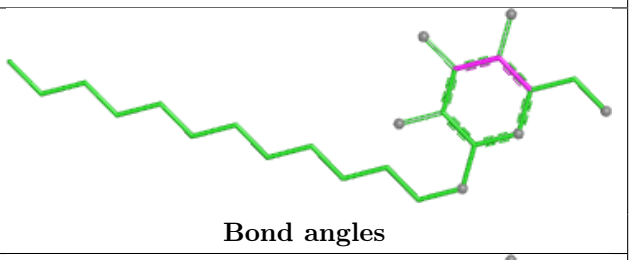


Rings

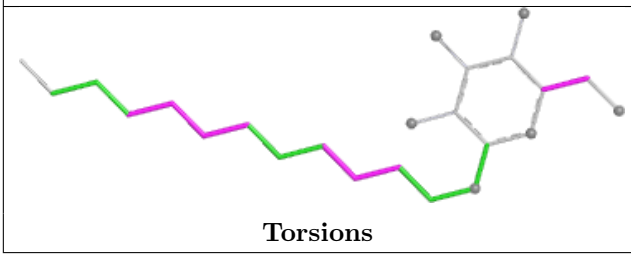
Ligand LMT J 103



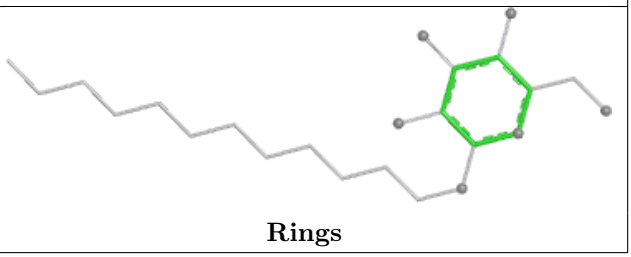
Bond lengths



Bond angles

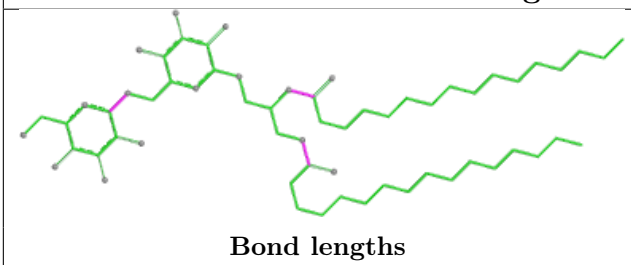


Torsions

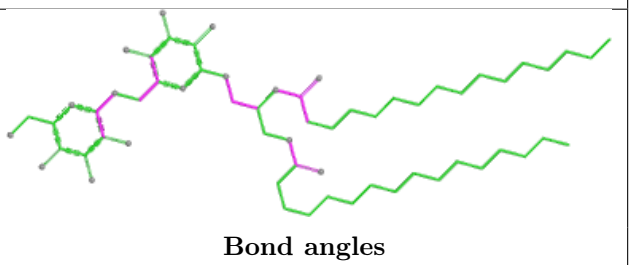


Rings

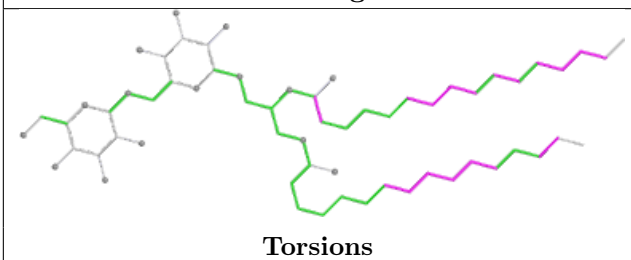
Ligand DGD h 101



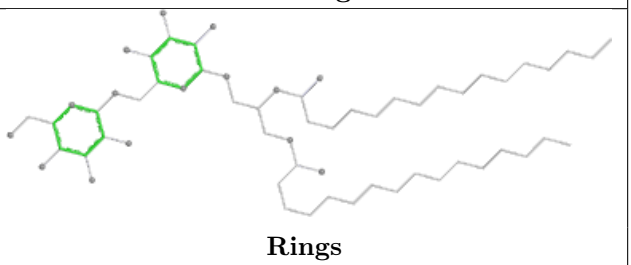
Bond lengths



Bond angles

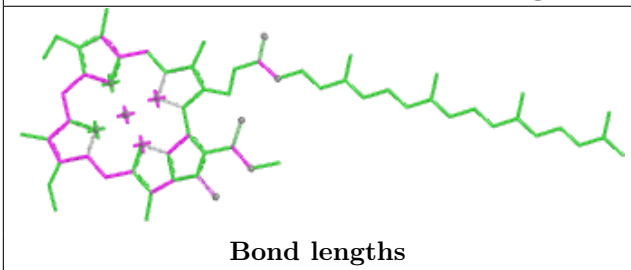


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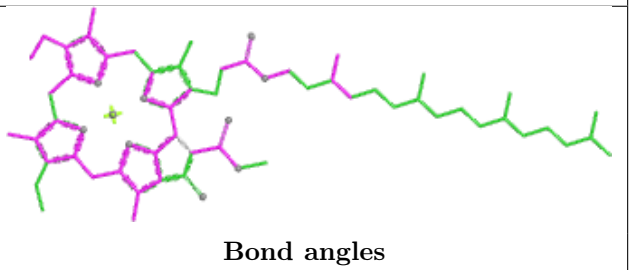


Rings

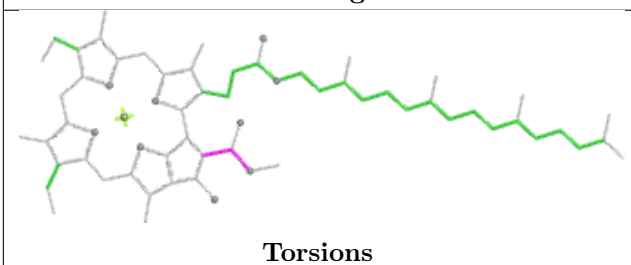
Ligand CLA c 501



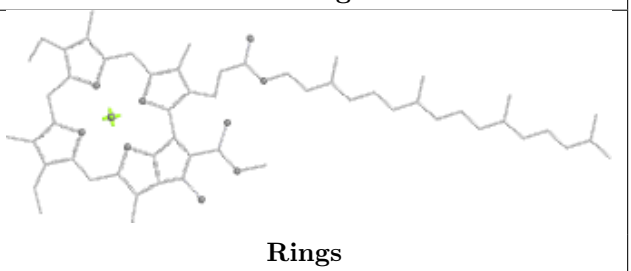
Bond lengths



Bond angles

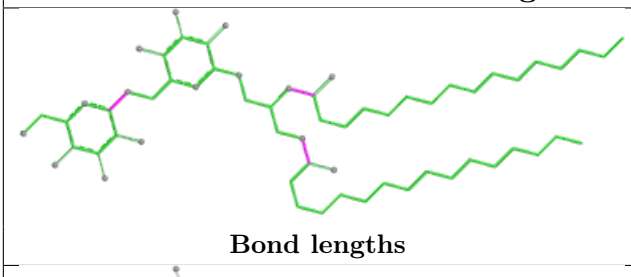


Torsions

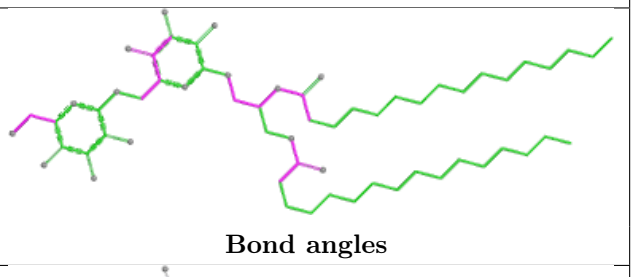


Rings

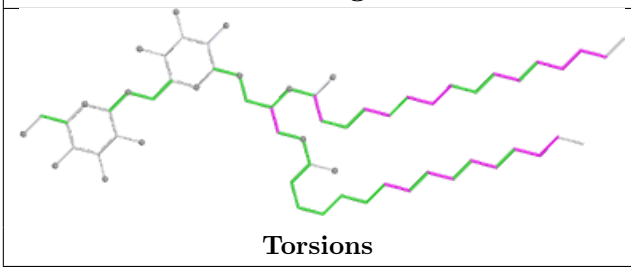
Ligand DGD H 102



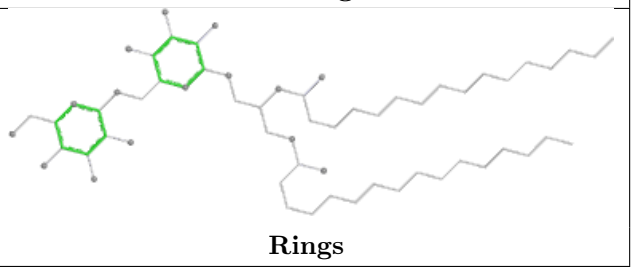
Bond lengths



Bond angles

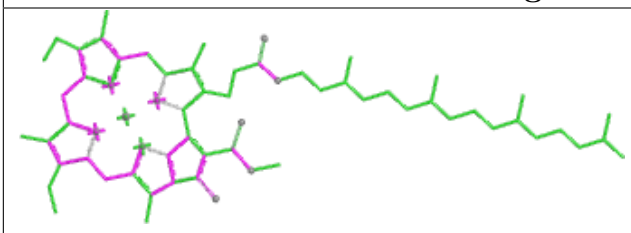


Torsions

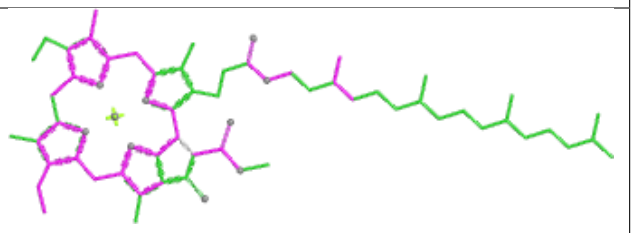


Rings

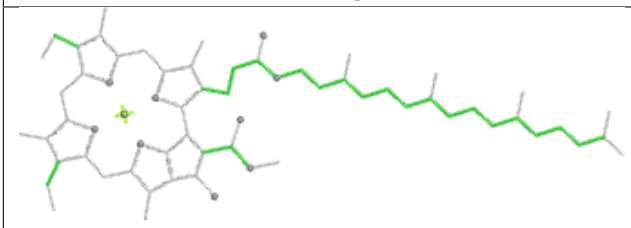
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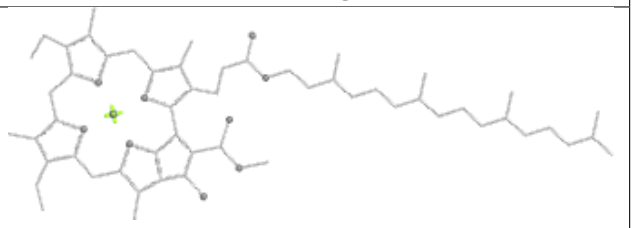
Bond lengths



Bond angles

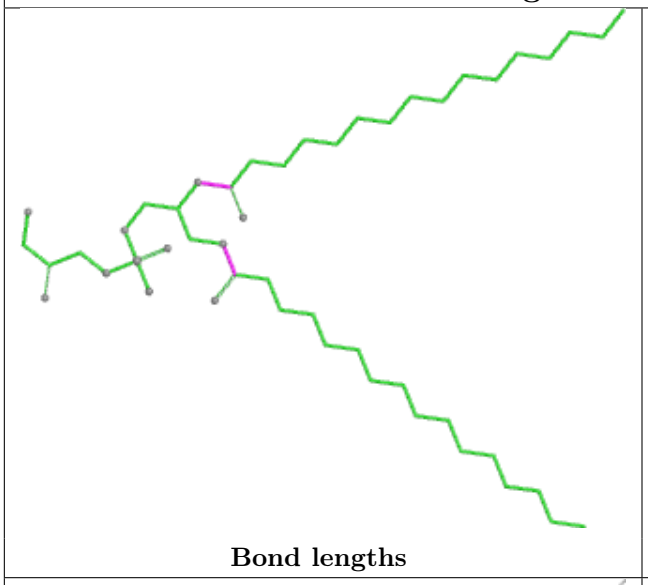


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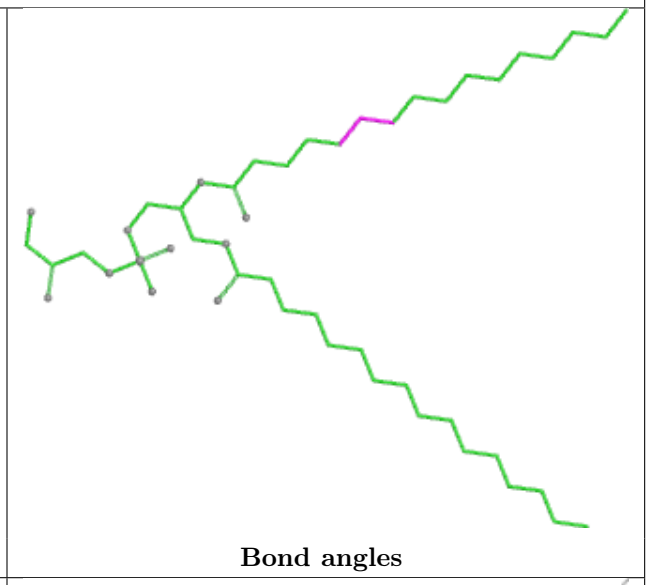


Rings

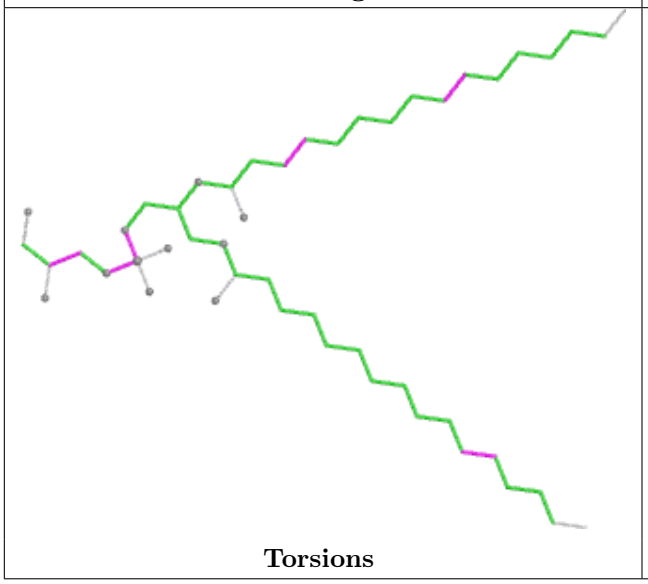
Ligand LHG D 408



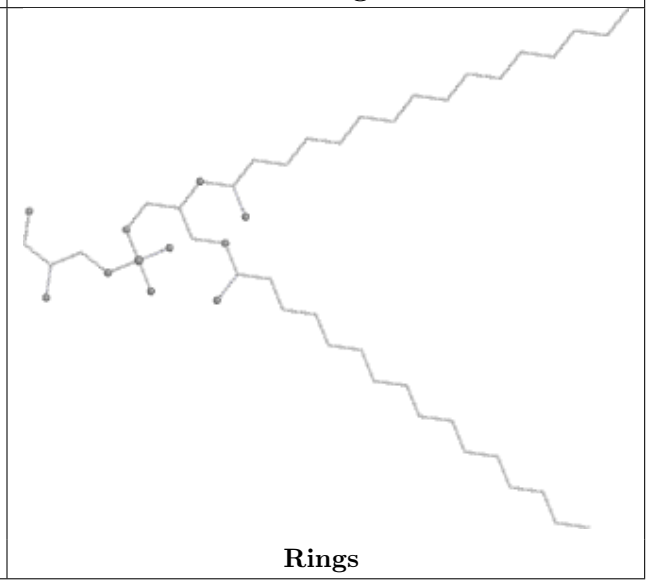
Bond lengths



Bond angles

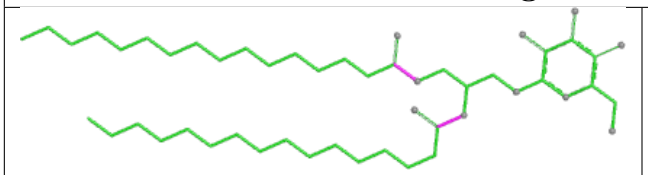


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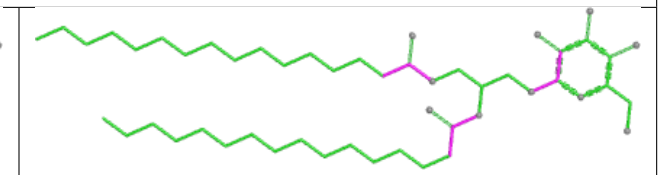


Rings

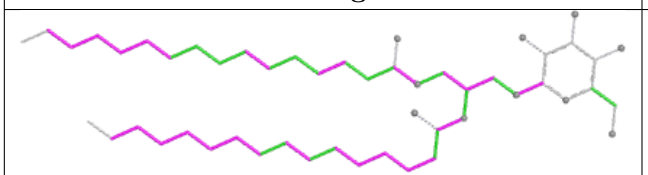
Ligand LMG A 407



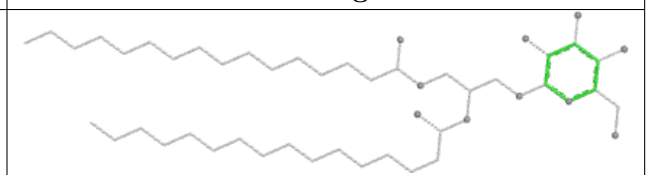
Bond lengths



Bond angles

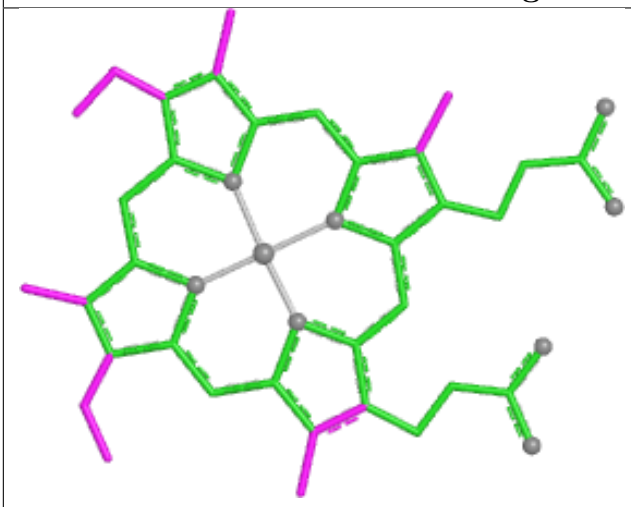


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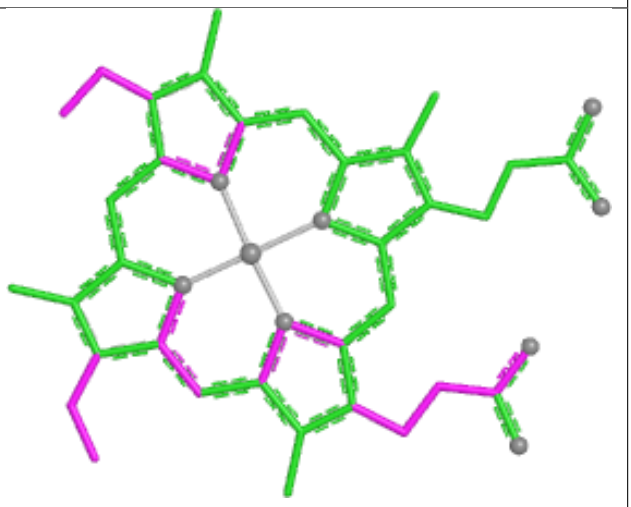


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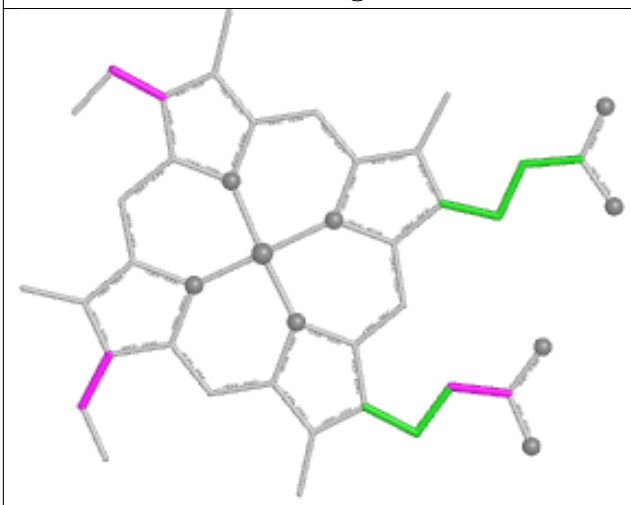
Ligand HEC V 201



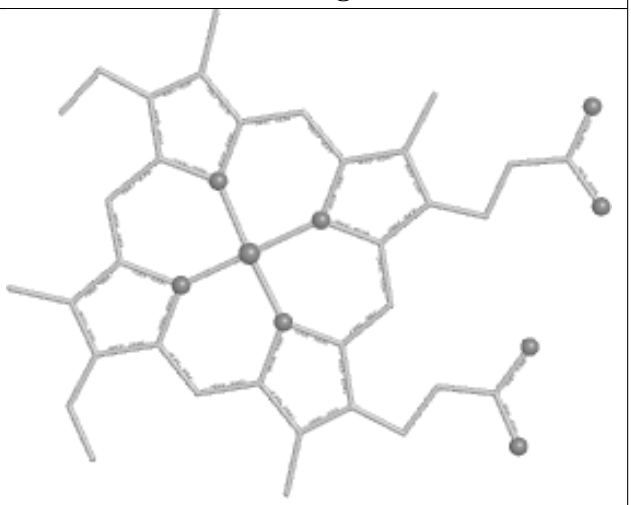
Bond lengths



Bond angles

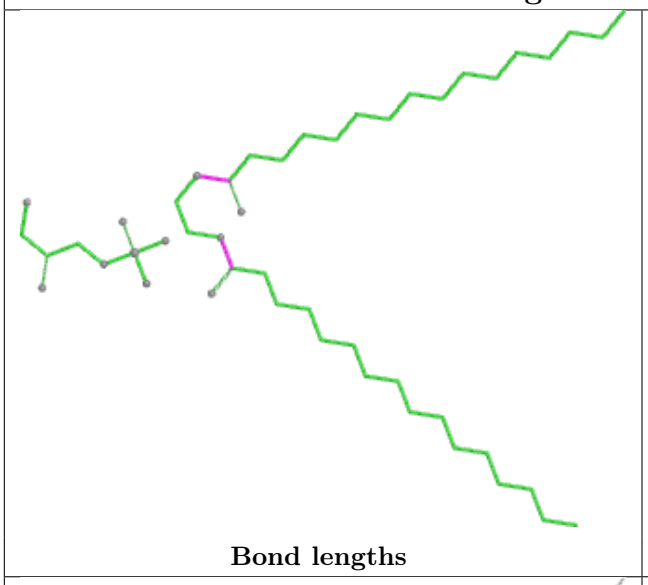


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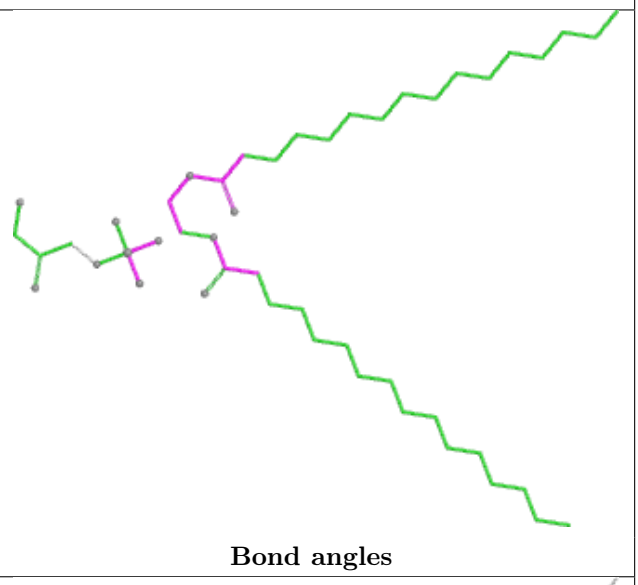


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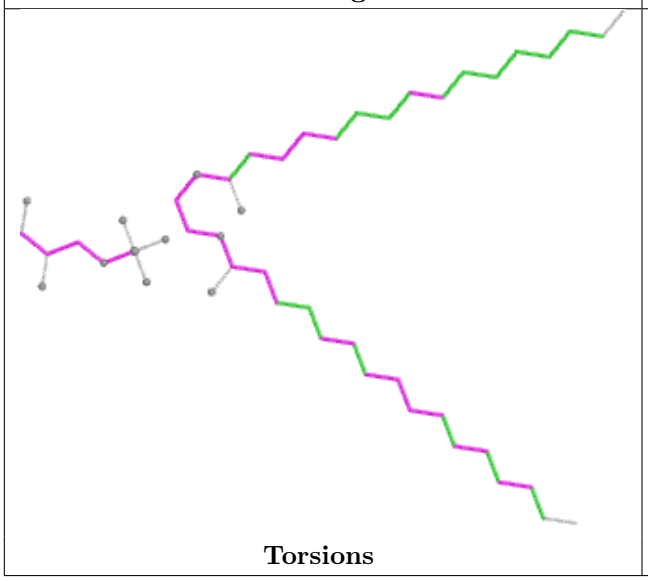
Ligand LHG E 103



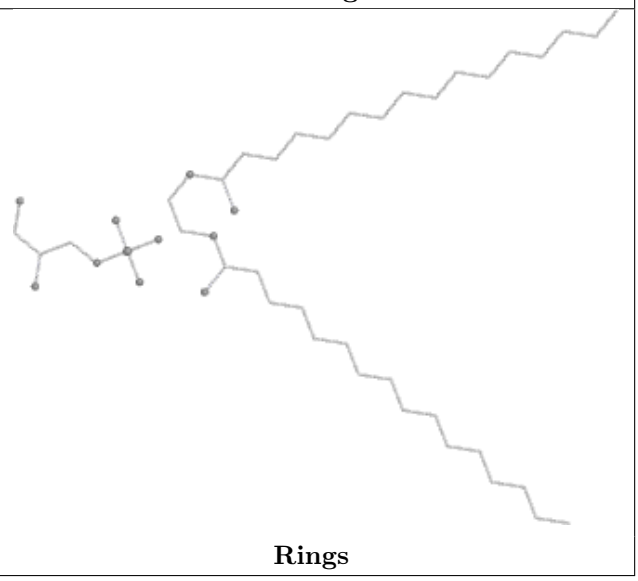
Bond lengths



Bond angles

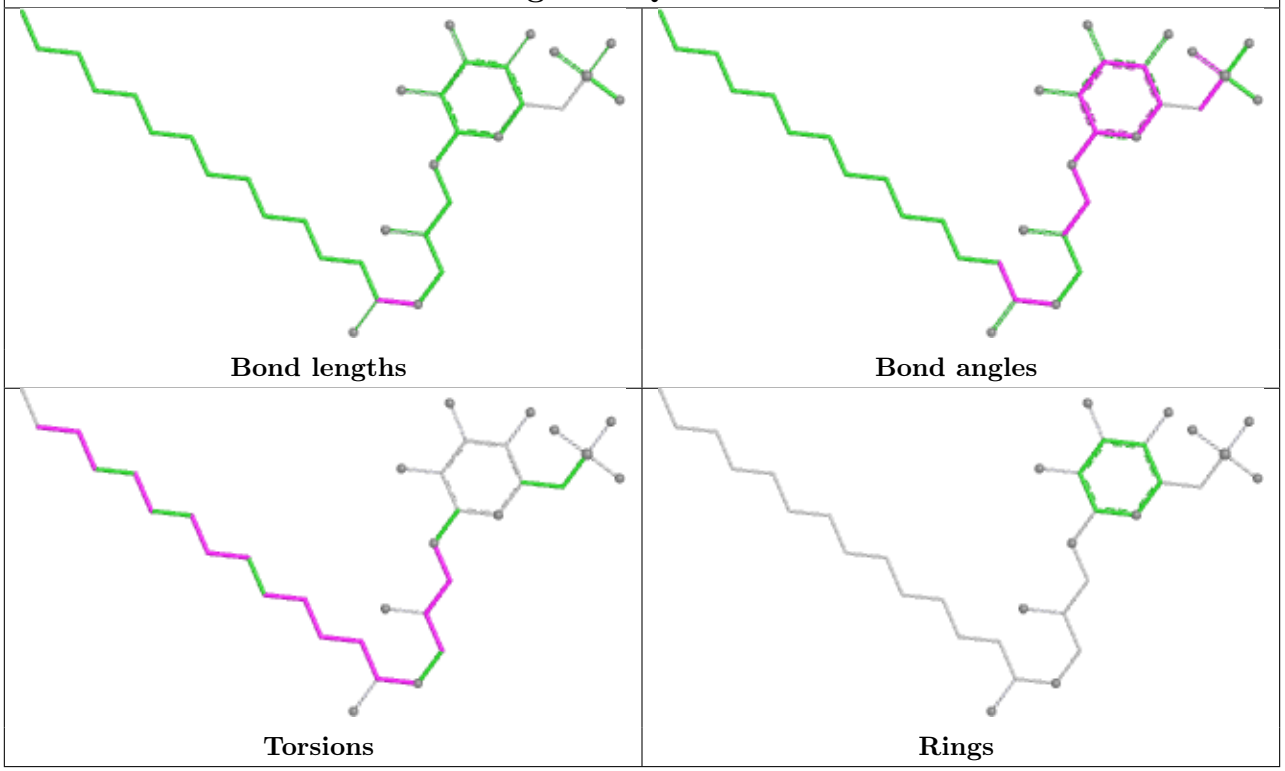


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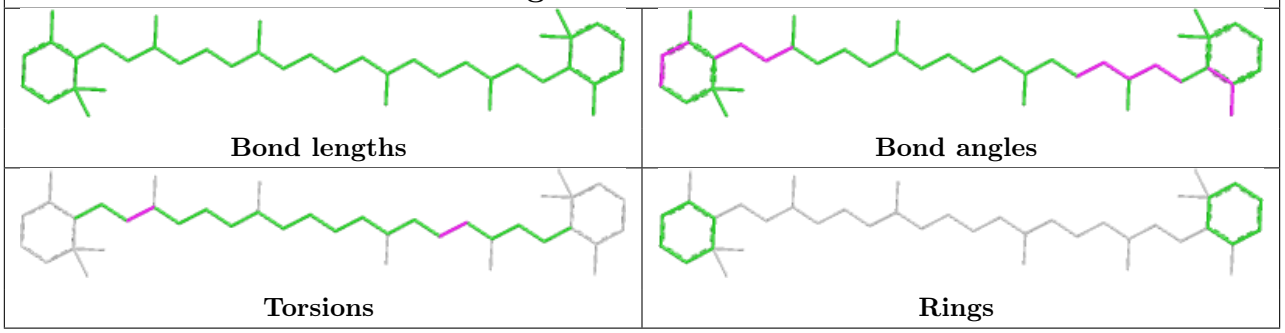


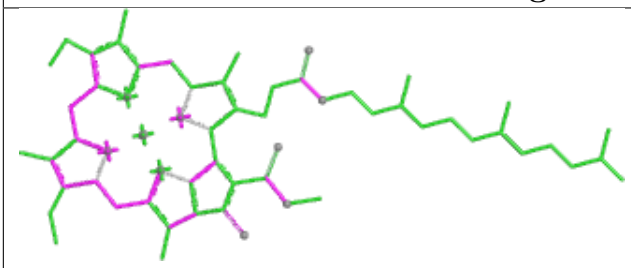
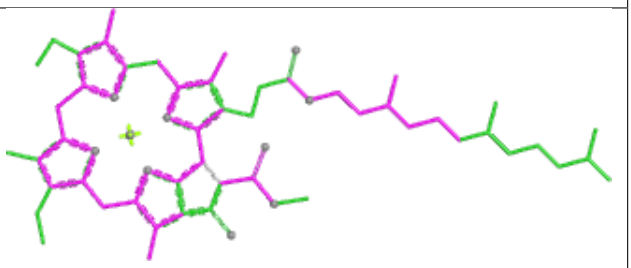
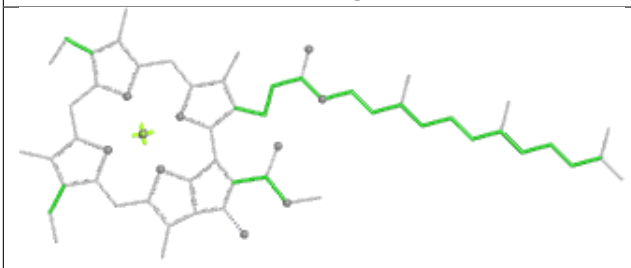
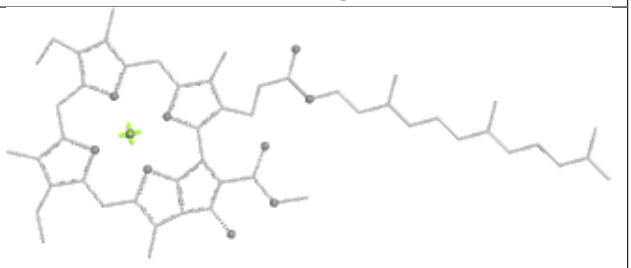
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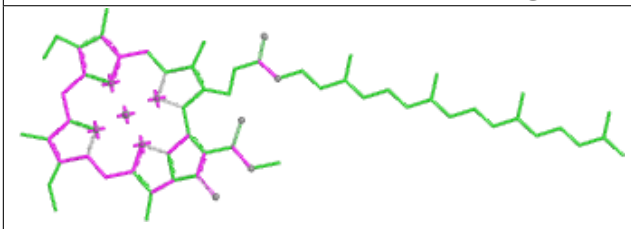
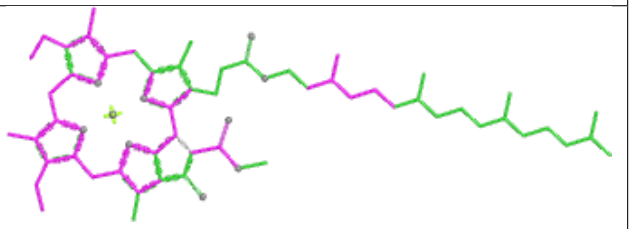
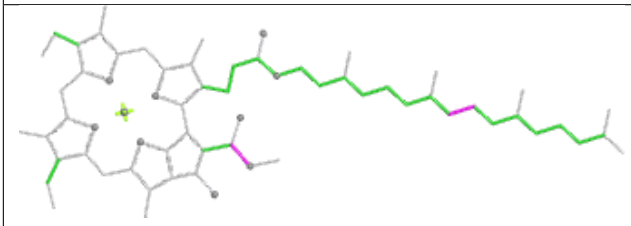
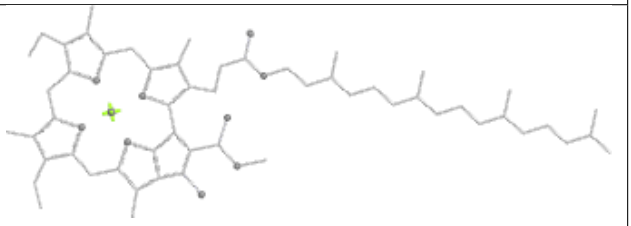
Ligand SQD F 101



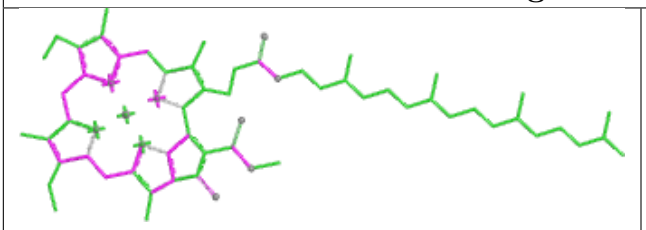
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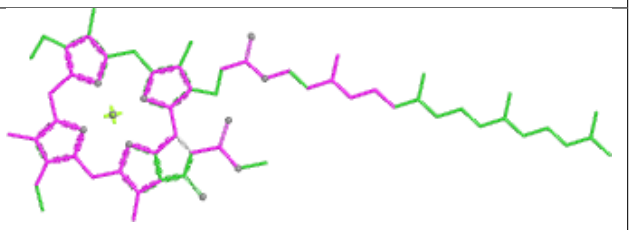
Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

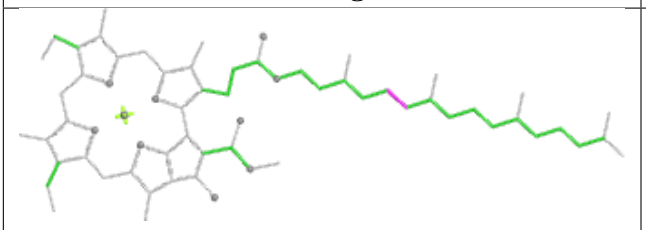
Ligand CLA b 605



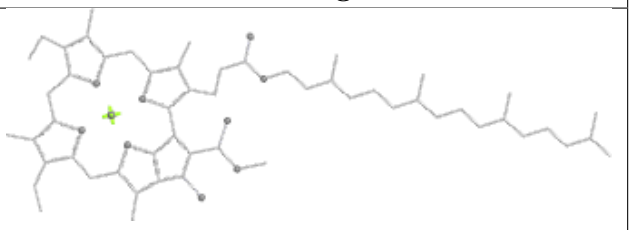
Bond lengths



Bond angles

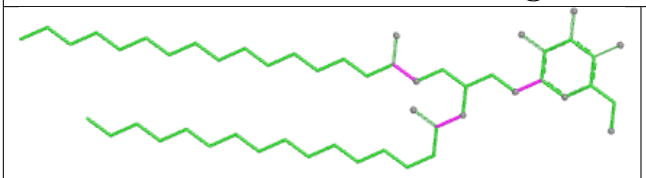


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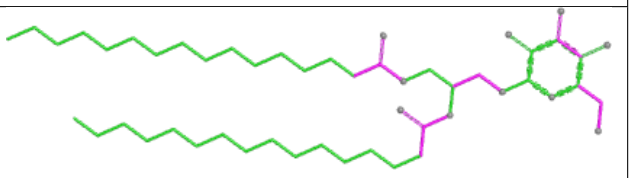


