Full wwPDB EM Validation Report ⓘ

Dec 11, 2023 – 02:14 PM JST

PDB ID	:	8J7Z
EMDB ID	:	EMD-36054
Title	:	Structure of FCP trimer in Cyclotella meneghiniana
Authors	:	Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on	:	2023-04-28
Resolution	:	2.72 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:

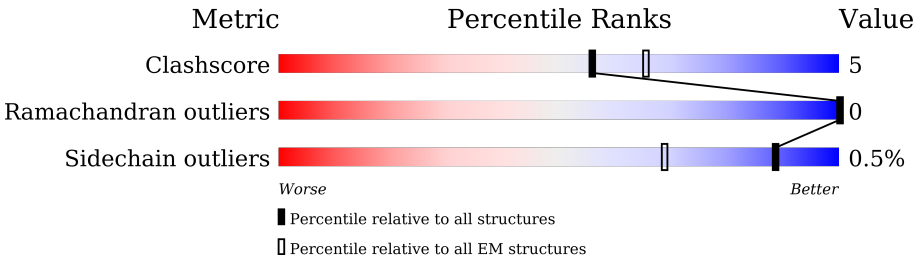
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.72 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	181	89% 11%
1	B	181	91% 8%
1	C	181	90% 10%

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
3	CLA	A	308	X	-	-	-
3	CLA	A	309	X	-	-	-
3	CLA	A	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	A	313	X	-	-	-
3	CLA	A	314	X	-	-	-
3	CLA	A	316	X	-	-	-
3	CLA	A	317	X	-	-	-
3	CLA	A	319	X	-	-	-
3	CLA	B	308	X	-	-	-
3	CLA	B	309	X	-	-	-
3	CLA	B	311	X	-	-	-
3	CLA	B	313	X	-	-	-
3	CLA	B	314	X	-	-	-
3	CLA	B	316	X	-	-	-
3	CLA	B	317	X	-	-	-
3	CLA	B	319	X	-	-	-
3	CLA	C	301	X	-	-	-
3	CLA	C	309	X	-	-	-
3	CLA	C	310	X	-	-	-
3	CLA	C	312	X	-	-	-
3	CLA	C	314	X	-	-	-
3	CLA	C	315	X	-	-	-
3	CLA	C	317	X	-	-	-
3	CLA	C	318	X	-	-	-

2 Entry composition

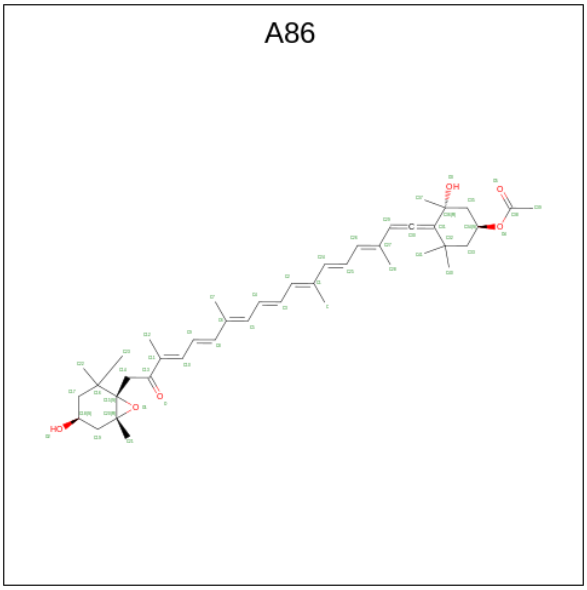
There are 6 unique types of molecules in this entry. The entry contains 7088 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	181	Total	C	N	O	S	0	0
			1396	895	236	258	7		
1	B	181	Total	C	N	O	S	0	0
			1396	895	236	258	7		
1	C	181	Total	C	N	O	S	0	0
			1396	895	236	258	7		

- Molecule 2 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (three-letter code: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			48	42	6	
2	A	1	Total	C	O	0
			48	42	6	
2	A	1	Total	C	O	0
			48	42	6	

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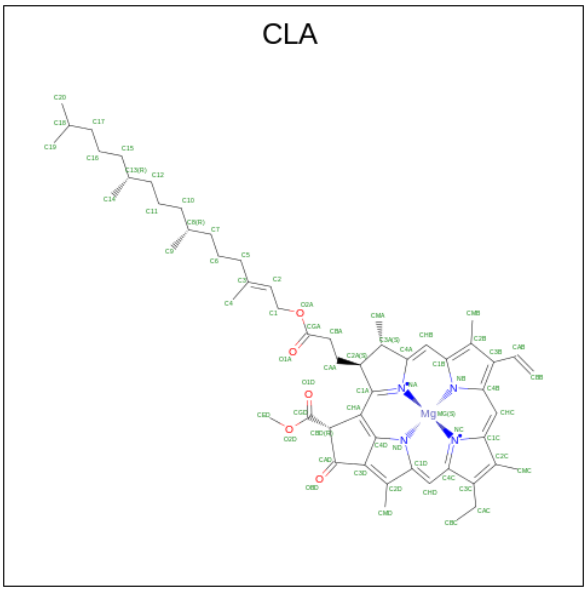
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O 48 42 6	0
2	A	1	Total C O 48 42 6	0
2	A	1	Total C O 48 42 6	0
2	A	1	Total C O 48 42 6	0
2	B	1	Total C O 48 42 6	0
2	B	1	Total C O 48 42 6	0
2	B	1	Total C O 48 42 6	0
2	B	1	Total C O 48 42 6	0
2	B	1	Total C O 48 42 6	0
2	B	1	Total C O 48 42 6	0
2	B	1	Total C O 48 42 6	0
2	C	1	Total C O 48 42 6	0
2	C	1	Total C O 48 42 6	0
2	C	1	Total C O 48 42 6	0
2	C	1	Total C O 48 42 6	0
2	C	1	Total C O 48 42 6	0
2	C	1	Total C O 48 42 6	0
2	C	1	Total C O 48 42 6	0

