Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID	:	7E0K / pdb_00007e0k
EMDB ID	:	EMD-30935
Title	:	LHCII-2 in the state transition supercomplex PSI-LHCI-LHCII from the double phosphatase mutant pph1;pbcp of Chlamydomonas reinhardti.
Authors	:	Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on	:	2021-01-28
Resolution	:	3.09 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

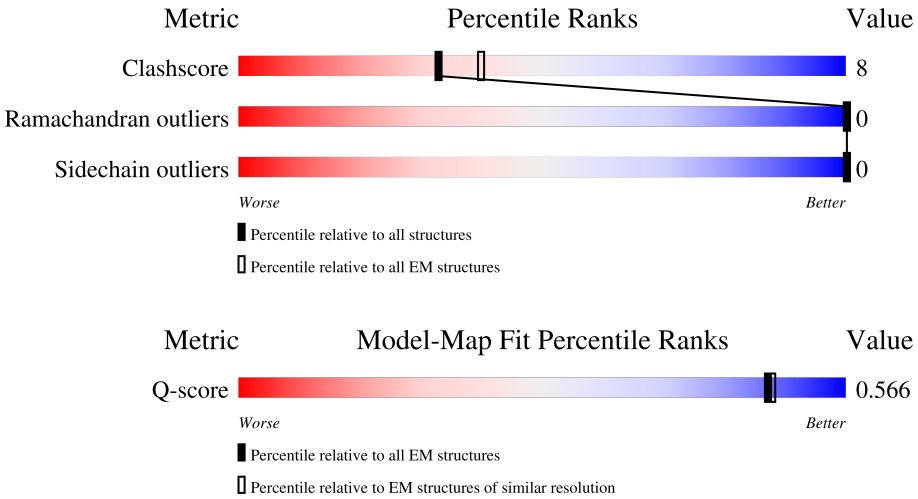
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14003 (2.59 - 3.59)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	U	257	74% 12% 15%
2	V	268	6% 82% 7% 11%
3	W	249	7% 79% 9% 12%

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
4	CHL	U	601	X	-	-	-
4	CHL	U	605	X	-	-	-
4	CHL	U	606	X	-	-	-
4	CHL	U	607	X	-	-	-
4	CHL	U	608	X	-	-	-
4	CHL	U	609	X	-	-	-
4	CHL	V	601	X	-	-	-
4	CHL	V	605	X	-	-	-
4	CHL	V	606	X	-	-	-
4	CHL	V	607	X	-	-	-
4	CHL	V	608	X	-	-	-
4	CHL	V	609	X	-	-	-
4	CHL	W	601	X	-	-	-
4	CHL	W	605	X	-	-	-
4	CHL	W	606	X	-	-	-
4	CHL	W	607	X	-	-	-
4	CHL	W	608	X	-	-	-
4	CHL	W	609	X	-	-	-
5	CLA	U	602	X	-	-	-
5	CLA	U	603	X	-	-	-
5	CLA	U	604	X	-	-	-
5	CLA	U	610	X	-	-	-
5	CLA	U	611	X	-	-	-
5	CLA	U	612	X	-	-	-
5	CLA	U	613	X	-	-	-
5	CLA	U	614	X	-	-	-
5	CLA	V	602	X	-	-	-
5	CLA	V	603	X	-	-	-
5	CLA	V	604	X	-	-	-
5	CLA	V	610	X	-	-	-
5	CLA	V	611	X	-	-	-
5	CLA	V	612	X	-	-	-
5	CLA	V	613	X	-	-	-
5	CLA	V	614	X	-	-	-
5	CLA	W	602	X	-	-	-
5	CLA	W	603	X	-	-	-
5	CLA	W	604	X	-	-	-
5	CLA	W	610	X	-	-	-
5	CLA	W	611	X	-	-	-
5	CLA	W	612	X	-	-	-
5	CLA	W	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	W	614	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8044 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	U	219	1670	1080	272	313	5	0	0

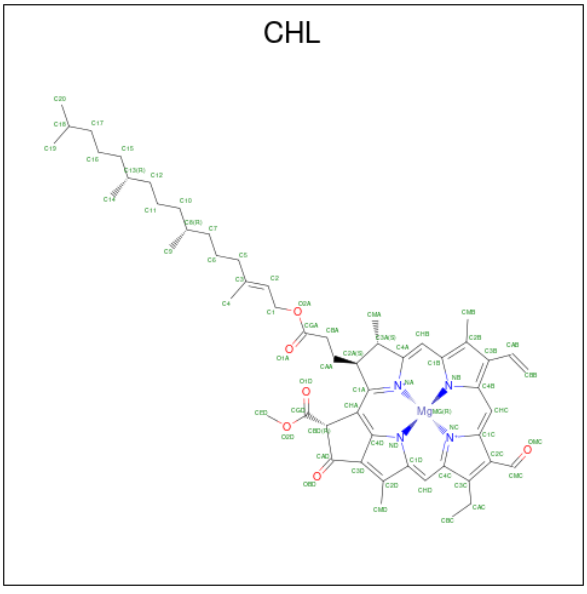
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
2	V	238	1815	1176	300	333	1	5	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

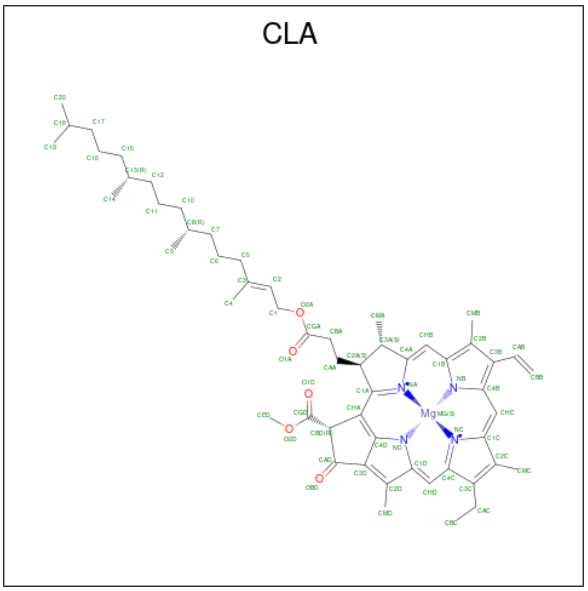
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	W	220	1671	1085	273	308	5	0	0

- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	U	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
4	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	U	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
4	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	V	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
4	V	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
4	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
4	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
4	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
5	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
5	U	1	Total	C	Mg	N	O	0
			48	39	1	4	4	
5	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
5	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
5	U	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
5	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
5	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
5	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
5	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
5	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
5	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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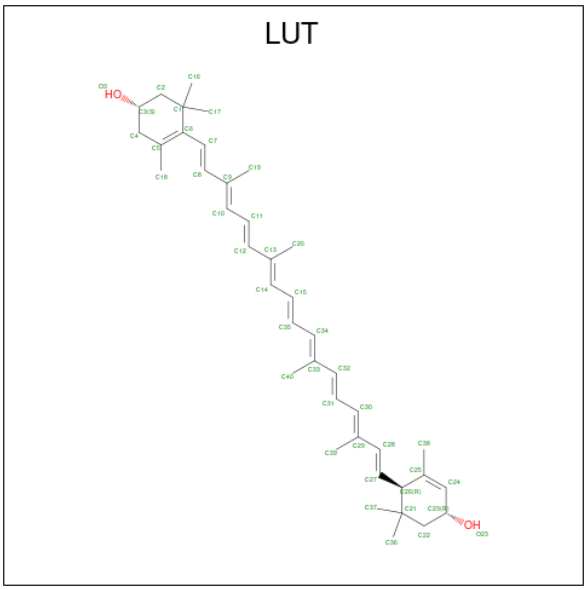
Mol	Chain	Residues	Atoms					AltConf
5	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
5	W	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
5	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	W	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
5	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 6 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3, 3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
6	U	1	Total	C	O	0
			42	40	2	

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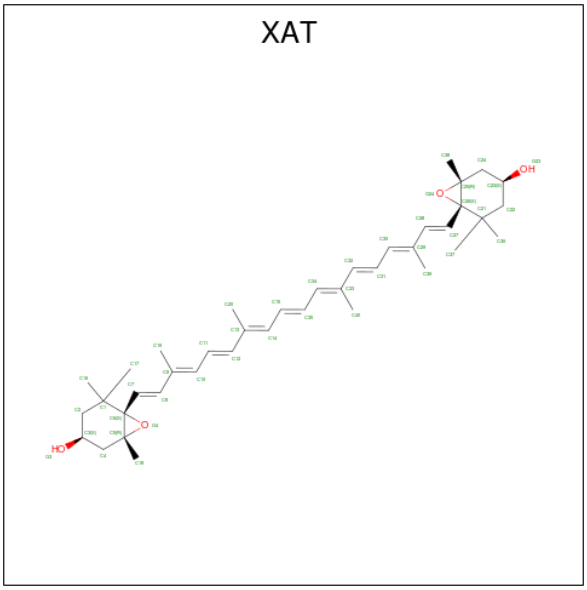
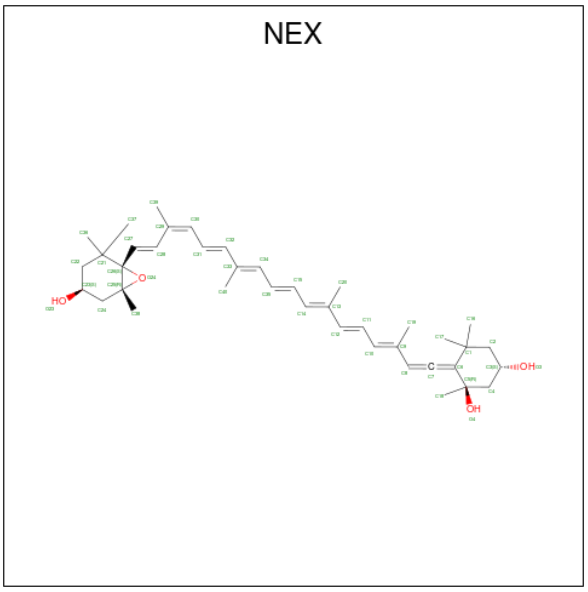
Mol	Chain	Residues	Atoms	AltConf
6	U	1	Total C O 42 40 2	0
6	V	1	Total C O 42 40 2	0
6	V	1	Total C O 42 40 2	0
6	W	1	Total C O 42 40 2	0
6	W	1	Total C O 42 40 2	0

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



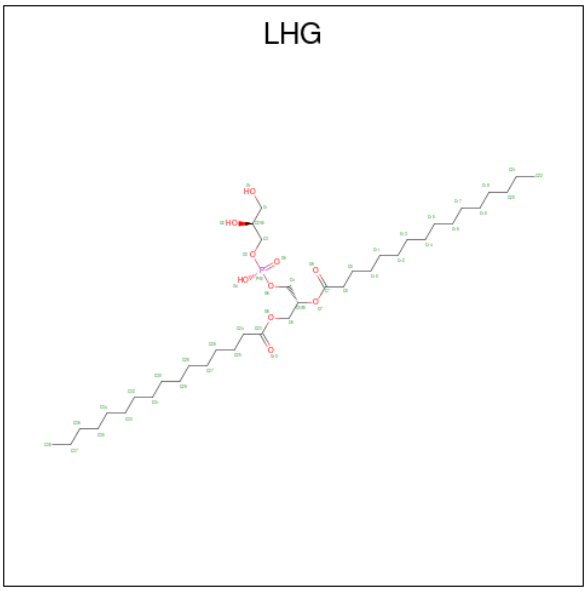
Mol	Chain	Residues	Atoms	AltConf
7	U	1	Total C O 44 40 4	0
7	V	1	Total C O 44 40 4	0
7	W	1	Total C O 44 40 4	0

- Molecule 8 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



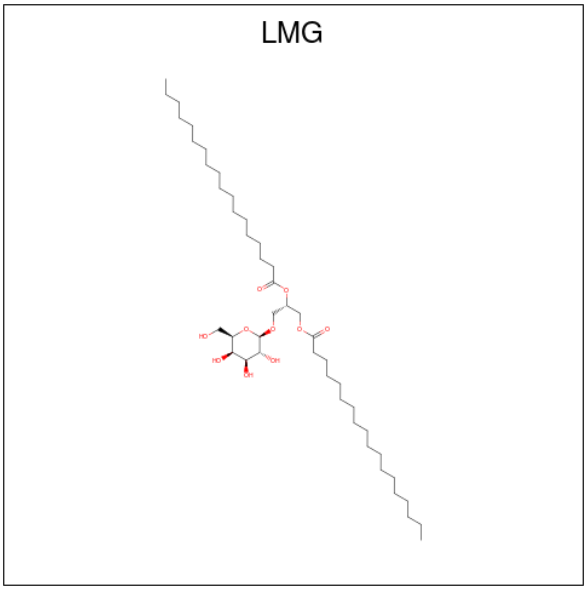
Mol	Chain	Residues	Atoms			AltConf
8	U	1	Total	C	O	0
			44	40	4	
8	V	1	Total	C	O	0
			44	40	4	
8	W	1	Total	C	O	0
			44	40	4	

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
9	U	1	Total	C	O	P	0
			49	38	10	1	
9	V	1	Total	C	O	P	0
			48	37	10	1	
9	W	1	Total	C	O	P	0
			44	33	10	1	

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



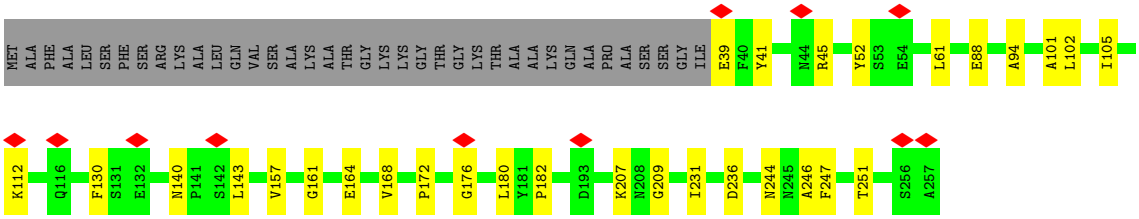
Mol	Chain	Residues	Atoms			AltConf
10	V	1	Total	C	O	0
			41	31	10	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

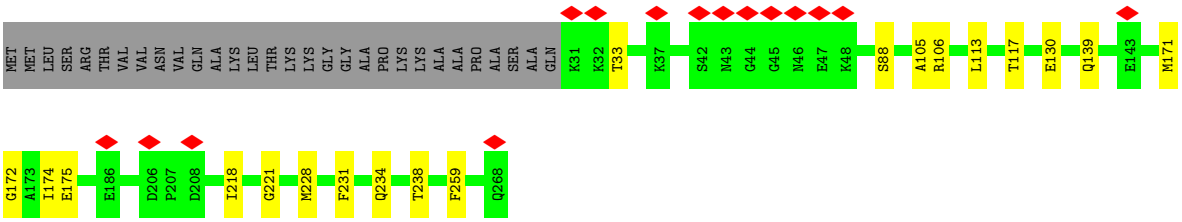
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain U:



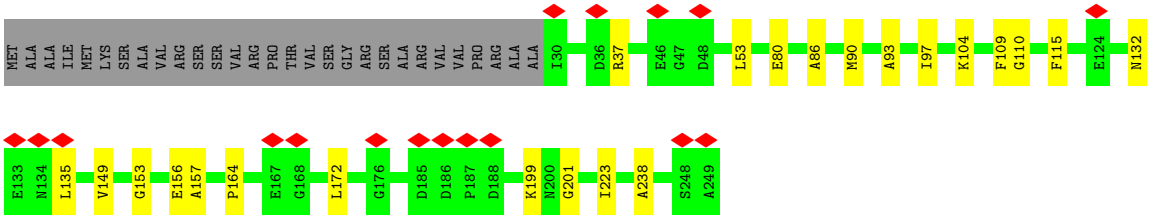
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain V:



• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, LUT, XAT, NEX, CLA, LHG, CHL, LMG

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	U	0.42	0/1718	0.50	1/2338 (0.0%)
2	V	0.40	0/1856	0.40	0/2518
3	W	0.39	0/1721	0.43	0/2341
All	All	0.40	0/5295	0.44	1/7197 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	176	GLY	N-CA-C	5.12	122.97	113.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1670	0	1604	33	0
2	V	1815	0	1765	30	0
3	W	1671	0	1604	26	0
4	U	303	0	248	13	0
4	V	309	0	253	26	0
4	W	336	0	298	18	0
5	U	401	0	344	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	415	0	365	3	0
5	W	426	0	377	4	0
6	U	84	0	112	2	0
6	V	84	0	112	2	0
6	W	84	0	112	2	0
7	U	44	0	56	5	0
7	V	44	0	56	0	0
7	W	44	0	56	4	0
8	U	44	0	56	0	0
8	V	44	0	56	1	0
8	W	44	0	56	2	0
9	U	49	0	74	1	0
9	V	48	0	69	2	0
9	W	44	0	61	0	0
10	V	41	0	52	0	0
All	All	8044	0	7786	132	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 8.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:140:ASN:CB	1:U:143:LEU:HD13	1.49	1.42
1:U:140:ASN:HB3	1:U:143:LEU:HD13	1.31	1.11
1:U:140:ASN:HB2	1:U:143:LEU:HD13	1.12	1.08
1:U:140:ASN:CB	1:U:143:LEU:CD1	2.35	1.03
2:V:174:ILE:HD11	4:V:608:CHL:C4A	1.93	0.98
1:U:140:ASN:HB3	1:U:143:LEU:CD1	1.97	0.91
2:V:174:ILE:HD11	4:V:608:CHL:CHB	2.00	0.90
2:V:171:MET:HA	2:V:174:ILE:HG22	1.50	0.90
2:V:171:MET:HA	2:V:174:ILE:CG2	2.03	0.88
3:W:132:ASN:HB2	3:W:135:LEU:CD1	2.07	0.85
1:U:140:ASN:HB2	1:U:143:LEU:CD1	2.01	0.82
2:V:171:MET:CA	2:V:174:ILE:HG22	2.10	0.82
2:V:174:ILE:HD11	4:V:608:CHL:CMA	2.10	0.81
2:V:171:MET:C	2:V:174:ILE:HG22	2.06	0.80
2:V:171:MET:O	2:V:174:ILE:HG22	1.82	0.79
2:V:174:ILE:CD1	4:V:608:CHL:CMA	2.65	0.74
2:V:174:ILE:CD1	4:V:608:CHL:CHB	2.67	0.72
3:W:238:ALA:N	5:W:613:CLA:O1A	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:132:ASN:HB2	3:W:135:LEU:HD12	1.73	0.69
2:V:174:ILE:CD1	4:V:608:CHL:HMA3	2.28	0.64
2:V:171:MET:O	2:V:174:ILE:CG2	2.47	0.63
3:W:132:ASN:CB	3:W:135:LEU:HG	2.29	0.63
2:V:174:ILE:HD11	4:V:608:CHL:HMA3	1.81	0.62
3:W:132:ASN:HB2	3:W:135:LEU:HG	1.82	0.62
3:W:199:LYS:NZ	5:W:611:CLA:O1D	2.28	0.62
2:V:174:ILE:CD1	4:V:608:CHL:HMA1	2.31	0.61
3:W:132:ASN:HB2	3:W:135:LEU:CG	2.32	0.60
2:V:171:MET:HA	2:V:174:ILE:HG21	1.84	0.59
1:U:251:THR:HA	4:W:607:CHL:HED3	1.85	0.58
2:V:106:ARG:NH1	4:V:608:CHL:OBD	2.37	0.56
1:U:157:VAL:HG13	4:U:609:CHL:HBB2	1.88	0.56
1:U:105:ILE:HG23	1:U:231:ILE:HD11	1.88	0.56
1:U:236:ASP:O	1:U:244:ASN:ND2	2.40	0.55
3:W:80:GLU:HA	3:W:172:LEU:HD21	1.90	0.54
4:V:605:CHL:HHD	4:V:606:CHL:OBD	2.07	0.54
3:W:97:ILE:HG23	3:W:223:ILE:HD11	1.88	0.54
1:U:88:GLU:HA	1:U:180:LEU:HD21	1.89	0.54
6:V:1620:LUT:H181	6:V:1620:LUT:C8	2.37	0.52
1:U:39:GLU:CD	1:U:41:TYR:O	2.53	0.52
2:V:105:ALA:HB1	2:V:221:GLY:HA3	1.92	0.51
3:W:153:GLY:CA	4:W:609:CHL:HAB	2.40	0.51
1:U:246:ALA:N	5:U:613:CLA:O1A	2.39	0.51
1:U:140:ASN:ND2	1:U:143:LEU:HD11	2.26	0.51
4:U:601:CHL:H161	4:W:607:CHL:H161	1.92	0.50
3:W:104:LYS:NZ	3:W:223:ILE:HG21	2.27	0.50
1:U:161:GLY:CA	4:U:609:CHL:HAB	2.42	0.50
1:U:94:ALA:HB1	1:U:209:GLY:HA3	1.93	0.50
3:W:156:GLU:OE1	4:W:609:CHL:NA	2.44	0.50
2:V:174:ILE:HG23	2:V:175:GLU:N	2.26	0.49
3:W:149:VAL:HG11	7:W:1622:XAT:C33	2.43	0.49
1:U:112:LYS:NZ	1:U:231:ILE:HG21	2.27	0.49
3:W:86:ALA:HB1	3:W:201:GLY:HA3	1.93	0.49
1:U:172:PRO:HG2	4:U:608:CHL:CBB	2.43	0.48
1:U:164:GLU:OE1	4:U:609:CHL:NA	2.45	0.48
4:W:607:CHL:H193	4:W:607:CHL:H162	1.74	0.48
1:U:140:ASN:HD22	1:U:143:LEU:HD11	1.76	0.48
1:U:157:VAL:HG11	7:U:1622:XAT:C33	2.44	0.47
3:W:149:VAL:HG13	4:W:609:CHL:HBB2	1.96	0.47
4:W:601:CHL:H101	4:W:601:CHL:H61	1.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:1622:XAT:H192	2:V:259:PHE:CE1	2.50	0.47
4:V:609:CHL:H111	4:V:609:CHL:H71	1.54	0.47
2:V:174:ILE:HD11	4:V:608:CHL:C3A	2.41	0.46
2:V:174:ILE:HD13	4:V:608:CHL:HMA3	1.98	0.46
3:W:115:PHE:HA	4:W:607:CHL:HMA2	1.96	0.46
3:W:132:ASN:HB3	3:W:135:LEU:HG	1.97	0.46
3:W:164:PRO:HG2	4:W:608:CHL:CBB	2.45	0.46
4:W:601:CHL:H3A	4:W:601:CHL:HBA1	1.53	0.46
4:U:601:CHL:H101	4:U:601:CHL:H61	1.51	0.45
8:V:1623:NEX:H201	8:V:1623:NEX:H15	1.75	0.45
1:U:207:LYS:NZ	5:U:611:CLA:O1D	2.37	0.45
3:W:90:MET:SD	5:W:610:CLA:HAB	2.57	0.45
1:U:164:GLU:O	1:U:168:VAL:HG13	2.17	0.45
4:U:609:CHL:H91	4:U:609:CHL:H111	1.62	0.45
7:U:1622:XAT:H31	7:U:1622:XAT:H391	1.77	0.45
4:V:605:CHL:HBB1	4:V:605:CHL:HHC	1.99	0.45
3:W:135:LEU:O	4:W:605:CHL:CGD	2.65	0.45
2:V:113:LEU:O	2:V:117:THR:OG1	2.28	0.44
4:V:608:CHL:HBB1	4:V:608:CHL:HHC	1.97	0.44
8:W:1623:NEX:H35	8:W:1623:NEX:H401	1.81	0.44
1:U:45:ARG:NH2	1:U:61:LEU:O	2.51	0.44
2:V:130:GLU:HB2	2:V:139:GLN:HG2	1.99	0.44
4:V:607:CHL:HBB2	4:V:609:CHL:HBC1	1.99	0.44
4:V:607:CHL:HBB2	4:V:609:CHL:CBC	2.48	0.44
8:W:1623:NEX:H15	8:W:1623:NEX:H201	1.76	0.44
7:W:1622:XAT:H31	7:W:1622:XAT:H391	1.77	0.44
5:U:613:CLA:HMB1	6:U:1620:LUT:H7	2.01	0.43
3:W:37:ARG:NH2	3:W:53:LEU:O	2.51	0.43
1:U:143:LEU:O	4:U:605:CHL:CGD	2.66	0.43
4:U:605:CHL:HHD	4:U:606:CHL:OBD	2.18	0.43
4:U:605:CHL:HBB1	4:U:605:CHL:HHC	2.00	0.43
9:U:2630:LHG:H202	7:W:1622:XAT:H10	2.00	0.43
4:W:605:CHL:HHD	4:W:606:CHL:OBD	2.18	0.43
4:V:601:CHL:HED3	9:V:2630:LHG:H282	2.01	0.43
1:U:130:PHE:HZ	2:V:259:PHE:HB3	1.84	0.43
4:W:605:CHL:HBB1	4:W:605:CHL:HHC	2.01	0.43
6:U:1620:LUT:H171	6:U:1620:LUT:C8	2.49	0.42
4:V:601:CHL:H141	4:V:601:CHL:H161	1.58	0.42
4:V:601:CHL:H61	4:V:601:CHL:H102	1.30	0.42
4:W:607:CHL:H92	4:W:607:CHL:H61	1.73	0.42
4:W:606:CHL:HBB1	4:W:606:CHL:HHC	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:234:GLN:O	2:V:238:THR:HB	2.19	0.42
4:U:606:CHL:HBB1	4:U:606:CHL:HHC	2.00	0.42
2:V:174:ILE:HG23	2:V:175:GLU:HG2	2.01	0.42
4:V:606:CHL:HBB1	4:V:606:CHL:HHC	2.01	0.42
5:W:613:CLA:HMB1	6:W:1620:LUT:H7	2.01	0.42
1:U:102:LEU:HD23	5:U:604:CLA:HMC1	2.01	0.42
3:W:153:GLY:HA2	4:W:609:CHL:HAB	2.02	0.42
6:W:1620:LUT:H171	6:W:1620:LUT:C8	2.49	0.42
1:U:164:GLU:OE1	4:U:609:CHL:C4A	2.67	0.42
7:U:1622:XAT:H201	7:U:1622:XAT:H15	1.70	0.42
4:V:607:CHL:HBB1	4:V:607:CHL:HHC	2.01	0.42
4:W:606:CHL:HBB1	4:W:607:CHL:HHC	2.02	0.42
4:U:601:CHL:H3A	4:U:601:CHL:HBA1	1.76	0.41
5:V:611:CLA:O1D	5:V:611:CLA:H2A	2.20	0.41
2:V:218:ILE:HD12	2:V:218:ILE:HA	1.91	0.41
4:V:601:CHL:H3A	4:V:601:CHL:HBA1	1.75	0.41
5:V:602:CLA:CGA	5:V:602:CLA:H3A	2.50	0.41
4:V:606:CHL:HBB2	4:V:607:CHL:CBB	2.49	0.41
3:W:109:PHE:O	3:W:110:GLY:C	2.63	0.41
2:V:88:SER:OG	5:V:602:CLA:O1A	2.34	0.41
1:U:101:ALA:O	1:U:105:ILE:HG13	2.21	0.41
2:V:172:GLY:HA2	4:V:609:CHL:HAB	2.03	0.41
1:U:182:PRO:HD2	5:U:610:CLA:OBD	2.22	0.40
1:U:247:PHE:CE1	7:W:1622:XAT:H192	2.57	0.40
6:V:1620:LUT:C8	6:V:1620:LUT:C18	2.98	0.40
3:W:93:ALA:O	3:W:97:ILE:HG13	2.21	0.40
7:U:1622:XAT:H12	9:V:2630:LHG:H332	2.04	0.40
3:W:156:GLU:OE1	4:W:609:CHL:C4A	2.69	0.40
1:U:52:TYR:CB	3:W:157:ALA:HB1	2.51	0.40
1:U:112:LYS:HZ3	1:U:231:ILE:HG21	1.87	0.40
2:V:228:MET:SD	2:V:231:PHE:CD2	3.15	0.40
4:V:601:CHL:H111	4:V:601:CHL:H151	1.73	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 PDB entries followed by that with respect to all EM

entries.

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	U	217/257 (84%)	198 (91%)	19 (9%)	0	100	100
2	V	235/268 (88%)	220 (94%)	15 (6%)	0	100	100
3	W	218/249 (88%)	204 (94%)	14 (6%)	0	100	100
All	All	670/774 (87%)	622 (93%)	48 (7%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	U	168/194 (87%)	168 (100%)	0	100	100
2	V	178/201 (89%)	178 (100%)	0	100	100
3	W	164/187 (88%)	164 (100%)	0	100	100
All	All	510/582 (88%)	510 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	169	ASN
2	V	156	HIS
2	V	158	GLN
3	W	161	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
2	TPO	V	33	2	8,10,11	1.60	1 (12%)	10,14,16	1.95	2 (20%)

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
2	TPO	V	33	2	-	5/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	33	TPO	P-O1P	3.33	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	33	TPO	P-OG1-CB	-5.15	109.32	123.33
2	V	33	TPO	CG2-CB-CA	-2.34	108.70	113.26

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	33	TPO	N-CA-CB-CG2
2	V	33	TPO	CB-OG1-P-O1P
2	V	33	TPO	CB-OG1-P-O2P
2	V	33	TPO	CB-OG1-P-O3P
2	V	33	TPO	O-C-CA-CB

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)

58 ligands 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	$\#\|Z\| > 2$
5	CLA	V	613	2	69,73,73	1.18	6 (8%)	82,113,113	1.16	5 (6%)
7	XAT	W	1622	-	41,47,47	0.93	2 (4%)	54,74,74	4.33	25 (46%)
4	CHL	W	607	-	59,73,74	3.22	19 (32%)	59,113,114	2.15	17 (28%)
6	LUT	V	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.79	13 (25%)
4	CHL	W	605	3	40,54,74	4.04	19 (47%)	34,90,114	3.22	17 (50%)
6	LUT	V	1621	-	42,43,43	0.98	2 (4%)	51,60,60	1.82	12 (23%)
5	CLA	U	614	-	46,50,73	1.39	8 (17%)	53,85,113	1.27	4 (7%)
8	NEX	U	1623	-	40,46,46	1.01	3 (7%)	50,70,70	2.35	17 (34%)
4	CHL	V	606	-	38,52,74	3.96	19 (50%)	31,87,114	3.19	13 (41%)
9	LHG	U	2630	5	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
4	CHL	U	605	1	37,51,74	4.11	18 (48%)	30,86,114	3.38	16 (53%)
4	CHL	V	609	2	55,69,74	3.59	19 (34%)	52,108,114	2.21	15 (28%)
4	CHL	U	608	-	38,52,74	4.01	18 (47%)	31,87,114	3.05	13 (41%)
5	CLA	W	610	3	59,63,73	1.26	8 (13%)	70,101,113	1.16	6 (8%)
8	NEX	W	1623	-	40,46,46	1.01	2 (5%)	50,70,70	2.35	17 (34%)
5	CLA	V	610	2	66,70,73	1.19	7 (10%)	78,109,113	1.14	6 (7%)
7	XAT	V	1622	-	41,47,47	0.94	4 (9%)	54,74,74	2.47	19 (35%)
4	CHL	V	607	-	40,54,74	3.94	19 (47%)	34,90,114	2.93	14 (41%)
4	CHL	W	608	-	41,55,74	3.93	19 (46%)	35,91,114	2.92	15 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CLA	U	604	-	52,56,73	1.43	8 (15%)	61,91,113	1.26	6 (9%)
6	LUT	W	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.82	14 (27%)
4	CHL	U	606	-	38,52,74	3.96	18 (47%)	31,87,114	3.21	16 (51%)
4	CHL	V	601	2	60,74,74	3.37	19 (31%)	58,114,114	2.40	14 (24%)
5	CLA	W	614	-	49,53,73	1.37	8 (16%)	58,89,113	1.31	4 (6%)
5	CLA	W	612	3	49,53,73	1.38	8 (16%)	58,89,113	1.30	4 (6%)
6	LUT	W	1620	-	42,43,43	0.88	1 (2%)	51,60,60	1.89	9 (17%)
9	LHG	W	2630	5	43,43,48	0.96	2 (4%)	46,49,54	0.97	2 (4%)
6	LUT	U	1621	-	42,43,43	0.97	2 (4%)	51,60,60	1.83	14 (27%)
5	CLA	W	602	3	64,68,73	1.20	8 (12%)	76,107,113	1.24	4 (5%)
5	CLA	W	603	-	56,60,73	1.29	8 (14%)	65,97,113	1.36	6 (9%)
5	CLA	V	602	2	64,68,73	1.21	8 (12%)	76,107,113	1.23	8 (10%)
4	CHL	W	601	3	60,74,74	3.39	20 (33%)	58,114,114	2.45	17 (29%)
5	CLA	U	613	1	63,67,73	1.20	6 (9%)	74,105,113	1.21	5 (6%)
5	CLA	U	602	1	63,67,73	1.21	7 (11%)	74,105,113	1.23	4 (5%)
5	CLA	U	610	1	60,64,73	1.26	8 (13%)	71,102,113	1.16	6 (8%)
4	CHL	V	608	-	42,56,74	3.80	19 (45%)	36,92,114	2.93	15 (41%)
5	CLA	V	614	-	49,53,73	1.38	8 (16%)	58,89,113	1.26	4 (6%)
4	CHL	U	609	1	54,68,74	3.58	20 (37%)	50,106,114	2.48	15 (30%)
5	CLA	V	612	2	49,53,73	1.37	8 (16%)	58,89,113	1.33	6 (10%)
5	CLA	W	611	9	61,65,73	1.21	8 (13%)	72,103,113	1.22	5 (6%)
6	LUT	U	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.89	10 (19%)
8	NEX	V	1623	-	40,46,46	0.97	3 (7%)	50,70,70	2.11	12 (24%)
4	CHL	V	605	2	38,52,74	4.05	18 (47%)	31,87,114	3.09	13 (41%)
5	CLA	U	603	-	56,60,73	1.29	8 (14%)	65,97,113	1.34	6 (9%)
5	CLA	W	604	-	51,55,73	1.33	7 (13%)	60,91,113	1.23	4 (6%)
4	CHL	U	601	1	60,74,74	3.40	19 (31%)	58,114,114	2.46	16 (27%)
10	LMG	V	2631	-	41,41,55	1.02	3 (7%)	49,49,63	1.17	4 (8%)
5	CLA	V	604	-	54,58,73	1.32	6 (11%)	64,95,113	1.25	4 (6%)
4	CHL	W	606	-	40,54,74	3.95	19 (47%)	34,90,114	5.43	19 (55%)
5	CLA	W	613	3	69,73,73	1.16	6 (8%)	82,113,113	1.17	5 (6%)
5	CLA	V	603	-	49,53,73	1.38	8 (16%)	58,89,113	1.39	3 (5%)
4	CHL	W	609	3	60,74,74	3.41	20 (33%)	58,114,114	2.34	16 (27%)
7	XAT	U	1622	-	41,47,47	0.94	2 (4%)	54,74,74	4.34	25 (46%)
9	LHG	V	2630	5	47,47,48	0.90	2 (4%)	50,53,54	1.13	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CLA	U	611	9	46,50,73	1.36	8 (17%)	53,85,113	1.32	4 (7%)
5	CLA	U	612	1	47,51,73	1.38	8 (17%)	55,86,113	1.30	4 (7%)
5	CLA	V	611	9	47,51,73	1.36	7 (14%)	55,86,113	1.34	4 (7%)
4	CHL	U	607	-	40,54,74	3.94	19 (47%)	34,90,114	3.01	15 (44%)

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
5	CLA	V	613	2	1/1/15/20	16/39/115/115	-
7	XAT	W	1622	-	-	4/31/93/93	0/4/4/4
4	CHL	W	607	-	3/3/20/26	25/37/135/137	-
6	LUT	V	1620	-	-	0/29/67/67	0/2/2/2
4	CHL	W	605	3	3/3/16/26	3/15/113/137	-
6	LUT	V	1621	-	-	2/29/67/67	0/2/2/2
5	CLA	U	614	-	1/1/10/20	5/12/88/115	-
8	NEX	U	1623	-	-	5/27/83/83	0/3/3/3
4	CHL	V	606	-	3/3/15/26	2/13/111/137	-
9	LHG	U	2630	5	-	12/53/53/53	-
4	CHL	U	605	1	3/3/15/26	0/12/110/137	-
4	CHL	V	609	2	3/3/19/26	17/33/131/137	-
4	CHL	U	608	-	3/3/15/26	3/13/111/137	-
5	CLA	W	610	3	1/1/13/20	8/27/103/115	-
8	NEX	W	1623	-	-	4/27/83/83	0/3/3/3
5	CLA	V	610	2	1/1/14/20	6/36/112/115	-
7	XAT	V	1622	-	-	0/31/93/93	0/4/4/4
4	CHL	V	607	-	3/3/16/26	2/15/113/137	-
4	CHL	W	608	-	3/3/16/26	5/17/115/137	-
5	CLA	U	604	-	1/1/10/20	6/20/92/115	-
6	LUT	W	1621	-	-	1/29/67/67	0/2/2/2
4	CHL	U	606	-	3/3/15/26	0/13/111/137	-
4	CHL	V	601	2	3/3/20/26	13/39/137/137	-
5	CLA	W	614	-	1/1/11/20	4/15/91/115	-
5	CLA	W	612	3	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LUT	W	1620	-	-	2/29/67/67	0/2/2/2
9	LHG	W	2630	5	-	10/48/48/53	-
6	LUT	U	1621	-	-	1/29/67/67	0/2/2/2
5	CLA	W	602	3	1/1/14/20	6/33/109/115	-
5	CLA	W	603	-	1/1/12/20	11/24/100/115	-
5	CLA	V	602	2	1/1/14/20	5/33/109/115	-
4	CHL	W	601	3	3/3/20/26	20/39/137/137	-
5	CLA	U	613	1	1/1/13/20	10/32/108/115	-
5	CLA	U	602	1	1/1/13/20	6/32/108/115	-
5	CLA	U	610	1	1/1/13/20	8/29/105/115	-
4	CHL	V	608	-	3/3/16/26	5/18/116/137	-
5	CLA	V	614	-	1/1/11/20	5/15/91/115	-
4	CHL	U	609	1	3/3/18/26	12/32/130/137	-
5	CLA	V	612	2	1/1/11/20	4/15/91/115	-
5	CLA	W	611	9	1/1/13/20	12/30/106/115	-
6	LUT	U	1620	-	-	2/29/67/67	0/2/2/2
8	NEX	V	1623	-	-	4/27/83/83	0/3/3/3
4	CHL	V	605	2	3/3/15/26	0/13/111/137	-
5	CLA	U	603	-	1/1/12/20	11/24/100/115	-
5	CLA	W	604	-	1/1/11/20	2/18/94/115	-
4	CHL	U	601	1	3/3/20/26	20/39/137/137	-
10	LMG	V	2631	-	-	9/36/56/70	0/1/1/1
5	CLA	V	604	-	1/1/12/20	5/21/97/115	-
4	CHL	W	606	-	3/3/16/26	2/15/113/137	-
5	CLA	W	613	3	1/1/15/20	12/39/115/115	-
5	CLA	V	603	-	1/1/11/20	4/15/91/115	-
4	CHL	W	609	3	3/3/20/26	15/39/137/137	-
7	XAT	U	1622	-	-	4/31/93/93	0/4/4/4
9	LHG	V	2630	5	-	7/52/52/53	-
5	CLA	U	611	9	1/1/10/20	6/12/88/115	-
5	CLA	U	612	1	1/1/10/20	4/13/89/115	-
5	CLA	V	611	9	1/1/10/20	4/13/89/115	-
4	CHL	U	607	-	3/3/16/26	4/15/113/137	-