Rings

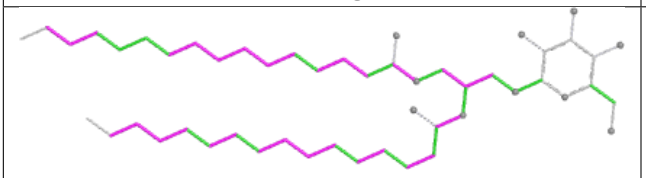
Ligand LMG c 519



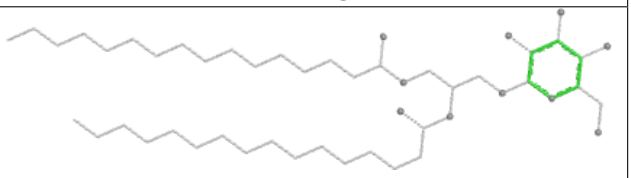
Bond lengths



Bond angles

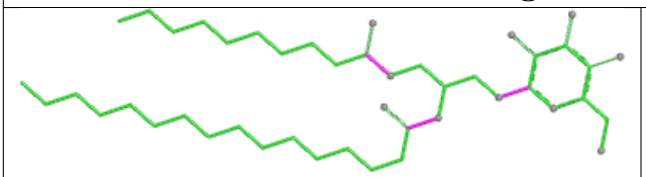


Torsions



Rings

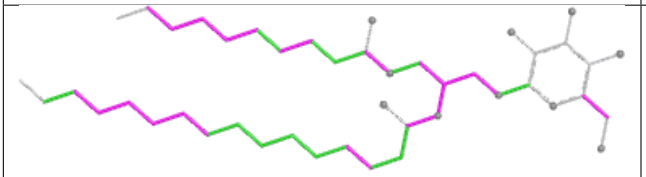
Ligand LMG C 524



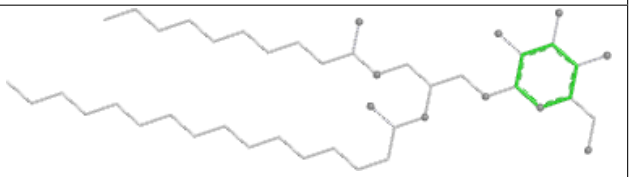
Bond lengths



Bond angles

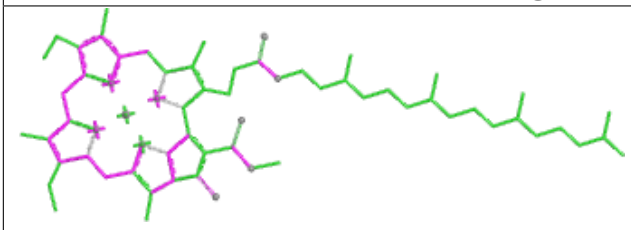


Torsions

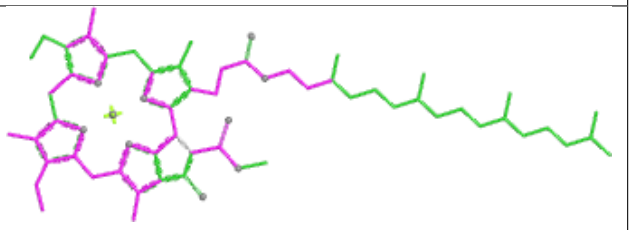


Rings

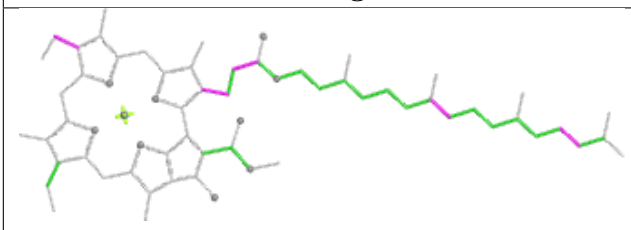
Ligand CLA c 512



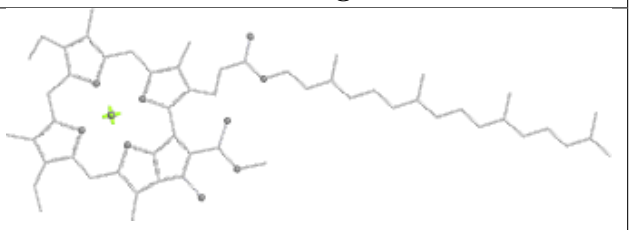
Bond lengths



Bond angles

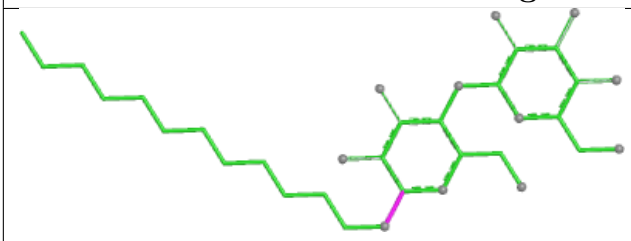


Torsions

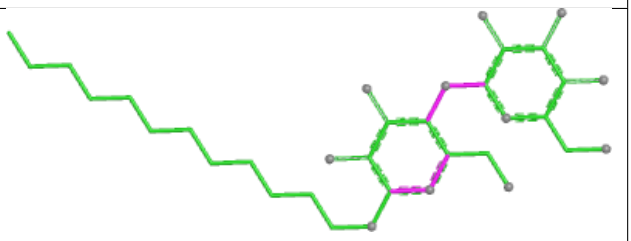


Rings

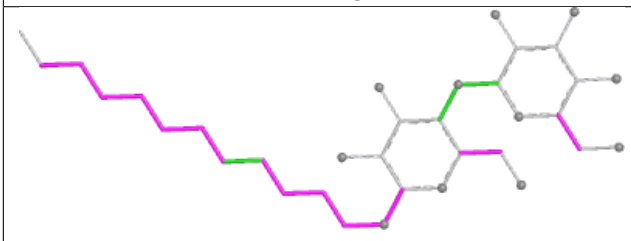
Ligand LMT m 101



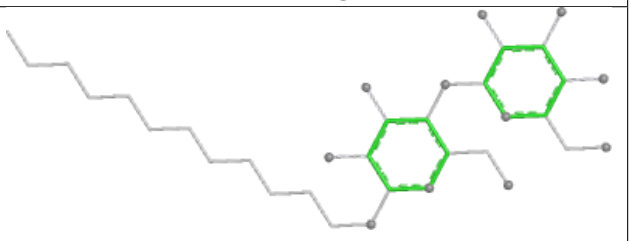
Bond lengths



Bond angles



Torsions

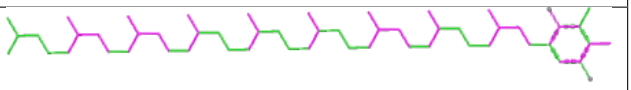


Rings

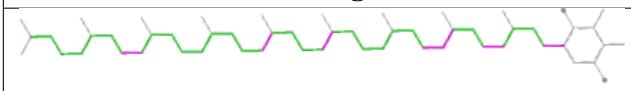
Ligand PL9 a 415



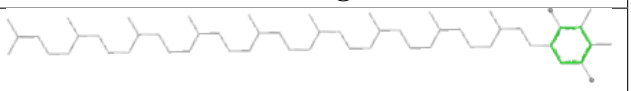
Bond lengths



Bond angles

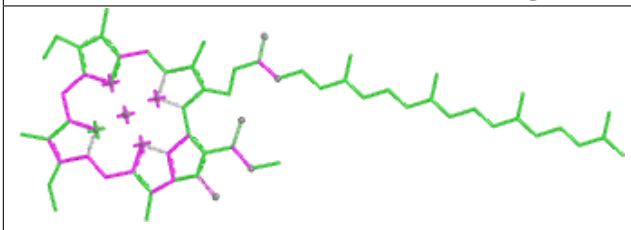


Torsions

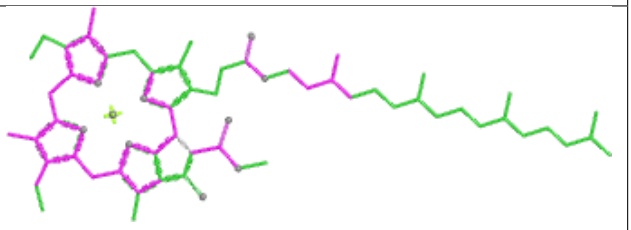


Rings

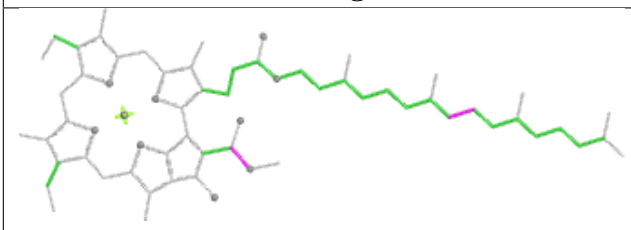
Ligand CLA C 510



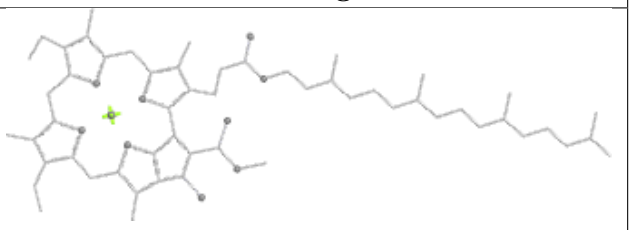
Bond lengths



Bond angles

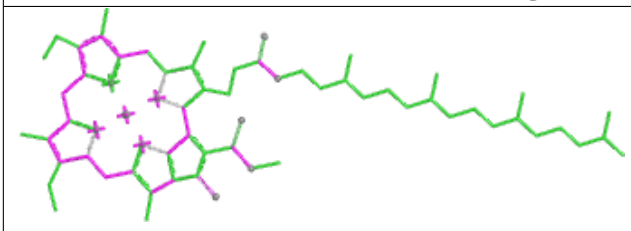


Torsions

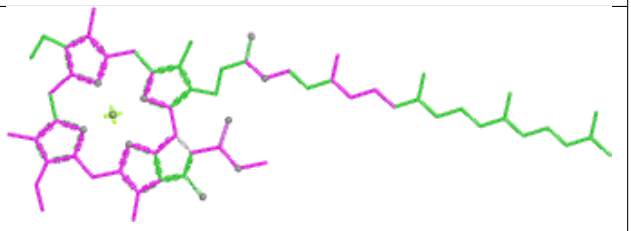


Rings

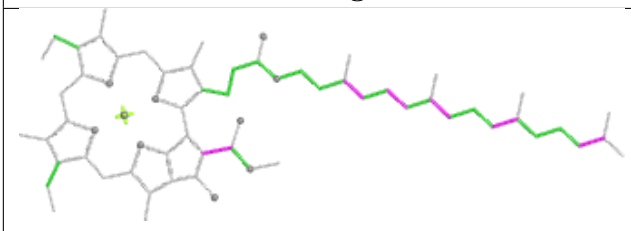
Ligand CLA C 507



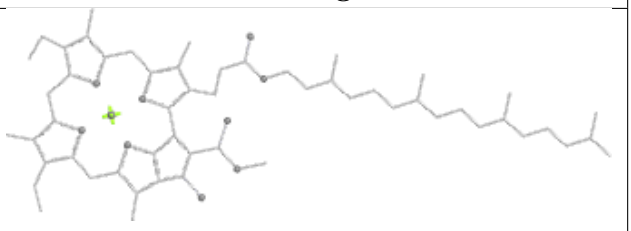
Bond lengths



Bond angles

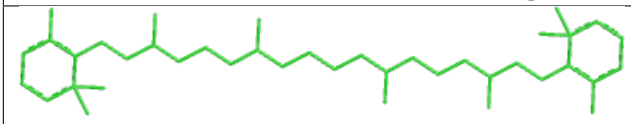


Torsions

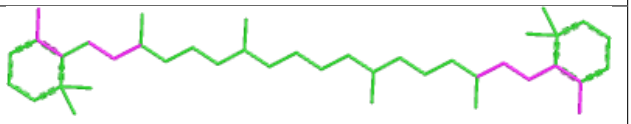


Rings

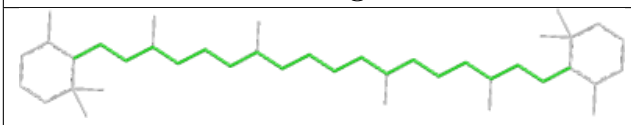
Ligand BCR C 515



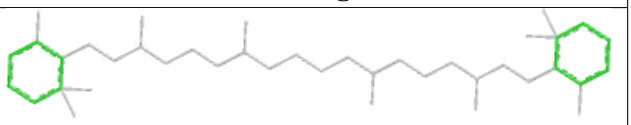
Bond lengths



Bond angles

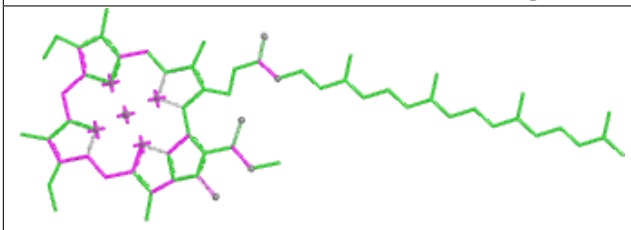


Torsions

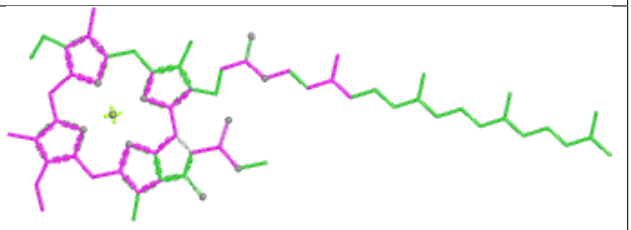


Rings

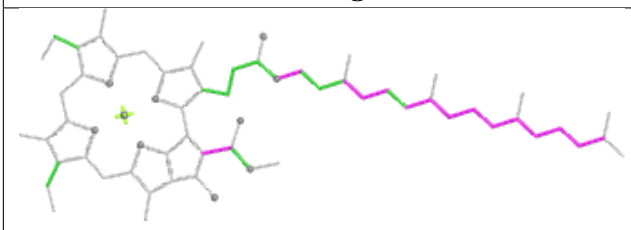
Ligand CLA B 601



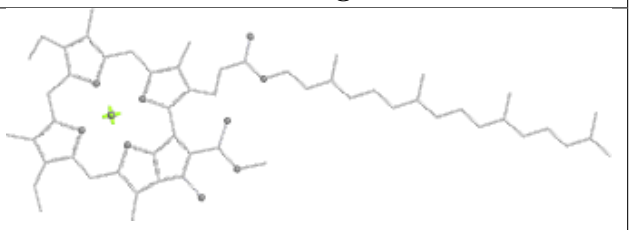
Bond lengths



Bond angles

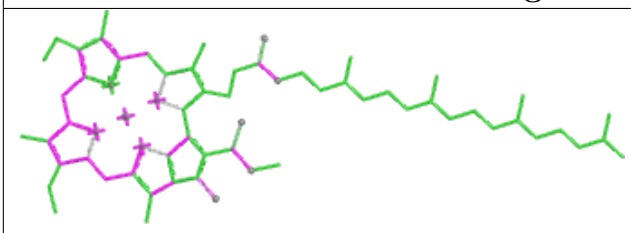


Torsions

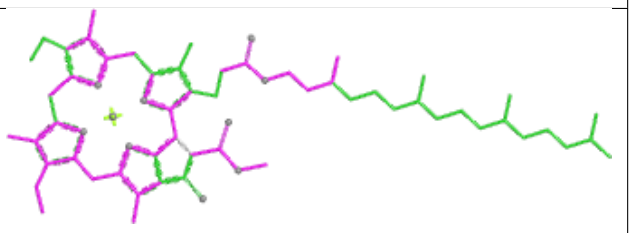


Rings

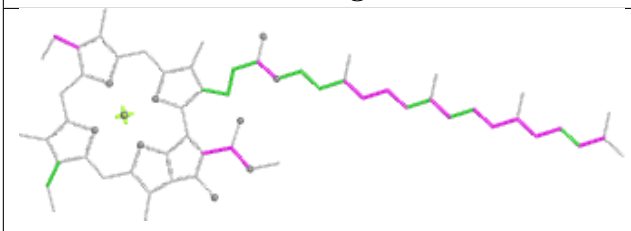
Ligand CLA B 602



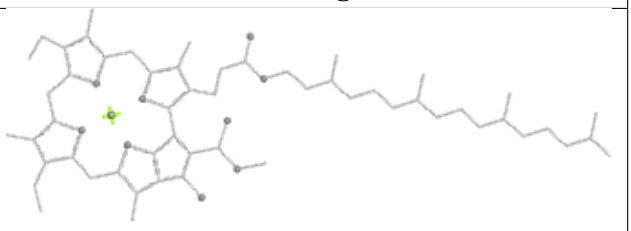
Bond lengths



Bond angles

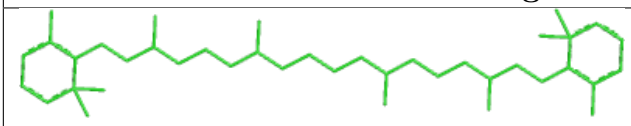


Torsions

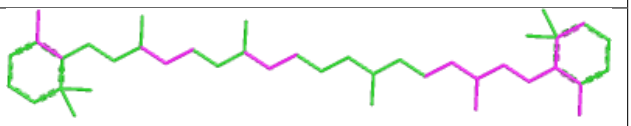


Rings

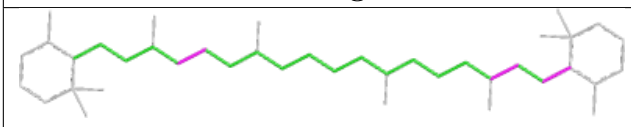
Ligand BCR C 514



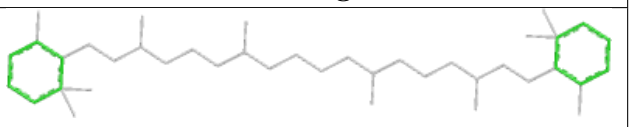
Bond lengths



Bond angles

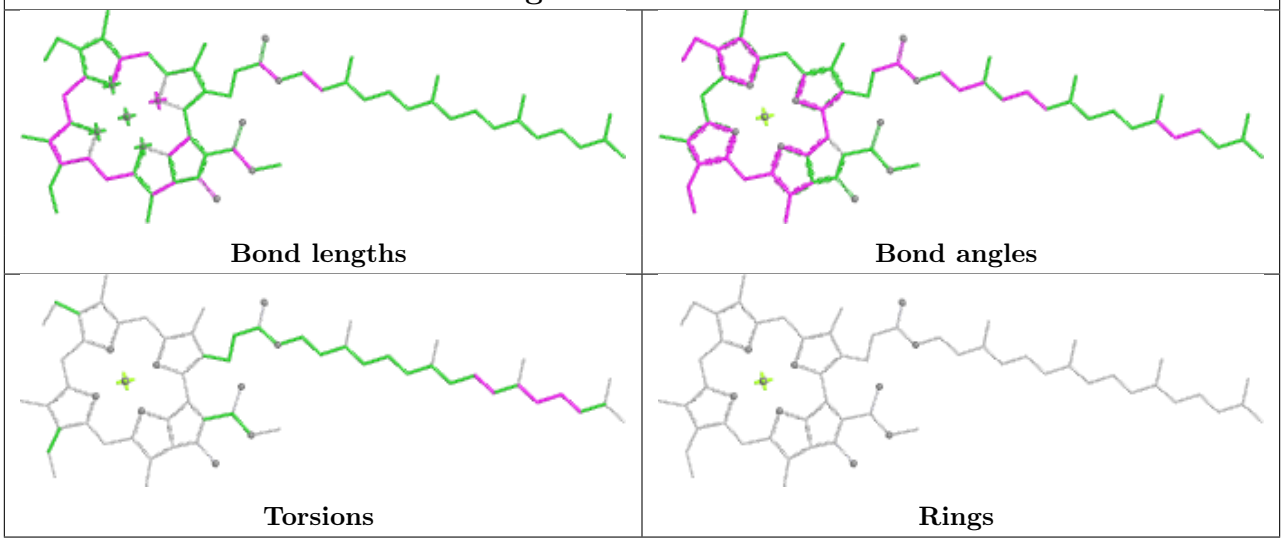


Torsions

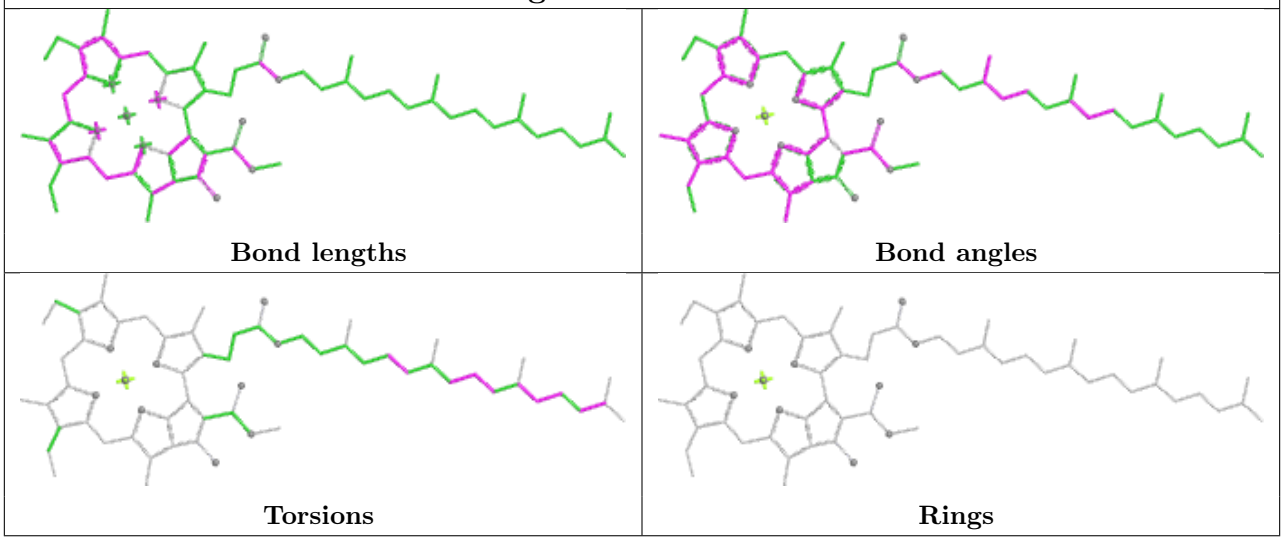


Rings

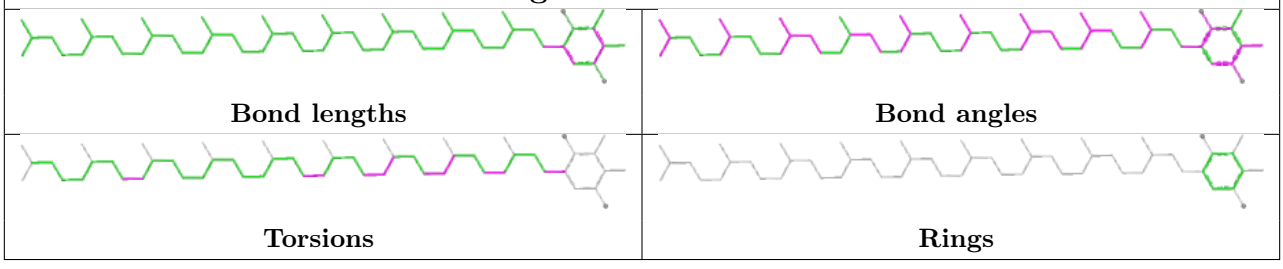
Ligand CLA B 614



Ligand CLA b 617



Ligand PL9 A 411



5.7 Other polymers

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%)	-0.66	2 (0%) 85 88	15, 23, 46, 68	3 (0%)
1	a	334/344 (97%)	-0.64	0 100 100	14, 23, 48, 78	4 (1%)
2	B	505/505 (100%)	-0.49	10 (1%) 65 68	15, 28, 54, 85	11 (2%)
2	b	495/505 (98%)	-0.42	13 (2%) 57 61	16, 27, 53, 95	4 (0%)
3	C	451/455 (99%)	-0.31	1 (0%) 91 93	21, 33, 49, 83	1 (0%)
3	c	455/455 (100%)	-0.34	0 100 100	22, 33, 46, 79	1 (0%)
4	D	342/342 (100%)	-0.66	1 (0%) 90 92	17, 24, 44, 90	1 (0%)
4	d	342/342 (100%)	-0.72	1 (0%) 90 92	18, 25, 42, 86	0
5	E	78/83 (93%)	0.44	6 (7%) 19 20	28, 47, 75, 87	1 (1%)
5	e	78/83 (93%)	0.20	2 (2%) 57 61	29, 43, 63, 81	2 (2%)
6	F	33/44 (75%)	-0.05	2 (6%) 27 29	28, 36, 63, 66	0
6	f	32/44 (72%)	-0.11	1 (3%) 51 55	28, 34, 72, 90	0
7	H	64/65 (98%)	0.07	2 (3%) 51 55	26, 36, 50, 78	1 (1%)
7	h	62/65 (95%)	-0.06	0 100 100	25, 36, 48, 58	1 (1%)
8	I	34/38 (89%)	-0.05	0 100 100	29, 36, 60, 78	0
8	i	35/38 (92%)	-0.14	0 100 100	29, 34, 47, 85	1 (2%)
9	J	36/40 (90%)	-0.01	1 (2%) 55 58	26, 41, 74, 90	0
9	j	40/40 (100%)	0.09	2 (5%) 34 37	27, 39, 56, 65	0
10	K	37/37 (100%)	-0.22	0 100 100	33, 40, 52, 59	0
10	k	37/37 (100%)	-0.06	0 100 100	32, 40, 56, 64	0
11	L	37/37 (100%)	-0.65	0 100 100	12, 22, 65, 81	1 (2%)
11	l	37/37 (100%)	-0.67	0 100 100	12, 22, 76, 91	1 (2%)
12	M	33/36 (91%)	-0.67	1 (3%) 52 56	15, 25, 39, 57	1 (3%)
12	m	34/36 (94%)	-0.64	0 100 100	16, 26, 53, 74	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.26	2 (0%) 82 86	17, 32, 56, 85	6 (2%)
13	o	243/244 (99%)	-0.21	2 (0%) 82 86	17, 35, 67, 89	2 (0%)
14	T	28/32 (87%)	-0.70	0 100 100	19, 23, 37, 54	1 (3%)
14	t	29/32 (90%)	-0.52	0 100 100	20, 23, 49, 74	0
15	U	97/104 (93%)	-0.38	0 100 100	22, 29, 49, 67	0
15	u	97/104 (93%)	-0.39	0 100 100	24, 29, 44, 75	0
16	V	137/137 (100%)	-0.55	0 100 100	17, 28, 43, 60	3 (2%)
16	v	137/137 (100%)	-0.18	0 100 100	25, 36, 53, 74	0
17	Y	29/30 (96%)	0.52	2 (6%) 23 25	41, 51, 72, 79	0
17	y	29/30 (96%)	0.30	0 100 100	41, 50, 66, 70	0
18	X	38/40 (95%)	0.38	1 (2%) 57 61	32, 42, 68, 72	0
18	x	35/40 (87%)	0.18	1 (2%) 53 57	33, 40, 63, 67	0
19	Z	62/62 (100%)	0.61	4 (6%) 25 27	38, 48, 86, 98	0
19	z	61/62 (98%)	0.88	6 (9%) 13 13	45, 54, 86, 96	0
All	All	5230/5350 (97%)	-0.36	63 (1%) 76 80	12, 30, 57, 98	47 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	5.1
7	H	65	LEU	4.9
2	b	495	PHE	4.3
2	b	499	VAL	4.3
2	b	502	VAL	3.9
19	Z	33	TRP	3.8
2	b	484	PRO	3.8
2	b	504	THR	3.6
5	e	61	ARG	3.4
19	z	61	VAL	3.4
5	E	73	LYS	3.3
2	B	495	PHE	3.2
5	e	83	LEU	3.0
3	C	23	ALA	3.0
7	H	64	ALA	3.0
2	B	486	LEU	2.9
5	E	80	LEU	2.9
19	z	36	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	494	GLY	2.9
2	b	503	THR	2.9
19	Z	32	ASP	2.9
13	O	60	ARG	2.8
6	f	14	PRO	2.8
19	z	33	TRP	2.7
2	b	491	VAL	2.6
2	B	479	PHE	2.6
2	b	479	PHE	2.6
17	Y	18	VAL	2.5
19	Z	30	PRO	2.5
1	A	262	TYR	2.5
2	B	500	GLY	2.5
2	b	500	GLY	2.5
5	E	79	PHE	2.4
2	b	497	GLN	2.4
17	Y	19	ILE	2.4
2	B	487	SER	2.4
5	E	4	THR	2.4
19	z	4	LEU	2.3
1	A	11	ALA	2.3
19	z	30	PRO	2.3
4	D	11	GLU	2.3
2	b	501	ASP	2.3
2	B	293	ALA	2.2
2	B	496	TYR	2.2
4	d	11	GLU	2.2
6	F	16	PHE	2.2
6	F	13	TYR	2.2
13	o	36	GLN	2.2
2	b	129	GLY	2.2
13	O	59	LYS	2.2
9	j	2	MET	2.1
2	B	499	VAL	2.1
18	X	2	THR	2.1
9	J	5	GLY	2.1
13	o	246	ALA	2.1
5	E	76	VAL	2.1
9	j	1	MET	2.1
18	x	2	THR	2.1
19	z	2	THR	2.1
2	B	501	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	61	ARG	2.1
19	Z	35	ARG	2.1
12	M	33	GLN	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	0.96	0.06	23,27,49,50	0
14	FME	T	1	10/11	0.97	0.06	23,29,48,51	0
8	FME	i	1	10/11	0.98	0.06	30,31,34,35	0
8	FME	I	1	10/11	0.98	0.05	26,32,36,37	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
26	UNL	b	642	13/-	0.59	0.14	71,80,87,90	0
35	DGD	D	406	51/66	0.62	0.16	57,74,100,108	0
26	UNL	B	646	16/-	0.64	0.14	85,89,93,94	0
28	DMS	j	105	4/4	0.66	0.18	70,74,75,88	0
26	UNL	B	629	10/-	0.66	0.15	54,69,74,74	0
28	DMS	O	308	4/4	0.67	0.17	66,74,76,87	0
26	UNL	Z	102	4/-	0.67	0.20	59,61,62,63	0
32	HTG	C	534	19/19	0.67	0.14	68,110,128,130	0
26	UNL	b	643	9/-	0.67	0.12	67,67,74,74	0
28	DMS	b	638	4/4	0.68	0.20	67,75,77,86	0
28	DMS	o	306	4/4	0.68	0.19	55,58,65,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	LMT	f	102	24/35	0.69	0.15	62,77,94,98	0
28	DMS	U	904	4/4	0.69	0.18	58,66,66,83	0
28	DMS	O	305	4/4	0.70	0.22	64,66,77,86	0
32	HTG	D	417	19/19	0.70	0.15	67,105,119,120	0
28	DMS	B	636	4/4	0.71	0.17	77,86,90,96	0
28	DMS	O	309	4/4	0.71	0.23	58,65,72,73	0
35	DGD	d	416	51/66	0.71	0.14	56,75,96,103	0
28	DMS	H	103	4/4	0.72	0.21	84,101,109,112	0
26	UNL	B	647	13/-	0.72	0.13	71,81,90,91	0
28	DMS	b	640	4/4	0.72	0.18	49,58,71,73	0
26	UNL	A	413	4/-	0.72	0.13	64,64,64,66	0
26	UNL	a	402	6/-	0.72	0.14	50,57,62,63	0
32	HTG	v	210	14/19	0.73	0.16	60,80,92,100	0
26	UNL	T	103	13/-	0.73	0.13	64,68,72,72	0
26	UNL	a	414	28/-	0.73	0.14	59,68,84,87	0
32	HTG	c	521	19/19	0.73	0.14	57,85,102,105	0
26	UNL	b	645	6/-	0.74	0.16	57,65,76,76	0
26	UNL	h	103	16/-	0.74	0.14	61,69,73,76	0
32	HTG	c	520	19/19	0.74	0.15	77,88,99,100	0
26	UNL	A	410	36/-	0.74	0.15	57,78,84,91	0
26	UNL	c	526	8/-	0.75	0.17	54,59,64,65	0
28	DMS	D	415	4/4	0.75	0.23	57,58,63,65	0
34	LMT	I	101	35/35	0.75	0.13	67,82,91,92	0
28	DMS	O	310	4/4	0.76	0.19	76,78,82,94	0
26	UNL	E	102	15/-	0.76	0.17	55,62,76,77	0
28	DMS	o	308	4/4	0.76	0.19	60,61,62,63	0
34	LMT	b	627	32/35	0.77	0.14	42,67,84,87	0
26	UNL	J	107	3/-	0.77	0.12	61,61,63,64	0
32	HTG	b	602	19/19	0.77	0.13	51,103,117,118	0
28	DMS	b	641	4/4	0.77	0.20	63,65,75,80	0
36	LHG	E	103	48/49	0.77	0.15	44,99,108,119	0
34	LMT	E	101	24/35	0.78	0.12	64,78,84,90	0
26	UNL	I	105	10/-	0.78	0.10	60,66,71,72	0
26	UNL	I	106	11/-	0.78	0.17	61,73,81,81	0
26	UNL	B	633	16/-	0.78	0.16	53,61,69,70	0
26	UNL	I	104	11/-	0.78	0.13	53,56,59,62	0
32	HTG	u	201	8/19	0.78	0.17	45,52,69,89	0
26	UNL	j	104	16/-	0.78	0.14	49,58,64,66	0
32	HTG	B	623	19/19	0.79	0.12	53,88,93,94	0
26	UNL	J	104	14/-	0.79	0.13	67,77,80,81	0
26	UNL	I	103	13/-	0.79	0.14	47,53,84,87	0
26	UNL	H	104	4/-	0.79	0.14	60,62,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	LMT	c	523	35/35	0.79	0.12	67,77,83,85	0
26	UNL	t	102	16/-	0.79	0.12	61,71,80,80	0
26	UNL	c	524	30/-	0.79	0.14	59,74,86,87	0
32	HTG	d	401	19/19	0.79	0.14	58,99,111,120	0
26	UNL	c	525	10/-	0.79	0.13	58,65,66,67	0
26	UNL	U	901	14/-	0.80	0.15	40,49,59,59	0
28	DMS	B	638	4/4	0.80	0.18	53,61,63,68	0
26	UNL	C	523	34/-	0.80	0.12	59,80,92,101	0
26	UNL	b	644	7/-	0.80	0.11	64,65,70,70	0
26	UNL	H	105	6/-	0.80	0.13	51,55,63,65	0
34	LMT	a	418	35/35	0.80	0.13	45,69,78,81	0
26	UNL	j	106	6/-	0.80	0.16	52,55,58,59	0
23	SQD	f	101	40/54	0.80	0.14	57,86,102,107	0
27	PL9	A	411	55/55	0.80	0.15	43,67,89,92	0
34	LMT	m	101	35/35	0.80	0.13	48,94,110,114	0
27	PL9	a	415	55/55	0.80	0.16	52,67,89,94	0
28	DMS	b	637	4/4	0.80	0.17	77,79,84,93	0
28	DMS	A	418	4/4	0.80	0.21	68,74,80,85	0
34	LMT	b	628	25/35	0.81	0.12	54,79,95,96	0
28	DMS	u	204	4/4	0.81	0.18	71,78,83,86	0
28	DMS	B	642	4/4	0.81	0.22	43,51,68,71	0
32	HTG	B	632	19/19	0.81	0.12	51,97,108,114	0
34	LMT	z	102	35/35	0.81	0.12	46,85,99,101	0
34	LMT	Z	101	35/35	0.81	0.14	44,90,107,109	0
24	LMG	C	524	45/55	0.81	0.20	22,46,51,56	45
26	UNL	b	630	11/-	0.81	0.13	55,60,67,68	0
28	DMS	d	415	4/4	0.82	0.17	68,71,71,72	0
28	DMS	O	306	4/4	0.82	0.18	66,73,73,75	0
32	HTG	C	521	19/19	0.82	0.12	46,78,89,90	0
28	DMS	V	205	4/4	0.82	0.15	67,76,77,79	0
28	DMS	B	639	4/4	0.82	0.18	65,70,71,76	0
28	DMS	c	533	4/4	0.82	0.16	73,75,77,87	0
26	UNL	M	102	12/-	0.83	0.13	49,53,95,98	0
26	UNL	B	630	14/-	0.83	0.12	67,74,83,84	0
26	UNL	a	416	11/-	0.83	0.14	66,68,76,78	0
34	LMT	J	103	24/35	0.83	0.12	53,61,81,85	0
26	UNL	x	102	9/-	0.83	0.14	56,68,72,72	0
26	UNL	L	102	14/-	0.84	0.15	56,60,84,84	0
24	LMG	c	518	51/55	0.84	0.11	37,72,84,87	0
23	SQD	l	101	54/54	0.84	0.13	47,68,101,106	0
28	DMS	b	636	4/4	0.84	0.18	66,71,72,79	0
26	UNL	d	409	36/-	0.84	0.12	36,60,91,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DMS	v	207	4/4	0.84	0.15	53,66,72,87	0
23	SQD	b	622	54/54	0.84	0.12	46,63,95,100	0
34	LMT	B	627	16/35	0.84	0.12	52,60,78,78	0
26	UNL	i	101	16/-	0.84	0.12	41,45,65,65	0
26	UNL	i	103	11/-	0.84	0.11	58,61,65,66	0
26	UNL	b	629	16/-	0.84	0.13	41,48,60,60	0
28	DMS	C	532	4/4	0.85	0.17	33,40,41,48	0
32	HTG	C	520	19/19	0.85	0.11	64,70,76,79	0
28	DMS	O	311	4/4	0.85	0.16	57,65,69,72	0
32	HTG	C	522	19/19	0.85	0.11	66,83,104,107	0
28	DMS	c	534	4/4	0.85	0.14	70,71,75,81	0
23	SQD	F	101	35/54	0.85	0.13	51,76,89,90	0
26	UNL	e	101	7/-	0.85	0.12	54,58,64,65	0
32	HTG	b	624	19/19	0.85	0.12	49,74,80,85	0
28	DMS	b	634	4/4	0.85	0.16	59,67,67,75	0
28	DMS	A	417	4/4	0.85	0.16	70,72,77,81	0
26	UNL	J	105	12/-	0.85	0.13	63,67,71,71	0
28	DMS	v	203	4/4	0.85	0.18	67,69,76,79	0
28	DMS	B	644	4/4	0.85	0.16	52,53,61,69	0
28	DMS	C	527	4/4	0.85	0.17	73,76,79,87	0
26	UNL	z	101	6/-	0.86	0.10	49,55,55,57	0
28	DMS	C	533	4/4	0.86	0.13	72,73,73,74	0
23	SQD	a	401	54/54	0.86	0.11	39,58,82,86	0
28	DMS	v	204	4/4	0.86	0.17	48,54,57,69	0
28	DMS	U	902	4/4	0.86	0.18	35,44,49,58	0
28	DMS	c	532	4/4	0.86	0.18	65,70,76,77	0
23	SQD	A	412	54/54	0.86	0.11	41,60,78,81	0
26	UNL	B	628	15/-	0.86	0.12	45,50,60,66	0
34	LMT	B	625	24/35	0.86	0.10	48,67,86,89	0
28	DMS	V	208	4/4	0.86	0.18	75,77,82,85	0
26	UNL	D	410	37/-	0.86	0.11	42,57,93,98	0
28	DMS	B	635	4/4	0.86	0.17	90,94,95,96	0
32	HTG	B	622	19/19	0.87	0.14	28,46,54,54	0
32	HTG	b	625	19/19	0.87	0.14	30,44,66,70	0
28	DMS	B	640	4/4	0.87	0.23	45,48,49,50	0
26	UNL	b	646	6/-	0.87	0.12	54,58,60,62	0
28	DMS	u	203	4/4	0.87	0.20	47,55,56,65	0
28	DMS	c	535	4/4	0.87	0.14	58,59,65,68	0
28	DMS	O	304	4/4	0.87	0.15	63,68,72,73	0
26	UNL	D	411	16/-	0.87	0.11	39,45,58,62	0
34	LMT	m	102	35/35	0.87	0.10	34,53,58,59	0
34	LMT	B	626	24/35	0.87	0.11	37,54,86,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DMS	o	303	4/4	0.87	0.15	66,69,75,79	0
32	HTG	V	202	13/19	0.87	0.10	45,49,70,82	0
28	DMS	v	208	4/4	0.87	0.17	89,92,92,95	0
34	LMT	T	102	24/35	0.88	0.12	36,53,78,85	0
28	DMS	o	305	4/4	0.88	0.14	73,75,77,87	0
28	DMS	C	529	4/4	0.88	0.15	70,73,74,74	0
28	DMS	C	531	4/4	0.88	0.17	53,54,58,74	0
24	LMG	a	410	51/55	0.88	0.09	44,55,65,67	0
28	DMS	B	643	4/4	0.88	0.13	51,53,62,71	0
28	DMS	A	415	4/4	0.88	0.15	55,58,65,71	0
28	DMS	D	416	4/4	0.88	0.14	83,87,89,91	0
26	UNL	I	102	16/-	0.88	0.11	38,47,63,64	0
28	DMS	O	303	4/4	0.88	0.14	63,72,77,78	0
28	DMS	v	209	4/4	0.88	0.13	71,78,79,79	0
28	DMS	o	304	4/4	0.88	0.15	68,79,82,83	0
34	LMT	M	101	35/35	0.88	0.10	34,53,63,64	0
26	UNL	i	102	11/-	0.89	0.10	48,54,64,65	0
26	UNL	d	411	16/-	0.89	0.09	33,42,55,55	0
26	UNL	J	106	4/-	0.89	0.12	57,60,61,67	0
24	LMG	B	620	51/55	0.89	0.09	33,43,55,58	0
28	DMS	v	205	4/4	0.89	0.12	67,70,72,73	0
26	UNL	X	101	16/-	0.89	0.11	37,40,59,59	0
28	DMS	C	525[A]	4/4	0.89	0.17	48,49,51,57	4
28	DMS	V	209	4/4	0.89	0.14	57,73,77,81	0
28	DMS	C	525[B]	4/4	0.89	0.17	32,33,35,35	4
24	LMG	c	519	51/55	0.90	0.11	29,59,86,88	0
28	DMS	O	307	4/4	0.90	0.15	69,76,77,88	0
24	LMG	C	519	51/55	0.90	0.11	31,67,83,84	0
28	DMS	B	645	4/4	0.90	0.13	56,59,64,71	0
20	CLA	C	513	65/65	0.90	0.09	40,48,72,77	0
28	DMS	A	416	4/4	0.90	0.12	59,60,69,77	0
24	LMG	A	407	51/55	0.90	0.09	40,55,70,78	0
28	DMS	U	903[A]	4/4	0.90	0.16	32,34,40,41	4
28	DMS	U	903[B]	4/4	0.90	0.16	26,28,29,32	4
28	DMS	B	641	4/4	0.90	0.12	68,69,75,80	0
28	DMS	V	204	4/4	0.90	0.12	58,64,64,72	0
20	CLA	C	506	65/65	0.90	0.09	32,45,86,87	0
28	DMS	c	536	4/4	0.90	0.18	33,33,45,46	0
28	DMS	V	207	4/4	0.91	0.14	62,63,63,70	0
20	CLA	b	603	65/65	0.91	0.10	30,45,75,82	0
24	LMG	b	623	49/55	0.91	0.09	33,42,54,61	0
33	CA	V	203	1/1	0.91	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DMS	v	206	4/4	0.91	0.13	52,53,61,66	0
28	DMS	u	202	4/4	0.91	0.18	40,46,52,54	0
28	DMS	b	639	4/4	0.91	0.13	46,49,49,50	0
23	SQD	A	406	54/54	0.91	0.10	34,59,71,76	0
28	DMS	o	307	4/4	0.92	0.13	53,58,63,65	0
22	BCR	C	514	40/40	0.92	0.07	36,45,49,50	0
28	DMS	V	206	4/4	0.92	0.12	59,61,63,65	0
26	UNL	d	410	16/-	0.92	0.10	33,45,63,63	0
28	DMS	d	413	4/4	0.92	0.14	47,53,55,57	0
28	DMS	d	414	4/4	0.92	0.17	57,62,64,68	0
20	CLA	B	602	65/65	0.92	0.10	29,42,77,81	0
28	DMS	B	637	4/4	0.92	0.14	53,53,54,60	0
28	DMS	b	632	4/4	0.92	0.12	55,58,66,70	0
32	HTG	b	601	19/19	0.92	0.09	45,61,67,80	0
28	DMS	c	529	4/4	0.92	0.11	79,82,86,87	0
28	DMS	C	530	4/4	0.92	0.17	44,44,46,50	0
28	DMS	b	635	4/4	0.92	0.12	58,62,69,73	0
28	DMS	h	102	4/4	0.93	0.15	50,51,53,62	0
33	CA	o	301	1/1	0.93	0.06	48,48,48,48	0
28	DMS	i	104	4/4	0.93	0.11	63,66,67,71	0
28	DMS	C	526	4/4	0.93	0.13	59,60,63,65	0
32	HTG	B	631	19/19	0.93	0.08	41,57,69,73	0
20	CLA	C	512	55/65	0.93	0.07	37,44,49,54	0
28	DMS	D	413	4/4	0.93	0.11	50,56,60,61	0
22	BCR	K	101	40/40	0.93	0.07	33,37,42,45	0
22	BCR	k	102	40/40	0.93	0.07	41,46,51,51	0
28	DMS	c	530	4/4	0.93	0.20	36,43,45,49	0
35	DGD	h	101	62/66	0.93	0.08	25,34,41,49	0
20	CLA	b	618	65/65	0.93	0.09	23,33,92,98	0
22	BCR	D	405	40/40	0.94	0.07	26,30,58,60	0
20	CLA	c	513	65/65	0.94	0.08	36,46,81,87	0
31	BCT	A	421	4/4	0.94	0.07	31,34,40,44	0
31	BCT	a	413	4/4	0.94	0.07	32,32,38,42	0
32	HTG	B	621	19/19	0.94	0.08	36,41,48,52	0
22	BCR	K	102	40/40	0.94	0.07	31,36,40,41	0
22	BCR	d	405	40/40	0.94	0.07	24,30,56,58	0
28	DMS	F	102	4/4	0.94	0.12	51,52,56,64	0
23	SQD	a	409	54/54	0.94	0.09	33,56,75,78	0
22	BCR	k	101	40/40	0.94	0.07	28,36,41,42	0
28	DMS	c	528	4/4	0.94	0.13	58,62,63,65	0
20	CLA	c	506	65/65	0.94	0.07	24,39,71,74	0
28	DMS	b	633	4/4	0.94	0.12	45,48,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	DGD	H	102	62/66	0.94	0.08	25,33,40,43	0
28	DMS	c	531	4/4	0.94	0.11	73,78,85,86	0
32	HTG	O	302	19/19	0.94	0.08	34,42,50,53	0
36	LHG	D	407	49/49	0.94	0.07	28,37,44,52	0
36	LHG	D	409	49/49	0.94	0.10	27,33,81,83	0
22	BCR	t	101	40/40	0.94	0.06	22,29,41,43	0
38	RRX	H	101	41/41	0.94	0.07	27,31,41,46	0
38	RRX	x	101	41/41	0.94	0.07	26,32,47,58	0
20	CLA	C	505	65/65	0.95	0.06	28,33,44,48	0
20	CLA	B	601	65/65	0.95	0.08	23,29,82,86	0
20	CLA	c	511	65/65	0.95	0.06	27,33,40,43	0
20	CLA	c	512	65/65	0.95	0.07	28,41,70,72	0
28	DMS	D	414	4/4	0.95	0.12	55,56,57,58	0
20	CLA	C	507	65/65	0.95	0.07	28,37,52,57	0
35	DGD	C	517	55/66	0.95	0.06	26,34,59,62	0
24	LMG	j	101	45/55	0.95	0.07	27,32,60,64	0
20	CLA	C	508	60/65	0.95	0.06	23,31,47,51	0
35	DGD	c	517	62/66	0.95	0.07	23,30,56,71	0
22	BCR	C	515	40/40	0.95	0.06	31,37,43,45	0
20	CLA	C	511	65/65	0.95	0.07	30,37,42,45	0
20	CLA	B	610	65/65	0.95	0.06	26,31,35,38	0
20	CLA	C	503	65/65	0.95	0.06	28,33,37,42	0
22	BCR	T	101	40/40	0.95	0.06	24,32,43,45	0
20	CLA	C	504	65/65	0.95	0.07	27,30,59,61	0
20	CLA	b	608	65/65	0.95	0.07	24,31,59,63	0
20	CLA	c	507	65/65	0.96	0.07	25,30,49,57	0
20	CLA	c	508	60/65	0.96	0.06	24,28,52,54	0
28	DMS	b	631	4/4	0.96	0.09	23,24,27,35	0
33	CA	O	301	1/1	0.96	0.05	47,47,47,47	0
20	CLA	c	509	65/65	0.96	0.07	25,30,53,58	0
20	CLA	C	509	65/65	0.96	0.07	29,34,52,55	0
28	DMS	v	202	4/4	0.96	0.11	50,51,53,55	0
20	CLA	C	510	65/65	0.96	0.06	26,31,38,44	0
20	CLA	C	502	65/65	0.96	0.06	24,29,41,48	0
22	BCR	A	405	40/40	0.96	0.05	21,26,32,35	0
22	BCR	B	618	40/40	0.96	0.06	21,28,42,45	0
24	LMG	J	101	45/55	0.96	0.07	27,32,64,70	0
22	BCR	B	619	40/40	0.96	0.06	22,30,42,44	0
20	CLA	B	607	65/65	0.96	0.07	22,29,55,62	0
20	CLA	B	603	65/65	0.96	0.06	23,28,35,39	0
27	PL9	D	412	55/55	0.96	0.05	19,23,29,34	0
20	CLA	B	611	65/65	0.96	0.06	21,26,34,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	PL9	d	412	55/55	0.96	0.05	18,23,29,35	0
20	CLA	b	604	65/65	0.96	0.06	23,27,33,35	0
20	CLA	B	615	65/65	0.96	0.07	20,24,70,79	0
20	CLA	b	611	65/65	0.96	0.06	24,30,34,41	0
22	BCR	a	408	40/40	0.96	0.05	21,25,30,31	0
22	BCR	b	619	40/40	0.96	0.05	23,26,32,35	0
35	DGD	C	516	62/66	0.96	0.07	22,32,74,79	0
22	BCR	b	620	40/40	0.96	0.05	22,27,43,46	0
35	DGD	C	518	62/66	0.96	0.07	24,30,62,73	0
22	BCR	c	514	40/40	0.96	0.06	28,36,39,39	0
20	CLA	b	612	65/65	0.96	0.06	21,27,36,41	0
35	DGD	c	515	62/66	0.96	0.07	23,32,71,75	0
35	DGD	c	516	57/66	0.96	0.06	27,32,62,68	0
22	BCR	j	102	40/40	0.96	0.06	30,35,42,45	0
20	CLA	b	616	65/65	0.96	0.07	20,26,73,80	0
20	CLA	B	616	65/65	0.96	0.06	25,29,48,52	0
20	CLA	c	501	65/65	0.96	0.06	26,30,41,48	0
20	CLA	c	503	65/65	0.96	0.06	25,35,40,43	0
20	CLA	c	504	65/65	0.96	0.06	25,29,55,60	0
36	LHG	d	406	49/49	0.96	0.06	29,36,43,48	0
36	LHG	d	408	49/49	0.96	0.09	24,31,83,88	0
20	CLA	c	505	65/65	0.96	0.06	25,30,46,50	0
20	CLA	C	501	65/65	0.96	0.06	27,33,45,52	0
21	PHO	A	403	64/64	0.97	0.04	18,22,24,25	0
21	PHO	D	403	64/64	0.97	0.04	18,24,29,35	0
21	PHO	a	405	64/64	0.97	0.04	17,20,22,25	0
21	PHO	a	406	64/64	0.97	0.04	19,24,29,32	0
20	CLA	b	610	65/65	0.97	0.05	20,26,31,33	0
22	BCR	B	617	40/40	0.97	0.05	22,26,32,33	0
20	CLA	B	608	65/65	0.97	0.05	18,21,34,39	0
20	CLA	B	609	65/65	0.97	0.04	22,25,31,33	0
20	CLA	b	613	65/65	0.97	0.05	20,22,38,44	0
20	CLA	b	614	65/65	0.97	0.05	21,25,31,37	0
20	CLA	A	402	59/65	0.97	0.05	18,22,52,58	0
20	CLA	b	617	65/65	0.97	0.05	23,30,44,50	0
20	CLA	B	604	65/65	0.97	0.05	21,24,33,39	0
20	CLA	B	612	65/65	0.97	0.05	19,22,36,42	0
20	CLA	c	502	65/65	0.97	0.06	22,26,39,48	0
20	CLA	D	401	65/65	0.97	0.05	16,20,35,41	0
20	CLA	D	404	65/65	0.97	0.07	26,29,77,81	0
22	BCR	b	621	40/40	0.97	0.05	27,32,42,44	0
20	CLA	a	403	65/65	0.97	0.05	17,20,29,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	a	407	47/65	0.97	0.05	19,22,41,48	0
20	CLA	B	613	65/65	0.97	0.05	21,25,30,34	0
20	CLA	B	606	65/65	0.97	0.05	19,24,35,37	0
33	CA	b	626	1/1	0.97	0.06	42,42,42,42	0
36	LHG	D	408	49/49	0.97	0.06	23,30,44,49	0
20	CLA	b	605	65/65	0.97	0.05	21,25,34,37	0
20	CLA	c	510	65/65	0.97	0.05	23,29,39,42	0
36	LHG	L	101	49/49	0.97	0.06	24,31,49,53	0
20	CLA	b	606	65/65	0.97	0.05	20,24,54,59	0
36	LHG	d	407	49/49	0.97	0.06	22,27,46,50	0
20	CLA	A	404	65/65	0.97	0.07	20,25,88,90	0
36	LHG	l	102	49/49	0.97	0.06	22,30,51,54	0
37	HEM	E	104	43/43	0.97	0.08	39,44,52,56	0
37	HEM	e	102	43/43	0.97	0.08	34,41,56,68	0
20	CLA	b	609	65/65	0.97	0.05	19,22,33,37	0
20	CLA	d	404	65/65	0.97	0.07	24,29,78,87	0
20	CLA	b	615	65/65	0.98	0.05	18,22,53,59	0
20	CLA	D	402	65/65	0.98	0.04	15,19,30,36	0
20	CLA	B	605	65/65	0.98	0.06	19,23,55,58	0
33	CA	c	522	1/1	0.98	0.05	41,41,41,41	0
28	DMS	B	634	4/4	0.98	0.07	23,24,25,26	0
20	CLA	d	402	65/65	0.98	0.04	16,20,35,41	0
20	CLA	d	403	65/65	0.98	0.04	17,19,27,34	0
20	CLA	B	614	65/65	0.98	0.04	19,22,48,53	0
28	DMS	c	527	4/4	0.98	0.06	33,33,34,38	0
20	CLA	a	404	60/65	0.98	0.06	18,22,66,75	0
20	CLA	b	607	65/65	0.98	0.05	20,24,33,35	0
28	DMS	C	528	4/4	0.98	0.07	33,37,39,41	0
28	DMS	o	302	4/4	0.98	0.08	20,28,31,36	0
20	CLA	A	401	65/65	0.98	0.04	16,19,30,36	0
33	CA	B	624	1/1	0.98	0.11	43,43,43,43	0
39	MG	J	102	1/1	0.98	0.05	33,33,33,33	0
40	HEC	v	201	43/43	0.98	0.06	25,29,34,37	0
25	CL	A	409	1/1	0.99	0.03	22,22,22,22	0
28	DMS	A	414	4/4	0.99	0.06	25,28,28,29	0
29	FE2	A	419	1/1	0.99	0.02	29,29,29,29	0
29	FE2	a	417	1/1	0.99	0.02	27,27,27,27	0
39	MG	j	103	1/1	0.99	0.08	31,31,31,31	0
40	HEC	V	201	43/43	0.99	0.04	21,23,27,31	0
25	CL	a	412	1/1	0.99	0.03	24,24,24,24	0
25	CL	A	408	1/1	1.00	0.01	22,22,22,22	0
30	OEX	A	420	10/10	1.00	0.03	21,23,24,24	0

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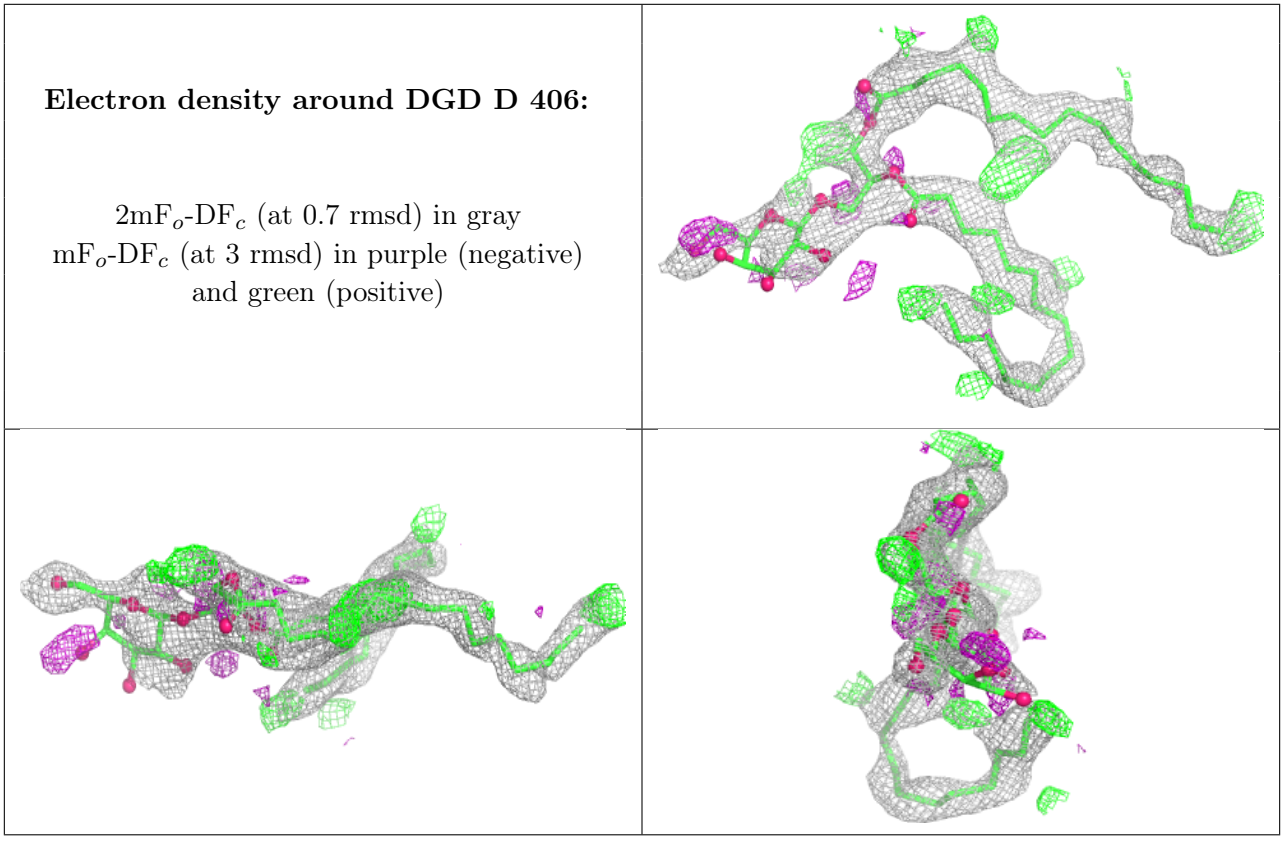
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	OEX	a	419	10/10	1.00	0.02	21,24,26,26	0
25	CL	a	411	1/1	1.00	0.03	22,22,22,22	0

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.