- Molecule 3 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
3	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
3	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
3	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
3	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
3	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
3	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
3	B	1	Total 41	C 33	Mg 1	N 4	O 3	0

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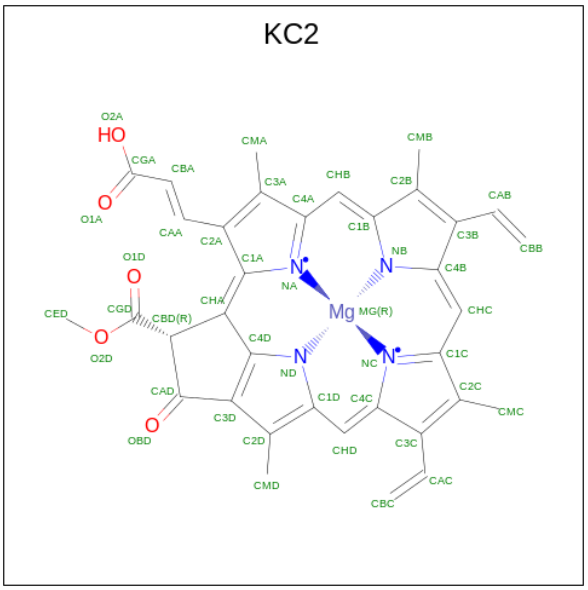
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	C	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

- Molecule 4 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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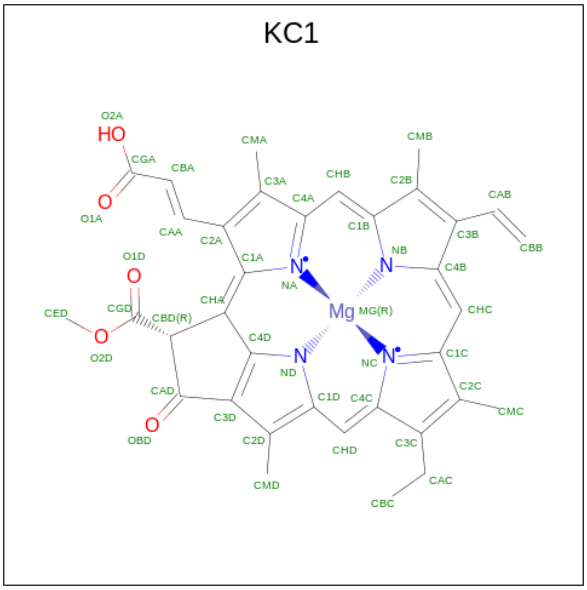
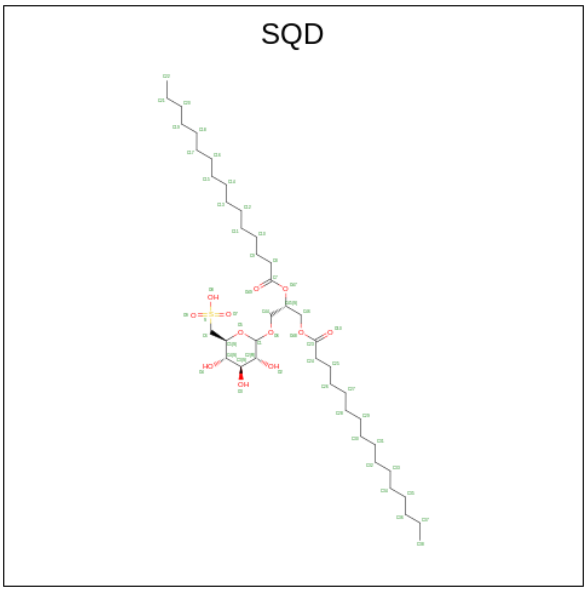
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 5 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 6 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



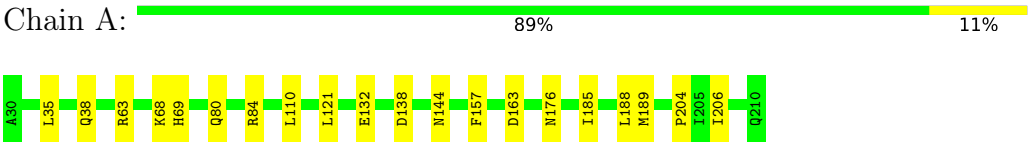
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	S	0
			43	30	12	1	
6	B	1	Total	C	O	S	0
			43	30	12	1	
6	C	1	Total	C	O	S	0
			43	30	12	1	

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.

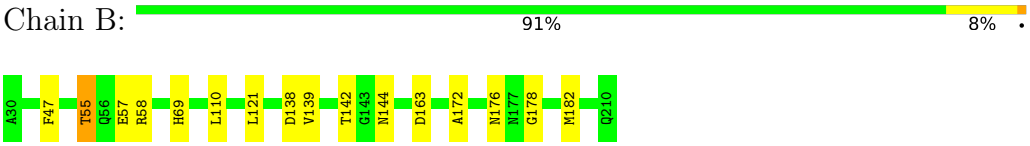
- Molecule 1: FCP

Chain A:



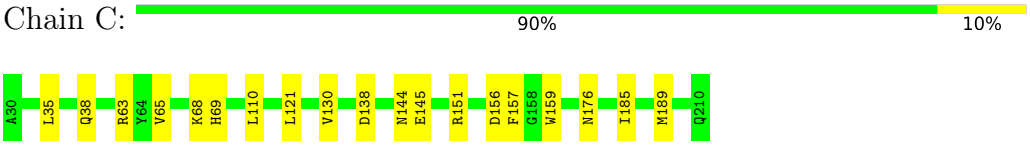
- Molecule 1: FCP

Chain B:



- Molecule 1: FCP

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	970425	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.821	Depositor
Minimum map value	-0.292	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.188	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, SQD, A86, KC2, KC1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/1431	0.45	0/1938
1	B	0.27	0/1431	0.44	0/1938
1	C	0.26	0/1431	0.45	0/1938
All	All	0.27	0/4293	0.45	0/5814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1396	0	1349	14	0
1	B	1396	0	1349	10	0
1	C	1396	0	1349	13	0
2	A	336	0	0	1	0
2	B	336	0	0	1	0
2	C	336	0	0	1	0
3	A	450	0	430	17	0
3	B	452	0	435	10	0
3	C	456	0	442	12	0
4	A	90	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	90	0	0	0	0
4	C	90	0	0	0	0
5	A	45	0	0	1	0
5	B	45	0	0	1	0
5	C	45	0	0	1	0
6	A	43	0	50	2	0
6	B	43	0	49	0	0
6	C	43	0	49	1	0
All	All	7088	0	5502	65	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 5.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLN:HE21	1:A:84:ARG:HE	1.29	0.79
1:C:176:ASN:ND2	3:C:309:CLA:O1D	2.23	0.72
1:A:80:GLN:HG2	1:A:188:LEU:HD13	1.72	0.72
1:A:176:ASN:ND2	3:A:308:CLA:O1D	2.24	0.69
3:C:301:CLA:H51	6:C:319:SQD:H112	1.77	0.66
1:B:138:ASP:OD1	1:B:144:ASN:ND2	2.30	0.64
1:B:172:ALA:O	1:B:176:ASN:ND2	2.31	0.64
1:A:138:ASP:OD1	1:A:144:ASN:ND2	2.31	0.62
1:B:176:ASN:ND2	3:B:308:CLA:O1D	2.38	0.55
1:A:157:PHE:HB2	3:A:314:CLA:H12	1.87	0.55
1:B:110:LEU:HD22	1:B:121:LEU:HD13	1.90	0.54
1:C:138:ASP:OD1	1:C:144:ASN:ND2	2.32	0.53
3:A:319:CLA:HAB	3:B:316:CLA:HMD1	1.92	0.51
1:C:185:ILE:O	1:C:189:MET:HG3	2.11	0.51
2:B:304:A86:O3	5:B:315:KC1:O1A	2.28	0.50
1:C:110:LEU:HD22	1:C:121:LEU:HD13	1.93	0.50
1:A:68:LYS:NZ	1:A:132:GLU:OE2	2.33	0.50
3:A:319:CLA:HMB1	3:A:319:CLA:HBB1	1.92	0.50
1:A:38:GLN:OE1	1:A:176:ASN:ND2	2.39	0.48
3:C:310:CLA:H111	3:C:310:CLA:H151	1.71	0.48
1:B:178:GLY:O	1:B:182:MET:HG3	2.14	0.47
1:C:151:ARG:NH1	1:C:156:ASP:OD2	2.43	0.47
2:A:304:A86:O3	5:A:315:KC1:O1A	2.33	0.47
3:A:309:CLA:H62	3:A:309:CLA:H41	1.61	0.47
1:A:110:LEU:HD22	1:A:121:LEU:HD13	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HB3	1:A:63:ARG:HH12	1.79	0.46
1:B:47:PHE:HE2	3:B:309:CLA:H112	1.80	0.46
3:C:315:CLA:HBA1	3:C:315:CLA:H3A	1.84	0.46
3:C:309:CLA:H12	3:C:309:CLA:H51	1.76	0.45
3:C:310:CLA:H111	3:C:310:CLA:H93	1.73	0.45
3:A:308:CLA:H41	3:A:308:CLA:H61	1.79	0.44
3:B:319:CLA:HBB1	3:B:319:CLA:HMB1	1.99	0.44
3:C:312:CLA:H91	3:C:312:CLA:H111	1.76	0.44
3:B:319:CLA:H61	3:B:319:CLA:H41	1.63	0.44
1:C:157:PHE:HB2	3:C:315:CLA:H12	1.99	0.44
3:B:309:CLA:H111	3:B:309:CLA:H151	1.69	0.43
1:A:204:PRO:O	1:A:206:ILE:N	2.47	0.43
1:B:55:THR:HG23	1:B:58:ARG:H	1.83	0.43
1:C:69:HIS:CE1	3:C:314:CLA:HMD1	2.54	0.43
1:B:163:ASP:OD1	1:B:163:ASP:N	2.52	0.43
2:C:305:A86:O3	5:C:316:KC1:O1A	2.37	0.43
6:A:318:SQD:H112	3:A:319:CLA:H51	2.01	0.43
1:B:139:VAL:O	1:B:142:THR:OG1	2.28	0.43
1:C:65:VAL:HG13	1:C:69:HIS:CE1	2.54	0.43
3:B:319:CLA:HAB	3:C:317:CLA:HMD1	1.99	0.42
1:C:145:GLU:OE2	1:C:159:TRP:NE1	2.41	0.42
3:A:314:CLA:HBA1	3:A:314:CLA:H3A	1.89	0.42
3:A:316:CLA:HMD1	3:C:301:CLA:HAB	2.01	0.42
1:A:69:HIS:CE1	3:A:313:CLA:HMD1	2.54	0.42
1:A:163:ASP:OD1	1:A:163:ASP:N	2.47	0.41
3:B:314:CLA:H52	3:B:314:CLA:H11	1.73	0.41
1:B:69:HIS:CE1	3:B:313:CLA:HMD1	2.55	0.41
1:C:35:LEU:HB3	1:C:63:ARG:HH12	1.84	0.41
1:A:68:LYS:HD3	3:A:313:CLA:CAD	2.50	0.41
1:C:68:LYS:HE2	3:C:314:CLA:C4D	2.51	0.41
3:A:309:CLA:H111	3:A:309:CLA:H93	1.72	0.41
3:A:311:CLA:H141	3:A:311:CLA:H162	1.87	0.41
1:A:185:ILE:O	1:A:189:MET:HG3	2.21	0.40
3:A:309:CLA:H152	1:C:130:VAL:HG23	2.03	0.40
6:A:318:SQD:H342	6:A:318:SQD:H311	1.85	0.40
3:A:309:CLA:H143	3:A:309:CLA:H161	1.75	0.40
3:B:311:CLA:H91	3:B:311:CLA:H111	1.80	0.40
1:C:38:GLN:OE1	1:C:176:ASN:ND2	2.31	0.40
3:A:309:CLA:H111	3:A:309:CLA:H151	1.71	0.40
3:A:311:CLA:H111	3:A:311:CLA:H91	1.78	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	A	179/181 (99%)	171 (96%)	8 (4%)	0	100	100
1	B	179/181 (99%)	171 (96%)	8 (4%)	0	100	100
1	C	179/181 (99%)	169 (94%)	10 (6%)	0	100	100
All	All	537/543 (99%)	511 (95%)	26 (5%)	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	A	144/144 (100%)	144 (100%)	0	100	100
1	B	144/144 (100%)	142 (99%)	2 (1%)	67	85
1	C	144/144 (100%)	144 (100%)	0	100	100
All	All	432/432 (100%)	430 (100%)	2 (0%)	89	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	THR
1	B	57	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	B	38	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