All (555) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	609	CHL	C2C-C3C	10.92	1.46	1.36
4	W	609	CHL	C2C-C3C	10.71	1.46	1.36
4	U	608	CHL	C2C-C3C	10.71	1.46	1.36
4	W	608	CHL	C2C-C3C	10.69	1.46	1.36
4	W	605	CHL	C2C-C3C	10.67	1.46	1.36
4	V	605	CHL	C2C-C3C	10.62	1.46	1.36
4	U	601	CHL	C2C-C3C	10.61	1.46	1.36
4	V	607	CHL	C2C-C3C	10.60	1.46	1.36
4	U	609	CHL	C2C-C3C	10.57	1.46	1.36
4	U	605	CHL	C2C-C3C	10.54	1.46	1.36
4	V	601	CHL	C2C-C3C	10.47	1.46	1.36
4	U	607	CHL	C2C-C3C	10.46	1.46	1.36
4	V	606	CHL	C2C-C3C	10.42	1.46	1.36
4	U	606	CHL	C2C-C3C	10.41	1.46	1.36
4	W	606	CHL	C2C-C3C	10.39	1.46	1.36
4	V	609	CHL	C1D-C2D	10.39	1.51	1.39
4	W	601	CHL	C2C-C3C	10.36	1.46	1.36
4	W	609	CHL	C1D-C2D	10.25	1.51	1.39
4	W	601	CHL	C1D-C2D	10.24	1.51	1.39
4	U	609	CHL	C1D-C2D	10.23	1.51	1.39
4	U	601	CHL	C1D-C2D	10.18	1.51	1.39
4	V	608	CHL	C2C-C3C	10.00	1.46	1.36
4	V	601	CHL	C1D-C2D	9.94	1.50	1.39
4	W	607	CHL	C1D-C2D	9.59	1.50	1.39
4	W	606	CHL	C3B-C4B	9.13	1.50	1.41
4	U	605	CHL	C3B-C4B	9.01	1.50	1.41
4	W	608	CHL	C3B-C4B	9.00	1.50	1.41
4	W	605	CHL	C3B-C4B	8.98	1.50	1.41
4	U	606	CHL	C3B-C4B	8.97	1.50	1.41
4	W	607	CHL	C1A-CHA	8.96	1.50	1.40
4	U	608	CHL	C3B-C4B	8.95	1.50	1.41
4	V	606	CHL	C3B-C4B	8.85	1.50	1.41
4	U	607	CHL	C3B-C4B	8.57	1.49	1.41
4	V	608	CHL	C3B-C4B	8.54	1.49	1.41
4	V	605	CHL	C3B-C4B	8.46	1.49	1.41
4	W	601	CHL	C1B-C2B	8.40	1.49	1.39
4	W	607	CHL	C1B-C2B	8.37	1.49	1.39
4	V	607	CHL	C3B-C4B	8.35	1.49	1.41
4	V	601	CHL	C1B-C2B	8.34	1.49	1.39
4	W	609	CHL	C1B-C2B	8.29	1.49	1.39
4	U	609	CHL	C1B-C2B	8.27	1.49	1.39
4	U	601	CHL	C1B-C2B	8.18	1.48	1.39
4	V	609	CHL	C1B-C2B	8.14	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	607	CHL	C1A-CHA	8.14	1.49	1.40
4	W	601	CHL	C1A-CHA	7.83	1.48	1.40
4	V	609	CHL	C1A-CHA	7.81	1.48	1.40
4	V	601	CHL	C1A-CHA	7.80	1.48	1.40
4	V	607	CHL	C1A-CHA	7.77	1.48	1.40
4	V	605	CHL	C1D-C2D	7.76	1.48	1.39
4	U	609	CHL	C1A-CHA	7.75	1.48	1.40
4	U	601	CHL	C1A-CHA	7.75	1.48	1.40
4	W	605	CHL	C1A-CHA	7.74	1.48	1.40
4	W	609	CHL	C1A-CHA	7.70	1.48	1.40
4	U	605	CHL	C1A-CHA	7.62	1.48	1.40
4	W	605	CHL	C1B-C2B	7.59	1.48	1.39
4	U	605	CHL	C1B-C2B	7.51	1.48	1.39
4	U	601	CHL	C3B-C4B	7.50	1.48	1.41
4	W	605	CHL	C1D-C2D	7.43	1.48	1.39
4	V	607	CHL	C1D-C2D	7.41	1.48	1.39
4	W	608	CHL	C1D-C2D	7.36	1.47	1.39
4	U	609	CHL	C3B-C4B	7.32	1.48	1.41
4	W	601	CHL	C3B-C4B	7.31	1.48	1.41
4	V	607	CHL	C1B-C2B	7.29	1.47	1.39
4	U	605	CHL	C1D-C2D	7.27	1.47	1.39
4	U	608	CHL	C1D-C2D	7.26	1.47	1.39
4	W	608	CHL	C1A-CHA	7.21	1.48	1.40
4	W	606	CHL	C1D-C2D	7.20	1.47	1.39
4	V	601	CHL	C3B-C4B	7.17	1.48	1.41
4	W	607	CHL	C3B-C4B	7.16	1.48	1.41
4	V	605	CHL	C1B-C2B	7.16	1.47	1.39
4	V	605	CHL	C1A-CHA	7.15	1.48	1.40
4	W	606	CHL	C1A-CHA	7.15	1.48	1.40
4	V	608	CHL	C1A-CHA	7.15	1.48	1.40
4	V	609	CHL	C3B-C4B	7.10	1.48	1.41
4	U	606	CHL	C1D-C2D	7.10	1.47	1.39
4	U	606	CHL	C1A-CHA	7.10	1.48	1.40
4	U	607	CHL	C1B-C2B	7.10	1.47	1.39
4	W	609	CHL	C3B-C4B	7.09	1.48	1.41
4	V	606	CHL	C1D-C2D	7.08	1.47	1.39
4	U	608	CHL	C1A-CHA	7.07	1.48	1.40
4	V	608	CHL	C1B-C2B	6.96	1.47	1.39
4	V	608	CHL	C1D-C2D	6.87	1.47	1.39
4	U	607	CHL	C1D-C2D	6.86	1.47	1.39
4	V	606	CHL	C1A-CHA	6.85	1.47	1.40
4	U	608	CHL	C1B-C2B	6.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	606	CHL	C1B-C2B	6.61	1.47	1.39
4	W	608	CHL	C1B-C2B	6.56	1.47	1.39
4	W	606	CHL	C1B-C2B	6.54	1.47	1.39
4	U	606	CHL	C1B-C2B	6.52	1.47	1.39
4	V	606	CHL	C3A-C2A	-6.34	1.49	1.54
4	W	608	CHL	C3A-C2A	-5.99	1.49	1.54
4	V	608	CHL	C3A-C2A	-5.97	1.49	1.54
4	W	605	CHL	C3A-C2A	-5.94	1.49	1.54
4	V	605	CHL	C3A-C2A	-5.93	1.49	1.54
4	U	608	CHL	C3A-C2A	-5.91	1.49	1.54
4	U	605	CHL	C3A-C2A	-5.75	1.49	1.54
4	W	606	CHL	C3A-C2A	-5.57	1.49	1.54
4	U	606	CHL	C3A-C2A	-5.55	1.49	1.54
4	U	606	CHL	CHB-C4A	-5.52	1.32	1.38
4	W	606	CHL	CHB-C4A	-5.52	1.32	1.38
4	V	601	CHL	C3D-C4D	-5.51	1.33	1.41
4	U	601	CHL	C3D-C4D	-5.47	1.33	1.41
4	U	609	CHL	C3D-C4D	-5.46	1.33	1.41
4	V	609	CHL	C3D-C4D	-5.43	1.33	1.41
4	W	609	CHL	C3D-C4D	-5.42	1.33	1.41
4	W	601	CHL	C3D-C4D	-5.36	1.33	1.41
4	V	609	CHL	C3B-C2B	5.33	1.47	1.40
4	W	607	CHL	C3D-C4D	-5.27	1.33	1.41
4	V	607	CHL	CHB-C4A	-5.24	1.32	1.38
4	V	606	CHL	CHB-C4A	-5.22	1.32	1.38
4	U	608	CHL	CHB-C4A	-5.21	1.32	1.38
4	W	608	CHL	CHB-C4A	-5.19	1.32	1.38
4	U	607	CHL	CHB-C4A	-5.16	1.32	1.38
4	U	609	CHL	C3B-C2B	5.15	1.47	1.40
4	U	607	CHL	C3A-C2A	-5.15	1.50	1.54
4	W	607	CHL	CHB-C4A	-5.15	1.32	1.38
4	V	605	CHL	CHB-C4A	-5.13	1.32	1.38
4	U	607	CHL	C3D-C2D	5.12	1.48	1.39
4	V	608	CHL	CHB-C4A	-5.12	1.32	1.38
4	W	609	CHL	O2D-CGD	5.11	1.45	1.33
4	U	605	CHL	C3B-C2B	5.10	1.47	1.40
4	W	601	CHL	O2D-CGD	5.08	1.45	1.33
4	W	607	CHL	O2D-CGD	5.06	1.45	1.33
4	U	601	CHL	O2D-CGD	5.06	1.45	1.33
4	W	605	CHL	C3B-C2B	5.05	1.47	1.40
4	W	609	CHL	C3B-C2B	5.05	1.47	1.40
4	U	609	CHL	O2D-CGD	5.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	605	CHL	C3B-C2B	5.03	1.47	1.40
4	V	601	CHL	O2D-CGD	5.01	1.45	1.33
4	V	606	CHL	CHC-C4B	5.00	1.47	1.39
4	W	605	CHL	C3D-C2D	4.99	1.48	1.39
4	U	601	CHL	C3A-C2A	-4.99	1.50	1.54
4	W	606	CHL	O2D-CGD	4.98	1.45	1.33
4	V	609	CHL	O2D-CGD	4.98	1.45	1.33
4	U	605	CHL	C3D-C2D	4.96	1.48	1.39
4	W	605	CHL	O2D-CGD	4.94	1.45	1.33
4	U	606	CHL	O2D-CGD	4.94	1.45	1.33
4	W	606	CHL	C3D-C2D	4.93	1.48	1.39
4	W	607	CHL	OBD-CAD	4.93	1.28	1.22
4	U	606	CHL	CHC-C4B	4.93	1.47	1.39
4	W	605	CHL	OBD-CAD	4.92	1.28	1.22
4	U	605	CHL	O2D-CGD	4.91	1.45	1.33
4	V	605	CHL	C3D-C2D	4.91	1.48	1.39
4	W	601	CHL	C3A-C2A	-4.90	1.50	1.54
4	V	606	CHL	C3D-C2D	4.90	1.48	1.39
4	V	607	CHL	C3D-C2D	4.89	1.48	1.39
4	U	608	CHL	OBD-CAD	4.89	1.28	1.22
4	U	605	CHL	OBD-CAD	4.87	1.28	1.22
4	W	608	CHL	OBD-CAD	4.87	1.28	1.22
4	U	606	CHL	C3D-C2D	4.86	1.47	1.39
4	V	609	CHL	CHB-C1B	4.86	1.47	1.39
4	V	605	CHL	OBD-CAD	4.86	1.28	1.22
4	V	605	CHL	O2D-CGD	4.85	1.45	1.33
4	W	606	CHL	CHC-C4B	4.85	1.47	1.39
4	V	606	CHL	O2D-CGD	4.85	1.45	1.33
4	V	607	CHL	OBD-CAD	4.84	1.28	1.22
4	V	609	CHL	CHC-C4B	4.84	1.47	1.39
4	U	607	CHL	OBD-CAD	4.84	1.28	1.22
4	V	608	CHL	C3D-C2D	4.83	1.47	1.39
4	W	607	CHL	C3B-C2B	4.82	1.46	1.40
4	W	609	CHL	CHB-C1B	4.82	1.47	1.39
4	V	608	CHL	OBD-CAD	4.81	1.28	1.22
4	W	601	CHL	OBD-CAD	4.81	1.28	1.22
4	V	601	CHL	C3B-C2B	4.80	1.46	1.40
4	U	605	CHL	CHB-C4A	-4.80	1.32	1.38
4	V	607	CHL	C3A-C2A	-4.80	1.50	1.54
4	W	608	CHL	C3D-C2D	4.80	1.47	1.39
4	U	608	CHL	C3D-C2D	4.79	1.47	1.39
4	U	601	CHL	C3B-C2B	4.79	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	601	CHL	C3B-C2B	4.78	1.46	1.40
4	W	608	CHL	O2D-CGD	4.76	1.44	1.33
4	U	608	CHL	O2D-CGD	4.75	1.44	1.33
4	V	607	CHL	O2D-CGD	4.75	1.44	1.33
4	U	601	CHL	CHB-C4A	-4.75	1.32	1.38
4	U	601	CHL	OBD-CAD	4.75	1.28	1.22
4	V	601	CHL	C3A-C2A	-4.73	1.50	1.54
4	U	609	CHL	CHB-C1B	4.73	1.47	1.39
4	V	609	CHL	CHD-C1D	4.72	1.47	1.39
4	W	607	CHL	C2C-C3C	4.72	1.46	1.37
4	V	608	CHL	O2D-CGD	4.71	1.44	1.33
4	V	609	CHL	CHD-C4C	4.71	1.48	1.39
4	V	608	CHL	C3B-C2B	4.70	1.46	1.40
4	V	601	CHL	OBD-CAD	4.70	1.28	1.22
4	W	609	CHL	CHD-C4C	4.68	1.48	1.39
4	W	607	CHL	CHD-C1D	4.66	1.47	1.39
4	W	609	CHL	C3A-C2A	-4.65	1.50	1.54
4	W	605	CHL	CHC-C4B	4.65	1.47	1.39
4	V	601	CHL	CHB-C1B	4.64	1.47	1.39
4	V	609	CHL	OBD-CAD	4.63	1.28	1.22
4	U	607	CHL	O2D-CGD	4.63	1.44	1.33
4	U	609	CHL	CHC-C4B	4.63	1.47	1.39
4	U	605	CHL	CHC-C4B	4.61	1.47	1.39
4	W	607	CHL	CHC-C4B	4.60	1.47	1.39
4	W	605	CHL	CHB-C4A	-4.60	1.33	1.38
4	W	608	CHL	C3B-C2B	4.60	1.46	1.40
4	U	609	CHL	CHD-C4C	4.57	1.48	1.39
4	W	609	CHL	OBD-CAD	4.57	1.28	1.22
4	V	601	CHL	CHC-C4B	4.57	1.47	1.39
4	U	609	CHL	CHD-C1D	4.56	1.47	1.39
4	W	609	CHL	CHC-C4B	4.56	1.47	1.39
4	U	601	CHL	CHD-C4C	4.56	1.48	1.39
4	U	607	CHL	O2A-CGA	4.55	1.45	1.30
4	V	607	CHL	O2A-CGA	4.55	1.45	1.30
4	U	601	CHL	CHC-C4B	4.53	1.47	1.39
4	U	608	CHL	C3B-C2B	4.52	1.46	1.40
4	W	605	CHL	O2A-CGA	4.52	1.45	1.30
4	W	601	CHL	CHC-C4B	4.52	1.46	1.39
4	W	601	CHL	CHD-C4C	4.52	1.48	1.39
4	W	606	CHL	O2A-CGA	4.51	1.45	1.30
4	W	601	CHL	CHB-C4A	-4.49	1.33	1.38
4	W	606	CHL	C3B-C2B	4.49	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	607	CHL	C3B-C2B	4.48	1.46	1.40
4	V	601	CHL	CHD-C4C	4.47	1.48	1.39
4	W	609	CHL	CHD-C1D	4.47	1.46	1.39
4	W	607	CHL	CHD-C4C	4.46	1.47	1.39
4	V	607	CHL	C3B-C2B	4.46	1.46	1.40
4	U	608	CHL	CHC-C4B	4.46	1.46	1.39
4	W	608	CHL	CHC-C4B	4.45	1.46	1.39
4	U	609	CHL	OBD-CAD	4.44	1.28	1.22
4	V	609	CHL	CHC-C1C	4.42	1.47	1.39
4	W	601	CHL	CHB-C1B	4.40	1.46	1.39
4	V	606	CHL	C3B-C2B	4.39	1.46	1.40
4	U	601	CHL	CHD-C1D	4.38	1.46	1.39
4	U	606	CHL	C3B-C2B	4.37	1.46	1.40
4	W	607	CHL	CHC-C1C	4.37	1.47	1.39
4	U	609	CHL	C3A-C2A	-4.37	1.50	1.54
4	U	601	CHL	CHB-C1B	4.37	1.46	1.39
4	U	609	CHL	CHC-C1C	4.37	1.47	1.39
4	V	608	CHL	CHC-C4B	4.36	1.46	1.39
4	V	605	CHL	CHC-C4B	4.34	1.46	1.39
4	W	607	CHL	CHB-C1B	4.34	1.46	1.39
4	W	606	CHL	OBD-CAD	4.32	1.28	1.22
4	V	607	CHL	CHC-C4B	4.31	1.46	1.39
4	W	607	CHL	O2A-CGA	4.31	1.45	1.33
4	U	606	CHL	OBD-CAD	4.31	1.27	1.22
4	V	601	CHL	CHD-C1D	4.31	1.46	1.39
4	W	601	CHL	CHD-C1D	4.31	1.46	1.39
4	V	601	CHL	CHB-C4A	-4.30	1.33	1.38
4	V	601	CHL	CHC-C1C	4.29	1.47	1.39
4	V	609	CHL	O2A-CGA	4.26	1.45	1.33
4	U	601	CHL	CHC-C1C	4.26	1.47	1.39
4	V	609	CHL	CHB-C4A	-4.25	1.33	1.38
4	W	601	CHL	O2A-CGA	4.25	1.45	1.33
4	U	609	CHL	O2A-CGA	4.25	1.45	1.33
4	V	608	CHL	O2A-CGA	4.25	1.45	1.33
4	W	609	CHL	O2A-CGA	4.22	1.45	1.33
4	V	606	CHL	CHC-C1C	4.22	1.47	1.39
4	W	601	CHL	CHC-C1C	4.22	1.47	1.39
4	U	607	CHL	CHC-C4B	4.21	1.46	1.39
4	V	605	CHL	CHB-C1B	4.20	1.46	1.39
4	W	609	CHL	CHC-C1C	4.20	1.47	1.39
4	U	601	CHL	O2A-CGA	4.19	1.45	1.33
4	V	601	CHL	O2A-CGA	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	609	CHL	C3D-C2D	4.18	1.46	1.39
4	U	608	CHL	CHD-C4C	4.15	1.47	1.39
4	W	609	CHL	C3D-C2D	4.14	1.46	1.39
4	V	607	CHL	CHD-C1D	4.14	1.46	1.39
4	W	608	CHL	CHD-C4C	4.14	1.47	1.39
4	W	609	CHL	CHB-C4A	-4.14	1.33	1.38
9	U	2630	LHG	O7-C7	4.12	1.45	1.34
4	W	608	CHL	O2A-CGA	4.12	1.45	1.33
4	U	605	CHL	CHB-C1B	4.11	1.46	1.39
4	V	605	CHL	CHD-C1D	4.09	1.46	1.39
4	U	609	CHL	CHB-C4A	-4.08	1.33	1.38
4	U	608	CHL	CHC-C1C	4.07	1.47	1.39
9	W	2630	LHG	O7-C7	4.06	1.45	1.34
4	W	608	CHL	CHC-C1C	4.05	1.47	1.39
4	V	607	CHL	CHD-C4C	4.05	1.47	1.39
4	W	606	CHL	CHD-C4C	4.05	1.47	1.39
4	W	605	CHL	CHB-C1B	4.04	1.46	1.39
4	V	608	CHL	CHB-C1B	4.03	1.46	1.39
10	V	2631	LMG	O8-C28	4.02	1.45	1.33
10	V	2631	LMG	O7-C10	4.02	1.45	1.34
9	V	2630	LHG	O7-C7	4.00	1.45	1.34
4	U	605	CHL	CHC-C1C	4.00	1.47	1.39
9	W	2630	LHG	O8-C23	4.00	1.45	1.33
4	W	605	CHL	CHC-C1C	4.00	1.47	1.39
4	W	607	CHL	C3D-C2D	4.00	1.46	1.39
4	U	606	CHL	CHD-C4C	3.99	1.47	1.39
4	U	609	CHL	C3D-C2D	3.99	1.46	1.39
9	U	2630	LHG	O8-C23	3.98	1.44	1.33
4	U	608	CHL	CHB-C1B	3.97	1.46	1.39
4	W	605	CHL	CHD-C4C	3.96	1.47	1.39
4	U	605	CHL	CHD-C1D	3.95	1.46	1.39
4	V	606	CHL	CHB-C1B	3.94	1.46	1.39
4	W	608	CHL	CHB-C1B	3.93	1.46	1.39
4	U	605	CHL	CHD-C4C	3.93	1.46	1.39
4	W	606	CHL	CHC-C1C	3.90	1.46	1.39
4	U	606	CHL	CHC-C1C	3.90	1.46	1.39
4	V	606	CHL	CHD-C4C	3.89	1.46	1.39
4	V	608	CHL	CHD-C4C	3.88	1.46	1.39
4	W	605	CHL	CHD-C1D	3.88	1.45	1.39
9	V	2630	LHG	O8-C23	3.86	1.44	1.33
4	V	601	CHL	C3D-C2D	3.85	1.46	1.39
4	V	606	CHL	OBD-CAD	3.85	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	609	CHL	C3A-C2A	-3.85	1.51	1.54
4	U	601	CHL	C3D-C2D	3.85	1.46	1.39
4	V	607	CHL	CHC-C1C	3.84	1.46	1.39
4	W	601	CHL	C3D-C2D	3.81	1.46	1.39
4	U	607	CHL	CHC-C1C	3.79	1.46	1.39
4	W	606	CHL	CHB-C1B	3.79	1.45	1.39
4	V	605	CHL	CHD-C4C	3.78	1.46	1.39
4	U	606	CHL	CHB-C1B	3.77	1.45	1.39
4	W	607	CHL	C3A-C2A	-3.77	1.51	1.54
4	U	607	CHL	CHB-C1B	3.77	1.45	1.39
4	U	607	CHL	CHD-C4C	3.77	1.46	1.39
4	U	607	CHL	CHD-C1D	3.77	1.45	1.39
4	W	608	CHL	CHD-C1D	3.76	1.45	1.39
4	V	608	CHL	CHD-C1D	3.75	1.45	1.39
4	U	608	CHL	CHD-C1D	3.74	1.45	1.39
4	V	605	CHL	CHC-C1C	3.72	1.46	1.39
5	U	604	CLA	CAD-C3D	-3.65	1.44	1.50
4	U	607	CHL	CHA-CBD	-3.63	1.47	1.51
4	V	608	CHL	CHC-C1C	3.60	1.46	1.39
4	W	608	CHL	CHA-CBD	-3.58	1.47	1.51
4	V	606	CHL	CHA-CBD	-3.57	1.47	1.51
4	W	606	CHL	CHD-C1D	3.55	1.45	1.39
4	V	605	CHL	CHA-CBD	-3.55	1.47	1.51
4	V	606	CHL	CHD-C1D	3.53	1.45	1.39
4	U	608	CHL	CHA-CBD	-3.52	1.47	1.51
4	W	606	CHL	CHA-CBD	-3.52	1.47	1.51
4	U	606	CHL	CHD-C1D	3.51	1.45	1.39
4	V	607	CHL	CHB-C1B	3.46	1.45	1.39
4	U	606	CHL	CHA-CBD	-3.45	1.47	1.51
4	V	608	CHL	CHA-CBD	-3.39	1.47	1.51
5	V	604	CLA	C1D-ND	3.39	1.42	1.37
5	U	604	CLA	C1D-ND	3.24	1.42	1.37
4	V	607	CHL	CHA-CBD	-3.22	1.47	1.51
5	W	604	CLA	C1D-ND	3.20	1.42	1.37
5	V	613	CLA	C1D-ND	3.12	1.42	1.37
5	V	611	CLA	C1D-ND	3.07	1.41	1.37
5	V	603	CLA	C1D-ND	3.05	1.41	1.37
5	U	610	CLA	C4B-NB	3.02	1.41	1.37
5	W	612	CLA	C1D-ND	3.01	1.41	1.37
5	U	614	CLA	C1D-ND	3.00	1.41	1.37
5	U	612	CLA	C1D-ND	2.99	1.41	1.37
5	W	614	CLA	C1D-ND	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	610	CLA	C1D-ND	2.96	1.41	1.37
5	U	603	CLA	C1D-ND	2.95	1.41	1.37
5	W	603	CLA	C1D-ND	2.93	1.41	1.37
8	V	1623	NEX	C7-C8	-2.92	1.27	1.31
5	V	614	CLA	C1D-ND	2.92	1.41	1.37
5	W	611	CLA	C1D-ND	2.91	1.41	1.37
4	U	607	CHL	CBD-CGD	-2.91	1.48	1.52
5	U	611	CLA	C1D-ND	2.91	1.41	1.37
5	W	613	CLA	C1D-ND	2.90	1.41	1.37
5	V	614	CLA	CMD-C2D	-2.89	1.44	1.50
5	U	614	CLA	C4B-NB	2.89	1.41	1.37
5	U	604	CLA	C4B-NB	2.88	1.41	1.37
6	V	1620	LUT	C22-C21	-2.87	1.51	1.54
5	V	611	CLA	C4B-NB	2.86	1.41	1.37
5	U	612	CLA	C4B-NB	2.85	1.41	1.37
5	W	610	CLA	C4B-NB	2.85	1.41	1.37
5	W	614	CLA	C4B-NB	2.84	1.41	1.37
5	W	604	CLA	C4B-NB	2.84	1.41	1.37
8	W	1623	NEX	C7-C6	-2.84	1.27	1.30
5	U	613	CLA	C1D-ND	2.83	1.41	1.37
5	U	613	CLA	C4B-NB	2.82	1.41	1.37
6	V	1621	LUT	C22-C21	-2.81	1.51	1.54
5	V	602	CLA	CMD-C2D	-2.81	1.45	1.50
8	U	1623	NEX	C7-C8	-2.80	1.27	1.31
5	W	612	CLA	C4B-NB	2.79	1.41	1.37
5	W	611	CLA	C4B-NB	2.78	1.41	1.37
4	W	605	CHL	CHA-CBD	-2.78	1.48	1.51
6	U	1620	LUT	C22-C21	-2.77	1.51	1.54
5	V	604	CLA	C4B-NB	2.76	1.41	1.37
8	W	1623	NEX	C7-C8	-2.76	1.27	1.31
5	V	610	CLA	CMD-C2D	-2.75	1.45	1.50
5	V	604	CLA	CMB-C2B	-2.74	1.45	1.50
5	V	614	CLA	C4B-NB	2.74	1.41	1.37
5	V	612	CLA	C1D-ND	2.73	1.41	1.37
6	W	1620	LUT	C22-C21	-2.72	1.51	1.54
5	W	602	CLA	CMD-C2D	-2.71	1.45	1.50
5	U	602	CLA	CMD-C2D	-2.71	1.45	1.50
8	U	1623	NEX	C7-C6	-2.70	1.27	1.30
6	W	1621	LUT	C22-C21	-2.70	1.51	1.54
5	W	613	CLA	C1B-C2B	2.70	1.49	1.43
5	U	611	CLA	C4B-NB	2.70	1.41	1.37
5	W	613	CLA	C4B-NB	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	612	CLA	C4B-NB	2.69	1.41	1.37
5	U	610	CLA	C1D-ND	2.68	1.41	1.37
5	W	613	CLA	CMC-C2C	-2.66	1.45	1.50
5	U	610	CLA	CMD-C2D	-2.65	1.45	1.50
5	U	602	CLA	C4B-NB	2.64	1.41	1.37
4	U	605	CHL	CHA-CBD	-2.64	1.48	1.51
5	U	603	CLA	CMD-C2D	-2.64	1.45	1.50
5	V	602	CLA	C4B-NB	2.63	1.41	1.37
5	W	603	CLA	CMD-C2D	-2.63	1.45	1.50
6	U	1621	LUT	C22-C21	-2.63	1.51	1.54
5	W	603	CLA	C4B-NB	2.63	1.41	1.37
5	W	602	CLA	C1D-ND	2.62	1.41	1.37
5	U	604	CLA	CMB-C2B	-2.61	1.45	1.50
5	V	613	CLA	CMD-C2D	-2.61	1.45	1.50
5	W	610	CLA	CMB-C2B	-2.61	1.45	1.50
5	U	614	CLA	CMD-C2D	-2.60	1.45	1.50
5	W	614	CLA	CMD-C2D	-2.60	1.45	1.50
5	V	612	CLA	CMB-C2B	-2.59	1.45	1.50
5	V	611	CLA	C1B-C2B	2.59	1.49	1.43
4	V	608	CHL	CBD-CGD	-2.58	1.49	1.52
5	U	610	CLA	CMB-C2B	-2.58	1.45	1.50
5	W	602	CLA	C4B-NB	2.58	1.41	1.37
5	W	610	CLA	CMD-C2D	-2.58	1.45	1.50
5	U	613	CLA	C1B-C2B	2.58	1.49	1.43
6	V	1621	LUT	C1-C6	-2.58	1.50	1.53
5	W	610	CLA	C1D-ND	2.58	1.41	1.37
5	U	613	CLA	CMC-C2C	-2.57	1.45	1.50
5	V	603	CLA	CMD-C2D	-2.57	1.45	1.50
5	U	603	CLA	C4B-NB	2.56	1.41	1.37
5	V	602	CLA	CMC-C2C	-2.56	1.45	1.50
5	U	602	CLA	C1D-ND	2.55	1.41	1.37
6	W	1621	LUT	C1-C6	-2.54	1.50	1.53
5	V	610	CLA	CMC-C2C	-2.53	1.45	1.50
5	V	614	CLA	CMB-C2B	-2.53	1.45	1.50
4	W	608	CHL	CBD-CGD	-2.53	1.49	1.52
5	W	604	CLA	CMB-C2B	-2.53	1.45	1.50
5	W	603	CLA	CMB-C2B	-2.53	1.45	1.50
4	U	608	CHL	CBD-CGD	-2.52	1.49	1.52
5	V	603	CLA	CMB-C2B	-2.52	1.45	1.50
5	V	602	CLA	CMB-C2B	-2.52	1.45	1.50
5	W	614	CLA	C1B-C2B	2.52	1.49	1.43
5	V	611	CLA	CMD-C2D	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	613	CLA	C4B-NB	2.51	1.41	1.37
5	U	603	CLA	CMB-C2B	-2.51	1.45	1.50
4	V	605	CHL	CBD-CGD	-2.50	1.49	1.52
5	W	612	CLA	C1B-C2B	2.49	1.49	1.43
5	V	603	CLA	C4B-NB	2.49	1.41	1.37
5	V	603	CLA	C1B-C2B	2.49	1.49	1.43
6	U	1621	LUT	C1-C6	-2.49	1.50	1.53
5	U	614	CLA	C1B-C2B	2.48	1.49	1.43
5	U	612	CLA	C1B-C2B	2.48	1.48	1.43
5	V	611	CLA	CMC-C2C	-2.47	1.45	1.50
5	U	612	CLA	CMB-C2B	-2.47	1.45	1.50
5	W	611	CLA	C1B-C2B	2.47	1.48	1.43
5	U	611	CLA	C1B-C2B	2.47	1.48	1.43
5	V	612	CLA	CMD-C2D	-2.47	1.45	1.50
4	V	607	CHL	CBD-CGD	-2.46	1.49	1.52
5	W	602	CLA	CMC-C2C	-2.45	1.45	1.50
5	V	610	CLA	C4B-NB	2.45	1.41	1.37
5	U	602	CLA	CMC-C2C	-2.45	1.45	1.50
5	V	604	CLA	C1B-C2B	2.44	1.48	1.43
5	W	602	CLA	CMB-C2B	-2.44	1.45	1.50
5	W	612	CLA	CMB-C2B	-2.44	1.45	1.50
5	V	613	CLA	C1B-C2B	2.43	1.48	1.43
5	U	602	CLA	CMB-C2B	-2.43	1.45	1.50
7	U	1622	XAT	O24-C25	-2.43	1.43	1.46
5	V	613	CLA	CMC-C2C	-2.43	1.45	1.50
5	W	604	CLA	C1B-C2B	2.42	1.48	1.43
4	W	607	CHL	CBD-CGD	-2.42	1.49	1.52
5	U	612	CLA	CMD-C2D	-2.40	1.45	1.50
5	V	614	CLA	CMC-C2C	-2.40	1.45	1.50
5	U	613	CLA	CMD-C2D	-2.40	1.45	1.50
5	U	604	CLA	C1B-C2B	2.40	1.48	1.43
5	U	611	CLA	CMD-C2D	-2.40	1.45	1.50
5	W	613	CLA	CMD-C2D	-2.40	1.45	1.50
5	W	612	CLA	CMD-C2D	-2.40	1.45	1.50
7	V	1622	XAT	O4-C5	-2.39	1.43	1.46
8	V	1623	NEX	O24-C25	-2.38	1.43	1.46
5	V	610	CLA	CMB-C2B	-2.38	1.45	1.50
4	V	606	CHL	CBD-CGD	-2.38	1.49	1.52
5	V	603	CLA	CMC-C2C	-2.37	1.45	1.50
5	U	604	CLA	CMD-C2D	-2.37	1.45	1.50
5	U	614	CLA	CMB-C2B	-2.37	1.45	1.50
5	V	613	CLA	CMB-C2B	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	603	CLA	C1B-C2B	2.36	1.48	1.43
5	V	602	CLA	C1D-ND	2.36	1.41	1.37
5	W	611	CLA	CMD-C2D	-2.34	1.46	1.50
4	W	606	CHL	CBD-CGD	-2.34	1.49	1.52
4	U	606	CHL	CBD-CGD	-2.34	1.49	1.52
5	W	614	CLA	CMB-C2B	-2.33	1.46	1.50
5	W	612	CLA	CMC-C2C	-2.33	1.46	1.50
7	W	1622	XAT	O24-C25	-2.33	1.43	1.46
5	U	602	CLA	C1B-C2B	2.33	1.48	1.43
5	U	603	CLA	C1B-C2B	2.31	1.48	1.43
5	W	602	CLA	C1B-C2B	2.31	1.48	1.43
4	U	605	CHL	CBD-CGD	-2.30	1.49	1.52
5	W	604	CLA	CMD-C2D	-2.30	1.46	1.50
5	V	611	CLA	CMB-C2B	-2.29	1.46	1.50
5	U	613	CLA	CMB-C2B	-2.27	1.46	1.50
5	W	613	CLA	CMB-C2B	-2.27	1.46	1.50
5	W	611	CLA	CMC-C2C	-2.26	1.46	1.50
5	V	612	CLA	C1B-C2B	2.26	1.48	1.43
5	W	603	CLA	MG-NB	-2.26	2.01	2.05
5	V	612	CLA	CMC-C2C	-2.25	1.46	1.50
5	U	611	CLA	CMC-C2C	-2.25	1.46	1.50
5	U	611	CLA	CMB-C2B	-2.25	1.46	1.50
5	U	612	CLA	CMC-C2C	-2.24	1.46	1.50
5	U	603	CLA	MG-NB	-2.23	2.01	2.05
5	V	614	CLA	C1B-C2B	2.23	1.48	1.43
5	W	610	CLA	CMC-C2C	-2.23	1.46	1.50
5	V	604	CLA	CMC-C2C	-2.23	1.46	1.50
5	V	604	CLA	CMD-C2D	-2.23	1.46	1.50
8	V	1623	NEX	C7-C6	-2.23	1.28	1.30
5	U	610	CLA	CMC-C2C	-2.23	1.46	1.50
5	V	610	CLA	C1B-C2B	2.23	1.48	1.43
5	U	614	CLA	CMC-C2C	-2.22	1.46	1.50
5	W	611	CLA	CMB-C2B	-2.21	1.46	1.50
5	V	603	CLA	MG-NB	-2.21	2.01	2.05
5	V	602	CLA	C1B-C2B	2.21	1.48	1.43
7	U	1622	XAT	O4-C5	-2.20	1.43	1.46
7	V	1622	XAT	C2-C1	-2.20	1.51	1.54
5	V	602	CLA	C3B-C4B	2.20	1.49	1.42
5	W	614	CLA	CMC-C2C	-2.20	1.46	1.50
7	W	1622	XAT	O4-C5	-2.19	1.43	1.46
5	V	614	CLA	C3B-C4B	2.19	1.49	1.42
5	U	610	CLA	C1B-C2B	2.19	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	609	CHL	CBD-CGD	-2.19	1.49	1.52
5	U	603	CLA	CMC-C2C	-2.19	1.46	1.50
5	U	612	CLA	C3B-C4B	2.18	1.49	1.42
5	V	612	CLA	C3B-C4B	2.18	1.49	1.42
4	U	601	CHL	CMC-C2C	2.18	1.49	1.44
5	W	610	CLA	C1B-C2B	2.18	1.48	1.43
8	U	1623	NEX	O24-C25	-2.17	1.43	1.46
5	W	610	CLA	C3B-C4B	2.17	1.49	1.42
5	U	614	CLA	MG-NB	-2.16	2.01	2.05
5	U	602	CLA	MG-NB	-2.15	2.01	2.05
5	W	603	CLA	CMC-C2C	-2.15	1.46	1.50
5	V	610	CLA	C3B-C4B	2.14	1.49	1.42
5	W	614	CLA	MG-NB	-2.14	2.01	2.05
4	W	605	CHL	CBD-CGD	-2.13	1.49	1.52
4	V	601	CHL	CMC-C2C	2.13	1.49	1.44
5	W	614	CLA	C3B-C4B	2.13	1.48	1.42
5	U	610	CLA	C3B-C4B	2.12	1.48	1.42
5	W	602	CLA	MG-NB	-2.11	2.01	2.05
5	U	604	CLA	CMC-C2C	-2.11	1.46	1.50
5	U	614	CLA	C3B-C4B	2.11	1.48	1.42
5	U	611	CLA	MG-NB	-2.10	2.01	2.05
4	W	601	CHL	CMC-C2C	2.10	1.49	1.44
5	W	612	CLA	C3B-C4B	2.10	1.48	1.42
5	V	602	CLA	MG-NB	-2.09	2.01	2.05
5	W	603	CLA	C1B-NB	-2.09	1.35	1.37
5	W	612	CLA	MG-NB	-2.08	2.01	2.05
5	U	611	CLA	C3B-C4B	2.08	1.48	1.42
5	V	614	CLA	MG-NB	-2.07	2.01	2.05
10	V	2631	LMG	O1-C1	2.07	1.43	1.40
5	V	611	CLA	C3B-C4B	2.06	1.48	1.42
5	U	612	CLA	MG-NB	-2.06	2.01	2.05
5	V	612	CLA	MG-NB	-2.06	2.01	2.05
4	U	609	CHL	CMC-C2C	2.06	1.49	1.44
5	W	611	CLA	MG-NB	-2.06	2.01	2.05
5	W	604	CLA	CMC-C2C	-2.05	1.46	1.50
4	W	609	CHL	CMC-C2C	2.05	1.49	1.44
5	U	604	CLA	C3B-C4B	2.05	1.48	1.42
7	V	1622	XAT	O24-C25	-2.04	1.43	1.46
4	W	609	CHL	CBD-CGD	-2.04	1.49	1.52
5	W	604	CLA	C3B-C4B	2.04	1.48	1.42
5	U	603	CLA	CAC-C3C	-2.04	1.45	1.51
5	W	602	CLA	C3B-C4B	2.04	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	610	CLA	MG-NB	-2.03	2.01	2.05
4	W	601	CHL	CBD-CGD	-2.02	1.50	1.52
5	W	611	CLA	C3B-C4B	2.02	1.48	1.42
4	U	609	CHL	CBD-CGD	-2.01	1.50	1.52
5	U	610	CLA	MG-NB	-2.01	2.01	2.05
4	V	606	CHL	CBD-CAD	-2.01	1.46	1.53
5	V	603	CLA	CAC-C3C	-2.01	1.46	1.51
7	V	1622	XAT	C22-C21	-2.01	1.51	1.54