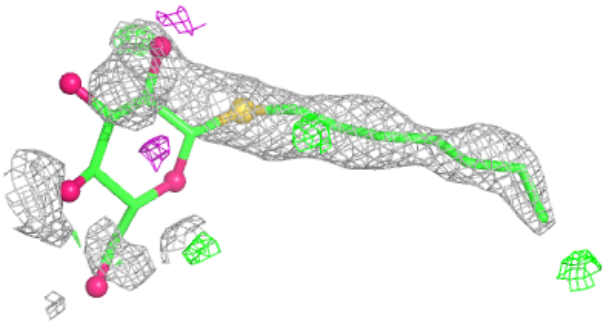
Electron density around DGD D 406:

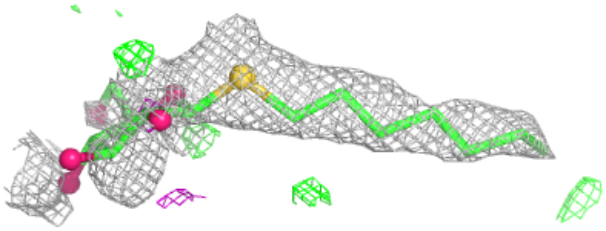
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

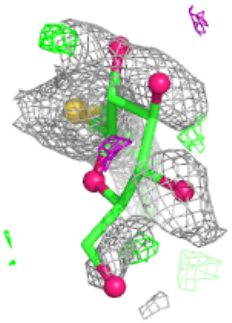


Electron density around HTG C 534:

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

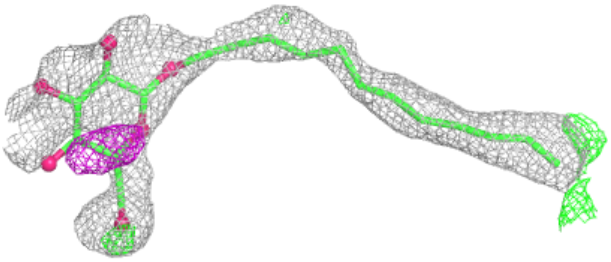


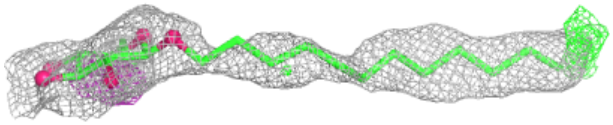


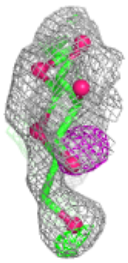


Electron density around LMT f 102:

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

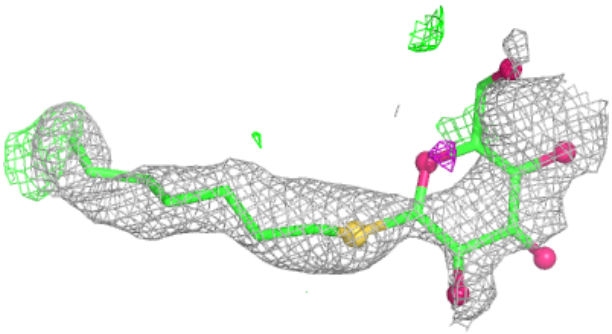


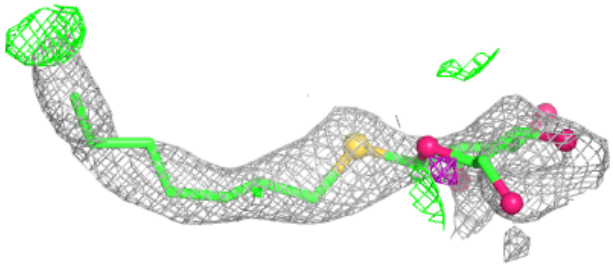


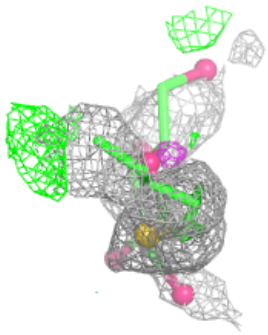


Electron density around HTG D 417:

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

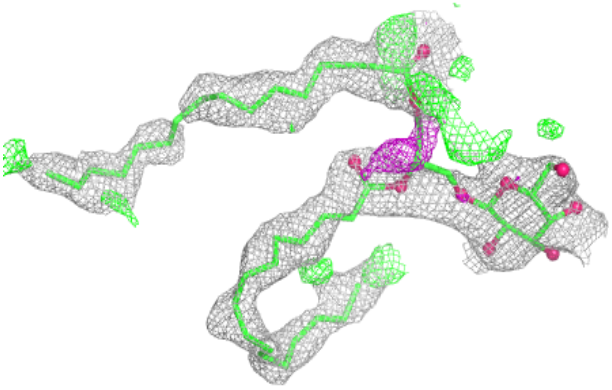


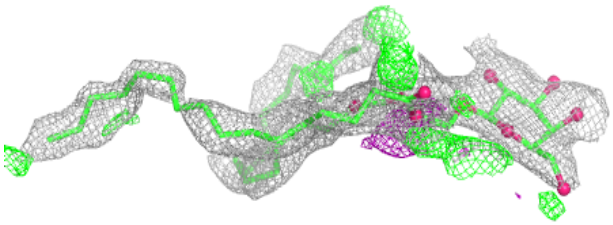


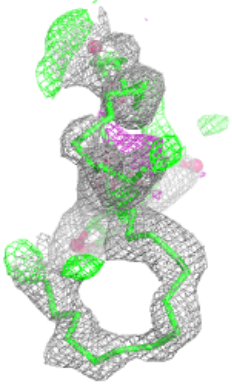


Electron density around DGD d 416:

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

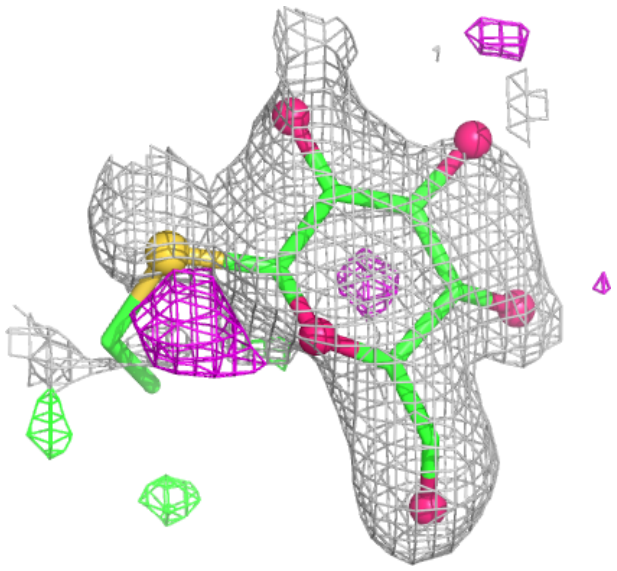


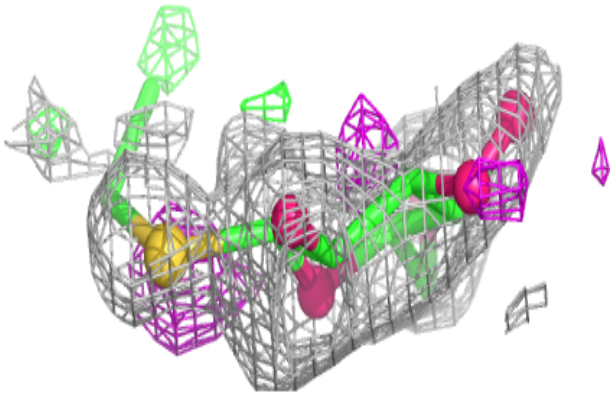


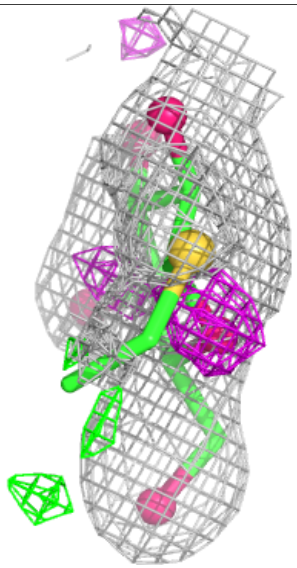


Electron density around HTG v 210:

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

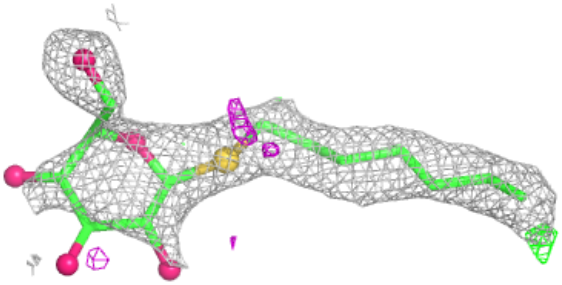


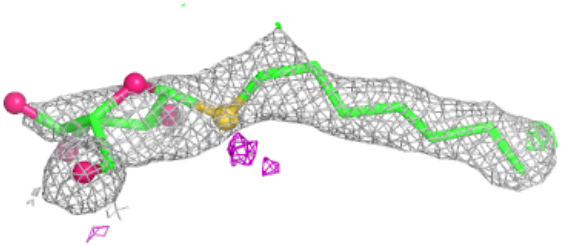


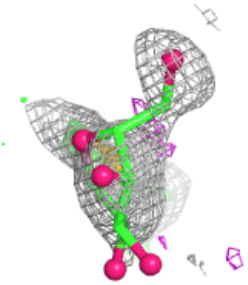


Electron density around HTG c 521:

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

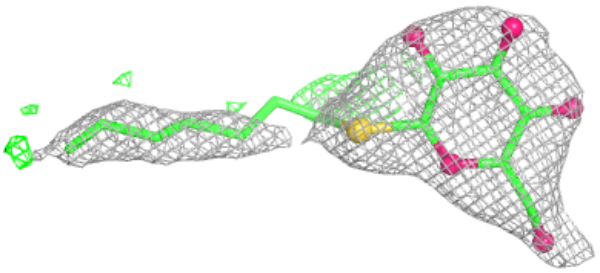


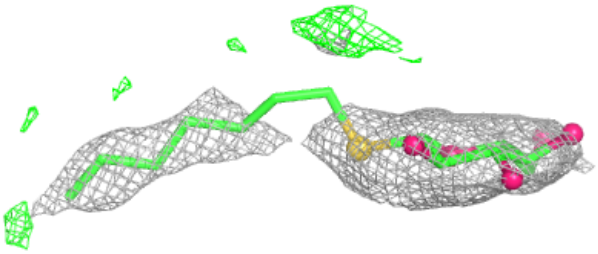


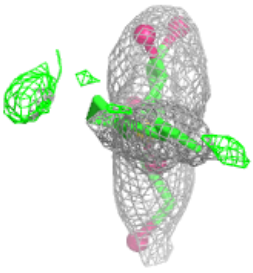


Electron density around HTG c 520:

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

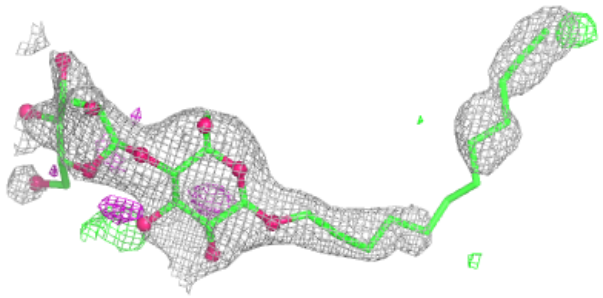


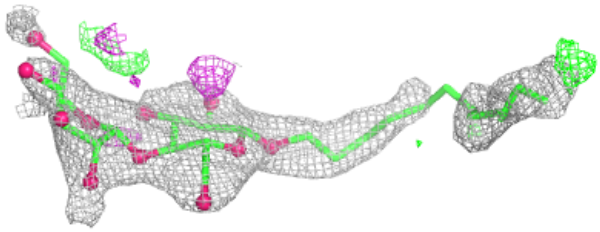


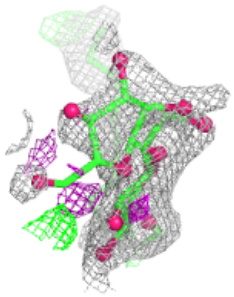


Electron density around LMT I 101:

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

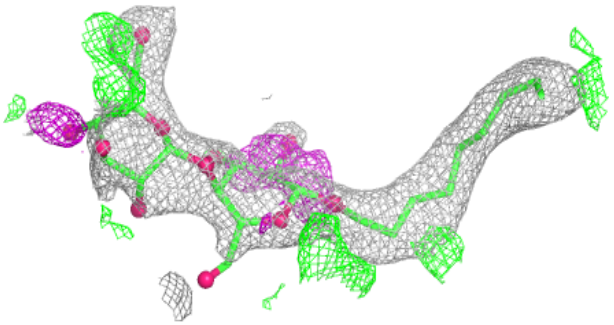


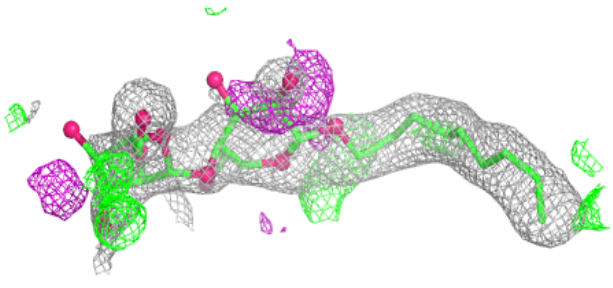


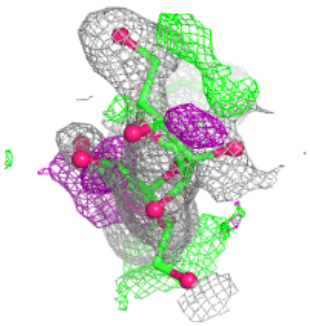


Electron density around LMT b 627:

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

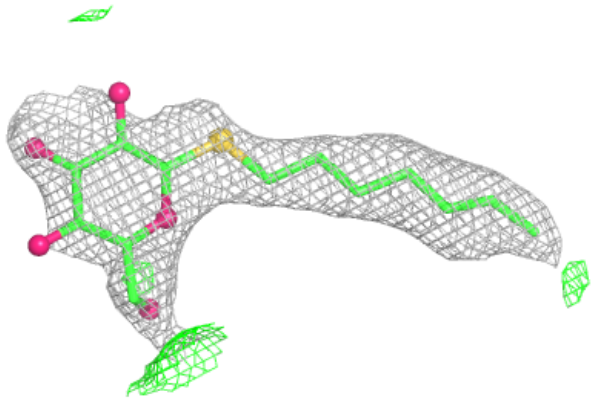


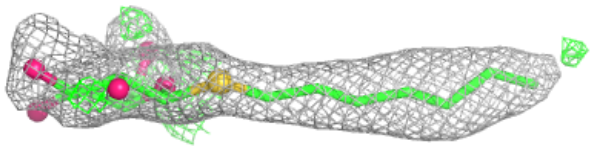


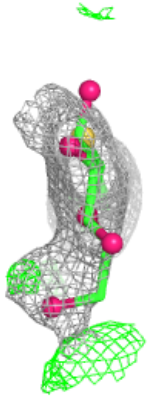


Electron density around HTG b 602:

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

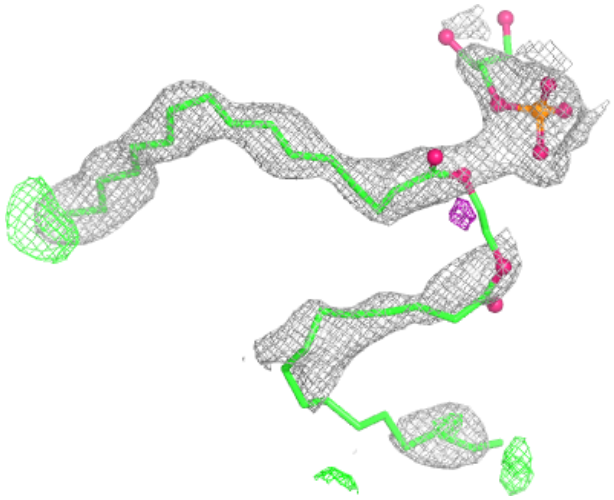


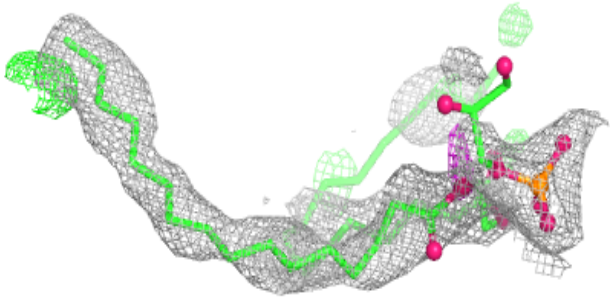


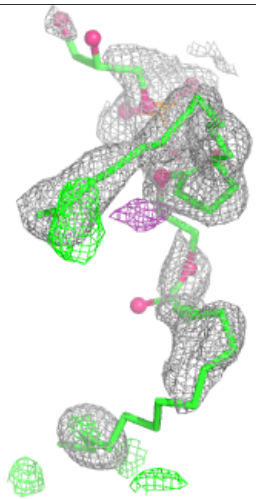


Electron density around LHG E 103:

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

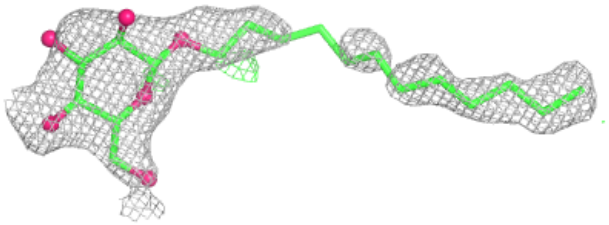


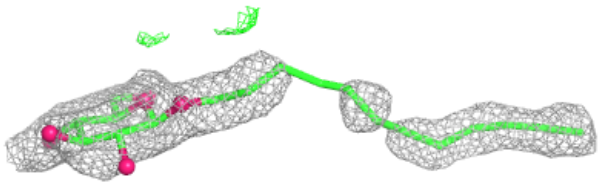


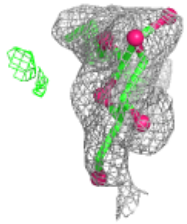


Electron density around LMT E 101:

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

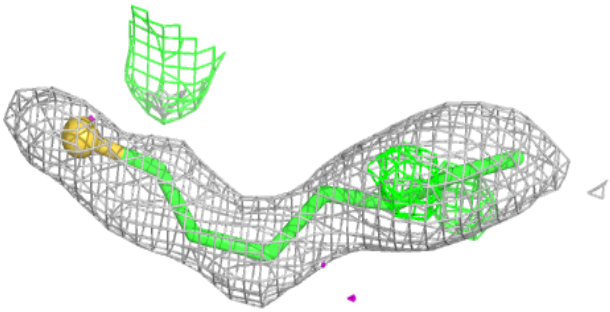


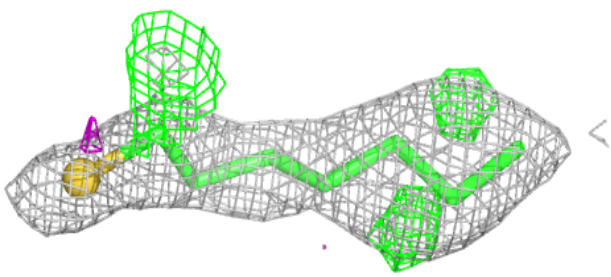


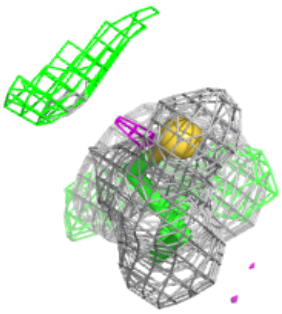


Electron density around HTG u 201:

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

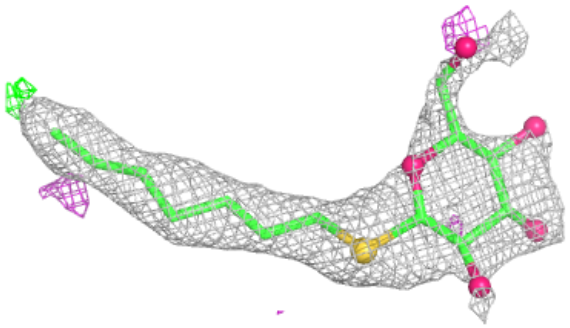


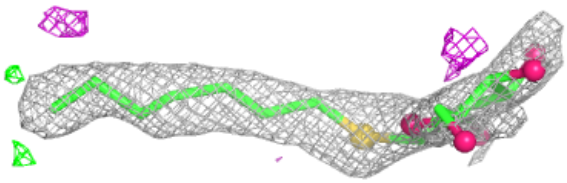


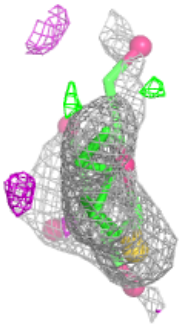


Electron density around HTG B 623:

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

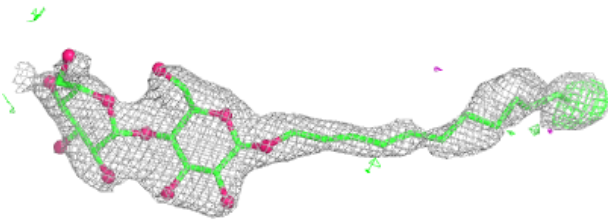


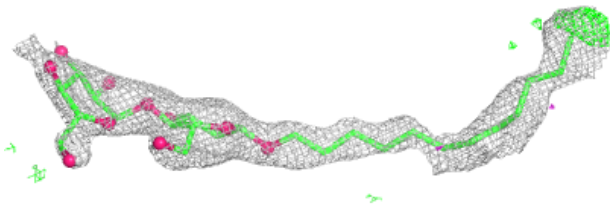


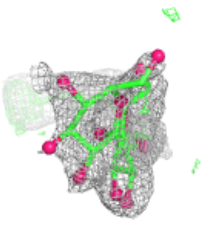


Electron density around LMT c 523:

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

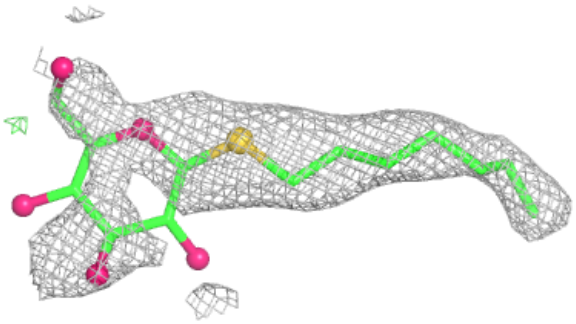


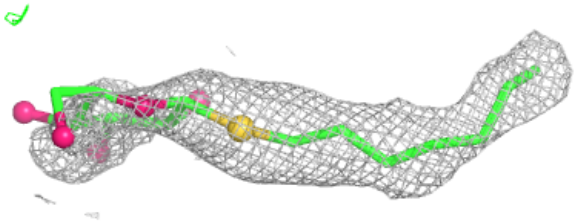


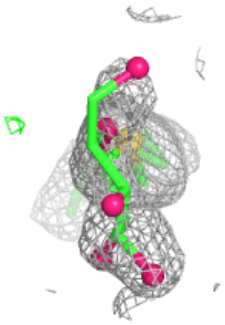


Electron density around HTG d 401:

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

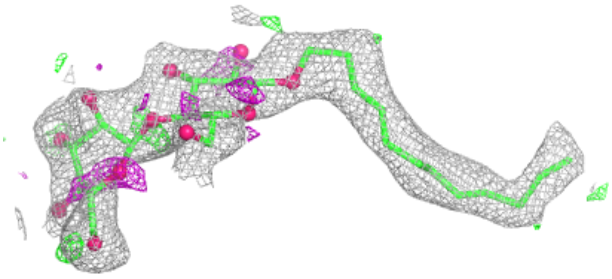


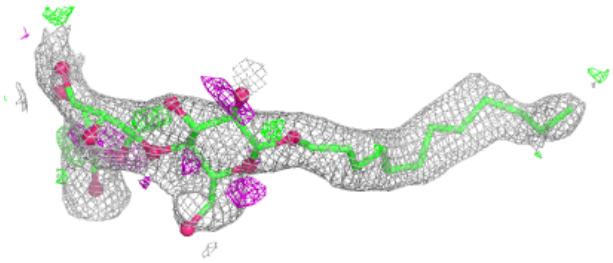


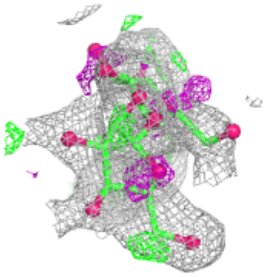


Electron density around LMT a 418:

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

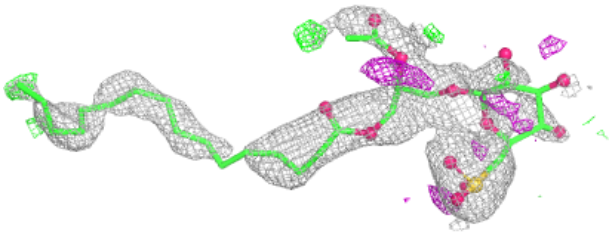


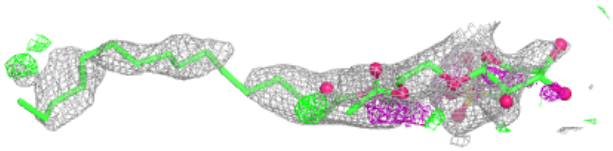




Electron density around SQD f 101:

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

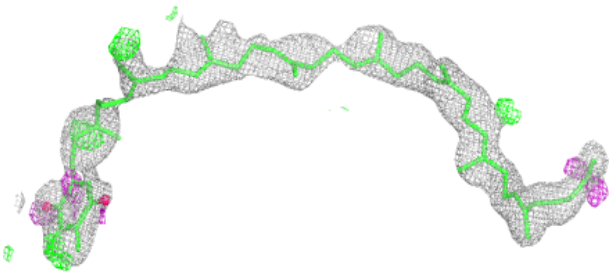


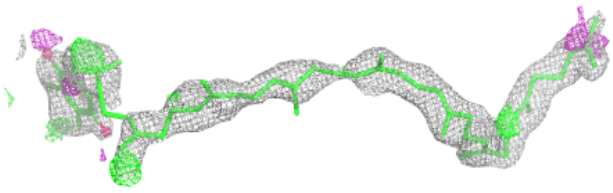


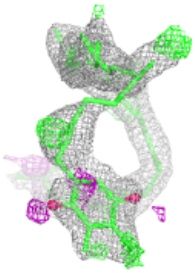


Electron density around PL9 A 411:

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

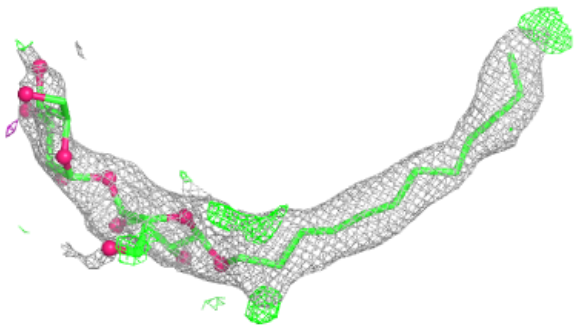


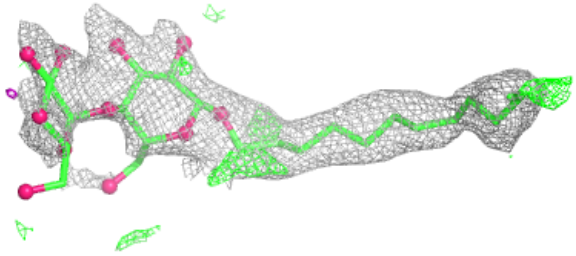


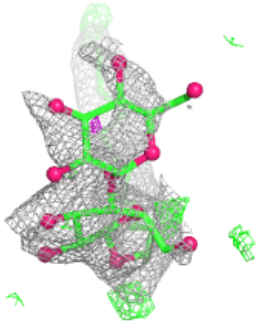


Electron density around LMT m 101:

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

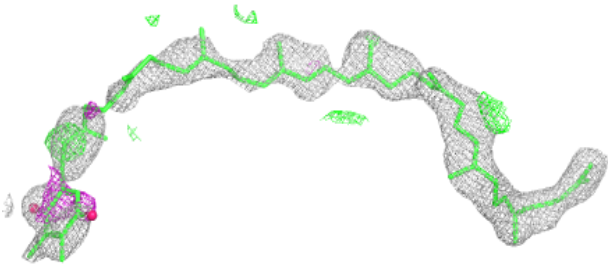


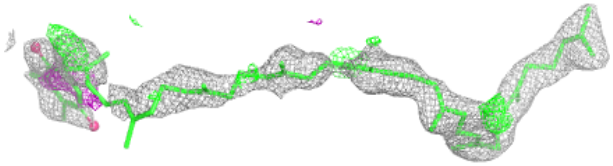


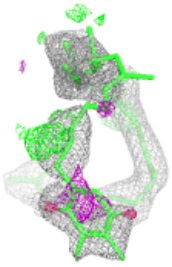


Electron density around PL9 a 415:

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

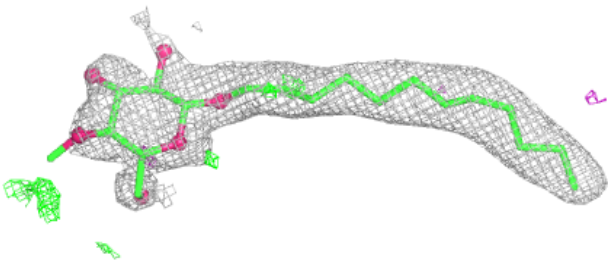


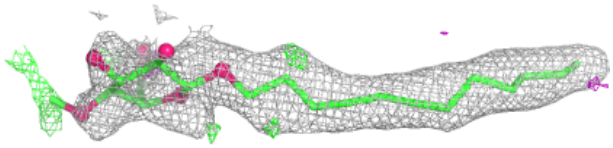




Electron density around LMT b 628:

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

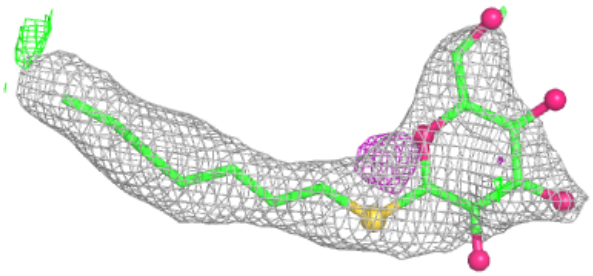


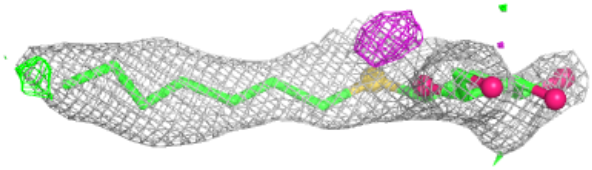


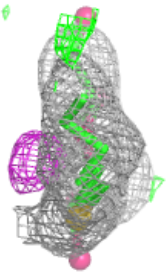


Electron density around HTG B 632:

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

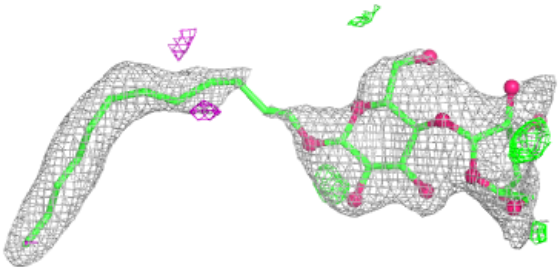


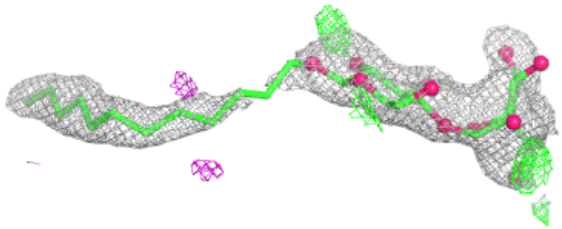


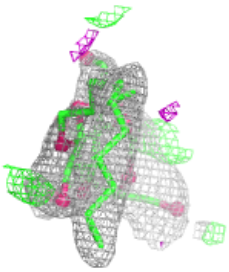


Electron density around LMT z 102:

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

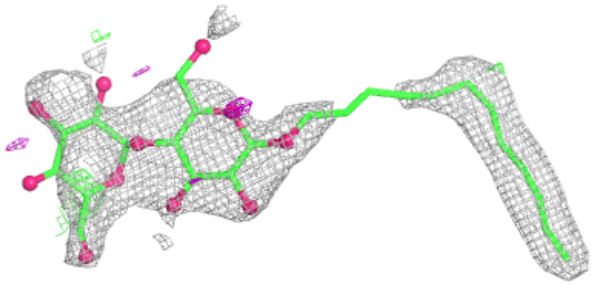


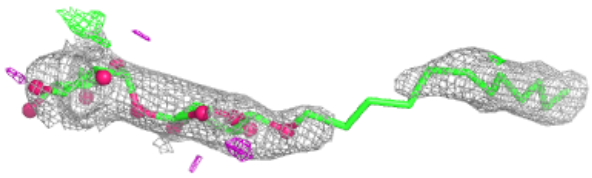


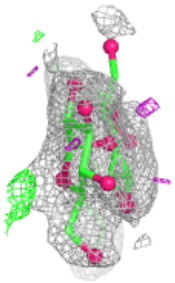


Electron density around LMT Z 101:

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

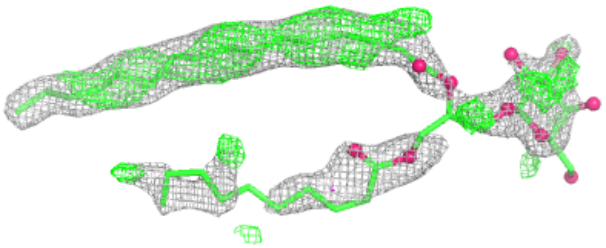


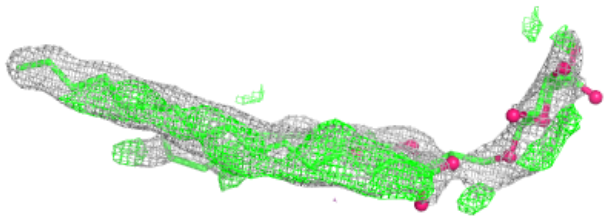


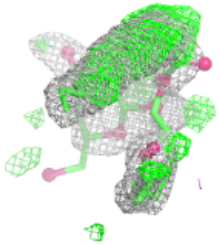


Electron density around LMG C 524:

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

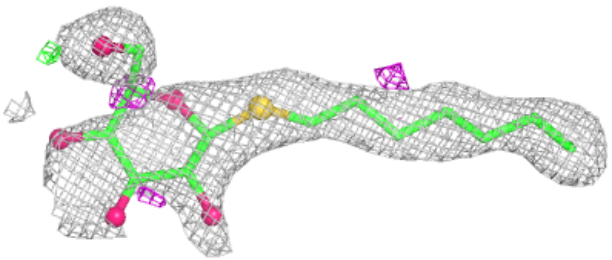


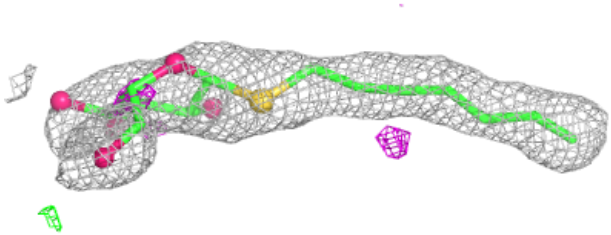


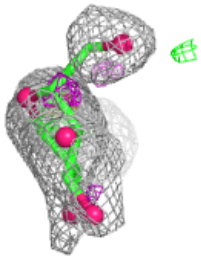


Electron density around HTG C 521:

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

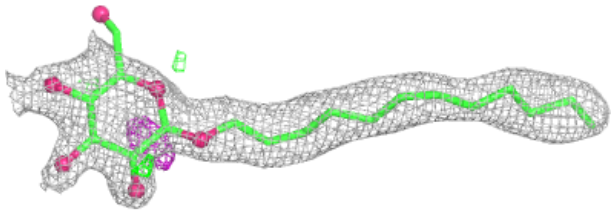


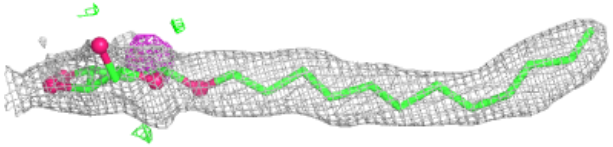


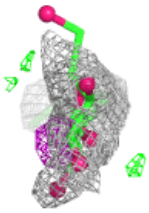


Electron density around LMT J 103:

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

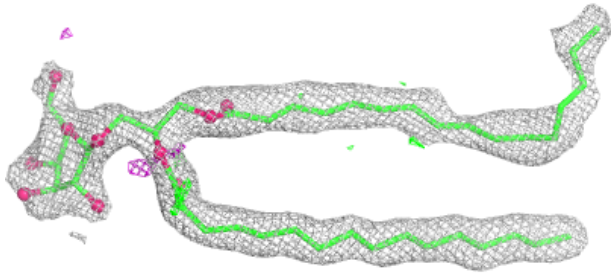


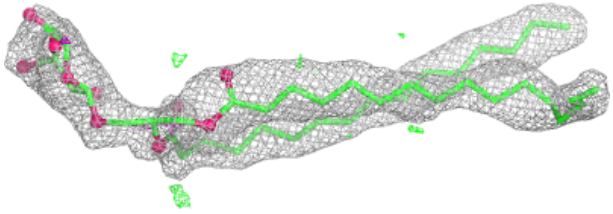


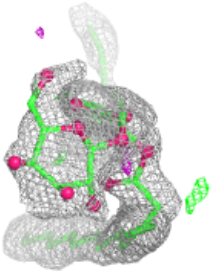


Electron density around LMG c 518:

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

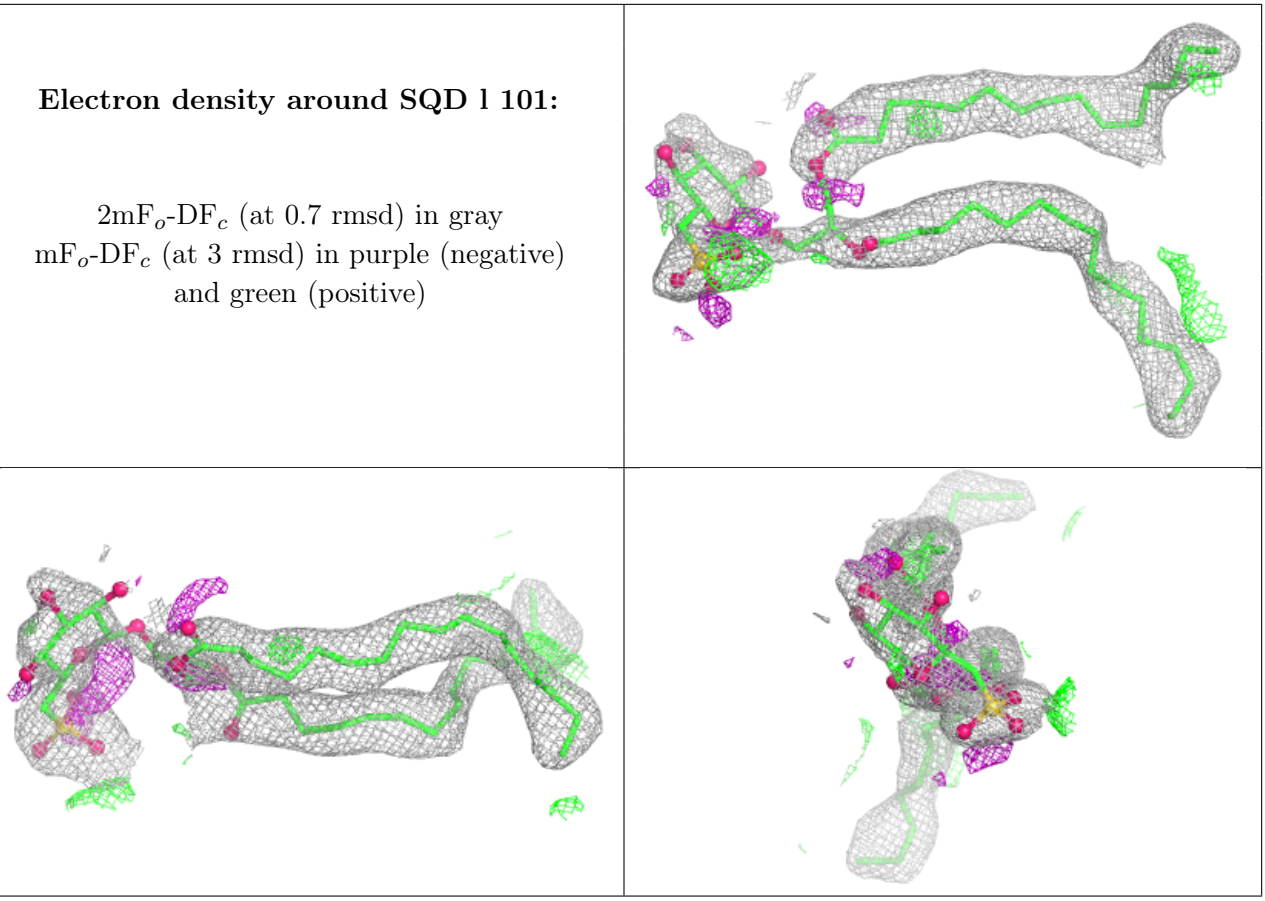






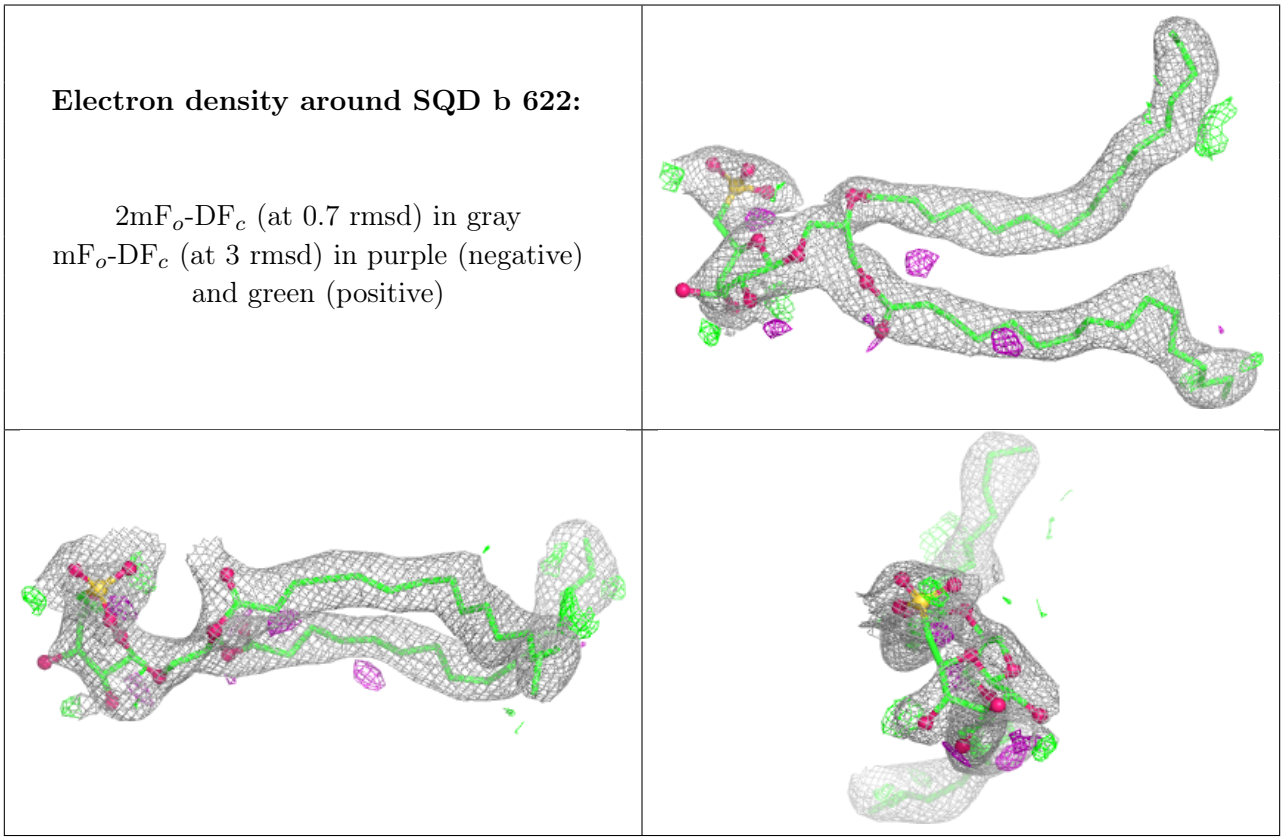
Electron density around SQD l 101:

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



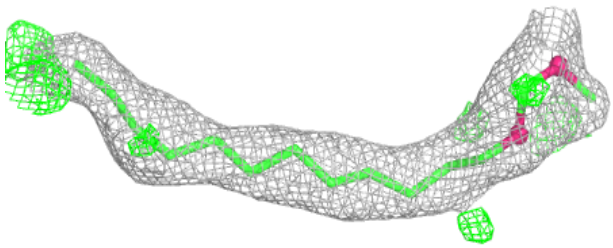
Electron density around SQD b 622:

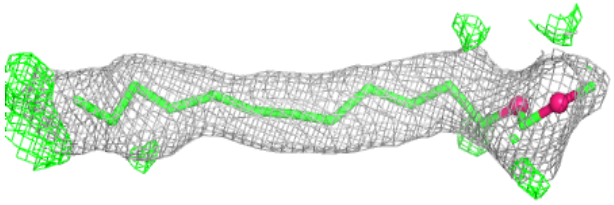
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

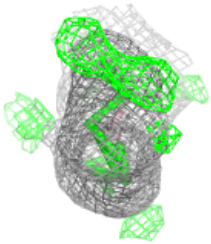


Electron density around LMT B 627:

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

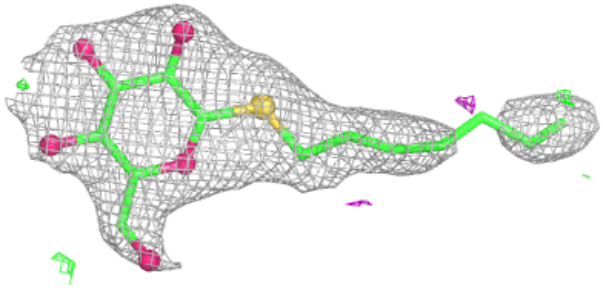


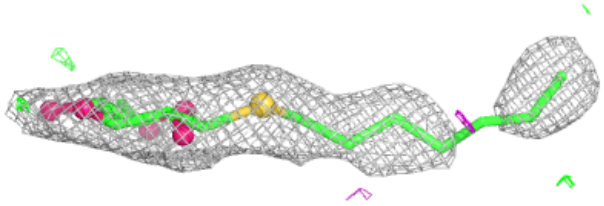


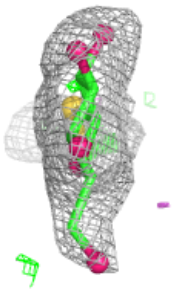


Electron density around HTG C 520:

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

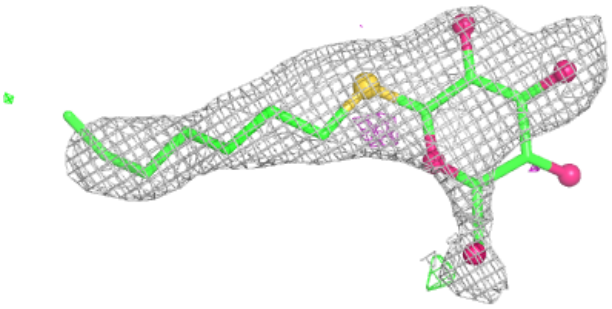


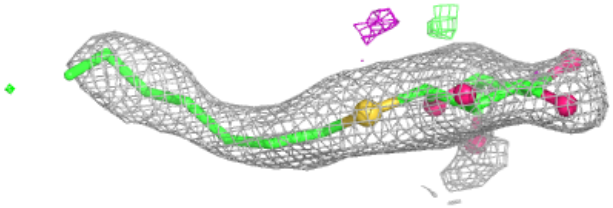


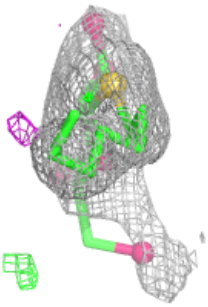


Electron density around HTG C 522:

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

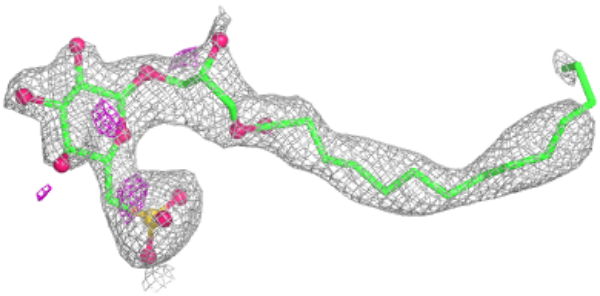


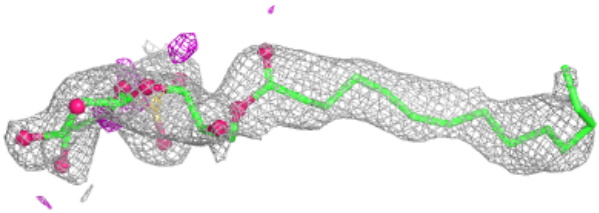


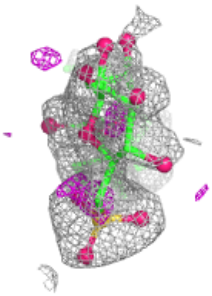


Electron density around SQD F 101:

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

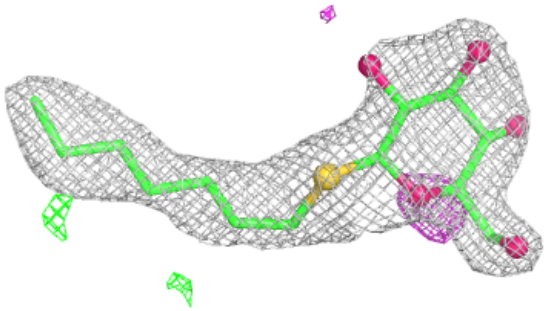


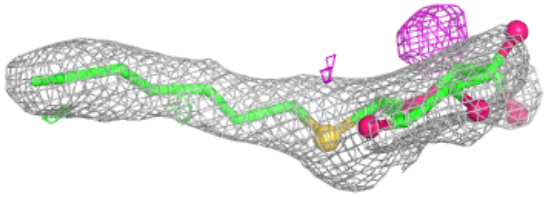


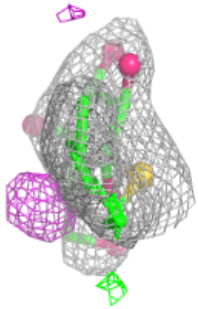


Electron density around HTG b 624:

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

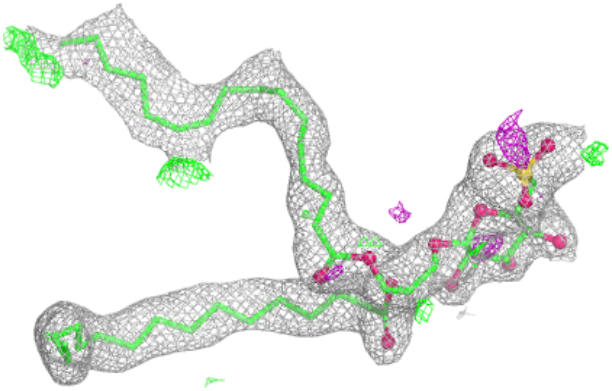


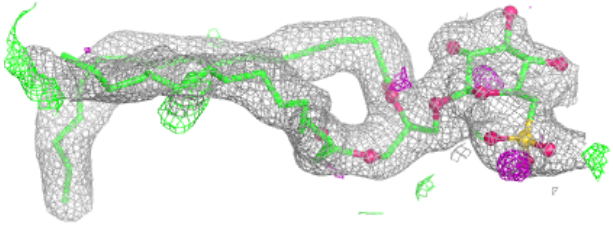


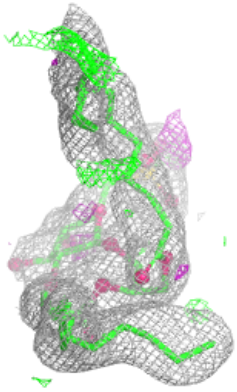


Electron density around SQD a 401:

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

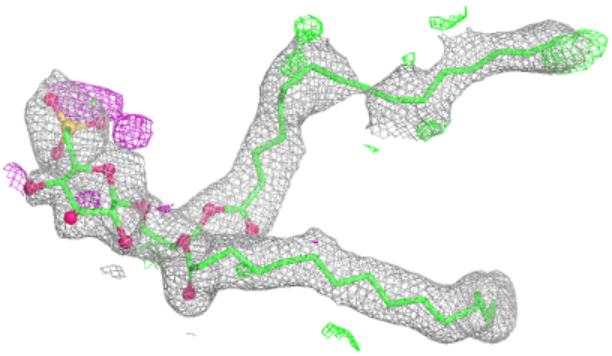


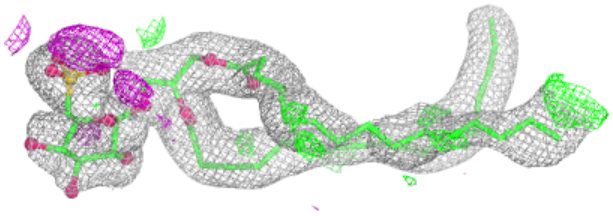


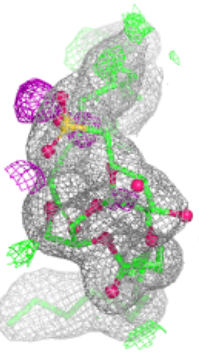


Electron density around SQD A 412:

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

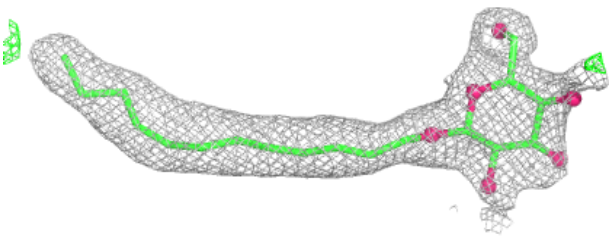


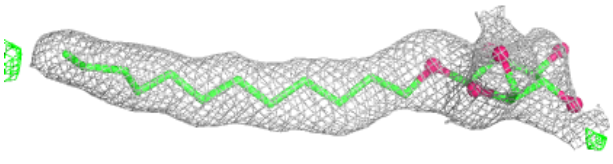


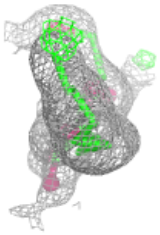


Electron density around LMT B 625:

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

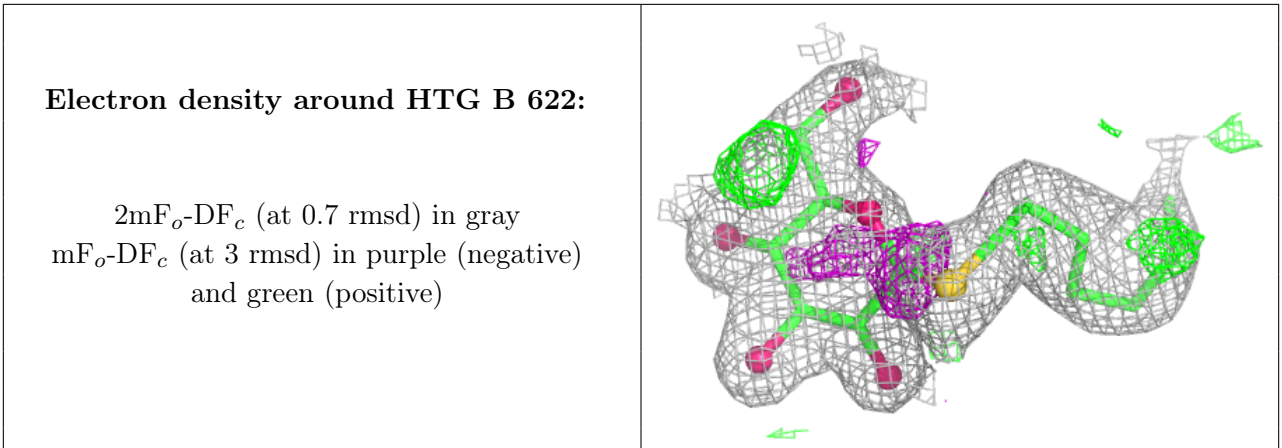






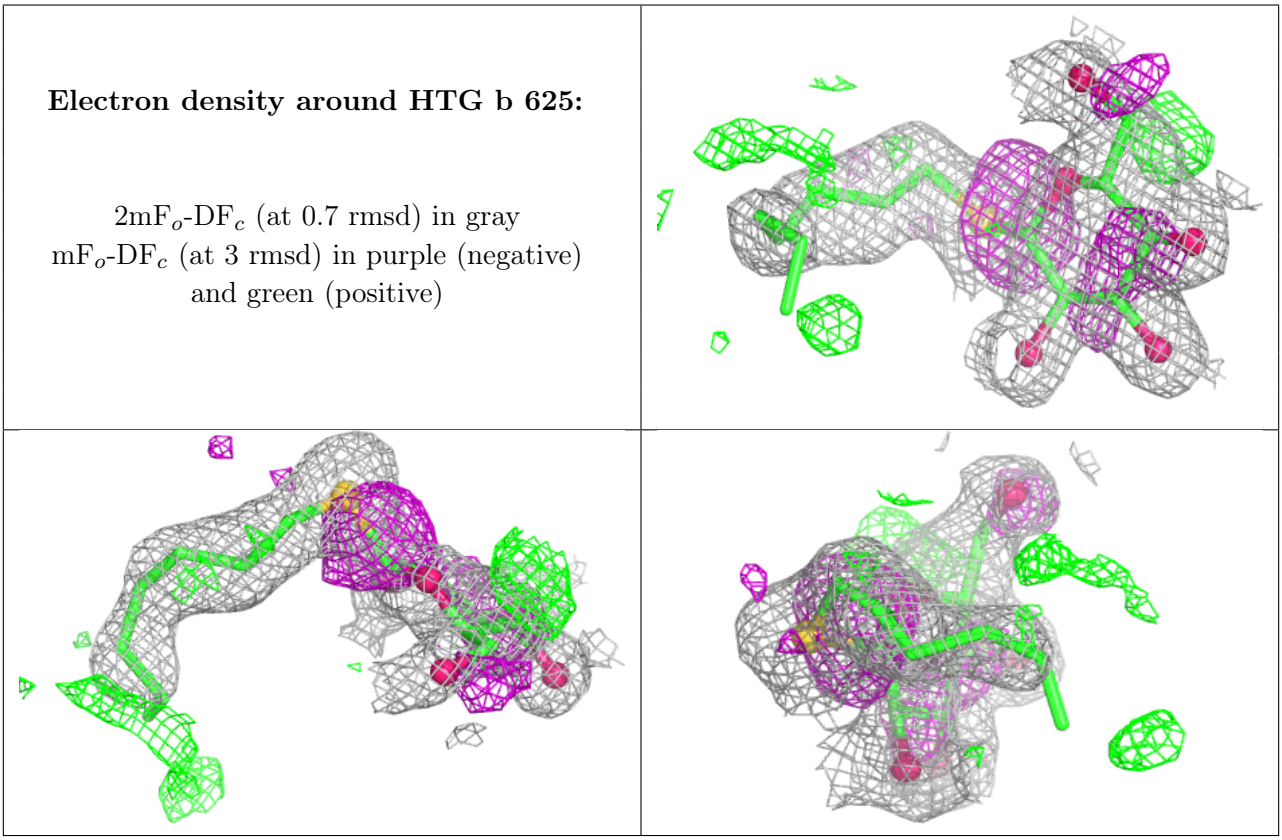
Electron density around HTG B 622:

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



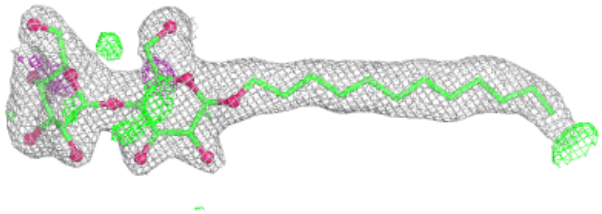
Electron density around HTG b 625:

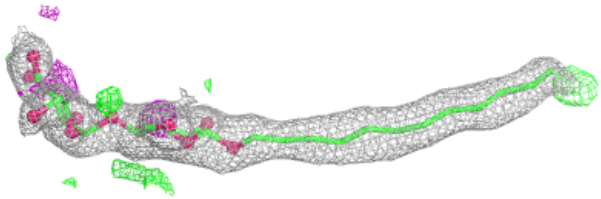
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

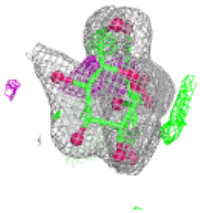


Electron density around LMT m 102:

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

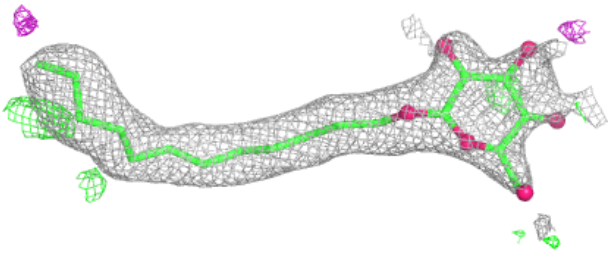


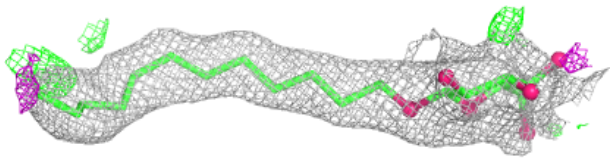


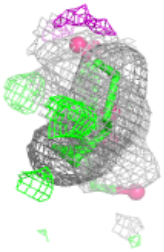


Electron density around LMT B 626:

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

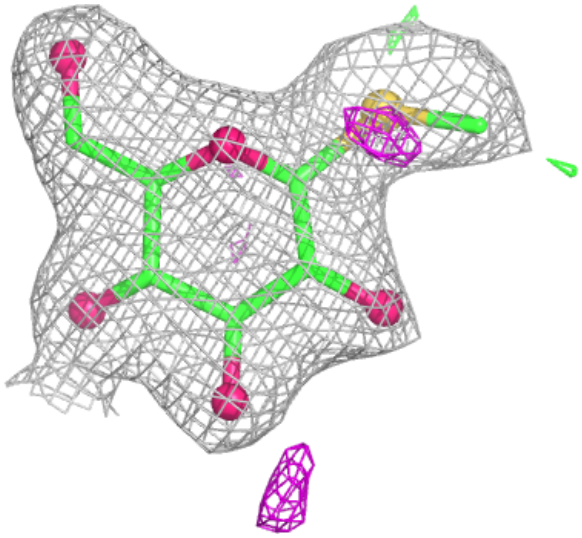


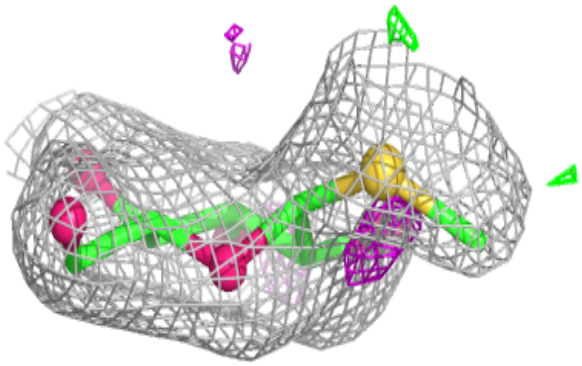


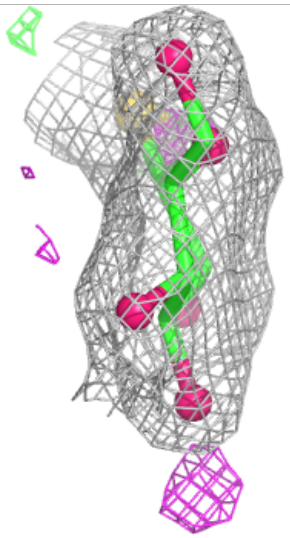


Electron density around HTG V 202:

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

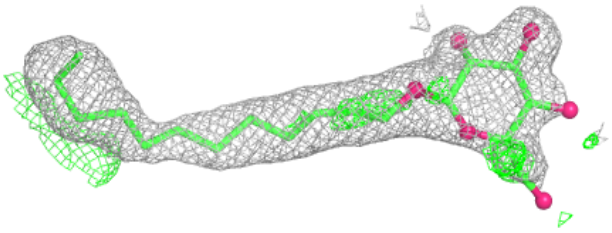


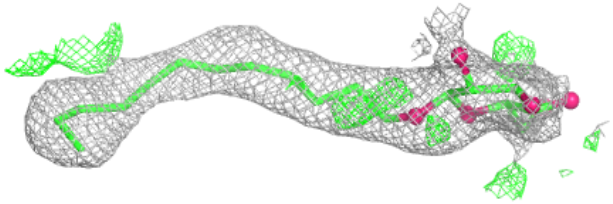


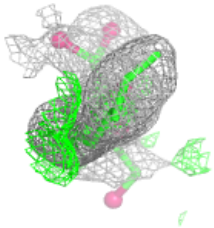


Electron density around LMT T 102:

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

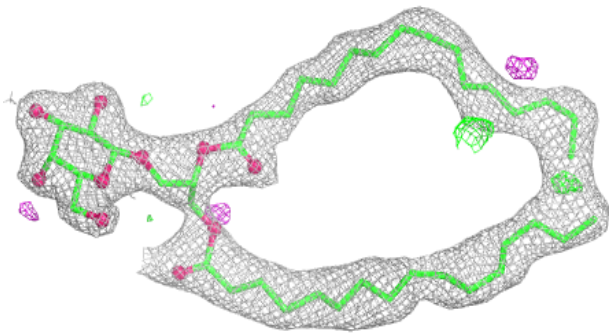


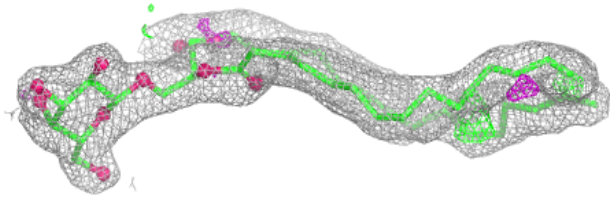


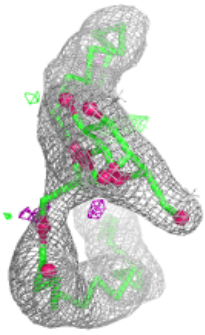


Electron density around LMG a 410:

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

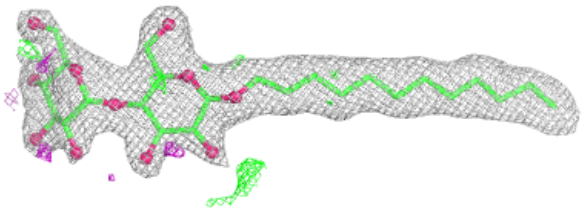


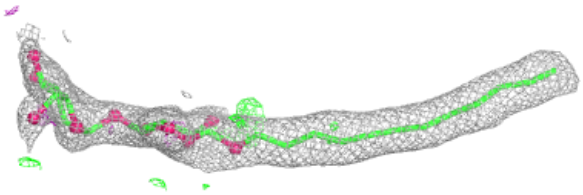


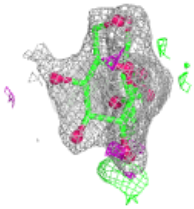


Electron density around LMT M 101:

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

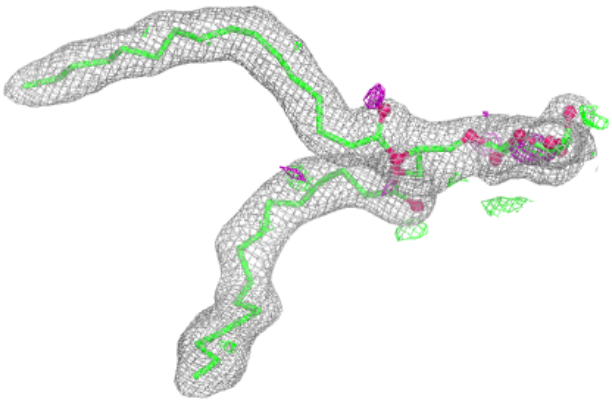


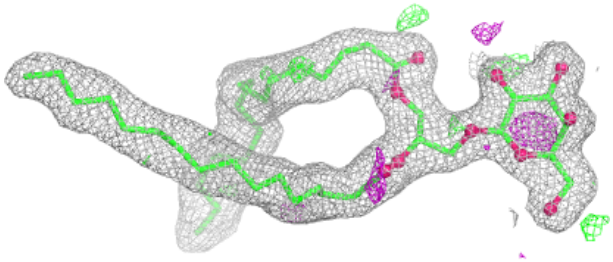


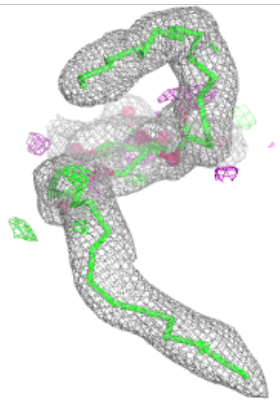


Electron density around LMG B 620:

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

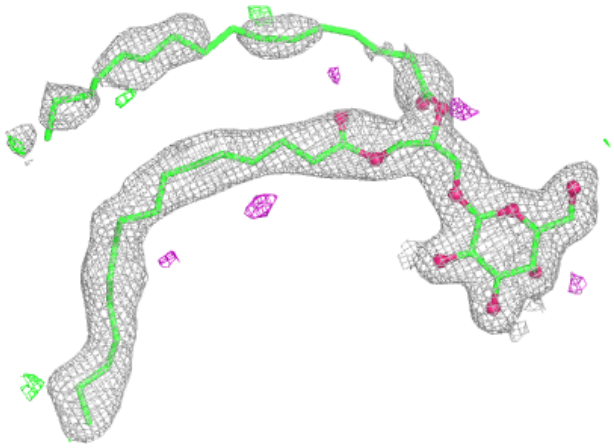


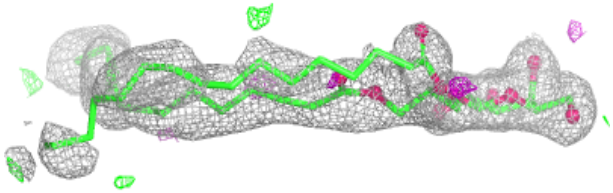


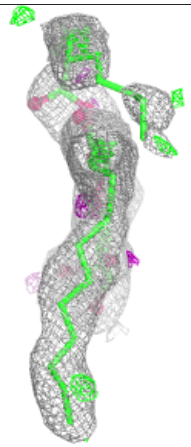


Electron density around LMG c 519:

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

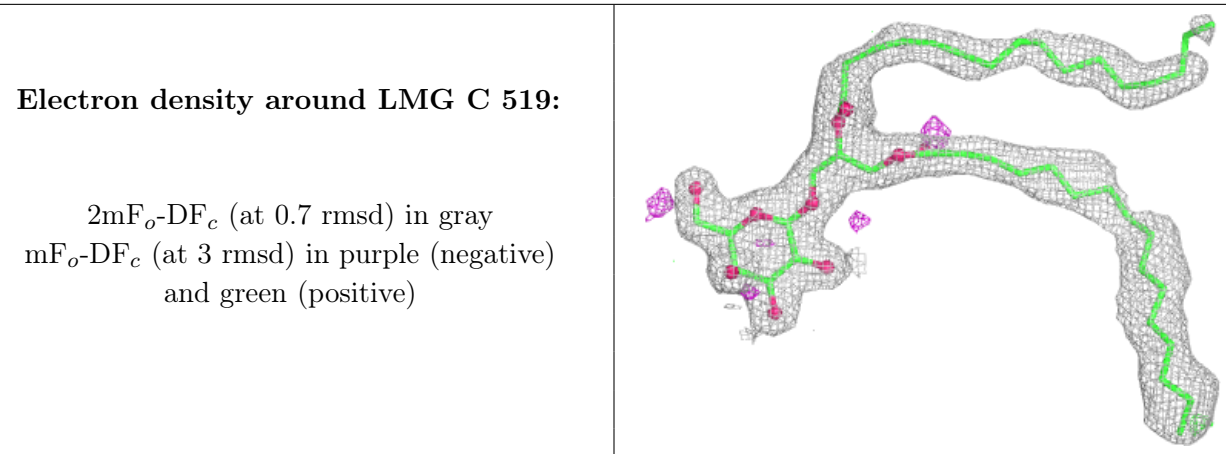






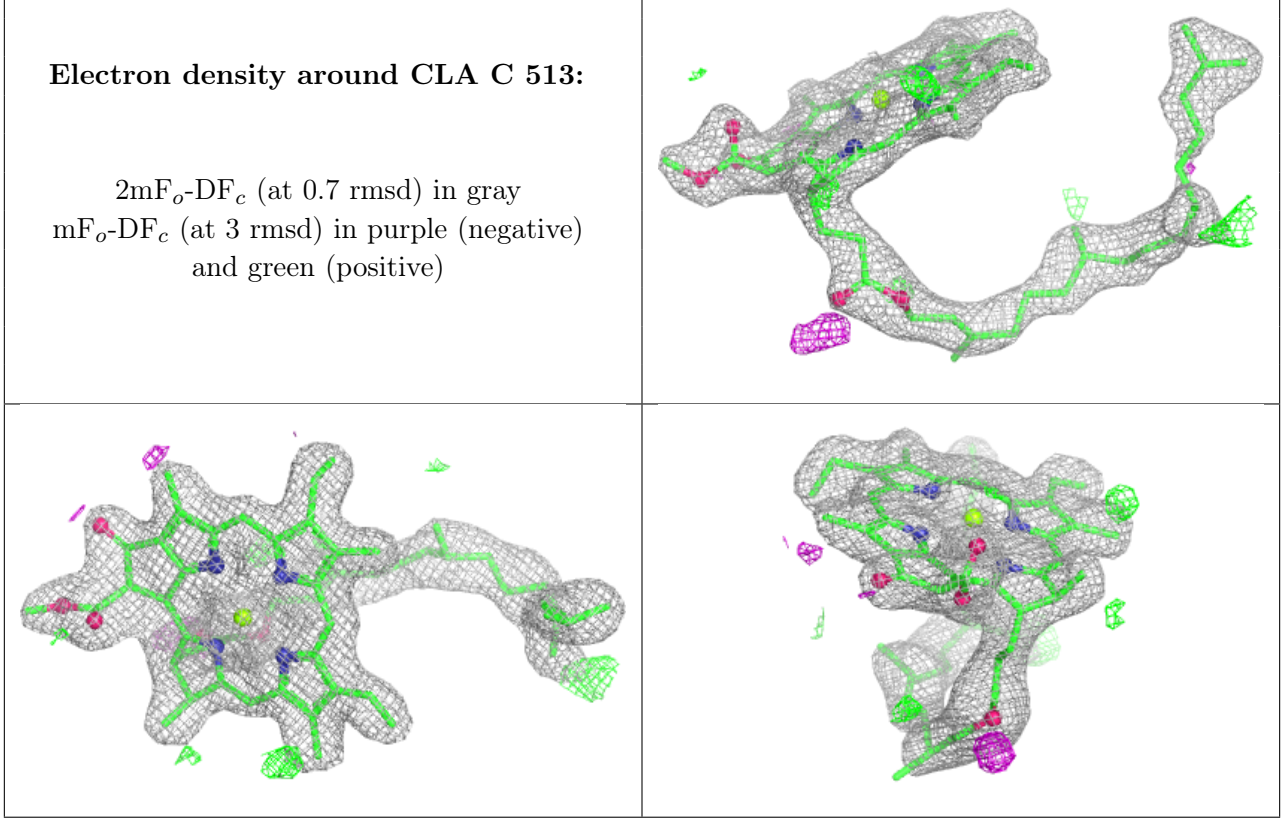
Electron density around LMG C 519:

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



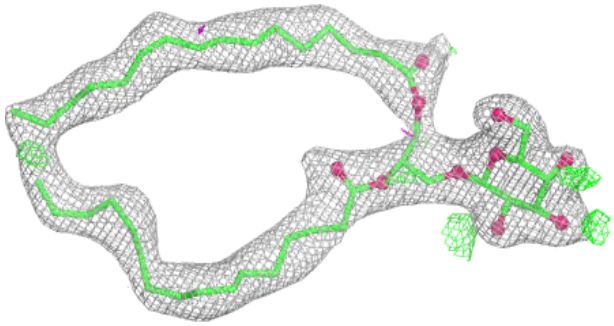
Electron density around CLA C 513:

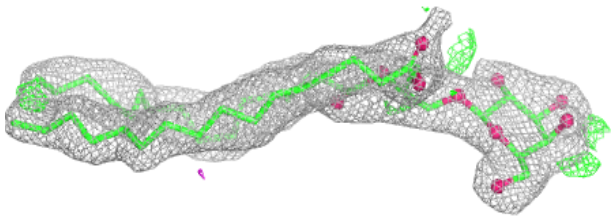
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

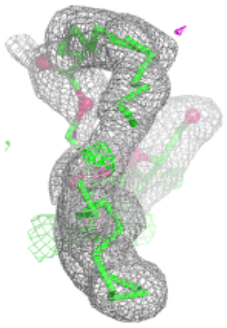


Electron density around LMG A 407:

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

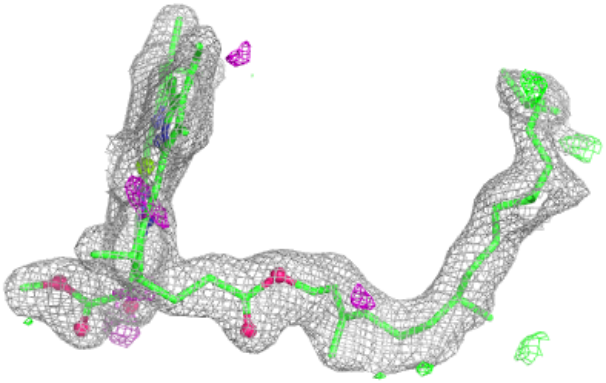


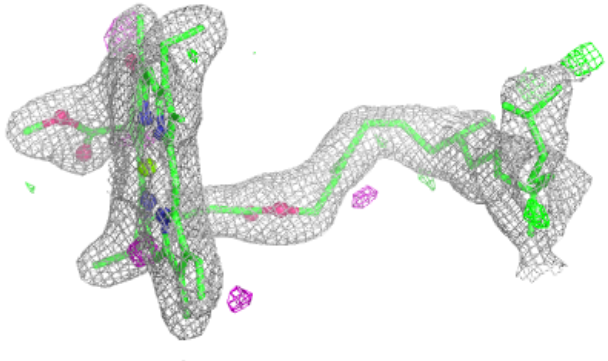


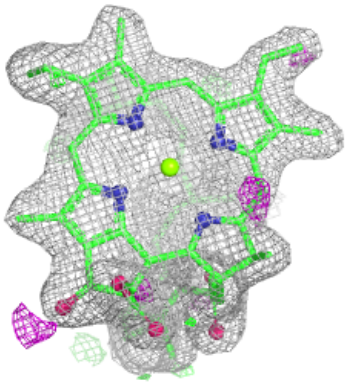


Electron density around CLA C 506:

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

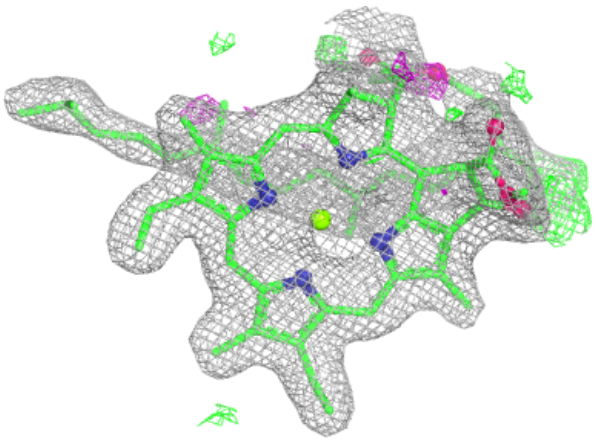


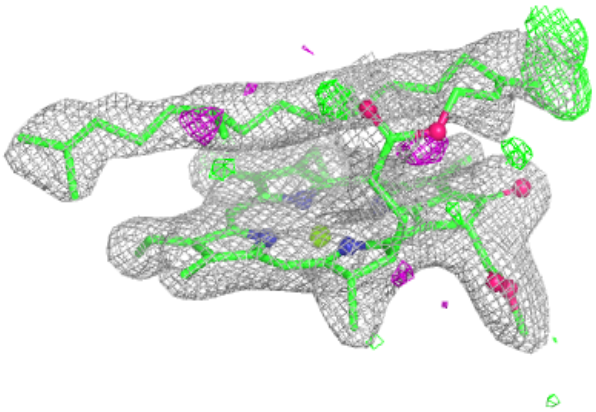


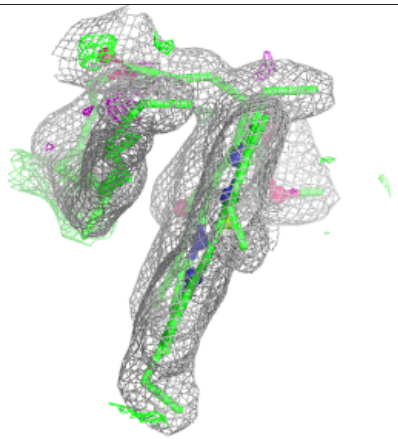


Electron density around CLA b 603:

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

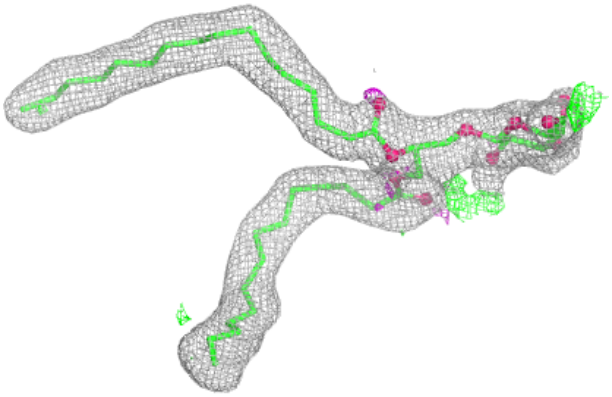


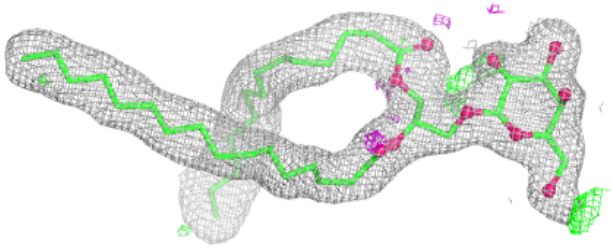


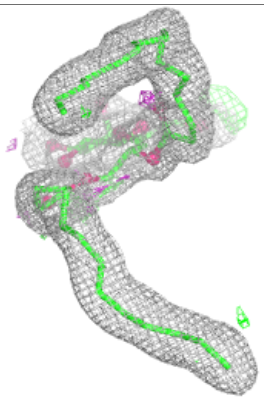


Electron density around LMG b 623:

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

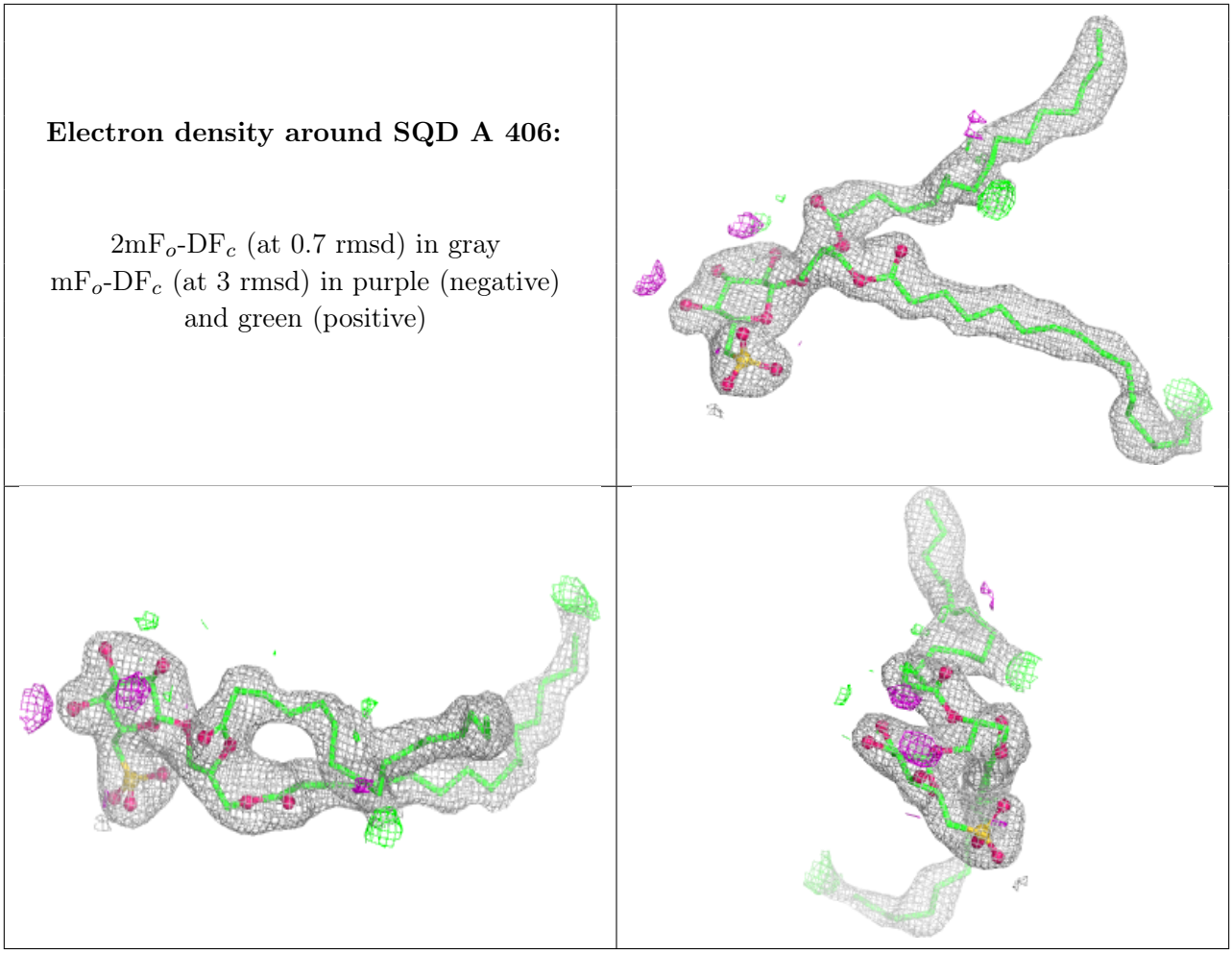






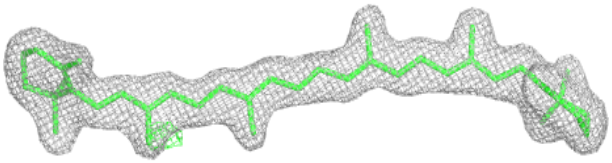
Electron density around SQD A 406:

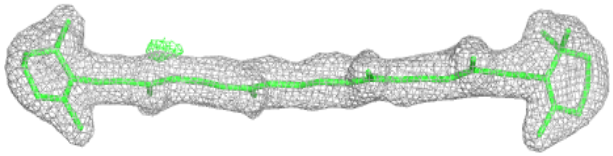
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

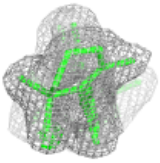


Electron density around BCR C 514:

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

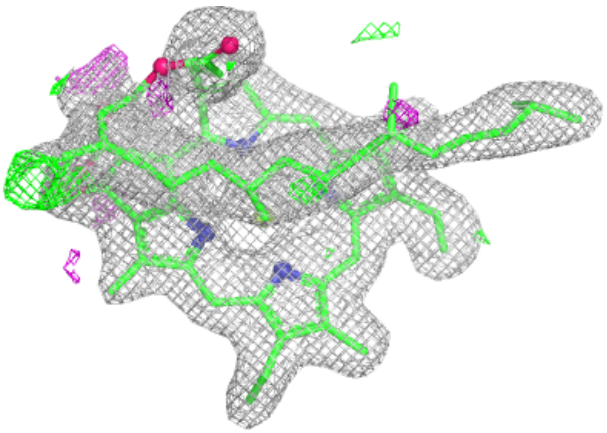


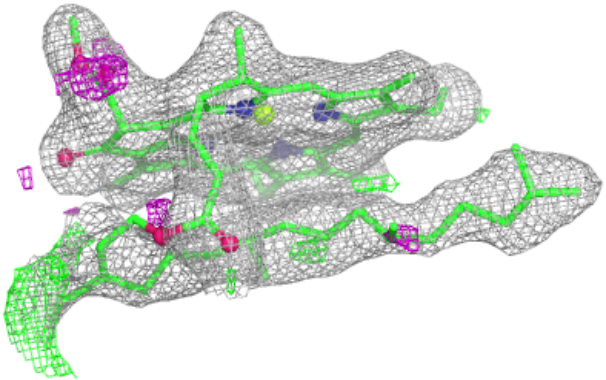


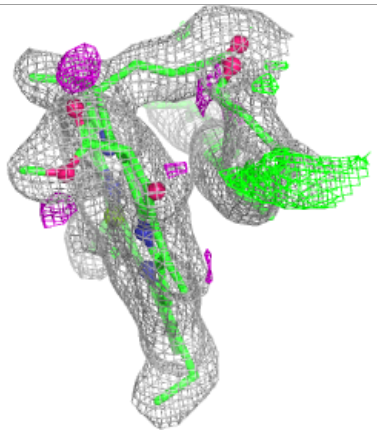


Electron density around CLA B 602:

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

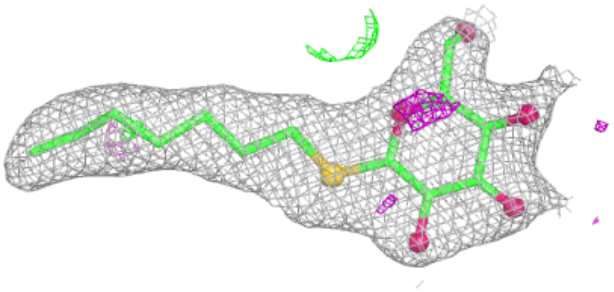


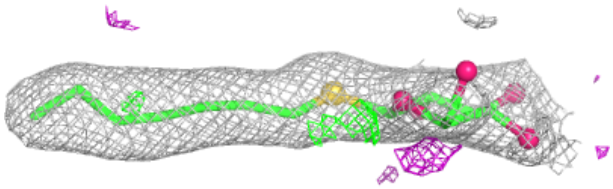


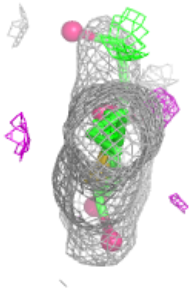


Electron density around HTG b 601:

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

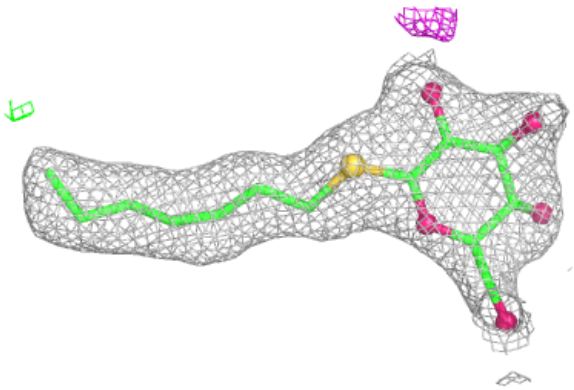


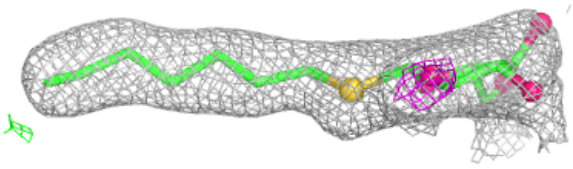


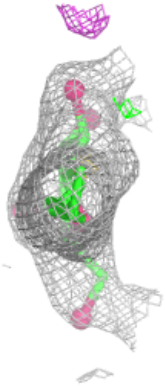


Electron density around HTG B 631:

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

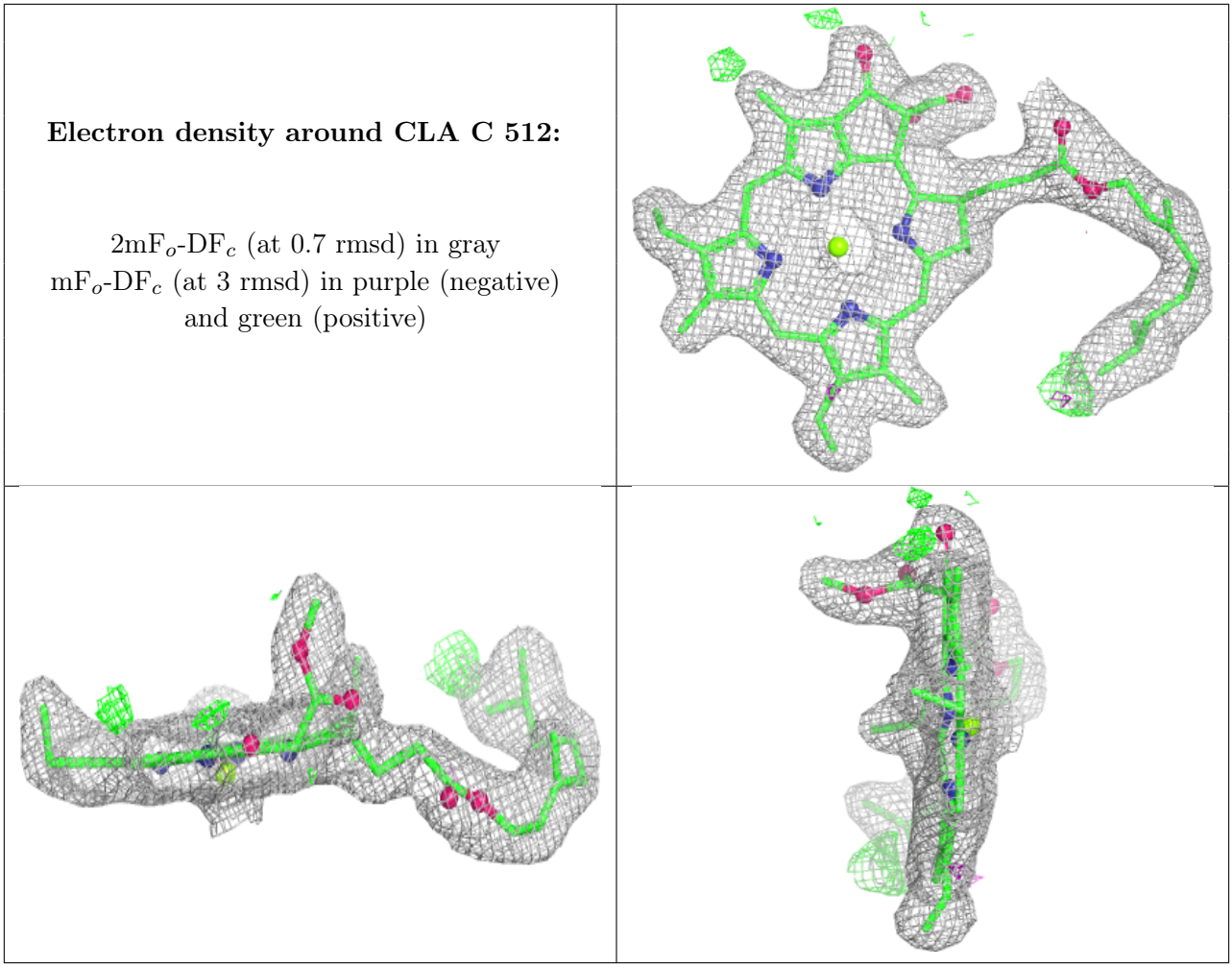






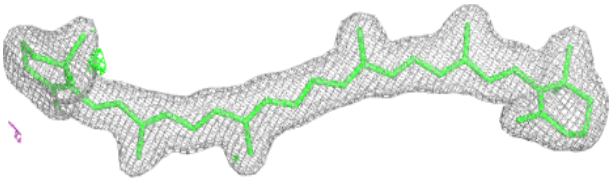
Electron density around CLA C 512:

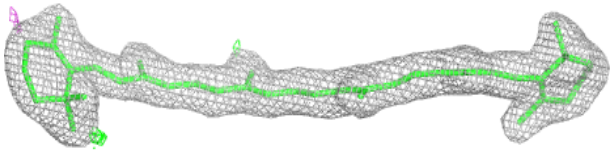
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

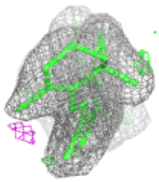


Electron density around BCR K 101:

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

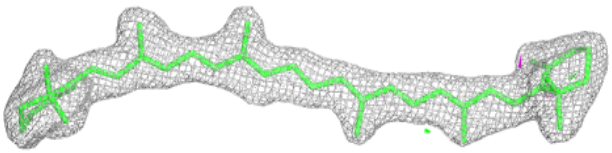


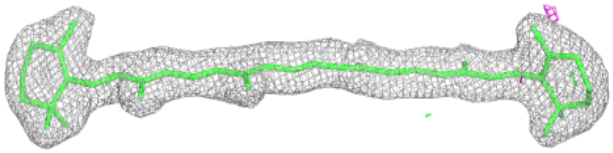


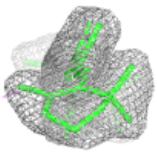


Electron density around BCR k 102:

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

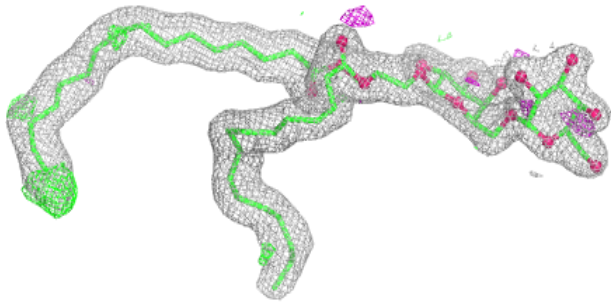


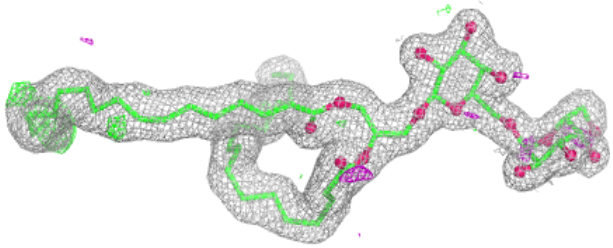




Electron density around DGD h 101:

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

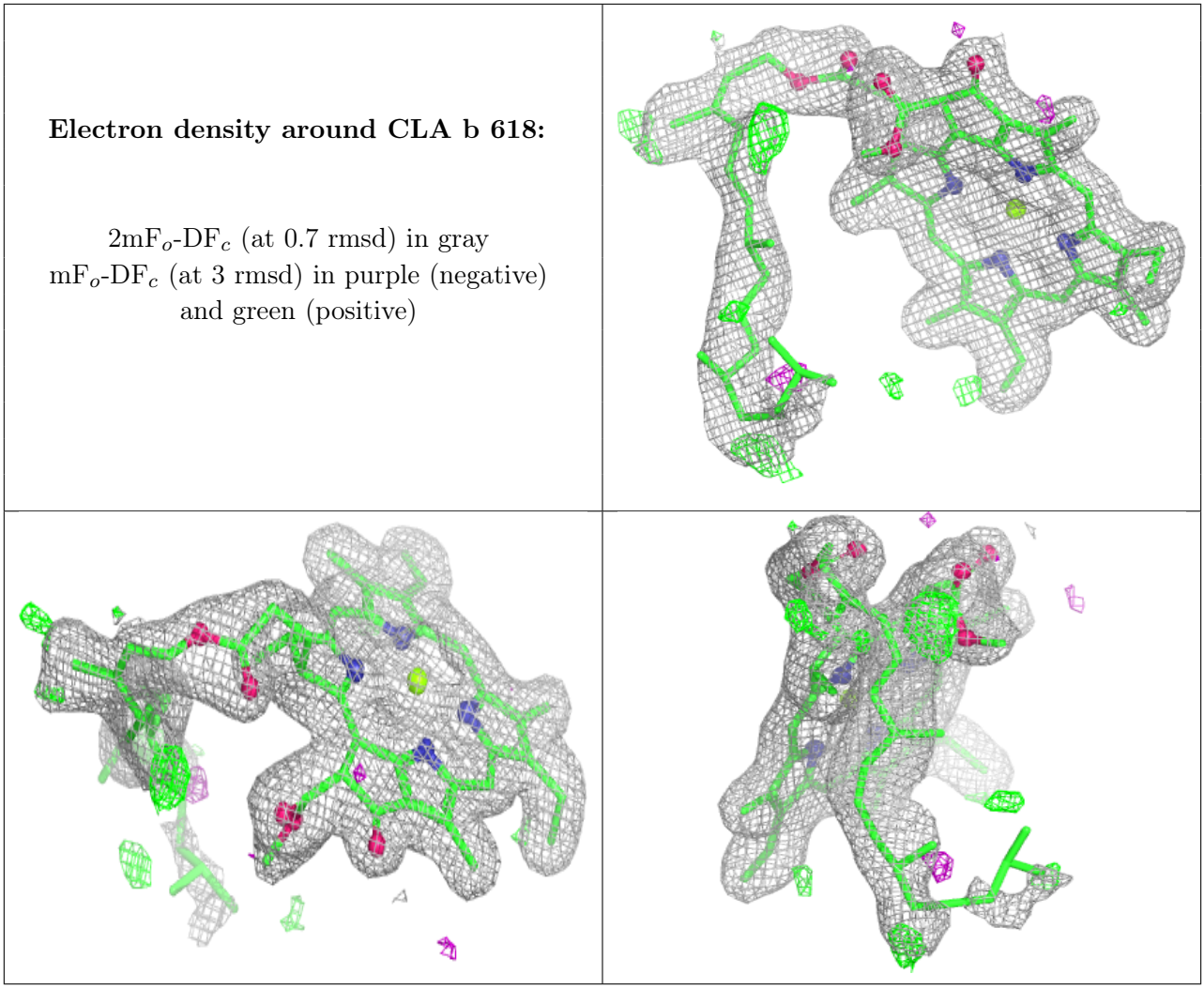






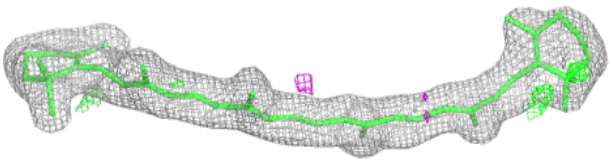
Electron density around CLA b 618:

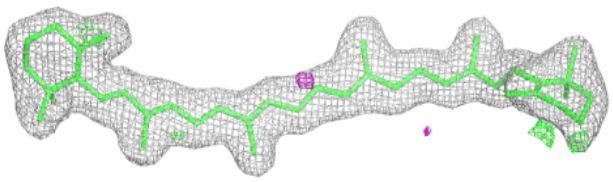
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

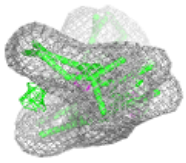


Electron density around BCR D 405:

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

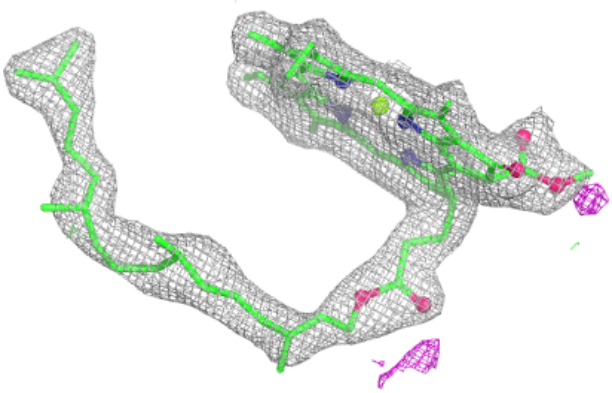


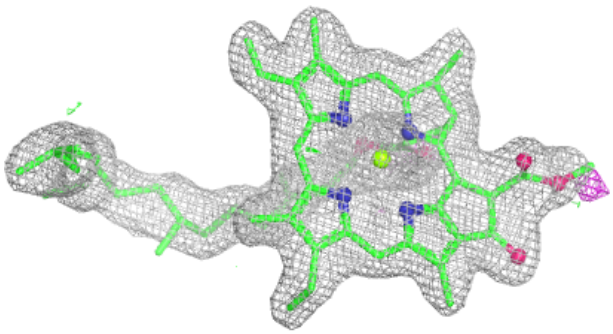


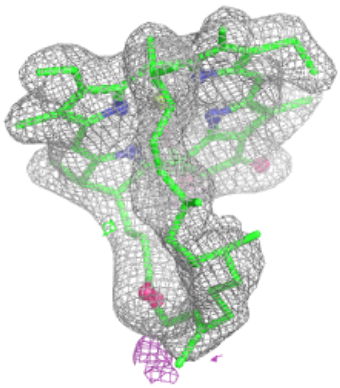


Electron density around CLA c 513:

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

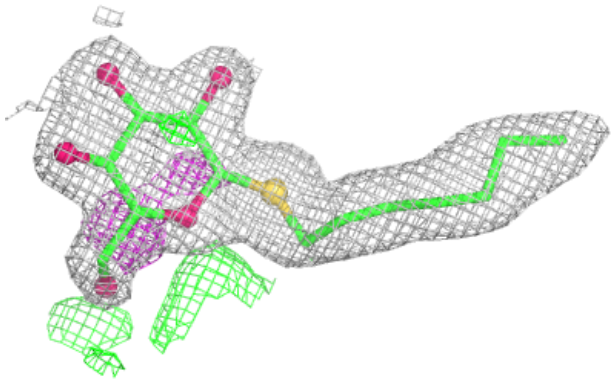


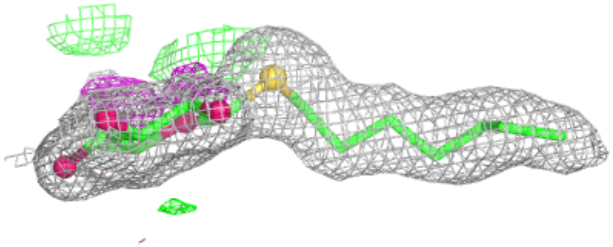


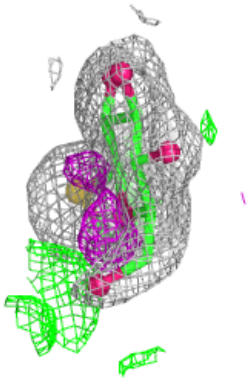


Electron density around HTG B 621:

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

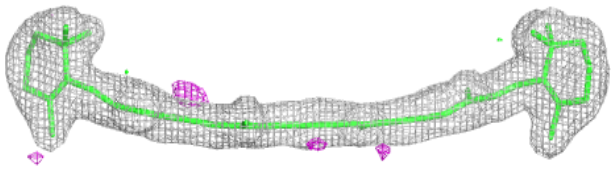


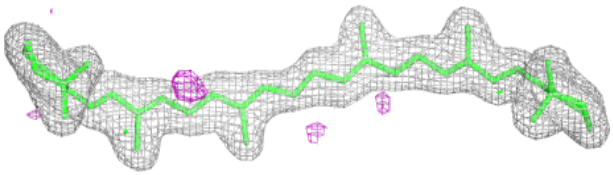


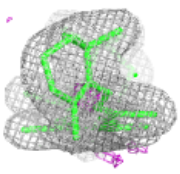


Electron density around BCR K 102:

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

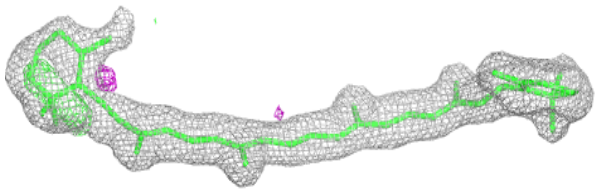


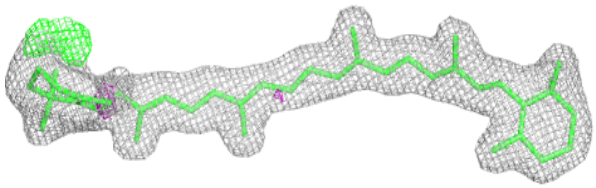


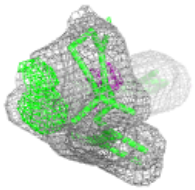


Electron density around BCR d 405:

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

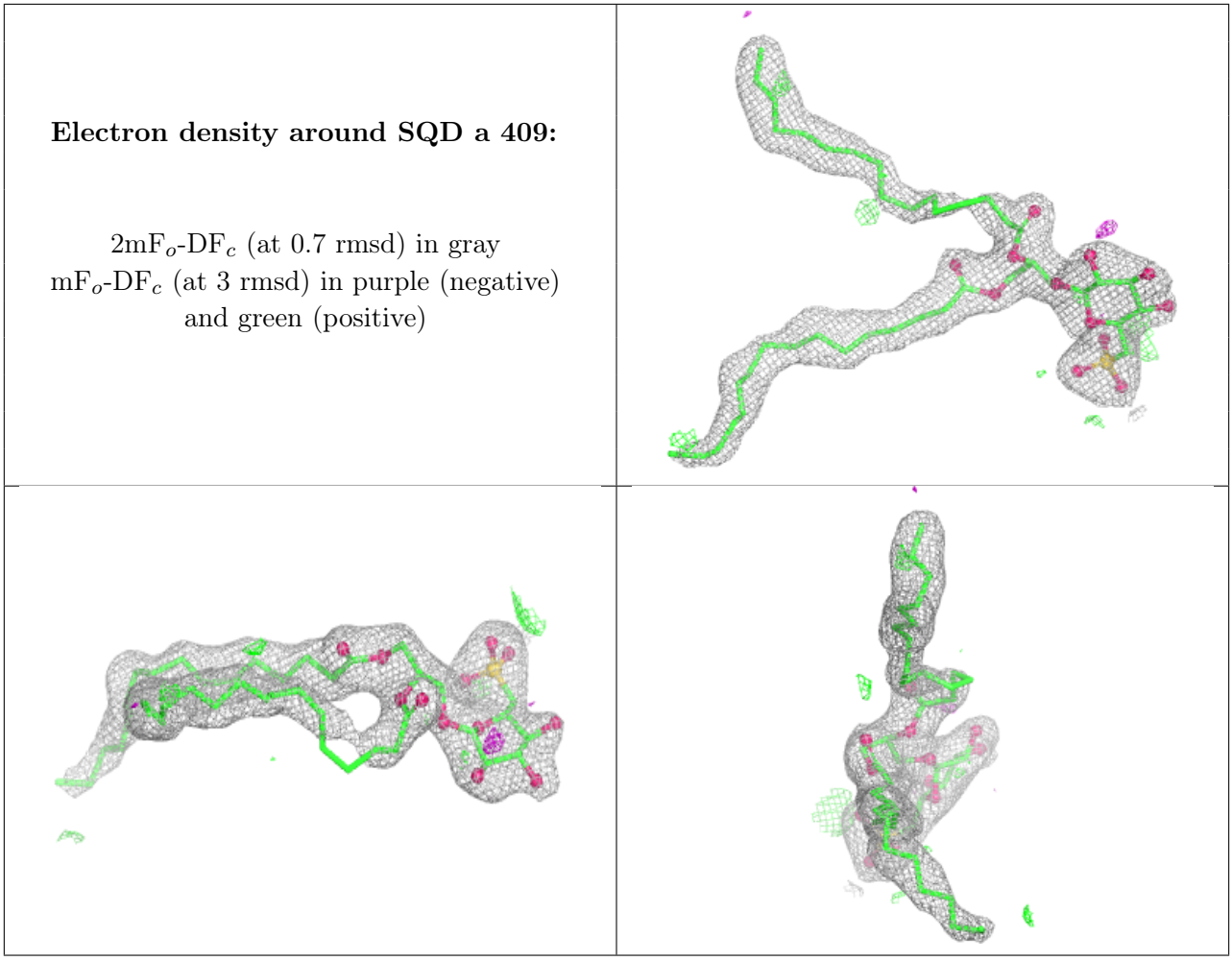






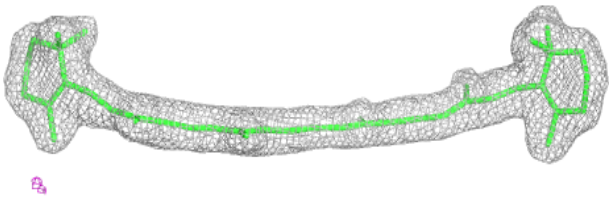
Electron density around SQD a 409:

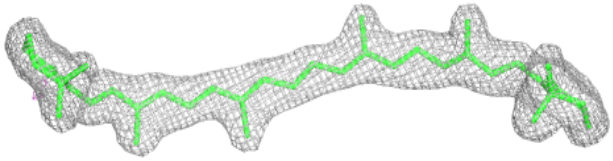
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCR k 101:

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

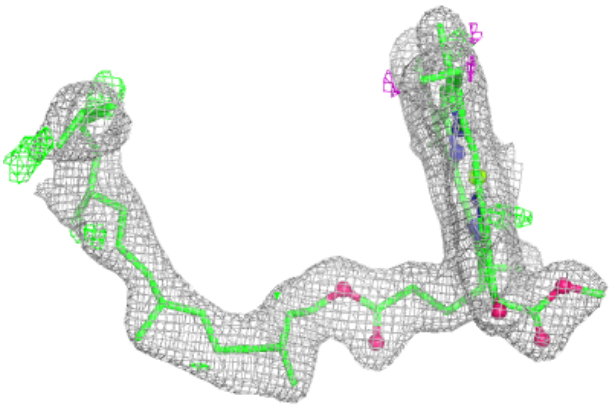


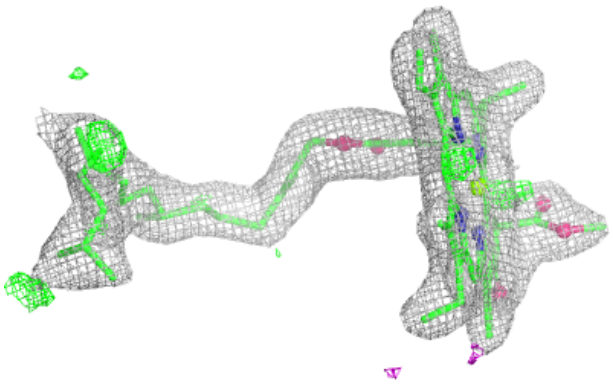


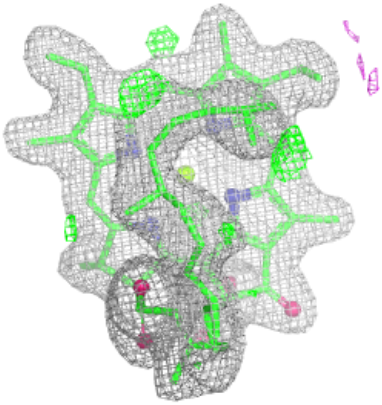


Electron density around CLA c 506:

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

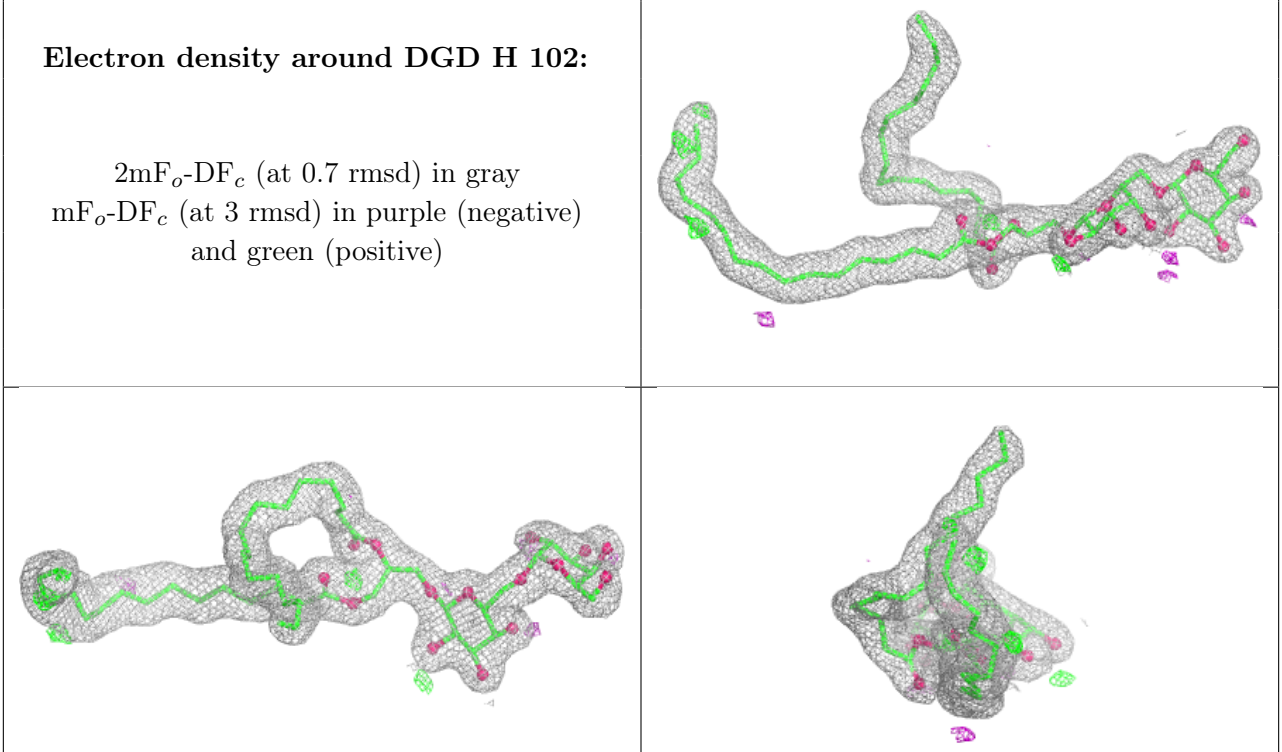






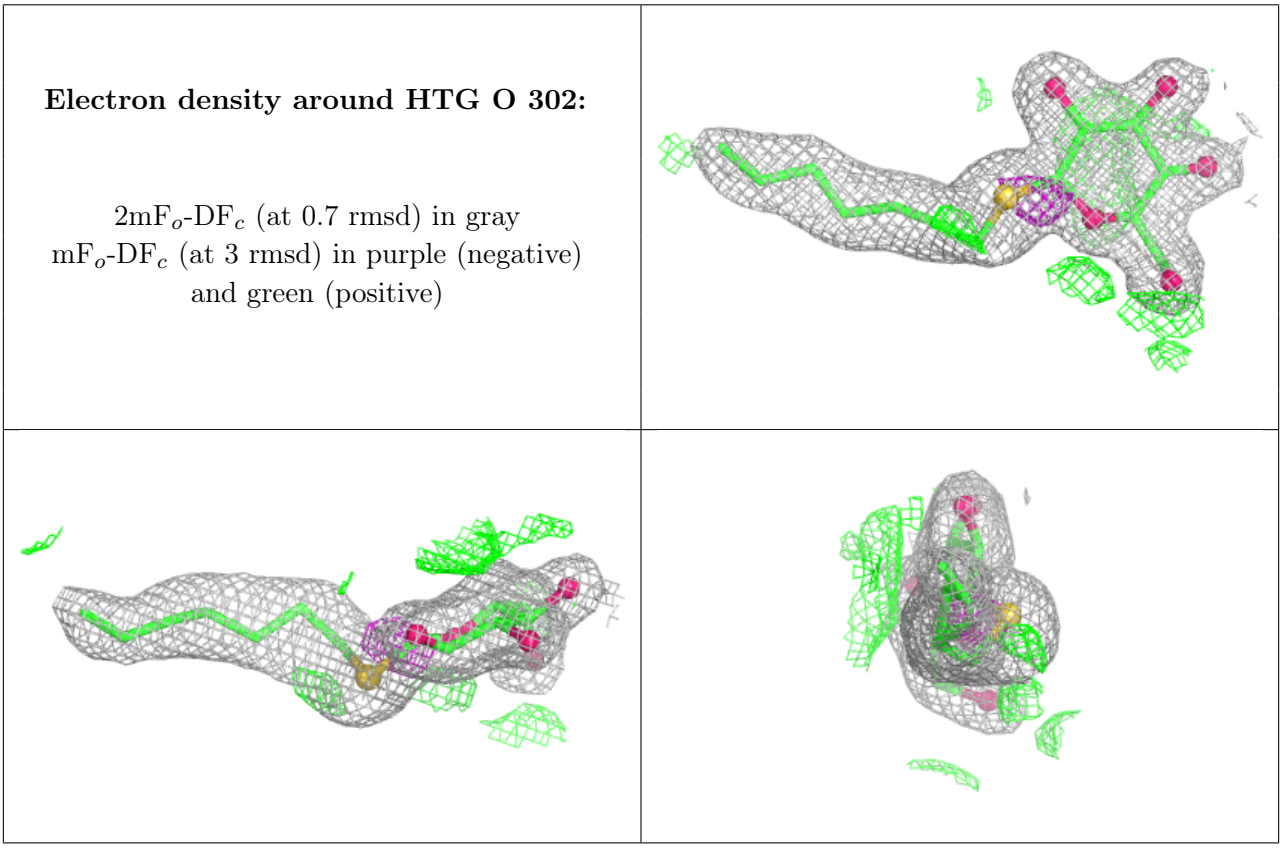
Electron density around DGD H 102:

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



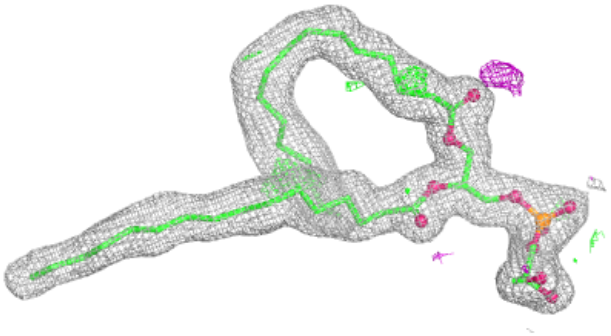
Electron density around HTG O 302:

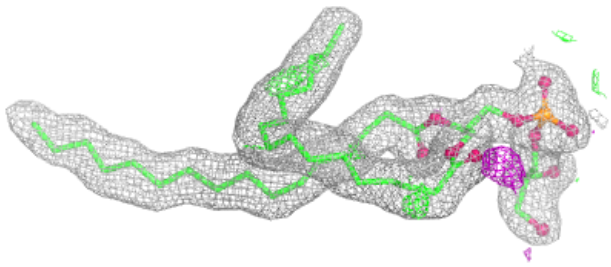
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

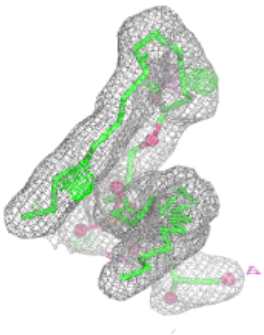


Electron density around LHG D 407:

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

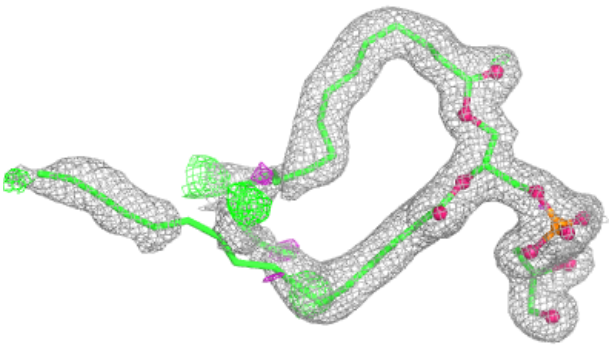


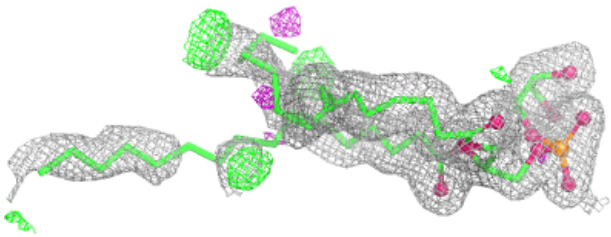


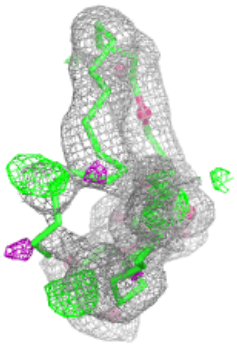


Electron density around LHG D 409:

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

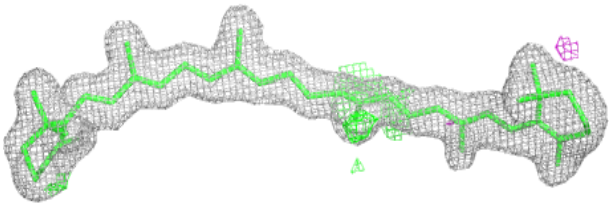


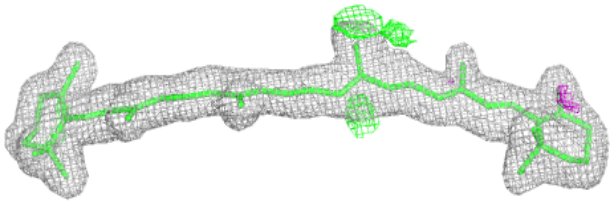


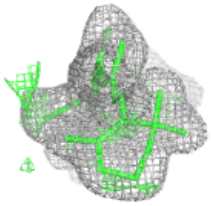


Electron density around BCR t 101:

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

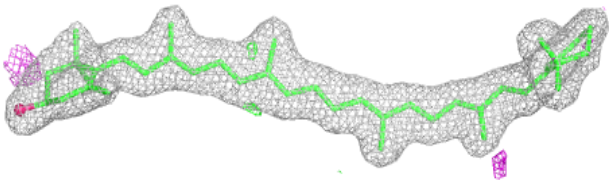


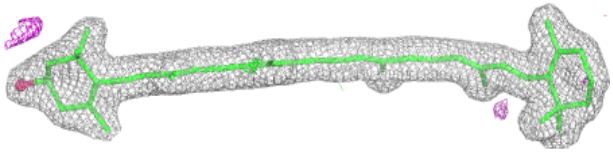


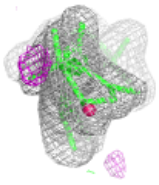


Electron density around RRX H 101:

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

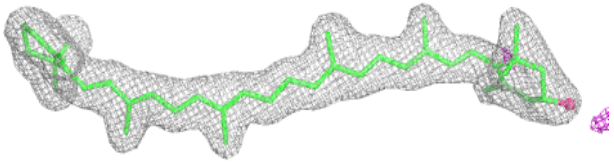


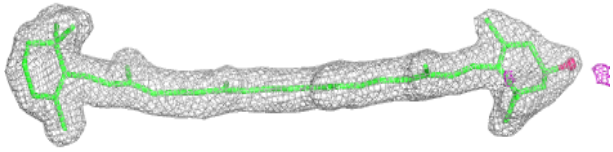


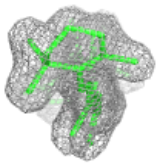


Electron density around RRX x 101:

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

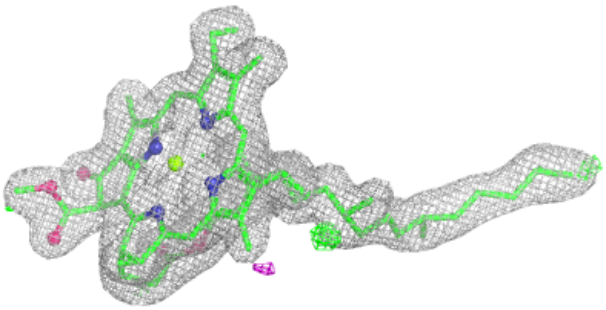


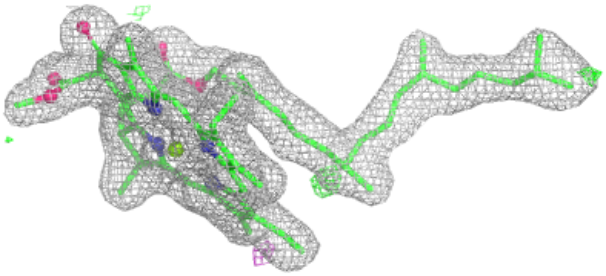


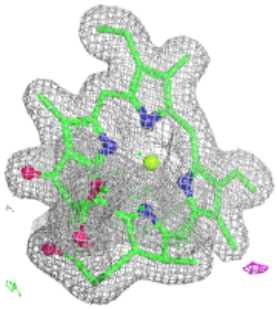


Electron density around CLA C 505:

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

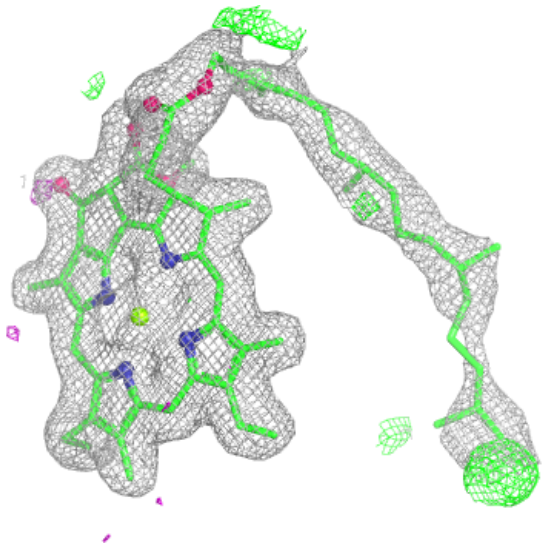


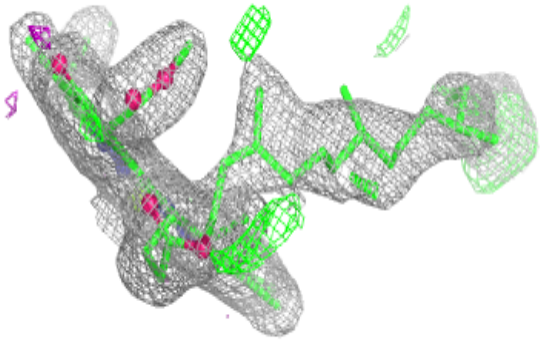


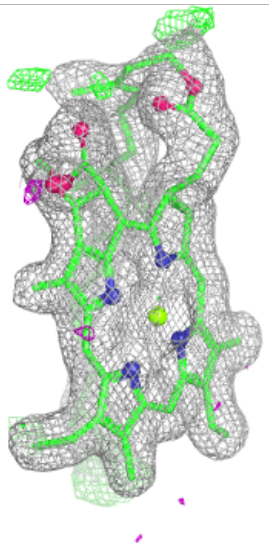


Electron density around CLA B 601:

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

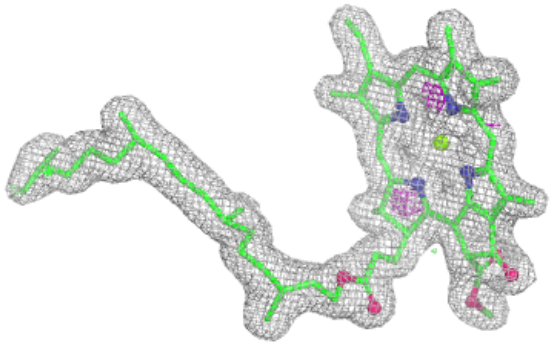


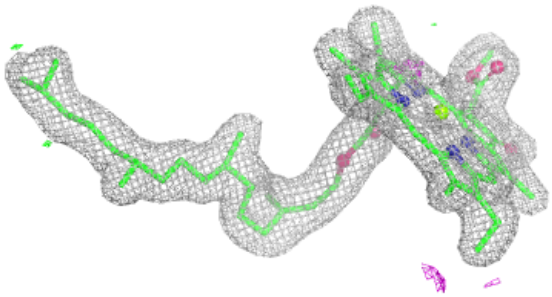


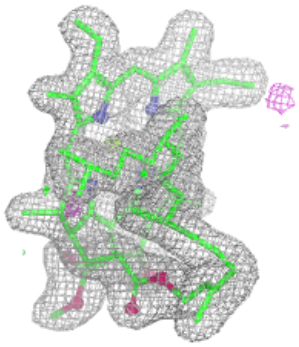


Electron density around CLA c 511:

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

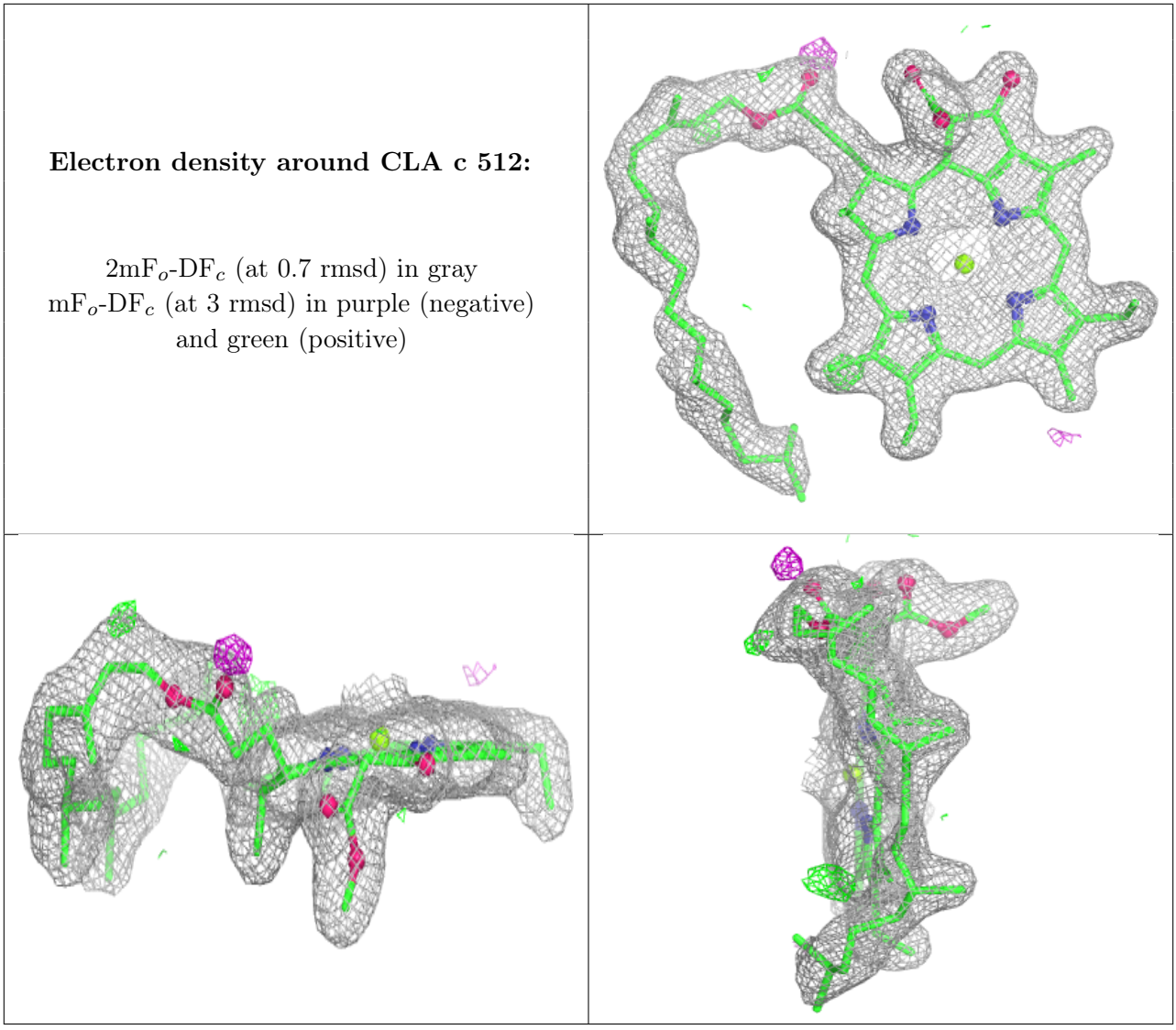






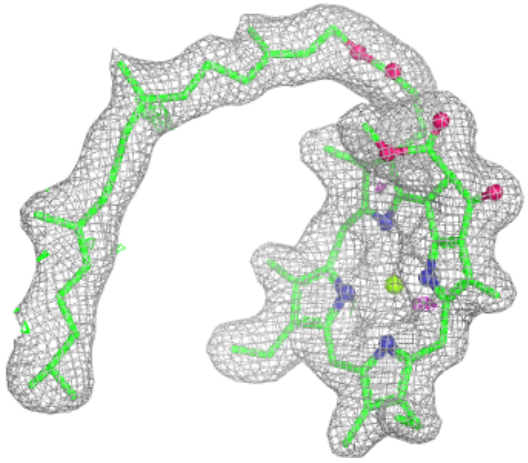
Electron density around CLA c 512:

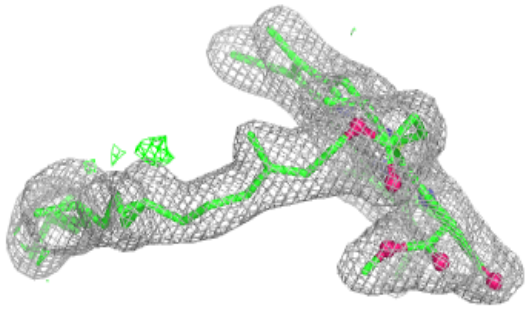
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

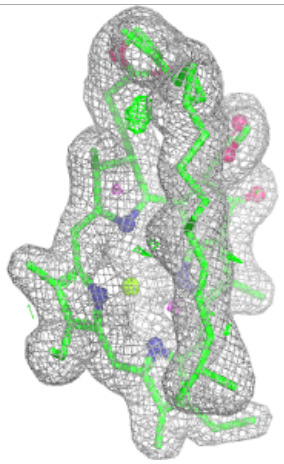


Electron density around CLA C 507:

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

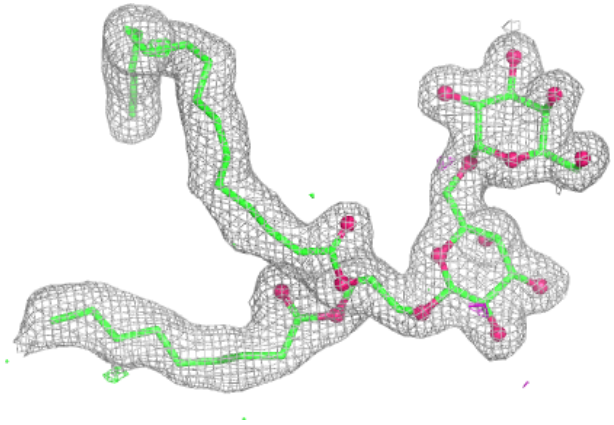


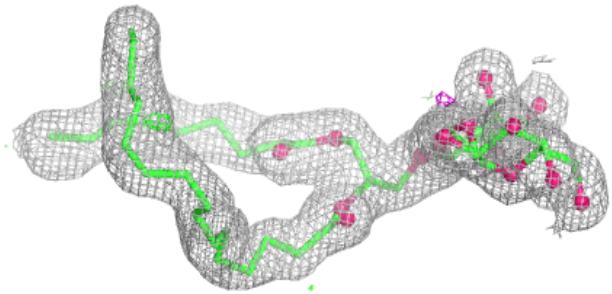




Electron density around DGD C 517:

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

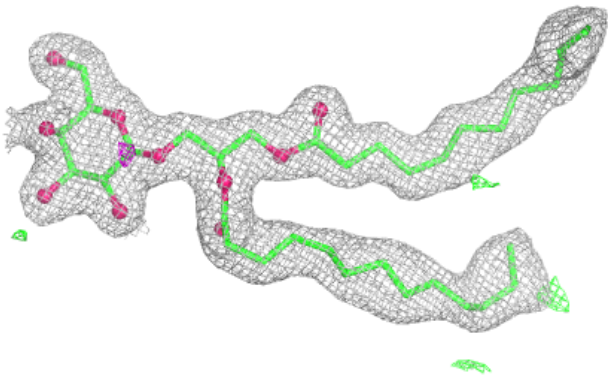


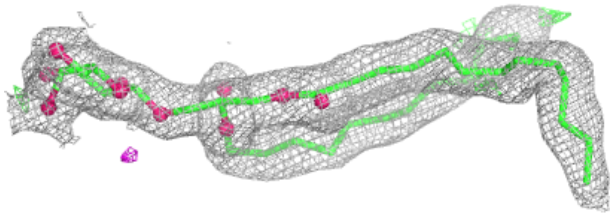


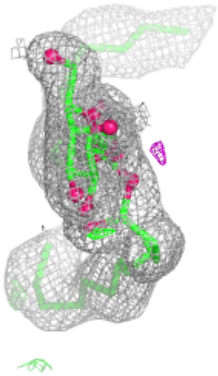


Electron density around LMG j 101:

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

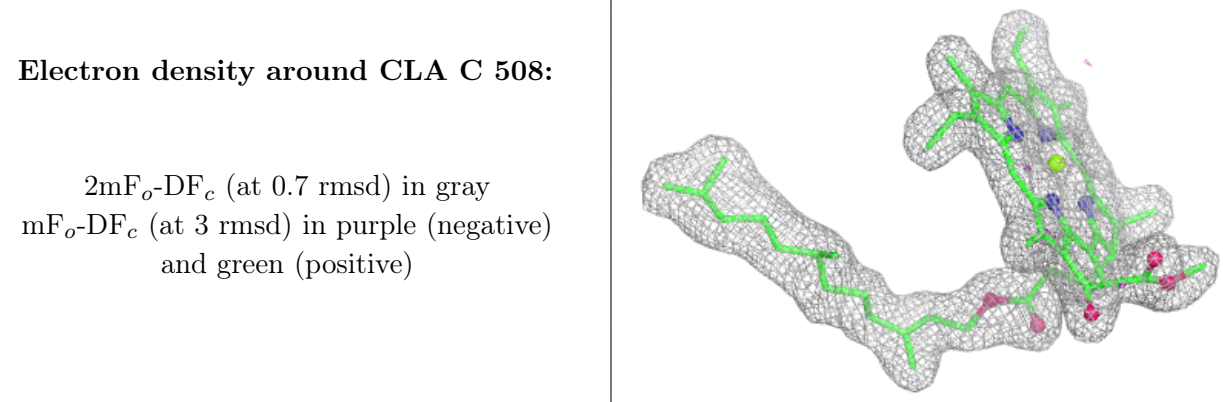






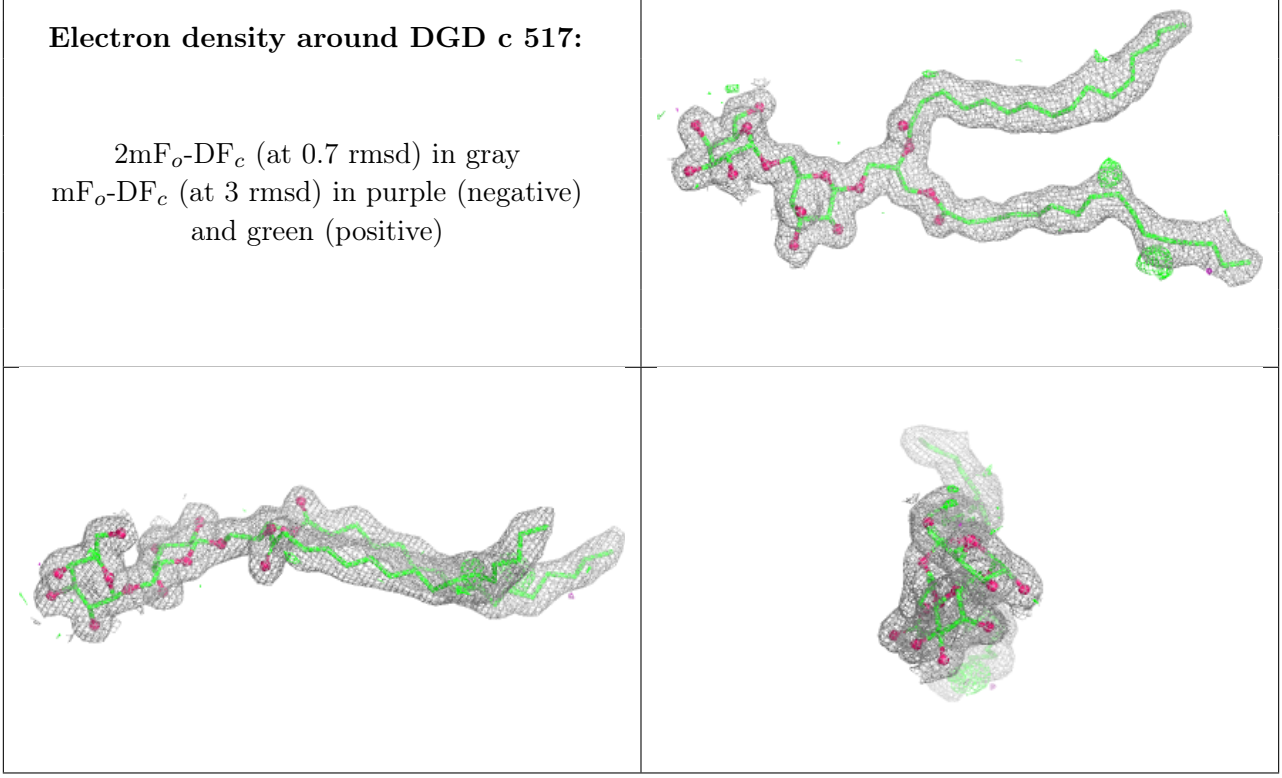
Electron density around CLA C 508:

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



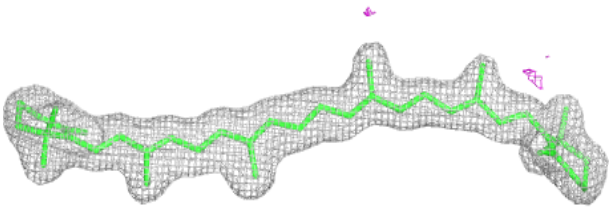
Electron density around DGD c 517:

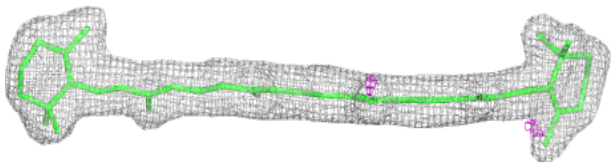
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

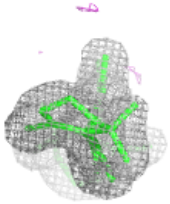


Electron density around BCR C 515:

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

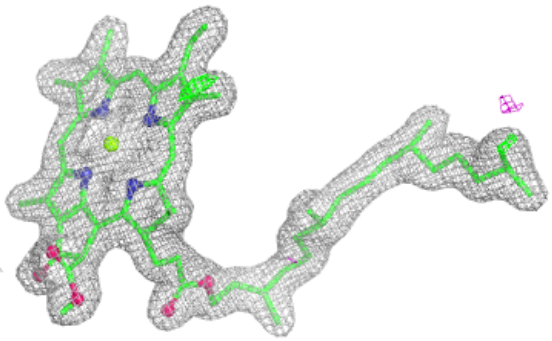


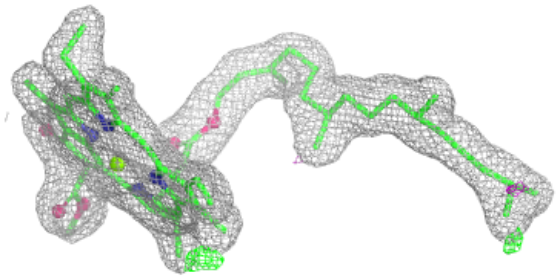


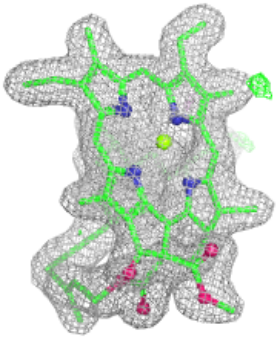


Electron density around CLA C 511:

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

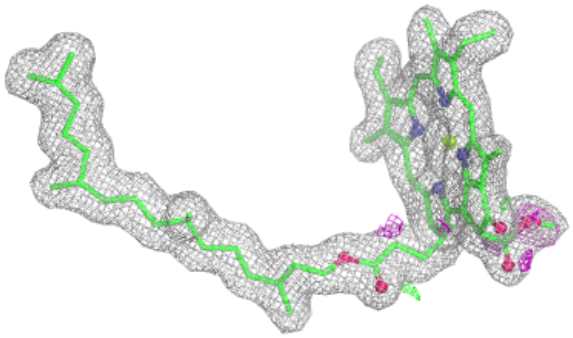


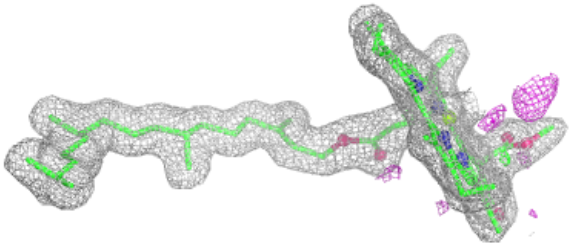




Electron density around CLA B 610:

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

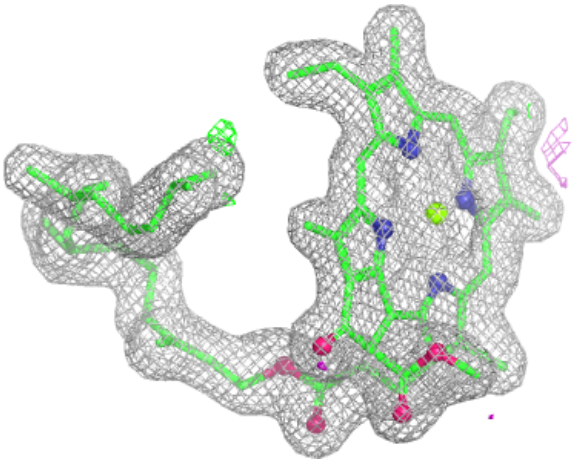


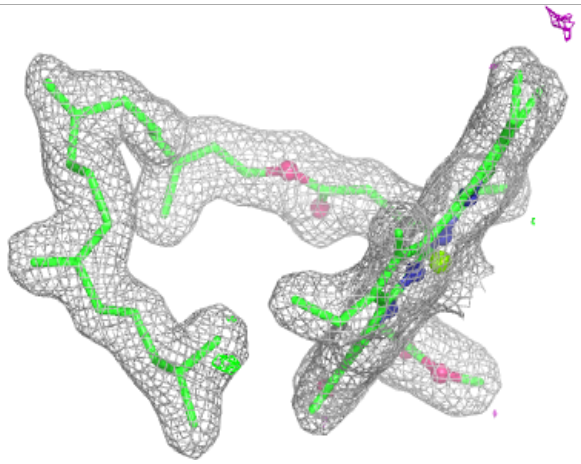


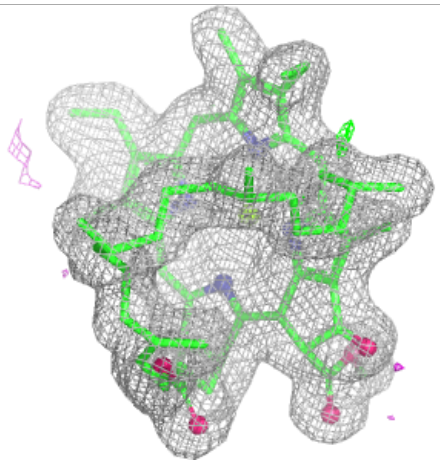


Electron density around CLA C 503:

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

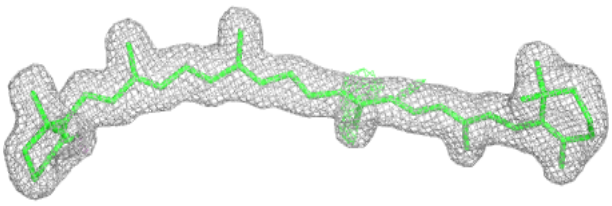


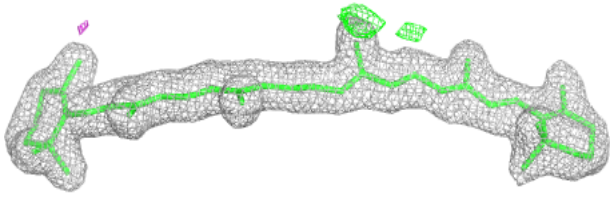


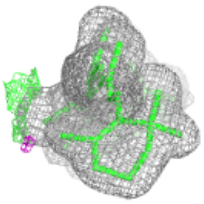


Electron density around BCR T 101:

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

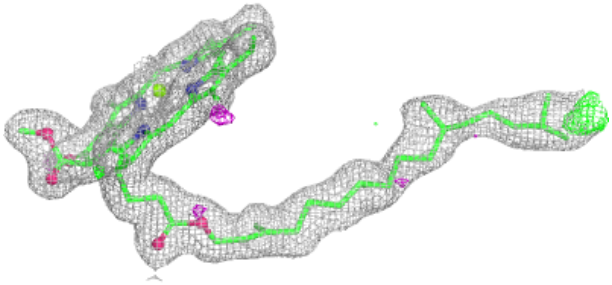


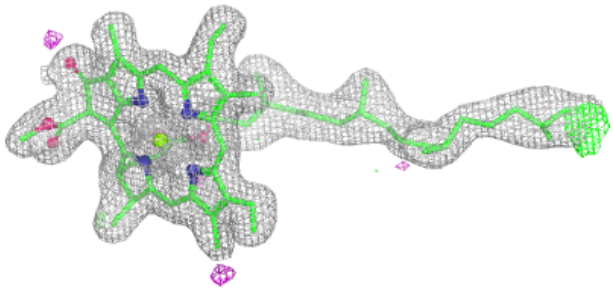


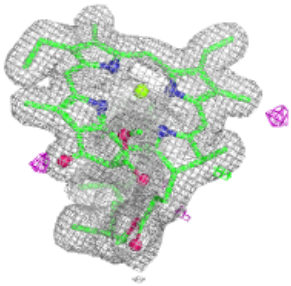


Electron density around CLA C 504:

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

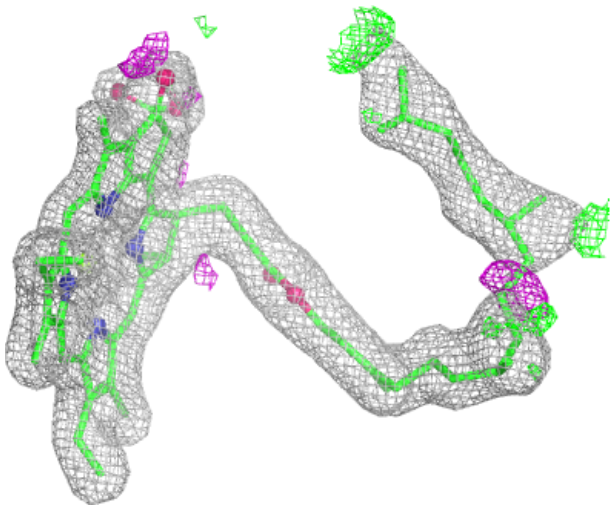


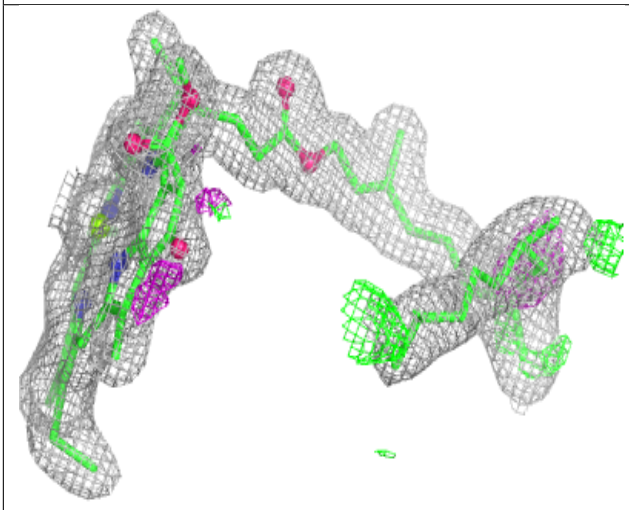


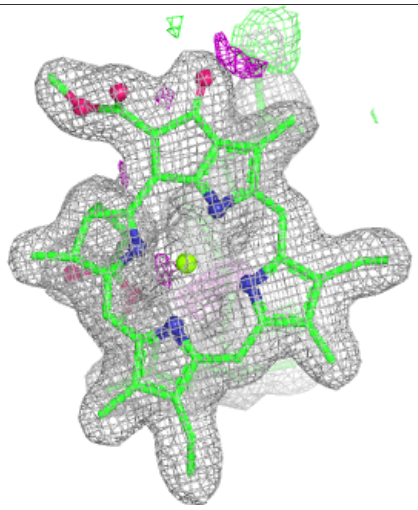


Electron density around CLA b 608:

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

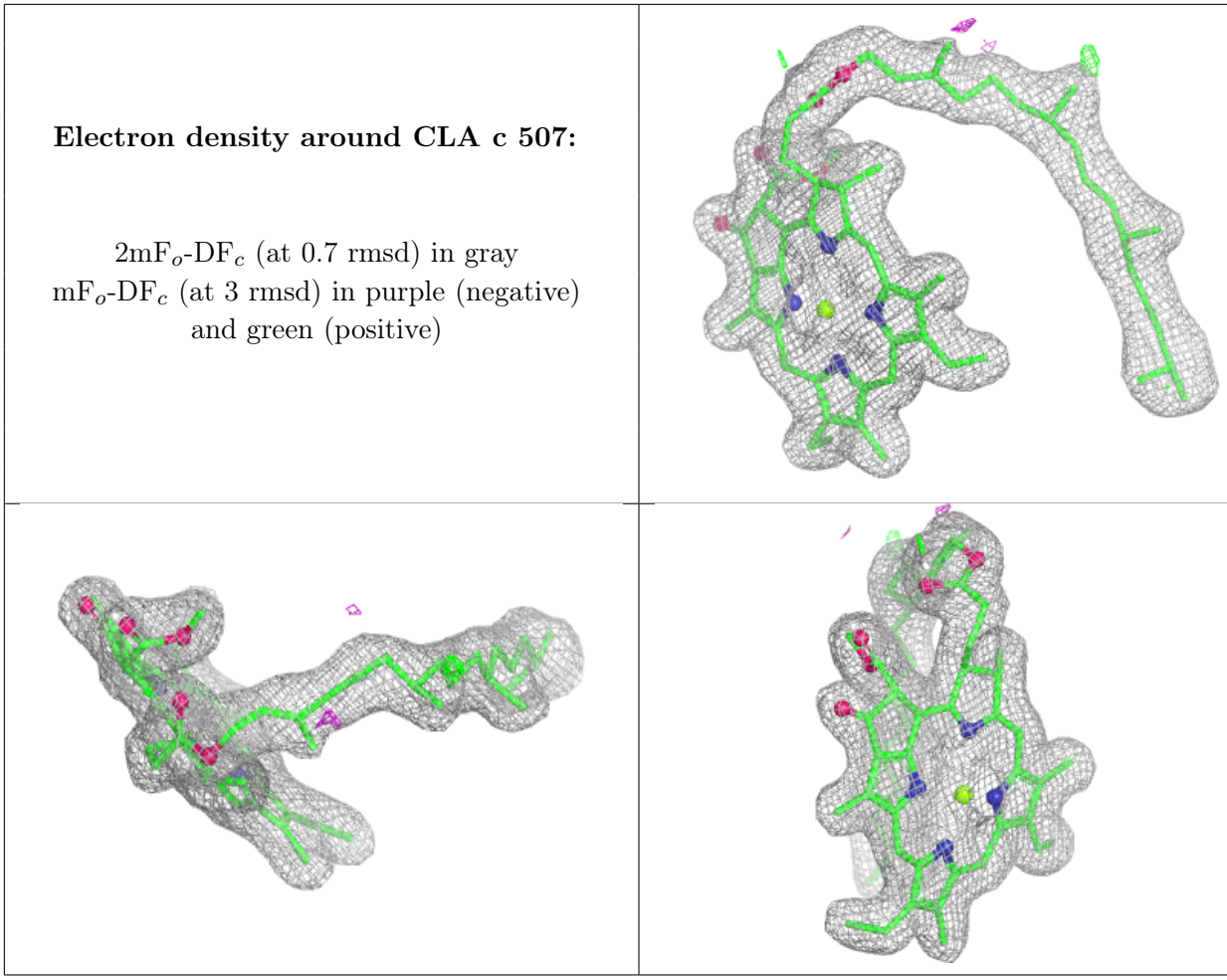






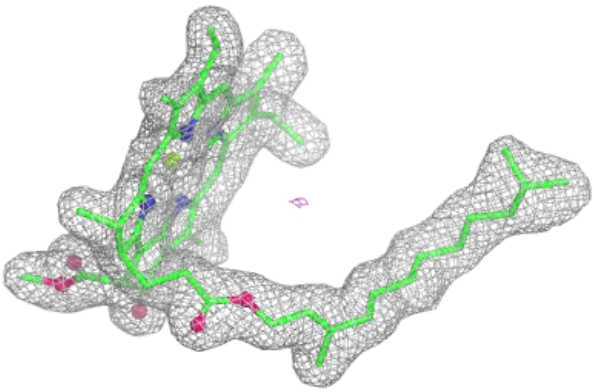
Electron density around CLA c 507:

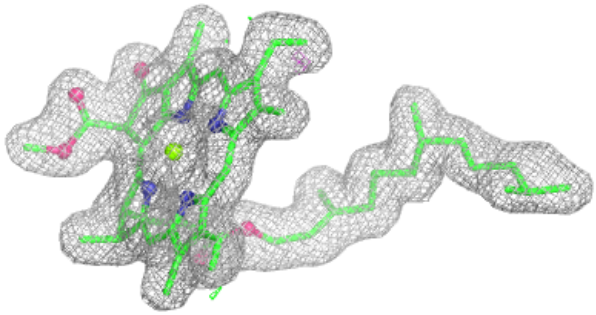
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

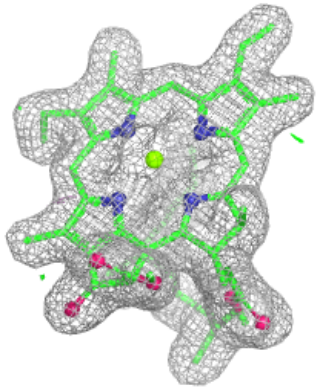


Electron density around CLA c 508:

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

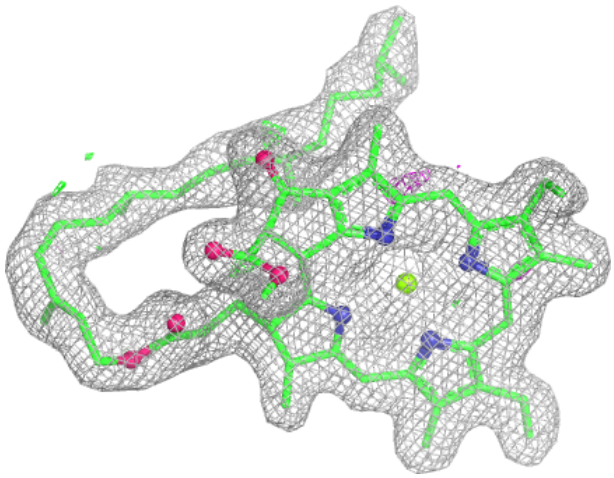


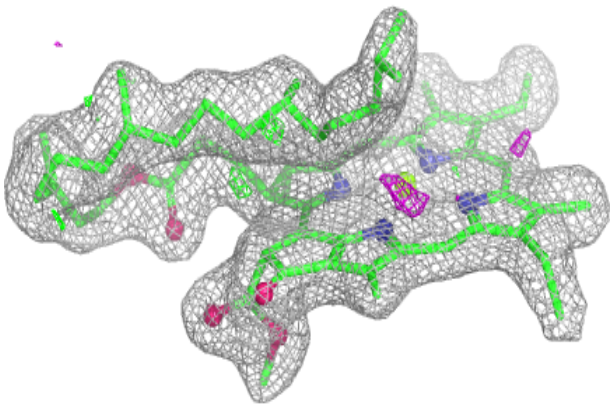


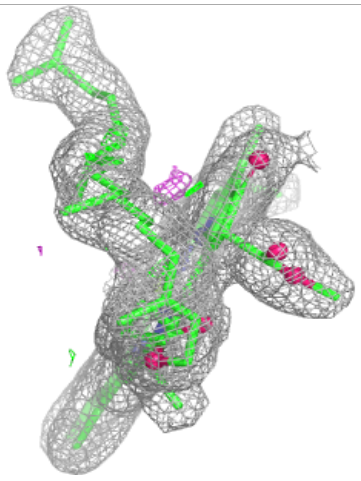


Electron density around CLA c 509:

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

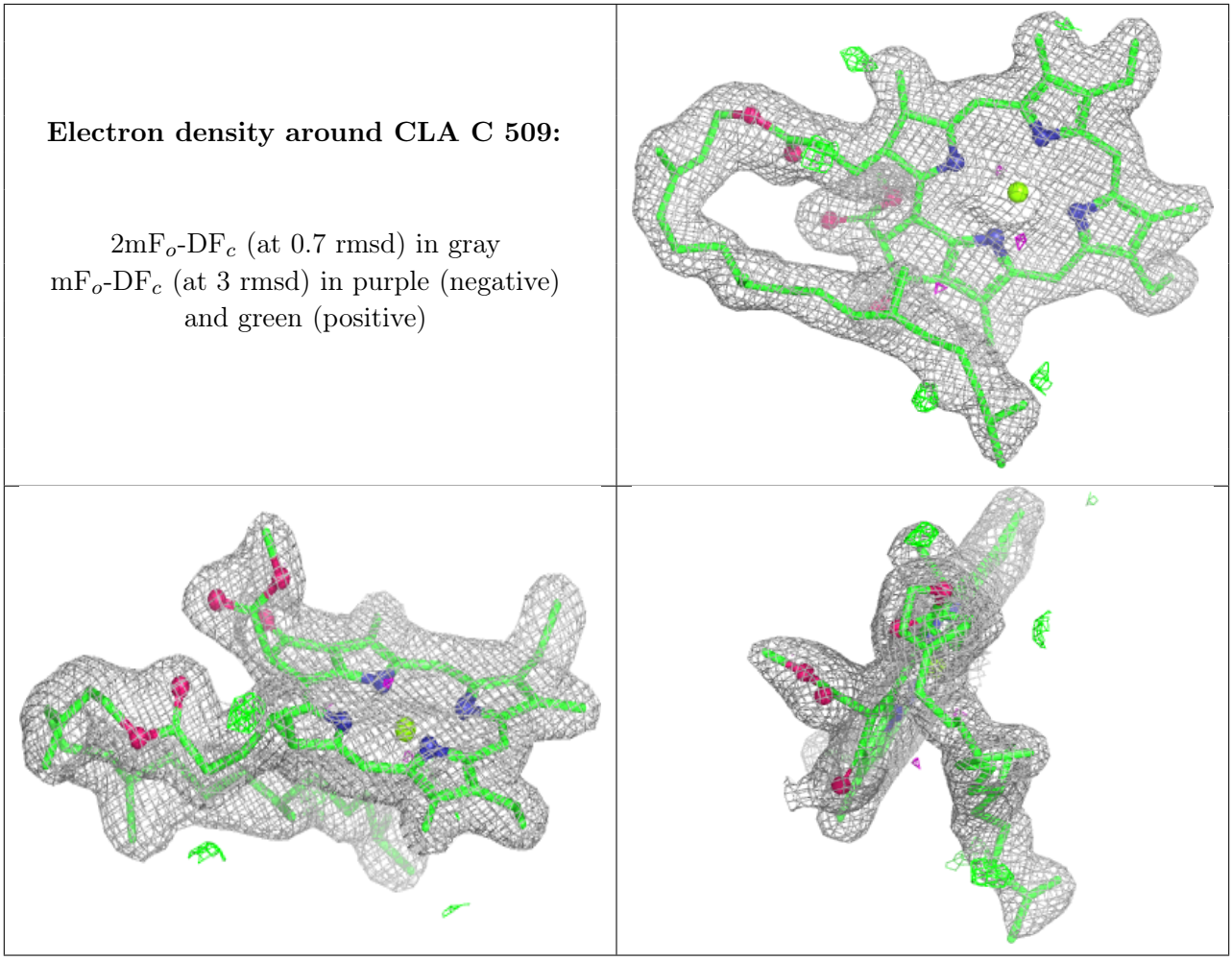






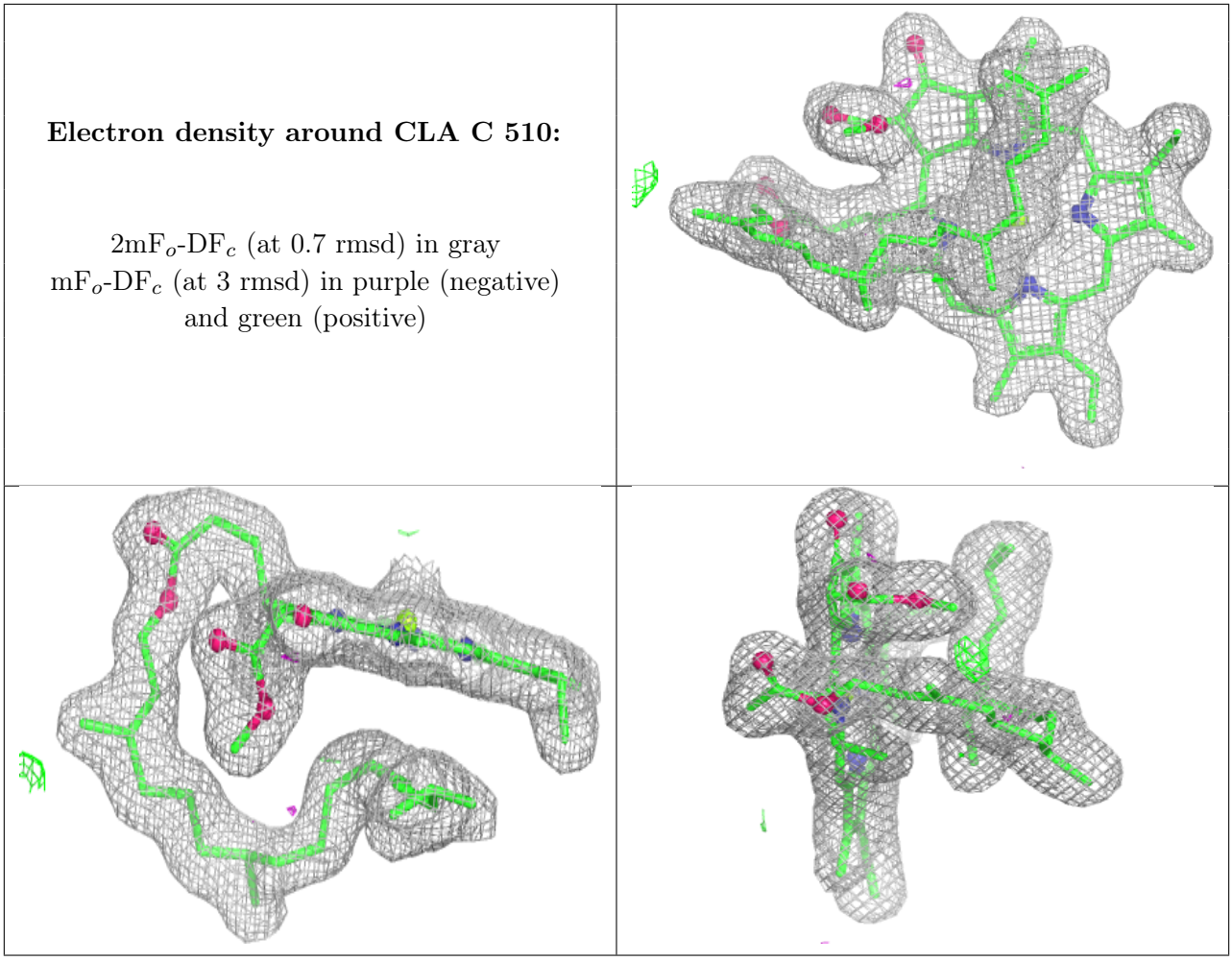
Electron density around CLA C 509:

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



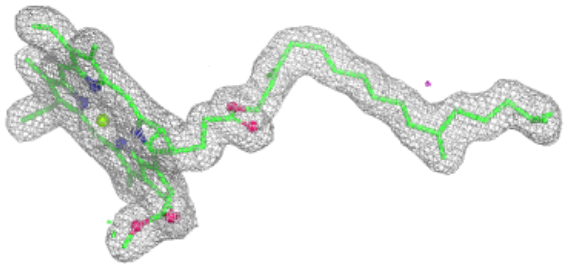
Electron density around CLA C 510:

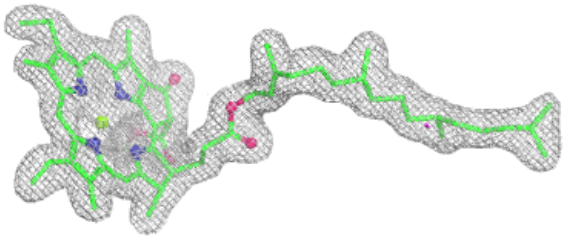
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

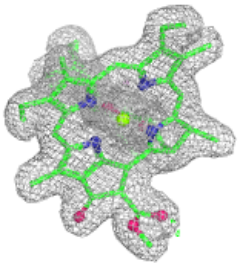


Electron density around CLA C 502:

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

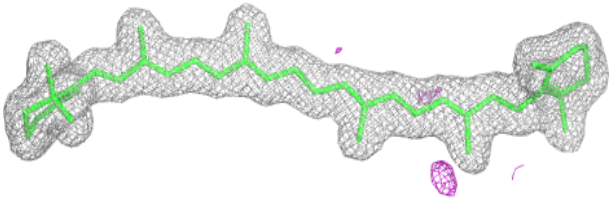


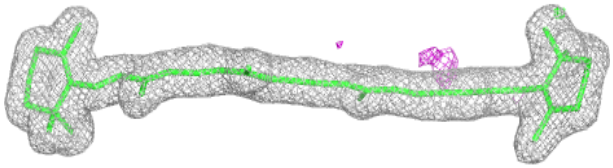


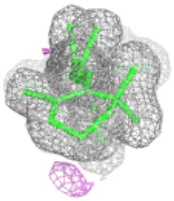


Electron density around BCR A 405:

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

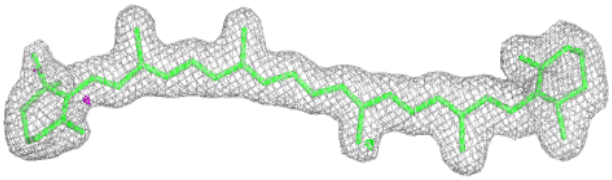


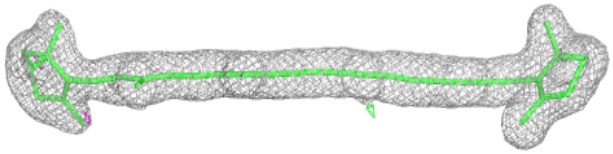


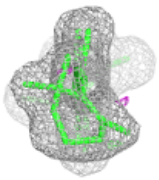


Electron density around BCR B 618:

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

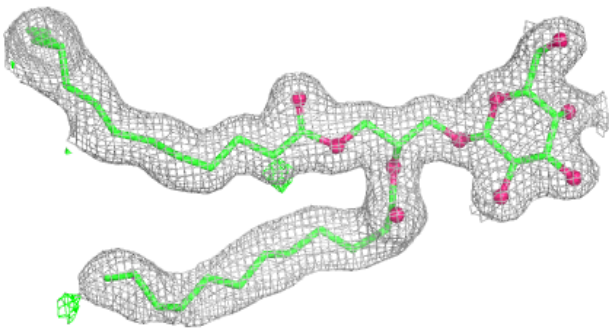


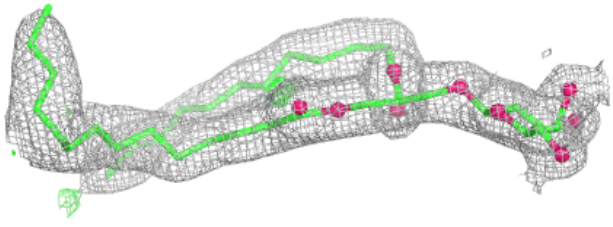


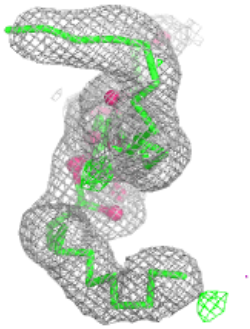


Electron density around LMG J 101:

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

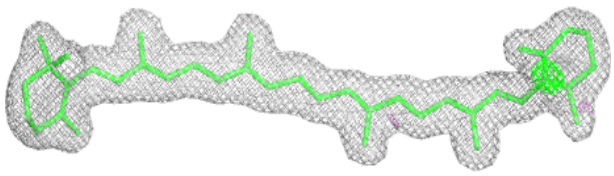


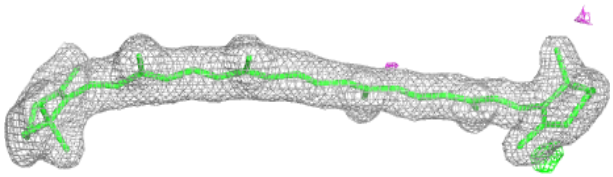


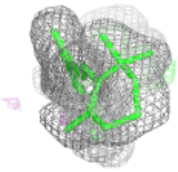


Electron density around BCR B 619:

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

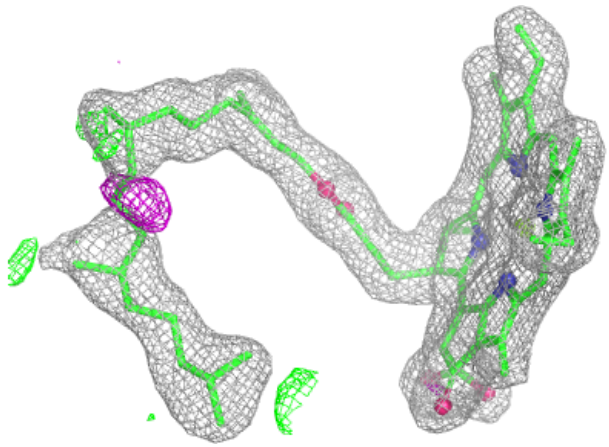


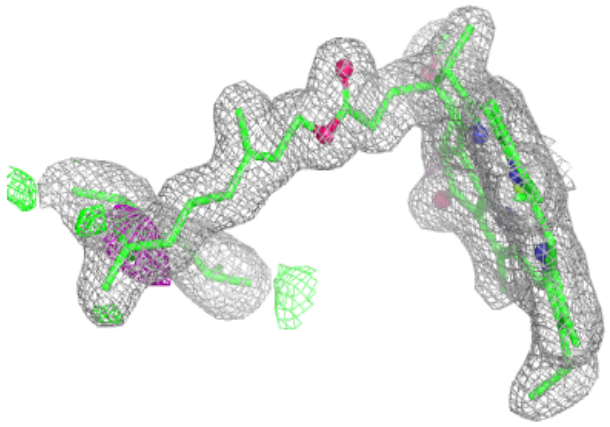


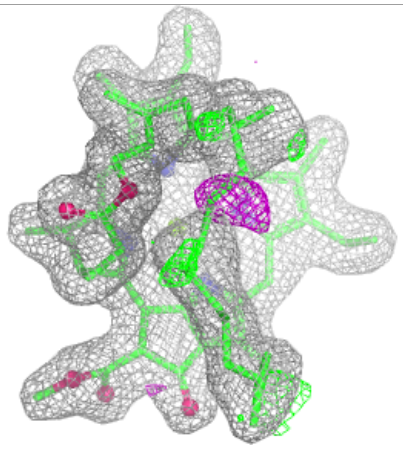


Electron density around CLA B 607:

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

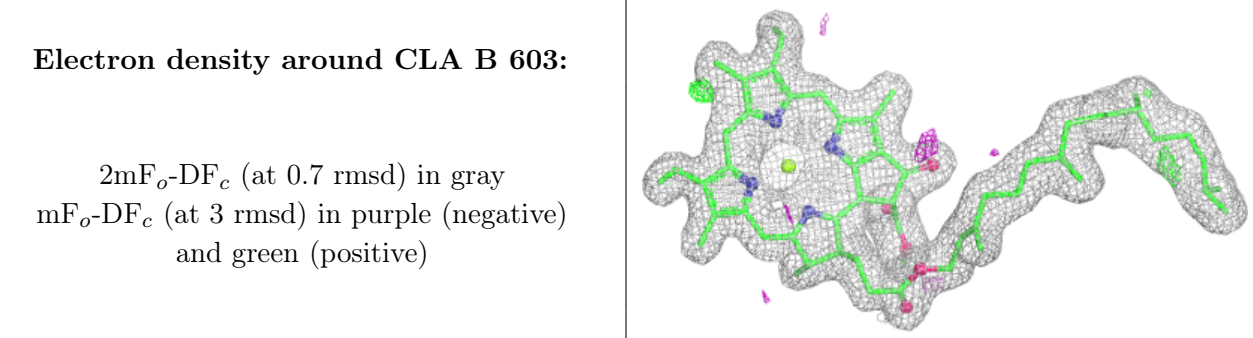


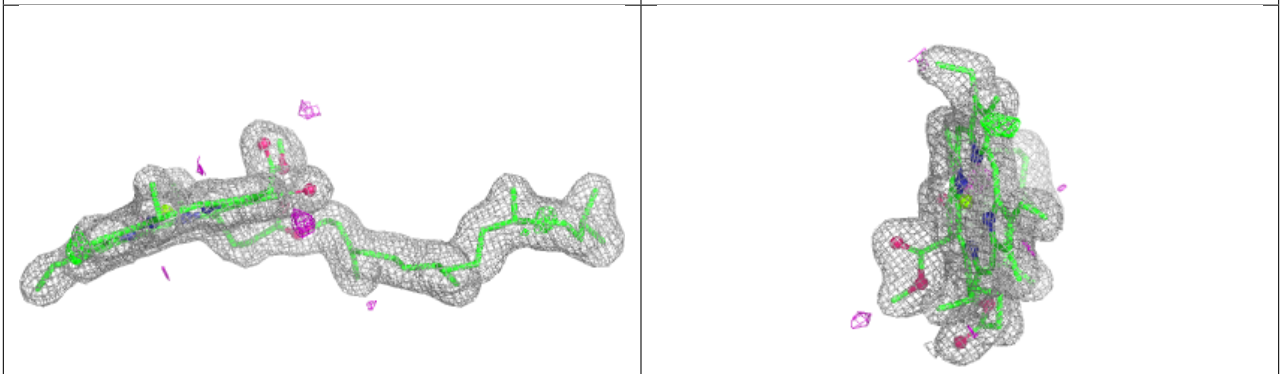




Electron density around CLA B 603:

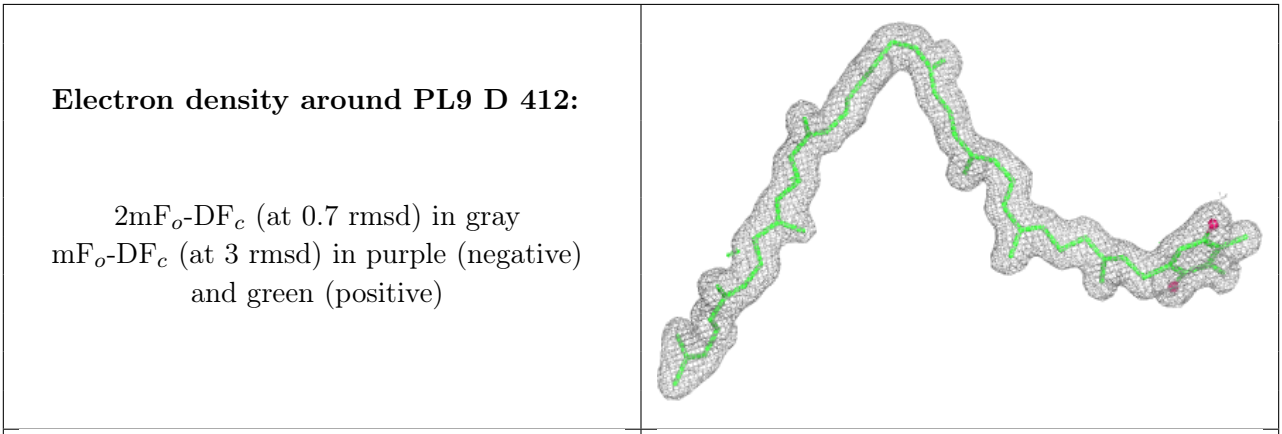
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

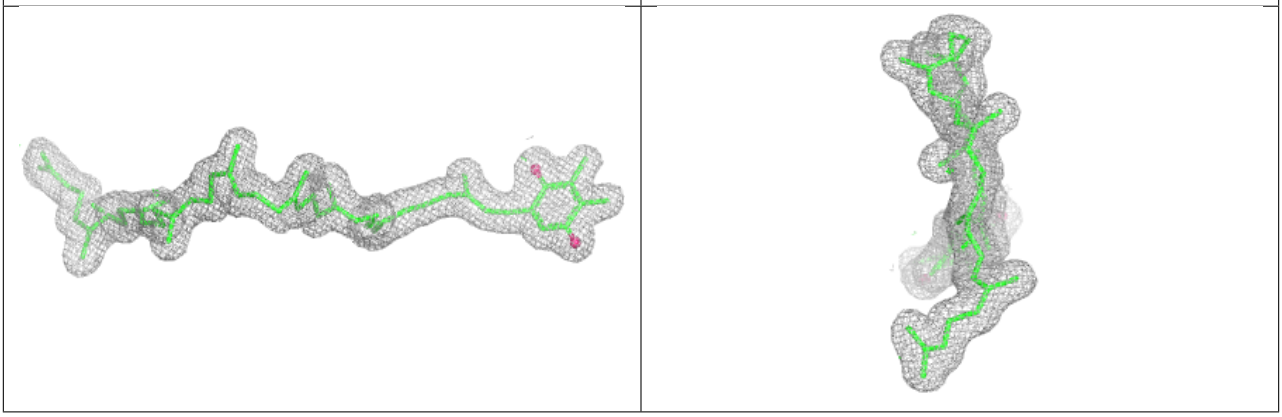




Electron density around PL9 D 412:

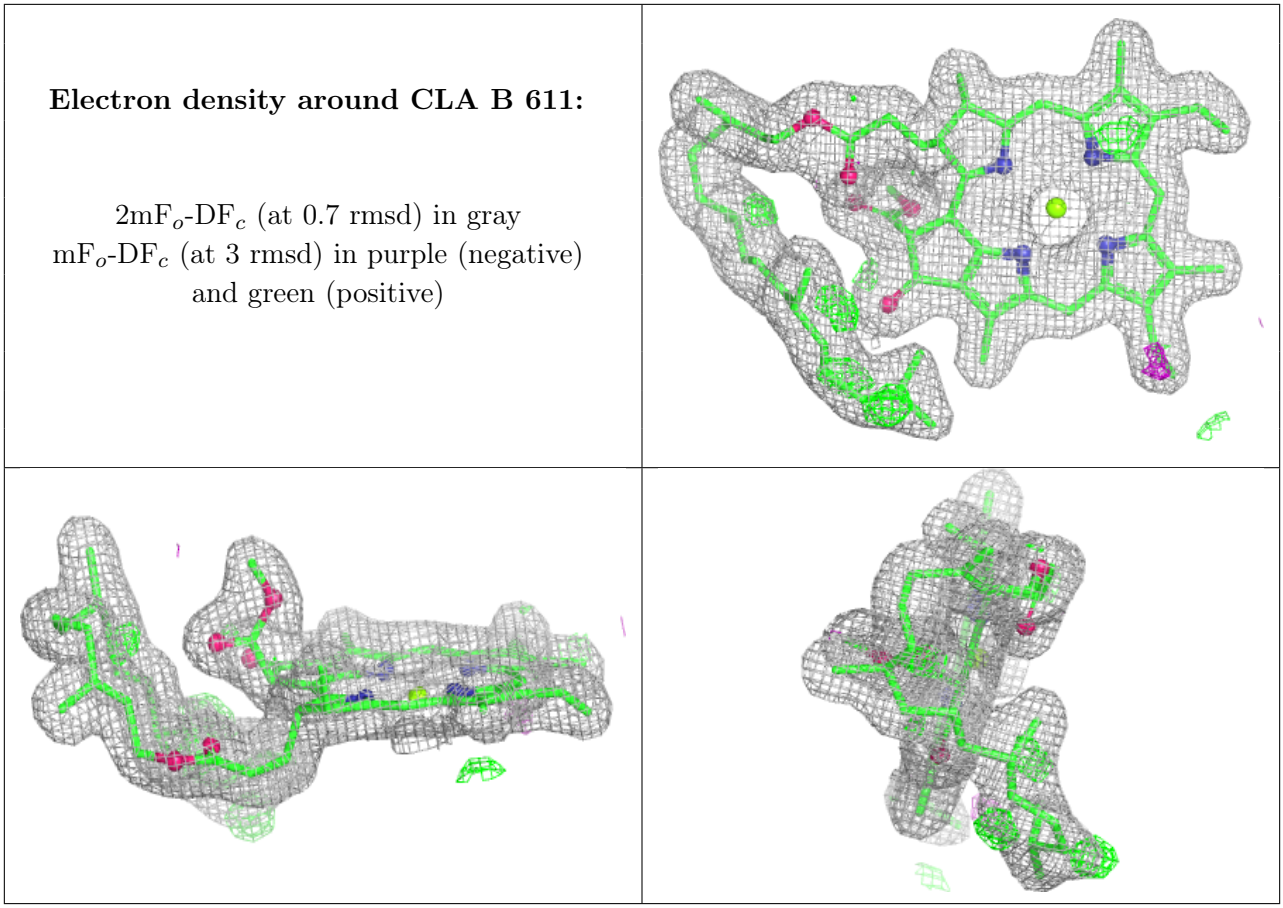
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





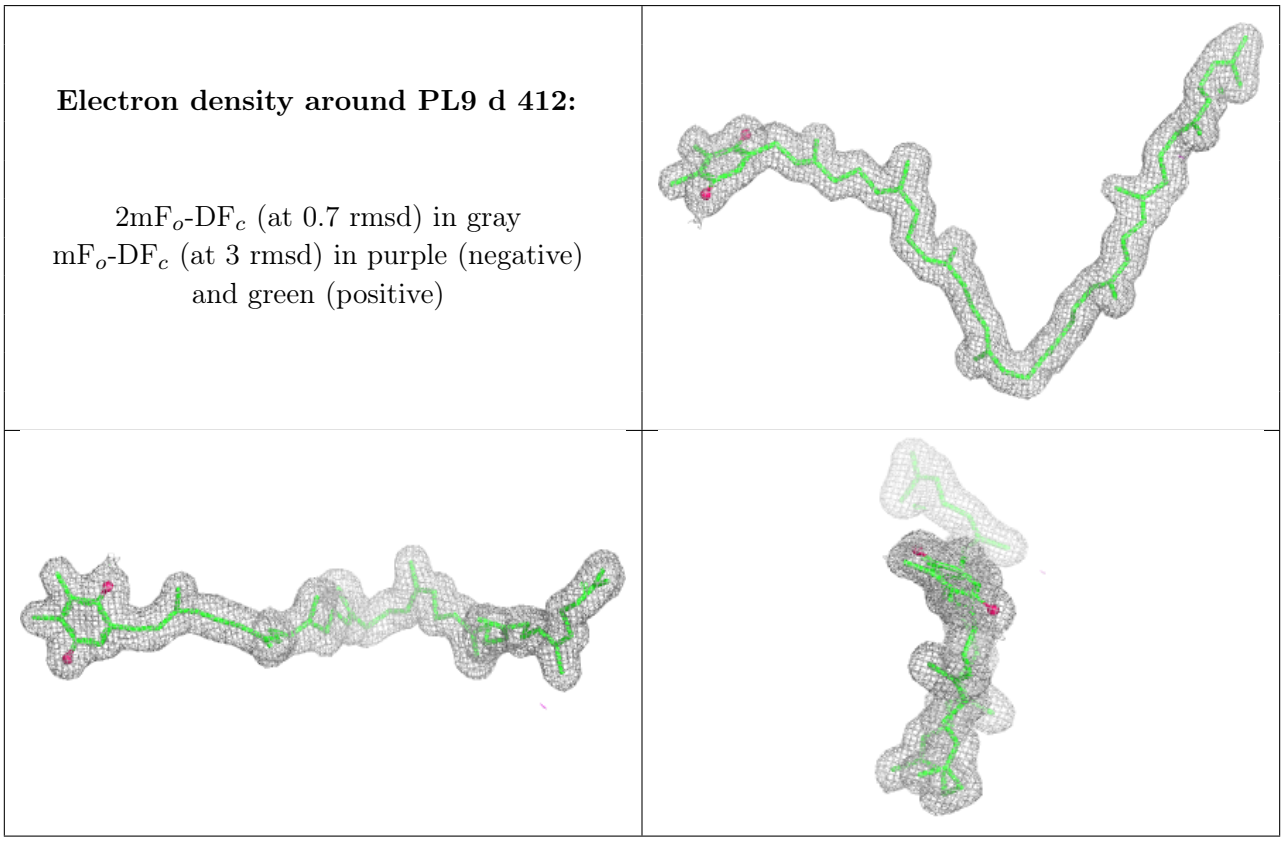
Electron density around CLA B 611:

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



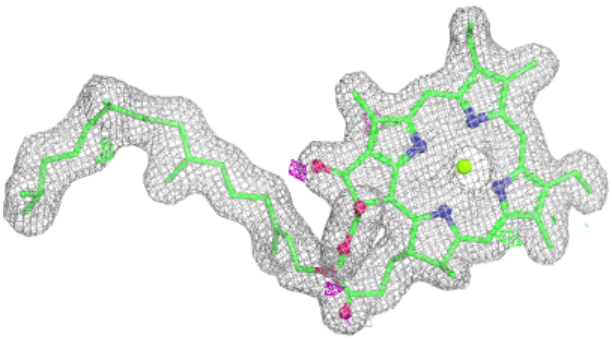
Electron density around PL9 d 412:

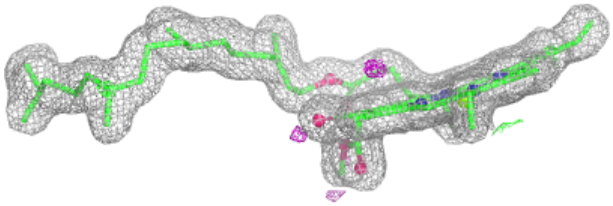
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

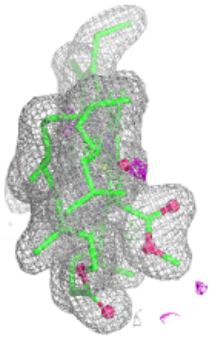


Electron density around CLA b 604:

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

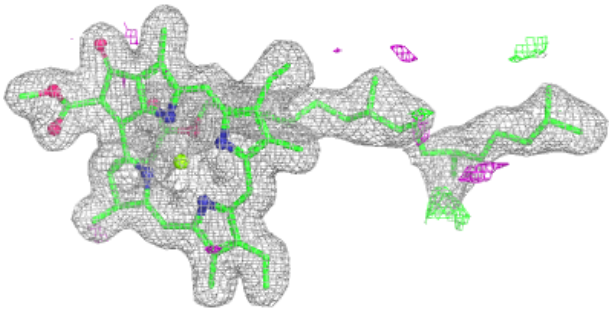


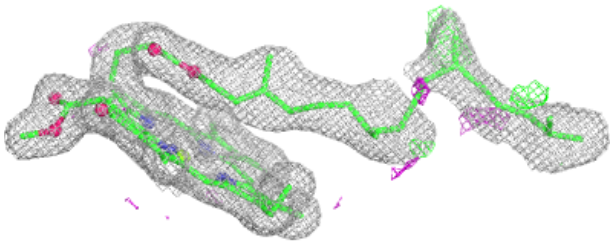


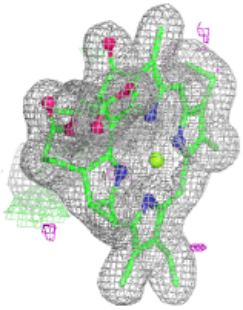


Electron density around CLA B 615:

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

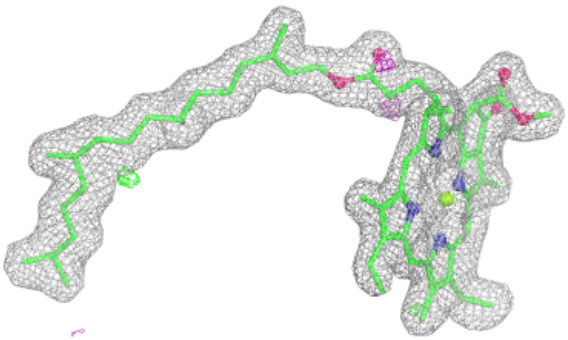


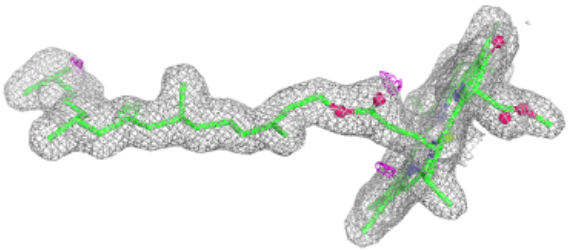


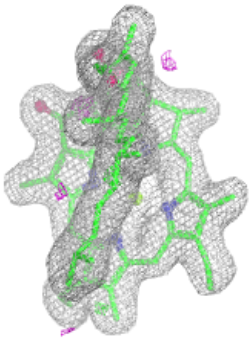


Electron density around CLA b 611:

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

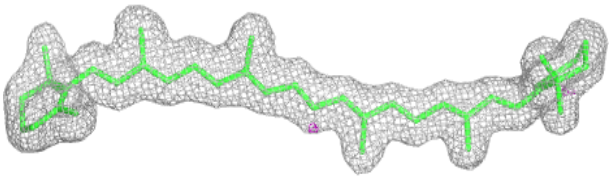


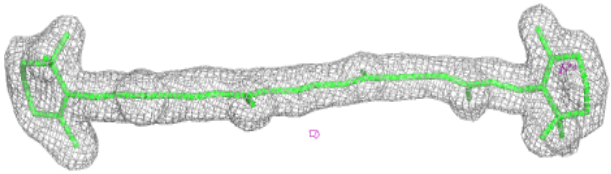


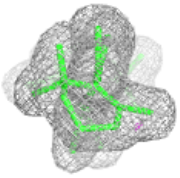


Electron density around BCR a 408:

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

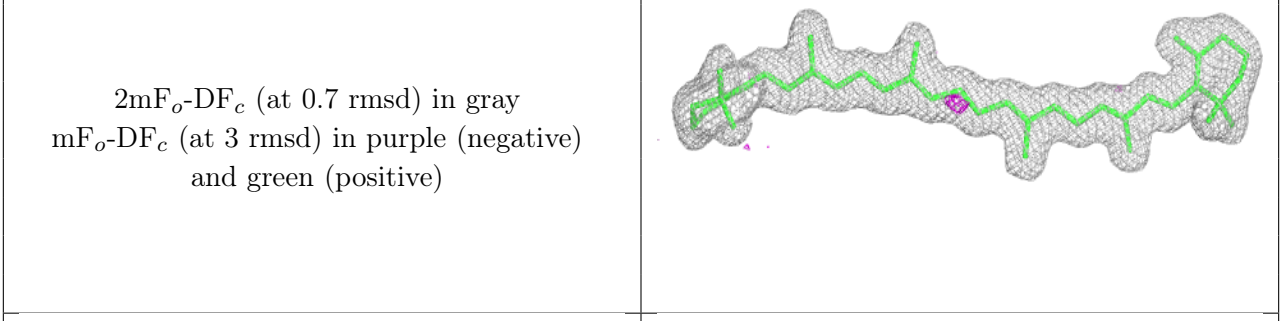


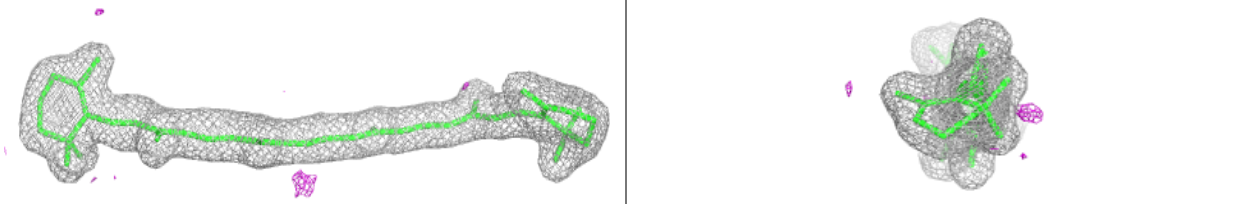




Electron density around BCR b 619:

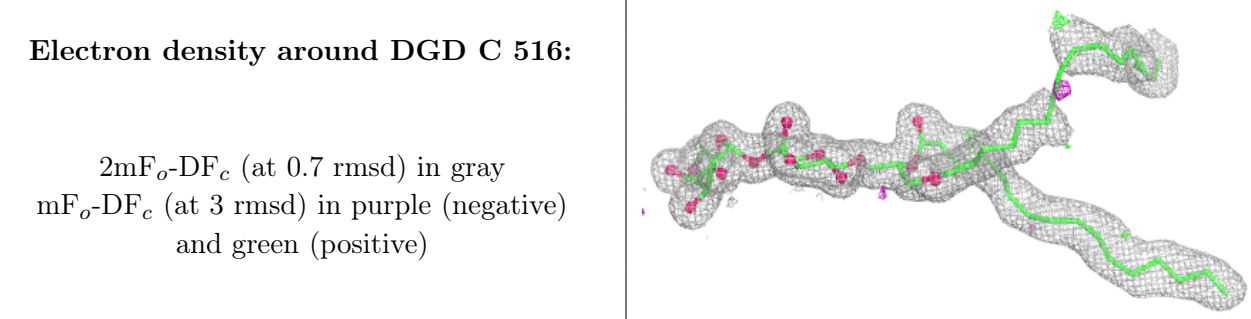
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

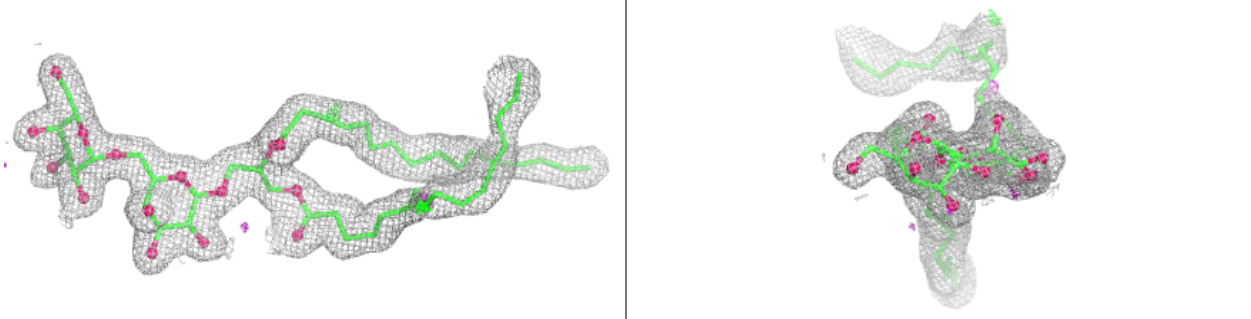




Electron density around DGD C 516:

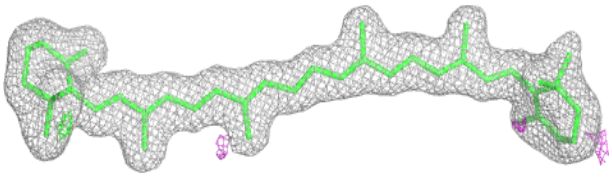
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

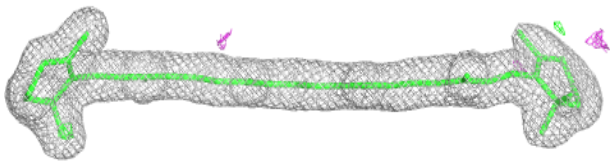


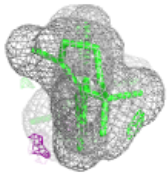


Electron density around BCR b 620:

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

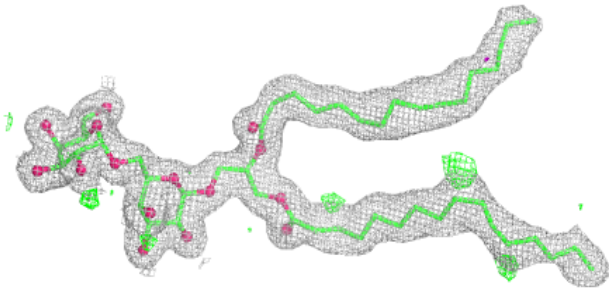


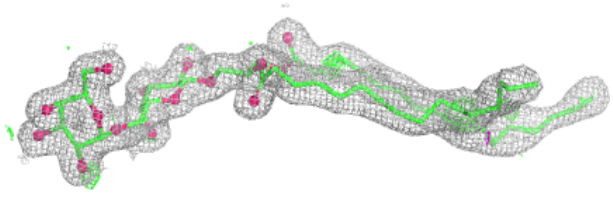


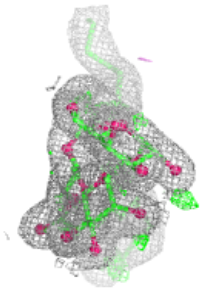


Electron density around DGD C 518:

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

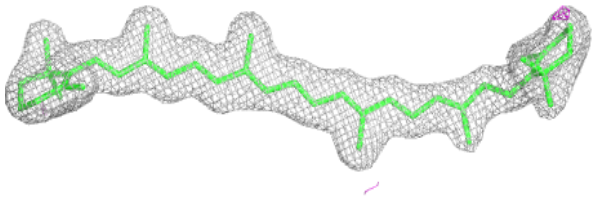


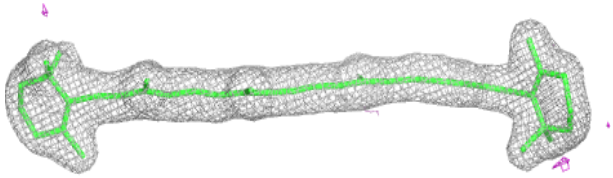


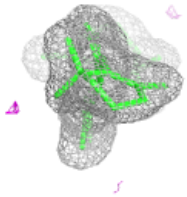


Electron density around BCR c 514:

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

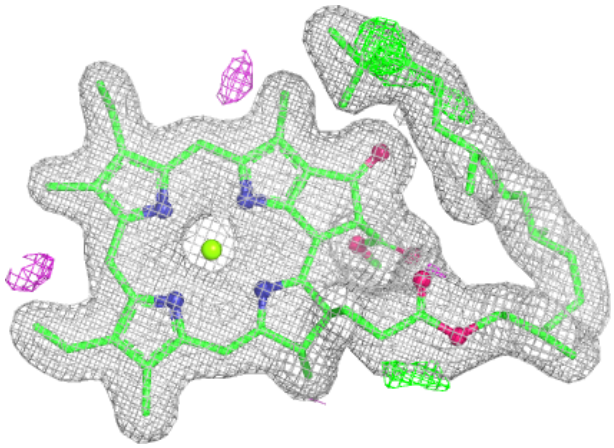


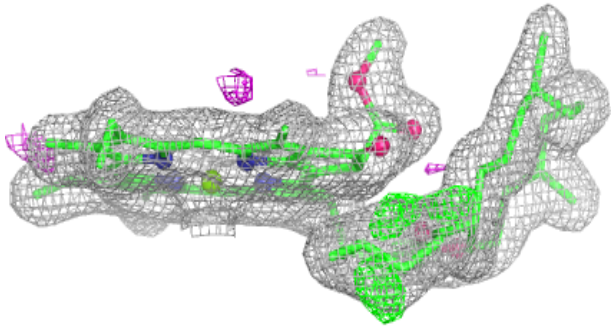


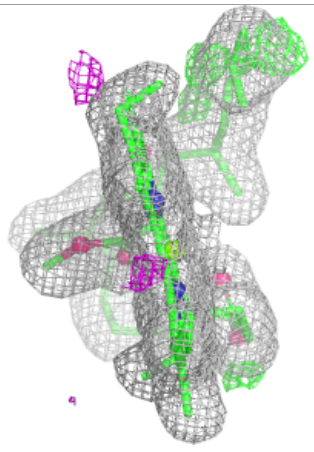


Electron density around CLA b 612:

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

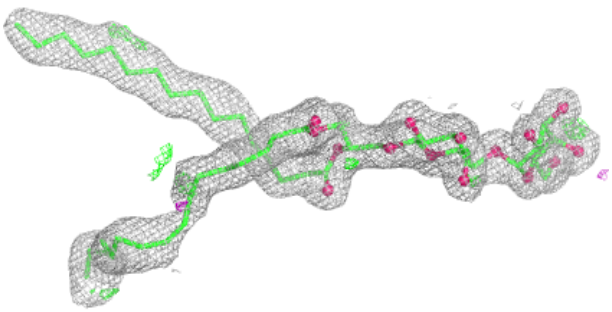


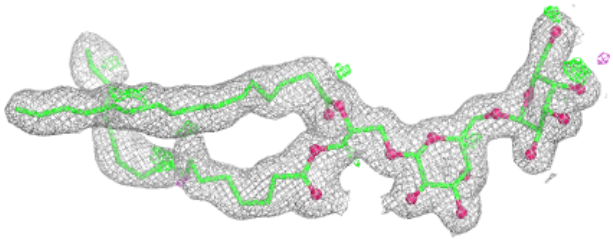


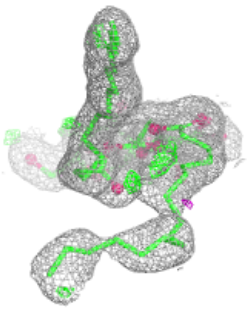


Electron density around DGD c 515:

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

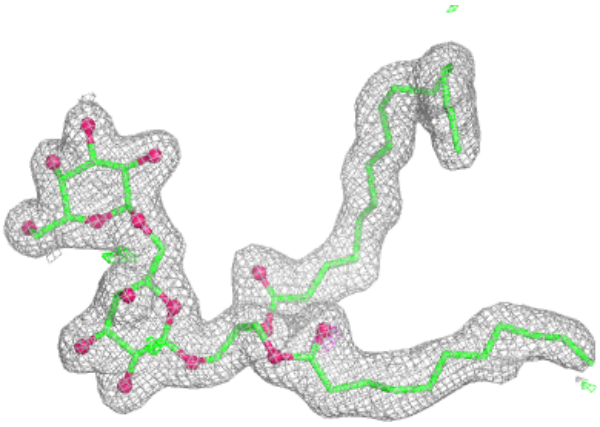


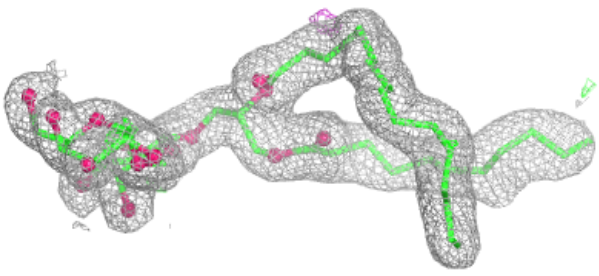




Electron density around DGD c 516:

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

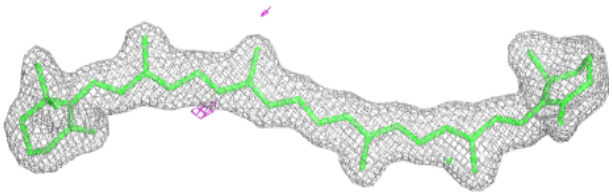


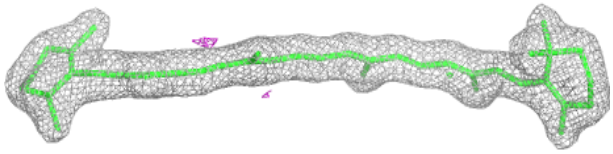


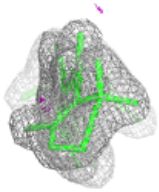


Electron density around BCR j 102:

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

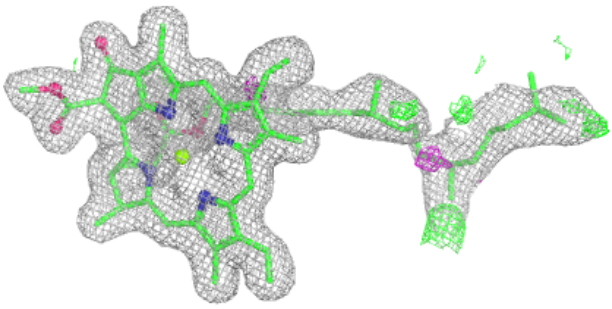


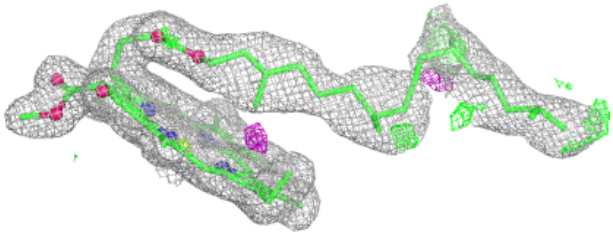


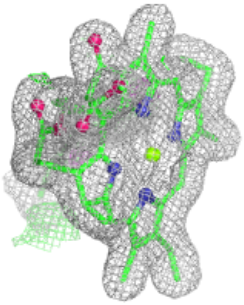


Electron density around CLA b 616:

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

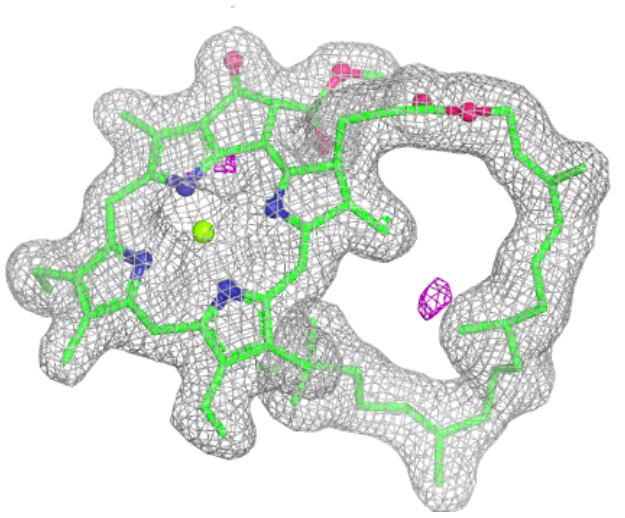


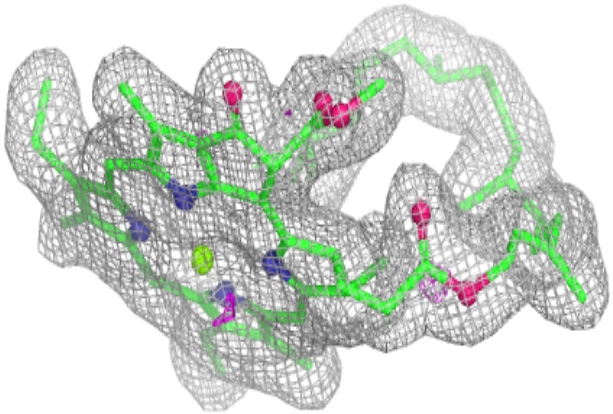


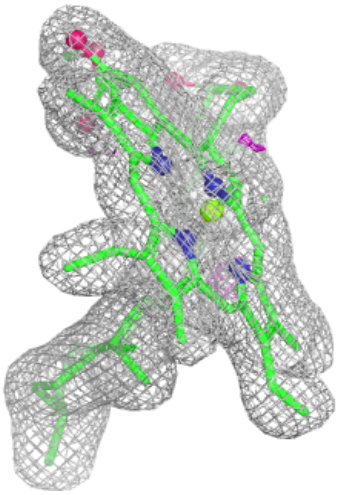


Electron density around CLA B 616:

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

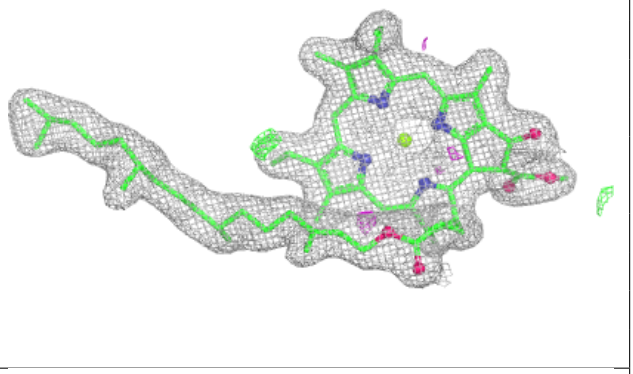


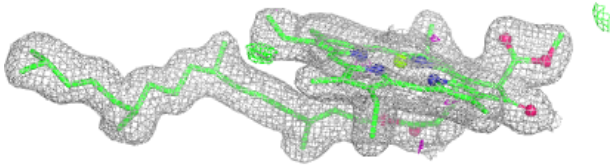


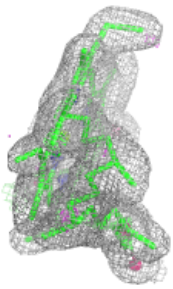


Electron density around CLA c 501:

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

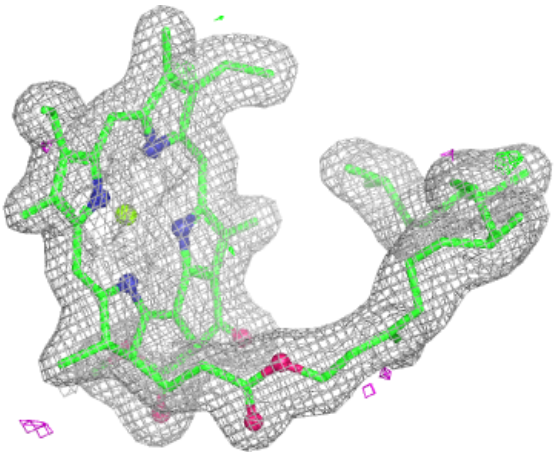


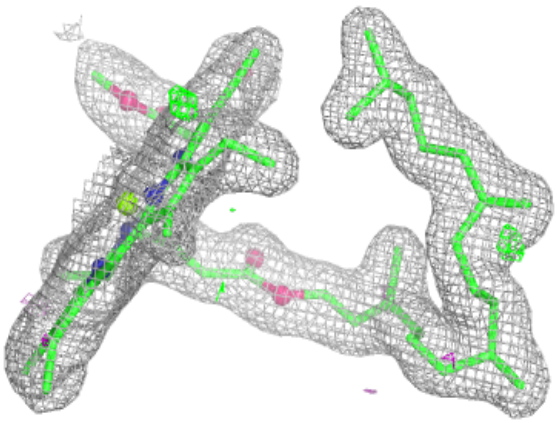


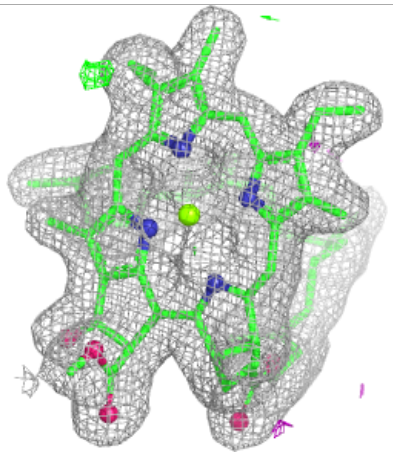


Electron density around CLA c 503:

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

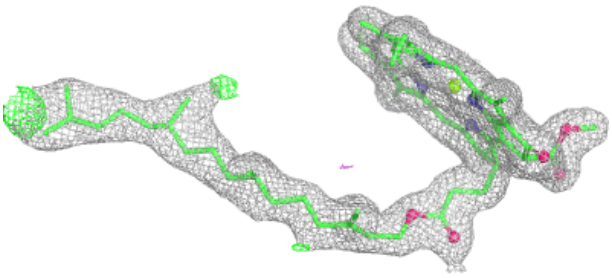


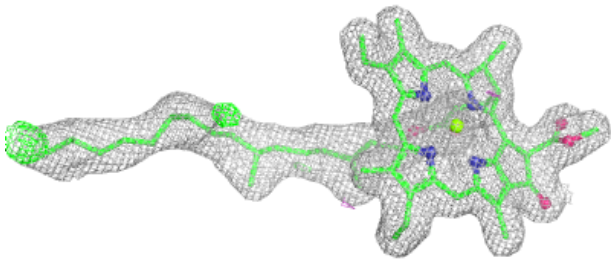


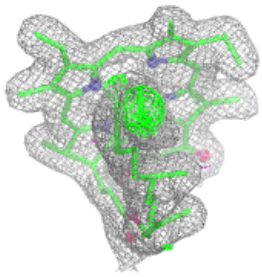


Electron density around CLA c 504:

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

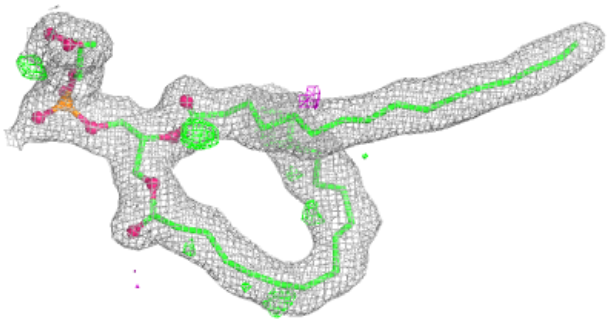


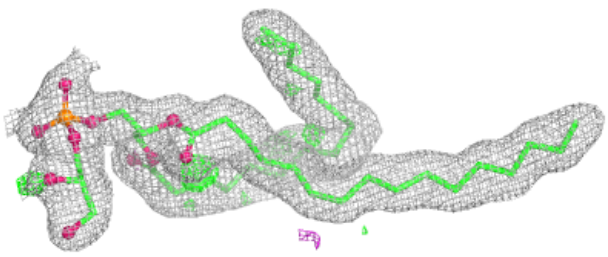




Electron density around LHG d 406:

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

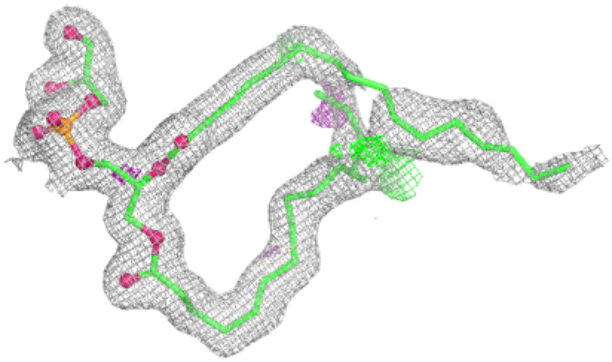


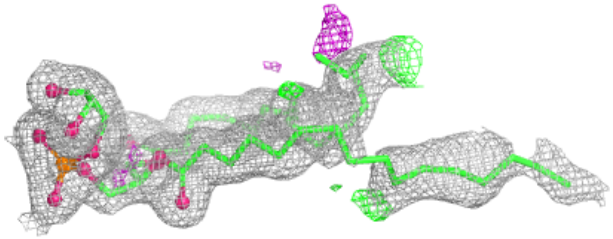


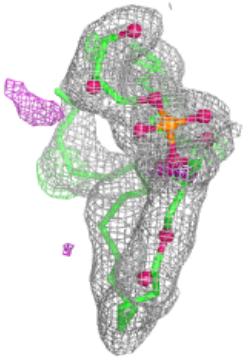


Electron density around LHG d 408:

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

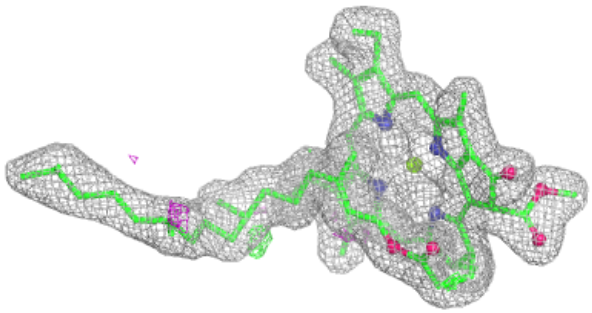


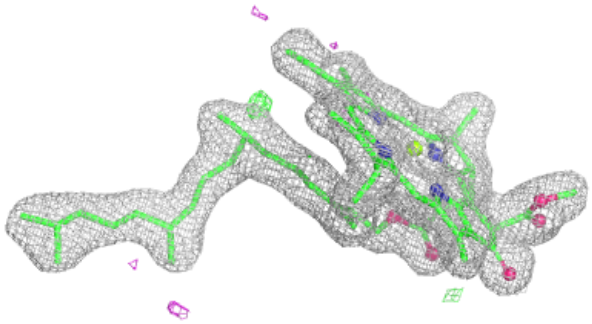


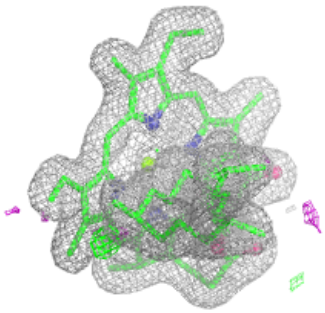


Electron density around CLA c 505:

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

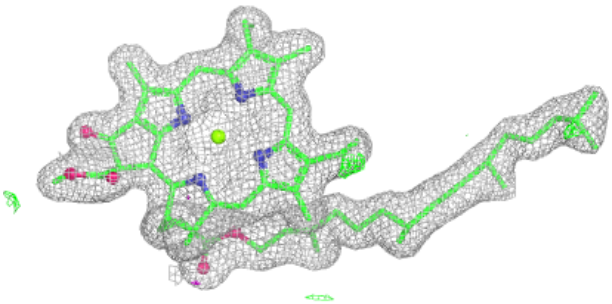


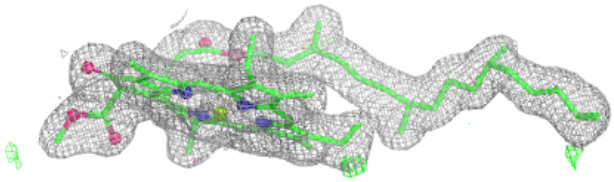


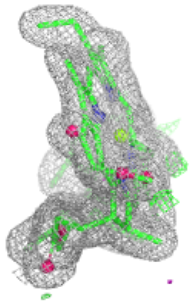


Electron density around CLA C 501:

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

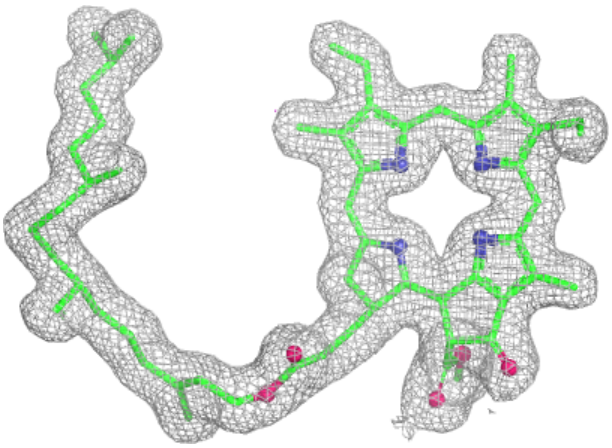


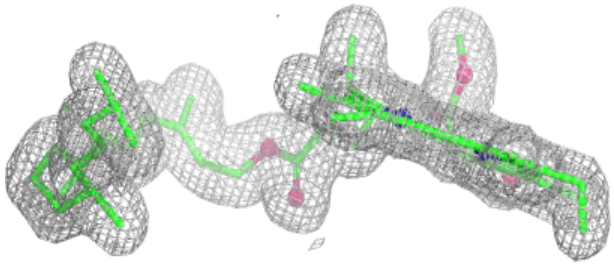


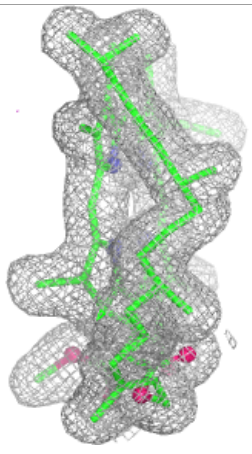


Electron density around PHO A 403:

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

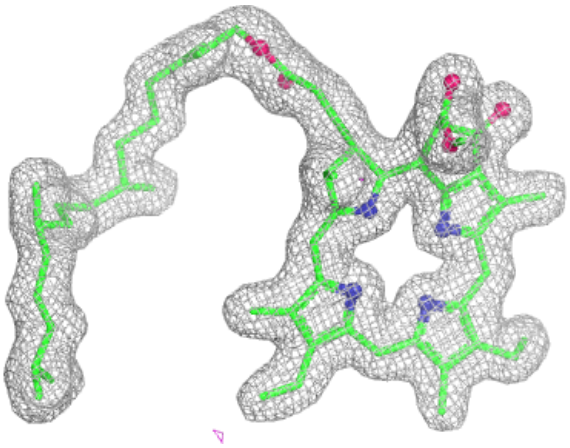


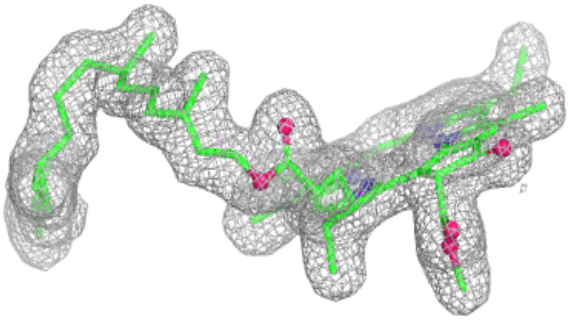


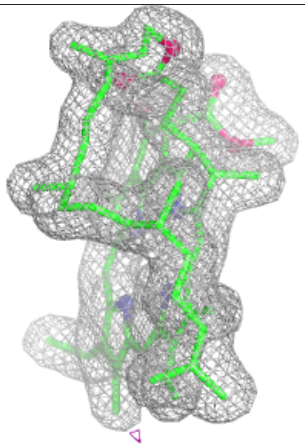


Electron density around PHO D 403:

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

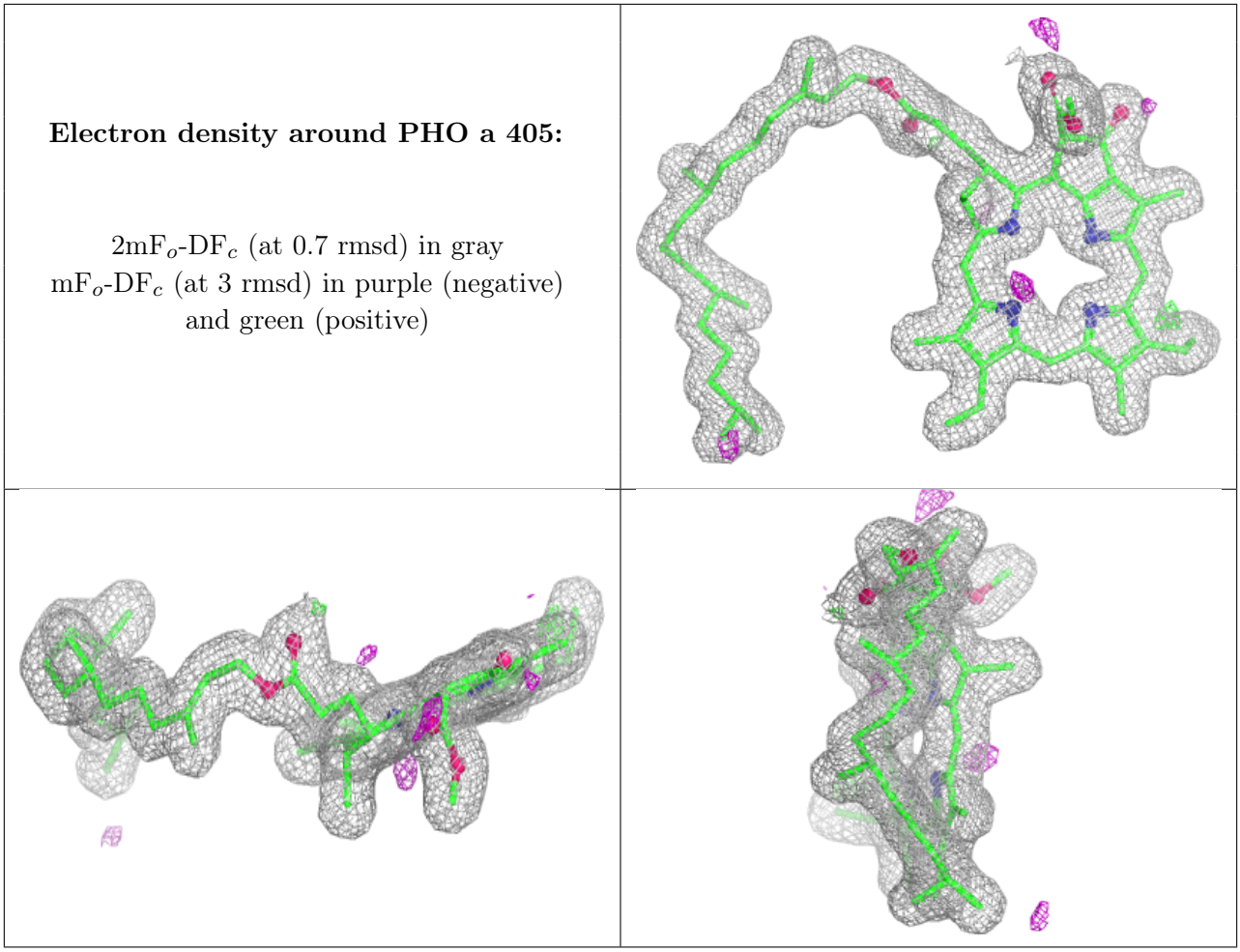






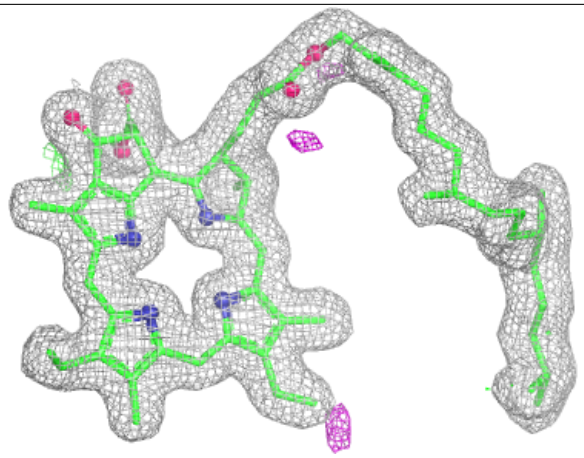
Electron density around PHO a 405:

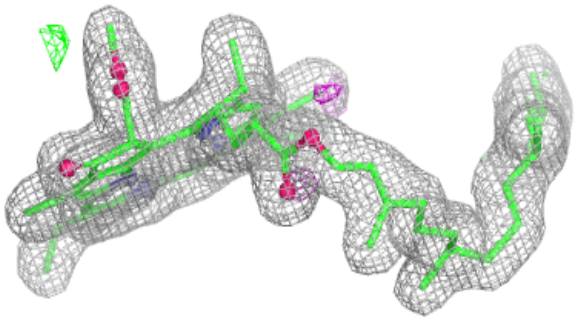
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

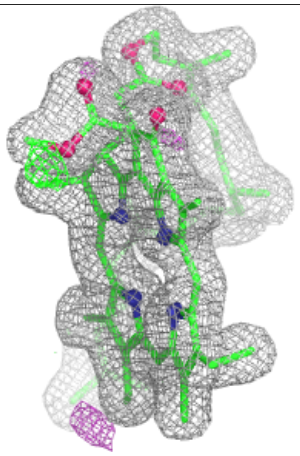


Electron density around PHO a 406:

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

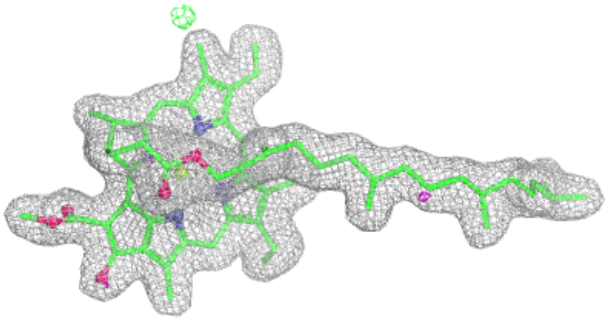


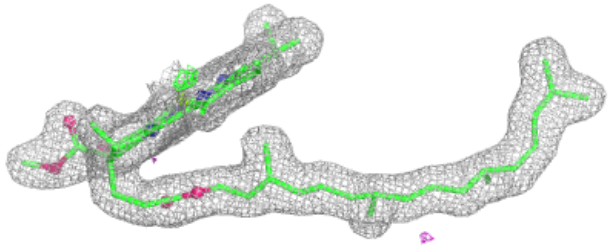


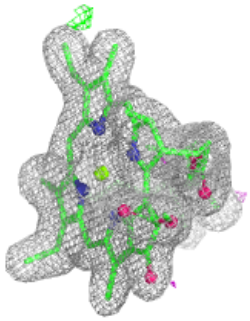


Electron density around CLA b 610:

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

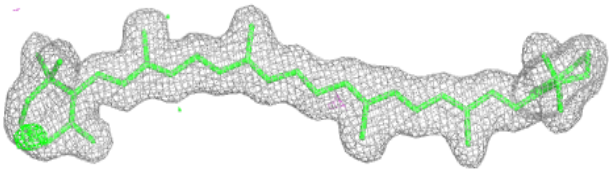


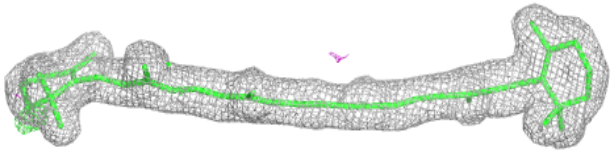


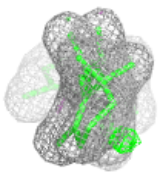


Electron density around BCR B 617:

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

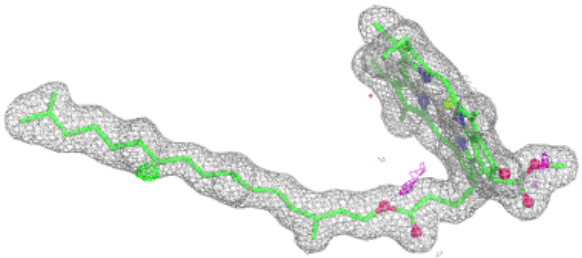


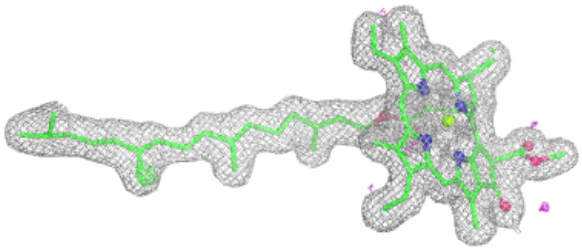


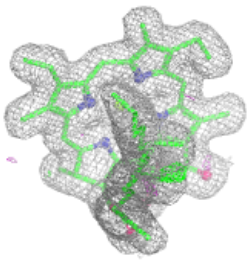


Electron density around CLA B 608:

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

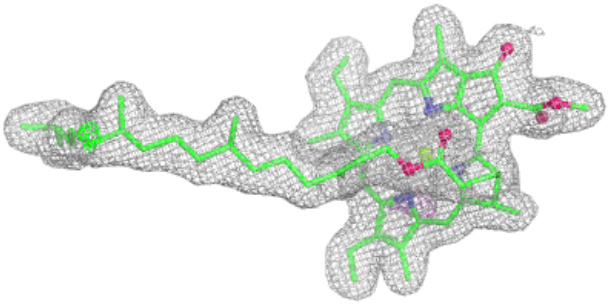


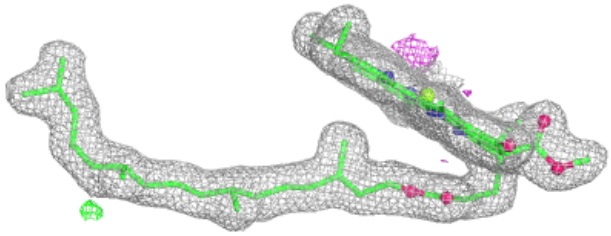




Electron density around CLA B 609:

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

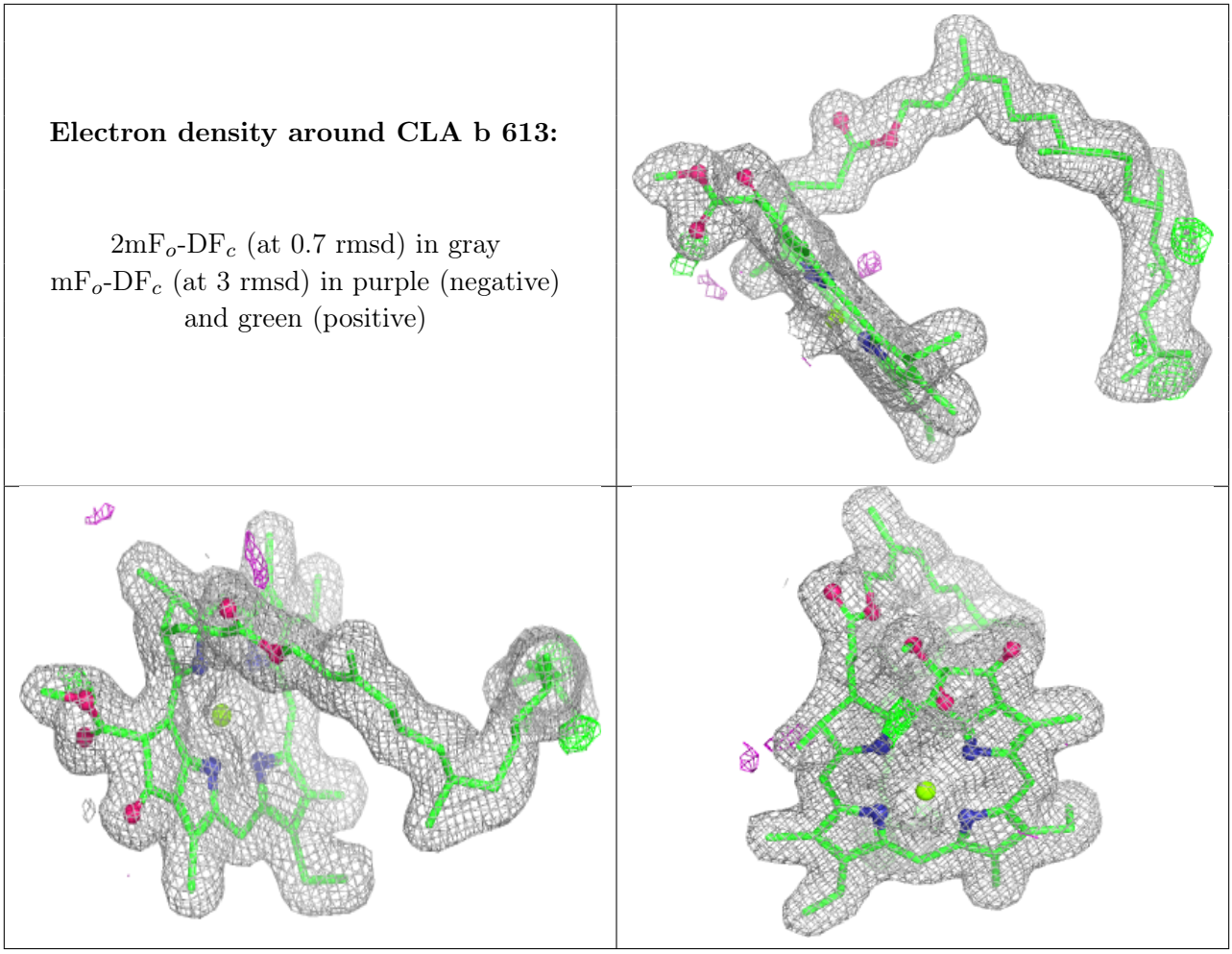






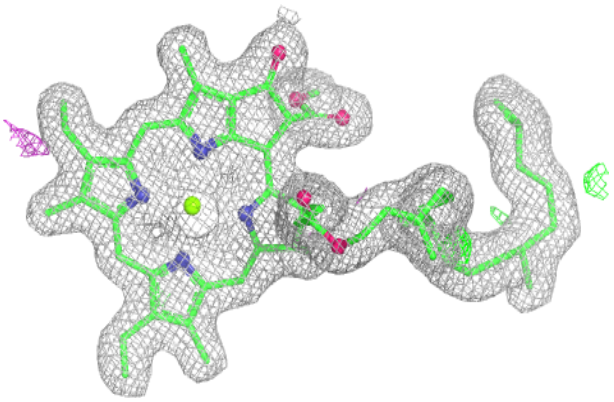
Electron density around CLA b 613:

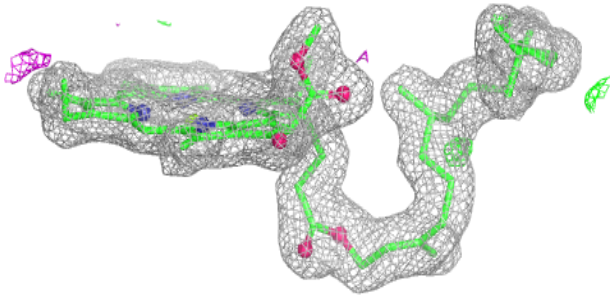
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

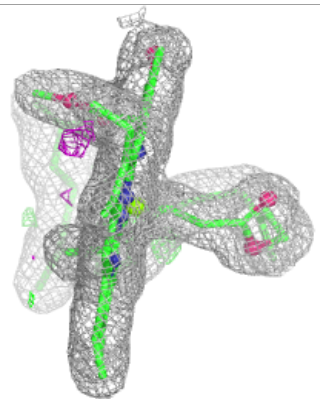


Electron density around CLA b 614:

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

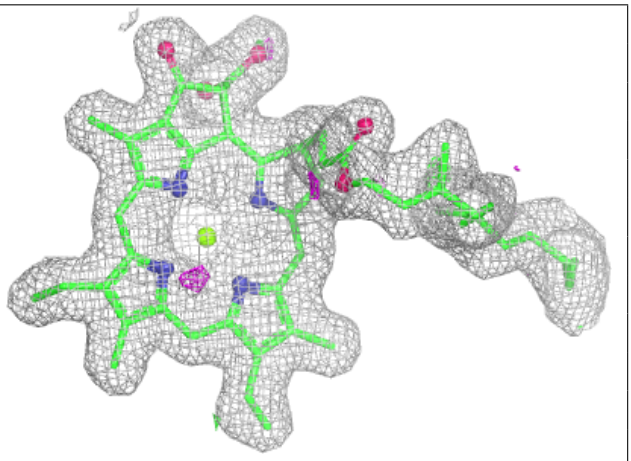


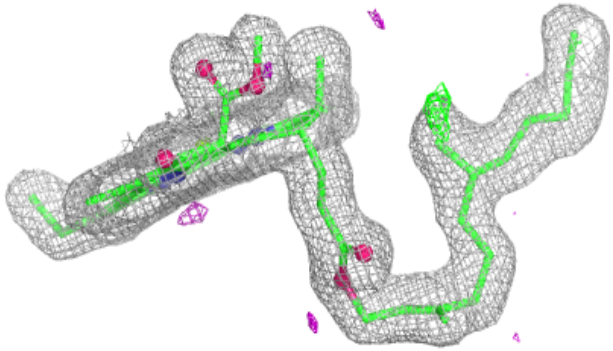


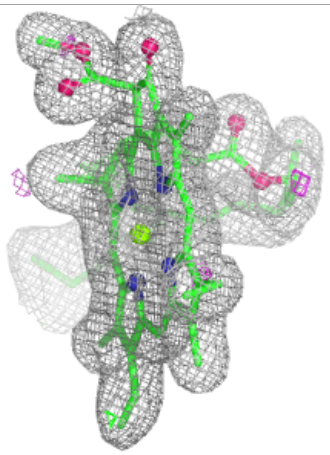


Electron density around CLA A 402:

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

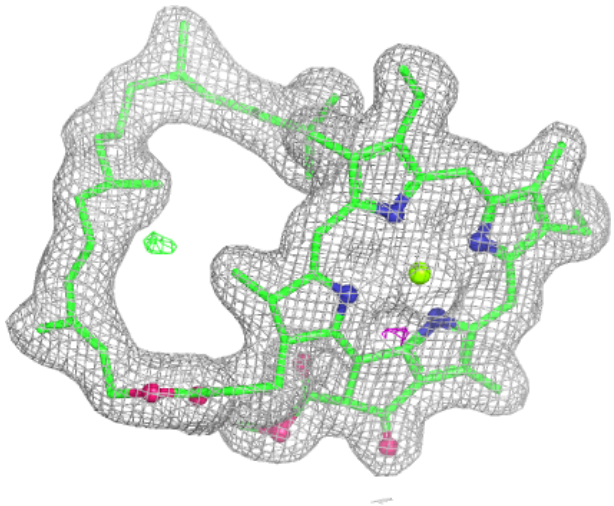


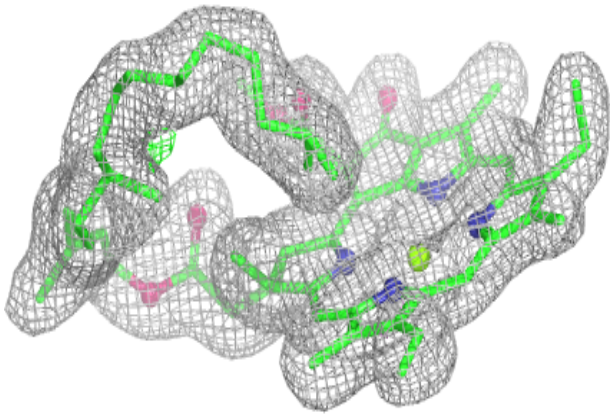


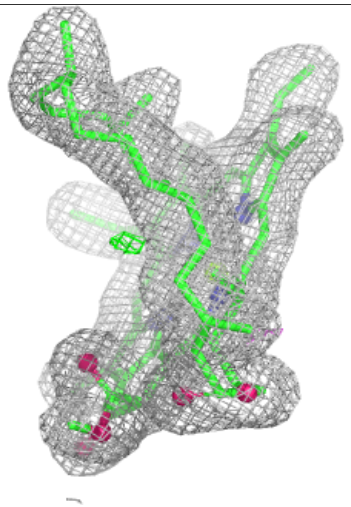


Electron density around CLA b 617:

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

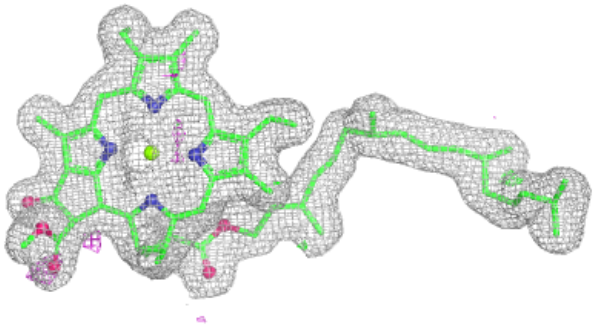


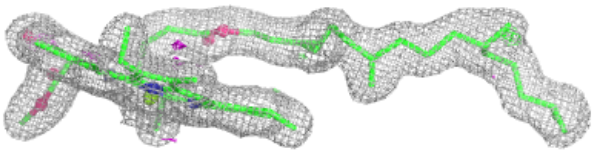


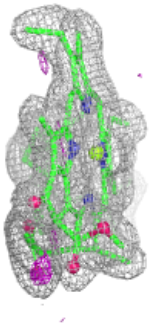


Electron density around CLA B 604:

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

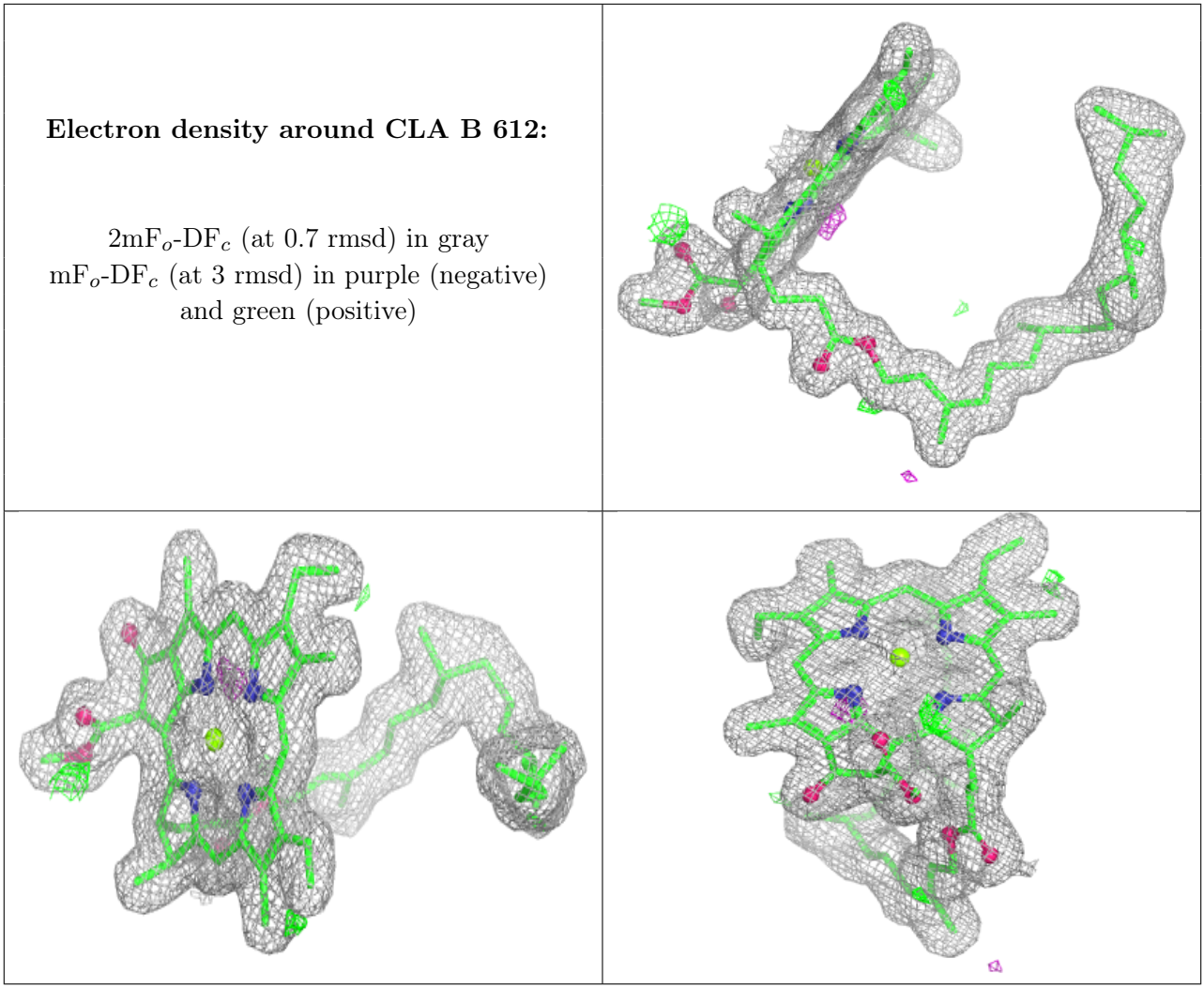






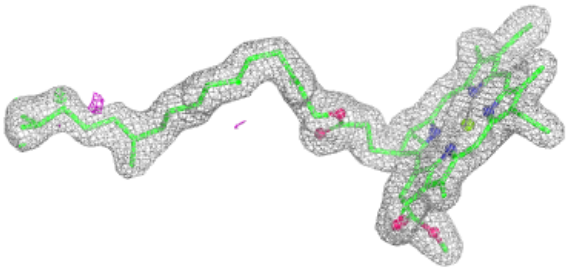
Electron density around CLA B 612:

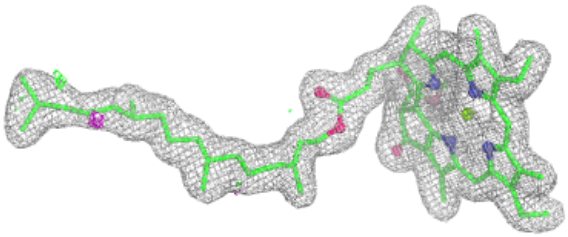
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

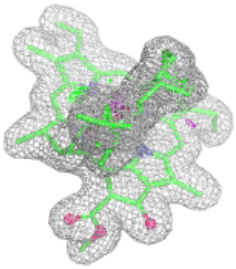


Electron density around CLA c 502:

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

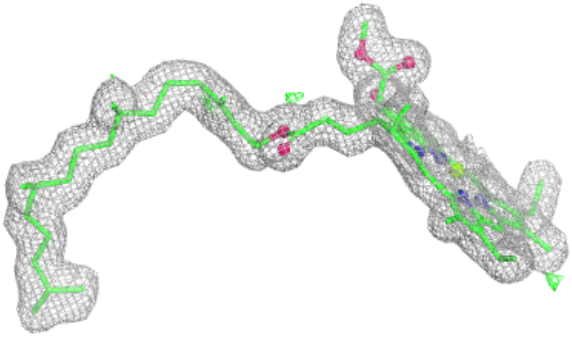


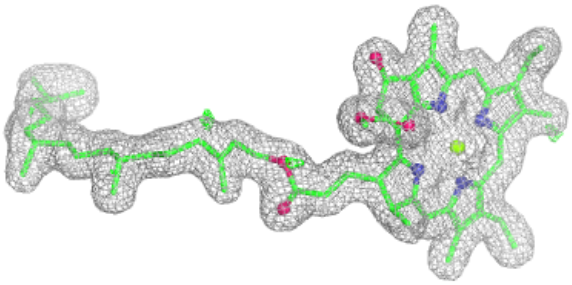


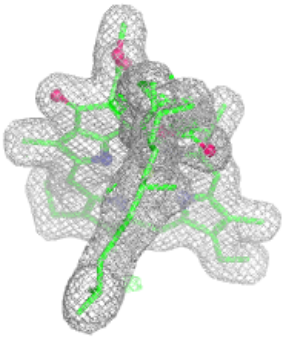


Electron density around CLA D 401:

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

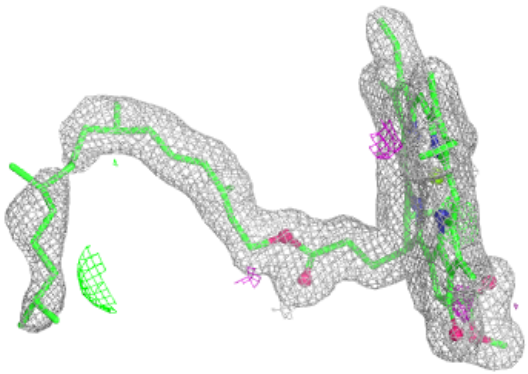


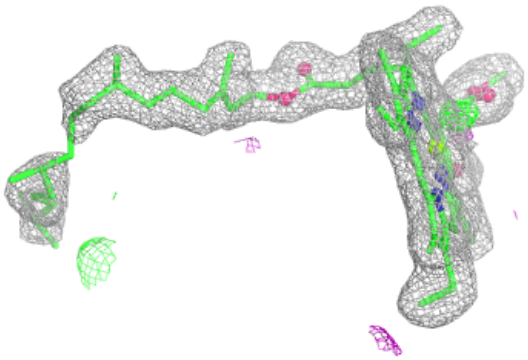


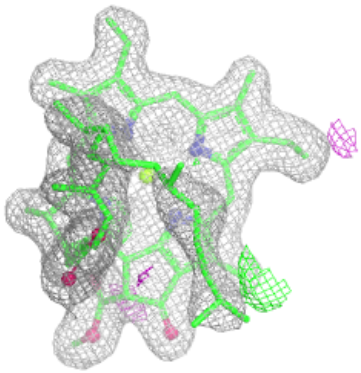


Electron density around CLA D 404:

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

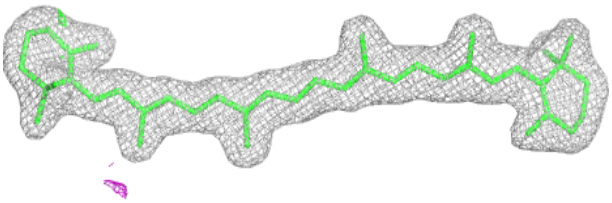


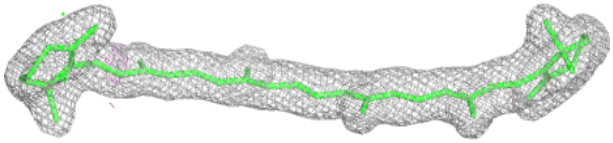


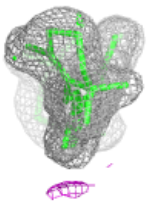


Electron density around BCR b 621:

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

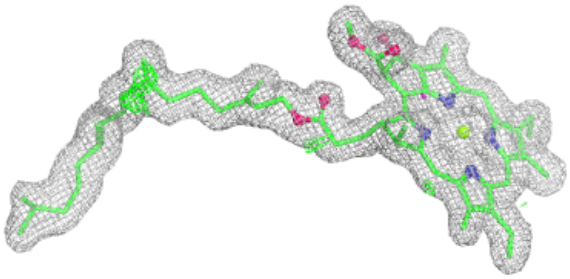


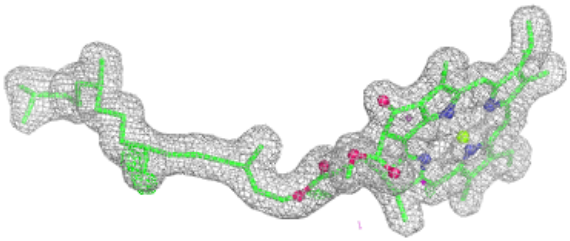


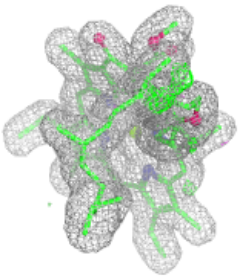


Electron density around CLA a 403:

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

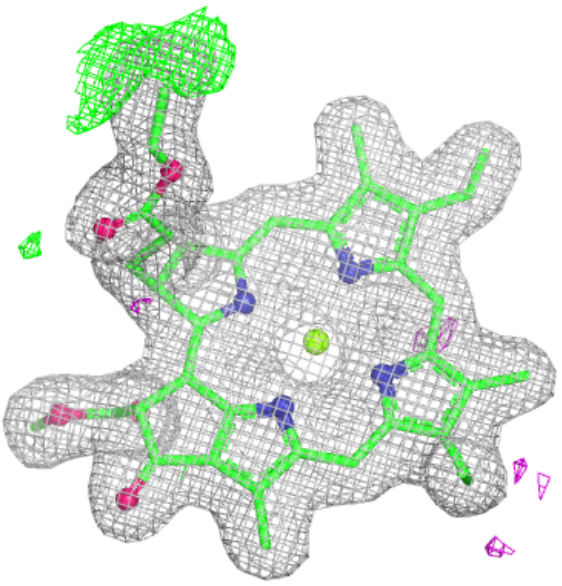


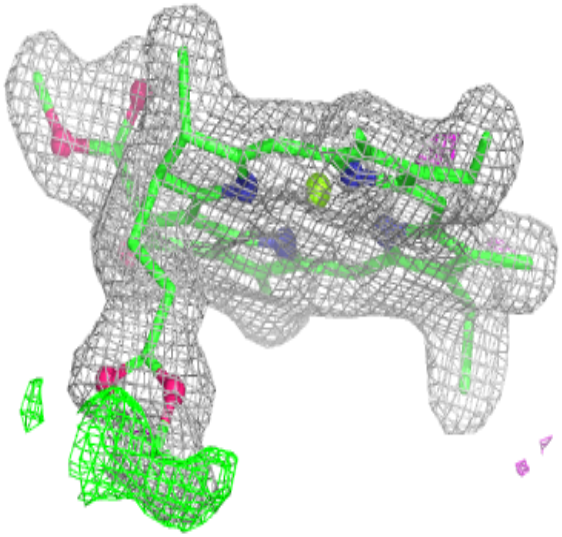




Electron density around CLA a 407:

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

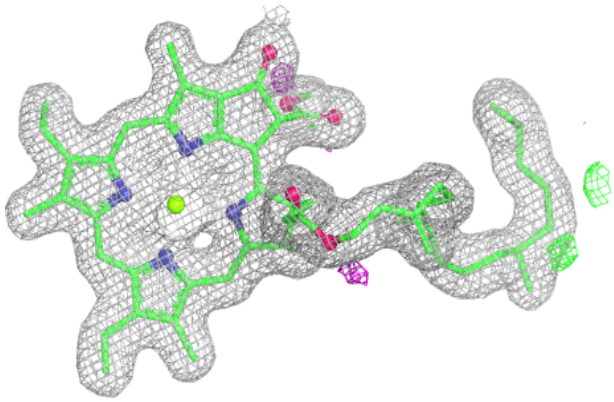


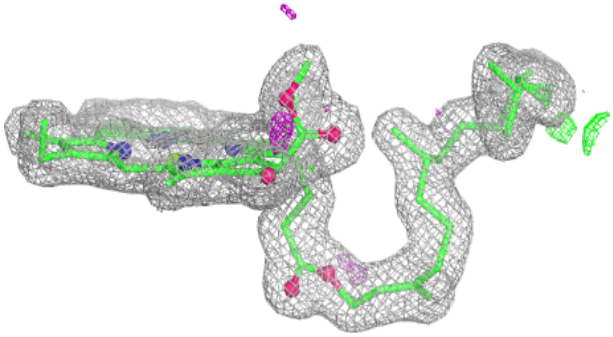


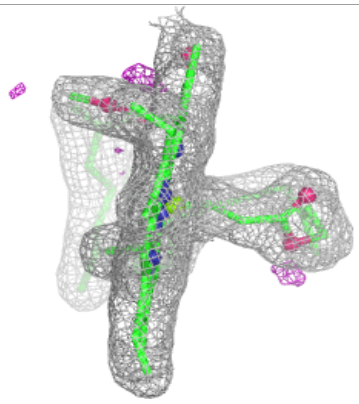


Electron density around CLA B 613:

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

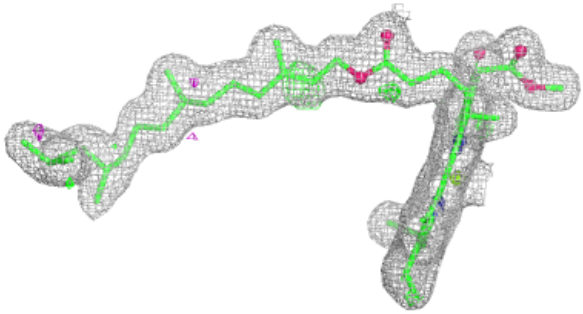


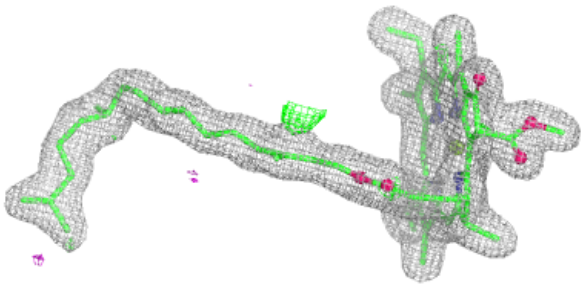


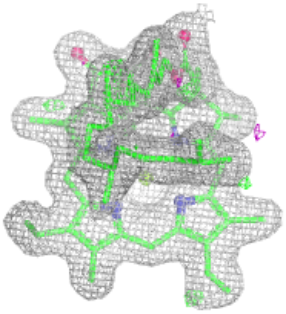


Electron density around CLA B 606:

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

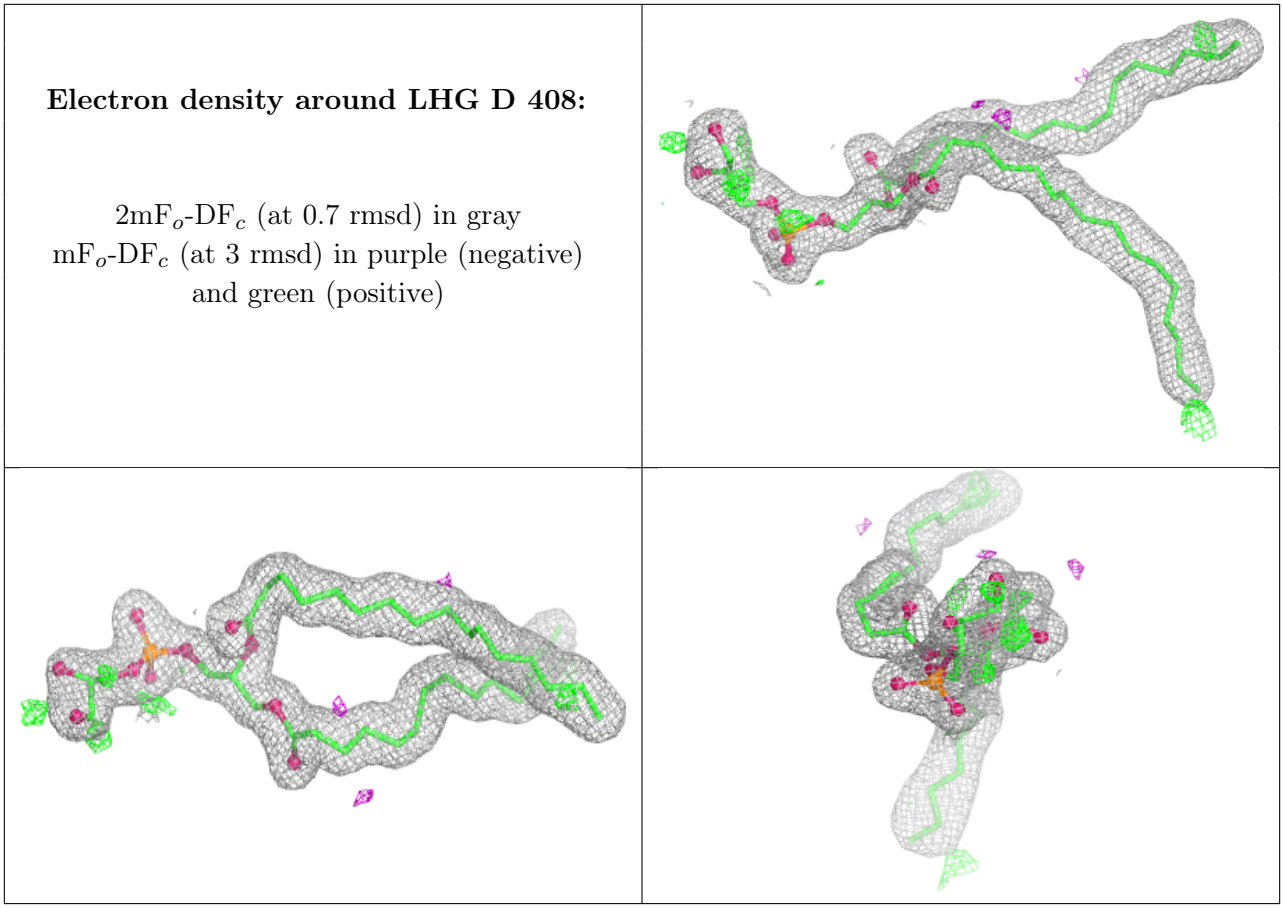






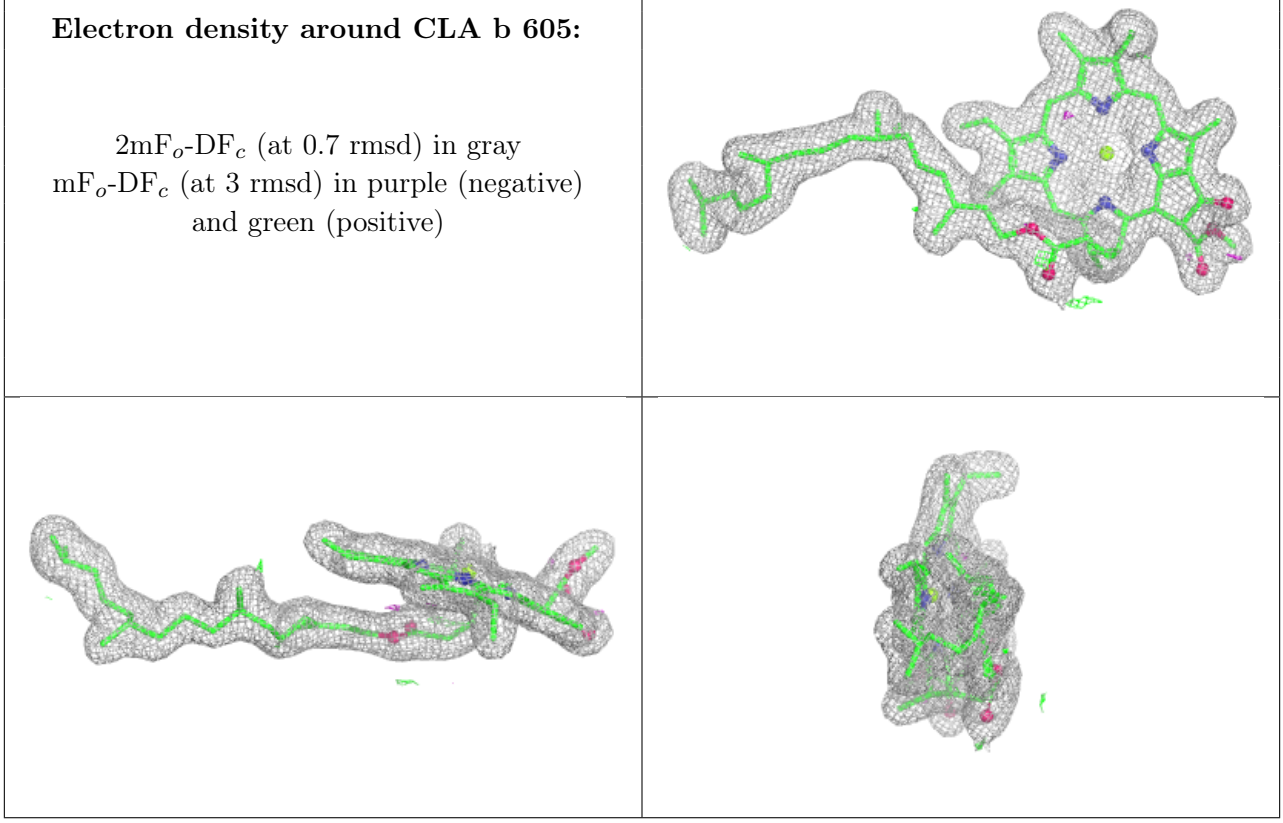
Electron density around LHG D 408:

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



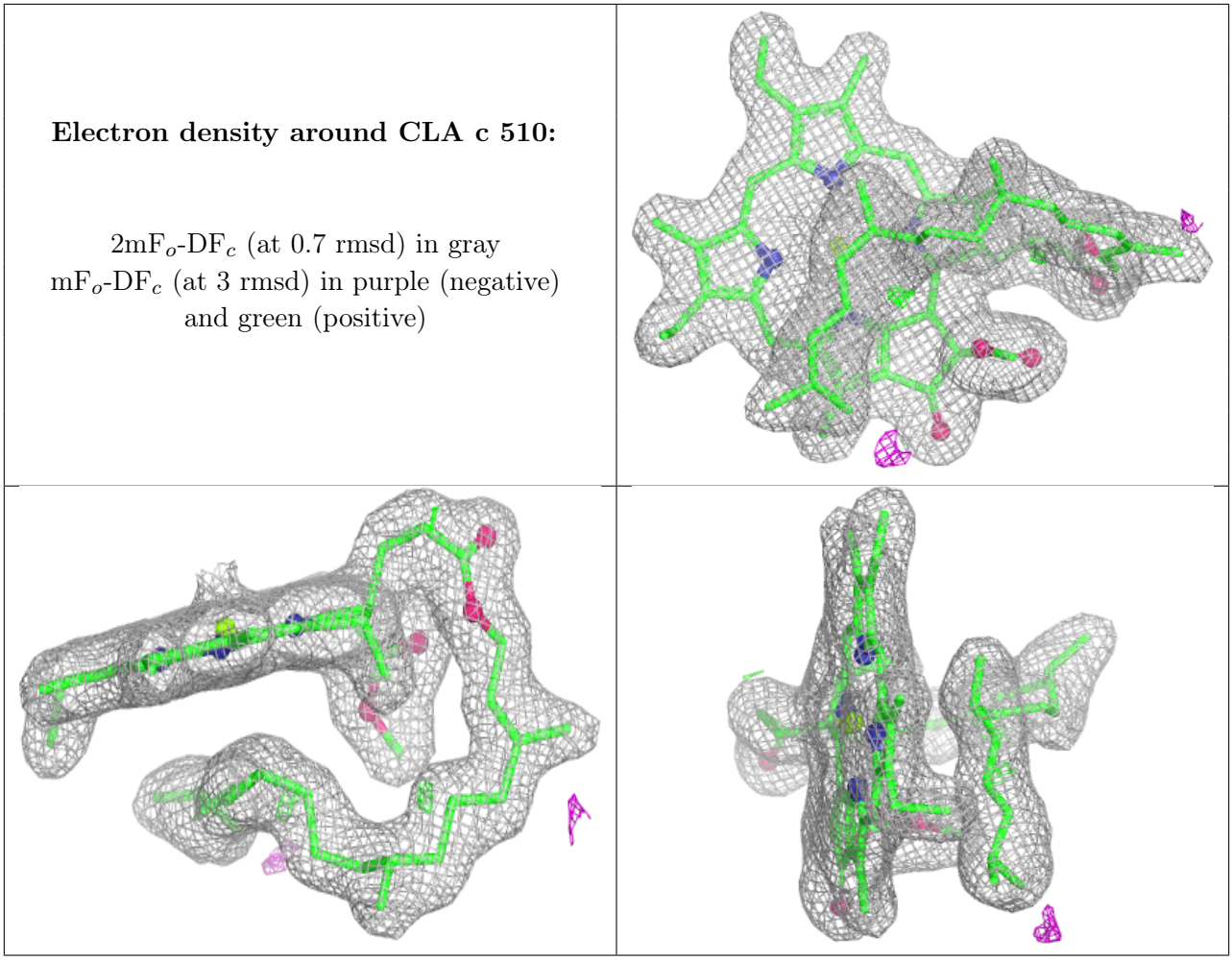
Electron density around CLA b 605:

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



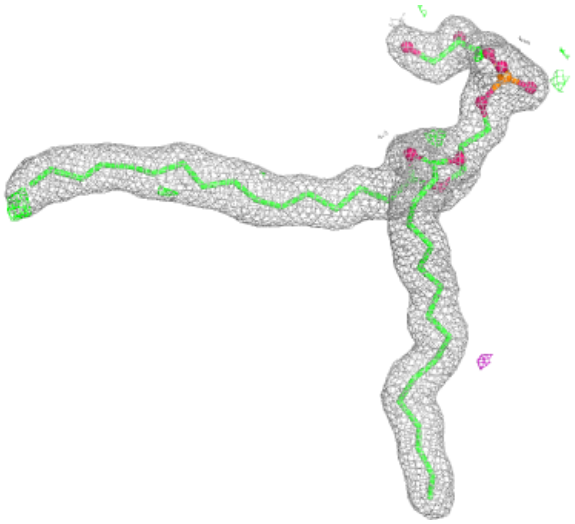
Electron density around CLA c 510:

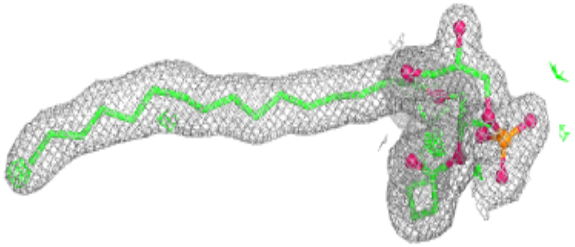
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

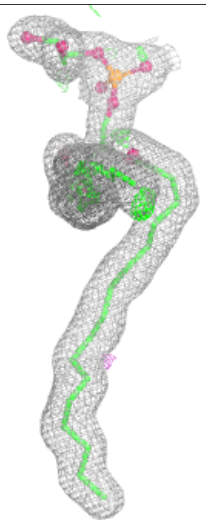


Electron density around LHG L 101:

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

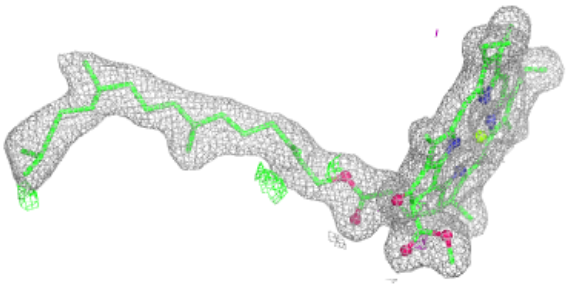


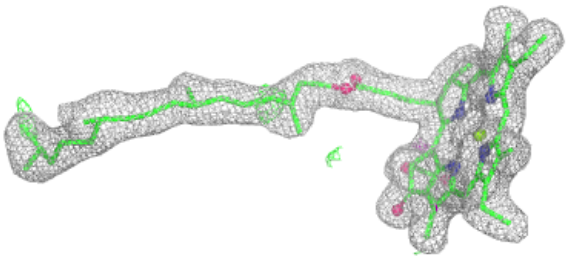


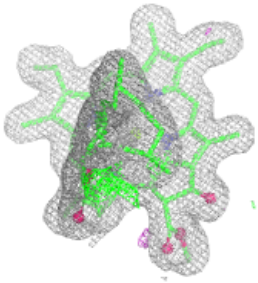


Electron density around CLA b 606:

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

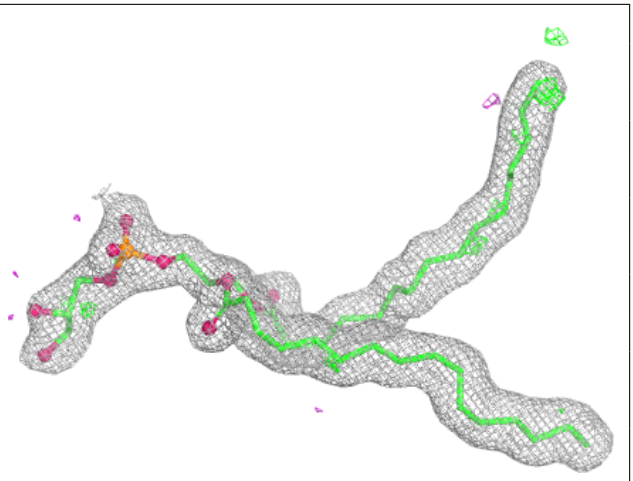


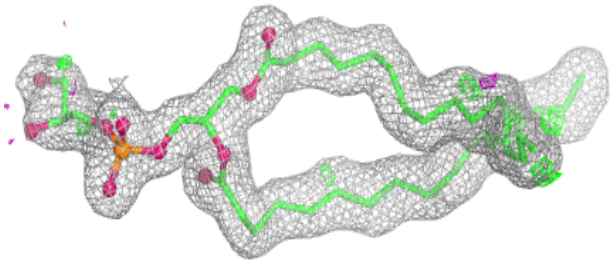


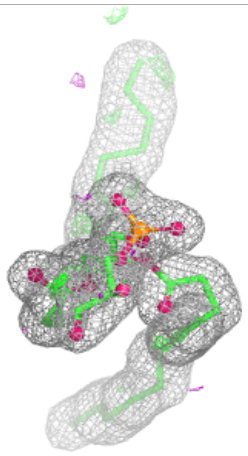


Electron density around LHG d 407:

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

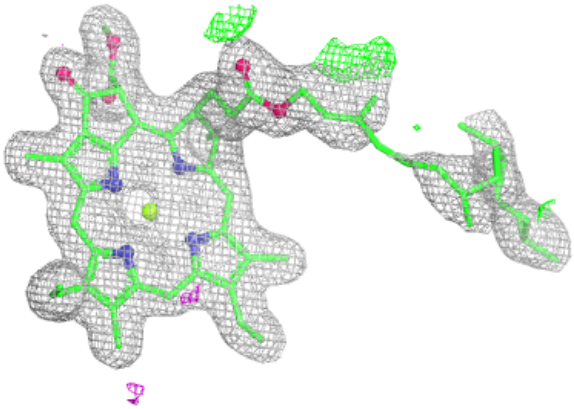


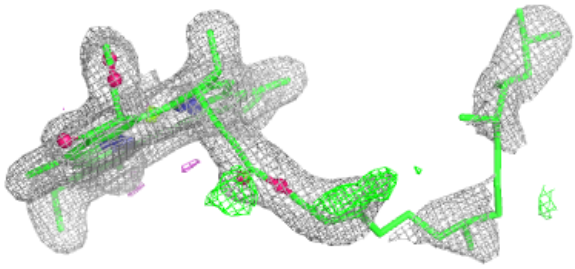


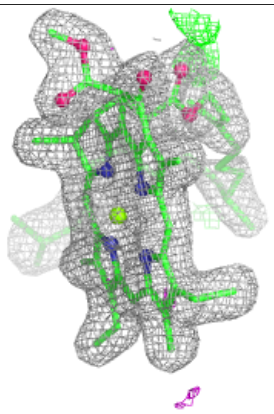


Electron density around CLA A 404:

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

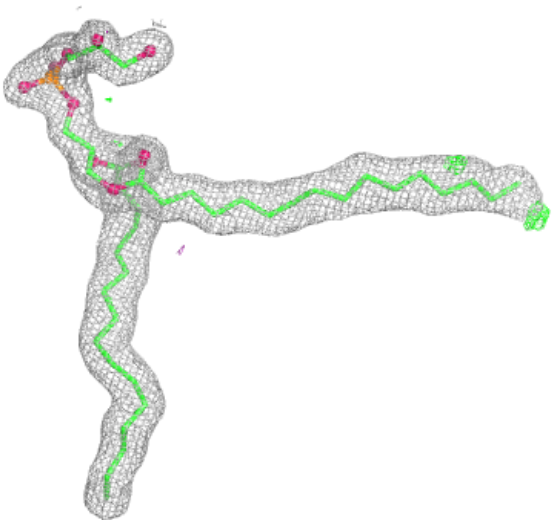


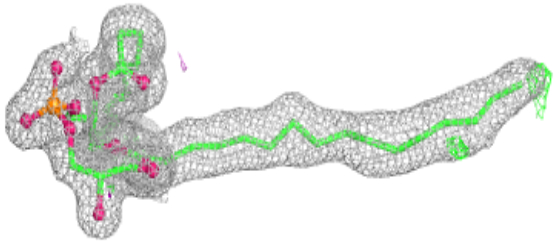


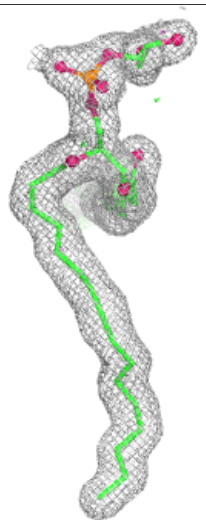


Electron density around LHG l 102:

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

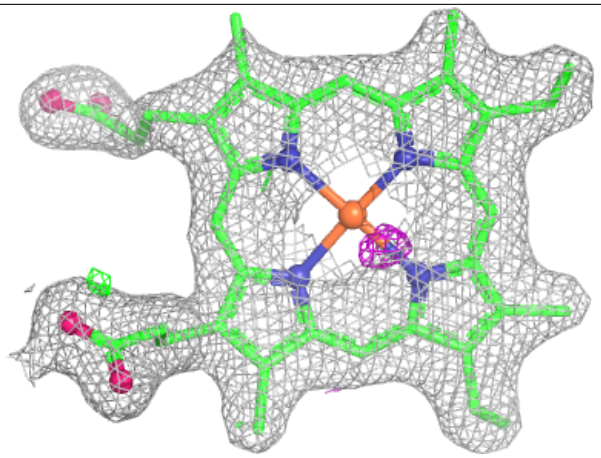


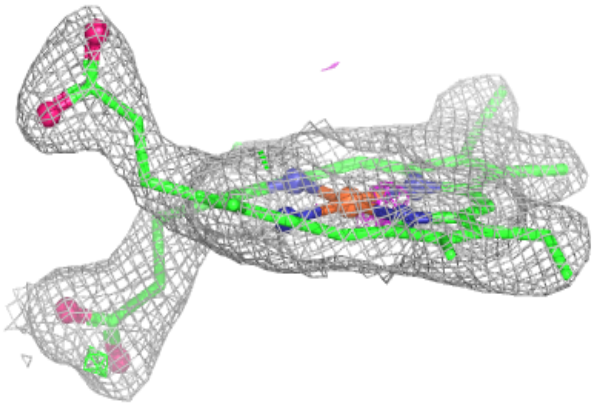


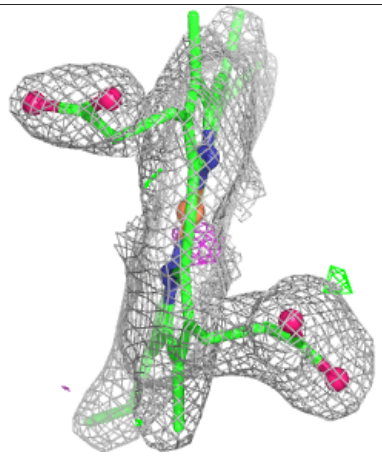


Electron density around HEM E 104:

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

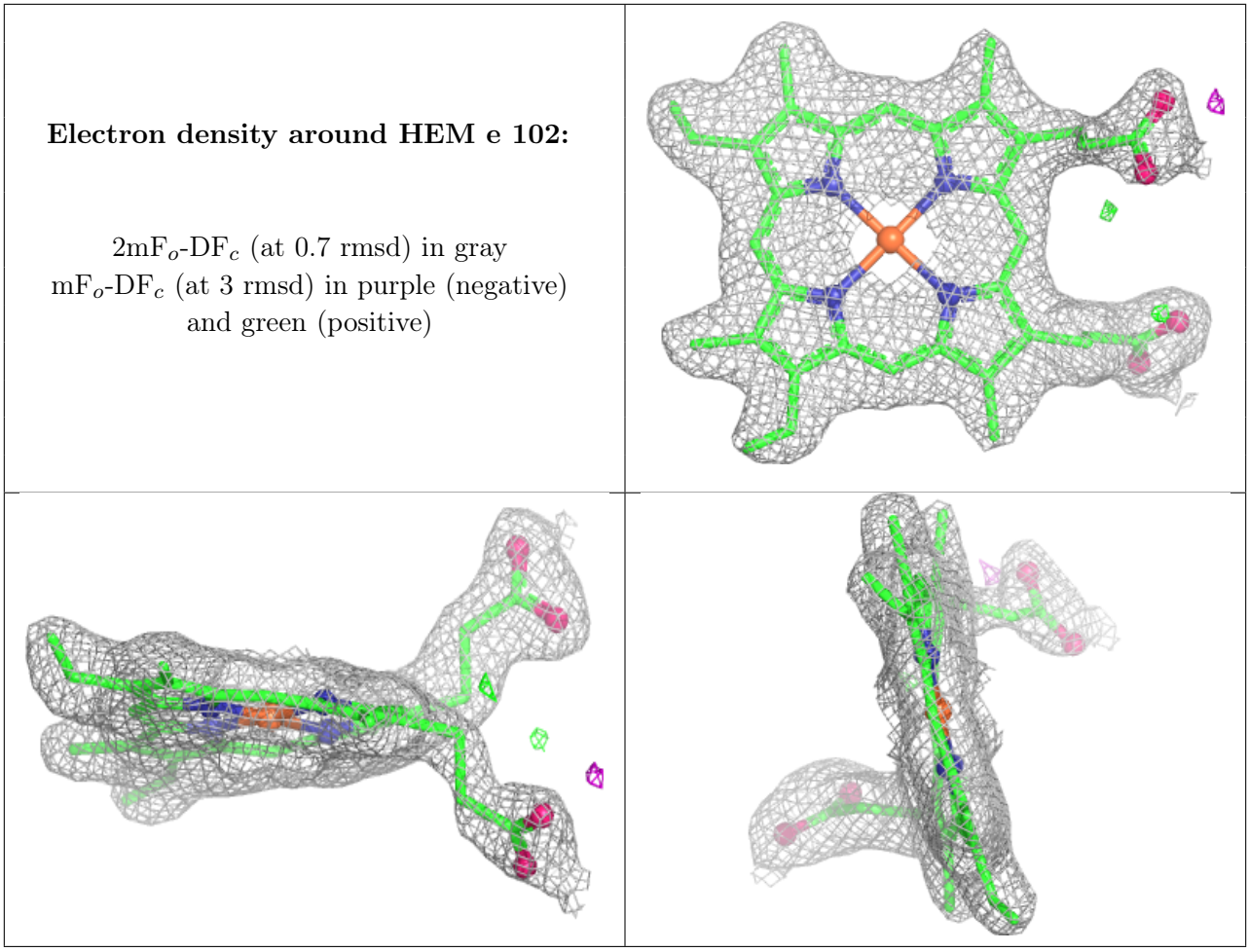






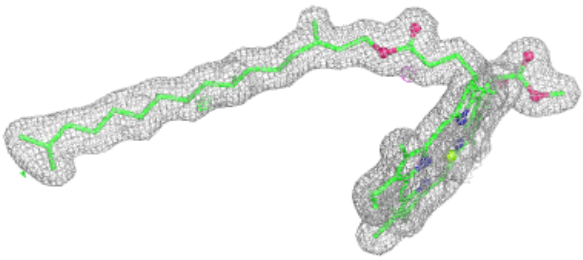
Electron density around HEM e 102:

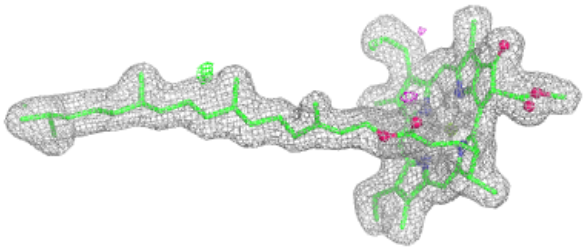
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

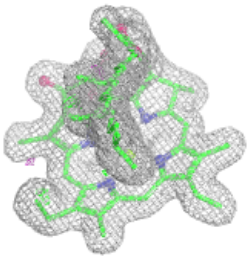


Electron density around CLA b 609:

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

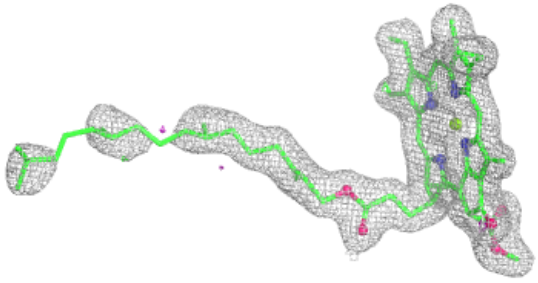


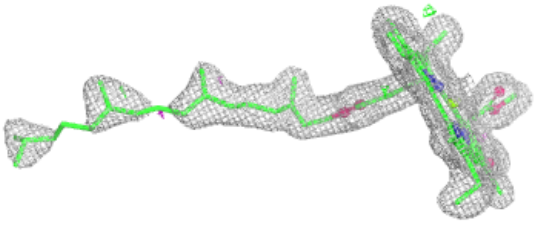


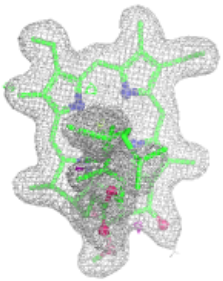


Electron density around CLA d 404:

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

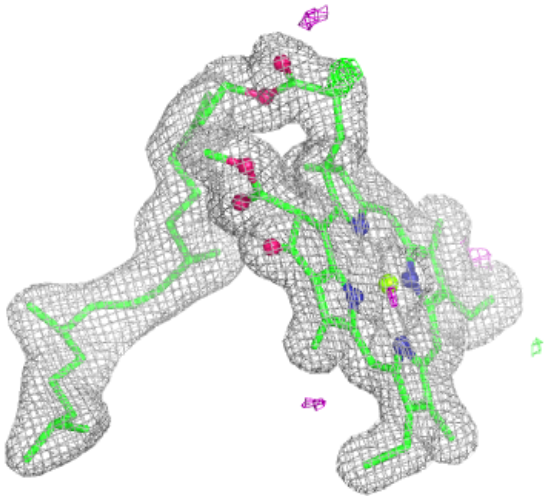


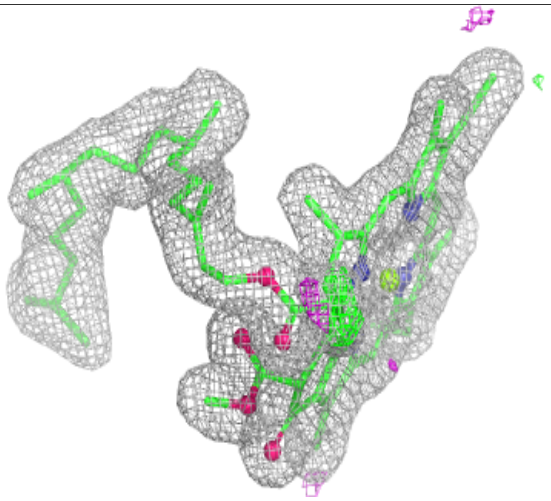


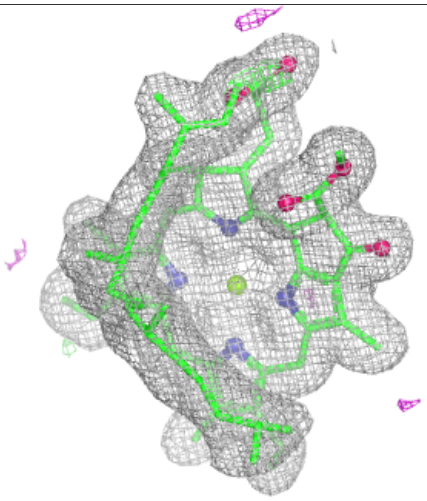


Electron density around CLA b 615:

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

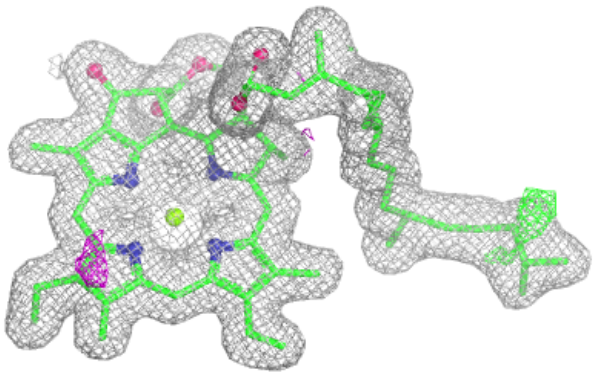


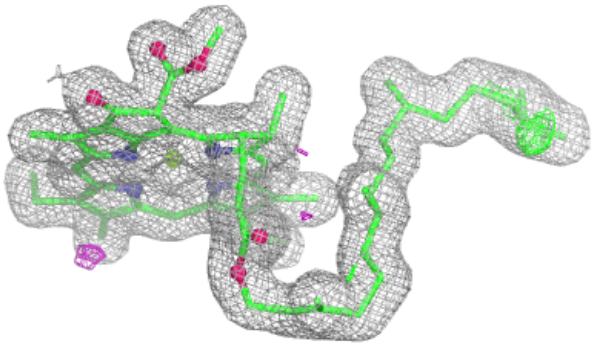




Electron density around CLA D 402:

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

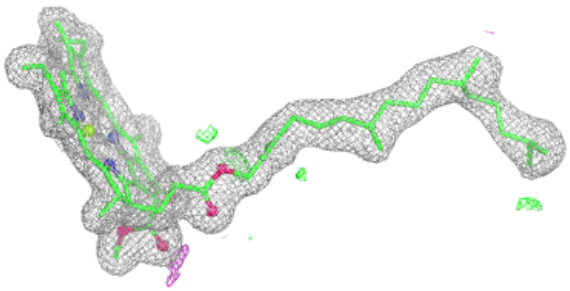


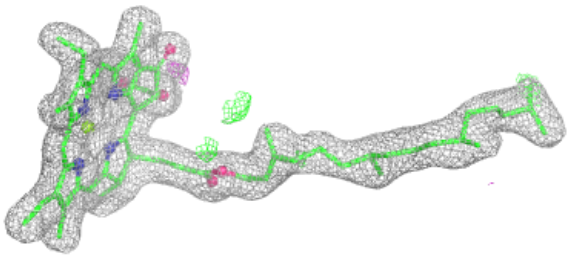


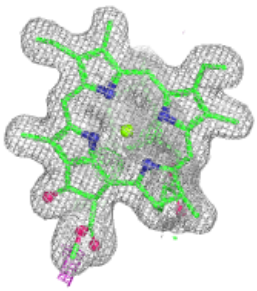


Electron density around CLA B 605:

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

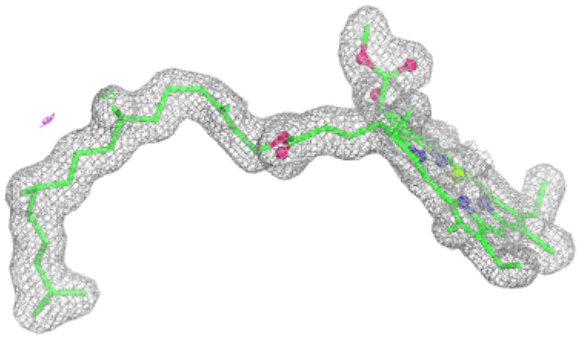


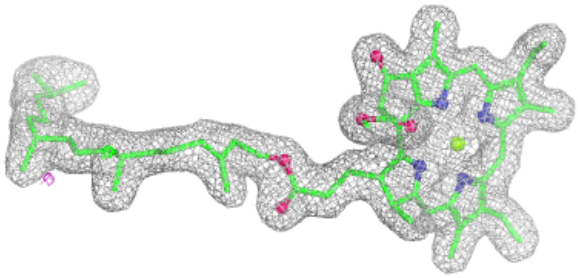


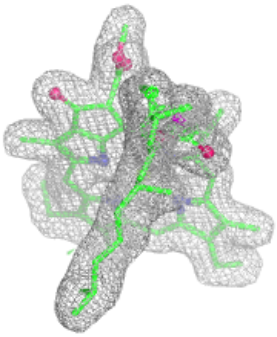


Electron density around CLA d 402:

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

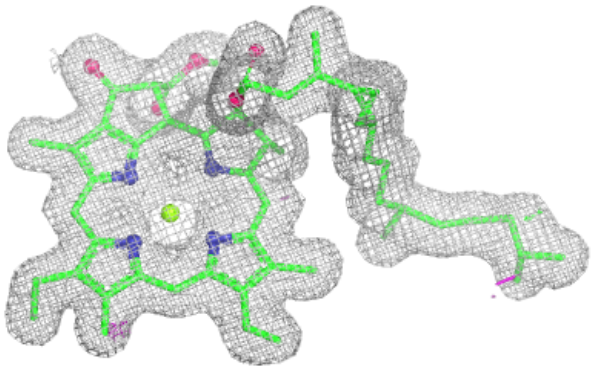


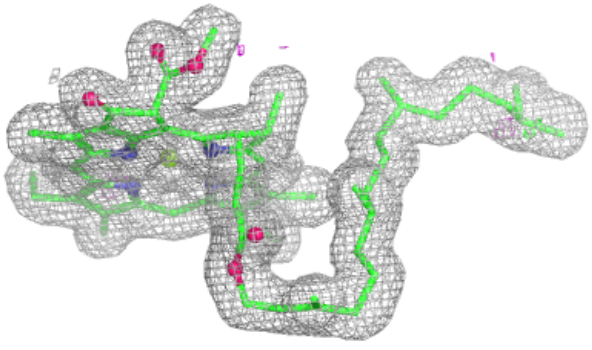


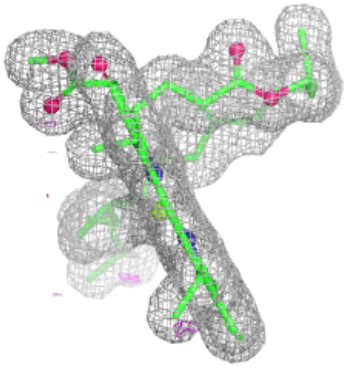


Electron density around CLA d 403:

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

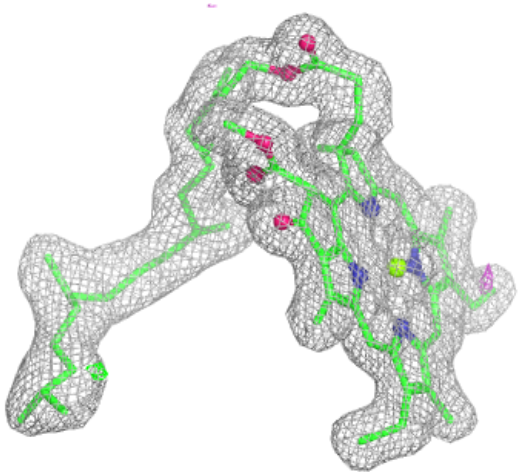


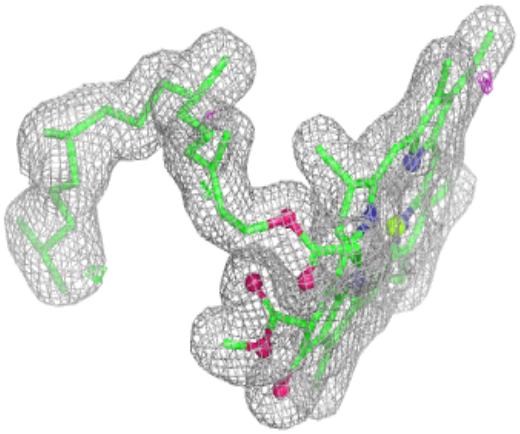


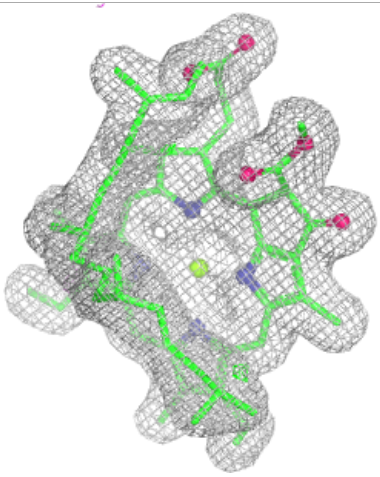


Electron density around CLA B 614:

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

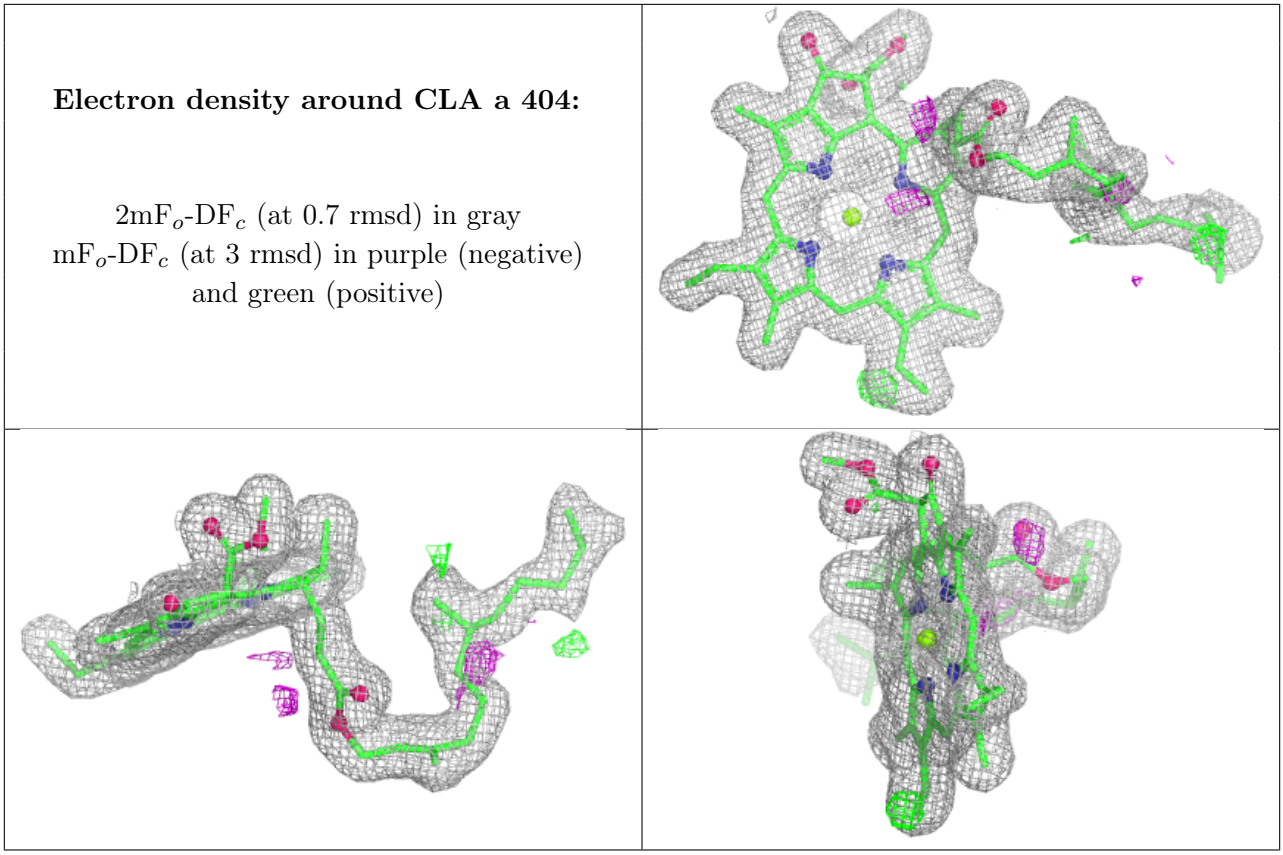






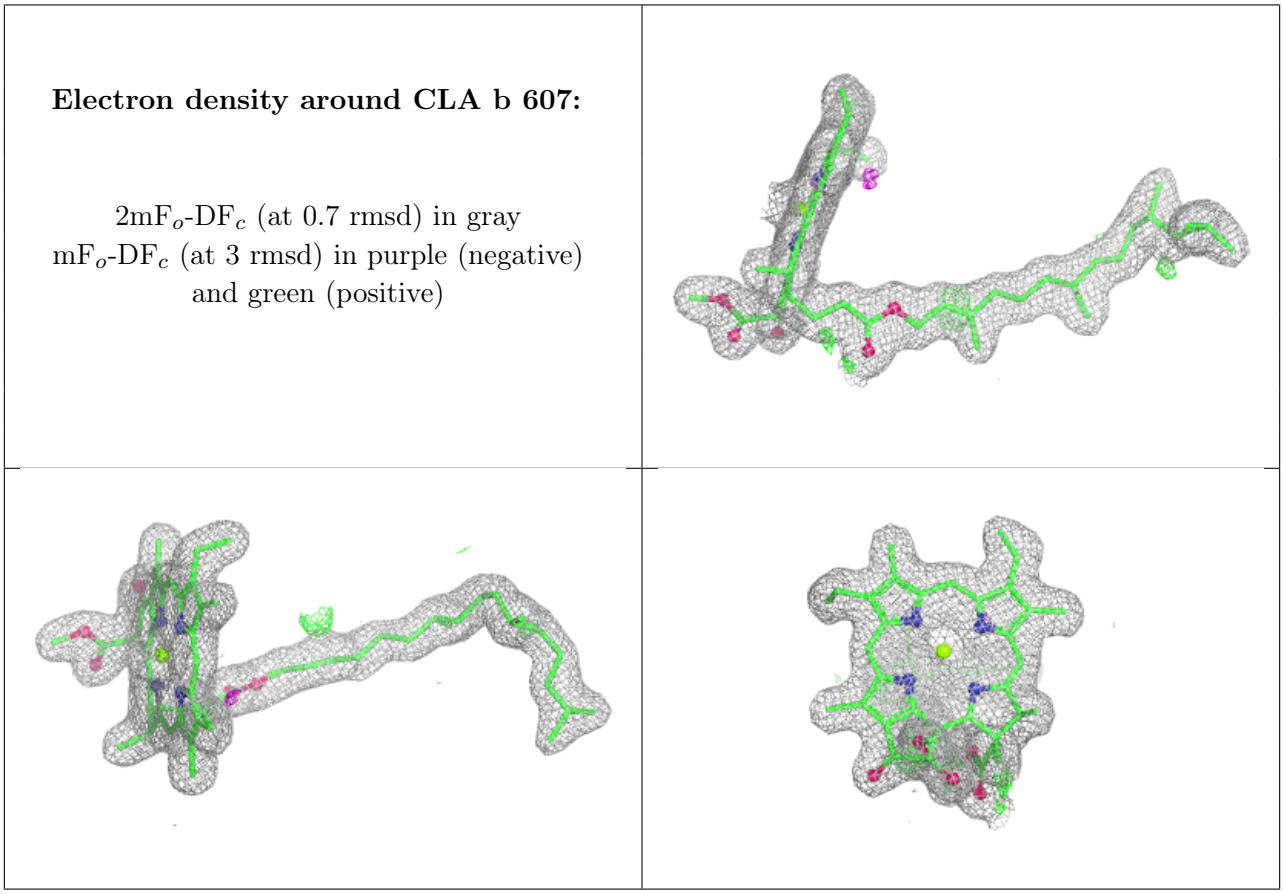
Electron density around CLA a 404:

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



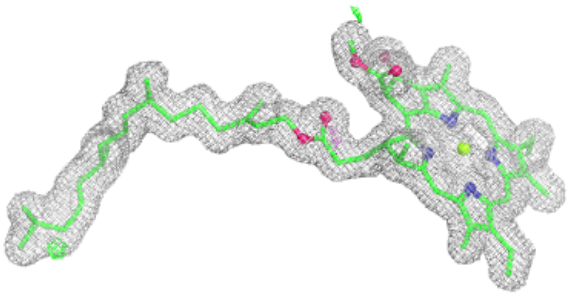
Electron density around CLA b 607:

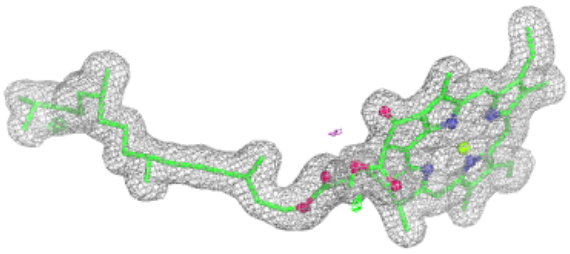
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

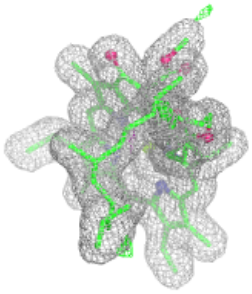


Electron density around CLA A 401:

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

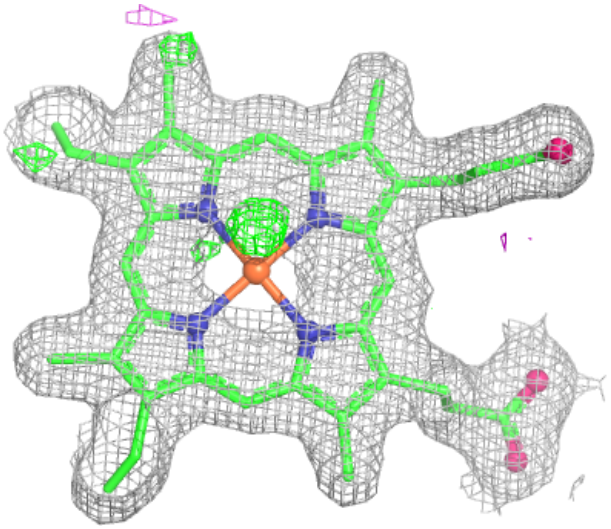


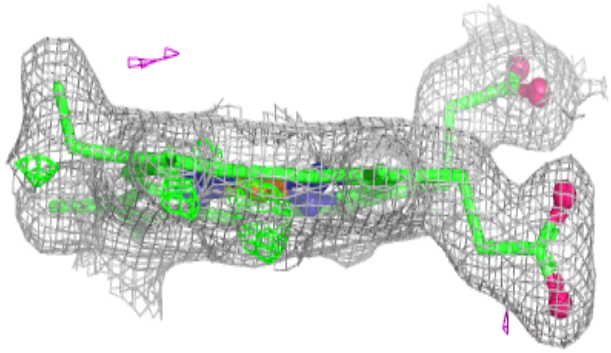


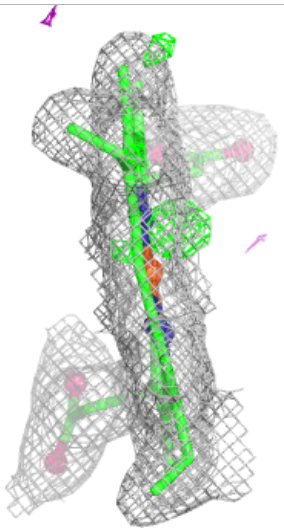


Electron density around HEC v 201:

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

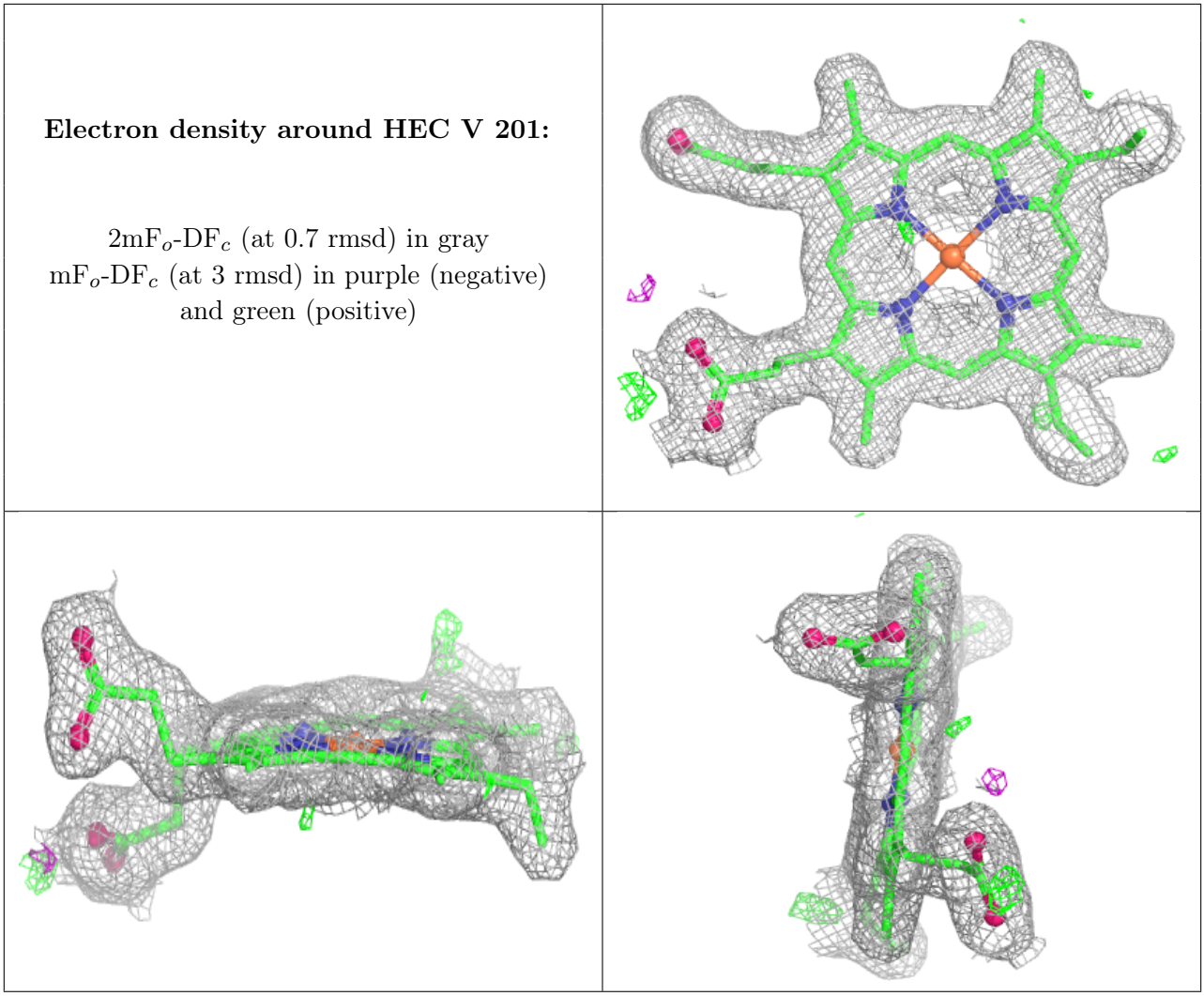






Electron density around HEC V 201:

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



6.5 Other polymers

There are no such residues in this entry.