57 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	$\#\|Z\| > 2$
3	CLA	A	311	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
2	A86	B	303	-	44,50,50	1.22	3 (6%)	51,76,76	5.60	15 (29%)
2	A86	A	305	-	44,50,50	1.24	3 (6%)	51,76,76	5.74	14 (27%)
2	A86	A	306	-	44,50,50	1.24	3 (6%)	51,76,76	6.25	18 (35%)
2	A86	B	302	-	44,50,50	1.23	3 (6%)	51,76,76	7.15	17 (33%)
3	CLA	A	308	-	53,61,73	1.64	6 (11%)	61,98,113	1.50	7 (11%)
4	KC2	A	310	-	48,53,53	1.87	10 (20%)	54,89,89	2.10	14 (25%)
2	A86	C	307	-	44,50,50	1.23	3 (6%)	51,76,76	6.22	19 (37%)
3	CLA	C	318	1	54,62,73	1.64	5 (9%)	62,99,113	1.45	7 (11%)
5	KC1	B	315	1	48,53,53	1.52	7 (14%)	55,89,89	1.81	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CLA	A	309	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	8 (10%)
3	CLA	A	317	1	54,62,73	1.65	6 (11%)	62,99,113	1.45	8 (12%)
3	CLA	B	314	-	53,61,73	1.64	6 (11%)	61,98,113	1.53	9 (14%)
2	A86	B	301	-	44,50,50	1.23	3 (6%)	51,76,76	6.05	17 (33%)
3	CLA	A	316	-	41,49,73	1.82	6 (14%)	47,84,113	1.67	7 (14%)
3	CLA	C	314	1	65,73,73	1.47	6 (9%)	76,113,113	1.36	6 (7%)
3	CLA	C	301	-	55,63,73	1.60	5 (9%)	64,101,113	1.48	9 (14%)
4	KC2	B	312	1	48,53,53	1.88	10 (20%)	54,89,89	2.10	14 (25%)
3	CLA	A	313	1	65,73,73	1.48	6 (9%)	76,113,113	1.38	6 (7%)
2	A86	B	304	-	44,50,50	1.23	3 (6%)	51,76,76	5.62	17 (33%)
4	KC2	C	311	-	48,53,53	1.87	10 (20%)	54,89,89	2.10	14 (25%)
2	A86	A	303	-	44,50,50	1.24	3 (6%)	51,76,76	7.17	15 (29%)
2	A86	C	305	-	44,50,50	1.24	3 (6%)	51,76,76	5.39	16 (31%)
3	CLA	C	310	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
2	A86	A	307	-	44,50,50	1.24	3 (6%)	51,76,76	6.77	17 (33%)
3	CLA	C	312	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
4	KC2	B	310	-	48,53,53	1.88	10 (20%)	54,89,89	2.11	14 (25%)
2	A86	C	303	-	44,50,50	1.23	3 (6%)	51,76,76	6.79	17 (33%)
3	CLA	C	317	-	41,49,73	1.81	6 (14%)	47,84,113	1.66	7 (14%)
2	A86	A	304	-	44,50,50	1.24	3 (6%)	51,76,76	5.51	15 (29%)
3	CLA	B	316	-	41,49,73	1.83	6 (14%)	47,84,113	1.67	7 (14%)
2	A86	A	302	-	44,50,50	1.24	3 (6%)	51,76,76	7.60	17 (33%)
2	A86	C	302	-	44,50,50	1.23	3 (6%)	51,76,76	5.88	17 (33%)
6	SQD	C	319	-	42,43,54	1.08	5 (11%)	51,54,65	1.65	10 (19%)
3	CLA	B	313	1	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
4	KC2	A	312	1	48,53,53	1.88	10 (20%)	54,89,89	2.11	14 (25%)
6	SQD	B	318	-	42,43,54	1.07	5 (11%)	51,54,65	1.63	10 (19%)
2	A86	B	307	-	44,50,50	1.23	3 (6%)	51,76,76	6.63	18 (35%)
2	A86	C	304	-	44,50,50	1.23	3 (6%)	51,76,76	7.22	16 (31%)
5	KC1	A	315	1	48,53,53	1.53	7 (14%)	55,89,89	1.82	10 (18%)
4	KC2	C	313	1	48,53,53	1.88	10 (20%)	54,89,89	2.10	13 (24%)
2	A86	C	306	-	44,50,50	1.24	3 (6%)	51,76,76	5.98	14 (27%)
2	A86	A	301	-	44,50,50	1.23	3 (6%)	51,76,76	5.98	17 (33%)
2	A86	C	308	-	44,50,50	1.23	3 (6%)	51,76,76	6.81	17 (33%)
3	CLA	A	319	-	55,63,73	1.59	6 (10%)	64,101,113	1.52	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CLA	B	308	-	54,62,73	1.61	6 (11%)	62,99,113	1.47	7 (11%)
3	CLA	B	311	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	8 (10%)
2	A86	B	305	-	44,50,50	1.24	3 (6%)	51,76,76	6.14	14 (27%)
2	A86	B	306	-	44,50,50	1.24	3 (6%)	51,76,76	6.28	17 (33%)
3	CLA	C	315	-	53,61,73	1.62	6 (11%)	61,98,113	1.53	9 (14%)
5	KC1	C	316	1	48,53,53	1.53	7 (14%)	55,89,89	1.81	11 (20%)
6	SQD	A	318	-	42,43,54	1.08	5 (11%)	51,54,65	1.64	10 (19%)
3	CLA	A	314	-	52,60,73	1.65	6 (11%)	60,97,113	1.55	9 (15%)
3	CLA	B	319	-	55,63,73	1.59	6 (10%)	64,101,113	1.51	9 (14%)
3	CLA	B	309	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
3	CLA	B	317	1	54,62,73	1.64	5 (9%)	62,99,113	1.45	8 (12%)
3	CLA	C	309	-	58,66,73	1.57	6 (10%)	67,104,113	1.45	7 (10%)