All (591) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	1622	XAT	C37-C21-C36	-17.56	81.86	107.37
7	W	1622	XAT	C37-C21-C36	-17.54	81.88	107.37
4	W	606	CHL	O2A-CGA-O1A	-17.10	79.35	123.33
7	U	1622	XAT	C37-C21-C22	-15.34	82.01	108.97
7	W	1622	XAT	C37-C21-C22	-15.33	82.03	108.97
4	W	606	CHL	O2A-CGA-CBA	14.66	160.33	114.00
4	W	606	CHL	O1A-CGA-CBA	-13.27	81.01	123.09
4	U	601	CHL	C1B-CHB-C4A	9.92	127.70	121.32
4	W	601	CHL	C1B-CHB-C4A	9.65	127.53	121.32
4	V	601	CHL	C1B-CHB-C4A	9.09	127.17	121.32
4	U	605	CHL	O2D-CGD-CBD	8.92	120.75	110.95
4	W	605	CHL	O2D-CGD-CBD	8.89	120.71	110.95
4	W	607	CHL	O2D-CGD-CBD	8.80	120.62	110.95
4	V	609	CHL	O2D-CGD-CBD	8.79	120.60	110.95
4	U	609	CHL	O2D-CGD-CBD	8.33	120.10	110.95
4	W	609	CHL	O2D-CGD-CBD	8.12	119.87	110.95
4	U	607	CHL	O2D-CGD-CBD	8.09	119.83	110.95
7	W	1622	XAT	C36-C21-C22	7.99	123.01	108.97
7	U	1622	XAT	C36-C21-C22	7.97	122.98	108.97
4	V	606	CHL	OBD-CAD-C3D	-7.85	115.64	127.89
4	V	601	CHL	O2D-CGD-CBD	7.79	119.51	110.95
4	V	606	CHL	CHA-C1A-C2A	-7.71	115.20	133.31
4	U	606	CHL	OBD-CAD-C3D	-7.67	115.92	127.89
4	W	601	CHL	O2D-CGD-CBD	7.65	119.35	110.95
4	U	605	CHL	CHA-C1A-C2A	-7.64	115.38	133.31
4	W	605	CHL	CHA-C1A-C2A	-7.63	115.40	133.31
4	W	606	CHL	OBD-CAD-C3D	-7.60	116.04	127.89
4	U	601	CHL	O2D-CGD-CBD	7.58	119.28	110.95
4	V	607	CHL	CHA-C1A-C2A	-7.51	115.68	133.31
4	V	608	CHL	CHA-C1A-C2A	-7.50	115.71	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	608	CHL	CHA-C1A-C2A	-7.50	115.71	133.31
4	V	605	CHL	O2D-CGD-CBD	7.49	119.18	110.95
4	U	608	CHL	CHA-C1A-C2A	-7.48	115.74	133.31
4	W	606	CHL	CHA-C1A-C2A	-7.46	115.79	133.31
4	U	606	CHL	CHA-C1A-C2A	-7.45	115.81	133.31
6	W	1620	LUT	C8-C7-C6	-7.38	107.28	127.00
6	U	1620	LUT	C8-C7-C6	-7.36	107.33	127.00
4	U	606	CHL	O2D-CGD-CBD	7.35	119.02	110.95
8	U	1623	NEX	O24-C25-C24	7.33	120.36	113.49
8	W	1623	NEX	O24-C25-C24	7.29	120.33	113.49
8	V	1623	NEX	O24-C25-C24	7.29	120.32	113.49
4	W	606	CHL	O2D-CGD-CBD	7.28	118.95	110.95
4	W	609	CHL	C1B-CHB-C4A	7.26	125.99	121.32
4	V	605	CHL	CHA-C1A-C2A	-7.23	116.33	133.31
4	W	605	CHL	OBD-CAD-C3D	-7.02	116.94	127.89
7	U	1622	XAT	O24-C25-C24	6.99	120.04	113.49
7	V	1622	XAT	C38-C25-C26	-6.97	110.82	122.30
4	U	605	CHL	OBD-CAD-C3D	-6.97	117.02	127.89
4	W	608	CHL	O2D-CGD-CBD	6.95	118.58	110.95
4	V	605	CHL	OBD-CAD-C3D	-6.94	117.06	127.89
4	U	608	CHL	O2D-CGD-CBD	6.93	118.56	110.95
4	V	607	CHL	OBD-CAD-C3D	-6.91	117.11	127.89
7	W	1622	XAT	O24-C25-C24	6.86	119.92	113.49
4	V	608	CHL	OBD-CAD-C3D	-6.85	117.21	127.89
4	V	606	CHL	O2D-CGD-CBD	6.82	118.44	110.95
4	V	608	CHL	O2D-CGD-CBD	6.82	118.44	110.95
4	U	609	CHL	C1B-CHB-C4A	6.78	125.68	121.32
4	V	607	CHL	O2D-CGD-CBD	6.72	118.33	110.95
4	U	607	CHL	CHA-C1A-C2A	-6.69	117.61	133.31
4	U	607	CHL	OBD-CAD-C3D	-6.68	117.47	127.89
4	W	608	CHL	OBD-CAD-C3D	-6.66	117.50	127.89
4	U	608	CHL	OBD-CAD-C3D	-6.65	117.52	127.89
5	V	603	CLA	C4A-NA-C1A	6.52	109.65	106.68
7	V	1622	XAT	O24-C25-C24	6.45	119.53	113.49
7	V	1622	XAT	C18-C5-C6	-6.13	112.21	122.30
4	W	601	CHL	C4D-ND-C1D	-6.10	100.59	105.22
4	V	601	CHL	C4D-ND-C1D	-6.09	100.60	105.22
4	U	601	CHL	C4D-ND-C1D	-6.01	100.66	105.22
7	W	1622	XAT	C15-C14-C13	-5.96	118.92	127.28
7	U	1622	XAT	C15-C14-C13	-5.94	118.94	127.28
5	W	614	CLA	C4A-NA-C1A	5.88	109.36	106.68
5	W	603	CLA	C4A-NA-C1A	5.87	109.36	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	U	601	CHL	CHA-C1A-C2A	-5.84	119.59	133.31
4	U	609	CHL	C4D-ND-C1D	-5.84	100.79	105.22
4	V	601	CHL	CHA-C1A-C2A	-5.75	119.81	133.31
4	W	609	CHL	C4D-ND-C1D	-5.74	100.86	105.22
4	W	601	CHL	CHA-C1A-C2A	-5.74	119.83	133.31
6	V	1620	LUT	C8-C7-C6	-5.67	111.84	127.00
5	U	611	CLA	C4A-NA-C1A	5.67	109.27	106.68
5	U	603	CLA	C4A-NA-C1A	5.66	109.26	106.68
6	U	1620	LUT	C21-C26-C27	-5.65	106.33	112.83
4	U	609	CHL	CHA-C1A-C2A	-5.64	120.07	133.31
6	W	1620	LUT	C21-C26-C27	-5.64	106.35	112.83
5	W	602	CLA	C4A-NA-C1A	5.62	109.24	106.68
4	W	609	CHL	CHA-C1A-C2A	-5.57	120.23	133.31
5	U	612	CLA	C4A-NA-C1A	5.54	109.21	106.68
5	U	614	CLA	C4A-NA-C1A	5.53	109.20	106.68
7	W	1622	XAT	O4-C5-C4	5.53	118.67	113.49
4	U	607	CHL	C4D-ND-C1D	5.53	109.41	105.22
7	U	1622	XAT	O4-C5-C4	5.52	118.66	113.49
5	U	602	CLA	C4A-NA-C1A	5.51	109.19	106.68
4	V	607	CHL	C4D-ND-C1D	5.44	109.35	105.22
5	W	612	CLA	C4A-NA-C1A	5.41	109.15	106.68
5	W	611	CLA	C4A-NA-C1A	5.35	109.12	106.68
4	V	606	CHL	C4D-ND-C1D	5.34	109.27	105.22
5	U	613	CLA	C4A-NA-C1A	5.34	109.12	106.68
4	V	605	CHL	C4D-ND-C1D	5.30	109.24	105.22
4	W	606	CHL	C4D-ND-C1D	5.24	109.20	105.22
6	W	1621	LUT	C7-C8-C9	-5.24	118.48	126.23
6	U	1621	LUT	C7-C8-C9	-5.22	118.51	126.23
5	W	613	CLA	C4A-NA-C1A	5.19	109.05	106.68
5	V	612	CLA	C4A-NA-C1A	5.17	109.04	106.68
4	V	609	CHL	C4D-ND-C1D	-5.15	101.31	105.22
4	U	606	CHL	OBD-CAD-CBD	5.15	133.38	125.82
5	V	611	CLA	C4A-NA-C1A	5.12	109.02	106.68
4	W	605	CHL	C4D-ND-C1D	5.12	109.10	105.22
4	U	606	CHL	C4D-ND-C1D	5.11	109.09	105.22
4	W	606	CHL	OBD-CAD-CBD	5.10	133.31	125.82
5	V	613	CLA	C4A-NA-C1A	5.05	108.98	106.68
4	V	606	CHL	OBD-CAD-CBD	5.04	133.22	125.82
4	U	605	CHL	C4D-ND-C1D	5.02	109.03	105.22
4	V	609	CHL	CHA-C1A-C2A	-5.02	121.52	133.31
4	V	608	CHL	C4D-ND-C1D	5.00	109.01	105.22
7	V	1622	XAT	O4-C5-C18	4.99	120.62	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	V	608	CHL	OBD-CAD-CBD	4.98	133.13	125.82
4	V	605	CHL	OBD-CAD-CBD	4.96	133.11	125.82
4	W	608	CHL	C4D-ND-C1D	4.96	108.98	105.22
4	U	608	CHL	C4D-ND-C1D	4.95	108.97	105.22
7	W	1622	XAT	C31-C30-C29	-4.94	120.35	127.28
7	U	1622	XAT	C31-C30-C29	-4.91	120.40	127.28
5	V	602	CLA	C4A-NA-C1A	4.90	108.91	106.68
7	U	1622	XAT	C38-C25-C26	-4.88	114.28	122.30
4	V	607	CHL	OBD-CAD-CBD	4.87	132.97	125.82
8	W	1623	NEX	C15-C14-C13	-4.86	120.46	127.28
8	U	1623	NEX	C38-C25-C26	-4.84	114.34	122.30
5	V	604	CLA	C4A-NA-C1A	4.83	108.88	106.68
8	W	1623	NEX	C38-C25-C26	-4.82	114.38	122.30
8	V	1623	NEX	C15-C14-C13	-4.82	120.53	127.28
4	U	607	CHL	OBD-CAD-CBD	4.81	132.89	125.82
7	W	1622	XAT	C38-C25-C26	-4.81	114.39	122.30
8	U	1623	NEX	C15-C14-C13	-4.79	120.57	127.28
5	U	604	CLA	C4A-NA-C1A	4.78	108.86	106.68
7	U	1622	XAT	C15-C35-C34	-4.77	113.76	123.52
7	W	1622	XAT	C15-C35-C34	-4.77	113.77	123.52
8	U	1623	NEX	C35-C34-C33	-4.76	120.60	127.28
7	V	1622	XAT	O4-C5-C4	4.75	117.95	113.49
5	W	604	CLA	C4A-NA-C1A	4.75	108.84	106.68
4	W	607	CHL	C4D-ND-C1D	-4.75	101.62	105.22
8	W	1623	NEX	C35-C34-C33	-4.74	120.63	127.28
4	W	608	CHL	OBD-CAD-CBD	4.74	132.77	125.82
4	U	608	CHL	OBD-CAD-CBD	4.73	132.76	125.82
4	W	605	CHL	OBD-CAD-CBD	4.72	132.75	125.82
7	U	1622	XAT	C37-C21-C26	-4.66	97.47	110.05
4	U	605	CHL	OBD-CAD-CBD	4.66	132.66	125.82
6	V	1621	LUT	C7-C8-C9	-4.63	119.38	126.23
7	W	1622	XAT	C37-C21-C26	-4.63	97.54	110.05
7	U	1622	XAT	C6-C7-C8	-4.61	116.25	125.99
7	U	1622	XAT	O4-C5-C18	4.59	120.17	115.05
7	W	1622	XAT	C6-C7-C8	-4.56	116.34	125.99
7	W	1622	XAT	O4-C5-C18	4.54	120.13	115.05
8	W	1623	NEX	C27-C28-C29	-4.54	118.49	125.53
8	U	1623	NEX	C27-C28-C29	-4.52	118.52	125.53
8	W	1623	NEX	C11-C10-C9	-4.50	120.97	127.28
8	U	1623	NEX	C11-C10-C9	-4.49	120.98	127.28
9	V	2630	LHG	O7-C7-C8	4.47	121.15	111.48
7	U	1622	XAT	C27-C28-C29	-4.41	118.68	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	V	1620	LUT	C26-C27-C28	-4.40	117.73	124.58
8	V	1623	NEX	C27-C28-C29	-4.40	118.70	125.53
7	W	1622	XAT	C27-C28-C29	-4.39	118.73	125.53
7	W	1622	XAT	C18-C5-C6	-4.38	115.09	122.30
7	U	1622	XAT	C18-C5-C6	-4.35	115.14	122.30
4	U	605	CHL	C1A-CHA-C4D	-4.34	111.74	118.98
8	V	1623	NEX	C38-C25-C26	-4.34	115.17	122.30
4	W	605	CHL	C1A-CHA-C4D	-4.32	111.77	118.98
6	V	1621	LUT	C8-C7-C6	-4.29	115.55	127.00
5	V	614	CLA	C4A-NA-C1A	4.17	108.58	106.68
4	W	601	CHL	C1-C2-C3	-4.10	119.48	126.20
4	V	605	CHL	C1A-CHA-C4D	-4.04	112.24	118.98
4	W	606	CHL	C1A-CHA-C4D	-4.02	112.27	118.98
10	V	2631	LMG	O7-C10-C11	4.02	120.18	111.48
5	V	610	CLA	C4A-NA-C1A	4.02	108.51	106.68
4	U	606	CHL	C1A-CHA-C4D	-3.99	112.33	118.98
6	V	1621	LUT	C17-C1-C6	-3.96	104.03	110.24
4	W	607	CHL	CHA-C1A-C2A	-3.96	124.00	133.31
4	W	607	CHL	CMA-C3A-C4A	-3.96	106.08	114.61
6	U	1621	LUT	C26-C27-C28	-3.96	118.42	124.58
6	W	1621	LUT	C26-C27-C28	-3.94	118.45	124.58
4	V	601	CHL	C1-C2-C3	-3.89	119.82	126.20
4	U	601	CHL	C1-C2-C3	-3.88	119.83	126.20
5	W	610	CLA	C4A-NA-C1A	3.88	108.45	106.68
8	V	1623	NEX	C35-C34-C33	-3.85	121.88	127.28
5	U	610	CLA	C4A-NA-C1A	3.84	108.43	106.68
4	V	608	CHL	CBC-CAC-C3C	-3.83	107.39	112.87
4	V	606	CHL	C1C-C2C-CMC	3.82	133.69	126.80
4	W	608	CHL	C1A-CHA-C4D	-3.82	112.61	118.98
7	V	1622	XAT	O24-C25-C38	3.81	119.31	115.05
4	V	606	CHL	C1A-CHA-C4D	-3.79	112.65	118.98
8	U	1623	NEX	C17-C1-C6	-3.79	107.08	110.47
6	V	1621	LUT	C26-C27-C28	-3.78	118.69	124.58
4	U	608	CHL	C1A-CHA-C4D	-3.78	112.68	118.98
5	V	611	CLA	O2D-CGD-O1D	-3.77	116.52	123.85
4	U	607	CHL	CMD-C2D-C3D	3.76	132.19	124.68
8	U	1623	NEX	O24-C25-C38	3.73	119.22	115.05
8	W	1623	NEX	C17-C1-C6	-3.72	107.15	110.47
7	W	1622	XAT	C35-C34-C33	-3.67	122.13	127.28
4	V	608	CHL	C1A-CHA-C4D	-3.65	112.89	118.98
8	W	1623	NEX	O24-C25-C38	3.65	119.13	115.05
7	U	1622	XAT	C35-C34-C33	-3.63	122.18	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	U	609	CHL	CBC-CAC-C3C	-3.62	107.69	112.87
4	V	606	CHL	CMD-C2D-C3D	3.61	131.90	124.68
6	V	1620	LUT	C17-C1-C6	-3.58	104.63	110.24
4	U	605	CHL	CMA-C3A-C4A	-3.58	106.91	114.61
4	W	605	CHL	CMA-C3A-C4A	-3.57	106.91	114.61
7	U	1622	XAT	C4-C3-C2	-3.57	104.11	110.79
4	U	608	CHL	CBC-CAC-C3C	-3.56	107.77	112.87
7	W	1622	XAT	C4-C3-C2	-3.56	104.14	110.79
4	W	608	CHL	CBC-CAC-C3C	-3.55	107.80	112.87
9	W	2630	LHG	O7-C7-C8	3.55	119.15	111.48
9	U	2630	LHG	O7-C7-C8	3.50	119.06	111.48
7	U	1622	XAT	C10-C11-C12	-3.50	113.06	123.20
4	V	607	CHL	C1A-CHA-C4D	-3.49	113.15	118.98
10	V	2631	LMG	O1-C1-C2	3.49	113.58	108.27
7	W	1622	XAT	C10-C11-C12	-3.49	113.10	123.20
6	U	1621	LUT	C17-C1-C6	-3.46	104.82	110.24
4	W	606	CHL	CMD-C2D-C3D	3.45	131.58	124.68
4	W	609	CHL	CBC-CAC-C3C	-3.42	107.97	112.87
4	V	608	CHL	C1C-C2C-CMC	3.42	132.97	126.80
4	U	606	CHL	CMD-C2D-C3D	3.41	131.50	124.68
6	W	1621	LUT	C1-C6-C5	-3.40	117.99	122.64
6	W	1621	LUT	C17-C1-C6	-3.40	104.91	110.24
6	U	1621	LUT	C1-C6-C5	-3.39	118.00	122.64
4	V	609	CHL	CBC-CAC-C3C	-3.39	108.02	112.87
4	W	607	CHL	C4C-C3C-C2C	-3.38	100.64	108.42
7	V	1622	XAT	C6-C7-C8	-3.36	118.88	125.99
7	W	1622	XAT	O24-C25-C38	3.35	118.80	115.05
4	W	605	CHL	C1C-C2C-CMC	3.35	132.84	126.80
4	U	601	CHL	C3D-C4D-ND	3.34	118.30	112.94
4	U	609	CHL	C3D-C4D-ND	3.34	118.29	112.94
4	U	605	CHL	C1C-C2C-CMC	3.33	132.80	126.80
7	U	1622	XAT	O24-C25-C38	3.33	118.77	115.05
4	V	601	CHL	C3D-C4D-ND	3.32	118.27	112.94
4	U	607	CHL	C1A-CHA-C4D	-3.31	113.45	118.98
4	W	601	CHL	C3D-C4D-ND	3.31	118.25	112.94
4	V	608	CHL	CMD-C2D-C3D	3.29	131.26	124.68
4	W	605	CHL	CMD-C2D-C3D	3.28	131.24	124.68
4	W	609	CHL	C3D-C4D-ND	3.28	118.20	112.94
6	V	1621	LUT	C21-C26-C27	-3.27	109.07	112.83
4	U	605	CHL	CMD-C2D-C3D	3.26	131.20	124.68
4	U	608	CHL	C1C-C2C-CMC	3.24	132.64	126.80
4	W	608	CHL	C1C-C2C-CMC	3.23	132.62	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	607	CHL	O1D-CGD-CBD	-3.20	119.87	124.72
6	U	1620	LUT	C26-C27-C28	-3.20	119.60	124.58
6	U	1620	LUT	C35-C15-C14	-3.19	116.98	123.52
7	V	1622	XAT	C31-C30-C29	-3.19	122.80	127.28
4	W	607	CHL	C4-C3-C5	3.18	120.74	115.23
8	V	1623	NEX	O24-C25-C38	3.17	118.59	115.05
6	W	1620	LUT	C35-C15-C14	-3.17	117.04	123.52
4	U	601	CHL	C1C-CHC-C4B	3.16	127.38	116.07
4	W	607	CHL	C1-C2-C3	-3.15	121.03	126.20
4	W	607	CHL	C1B-CHB-C4A	3.15	123.35	121.32
7	V	1622	XAT	C15-C35-C34	-3.15	117.08	123.52
6	W	1620	LUT	C26-C27-C28	-3.15	119.68	124.58
4	V	609	CHL	C3D-C4D-ND	3.14	117.97	112.94
6	V	1620	LUT	C7-C8-C9	-3.13	121.61	126.23
7	V	1622	XAT	C27-C28-C29	-3.12	120.69	125.53
4	W	601	CHL	C1C-CHC-C4B	3.12	127.23	116.07
4	V	605	CHL	C1C-C2C-CMC	3.10	132.38	126.80
4	U	607	CHL	O1D-CGD-CBD	-3.10	120.03	124.72
8	W	1623	NEX	C11-C12-C13	-3.09	117.88	126.36
4	W	609	CHL	C1C-CHC-C4B	3.09	127.14	116.07
7	W	1622	XAT	C11-C10-C9	-3.09	122.95	127.28
8	U	1623	NEX	C11-C12-C13	-3.08	117.91	126.36
4	W	606	CHL	OMC-CMC-C2C	-3.08	119.77	125.12
7	U	1622	XAT	C11-C10-C9	-3.08	122.95	127.28
4	U	609	CHL	C1C-CHC-C4B	3.08	127.10	116.07
4	V	607	CHL	C1C-C2C-CMC	3.07	132.34	126.80
4	U	609	CHL	CMA-C3A-C4A	-3.07	108.00	114.61
8	V	1623	NEX	C31-C30-C29	-3.05	123.00	127.28
4	U	606	CHL	OMC-CMC-C2C	-3.04	119.84	125.12
4	W	609	CHL	C1-C2-C3	-3.03	121.24	126.20
5	V	614	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
6	W	1621	LUT	C8-C7-C6	-3.02	118.92	127.00
4	V	601	CHL	C1C-CHC-C4B	3.02	126.88	116.07
6	U	1621	LUT	C8-C7-C6	-3.02	118.94	127.00
4	V	601	CHL	C4-C3-C5	3.01	120.44	115.23
4	V	608	CHL	OMC-CMC-C2C	-3.00	119.91	125.12
4	W	609	CHL	C4-C3-C5	3.00	120.44	115.23
9	V	2630	LHG	O8-C23-C24	3.00	120.98	111.83
4	V	605	CHL	OMC-CMC-C2C	-3.00	119.91	125.12
4	W	605	CHL	OMC-CMC-C2C	-2.98	119.95	125.12
4	U	605	CHL	OMC-CMC-C2C	-2.97	119.96	125.12
4	U	607	CHL	C1C-C2C-CMC	2.97	132.16	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	1620	LUT	C11-C10-C9	-2.97	123.11	127.28
4	U	608	CHL	CMD-C2D-C3D	2.97	130.61	124.68
4	V	609	CHL	C4-C3-C5	2.96	120.37	115.23
7	W	1622	XAT	C36-C21-C26	2.95	118.00	110.05
7	U	1622	XAT	C36-C21-C26	2.95	118.00	110.05
5	U	611	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
4	V	606	CHL	OMC-CMC-C2C	-2.93	120.02	125.12
4	W	608	CHL	CMD-C2D-C3D	2.93	130.54	124.68
4	U	608	CHL	CMB-C2B-C3B	2.91	130.49	124.68
4	W	606	CHL	CBC-CAC-C3C	-2.90	108.73	112.87
6	U	1620	LUT	C11-C10-C9	-2.90	123.22	127.28
4	U	606	CHL	C1C-C2C-CMC	2.90	132.02	126.80
5	V	602	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
4	W	606	CHL	C1C-C2C-CMC	2.89	132.02	126.80
4	W	605	CHL	O1D-CGD-CBD	-2.89	120.35	124.72
4	U	608	CHL	OMC-CMC-C2C	-2.88	120.11	125.12
5	U	613	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
5	W	602	CLA	CHB-C4A-NA	2.87	128.54	124.40
6	V	1621	LUT	C1-C6-C5	-2.87	118.72	122.64
4	W	608	CHL	CMB-C2B-C3B	2.87	130.41	124.68
4	U	605	CHL	O1D-CGD-CBD	-2.87	120.38	124.72
4	V	609	CHL	C1C-CHC-C4B	2.86	126.31	116.07
4	V	607	CHL	CMD-C2D-C3D	2.86	130.40	124.68
4	U	601	CHL	C4-C3-C5	2.86	120.20	115.23
4	U	606	CHL	CBC-CAC-C3C	-2.86	108.78	112.87
4	U	609	CHL	C4-C3-C5	2.85	120.18	115.23
5	W	610	CLA	C3B-C4B-NB	-2.85	107.99	110.53
5	V	610	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
4	W	608	CHL	OMC-CMC-C2C	-2.84	120.19	125.12
5	W	611	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
5	U	602	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
9	W	2630	LHG	O8-C23-C24	2.83	120.47	111.83
7	V	1622	XAT	C7-C8-C9	-2.83	121.14	125.53
9	U	2630	LHG	O8-C23-C24	2.83	120.45	111.83
4	U	609	CHL	O2A-CGA-CBA	2.82	120.44	111.83
5	W	602	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
5	U	610	CLA	C3B-C4B-NB	-2.82	108.02	110.53
4	W	607	CHL	O2A-CGA-CBA	2.81	120.41	111.83
8	W	1623	NEX	C24-C23-C22	-2.81	105.53	110.79
5	W	613	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
7	W	1622	XAT	C31-C32-C33	-2.81	118.67	126.36
4	V	608	CHL	CMB-C2B-C3B	2.81	130.29	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	609	CHL	O2A-CGA-CBA	2.80	120.38	111.83
8	U	1623	NEX	C24-C23-C22	-2.80	105.56	110.79
5	U	602	CLA	CHB-C4A-NA	2.79	128.43	124.40
5	V	611	CLA	O2D-CGD-CBD	2.79	116.11	111.23
7	U	1622	XAT	C31-C32-C33	-2.79	118.71	126.36
6	V	1621	LUT	C3-C4-C5	-2.79	105.24	112.18
4	W	607	CHL	CAC-C3C-C4C	2.79	129.75	124.73
5	V	613	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
7	V	1622	XAT	C38-C25-C24	2.79	117.37	114.24
4	V	609	CHL	CMB-C2B-C3B	2.78	130.25	124.68
5	V	612	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
4	W	607	CHL	C3D-C4D-ND	2.77	117.38	112.94
4	V	609	CHL	O1D-CGD-CBD	-2.77	120.53	124.72
4	V	609	CHL	O2A-CGA-CBA	2.76	120.26	111.83
5	U	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
7	V	1622	XAT	C26-C27-C28	-2.76	120.16	125.99
5	V	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
5	W	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
4	W	607	CHL	C1C-CHC-C4B	2.75	125.90	116.07
5	U	603	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
5	W	612	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
8	V	1623	NEX	C24-C23-C22	-2.75	105.65	110.79
5	U	612	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
5	U	610	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
4	V	606	CHL	CMB-C2B-C3B	2.73	130.13	124.68
4	W	601	CHL	C4-C3-C5	2.73	119.96	115.23
5	W	603	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
5	U	611	CLA	CHB-C4A-NA	2.70	128.30	124.40
5	W	610	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
4	U	605	CHL	C1A-CHA-CBD	2.69	139.24	132.36
8	W	1623	NEX	C39-C29-C30	-2.69	118.46	122.82
4	W	605	CHL	C1A-CHA-CBD	2.68	139.24	132.36
5	W	614	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
5	U	612	CLA	CHB-C4A-NA	2.68	128.27	124.40
4	V	606	CHL	C3D-CAD-CBD	2.68	111.13	107.61
4	U	609	CHL	CMB-C2B-C3B	2.67	130.03	124.68
4	W	601	CHL	O2A-CGA-CBA	2.67	119.99	111.83
5	W	611	CLA	CHB-C4A-NA	2.67	128.25	124.40
8	U	1623	NEX	C39-C29-C30	-2.67	118.50	122.82
4	W	607	CHL	OMC-CMC-C2C	-2.66	120.50	125.12
5	W	603	CLA	CHB-C4A-NA	2.65	128.23	124.40
6	V	1620	LUT	C11-C10-C9	-2.65	123.57	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	1623	NEX	C11-C10-C9	-2.65	123.57	127.28
5	U	613	CLA	CHB-C4A-NA	2.64	128.21	124.40
4	U	607	CHL	C1A-CHA-CBD	2.63	139.10	132.36
5	V	602	CLA	C3B-C4B-NB	-2.63	108.19	110.53
5	U	613	CLA	C1-C2-C3	-2.62	121.90	126.20
5	V	610	CLA	CHB-C4A-NA	2.62	128.19	124.40
5	V	602	CLA	CHB-C4A-NA	2.62	128.18	124.40
5	W	612	CLA	CHB-C4A-NA	2.62	128.18	124.40
4	W	609	CHL	CMA-C3A-C4A	-2.62	108.97	114.61
5	U	614	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
6	W	1621	LUT	C11-C10-C9	-2.61	123.62	127.28
4	V	605	CHL	C1A-CHA-CBD	2.61	139.04	132.36
4	W	609	CHL	CMB-C2B-C3B	2.61	129.89	124.68
6	U	1621	LUT	C11-C10-C9	-2.61	123.62	127.28
6	U	1621	LUT	C18-C5-C6	-2.60	121.65	124.48
5	W	613	CLA	C1-C2-C3	-2.60	121.94	126.20
6	W	1621	LUT	C18-C5-C6	-2.59	121.66	124.48
4	V	601	CHL	O2A-CGA-CBA	2.59	119.72	111.83
4	V	605	CHL	CMB-C2B-C3B	2.58	129.84	124.68
4	V	608	CHL	O2A-CGA-CBA	2.58	119.70	111.83
4	V	609	CHL	C1B-CHB-C4A	2.58	122.98	121.32
5	U	603	CLA	CHB-C4A-NA	2.58	128.12	124.40
4	U	609	CHL	O1D-CGD-CBD	-2.57	120.83	124.72
4	U	605	CHL	O2D-CGD-O1D	-2.57	118.85	123.85
6	V	1621	LUT	C11-C10-C9	-2.57	123.68	127.28
4	U	607	CHL	OMC-CMC-C2C	-2.56	120.67	125.12
4	V	609	CHL	O2D-CGD-O1D	-2.56	118.87	123.85
5	W	613	CLA	CHB-C4A-NA	2.56	128.09	124.40
4	U	606	CHL	C1A-CHA-CBD	2.55	138.90	132.36
5	V	612	CLA	CHB-C4A-NA	2.55	128.08	124.40
5	W	610	CLA	CHB-C4A-NA	2.55	128.08	124.40
4	V	607	CHL	OMC-CMC-C2C	-2.54	120.70	125.12
4	W	606	CHL	C1A-CHA-CBD	2.54	138.88	132.36
5	U	610	CLA	CHB-C4A-NA	2.54	128.07	124.40
5	W	610	CLA	C1-C2-C3	-2.54	122.04	126.20
4	W	605	CHL	O2D-CGD-O1D	-2.53	118.91	123.85
7	V	1622	XAT	C15-C14-C13	-2.53	123.72	127.28
4	U	601	CHL	O2A-CGA-CBA	2.53	119.55	111.83
4	V	605	CHL	CMD-C2D-C3D	2.53	129.73	124.68
4	U	607	CHL	O2A-CGA-CBA	2.52	121.98	114.00
5	W	614	CLA	C3B-C4B-NB	-2.52	108.28	110.53
5	U	610	CLA	C1-C2-C3	-2.52	122.07	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	V	1620	LUT	C28-C29-C30	-2.51	115.06	119.01
4	W	605	CHL	CMB-C2B-C3B	2.51	129.69	124.68
4	W	608	CHL	C1A-CHA-CBD	2.51	138.78	132.36
4	V	608	CHL	C1A-CHA-CBD	2.51	138.78	132.36
6	W	1621	LUT	C3-C4-C5	-2.50	105.94	112.18
4	U	608	CHL	C1A-CHA-CBD	2.50	138.76	132.36
4	U	609	CHL	C1-C2-C3	-2.50	122.11	126.20
8	V	1623	NEX	C15-C35-C34	-2.49	118.42	123.52
4	U	605	CHL	CMB-C2B-C3B	2.49	129.66	124.68
6	V	1620	LUT	C38-C25-C24	-2.49	117.48	123.36
6	U	1621	LUT	C3-C4-C5	-2.48	106.00	112.18
4	W	601	CHL	CMB-C2B-C3B	2.47	129.62	124.68
4	V	601	CHL	O2D-CGD-O1D	-2.47	119.04	123.85
4	V	609	CHL	C1-C2-C3	-2.47	122.15	126.20
4	U	606	CHL	CMB-C2B-C3B	2.47	129.61	124.68
8	V	1623	NEX	C39-C29-C30	-2.47	118.82	122.82
4	W	606	CHL	CMB-C2B-C3B	2.46	129.61	124.68
4	U	601	CHL	CMB-C2B-C3B	2.46	129.60	124.68
6	U	1621	LUT	C18-C5-C4	2.46	118.94	114.42
4	U	609	CHL	O2D-CGD-O1D	-2.45	119.07	123.85
7	V	1622	XAT	C31-C32-C33	-2.45	119.64	126.36
4	U	601	CHL	CMA-C3A-C4A	-2.45	109.34	114.61
6	U	1620	LUT	C11-C12-C13	-2.44	119.66	126.36
4	W	609	CHL	O1D-CGD-CBD	-2.44	121.02	124.72
5	W	614	CLA	CHB-C4A-NA	2.44	127.92	124.40
5	V	610	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
4	W	609	CHL	O2D-CGD-O1D	-2.44	119.11	123.85
6	W	1620	LUT	C11-C12-C13	-2.43	119.71	126.36
5	U	614	CLA	C3B-C4B-NB	-2.43	108.36	110.53
4	U	607	CHL	CMB-C2B-C3B	2.42	129.52	124.68
5	V	603	CLA	CHB-C4A-NA	2.42	127.89	124.40
6	V	1620	LUT	C35-C15-C14	-2.42	118.58	123.52
4	V	601	CHL	CMB-C2B-C3B	2.41	129.49	124.68
6	W	1621	LUT	C18-C5-C4	2.41	118.85	114.42
7	W	1622	XAT	C26-C27-C28	-2.40	120.91	125.99
5	V	610	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
7	U	1622	XAT	C26-C27-C28	-2.40	120.92	125.99
8	U	1623	NEX	C31-C30-C29	-2.39	123.92	127.28
4	V	607	CHL	CMB-C2B-C3B	2.39	129.47	124.68
5	W	603	CLA	C1-C2-C3	-2.39	122.29	126.20
5	U	614	CLA	CHB-C4A-NA	2.38	127.84	124.40
8	W	1623	NEX	C31-C30-C29	-2.38	123.94	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	U	1620	LUT	C17-C1-C6	2.38	113.98	110.24
4	V	606	CHL	C1A-CHA-CBD	2.38	138.45	132.36
4	W	601	CHL	O1D-CGD-CBD	-2.37	121.12	124.72
6	W	1620	LUT	C17-C1-C6	2.37	113.96	110.24
5	V	613	CLA	CHB-C4A-NA	2.37	127.82	124.40
5	V	614	CLA	C3B-C4B-NB	-2.36	108.42	110.53
5	W	610	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
4	V	605	CHL	O1D-CGD-CBD	-2.36	121.15	124.72
6	U	1621	LUT	O23-C23-C22	-2.36	105.88	110.06
8	W	1623	NEX	C2-C1-C6	2.35	111.50	109.21
4	U	606	CHL	C3D-CAD-CBD	2.35	110.70	107.61
5	W	602	CLA	C3B-C4B-NB	-2.35	108.43	110.53
5	U	610	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
10	V	2631	LMG	O8-C28-C29	2.34	118.98	111.83
5	V	603	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
6	V	1620	LUT	C35-C34-C33	-2.34	124.00	127.28
5	V	604	CLA	CHB-C4A-NA	2.34	127.78	124.40
8	U	1623	NEX	C2-C1-C6	2.34	111.48	109.21
6	W	1621	LUT	O23-C23-C22	-2.34	105.91	110.06
4	V	607	CHL	C1A-CHA-CBD	2.33	138.32	132.36
5	W	603	CLA	C3B-C4B-NB	-2.33	108.45	110.53
6	U	1621	LUT	C15-C14-C13	-2.33	124.01	127.28
5	U	603	CLA	C1-C2-C3	-2.33	122.39	126.20
5	V	610	CLA	CMB-C2B-C3B	2.32	132.01	126.55
5	U	603	CLA	C3B-C4B-NB	-2.32	108.46	110.53
4	W	601	CHL	CBC-CAC-C3C	-2.32	109.56	112.87
5	W	604	CLA	CHB-C4A-NA	2.32	127.74	124.40
6	V	1621	LUT	C15-C35-C34	-2.31	118.78	123.52
4	W	606	CHL	C3D-CAD-CBD	2.31	110.65	107.61
4	U	606	CHL	O1D-CGD-CBD	-2.31	121.23	124.72
6	W	1621	LUT	C15-C14-C13	-2.30	124.05	127.28
5	W	611	CLA	C3B-C4B-NB	-2.30	108.48	110.53
4	V	601	CHL	CMA-C3A-C4A	-2.30	109.66	114.61
5	U	604	CLA	CBD-CHA-C1A	2.30	131.84	127.58
5	U	604	CLA	CHB-C4A-NA	2.30	127.71	124.40
5	U	602	CLA	C3B-C4B-NB	-2.30	108.48	110.53
6	U	1621	LUT	C15-C35-C34	-2.30	118.82	123.52
4	W	607	CHL	CMB-C2B-C3B	2.28	129.24	124.68
7	V	1622	XAT	C24-C23-C22	-2.28	106.53	110.79
4	U	601	CHL	O1D-CGD-CBD	-2.27	121.28	124.72
4	U	601	CHL	C4C-CHD-C1D	2.26	124.17	116.07
4	U	601	CHL	O2D-CGD-O1D	-2.26	119.45	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	1622	XAT	C35-C34-C33	-2.26	124.11	127.28
4	W	606	CHL	O1D-CGD-CBD	-2.26	121.30	124.72
6	V	1620	LUT	C1-C6-C5	-2.25	119.56	122.64
5	V	602	CLA	C1-C2-C3	-2.25	122.51	126.20
7	V	1622	XAT	C11-C10-C9	-2.25	124.13	127.28
4	W	601	CHL	C6-C7-C8	-2.24	108.51	115.97
5	U	603	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
5	U	611	CLA	C3B-C4B-NB	-2.23	108.54	110.53
6	W	1621	LUT	C15-C35-C34	-2.23	118.96	123.52
4	W	607	CHL	O2D-CGD-O1D	-2.23	119.51	123.85
5	V	611	CLA	CHB-C4A-NA	2.22	127.61	124.40
4	W	601	CHL	O2D-CGD-O1D	-2.22	119.53	123.85
5	W	611	CLA	CAA-CBA-CGA	-2.22	106.91	113.21
4	W	608	CHL	O2A-CGA-CBA	2.22	120.51	112.14
6	V	1621	LUT	C15-C14-C13	-2.21	124.18	127.28
6	V	1620	LUT	C15-C14-C13	-2.21	124.18	127.28
5	U	612	CLA	C3B-C4B-NB	-2.21	108.56	110.53
4	V	607	CHL	CAA-C2A-C3A	2.21	118.97	113.00
5	W	603	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
9	V	2630	LHG	O8-C23-O10	-2.20	118.13	123.63
7	V	1622	XAT	C18-C5-C4	2.19	116.70	114.24
5	V	614	CLA	O2A-CGA-O1A	-2.19	117.70	123.33
4	W	606	CHL	C1B-CHB-C4A	-2.19	119.92	121.32
4	W	601	CHL	C4C-CHD-C1D	2.19	123.89	116.07
4	U	601	CHL	CBC-CAC-C3C	-2.17	109.77	112.87
6	U	1621	LUT	C21-C26-C27	-2.16	110.34	112.83
4	U	607	CHL	O2A-CGA-O1A	-2.16	117.77	123.33
5	V	613	CLA	C3B-C4B-NB	-2.16	108.60	110.53
5	W	612	CLA	C3B-C4B-NB	-2.16	108.60	110.53
4	V	601	CHL	O1D-CGD-CBD	-2.16	121.45	124.72
4	W	601	CHL	CED-O2D-CGD	2.15	120.80	115.92
7	W	1622	XAT	C40-C33-C32	2.15	121.37	118.09
4	V	605	CHL	O2D-CGD-O1D	-2.15	119.67	123.85
4	U	608	CHL	O1D-CGD-CBD	-2.14	121.47	124.72
5	V	613	CLA	C1-C2-C3	-2.14	122.69	126.20
6	W	1621	LUT	C21-C26-C27	-2.14	110.37	112.83
8	W	1623	NEX	O24-C25-C26	-2.14	57.24	58.93
4	V	607	CHL	O2D-CGD-O1D	-2.13	119.69	123.85
7	W	1622	XAT	C19-C9-C8	2.13	121.34	118.09
4	V	609	CHL	CMA-C3A-C4A	-2.13	110.03	114.61
5	V	604	CLA	CHD-C1D-ND	-2.12	121.82	124.80
7	U	1622	XAT	C19-C9-C8	2.11	121.32	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	606	CHL	O2D-CGD-O1D	-2.11	119.74	123.85
4	U	606	CHL	O2D-CGD-O1D	-2.11	119.74	123.85
4	V	609	CHL	C4C-CHD-C1D	2.11	123.62	116.07
4	W	601	CHL	CMA-C3A-C4A	-2.11	110.07	114.61
6	V	1620	LUT	C15-C35-C34	-2.11	119.21	123.52
8	W	1623	NEX	C26-C27-C28	-2.10	121.54	125.99
10	V	2631	LMG	C8-O7-C10	-2.10	112.76	117.80
4	W	607	CHL	C4C-CHD-C1D	2.10	123.59	116.07
4	V	606	CHL	O1D-CGD-CBD	-2.10	121.54	124.72
5	V	612	CLA	C3B-C4B-NB	-2.10	108.66	110.53
4	W	608	CHL	O1D-CGD-CBD	-2.10	121.54	124.72
4	U	606	CHL	C1B-CHB-C4A	-2.10	119.97	121.32
6	V	1621	LUT	C31-C30-C29	-2.10	124.34	127.28
7	U	1622	XAT	C40-C33-C32	2.10	121.29	118.09
4	W	605	CHL	CAC-C3C-C4C	2.09	129.41	124.03
6	U	1620	LUT	C28-C29-C30	-2.09	115.72	119.01
5	V	612	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
4	U	601	CHL	CED-O2D-CGD	2.08	120.64	115.92
4	U	609	CHL	C4C-CHD-C1D	2.08	123.52	116.07
8	U	1623	NEX	C15-C35-C34	-2.08	119.26	123.52
4	U	607	CHL	CBC-CAC-C3C	-2.08	109.89	112.87
8	U	1623	NEX	C26-C27-C28	-2.08	121.60	125.99
4	U	605	CHL	CAC-C3C-C4C	2.08	129.37	124.03
5	U	604	CLA	O1D-CGD-CBD	2.08	128.57	124.50
4	W	609	CHL	C4C-CHD-C1D	2.07	123.49	116.07
4	V	601	CHL	C4C-CHD-C1D	2.07	123.49	116.07
5	W	604	CLA	O1D-CGD-CBD	2.07	128.60	124.52
6	V	1620	LUT	C30-C31-C32	-2.07	117.20	123.20
8	V	1623	NEX	O24-C25-C26	-2.06	57.29	58.93
6	W	1621	LUT	C31-C30-C29	-2.06	124.39	127.28
4	U	605	CHL	C3D-CAD-CBD	2.06	110.32	107.61
5	V	612	CLA	O1D-CGD-CBD	2.06	128.59	124.52
5	W	613	CLA	C6-C5-C3	2.06	118.49	113.47
8	W	1623	NEX	C15-C35-C34	-2.06	119.30	123.52
5	U	613	CLA	C6-C5-C3	2.06	118.48	113.47
4	V	608	CHL	O1D-CGD-CBD	-2.06	121.61	124.72
6	W	1620	LUT	C28-C29-C30	-2.05	115.78	119.01
6	W	1620	LUT	C38-C25-C24	-2.05	118.50	123.36
8	U	1623	NEX	C30-C31-C32	-2.05	117.27	123.20
4	W	609	CHL	CAC-C3C-C4C	2.05	129.29	124.03
4	W	605	CHL	C3D-CAD-CBD	2.05	110.30	107.61
5	V	602	CLA	CMB-C2B-C1B	-2.04	122.31	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	1623	NEX	C30-C31-C32	-2.04	117.29	123.20
6	V	1621	LUT	O23-C23-C22	-2.04	106.44	110.06
4	W	608	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
4	V	607	CHL	CAC-C3C-C4C	2.04	129.27	124.03
4	W	605	CHL	O2A-CGA-CBA	2.04	120.44	114.00
7	U	1622	XAT	C7-C8-C9	-2.04	122.37	125.53
5	V	602	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
6	U	1621	LUT	C31-C30-C29	-2.03	124.43	127.28
6	U	1620	LUT	C38-C25-C24	-2.03	118.56	123.36
5	U	604	CLA	CHD-C1D-ND	-2.02	121.96	124.80
7	W	1622	XAT	C7-C8-C9	-2.02	122.39	125.53
8	U	1623	NEX	O24-C25-C26	-2.02	57.33	58.93
6	U	1620	LUT	C35-C34-C33	-2.01	124.47	127.28
5	V	602	CLA	O1D-CGD-CBD	2.00	128.47	124.52
4	V	608	CHL	O2D-CGD-O1D	-2.00	119.95	123.85