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
3	CLA	A	311	-	1/1/15/20	11/37/115/115	-
3	CLA	A	308	-	1/1/12/20	5/23/101/115	-
2	A86	A	305	-	-	3/34/90/90	0/3/3/3
2	A86	A	306	-	-	3/34/90/90	0/3/3/3
2	A86	B	302	-	-	3/34/90/90	0/3/3/3
2	A86	B	303	-	-	3/34/90/90	0/3/3/3
4	KC2	A	310	-	-	7/15/71/71	-
2	A86	C	307	-	-	3/34/90/90	0/3/3/3
3	CLA	C	318	1	1/1/12/20	6/24/102/115	-
5	KC1	B	315	1	-	3/15/71/71	-
3	CLA	A	309	-	1/1/15/20	14/37/115/115	-
3	CLA	A	317	1	1/1/12/20	6/24/102/115	-
3	CLA	B	314	-	1/1/12/20	7/23/101/115	-
2	A86	B	301	-	-	3/34/90/90	0/3/3/3
3	CLA	A	316	-	1/1/10/20	2/8/86/115	-
3	CLA	C	314	1	1/1/15/20	5/37/115/115	-
3	CLA	C	301	-	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KC2	B	312	1	-	6/15/71/71	-
3	CLA	A	313	1	1/1/15/20	8/37/115/115	-
2	A86	B	304	-	-	4/34/90/90	0/3/3/3
4	KC2	C	311	-	-	6/15/71/71	-
2	A86	A	303	-	-	3/34/90/90	0/3/3/3
3	CLA	C	310	-	1/1/15/20	14/37/115/115	-
3	CLA	C	312	-	1/1/15/20	10/37/115/115	-
2	A86	A	307	-	-	3/34/90/90	0/3/3/3
2	A86	C	305	-	-	4/34/90/90	0/3/3/3
4	KC2	B	310	-	-	7/15/71/71	-
2	A86	C	303	-	-	3/34/90/90	0/3/3/3
3	CLA	C	317	-	1/1/10/20	2/8/86/115	-
2	A86	A	304	-	-	4/34/90/90	0/3/3/3
3	CLA	B	316	-	1/1/10/20	4/8/86/115	-
2	A86	A	302	-	-	5/34/90/90	0/3/3/3
2	A86	C	302	-	-	4/34/90/90	0/3/3/3
6	SQD	C	319	-	-	14/38/58/69	0/1/1/1
3	CLA	B	313	1	1/1/15/20	7/37/115/115	-
4	KC2	A	312	1	-	3/15/71/71	-
6	SQD	B	318	-	-	14/38/58/69	0/1/1/1
2	A86	B	307	-	-	3/34/90/90	0/3/3/3
2	A86	C	304	-	-	3/34/90/90	0/3/3/3
5	KC1	A	315	1	-	3/15/71/71	-
4	KC2	C	313	1	-	4/15/71/71	-
2	A86	A	301	-	-	5/34/90/90	0/3/3/3
2	A86	C	306	-	-	3/34/90/90	0/3/3/3
2	A86	C	308	-	-	3/34/90/90	0/3/3/3
3	CLA	A	319	-	1/1/13/20	7/25/103/115	-
3	CLA	B	308	-	1/1/12/20	4/24/102/115	-
3	CLA	B	311	-	1/1/15/20	12/37/115/115	-
2	A86	B	305	-	-	3/34/90/90	0/3/3/3
2	A86	B	306	-	-	3/34/90/90	0/3/3/3
3	CLA	C	315	-	1/1/12/20	7/23/101/115	-
5	KC1	C	316	1	-	3/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SQD	A	318	-	-	13/38/58/69	0/1/1/1
3	CLA	A	314	-	1/1/12/20	6/22/100/115	-
3	CLA	B	319	-	1/1/13/20	8/25/103/115	-
3	CLA	B	309	-	1/1/15/20	13/37/115/115	-
3	CLA	B	317	1	1/1/12/20	4/24/102/115	-
3	CLA	C	309	-	1/1/13/20	8/29/107/115	-

All (302) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	317	CLA	C4B-NB	7.70	1.42	1.35
3	B	317	CLA	C4B-NB	7.56	1.42	1.35
3	C	318	CLA	C4B-NB	7.54	1.41	1.35
3	A	311	CLA	C4B-NB	7.43	1.41	1.35
3	A	308	CLA	C4B-NB	7.38	1.41	1.35
3	C	309	CLA	C4B-NB	7.36	1.41	1.35
3	B	311	CLA	C4B-NB	7.33	1.41	1.35
3	A	313	CLA	C4B-NB	7.31	1.41	1.35
3	B	314	CLA	C4B-NB	7.31	1.41	1.35
3	A	314	CLA	C4B-NB	7.31	1.41	1.35
3	B	313	CLA	C4B-NB	7.30	1.41	1.35
3	B	316	CLA	C4B-NB	7.28	1.41	1.35
3	A	309	CLA	C4B-NB	7.27	1.41	1.35
3	C	301	CLA	C4B-NB	7.27	1.41	1.35
3	C	310	CLA	C4B-NB	7.27	1.41	1.35
3	C	312	CLA	C4B-NB	7.26	1.41	1.35
3	A	316	CLA	C4B-NB	7.24	1.41	1.35
3	B	319	CLA	C4B-NB	7.22	1.41	1.35
3	C	315	CLA	C4B-NB	7.22	1.41	1.35
3	B	309	CLA	C4B-NB	7.22	1.41	1.35
3	B	308	CLA	C4B-NB	7.22	1.41	1.35
3	C	317	CLA	C4B-NB	7.20	1.41	1.35
3	C	314	CLA	C4B-NB	7.20	1.41	1.35
3	A	319	CLA	C4B-NB	7.20	1.41	1.35
4	A	312	KC2	C4D-CHA	-6.82	1.36	1.45
4	C	313	KC2	C4D-CHA	-6.79	1.36	1.45
5	A	315	KC1	C4D-CHA	-6.75	1.36	1.45
4	B	312	KC2	C4D-CHA	-6.75	1.36	1.45
5	C	316	KC1	C4D-CHA	-6.73	1.36	1.45
4	C	311	KC2	C4D-CHA	-6.71	1.36	1.45
5	B	315	KC1	C4D-CHA	-6.70	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	310	KC2	C4D-CHA	-6.68	1.36	1.45
4	A	310	KC2	C4D-CHA	-6.66	1.36	1.45
4	A	310	KC2	CHD-C4C	5.46	1.49	1.35
4	A	312	KC2	CHD-C4C	5.45	1.48	1.35
4	C	313	KC2	CHD-C4C	5.44	1.48	1.35
4	B	312	KC2	CHD-C4C	5.44	1.48	1.35
4	C	311	KC2	CHD-C4C	5.43	1.48	1.35
4	B	310	KC2	CHD-C4C	5.43	1.48	1.35
2	A	307	A86	O4-C38	4.72	1.45	1.35
2	B	307	A86	O4-C38	4.70	1.45	1.35
2	C	308	A86	O4-C38	4.70	1.45	1.35
2	C	306	A86	O4-C38	4.69	1.45	1.35
2	A	304	A86	O4-C38	4.67	1.45	1.35
2	B	304	A86	O4-C38	4.67	1.45	1.35
5	C	316	KC1	MG-NB	-4.67	1.96	2.05
2	C	305	A86	O4-C38	4.67	1.45	1.35
2	C	303	A86	O4-C38	4.67	1.45	1.35
5	A	315	KC1	MG-NB	-4.66	1.96	2.05
2	A	301	A86	O4-C38	4.66	1.45	1.35
2	A	302	A86	O4-C38	4.66	1.45	1.35
2	A	305	A86	O4-C38	4.66	1.45	1.35
2	A	303	A86	O4-C38	4.66	1.45	1.35
2	C	302	A86	O4-C38	4.66	1.45	1.35
2	B	305	A86	O4-C38	4.65	1.45	1.35
2	B	301	A86	O4-C38	4.63	1.45	1.35
2	B	302	A86	O4-C38	4.63	1.45	1.35
5	B	315	KC1	MG-NB	-4.63	1.96	2.05
2	C	304	A86	O4-C38	4.63	1.45	1.35
2	C	307	A86	O4-C38	4.60	1.45	1.35
2	A	306	A86	O4-C38	4.59	1.45	1.35
2	B	306	A86	O4-C38	4.59	1.45	1.35
2	B	303	A86	O4-C38	4.58	1.45	1.35
4	B	310	KC2	MG-NB	-4.17	1.97	2.05
4	C	311	KC2	CHC-C1C	4.15	1.48	1.39
4	C	311	KC2	MG-NB	-4.14	1.97	2.05
4	B	312	KC2	CHC-C1C	4.13	1.48	1.39
4	A	310	KC2	MG-NB	-4.13	1.97	2.05
4	A	310	KC2	CHC-C1C	4.13	1.48	1.39
4	B	310	KC2	CHC-C1C	4.10	1.48	1.39
4	A	312	KC2	CHC-C1C	4.07	1.48	1.39
4	C	313	KC2	CHC-C1C	4.07	1.48	1.39
4	B	312	KC2	CHC-C4B	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	312	KC2	MG-NB	-4.05	1.97	2.05
4	A	312	KC2	MG-NB	-4.05	1.97	2.05
4	C	313	KC2	MG-NB	-4.05	1.97	2.05
4	A	310	KC2	CHC-C4B	4.04	1.46	1.38
4	B	310	KC2	CHC-C4B	4.03	1.46	1.38
4	C	313	KC2	CHC-C4B	4.01	1.46	1.38
4	C	311	KC2	CHC-C4B	4.00	1.46	1.38
4	A	312	KC2	CHC-C4B	3.99	1.46	1.38
3	A	308	CLA	C1D-ND	3.89	1.42	1.37
3	C	309	CLA	C1D-ND	3.88	1.42	1.37
3	B	317	CLA	C1D-ND	3.86	1.42	1.37
3	A	317	CLA	C1D-ND	3.86	1.42	1.37
3	C	318	CLA	C1D-ND	3.82	1.42	1.37
3	B	311	CLA	C1D-ND	3.81	1.42	1.37
3	A	319	CLA	C1D-ND	3.81	1.42	1.37
3	B	319	CLA	C1D-ND	3.81	1.42	1.37
3	C	315	CLA	C1D-ND	3.80	1.42	1.37