All (78) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	U	601	CHL	NC
4	U	601	CHL	ND
4	U	601	CHL	NA
4	U	605	CHL	NC
4	U	605	CHL	ND
4	U	605	CHL	NA
4	U	606	CHL	NC
4	U	606	CHL	ND
4	U	606	CHL	NA
4	U	607	CHL	NC
4	U	607	CHL	ND
4	U	607	CHL	NA
4	U	608	CHL	NC
4	U	608	CHL	ND
4	U	608	CHL	NA
4	U	609	CHL	NC
4	U	609	CHL	ND
4	U	609	CHL	NA
4	V	601	CHL	NC
4	V	601	CHL	ND
4	V	601	CHL	NA
4	V	605	CHL	NC
4	V	605	CHL	ND

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Mol	Chain	Res	Type	Atom
4	V	605	CHL	NA
4	V	606	CHL	NC
4	V	606	CHL	ND
4	V	606	CHL	NA
4	V	607	CHL	NC
4	V	607	CHL	ND
4	V	607	CHL	NA
4	V	608	CHL	NC
4	V	608	CHL	ND
4	V	608	CHL	NA
4	V	609	CHL	NC
4	V	609	CHL	ND
4	V	609	CHL	NA
4	W	601	CHL	NC
4	W	601	CHL	ND
4	W	601	CHL	NA
4	W	605	CHL	NC
4	W	605	CHL	ND
4	W	605	CHL	NA
4	W	606	CHL	NC
4	W	606	CHL	ND
4	W	606	CHL	NA
4	W	607	CHL	NC
4	W	607	CHL	ND
4	W	607	CHL	NA
4	W	608	CHL	NC
4	W	608	CHL	ND
4	W	608	CHL	NA
4	W	609	CHL	NC
4	W	609	CHL	ND
4	W	609	CHL	NA
5	U	602	CLA	ND
5	U	603	CLA	ND
5	U	604	CLA	ND
5	U	610	CLA	ND
5	U	611	CLA	ND
5	U	612	CLA	ND
5	U	613	CLA	ND
5	U	614	CLA	ND
5	V	602	CLA	ND
5	V	603	CLA	ND
5	V	604	CLA	ND

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Mol	Chain	Res	Type	Atom
5	V	610	CLA	ND
5	V	611	CLA	ND
5	V	612	CLA	ND
5	V	613	CLA	ND
5	V	614	CLA	ND
5	W	602	CLA	ND
5	W	603	CLA	ND
5	W	604	CLA	ND
5	W	610	CLA	ND
5	W	611	CLA	ND
5	W	612	CLA	ND
5	W	613	CLA	ND
5	W	614	CLA	ND

All (381) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	608	CHL	CBD-CGD-O2D-CED
4	V	607	CHL	C1A-C2A-CAA-CBA
4	V	607	CHL	C3A-C2A-CAA-CBA
4	V	609	CHL	C1C-C2C-CMC-OMC
4	V	609	CHL	C3C-C2C-CMC-OMC
4	W	601	CHL	C6-C7-C8-C10
4	W	607	CHL	C1C-C2C-CMC-OMC
4	W	607	CHL	C3C-C2C-CMC-OMC
4	W	607	CHL	CBD-CGD-O2D-CED
4	W	608	CHL	CBD-CGD-O2D-CED
4	W	609	CHL	C3A-C2A-CAA-CBA
5	U	610	CLA	CBD-CGD-O2D-CED
5	U	611	CLA	C1A-C2A-CAA-CBA
5	U	611	CLA	C3A-C2A-CAA-CBA
5	U	611	CLA	C2B-C3B-CAB-CBB
5	U	611	CLA	C4B-C3B-CAB-CBB
5	U	612	CLA	CHA-CBD-CGD-O1D
5	U	612	CLA	CHA-CBD-CGD-O2D
5	U	614	CLA	CBD-CGD-O2D-CED
5	V	604	CLA	CBD-CGD-O2D-CED
5	V	611	CLA	CAD-CBD-CGD-O1D
5	V	611	CLA	CAD-CBD-CGD-O2D
5	V	614	CLA	C2B-C3B-CAB-CBB
5	V	614	CLA	C4B-C3B-CAB-CBB
5	W	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
5	W	611	CLA	C1A-C2A-CAA-CBA
5	W	611	CLA	C3A-C2A-CAA-CBA
5	W	611	CLA	C2B-C3B-CAB-CBB
5	W	611	CLA	C4B-C3B-CAB-CBB
5	W	612	CLA	CHA-CBD-CGD-O1D
5	W	612	CLA	CHA-CBD-CGD-O2D
5	W	614	CLA	CBD-CGD-O2D-CED
6	V	1621	LUT	C7-C8-C9-C10
7	U	1622	XAT	C11-C12-C13-C14
7	U	1622	XAT	C31-C32-C33-C34
7	W	1622	XAT	C11-C12-C13-C14
7	W	1622	XAT	C31-C32-C33-C34
8	V	1623	NEX	O24-C26-C27-C28
9	U	2630	LHG	C3-O3-P-O4
9	U	2630	LHG	C3-O3-P-O6
9	U	2630	LHG	C4-O6-P-O3
9	U	2630	LHG	C4-O6-P-O5
9	V	2630	LHG	C4-O6-P-O3
9	W	2630	LHG	C3-O3-P-O4
9	W	2630	LHG	C3-O3-P-O6
9	W	2630	LHG	C4-O6-P-O3
9	W	2630	LHG	C4-O6-P-O5
4	U	607	CHL	CBD-CGD-O2D-CED
4	V	608	CHL	CBD-CGD-O2D-CED
5	V	610	CLA	CBD-CGD-O2D-CED
5	V	613	CLA	CBD-CGD-O2D-CED
4	U	607	CHL	O1D-CGD-O2D-CED
4	W	607	CHL	O1D-CGD-O2D-CED
4	U	608	CHL	O1D-CGD-O2D-CED
4	W	608	CHL	O1D-CGD-O2D-CED
5	U	610	CLA	O1D-CGD-O2D-CED
5	W	610	CLA	O1D-CGD-O2D-CED
4	V	606	CHL	CBD-CGD-O2D-CED
4	V	609	CHL	CBD-CGD-O2D-CED
5	U	602	CLA	CBD-CGD-O2D-CED
5	U	611	CLA	CBD-CGD-O2D-CED
5	W	602	CLA	CBD-CGD-O2D-CED
5	W	611	CLA	CBD-CGD-O2D-CED
5	U	614	CLA	O1D-CGD-O2D-CED
5	V	604	CLA	O1D-CGD-O2D-CED
5	W	614	CLA	O1D-CGD-O2D-CED
4	U	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
4	W	601	CHL	C4-C3-C5-C6
4	U	601	CHL	C2-C3-C5-C6
4	W	601	CHL	C2-C3-C5-C6
4	W	601	CHL	CBD-CGD-O2D-CED
5	V	613	CLA	O1D-CGD-O2D-CED
5	U	613	CLA	C3-C5-C6-C7
5	W	613	CLA	C3-C5-C6-C7
5	V	602	CLA	C3-C5-C6-C7
4	V	608	CHL	O1D-CGD-O2D-CED
4	U	601	CHL	CBA-CGA-O2A-C1
4	U	601	CHL	O1A-CGA-O2A-C1
5	V	610	CLA	O1D-CGD-O2D-CED
4	U	601	CHL	CBD-CGD-O2D-CED
5	V	614	CLA	CBD-CGD-O2D-CED
5	U	604	CLA	CBA-CGA-O2A-C1
5	W	604	CLA	CBA-CGA-O2A-C1
4	U	609	CHL	C6-C7-C8-C9
4	U	609	CHL	C11-C10-C8-C9
4	V	601	CHL	C14-C13-C15-C16
4	W	607	CHL	C6-C7-C8-C9
4	W	609	CHL	C11-C10-C8-C9
4	W	609	CHL	C11-C12-C13-C14
5	U	602	CLA	O1D-CGD-O2D-CED
5	W	602	CLA	O1D-CGD-O2D-CED
4	V	606	CHL	O1D-CGD-O2D-CED
4	V	609	CHL	O1D-CGD-O2D-CED
7	U	1622	XAT	C11-C12-C13-C20
7	U	1622	XAT	C31-C32-C33-C40
7	W	1622	XAT	C11-C12-C13-C20
7	W	1622	XAT	C31-C32-C33-C40
4	W	607	CHL	C2A-CAA-CBA-CGA
5	U	604	CLA	O1A-CGA-O2A-C1
5	W	604	CLA	O1A-CGA-O2A-C1
4	W	601	CHL	C10-C11-C12-C13
5	W	611	CLA	C3-C5-C6-C7
4	U	601	CHL	C6-C7-C8-C10
4	V	601	CHL	C6-C7-C8-C10
5	V	613	CLA	C6-C7-C8-C10
5	V	613	CLA	C3-C5-C6-C7
5	U	611	CLA	O1D-CGD-O2D-CED
5	W	611	CLA	O1D-CGD-O2D-CED
4	U	601	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	W	601	CHL	C8-C10-C11-C12
4	U	607	CHL	C2A-CAA-CBA-CGA
4	W	605	CHL	C2A-CAA-CBA-CGA
4	V	601	CHL	C13-C15-C16-C17
4	V	601	CHL	C15-C16-C17-C18
4	V	609	CHL	C8-C10-C11-C12
4	W	607	CHL	C8-C10-C11-C12
10	V	2631	LMG	C10-C11-C12-C13
4	V	601	CHL	C5-C6-C7-C8
4	W	607	CHL	C15-C16-C17-C18
4	W	609	CHL	C15-C16-C17-C18
4	W	607	CHL	C13-C15-C16-C17
4	W	601	CHL	O1D-CGD-O2D-CED
5	U	602	CLA	C8-C10-C11-C12
5	V	610	CLA	C5-C6-C7-C8
5	W	602	CLA	C8-C10-C11-C12
5	V	610	CLA	C13-C15-C16-C17
5	U	613	CLA	CBA-CGA-O2A-C1
5	W	613	CLA	CBA-CGA-O2A-C1
5	V	613	CLA	C13-C15-C16-C17
4	W	609	CHL	C13-C15-C16-C17
4	U	601	CHL	C13-C15-C16-C17
5	U	610	CLA	C5-C6-C7-C8
5	W	602	CLA	C10-C11-C12-C13
5	W	610	CLA	C5-C6-C7-C8
4	W	607	CHL	C10-C11-C12-C13
4	W	609	CHL	C8-C10-C11-C12
4	W	607	CHL	C16-C17-C18-C20
5	V	613	CLA	C16-C17-C18-C20
4	U	601	CHL	C16-C17-C18-C19
4	V	609	CHL	C11-C12-C13-C15
4	W	601	CHL	C16-C17-C18-C20
4	U	601	CHL	C10-C11-C12-C13
4	W	607	CHL	CBA-CGA-O2A-C1
5	U	603	CLA	C4B-C3B-CAB-CBB
5	U	612	CLA	C4B-C3B-CAB-CBB
5	W	603	CLA	C4B-C3B-CAB-CBB
5	W	612	CLA	C4B-C3B-CAB-CBB
5	U	602	CLA	C10-C11-C12-C13
4	V	601	CHL	C16-C17-C18-C19
4	V	601	CHL	C16-C17-C18-C20
4	V	609	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	W	609	CHL	C16-C17-C18-C19
5	V	613	CLA	C16-C17-C18-C19
5	V	614	CLA	O1D-CGD-O2D-CED
5	U	613	CLA	C2A-CAA-CBA-CGA
5	W	613	CLA	C2A-CAA-CBA-CGA
4	V	601	CHL	C11-C12-C13-C15
5	U	613	CLA	C11-C10-C8-C7
5	W	613	CLA	C11-C10-C8-C7
4	W	601	CHL	C15-C16-C17-C18
4	U	601	CHL	O1D-CGD-O2D-CED
4	U	601	CHL	C16-C17-C18-C20
4	W	609	CHL	C16-C17-C18-C20
5	U	613	CLA	O1A-CGA-O2A-C1
5	W	613	CLA	O1A-CGA-O2A-C1
4	W	601	CHL	C3-C5-C6-C7
5	U	603	CLA	C2B-C3B-CAB-CBB
5	U	612	CLA	C2B-C3B-CAB-CBB
5	W	603	CLA	C2B-C3B-CAB-CBB
5	W	612	CLA	C2B-C3B-CAB-CBB
6	U	1620	LUT	C1-C6-C7-C8
6	W	1620	LUT	C1-C6-C7-C8
4	U	609	CHL	C11-C12-C13-C14
9	U	2630	LHG	C26-C27-C28-C29
9	W	2630	LHG	C26-C27-C28-C29
4	W	607	CHL	O1A-CGA-O2A-C1
9	V	2630	LHG	C11-C12-C13-C14
4	W	601	CHL	CBA-CGA-O2A-C1
4	U	601	CHL	C3-C5-C6-C7
10	V	2631	LMG	C15-C16-C17-C18
4	W	601	CHL	C13-C15-C16-C17
4	U	608	CHL	C2A-CAA-CBA-CGA
4	U	609	CHL	C8-C10-C11-C12
9	U	2630	LHG	C17-C18-C19-C20
9	W	2630	LHG	C17-C18-C19-C20
4	U	601	CHL	C5-C6-C7-C8
9	U	2630	LHG	C16-C17-C18-C19
9	W	2630	LHG	C16-C17-C18-C19
4	W	601	CHL	C16-C17-C18-C19
5	V	613	CLA	C2A-CAA-CBA-CGA
5	V	611	CLA	CBD-CGD-O2D-CED
4	W	601	CHL	O1A-CGA-O2A-C1
4	V	609	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
4	W	609	CHL	C11-C12-C13-C15
4	W	609	CHL	C12-C13-C15-C16
5	U	602	CLA	C6-C7-C8-C10
5	W	602	CLA	C6-C7-C8-C10
4	U	601	CHL	C15-C16-C17-C18
4	U	601	CHL	C6-C7-C8-C9
5	U	613	CLA	C11-C10-C8-C9
5	W	613	CLA	C11-C10-C8-C9
4	U	609	CHL	CHA-CBD-CGD-O1D
4	U	609	CHL	CHA-CBD-CGD-O2D
4	W	609	CHL	CHA-CBD-CGD-O1D
4	W	608	CHL	CBA-CGA-O2A-C1
5	V	613	CLA	C2-C3-C5-C6
4	W	609	CHL	C3-C5-C6-C7
9	U	2630	LHG	C31-C32-C33-C34
5	U	610	CLA	CBA-CGA-O2A-C1
5	V	613	CLA	CBA-CGA-O2A-C1
5	W	610	CLA	CBA-CGA-O2A-C1
5	V	613	CLA	C4-C3-C5-C6
4	V	608	CHL	CBA-CGA-O2A-C1
4	V	601	CHL	C6-C7-C8-C9
4	W	601	CHL	C11-C10-C8-C9
4	W	609	CHL	C14-C13-C15-C16
5	U	602	CLA	C6-C7-C8-C9
5	W	602	CLA	C6-C7-C8-C9
5	U	613	CLA	C5-C6-C7-C8
5	U	610	CLA	C4B-C3B-CAB-CBB
5	U	614	CLA	C4B-C3B-CAB-CBB
5	V	603	CLA	C4B-C3B-CAB-CBB
5	W	610	CLA	C4B-C3B-CAB-CBB
5	W	614	CLA	C4B-C3B-CAB-CBB
5	W	613	CLA	C5-C6-C7-C8
4	U	609	CHL	C3A-C2A-CAA-CBA
4	V	609	CHL	C3A-C2A-CAA-CBA
4	W	601	CHL	C3A-C2A-CAA-CBA
4	W	607	CHL	C16-C17-C18-C19
5	U	603	CLA	C4-C3-C5-C6
5	W	603	CLA	C4-C3-C5-C6
5	W	611	CLA	C4-C3-C5-C6
4	V	609	CHL	C3-C5-C6-C7
4	W	608	CHL	C2A-CAA-CBA-CGA
5	W	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
4	W	601	CHL	C6-C7-C8-C9
5	U	614	CLA	C1A-C2A-CAA-CBA
5	U	603	CLA	CAA-CBA-CGA-O2A
5	W	603	CLA	CAA-CBA-CGA-O2A
6	V	1621	LUT	C7-C8-C9-C19
4	U	601	CHL	C12-C13-C15-C16
4	W	607	CHL	C12-C13-C15-C16
5	W	613	CLA	C12-C13-C15-C16
6	U	1621	LUT	C7-C8-C9-C10
4	W	607	CHL	CAA-CBA-CGA-O2A
4	V	608	CHL	O1A-CGA-O2A-C1
5	U	603	CLA	C2-C3-C5-C6
5	W	603	CLA	C2-C3-C5-C6
9	W	2630	LHG	C29-C30-C31-C32
9	U	2630	LHG	C29-C30-C31-C32
5	U	610	CLA	O1A-CGA-O2A-C1
5	V	613	CLA	O1A-CGA-O2A-C1
5	W	610	CLA	O1A-CGA-O2A-C1
9	V	2630	LHG	C24-C25-C26-C27
5	U	604	CLA	CAD-CBD-CGD-O2D
4	W	607	CHL	C2-C1-O2A-CGA
4	U	601	CHL	C4C-C3C-CAC-CBC
4	W	607	CHL	C3-C5-C6-C7
6	W	1621	LUT	C7-C8-C9-C10
5	V	613	CLA	C10-C11-C12-C13
4	U	609	CHL	C11-C10-C8-C7
4	W	607	CHL	C6-C7-C8-C10
4	W	607	CHL	C11-C12-C13-C15
4	W	609	CHL	C11-C10-C8-C7
5	U	613	CLA	C4-C3-C5-C6
5	W	613	CLA	C4-C3-C5-C6
4	U	601	CHL	C14-C13-C15-C16
4	W	607	CHL	C14-C13-C15-C16
5	W	613	CLA	C14-C13-C15-C16
5	U	604	CLA	C1-C2-C3-C4
4	V	609	CHL	CHA-CBD-CGD-O1D
4	V	609	CHL	CHA-CBD-CGD-O2D
4	W	609	CHL	CHA-CBD-CGD-O2D
5	U	603	CLA	CHA-CBD-CGD-O1D
5	U	603	CLA	CHA-CBD-CGD-O2D
5	U	610	CLA	CHA-CBD-CGD-O1D
5	V	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	V	602	CLA	CHA-CBD-CGD-O2D
5	V	604	CLA	CHA-CBD-CGD-O2D
5	V	614	CLA	CHA-CBD-CGD-O1D
5	W	603	CLA	CHA-CBD-CGD-O1D
5	W	603	CLA	CHA-CBD-CGD-O2D
5	W	610	CLA	CHA-CBD-CGD-O1D
9	U	2630	LHG	C4-O6-P-O4
9	V	2630	LHG	C4-O6-P-O5
9	W	2630	LHG	C4-O6-P-O4
5	U	613	CLA	C2-C3-C5-C6
5	W	613	CLA	C2-C3-C5-C6
4	V	609	CHL	C10-C11-C12-C13
4	W	608	CHL	O1A-CGA-O2A-C1
5	V	613	CLA	C6-C7-C8-C9
4	U	609	CHL	C6-C7-C8-C10
5	V	602	CLA	C11-C10-C8-C7
5	U	613	CLA	C8-C10-C11-C12
5	V	611	CLA	O1D-CGD-O2D-CED
5	W	613	CLA	C8-C10-C11-C12
9	W	2630	LHG	C27-C28-C29-C30
9	U	2630	LHG	C27-C28-C29-C30
4	W	607	CHL	C11-C12-C13-C14
5	V	612	CLA	C4B-C3B-CAB-CBB
4	W	607	CHL	C4-C3-C5-C6
4	V	601	CHL	C11-C10-C8-C7
10	V	2631	LMG	C18-C19-C20-C21
5	V	604	CLA	C3A-C2A-CAA-CBA
8	U	1623	NEX	C39-C29-C30-C31
8	V	1623	NEX	C39-C29-C30-C31
8	W	1623	NEX	C39-C29-C30-C31
10	V	2631	LMG	C29-C30-C31-C32
4	V	601	CHL	C11-C10-C8-C9
4	W	601	CHL	C1A-C2A-CAA-CBA
5	W	612	CLA	CAA-CBA-CGA-O1A
5	V	604	CLA	C1A-C2A-CAA-CBA
8	U	1623	NEX	C28-C29-C30-C31
8	V	1623	NEX	C28-C29-C30-C31
8	W	1623	NEX	C28-C29-C30-C31
5	U	614	CLA	C2B-C3B-CAB-CBB
5	V	603	CLA	C2B-C3B-CAB-CBB
5	V	612	CLA	C2B-C3B-CAB-CBB
5	W	614	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	V	603	CLA	CAA-CBA-CGA-O2A
4	V	609	CHL	C4-C3-C5-C6
10	V	2631	LMG	O9-C10-O7-C8
5	V	610	CLA	C12-C13-C15-C16
5	V	612	CLA	CAA-CBA-CGA-O2A
9	U	2630	LHG	C33-C34-C35-C36
5	W	612	CLA	CAA-CBA-CGA-O2A
4	U	609	CHL	C4-C3-C5-C6
4	W	607	CHL	C2-C3-C5-C6
4	V	609	CHL	C2-C1-O2A-CGA
5	V	603	CLA	CAA-CBA-CGA-O1A
5	V	613	CLA	C8-C10-C11-C12
4	W	606	CHL	CAA-CBA-CGA-O2A
5	V	612	CLA	CAA-CBA-CGA-O1A
5	W	603	CLA	O1A-CGA-O2A-C1
5	U	603	CLA	O1A-CGA-O2A-C1
4	W	605	CHL	CAA-CBA-CGA-O2A
4	W	606	CHL	CAA-CBA-CGA-O1A
4	V	608	CHL	C2-C1-O2A-CGA
10	V	2631	LMG	C13-C14-C15-C16
4	U	601	CHL	CHA-CBD-CGD-O2D
4	V	601	CHL	CHA-CBD-CGD-O2D
4	W	601	CHL	CHA-CBD-CGD-O1D
4	W	601	CHL	CHA-CBD-CGD-O2D
9	V	2630	LHG	C33-C34-C35-C36
10	V	2631	LMG	C11-C10-O7-C8
5	V	613	CLA	C15-C16-C17-C18
8	V	1623	NEX	C29-C30-C31-C32
4	W	605	CHL	CAA-CBA-CGA-O1A
4	V	609	CHL	C6-C7-C8-C9
5	U	604	CLA	CHA-CBD-CGD-O1D
5	U	603	CLA	CBA-CGA-O2A-C1
5	W	603	CLA	CBA-CGA-O2A-C1
4	U	609	CHL	C2-C3-C5-C6
8	U	1623	NEX	O24-C26-C27-C28
8	W	1623	NEX	O24-C26-C27-C28
9	V	2630	LHG	O6-C4-C5-O7
8	U	1623	NEX	C9-C10-C11-C12
8	W	1623	NEX	C9-C10-C11-C12
5	U	603	CLA	CAA-CBA-CGA-O1A
5	W	603	CLA	CAA-CBA-CGA-O1A
9	V	2630	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	U	610	CLA	C2B-C3B-CAB-CBB
5	W	610	CLA	C2B-C3B-CAB-CBB
6	U	1620	LUT	C5-C6-C7-C8
6	W	1620	LUT	C5-C6-C7-C8
4	U	609	CHL	C2-C1-O2A-CGA
5	W	603	CLA	C3-C5-C6-C7
10	V	2631	LMG	C17-C18-C19-C20
5	W	611	CLA	CAA-CBA-CGA-O2A
5	W	611	CLA	C5-C6-C7-C8
5	V	610	CLA	C14-C13-C15-C16
4	W	607	CHL	CAA-CBA-CGA-O1A
5	U	603	CLA	C3-C5-C6-C7
10	V	2631	LMG	C11-C12-C13-C14
5	U	604	CLA	O2A-C1-C2-C3
5	W	611	CLA	CAA-CBA-CGA-O1A
4	V	609	CHL	C11-C10-C8-C9
5	V	602	CLA	C8-C10-C11-C12
4	V	601	CHL	C3-C5-C6-C7
8	U	1623	NEX	C29-C30-C31-C32
4	U	607	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

35 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	W	1622	XAT	4	0
4	W	607	CHL	6	0
6	V	1620	LUT	2	0
4	W	605	CHL	3	0
4	V	606	CHL	3	0
9	U	2630	LHG	1	0
4	U	605	CHL	3	0
4	V	609	CHL	4	0
4	U	608	CHL	1	0
5	W	610	CLA	1	0
8	W	1623	NEX	2	0
4	V	607	CHL	4	0
4	W	608	CHL	1	0
5	U	604	CLA	1	0
4	U	606	CHL	2	0
4	V	601	CHL	5	0
6	W	1620	LUT	2	0

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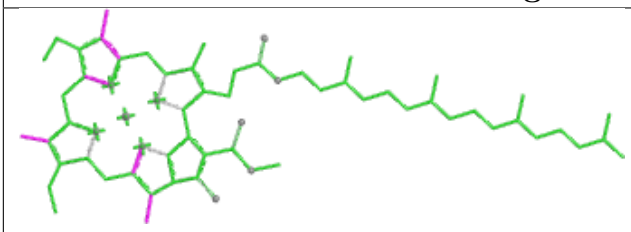
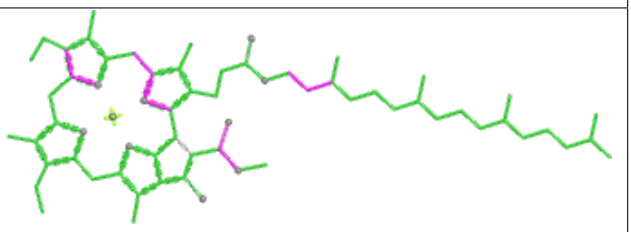
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	602	CLA	2	0
4	W	601	CHL	2	0
5	U	613	CLA	2	0
5	U	610	CLA	1	0
4	V	608	CHL	12	0
4	U	609	CHL	5	0
5	W	611	CLA	1	0
6	U	1620	LUT	2	0
8	V	1623	NEX	1	0
4	V	605	CHL	2	0
4	U	601	CHL	3	0
4	W	606	CHL	3	0
5	W	613	CLA	2	0
4	W	609	CHL	5	0
7	U	1622	XAT	5	0
9	V	2630	LHG	2	0
5	U	611	CLA	1	0
5	V	611	CLA	1	0

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

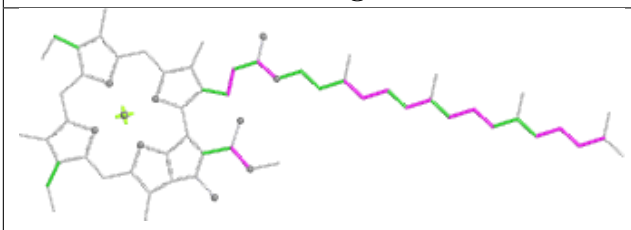
Ligand CLA V 613



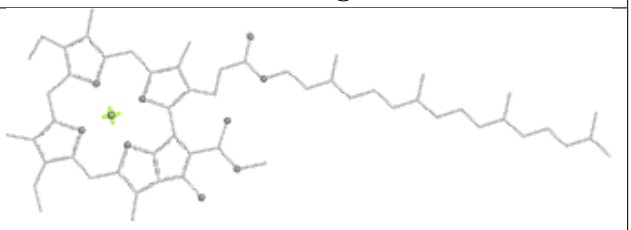
Bond lengths



Bond angles



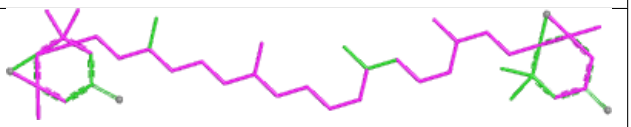
Torsions



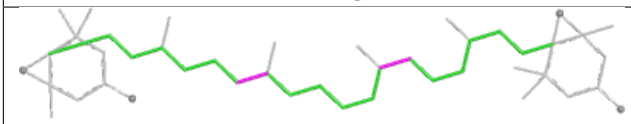
Rings

Ligand XAT W 1622

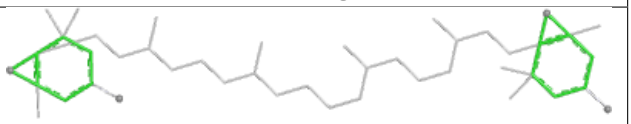
Bond lengths



Bond angles

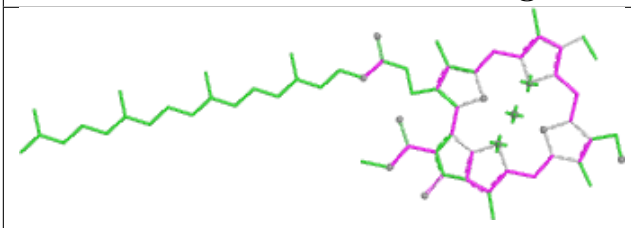


Torsions

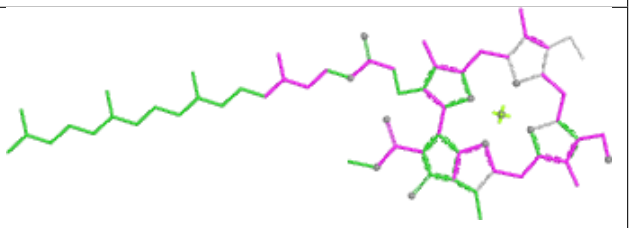


Rings

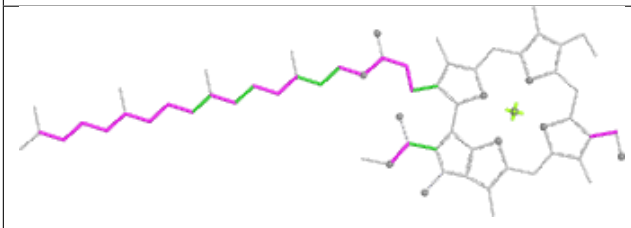
Ligand CHL W 607



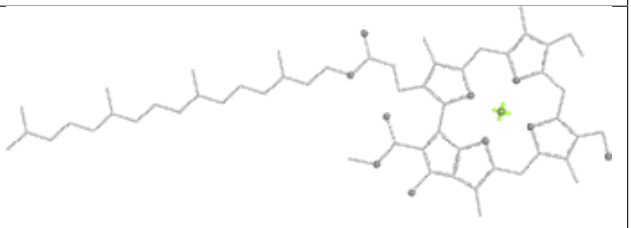
Bond lengths



Bond angles

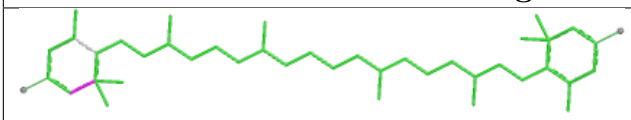


Torsions

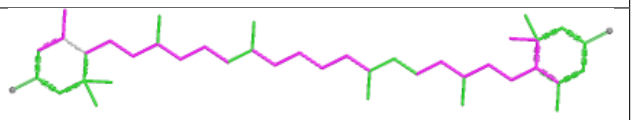


Rings

Ligand LUT V 1620

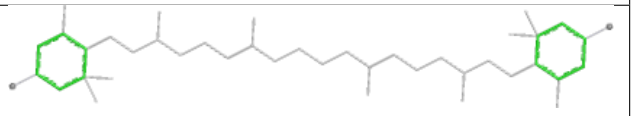


Bond lengths



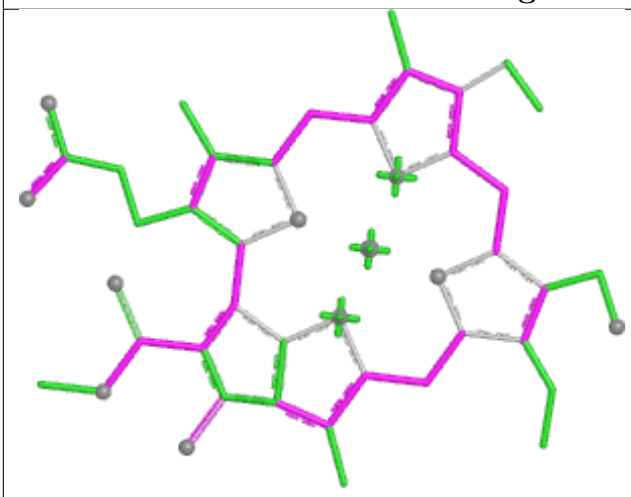
Bond angles

Torsions



Rings

Ligand CHL W 605



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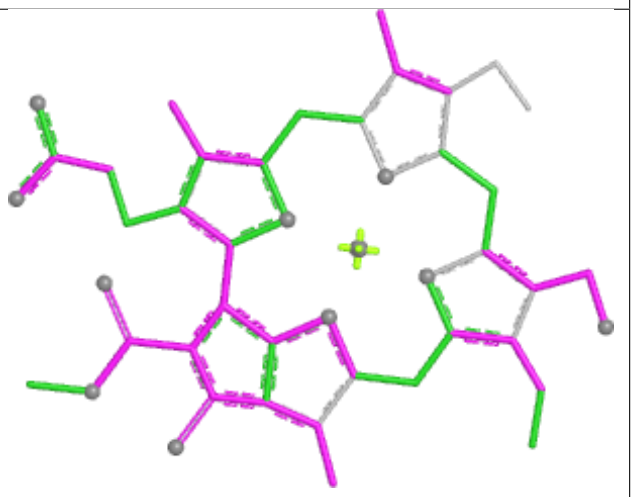
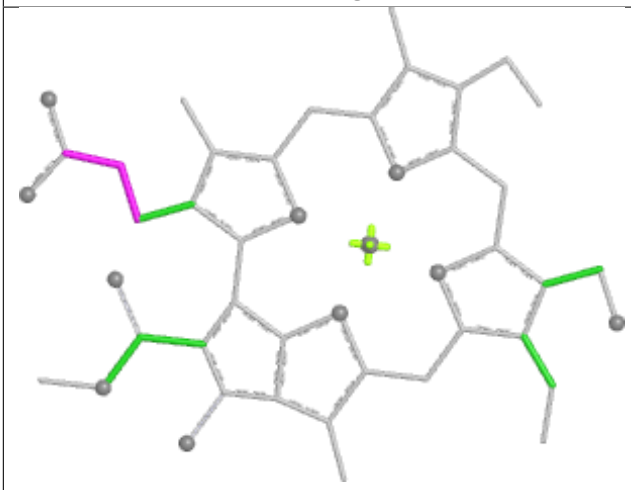


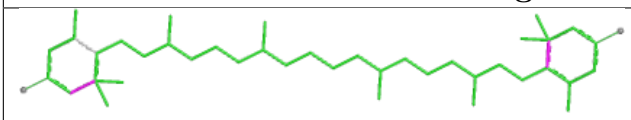
Bond angles



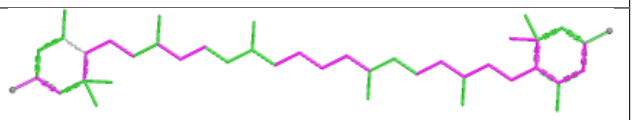
Torsions

Rings

Ligand LUT V 1621

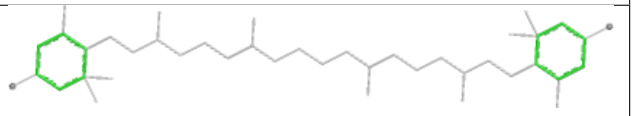


Bond lengths



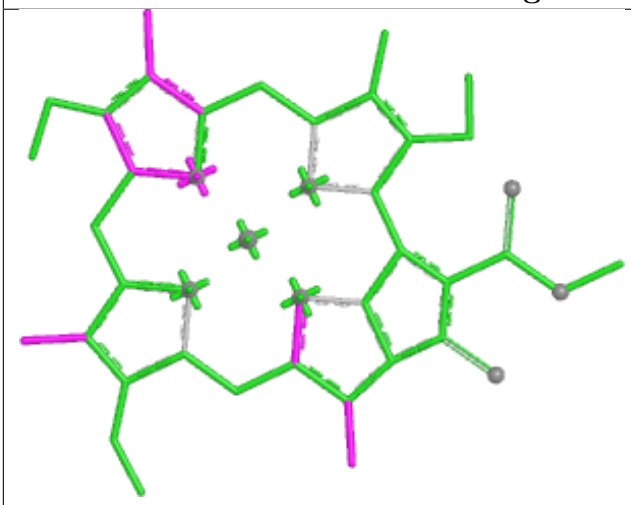
Bond angles

Torsions

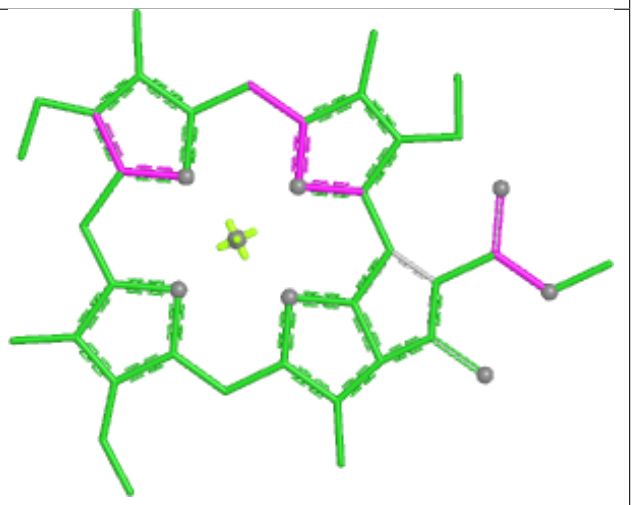


Rings

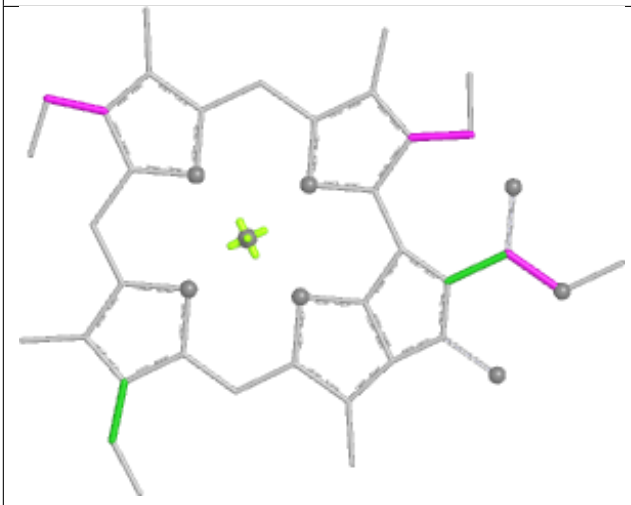
Ligand CLA U 614



Bond lengths



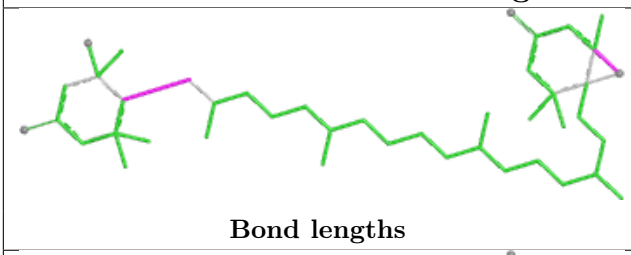
Bond angles



Torsions

Rings

Ligand NEX U 1623



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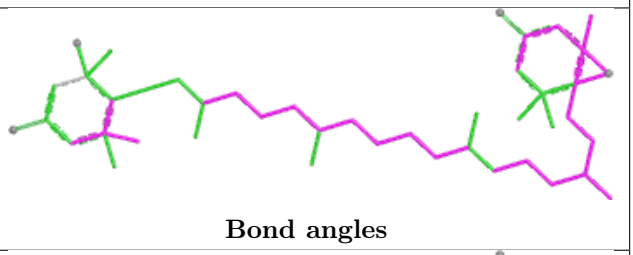
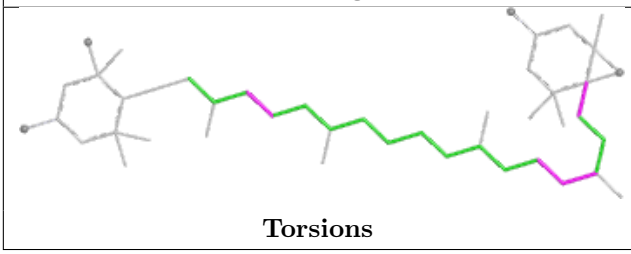


Bond angles



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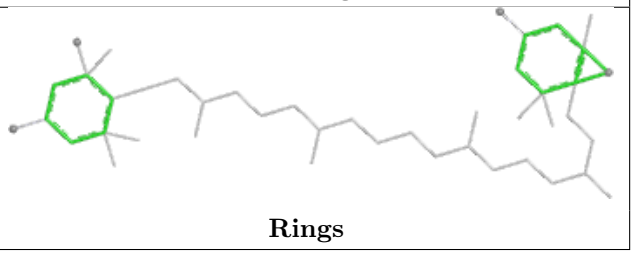
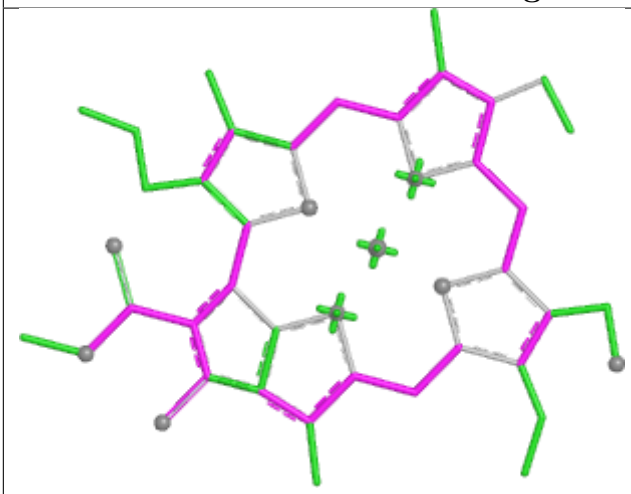