3	B	309	CLA	C1D-ND	3.80	1.42	1.37
3	C	301	CLA	C1D-ND	3.79	1.42	1.37
3	C	310	CLA	C1D-ND	3.78	1.42	1.37
3	B	308	CLA	C1D-ND	3.78	1.42	1.37
3	A	311	CLA	C1D-ND	3.78	1.42	1.37
3	A	316	CLA	C1D-ND	3.77	1.42	1.37
3	A	309	CLA	C1D-ND	3.76	1.42	1.37
3	B	316	CLA	C1D-ND	3.76	1.42	1.37
3	C	312	CLA	C1D-ND	3.74	1.42	1.37
3	C	317	CLA	C1D-ND	3.73	1.42	1.37
3	A	314	CLA	C1D-ND	3.71	1.42	1.37
3	B	314	CLA	C1D-ND	3.70	1.42	1.37
3	C	314	CLA	C1D-ND	3.69	1.42	1.37
3	A	313	CLA	C1D-ND	3.69	1.42	1.37
3	B	313	CLA	C1D-ND	3.67	1.42	1.37
2	A	306	A86	C30-C29	-3.64	1.25	1.32
2	B	305	A86	C30-C29	-3.62	1.25	1.32
2	C	306	A86	C30-C29	-3.59	1.26	1.32
2	C	304	A86	C30-C29	-3.57	1.26	1.32
2	B	306	A86	C30-C29	-3.56	1.26	1.32
2	A	303	A86	C30-C29	-3.55	1.26	1.32
2	C	307	A86	C30-C29	-3.55	1.26	1.32
2	A	307	A86	C30-C29	-3.54	1.26	1.32
2	A	302	A86	C30-C29	-3.53	1.26	1.32
2	C	303	A86	C30-C29	-3.53	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	A86	C30-C29	-3.53	1.26	1.32
2	A	301	A86	C30-C29	-3.52	1.26	1.32
2	B	307	A86	C30-C29	-3.52	1.26	1.32
2	C	308	A86	C30-C29	-3.52	1.26	1.32
2	A	305	A86	C30-C29	-3.51	1.26	1.32
2	C	302	A86	C30-C29	-3.49	1.26	1.32
2	B	302	A86	C30-C29	-3.49	1.26	1.32
2	C	305	A86	C30-C29	-3.48	1.26	1.32
2	B	303	A86	C30-C29	-3.48	1.26	1.32
2	B	304	A86	C30-C29	-3.46	1.26	1.32
2	A	304	A86	C30-C29	-3.46	1.26	1.32
3	B	319	CLA	CHC-C1C	3.16	1.43	1.35
3	C	301	CLA	CHC-C1C	3.16	1.43	1.35
3	A	319	CLA	CHC-C1C	3.15	1.43	1.35
3	A	313	CLA	CHC-C1C	3.15	1.43	1.35
3	A	311	CLA	CHC-C1C	3.14	1.43	1.35
3	B	313	CLA	CHC-C1C	3.13	1.43	1.35
3	B	314	CLA	CHC-C1C	3.13	1.43	1.35
6	B	318	SQD	O48-C23	3.13	1.42	1.33
3	C	314	CLA	CHC-C1C	3.13	1.43	1.35
3	B	308	CLA	CHC-C1C	3.12	1.43	1.35
6	A	318	SQD	O48-C23	3.12	1.42	1.33
3	B	316	CLA	CHC-C1C	3.11	1.42	1.35
3	B	311	CLA	CHC-C1C	3.11	1.42	1.35
6	C	319	SQD	O48-C23	3.10	1.42	1.33
3	A	308	CLA	CHC-C1C	3.10	1.42	1.35
3	C	310	CLA	CHC-C1C	3.10	1.42	1.35
3	C	312	CLA	CHC-C1C	3.10	1.42	1.35
3	A	314	CLA	CHC-C1C	3.09	1.42	1.35
3	C	309	CLA	CHC-C1C	3.09	1.42	1.35
3	A	309	CLA	CHC-C1C	3.09	1.42	1.35
3	C	317	CLA	CHC-C1C	3.09	1.42	1.35
3	C	318	CLA	CHC-C1C	3.09	1.42	1.35
3	B	309	CLA	CHC-C1C	3.08	1.42	1.35
3	C	315	CLA	CHC-C1C	3.08	1.42	1.35
3	A	316	CLA	CHC-C1C	3.08	1.42	1.35
3	A	317	CLA	CHC-C1C	3.07	1.42	1.35
3	B	317	CLA	CHC-C1C	3.07	1.42	1.35
3	B	314	CLA	C4D-ND	-3.04	1.33	1.37
3	B	309	CLA	C4D-ND	-3.02	1.33	1.37
3	C	315	CLA	C4D-ND	-3.02	1.33	1.37
3	C	310	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	309	CLA	C4D-ND	-2.98	1.33	1.37
3	A	314	CLA	C4D-ND	-2.97	1.33	1.37
3	A	308	CLA	C4D-ND	-2.97	1.33	1.37
3	C	314	CLA	C4D-ND	-2.97	1.33	1.37
3	B	316	CLA	C4D-ND	-2.96	1.33	1.37
3	A	316	CLA	C4D-ND	-2.96	1.33	1.37
3	A	313	CLA	C4D-ND	-2.95	1.33	1.37
3	C	312	CLA	C4D-ND	-2.94	1.33	1.37
3	B	319	CLA	C4D-ND	-2.94	1.33	1.37
3	B	311	CLA	C4D-ND	-2.94	1.33	1.37
3	B	308	CLA	C4D-ND	-2.93	1.33	1.37
3	A	319	CLA	C4D-ND	-2.92	1.33	1.37
3	C	318	CLA	C4D-ND	-2.92	1.33	1.37
3	A	311	CLA	C4D-ND	-2.91	1.33	1.37
3	C	317	CLA	C4D-ND	-2.91	1.33	1.37
3	C	309	CLA	C4D-ND	-2.91	1.33	1.37
3	B	313	CLA	C4D-ND	-2.91	1.33	1.37
3	A	317	CLA	C4D-ND	-2.89	1.33	1.37
3	C	301	CLA	C4D-ND	-2.88	1.33	1.37
3	B	317	CLA	C4D-ND	-2.87	1.33	1.37
5	A	315	KC1	CBA-CGA	-2.86	1.41	1.48
4	A	312	KC2	CBA-CGA	-2.84	1.41	1.48
6	C	319	SQD	O47-C7	2.83	1.42	1.34