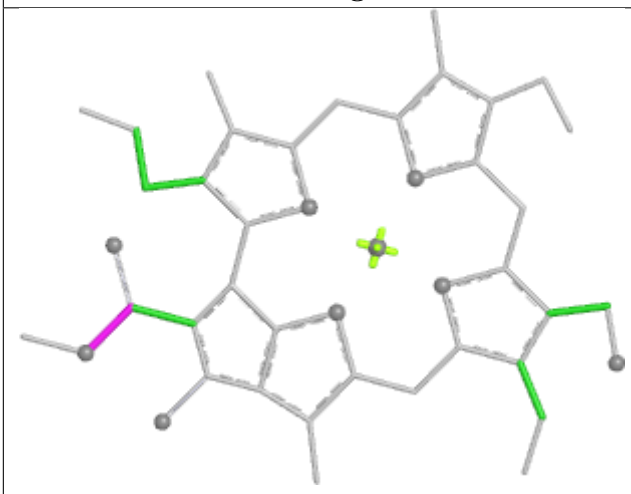
Rings

Ligand CHL V 606

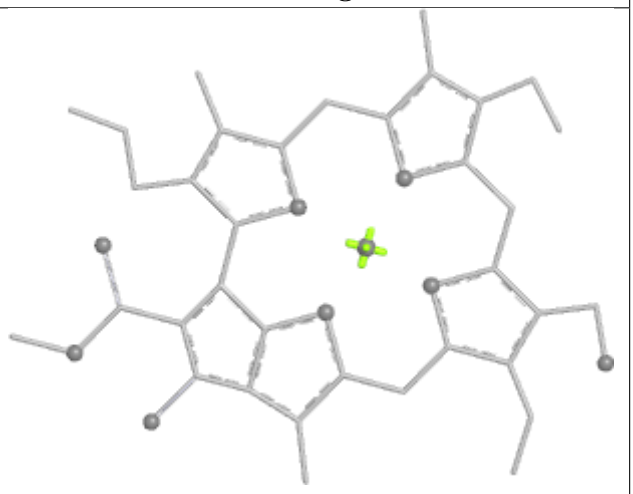


Bond lengths

Bond angles

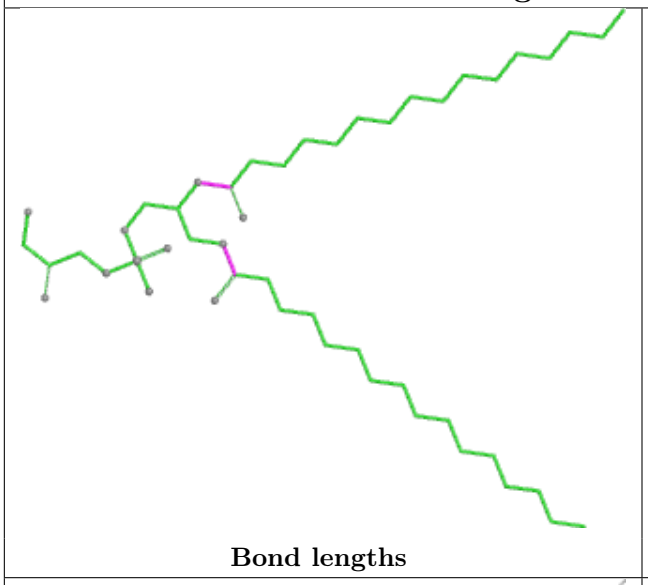


Torsions



Rings

Ligand LHG U 2630



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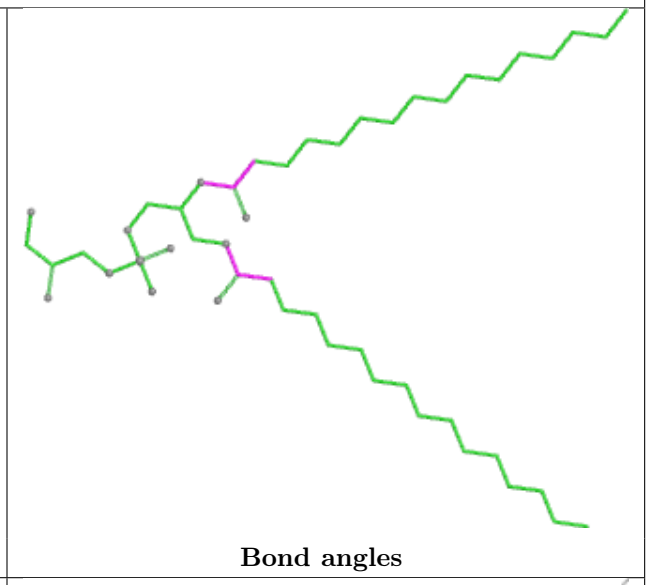
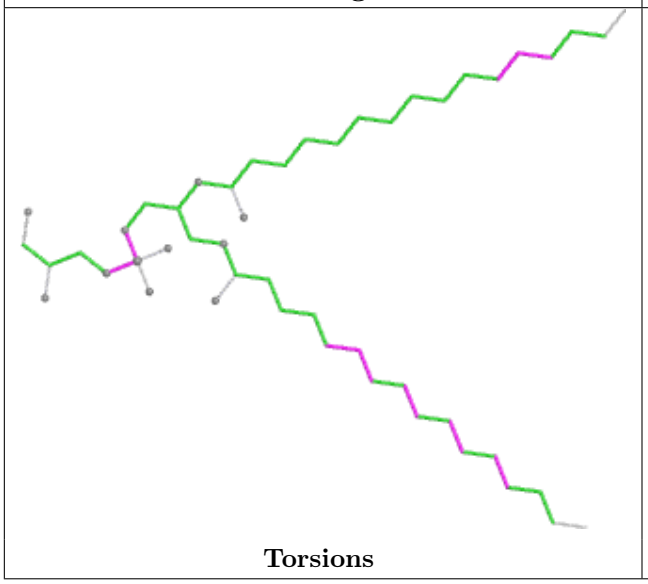
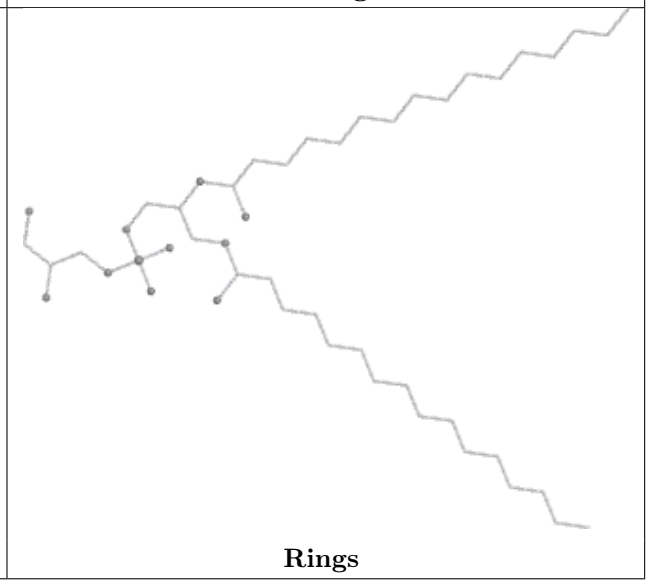


Bond angles

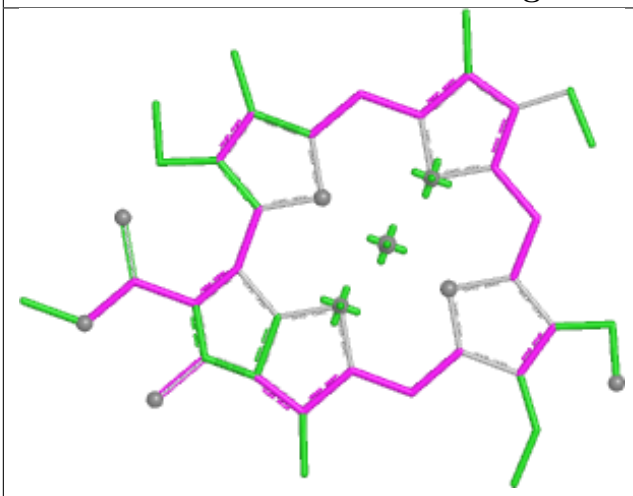


Torsions



Rings

Ligand CHL U 605



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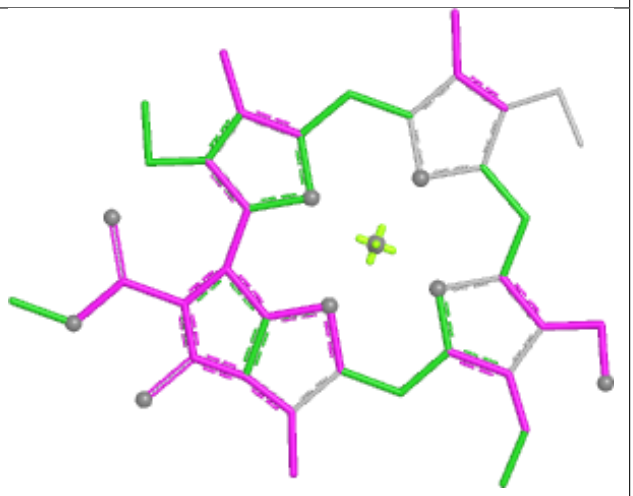
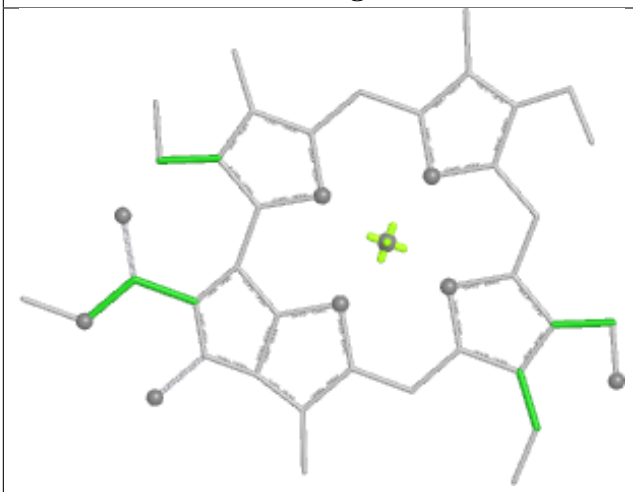
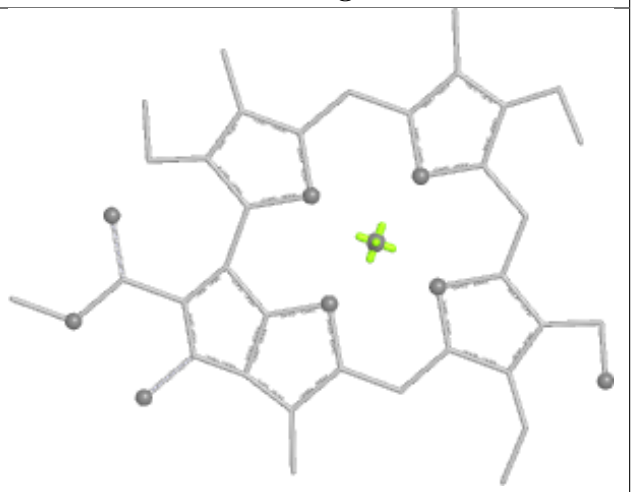


Bond angles

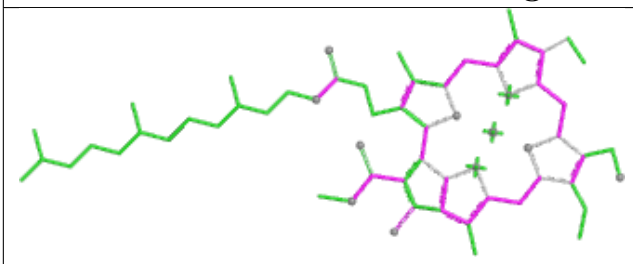


Torsions



Rings

Ligand CHL V 609



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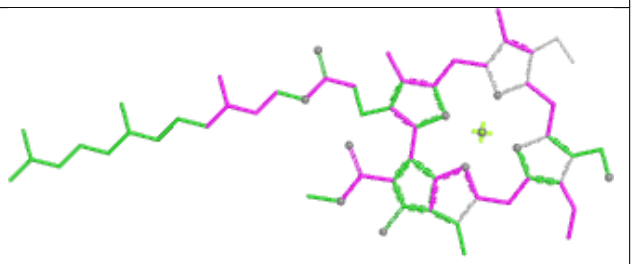
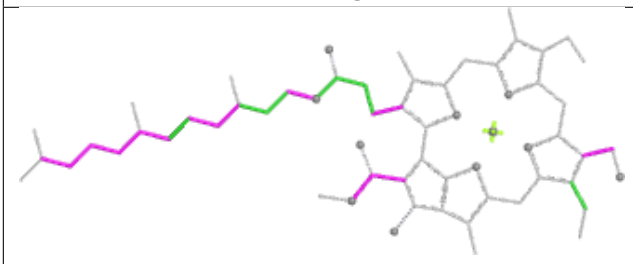
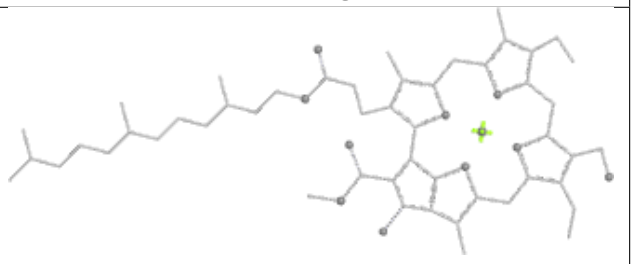


Bond angles



Torsions



Rings

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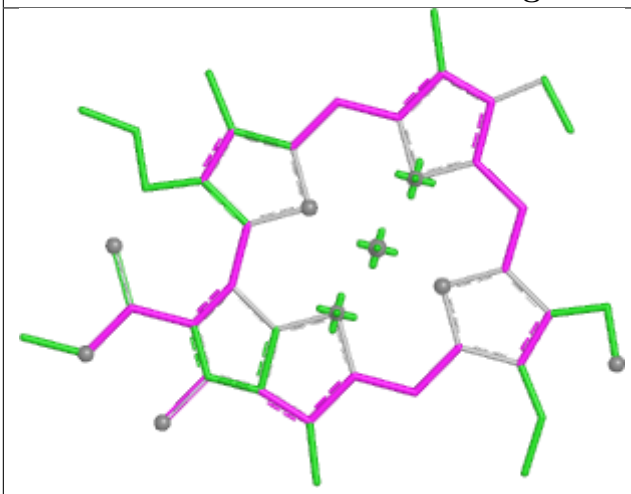

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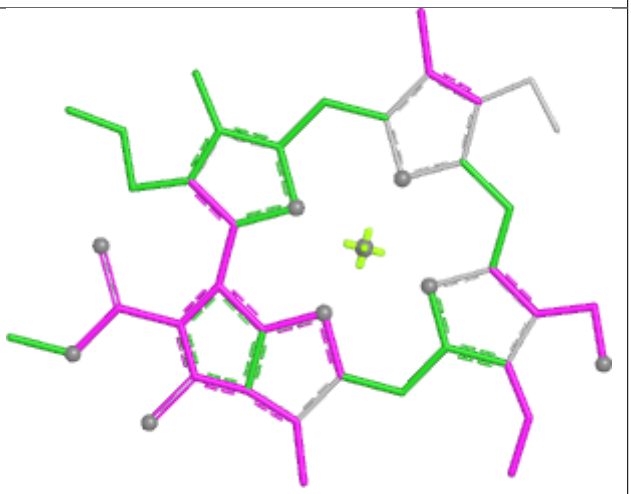
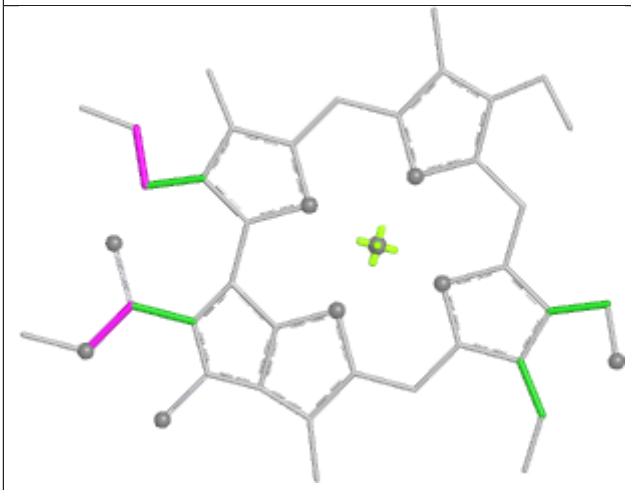
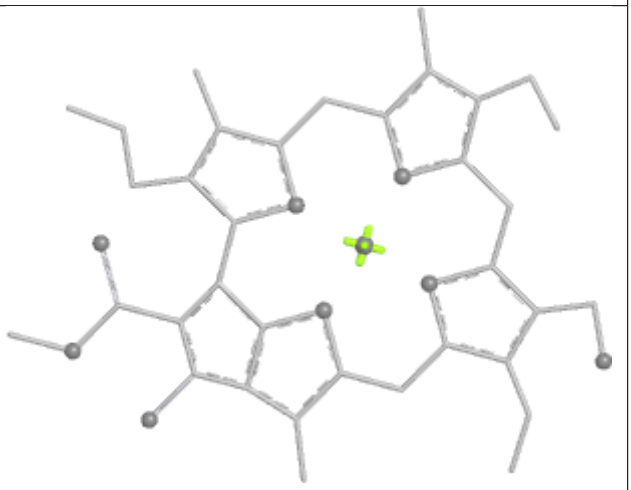


Bond angles

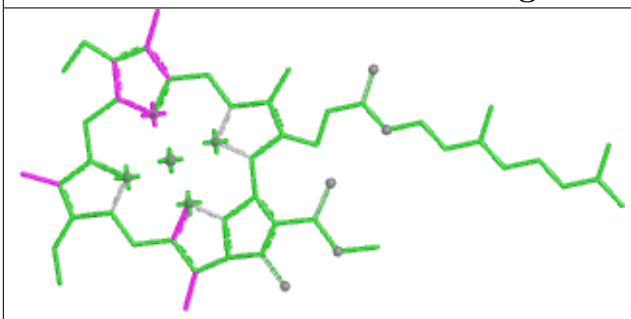


Torsions



Rings

Ligand CLA W 610



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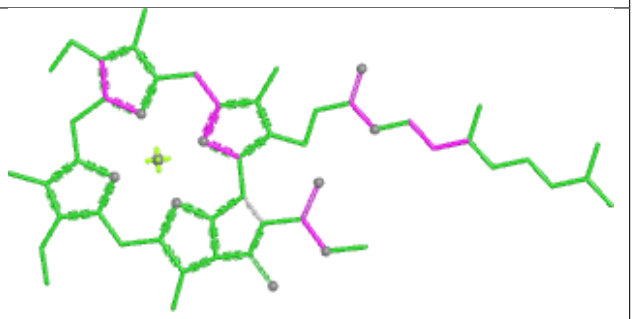
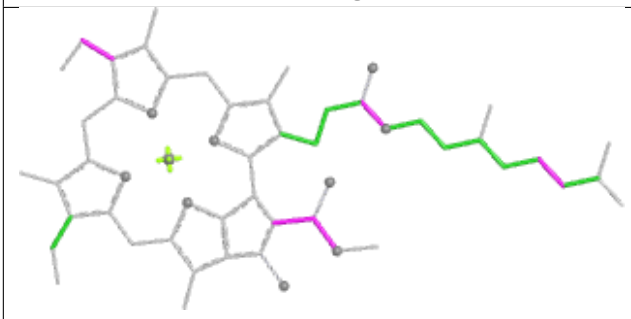
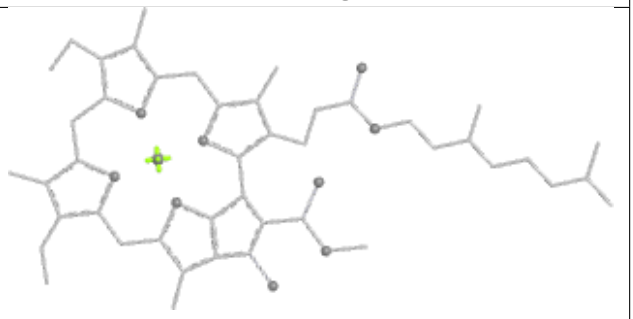


Bond angles

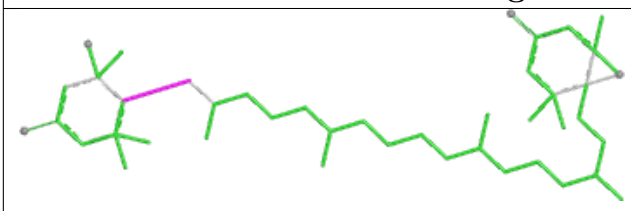


Torsions

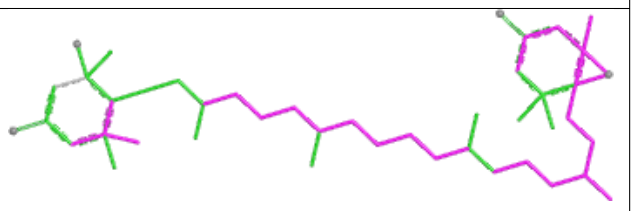


Rings

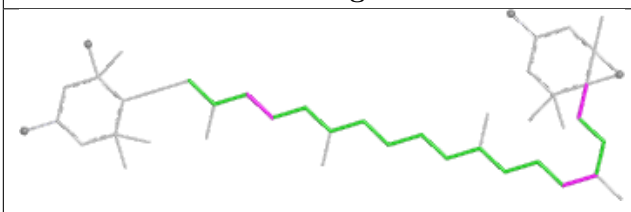
Ligand NEX W 1623



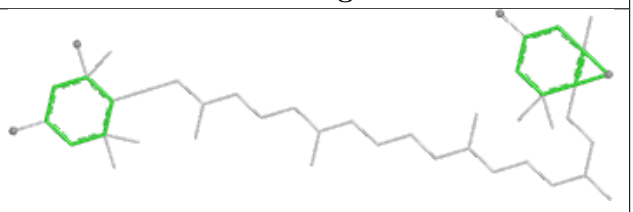
Bond lengths



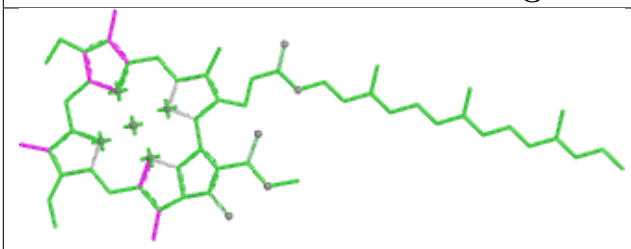
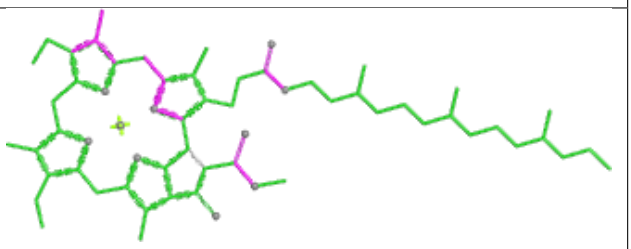
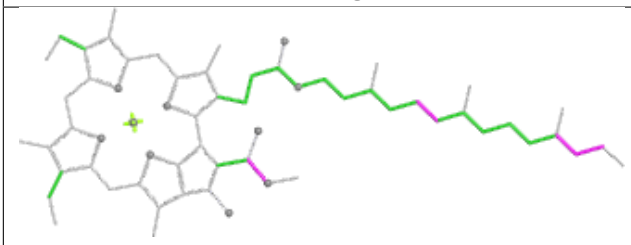
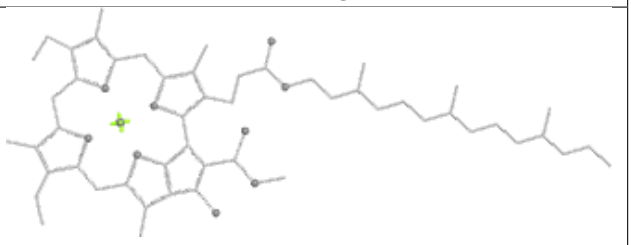
Bond angles

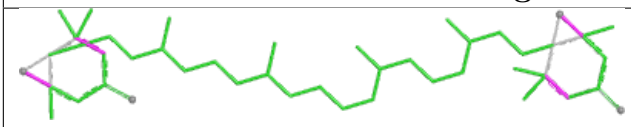
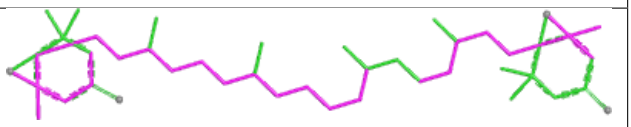
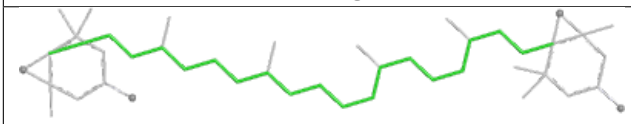
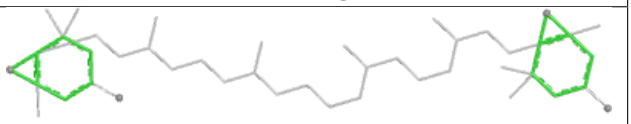


Torsions

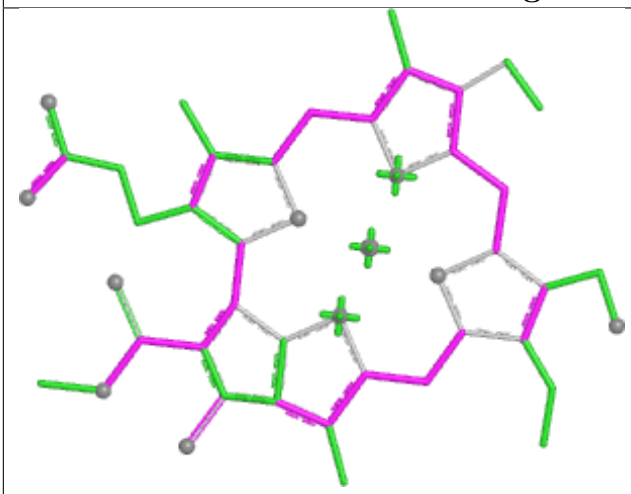


Rings

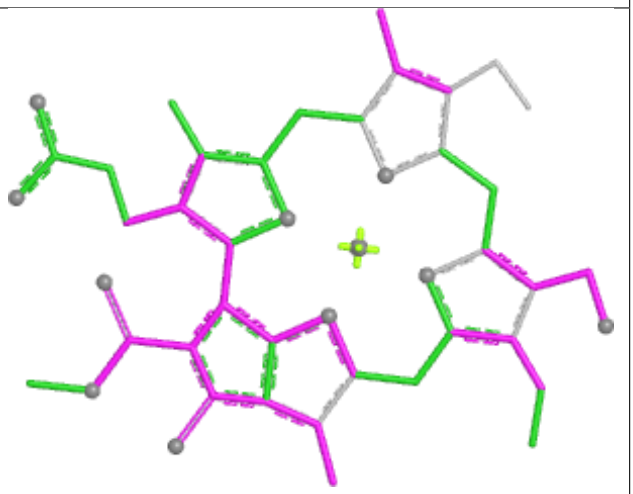
Ligand CLA V 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT V 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

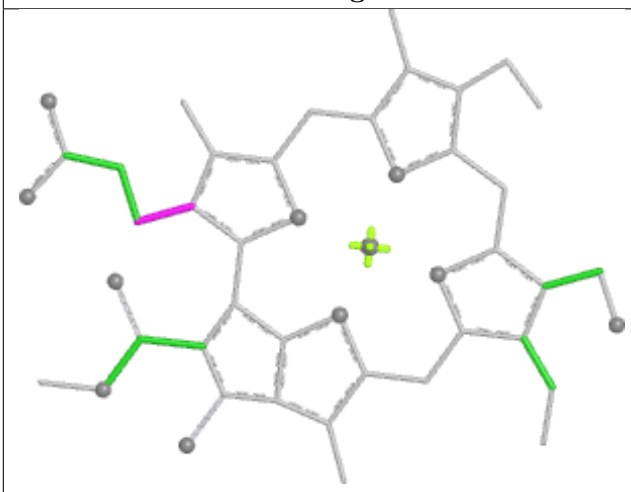
Ligand CHL V 607



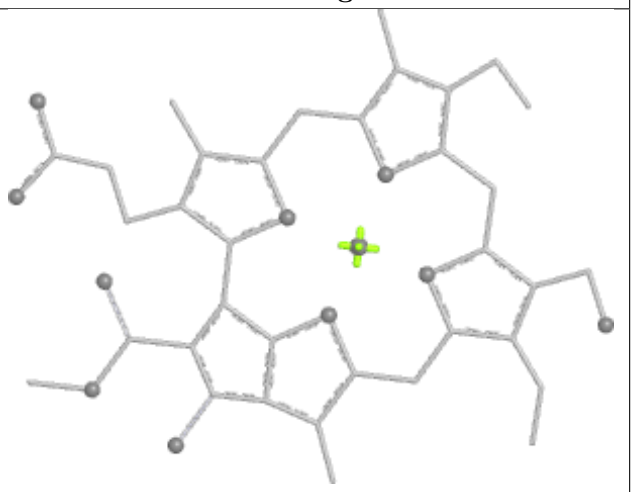
Bond lengths



Bond angles

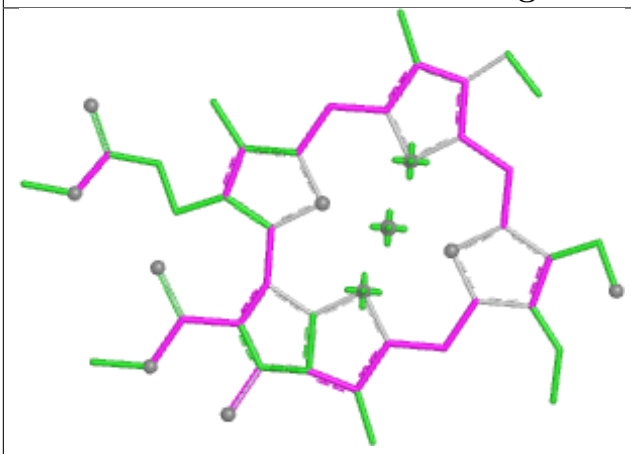


Torsions

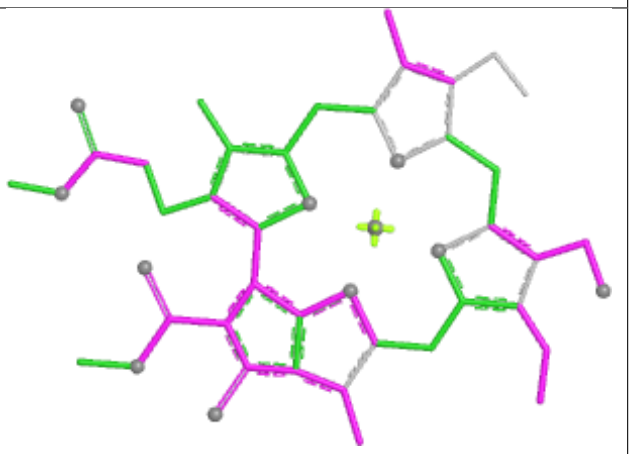


Rings

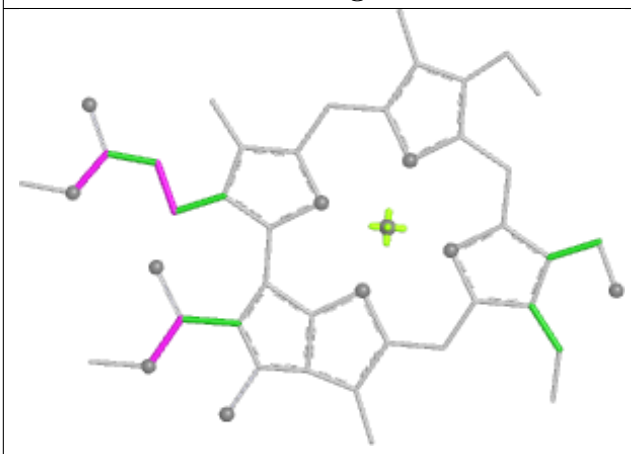
Ligand CHL W 608



Bond lengths



Bond angles



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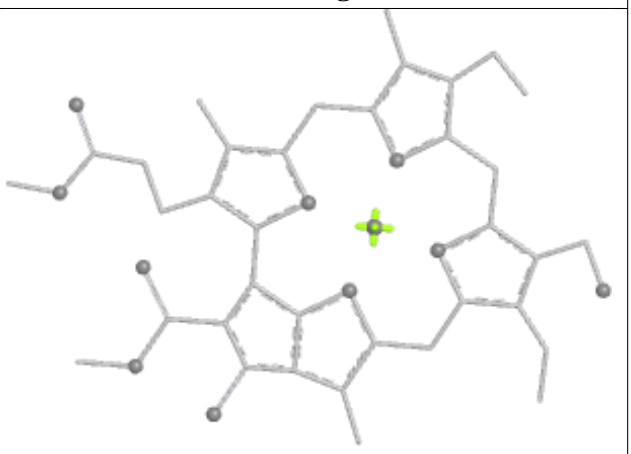
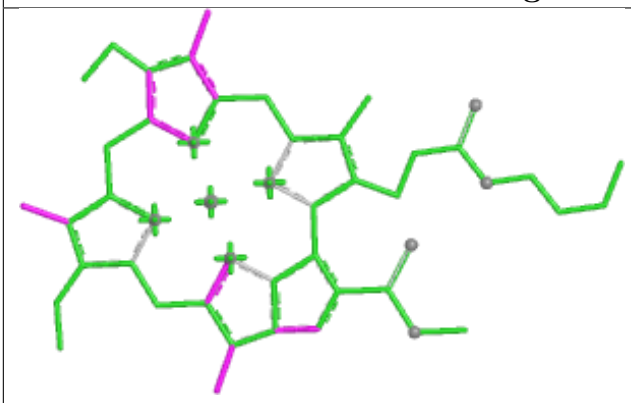
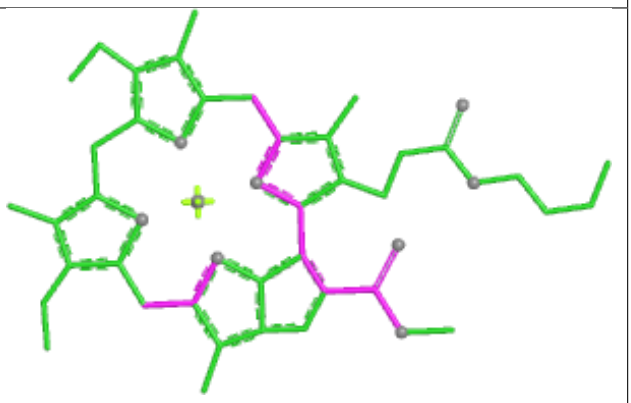


Rings

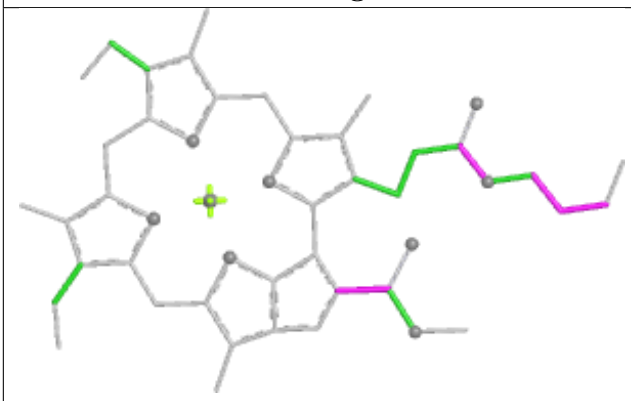
Ligand CLA U 604



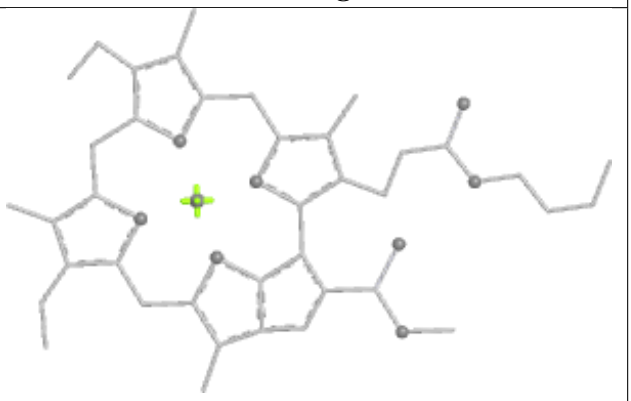
Bond lengths



Bond angles



Torsions

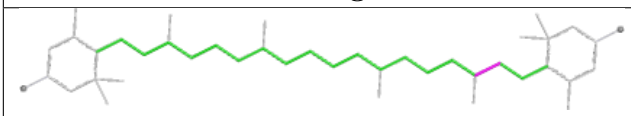


Rings

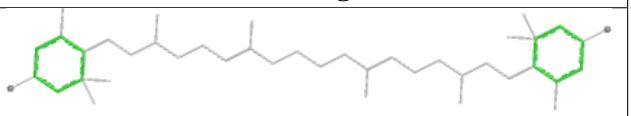
Ligand LUT W 1621

Bond lengths

Bond angles

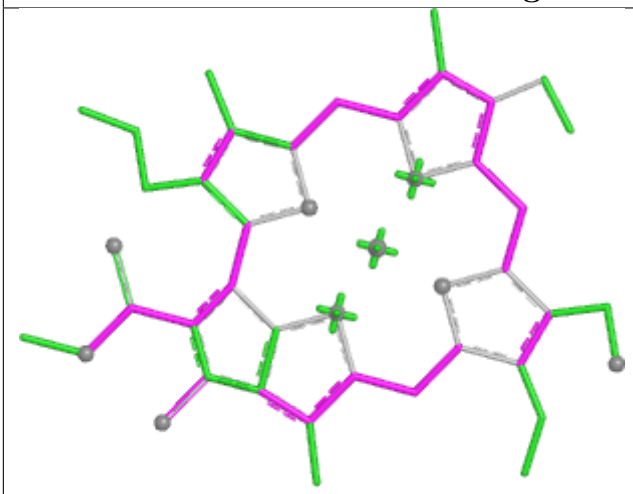


Torsions

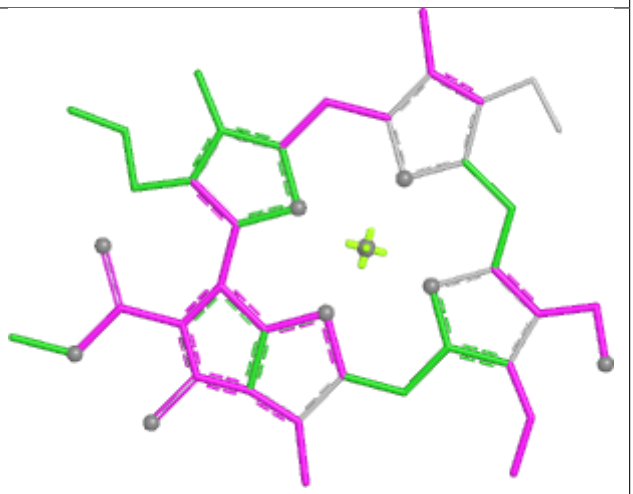


Rings

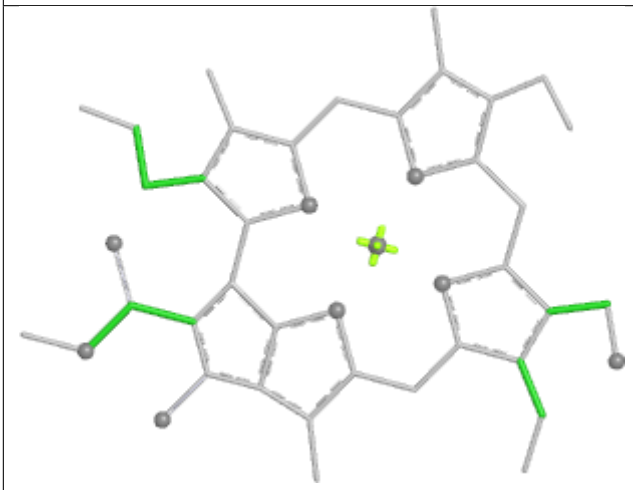
Ligand CHL U 606



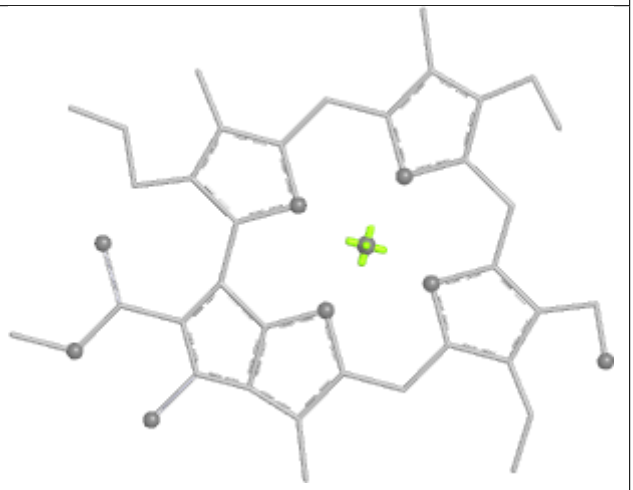
Bond lengths



Bond angles

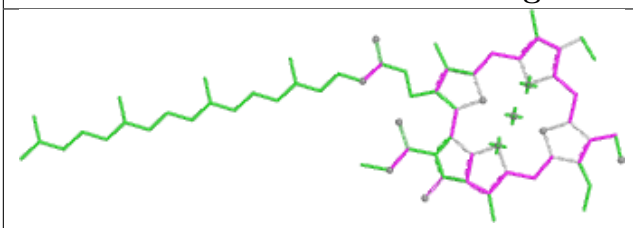


Torsions

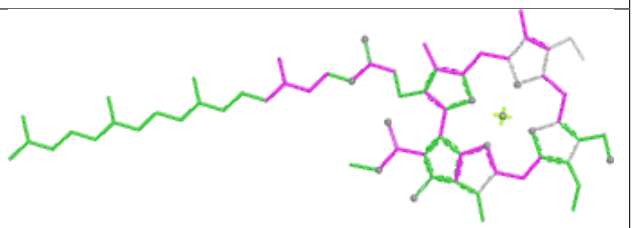


Rings

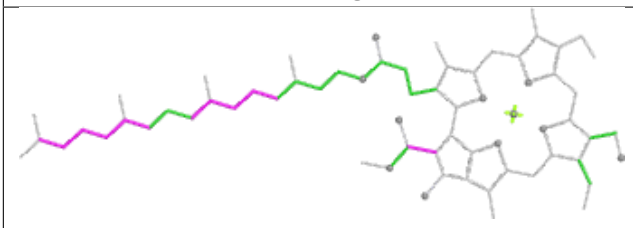
Ligand CHL V 601



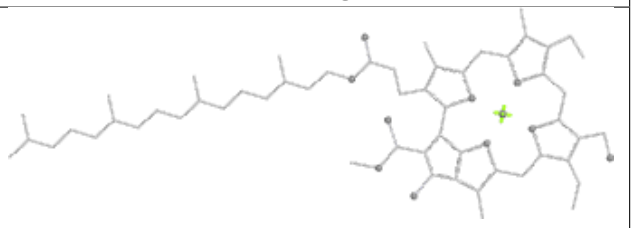
Bond lengths



Bond angles

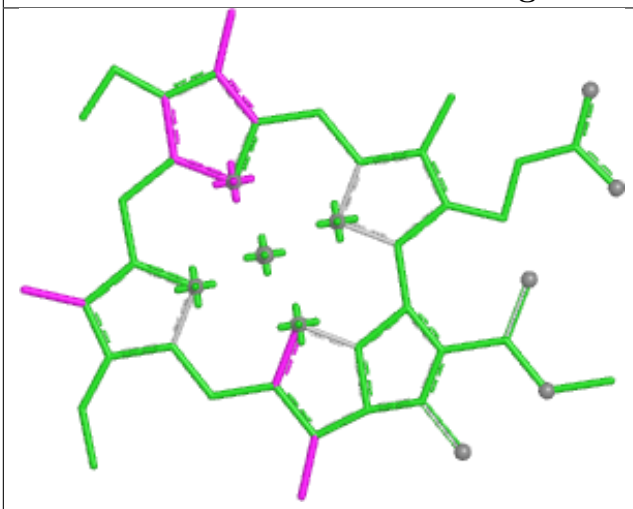


Torsions

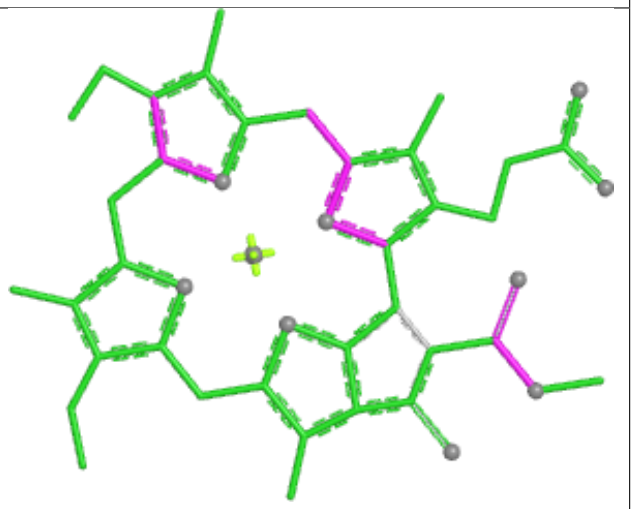


Rings

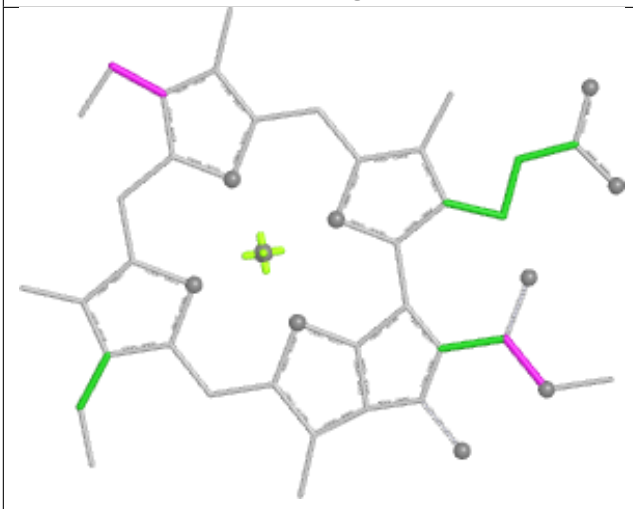
Ligand CLA W 614



Bond lengths



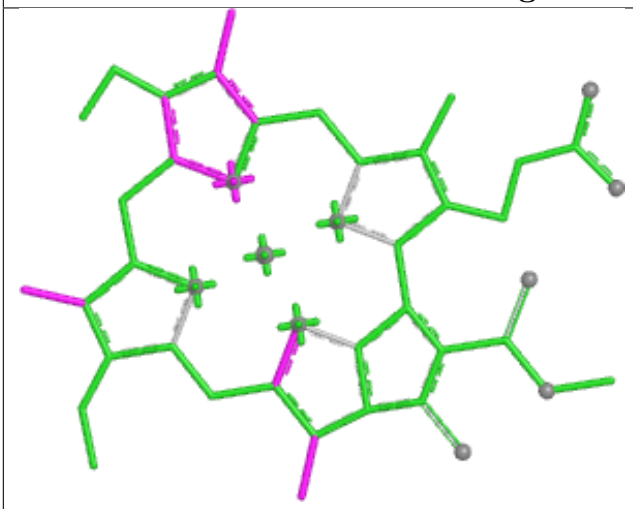
Bond angles



Torsions

Rings

Ligand CLA W 612



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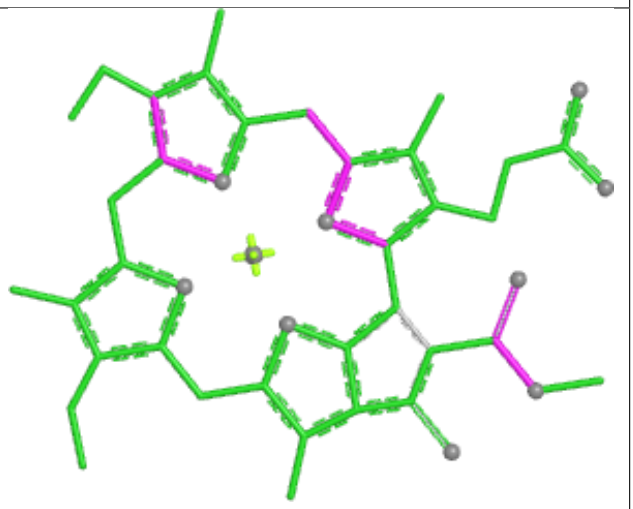
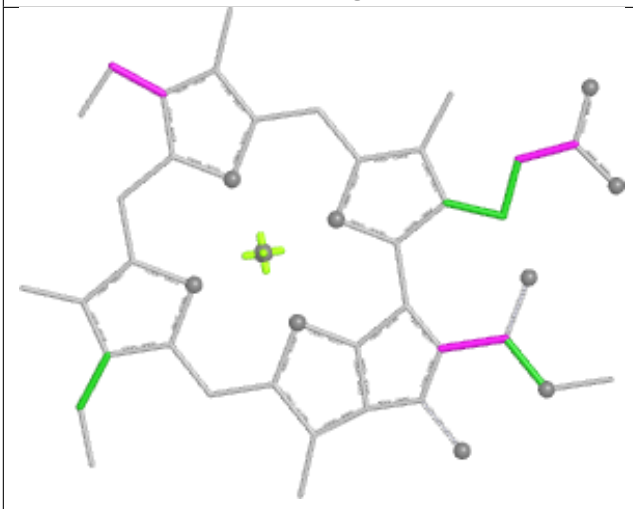


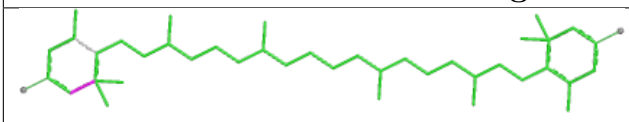
Bond angles



Torsions

Rings

Ligand LUT W 1620



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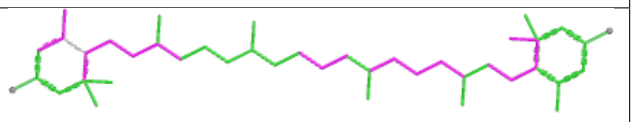
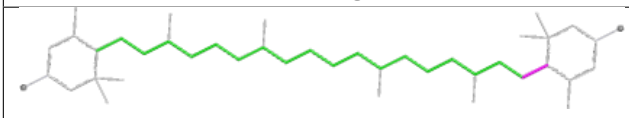
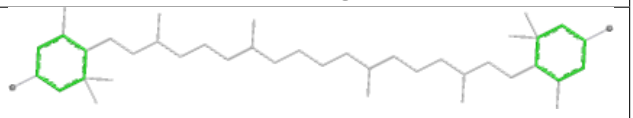


Bond angles

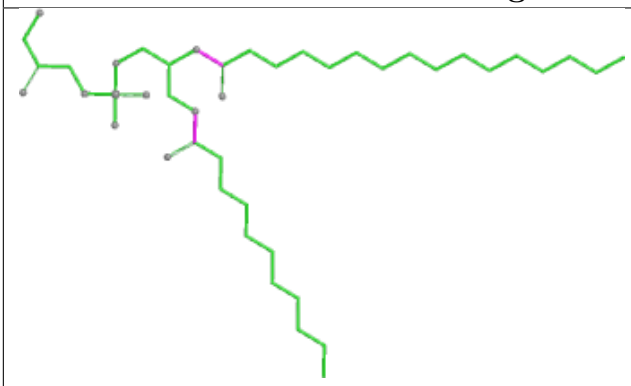


Torsions

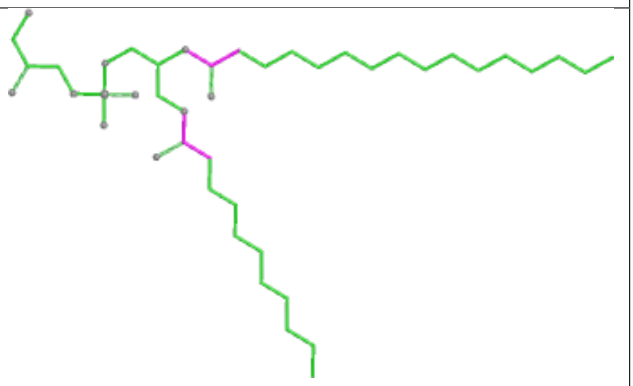


Rings

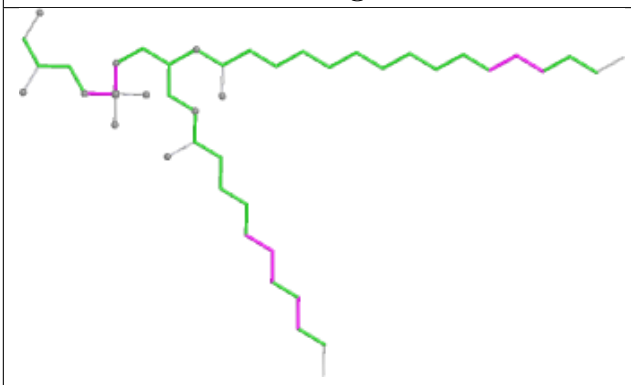
Ligand LHG W 2630



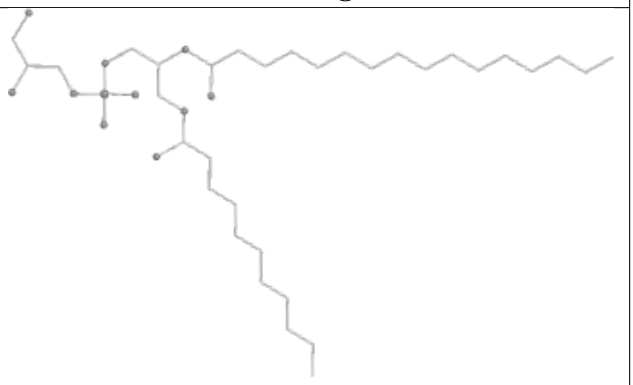
Bond lengths



Bond angles

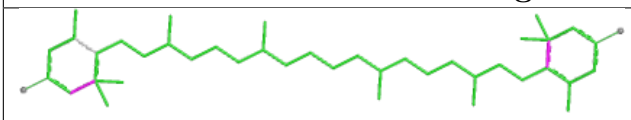


Torsions

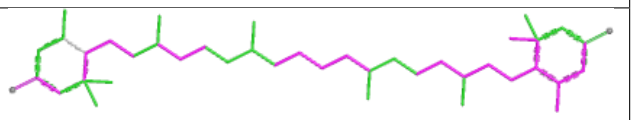


Rings

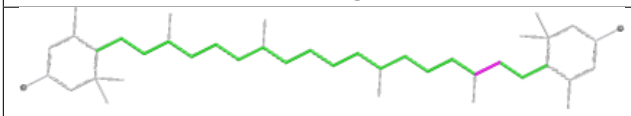
Ligand LUT U 1621



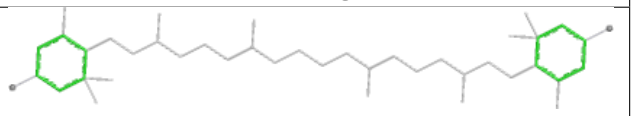
Bond lengths



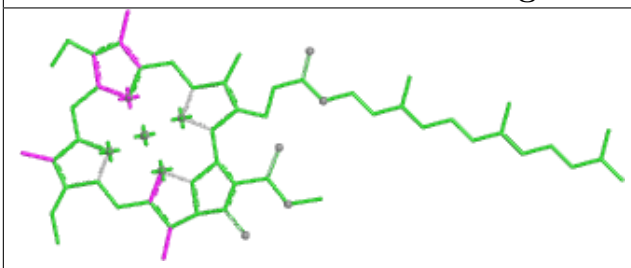
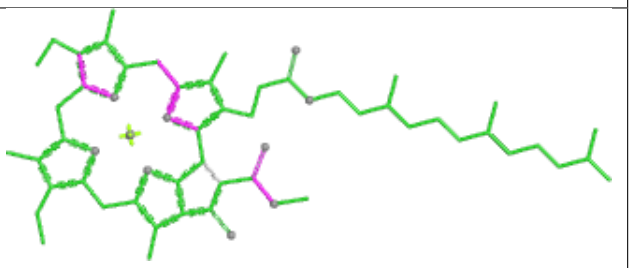
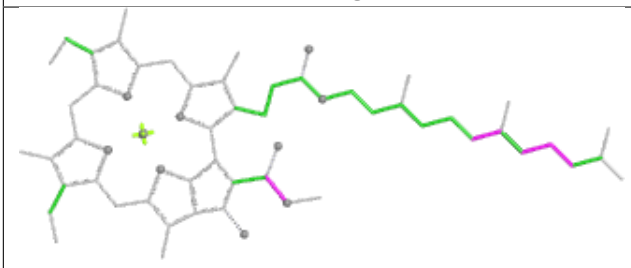
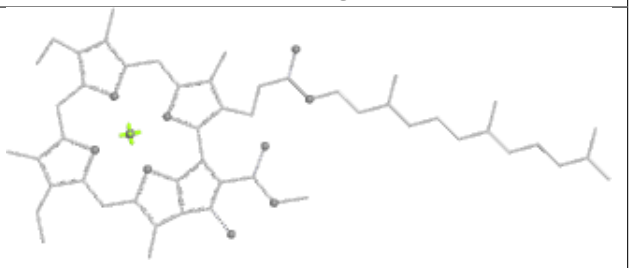
Bond angles

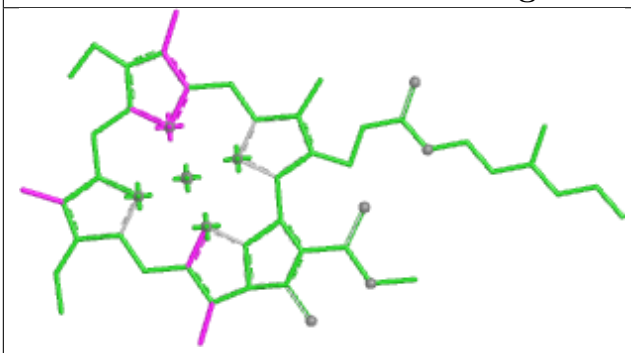
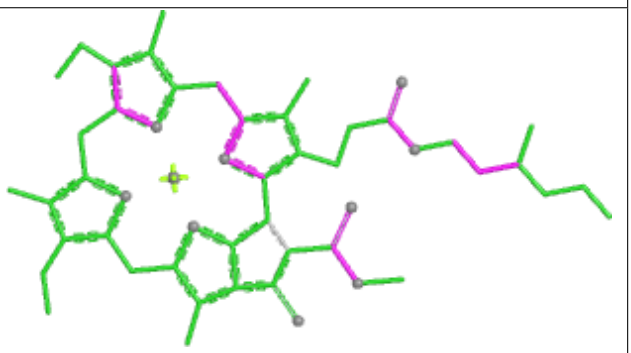
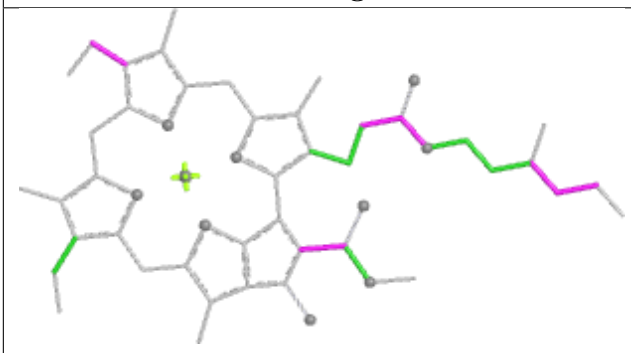
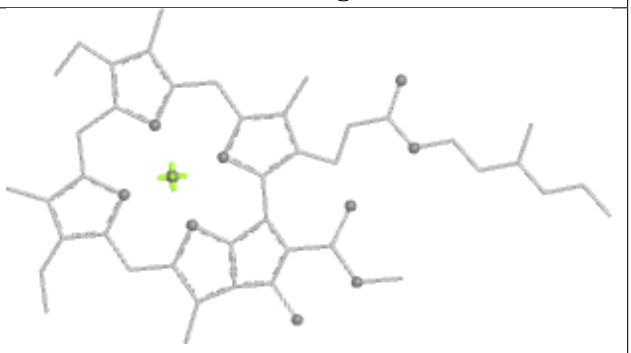


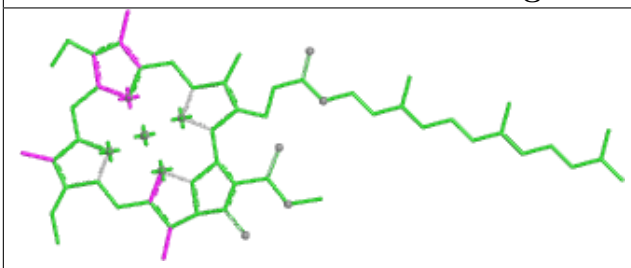
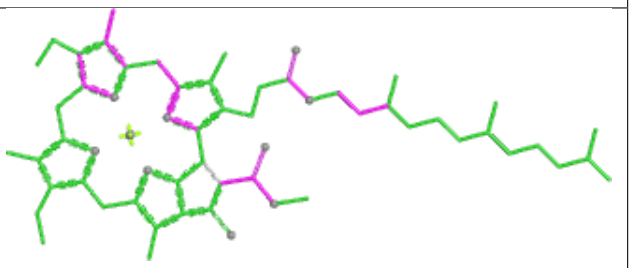
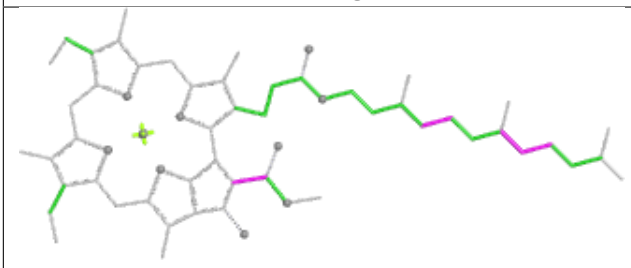
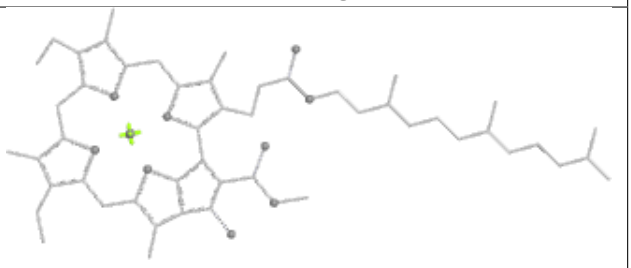
Torsions

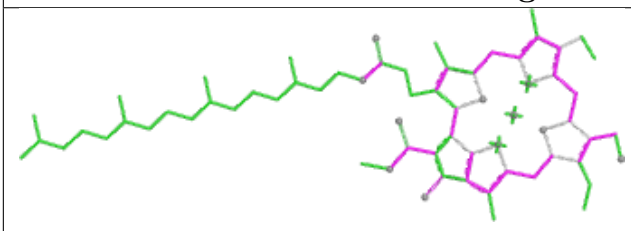
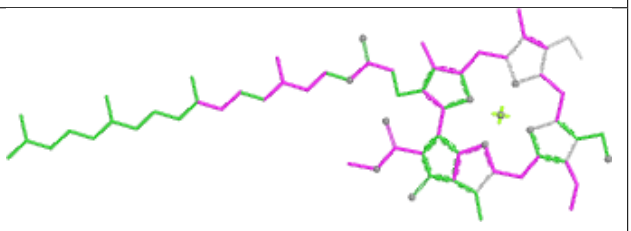
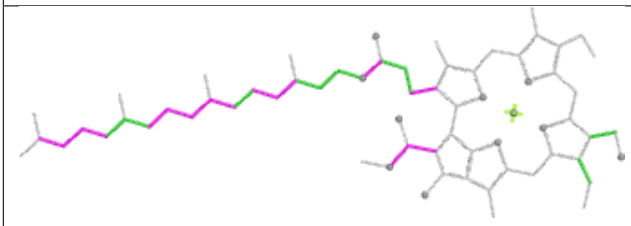
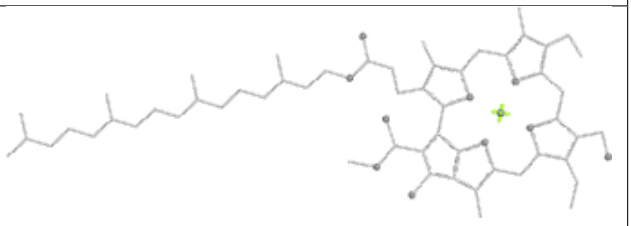


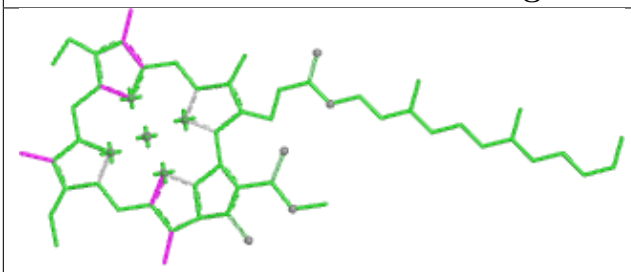
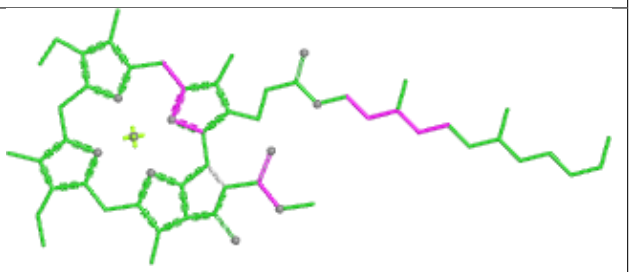
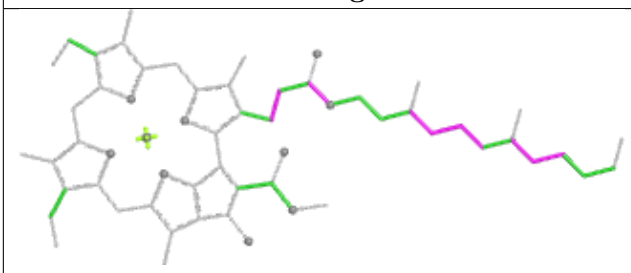
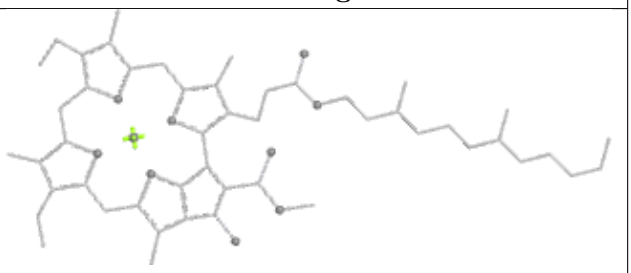
Rings

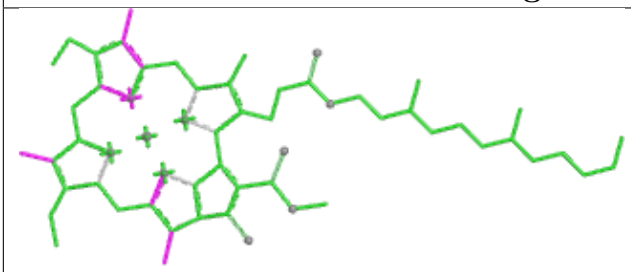
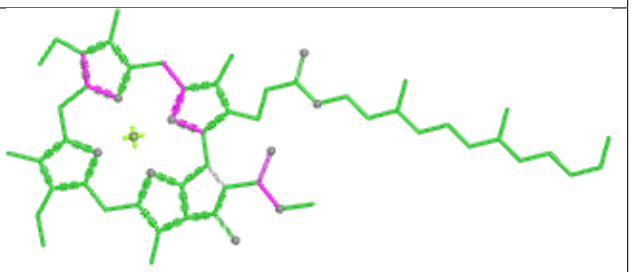
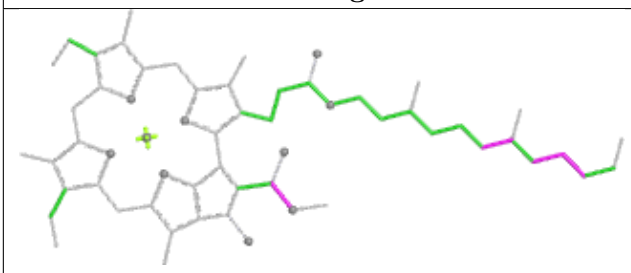
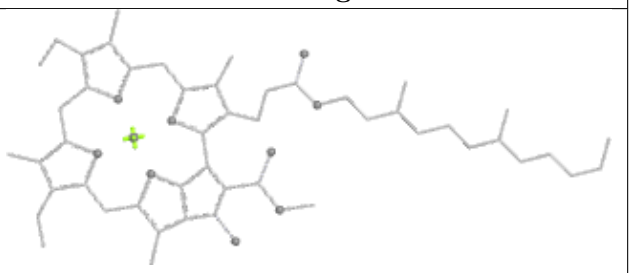
Ligand CLA W 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

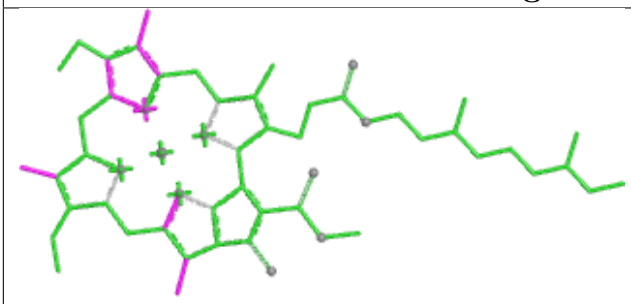
Ligand CLA V 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL W 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

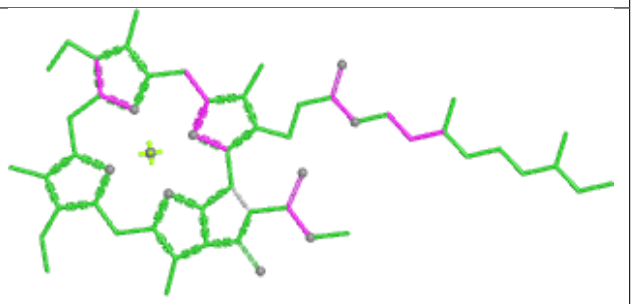
Ligand CLA U 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA U 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

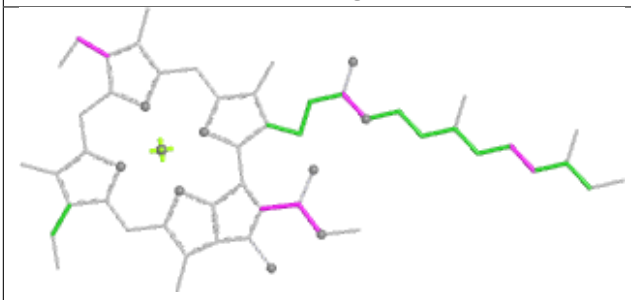
Ligand CLA U 610



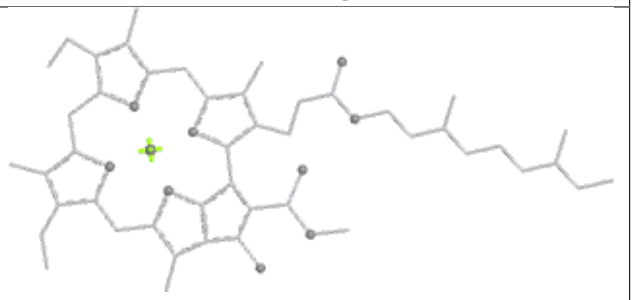
Bond lengths



Bond angles

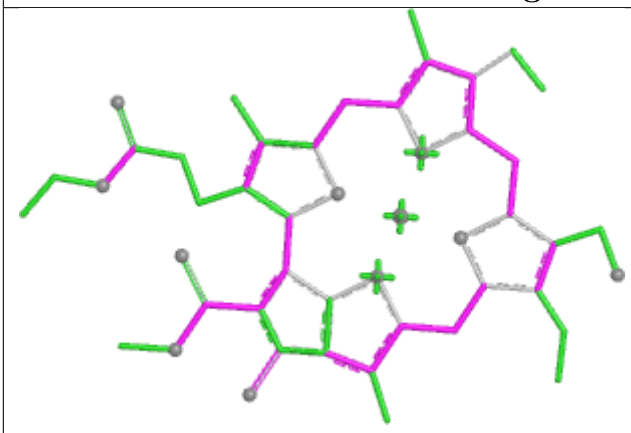


Torsions

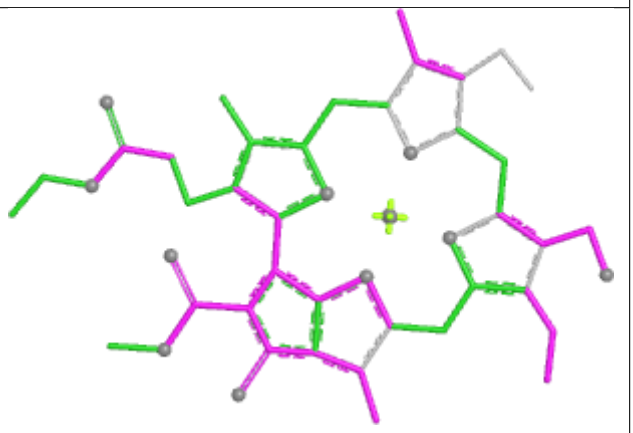


Rings

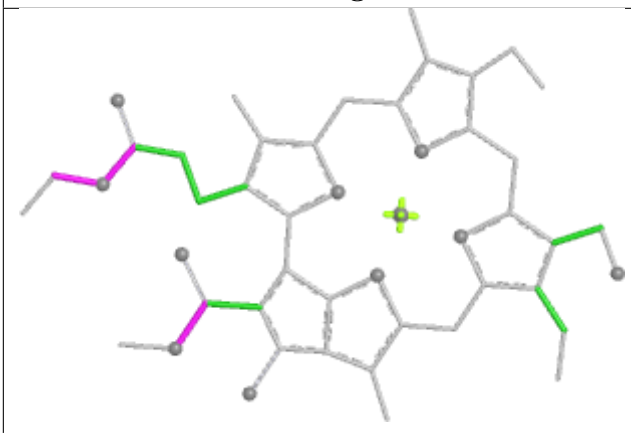
Ligand CHL V 608



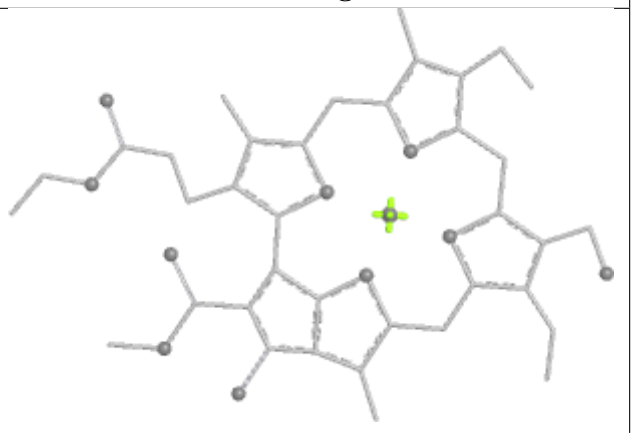
Bond lengths



Bond angles

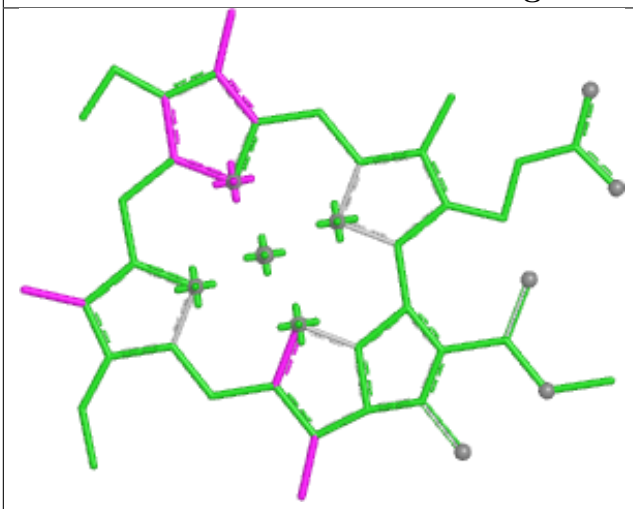


Torsions

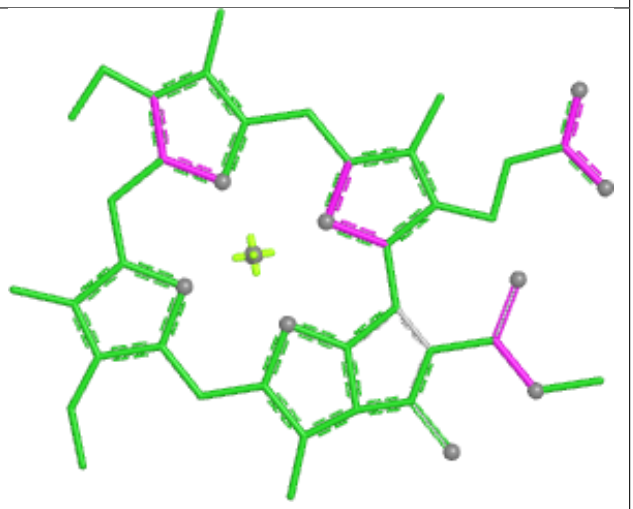


Rings

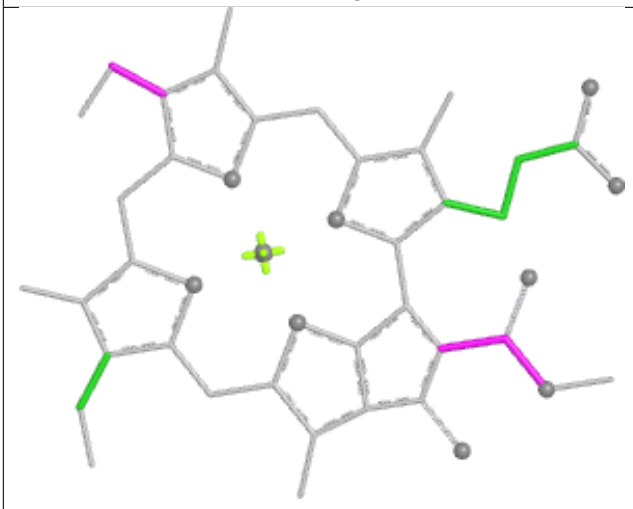
Ligand CLA V 614



Bond lengths



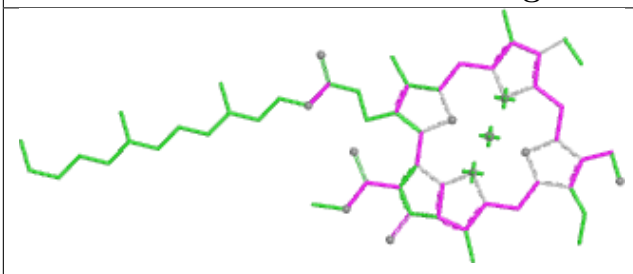
Bond angles



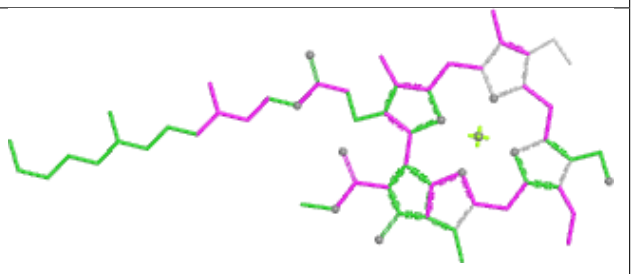
Torsions

Rings

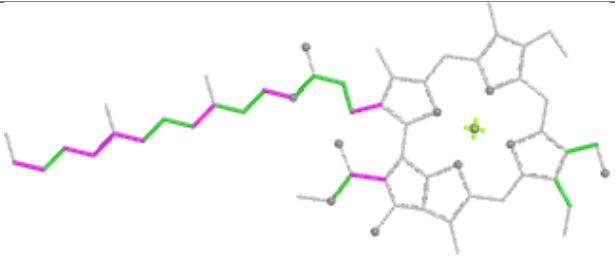
Ligand CHL U 609



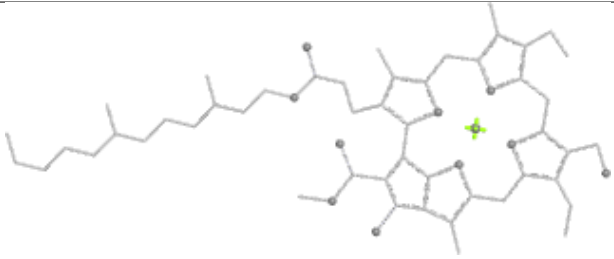
Bond lengths



Bond angles

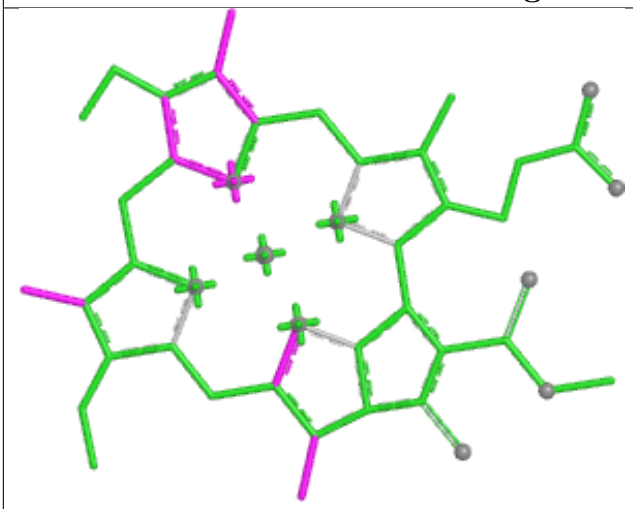


Torsions

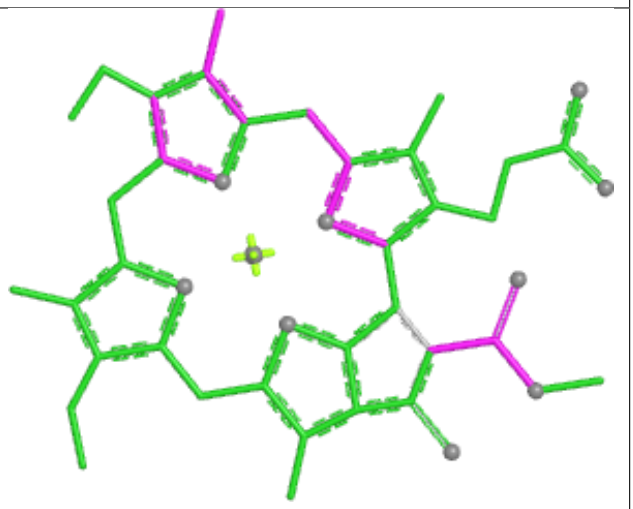


Rings

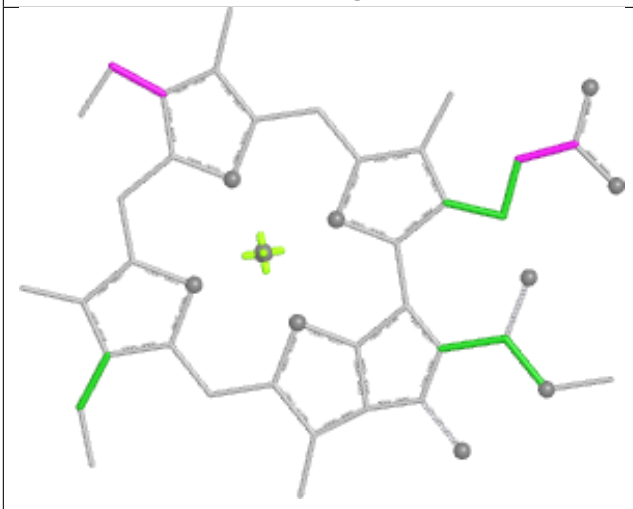
Ligand CLA V 612



Bond lengths



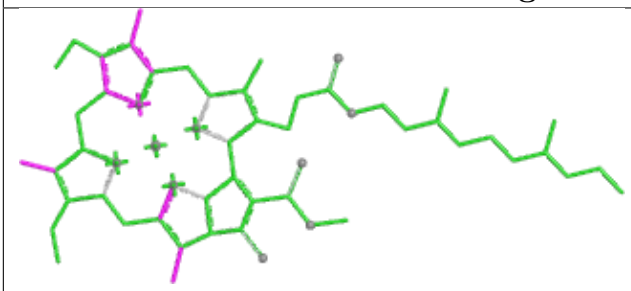
Bond angles



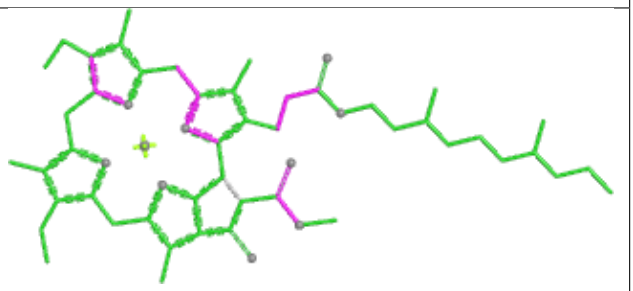
Torsions

Rings

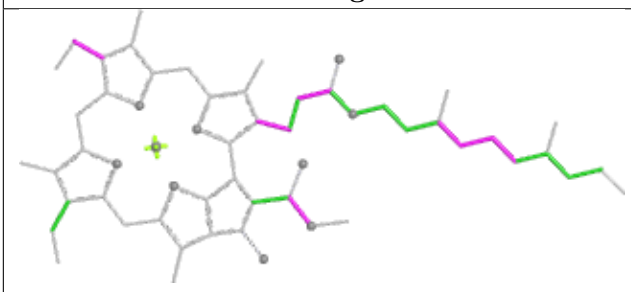
Ligand CLA W 611



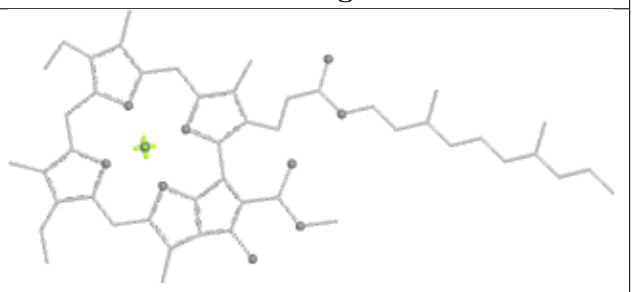
Bond lengths



Bond angles



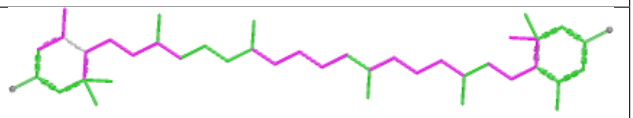
Torsions



Rings

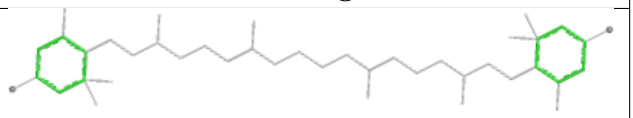
Ligand LUT U 1620

Bond lengths



Bond angles

Torsions

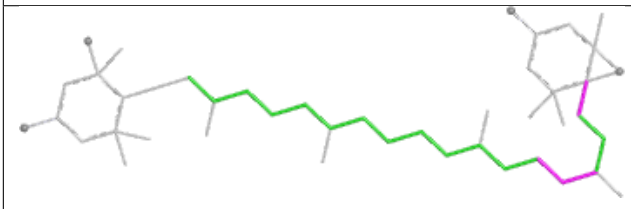


Rings

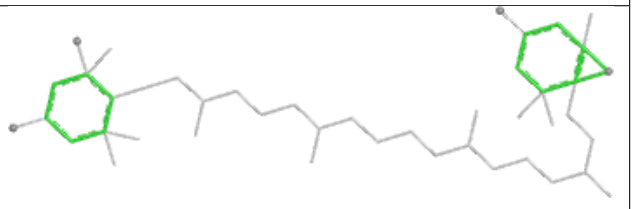
Ligand NEX V 1623

Bond lengths

Bond angles

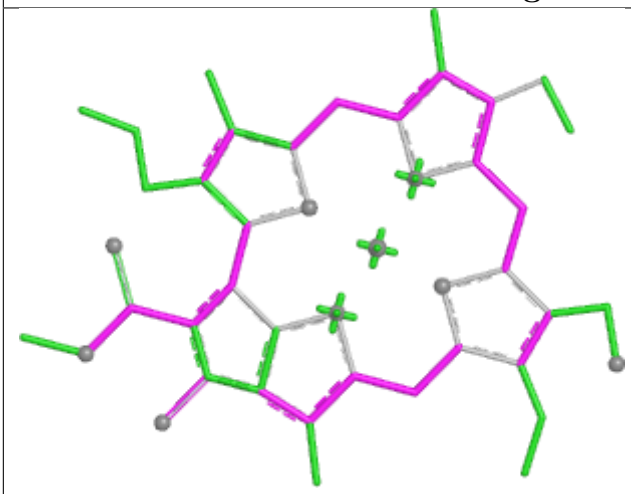


Torsions

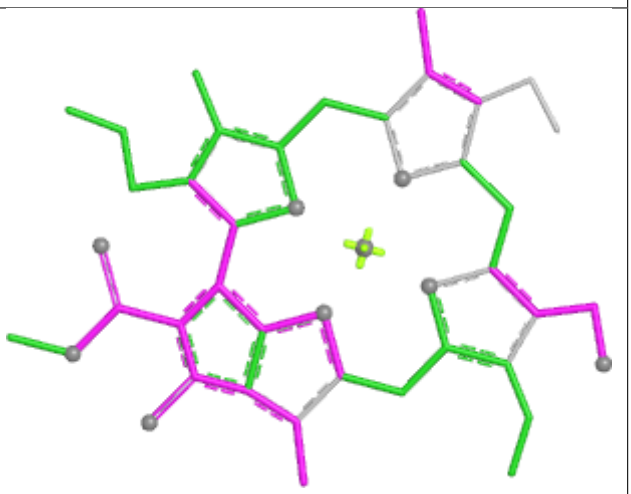


Rings

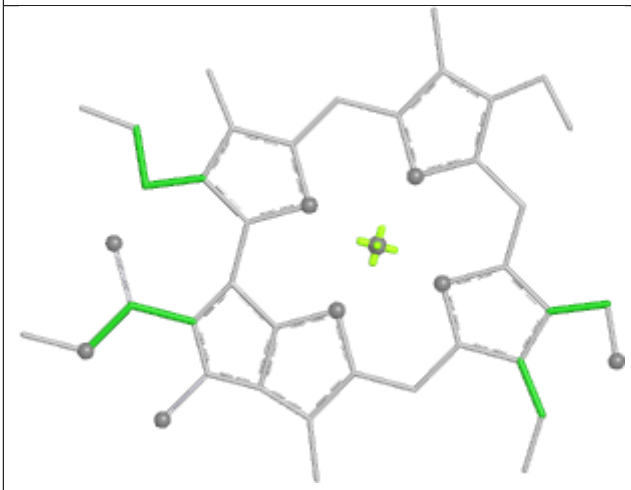
Ligand CHL V 605



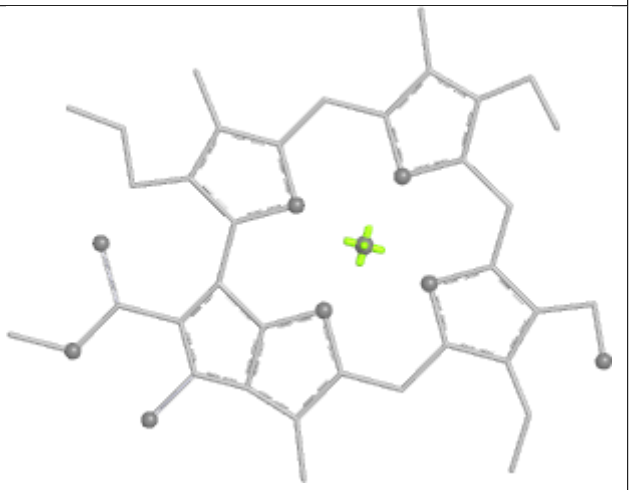
Bond lengths



Bond angles

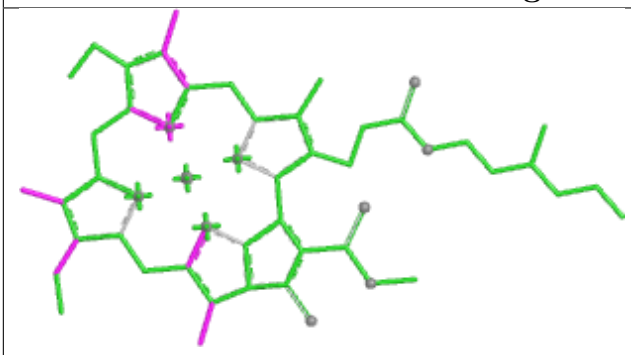


Torsions

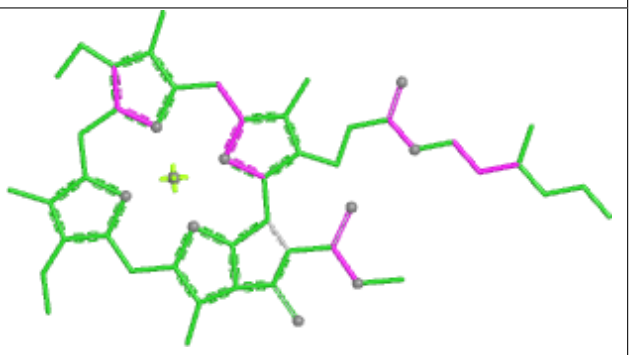


Rings

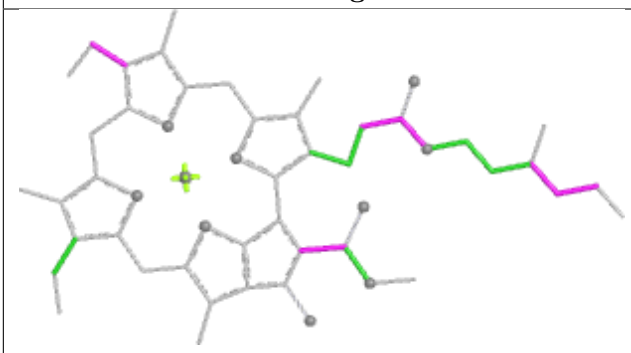
Ligand CLA U 603



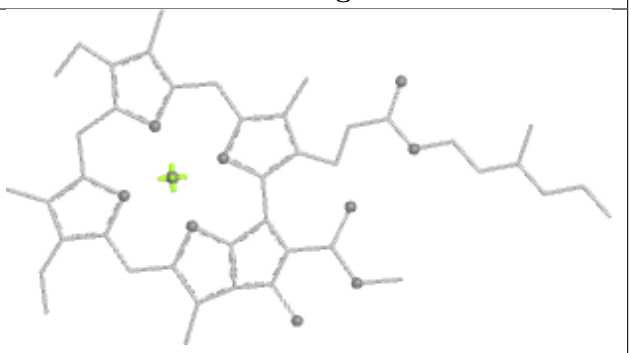
Bond lengths



Bond angles

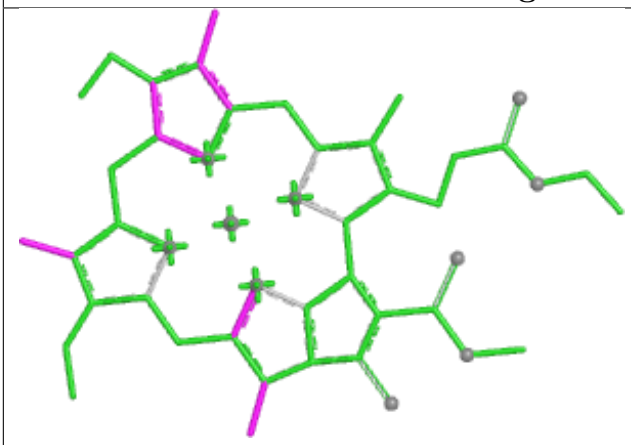


Torsions

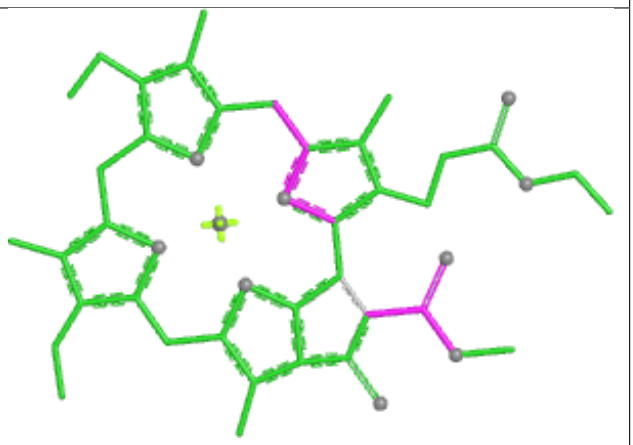


Rings

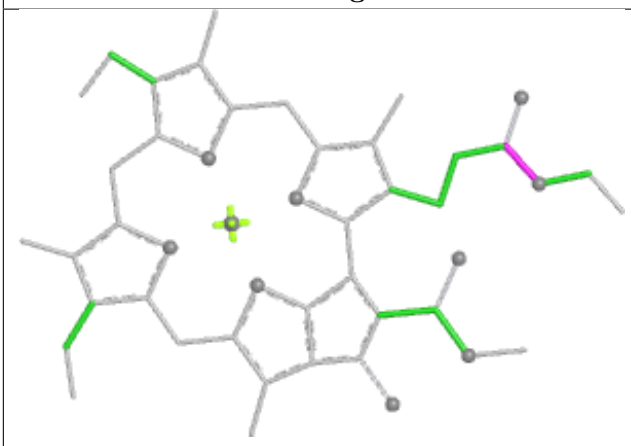
Ligand CLA W 604



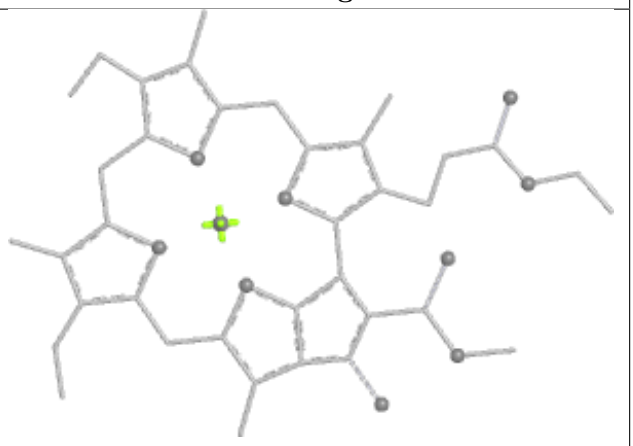
Bond lengths



Bond angles

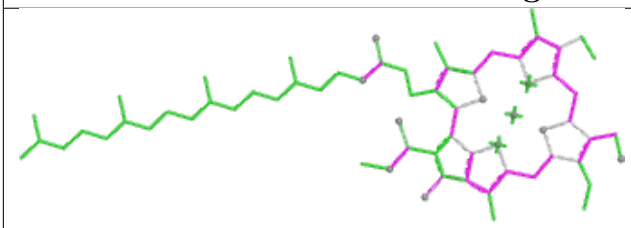


Torsions



Rings

Ligand CHL U 601



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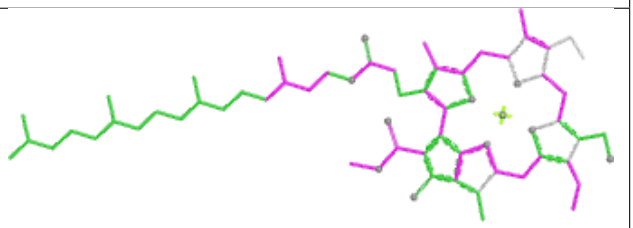
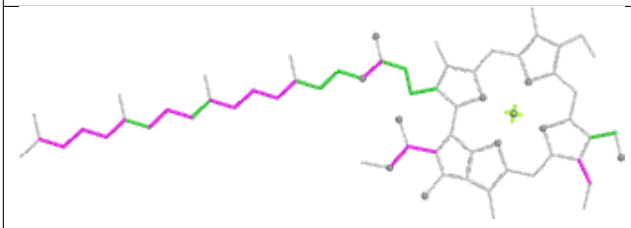
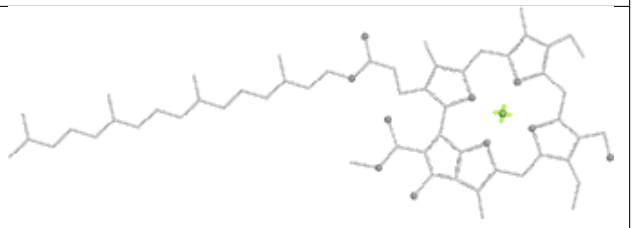


Bond angles

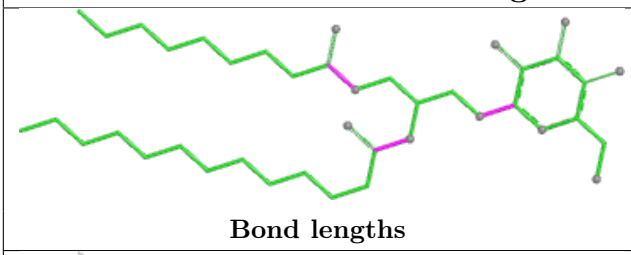


Torsions



Rings

Ligand LMG V 2631



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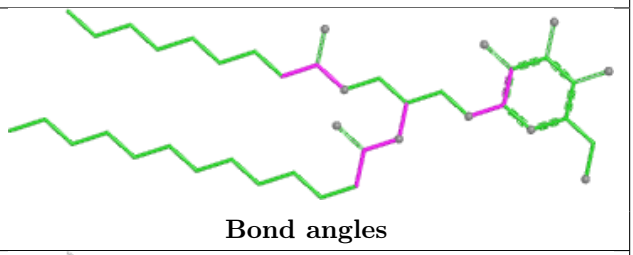
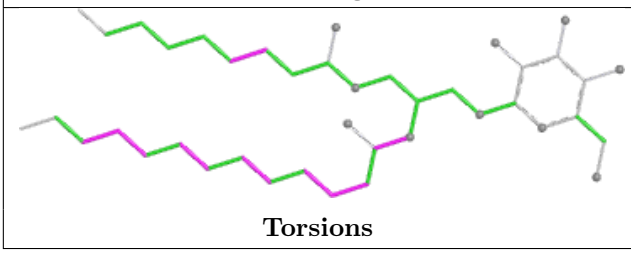
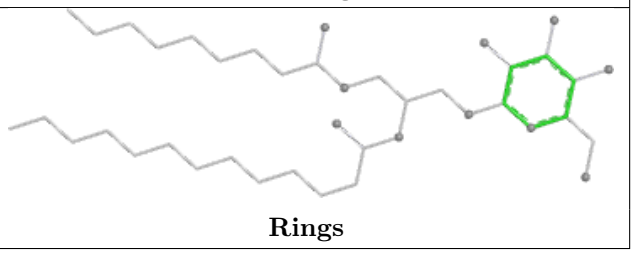


Bond angles

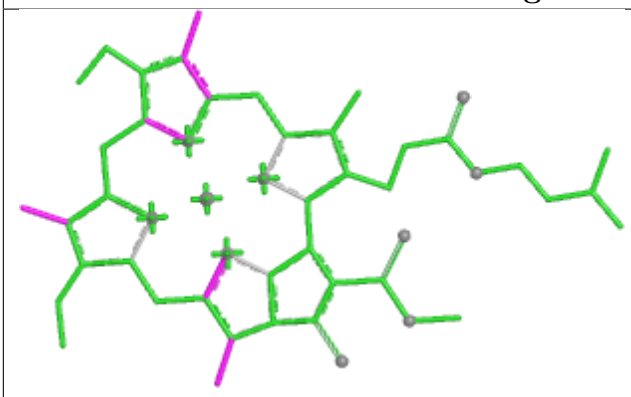


Torsions

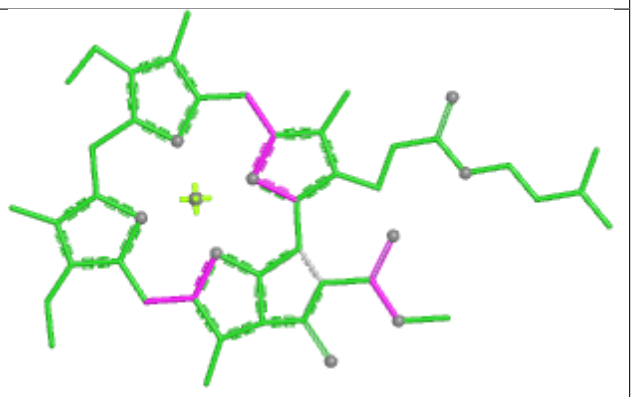


Rings

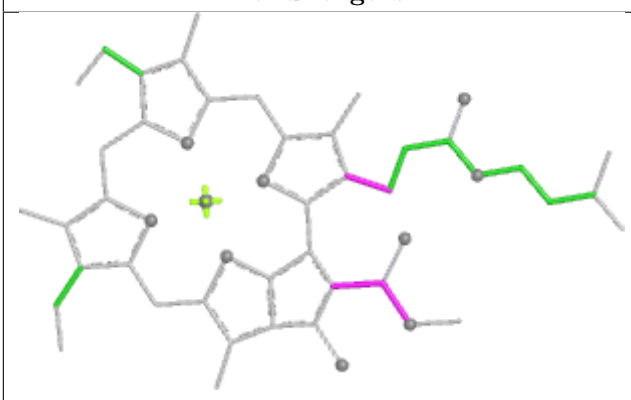
Ligand CLA V 604



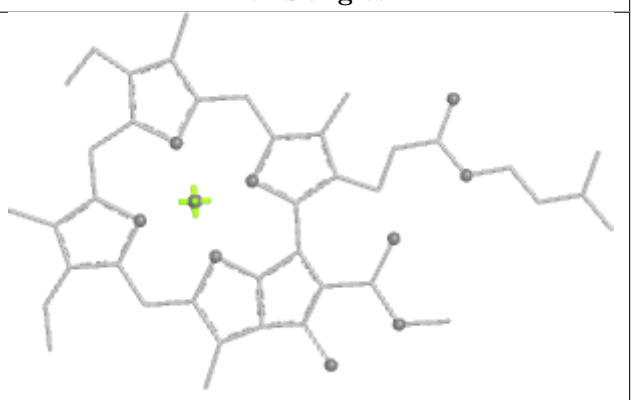
Bond lengths



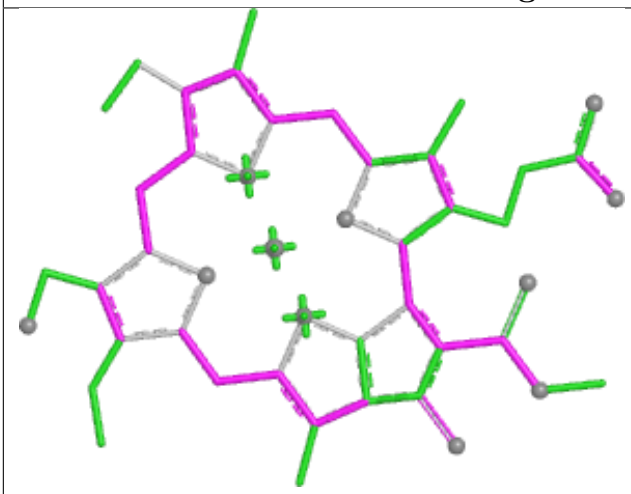
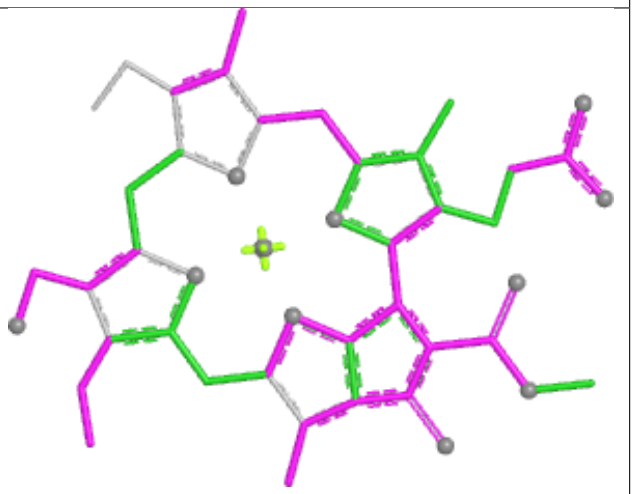
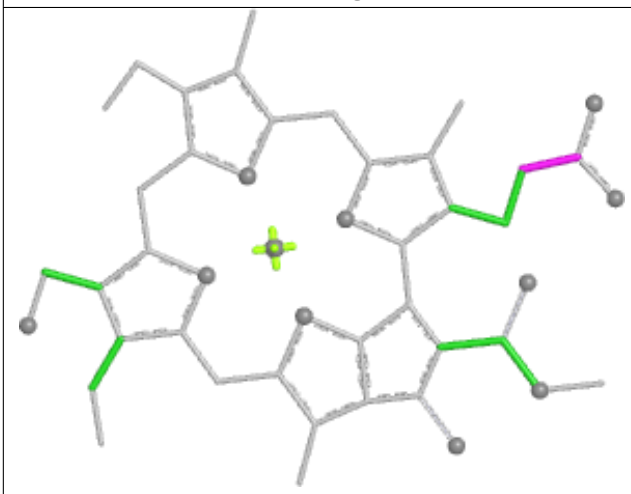
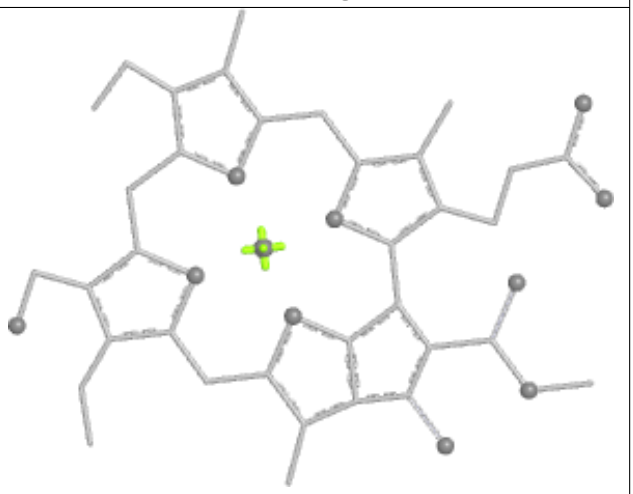
Bond angles

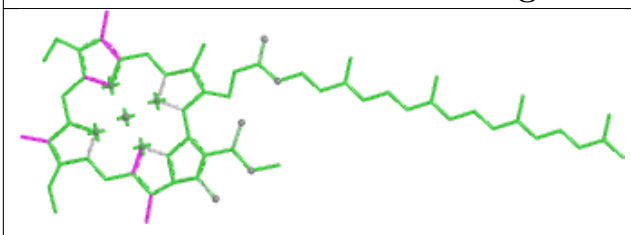
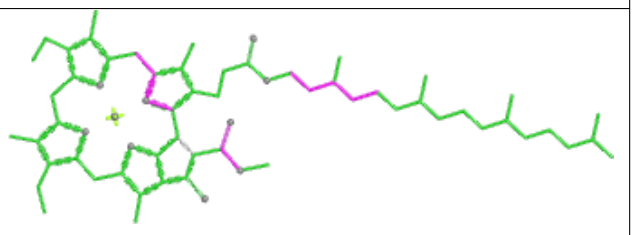
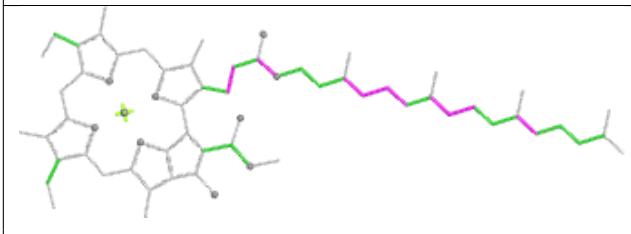
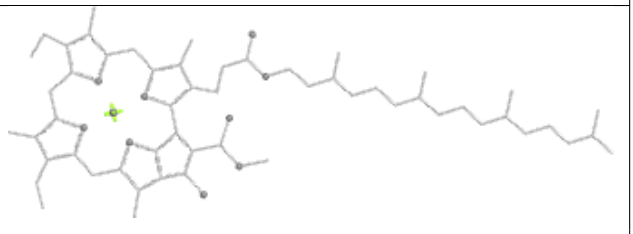


Torsions

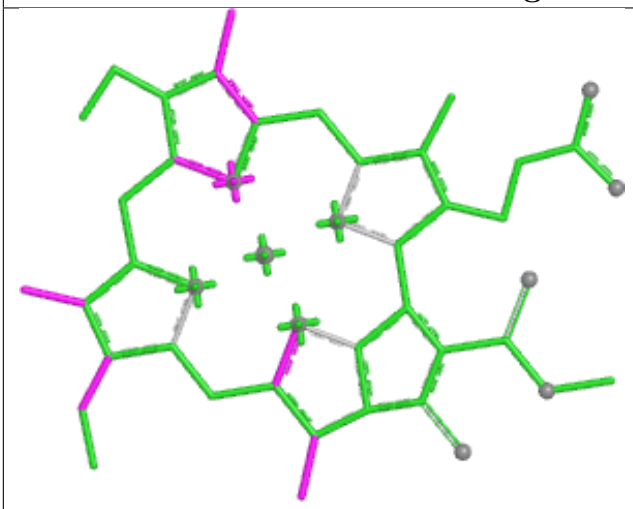


Rings

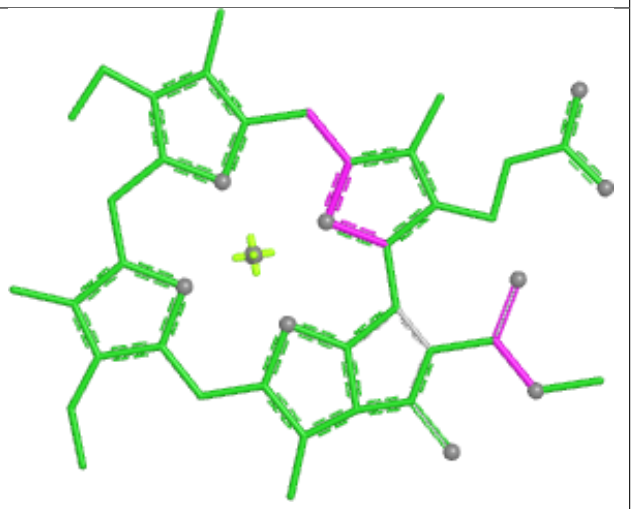
Ligand CHL W 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

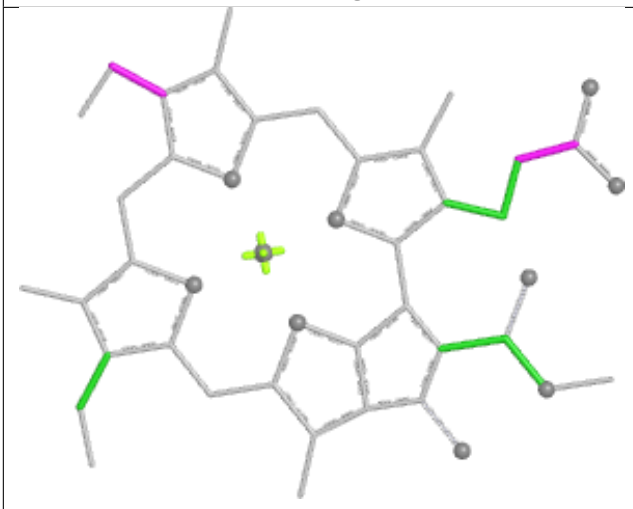
Ligand CLA V 603



Bond lengths



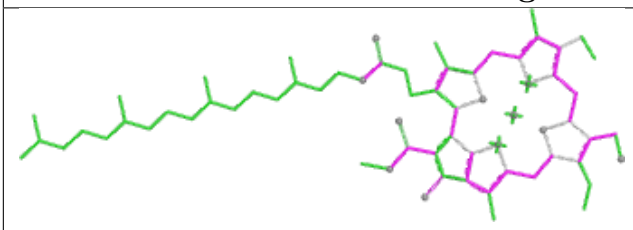
Bond angles



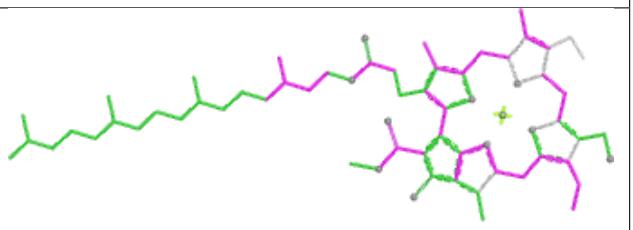
Torsions

Rings

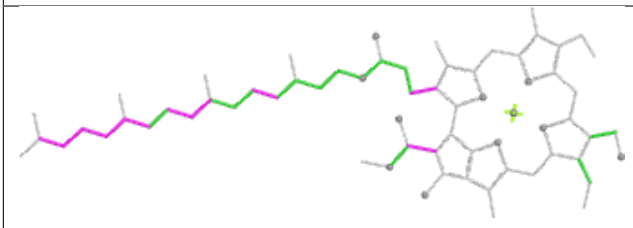
Ligand CHL W 609



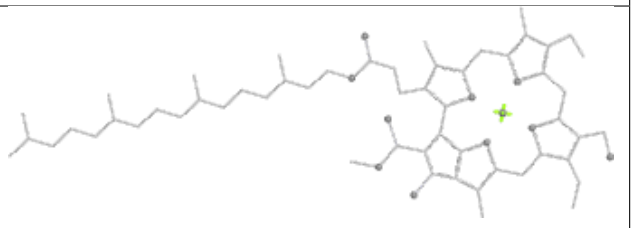
Bond lengths



Bond angles

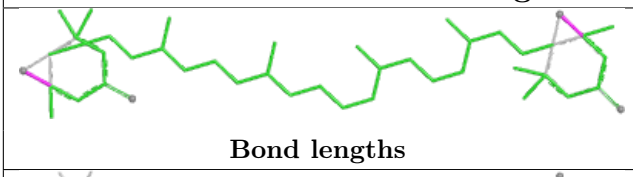


Torsions

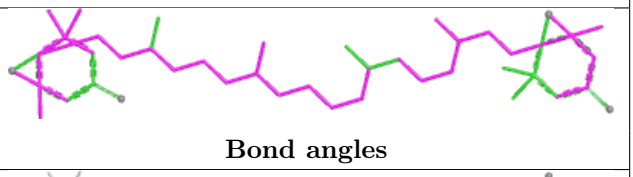


Rings

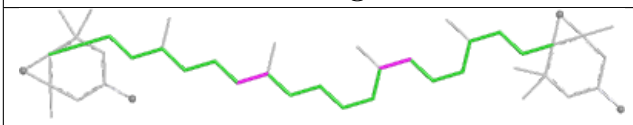
Ligand XAT U 1622



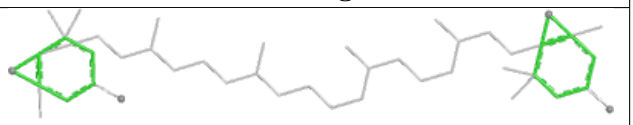
Bond lengths



Bond angles

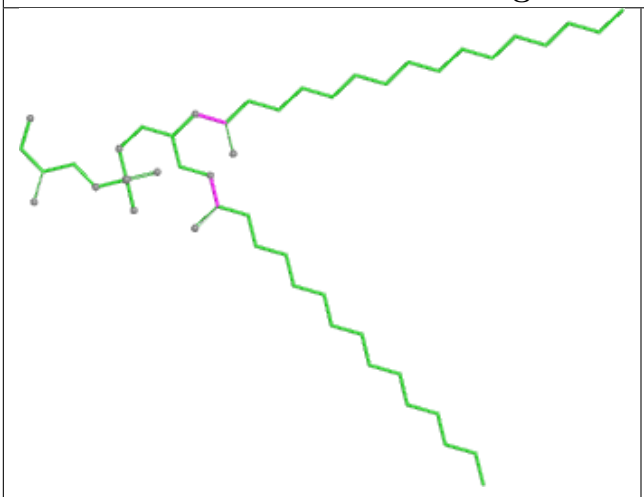


Torsions

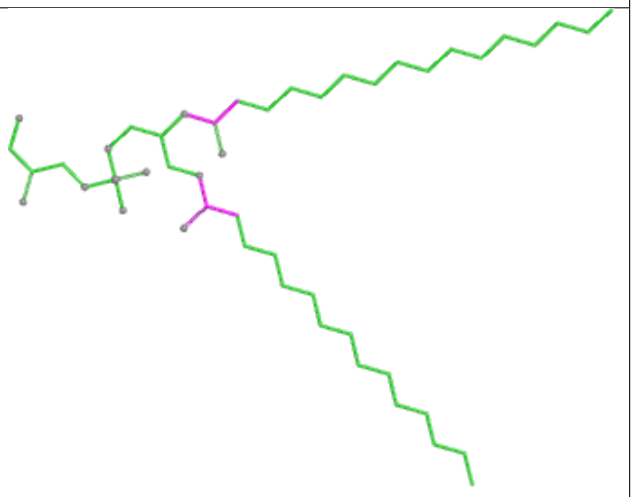


Rings

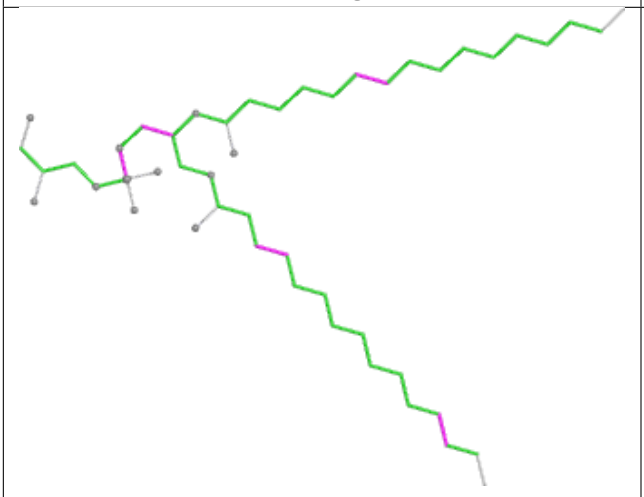
Ligand LHG V 2630



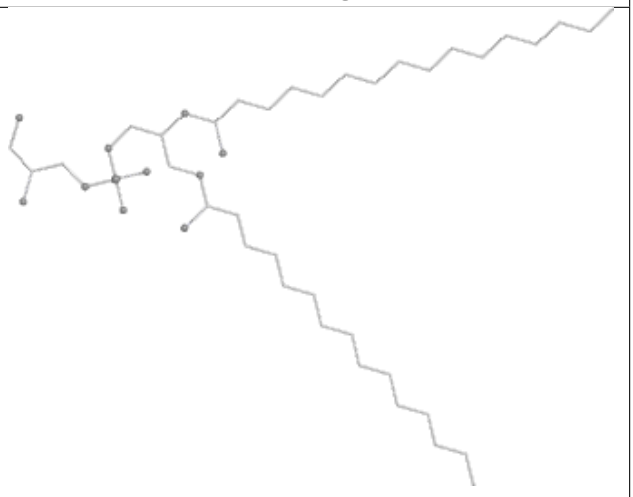
Bond lengths



Bond angles

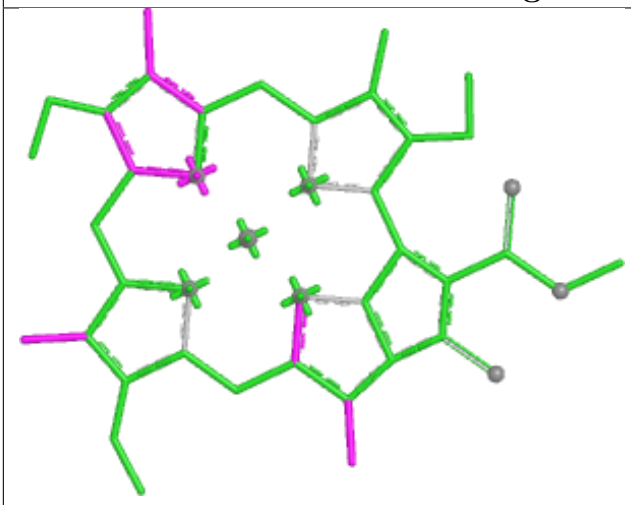


Torsions

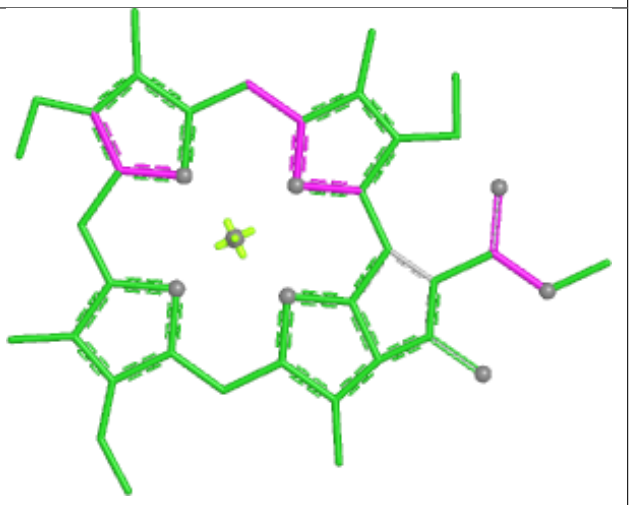


Rings

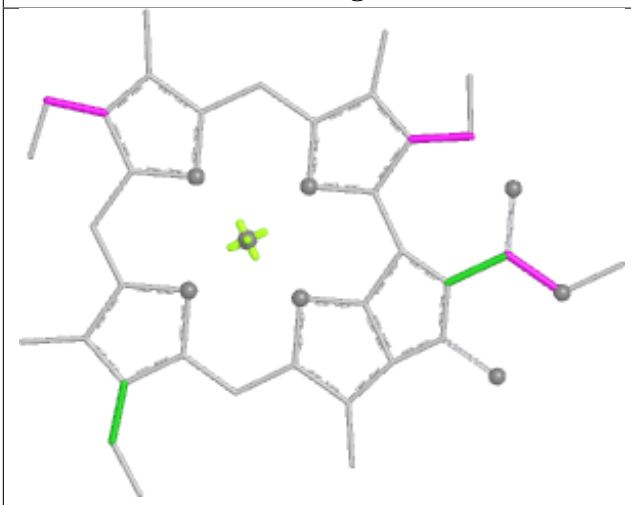
Ligand CLA U 611



Bond lengths



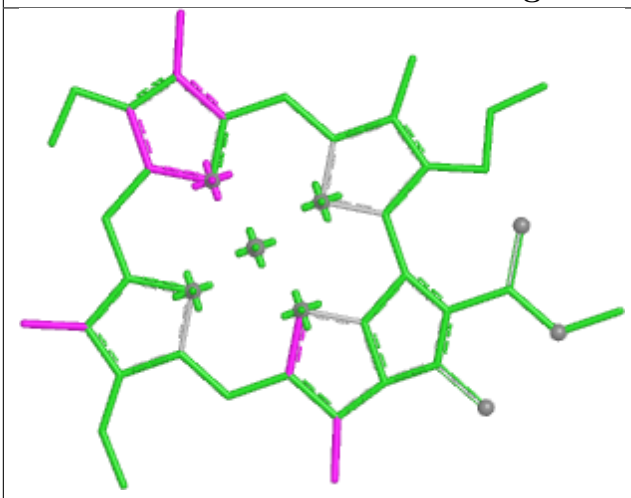
Bond angles



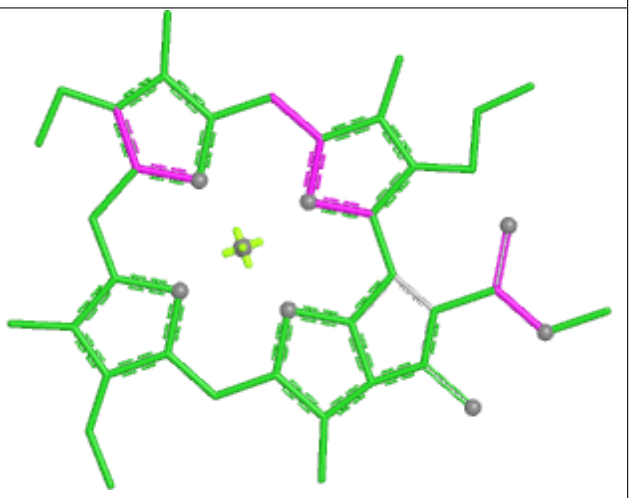
Torsions

Rings

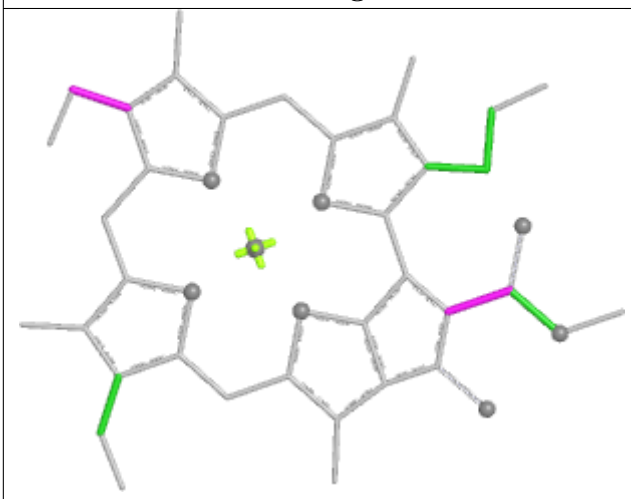
Ligand CLA U 612



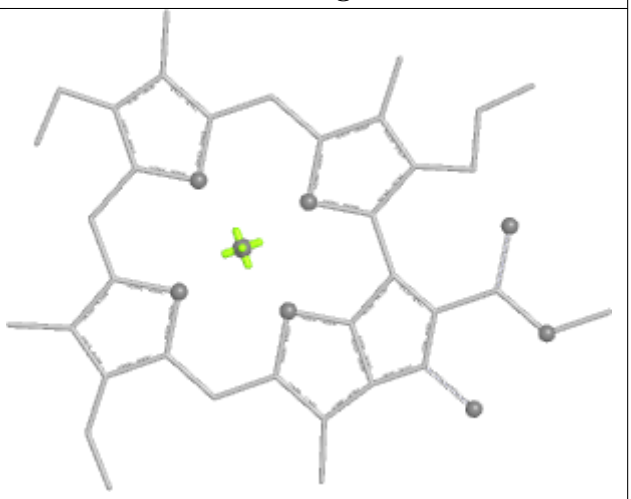
Bond lengths



Bond angles

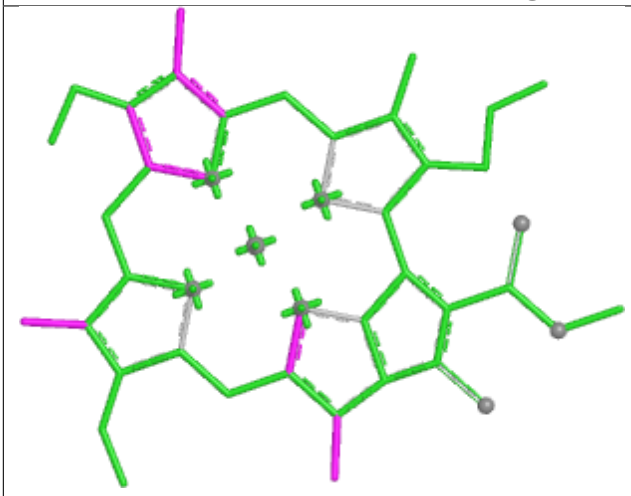


Torsions

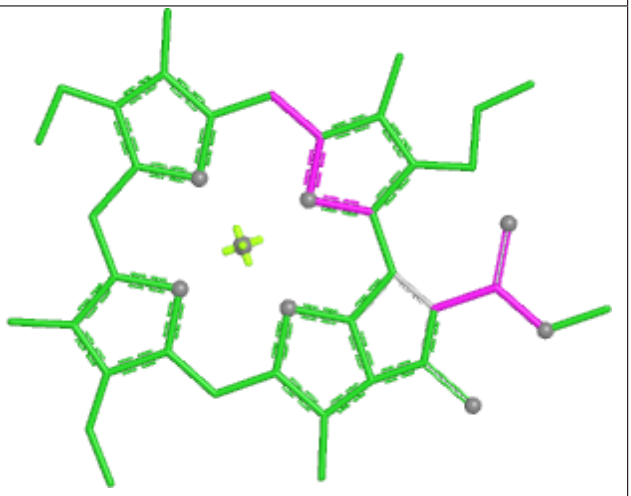


Rings

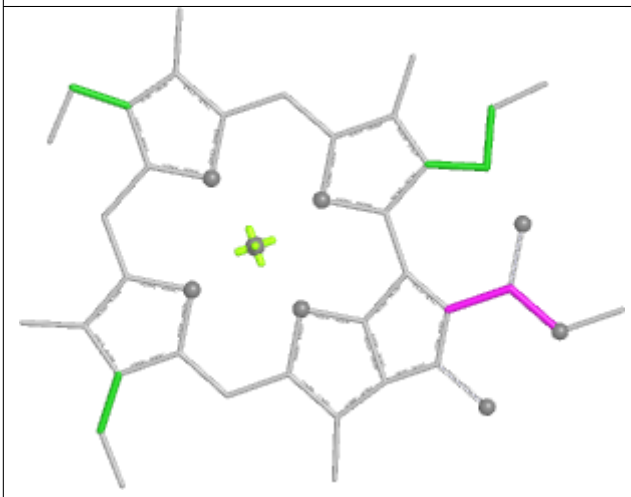
Ligand CLA V 611



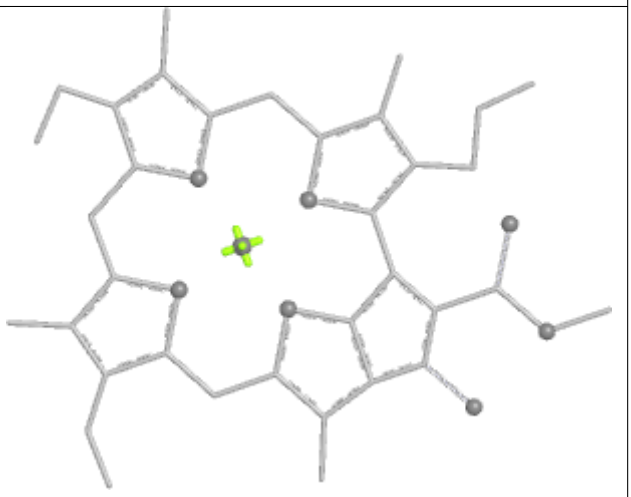
Bond lengths



Bond angles

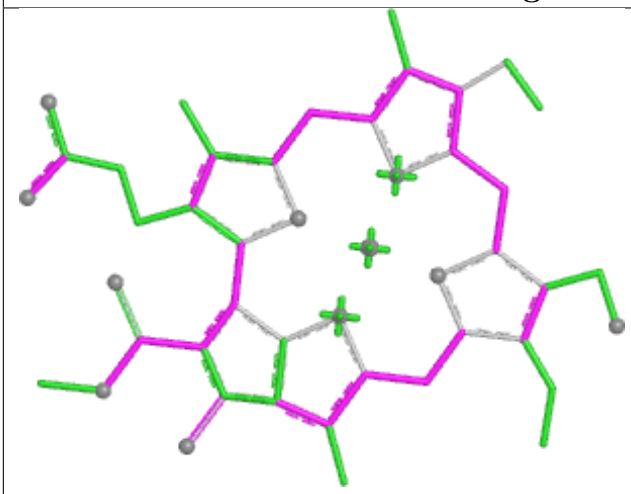


Torsions

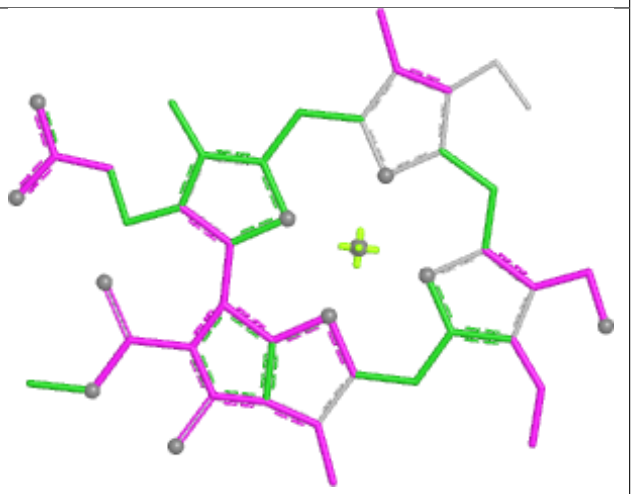


Rings

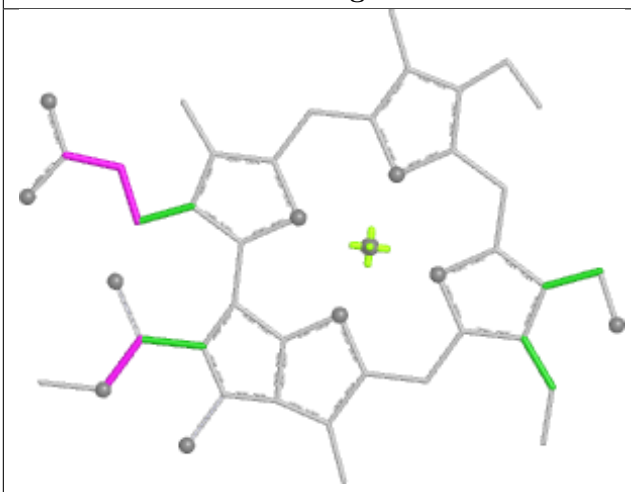
Ligand CHL U 607



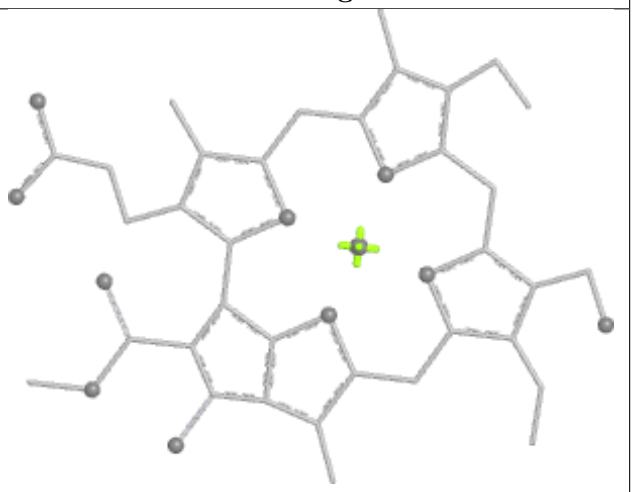
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

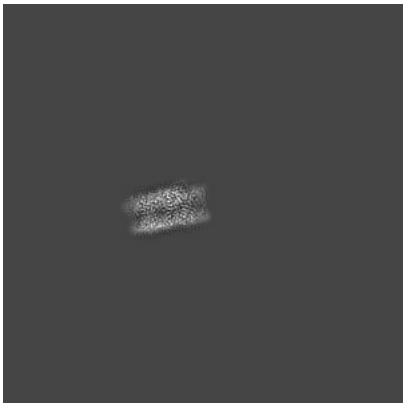
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30935. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

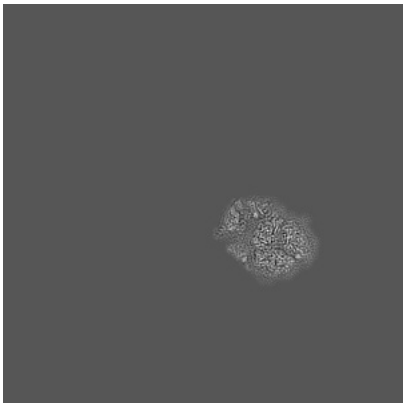
6.1 Orthogonal projections

6.1.1 Primary map



X

Y

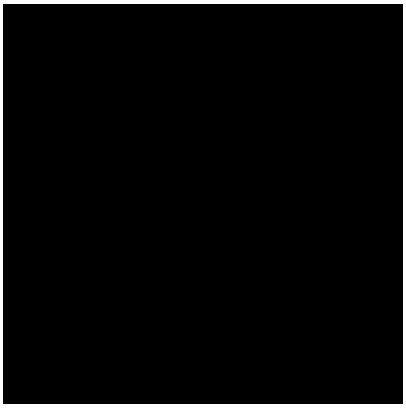


Z

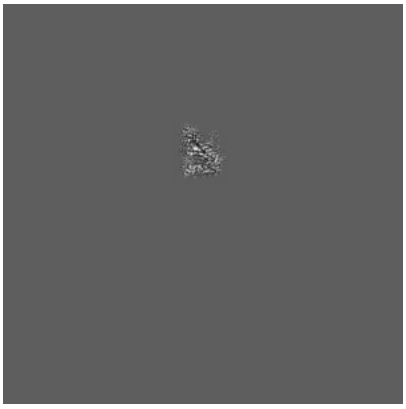
The images above show the map projected in three orthogonal directions.

6.2 Central slices

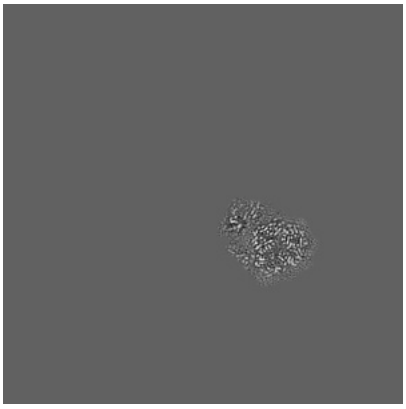
6.2.1 Primary map



X Index: 240



Y Index: 240

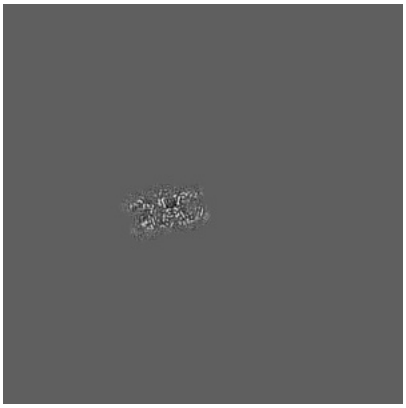


Z Index: 240

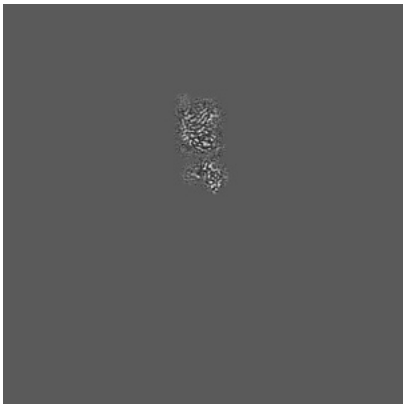
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

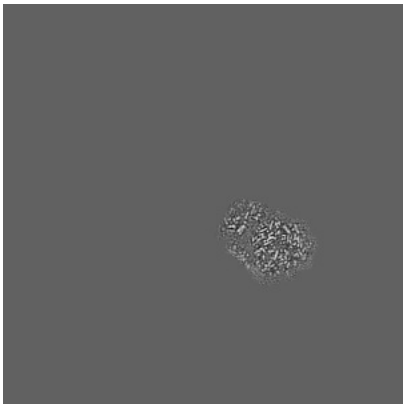
6.3.1 Primary map



X Index: 315



Y Index: 208

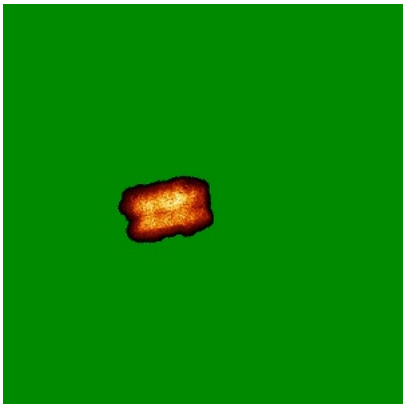


Z Index: 242

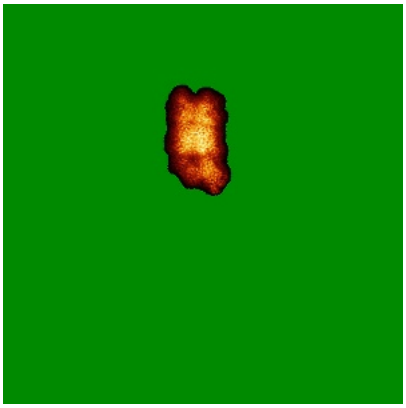
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

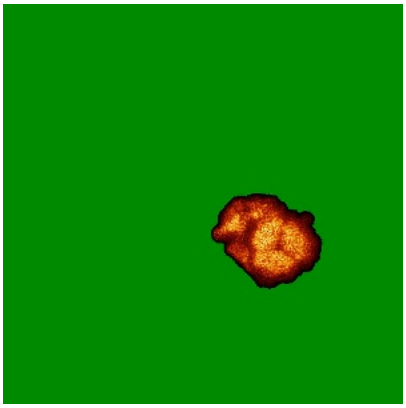
6.4.1 Primary map



X



Y

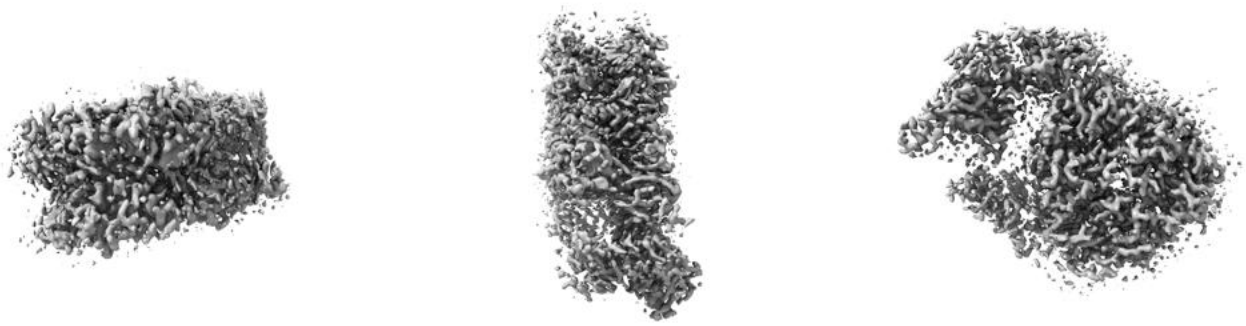


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

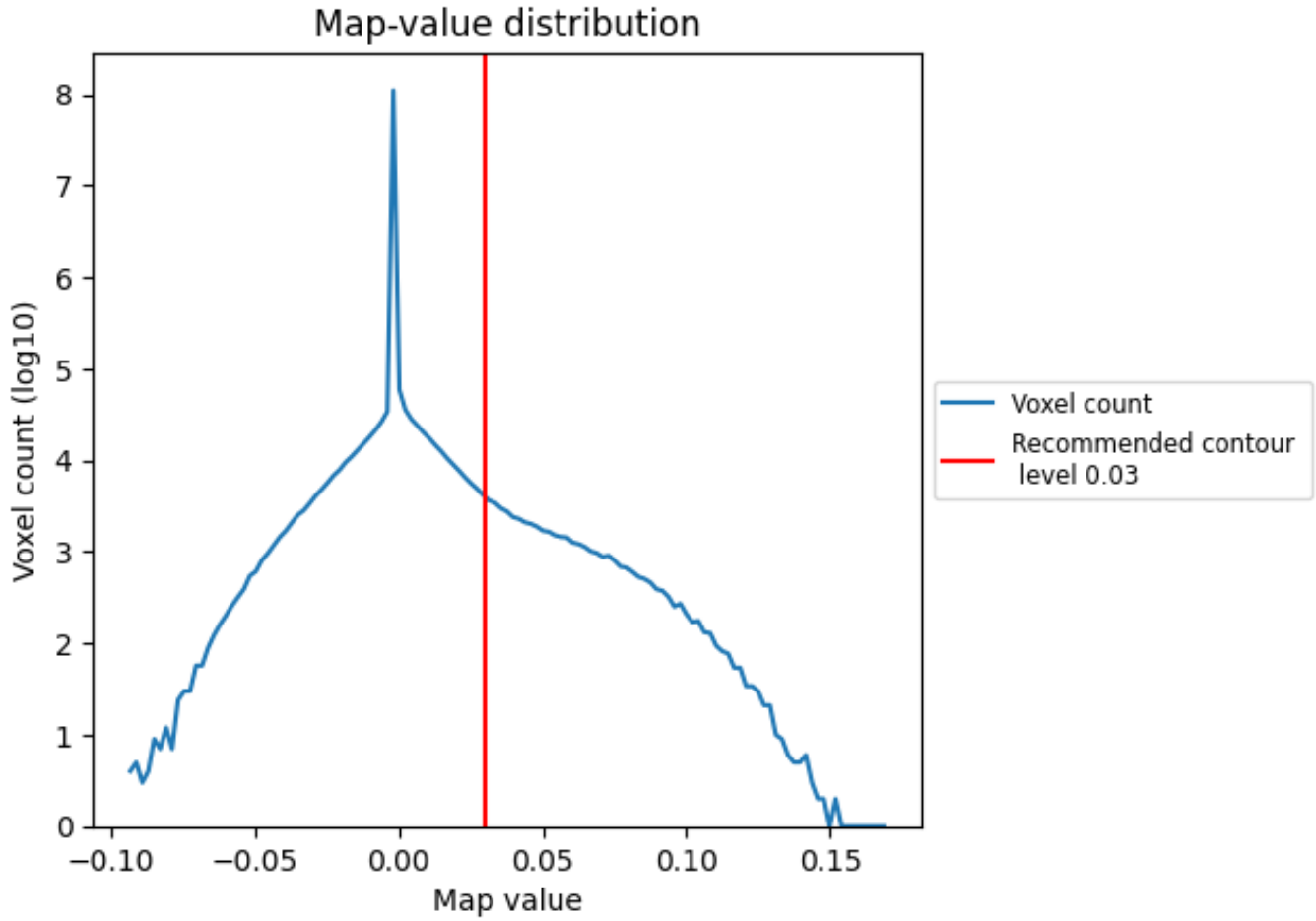
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

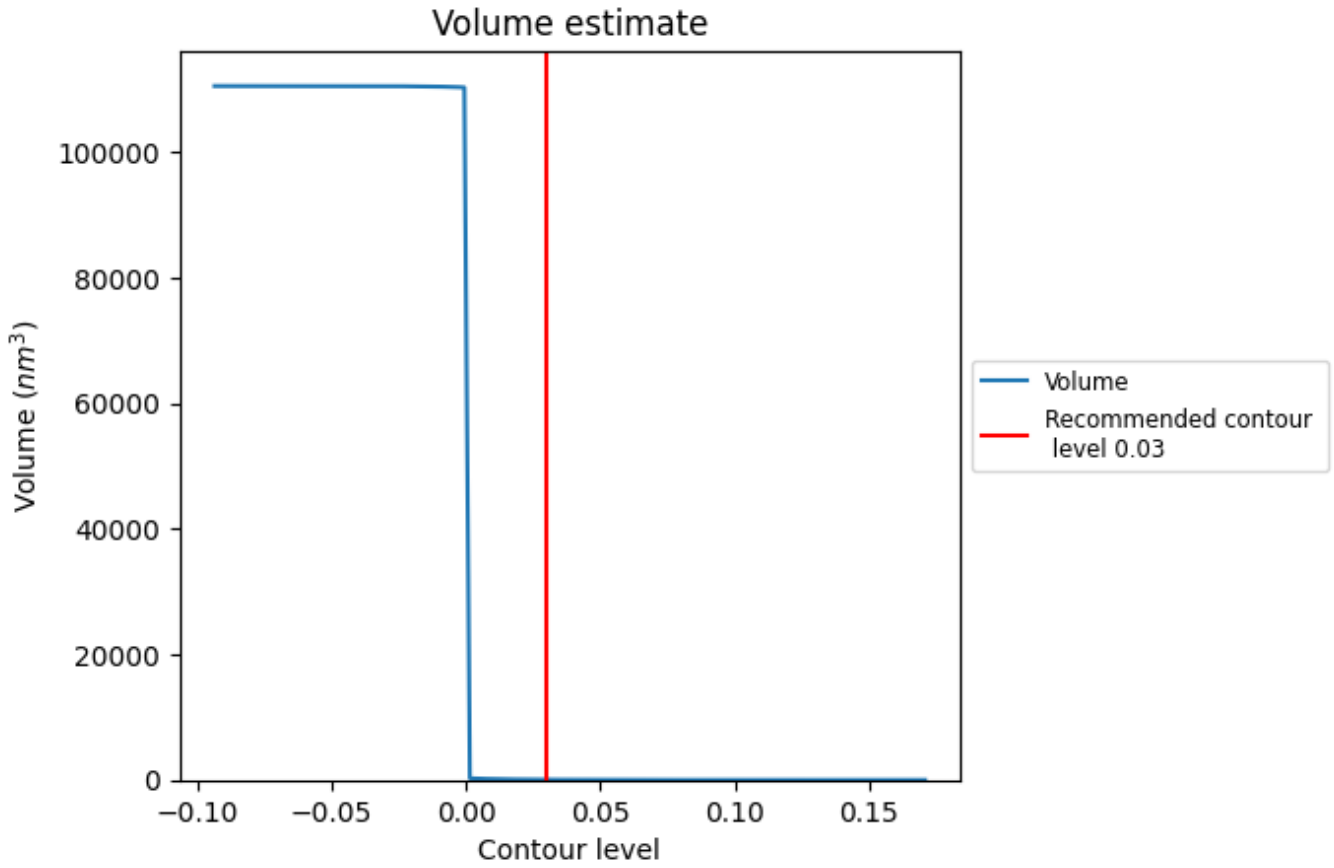
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

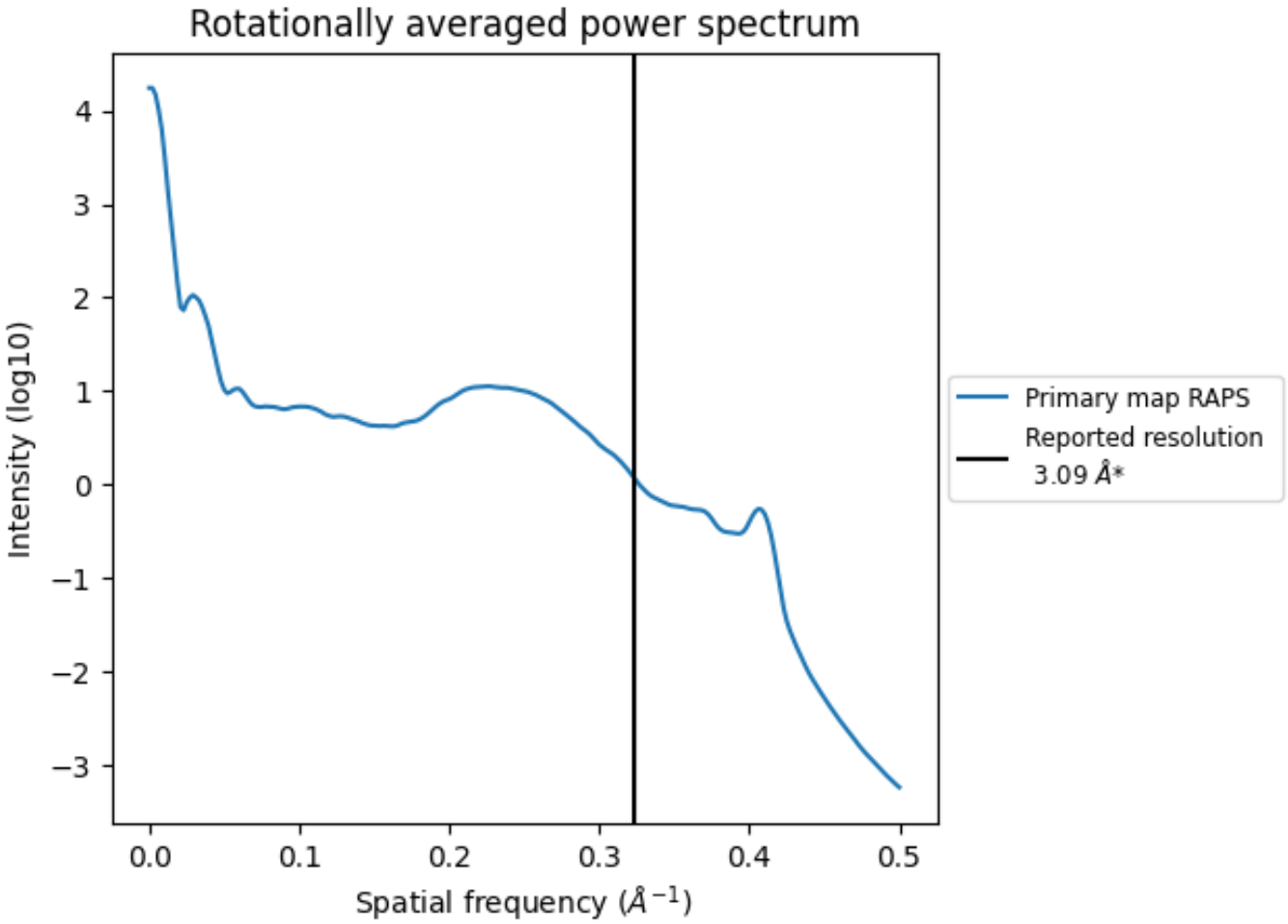
7.2 Volume estimate



The volume at the recommended contour level is 48 nm^3; this corresponds to an approximate mass of 44 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

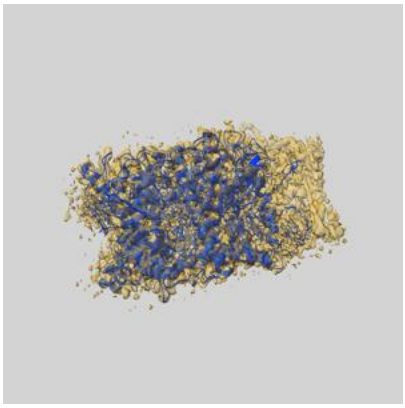
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

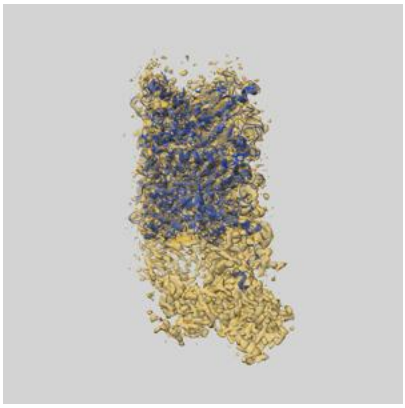
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30935 and PDB model 7E0K. Per-residue inclusion information can be found in section 3 on page 12.

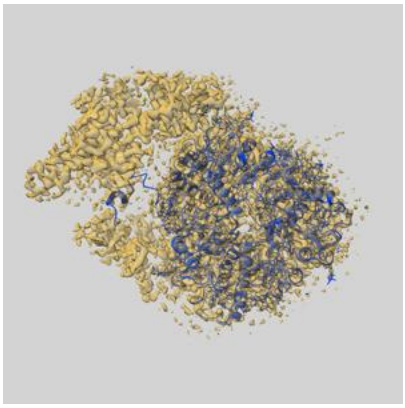
9.1 Map-model overlay



X



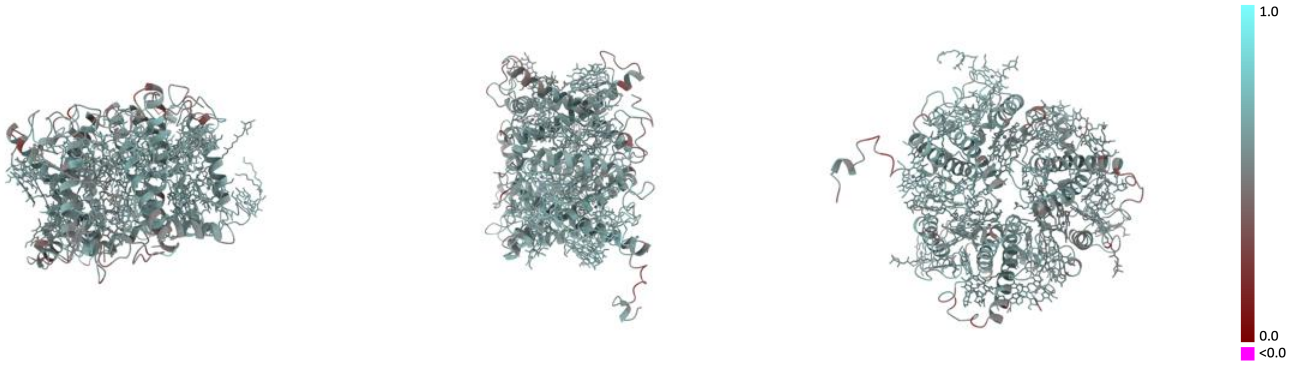
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

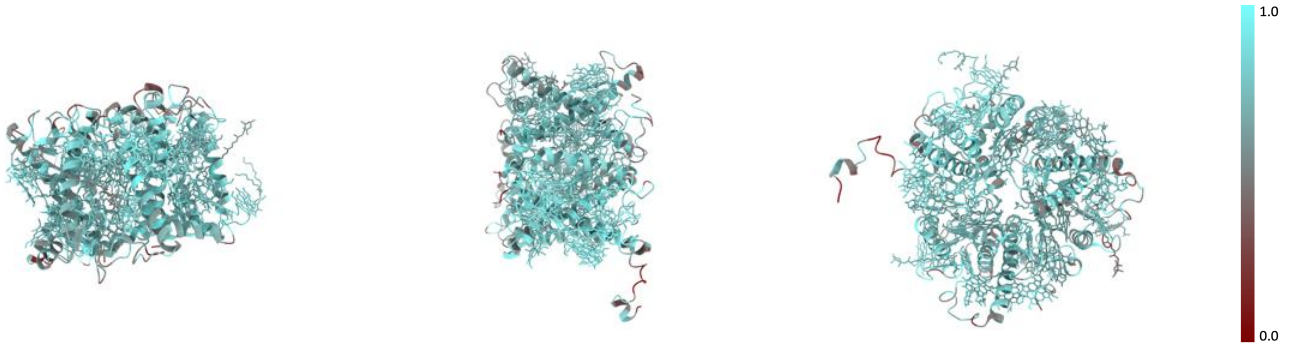
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

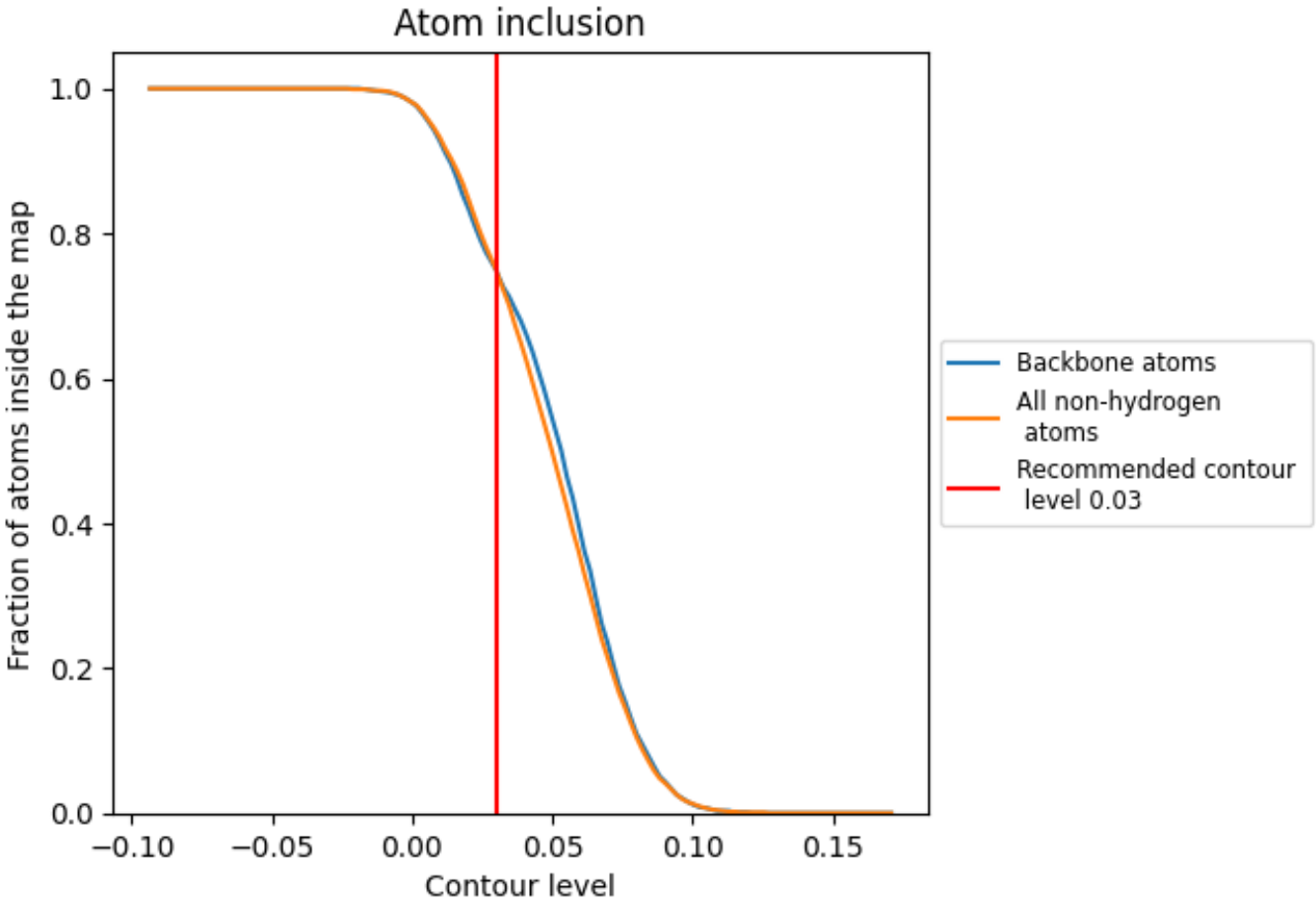
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7490	0.5660
U	0.7550	0.5650
V	0.7710	0.5850
W	0.7190	0.5470