5	B	315	KC1	C4B-NB	-2.82	1.34	1.37
4	B	312	KC2	CBA-CGA	-2.82	1.42	1.48
5	C	316	KC1	CBA-CGA	-2.82	1.42	1.48
5	A	315	KC1	C4B-NB	-2.81	1.34	1.37
5	B	315	KC1	CBA-CGA	-2.81	1.42	1.48
6	A	318	SQD	O47-C7	2.80	1.42	1.34
4	C	311	KC2	CBA-CGA	-2.80	1.42	1.48
4	B	310	KC2	CBA-CGA	-2.80	1.42	1.48
5	C	316	KC1	C4B-NB	-2.80	1.34	1.37
6	B	318	SQD	O47-C7	2.79	1.42	1.34
4	A	310	KC2	CBA-CGA	-2.79	1.42	1.48
4	C	313	KC2	CBA-CGA	-2.78	1.42	1.48
4	A	312	KC2	C4B-NB	-2.51	1.34	1.37
4	B	310	KC2	C4B-NB	-2.51	1.34	1.37
4	B	312	KC2	C4B-NB	-2.51	1.34	1.37
3	B	313	CLA	CMB-C2B	-2.50	1.46	1.51
4	A	310	KC2	C4B-NB	-2.49	1.34	1.37
3	C	315	CLA	CMB-C2B	-2.48	1.46	1.51
3	C	318	CLA	CMB-C2B	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	311	CLA	CMB-C2B	-2.48	1.46	1.51
3	A	313	CLA	CMB-C2B	-2.48	1.46	1.51
3	C	314	CLA	CMB-C2B	-2.48	1.46	1.51
4	C	313	KC2	C4B-NB	-2.48	1.34	1.37
3	A	314	CLA	CMB-C2B	-2.47	1.46	1.51
4	C	311	KC2	C4B-NB	-2.47	1.34	1.37
3	B	317	CLA	CMB-C2B	-2.46	1.46	1.51
3	B	309	CLA	CMB-C2B	-2.46	1.46	1.51
3	B	316	CLA	CMB-C2B	-2.46	1.46	1.51
3	A	317	CLA	CMB-C2B	-2.45	1.46	1.51
3	C	301	CLA	CMB-C2B	-2.44	1.46	1.51
3	B	308	CLA	CMB-C2B	-2.43	1.46	1.51
3	C	310	CLA	CMB-C2B	-2.43	1.46	1.51
5	B	315	KC1	C1B-NB	-2.43	1.34	1.37
3	A	309	CLA	CMB-C2B	-2.43	1.46	1.51
3	B	314	CLA	CMB-C2B	-2.43	1.46	1.51
5	C	316	KC1	C1B-NB	-2.42	1.34	1.37
3	A	308	CLA	CMB-C2B	-2.42	1.46	1.51
3	C	312	CLA	CMB-C2B	-2.42	1.46	1.51
3	B	311	CLA	CMB-C2B	-2.42	1.46	1.51
3	C	309	CLA	CMB-C2B	-2.42	1.46	1.51
3	B	319	CLA	CMB-C2B	-2.41	1.46	1.51
3	C	317	CLA	CMB-C2B	-2.41	1.46	1.51
5	A	315	KC1	C1B-NB	-2.41	1.34	1.37
3	A	316	CLA	CMB-C2B	-2.39	1.46	1.51
3	A	319	CLA	CMB-C2B	-2.39	1.46	1.51
5	A	315	KC1	CHD-C4C	2.38	1.41	1.35
5	C	316	KC1	CHD-C4C	2.37	1.41	1.35
2	A	303	A86	O1-C20	-2.35	1.42	1.46
2	A	301	A86	O1-C20	-2.35	1.42	1.46
5	B	315	KC1	CHD-C4C	2.34	1.41	1.35
2	A	305	A86	O1-C20	-2.34	1.42	1.46
2	A	304	A86	O1-C20	-2.34	1.42	1.46
2	C	302	A86	O1-C20	-2.33	1.42	1.46
2	B	305	A86	O1-C20	-2.33	1.42	1.46
2	B	302	A86	O1-C20	-2.33	1.42	1.46
2	B	301	A86	O1-C20	-2.32	1.42	1.46
2	C	305	A86	O1-C20	-2.29	1.42	1.46
2	B	303	A86	O1-C20	-2.29	1.42	1.46
2	A	302	A86	O1-C20	-2.29	1.42	1.46
2	A	306	A86	O1-C20	-2.29	1.42	1.46
2	C	303	A86	O1-C20	-2.28	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	306	A86	O1-C20	-2.28	1.42	1.46
2	C	307	A86	O1-C20	-2.27	1.43	1.46
2	A	307	A86	O1-C20	-2.27	1.43	1.46
2	B	304	A86	O1-C20	-2.27	1.43	1.46
2	B	306	A86	O1-C20	-2.26	1.43	1.46
2	B	307	A86	O1-C20	-2.25	1.43	1.46
2	C	304	A86	O1-C20	-2.25	1.43	1.46
5	C	316	KC1	C4A-C3A	-2.24	1.40	1.44
4	B	310	KC2	C4A-C3A	-2.24	1.40	1.44
4	C	313	KC2	C4A-C3A	-2.23	1.40	1.44
2	C	308	A86	O1-C20	-2.22	1.43	1.46
4	B	312	KC2	C4A-C3A	-2.22	1.40	1.44
4	A	312	KC2	C4A-C3A	-2.20	1.40	1.44
4	A	310	KC2	C4A-C3A	-2.18	1.40	1.44
6	C	319	SQD	O2-C2	-2.18	1.37	1.43
5	A	315	KC1	C4A-C3A	-2.17	1.40	1.44
4	C	311	KC2	C4A-C3A	-2.17	1.40	1.44
6	B	318	SQD	O2-C2	-2.17	1.37	1.43
6	A	318	SQD	O2-C2	-2.16	1.37	1.43
3	A	314	CLA	CMD-C2D	-2.16	1.46	1.50
3	B	314	CLA	CMD-C2D	-2.15	1.46	1.50
3	A	313	CLA	CMD-C2D	-2.14	1.46	1.50
5	B	315	KC1	C4A-C3A	-2.14	1.40	1.44
4	A	312	KC2	C1C-C2C	-2.13	1.40	1.44
4	B	312	KC2	C1D-CHD	2.12	1.46	1.41
4	B	312	KC2	C1C-C2C	-2.12	1.40	1.44
4	B	310	KC2	C1D-CHD	2.11	1.46	1.41
4	A	310	KC2	C1D-CHD	2.11	1.46	1.41
4	C	313	KC2	C1D-CHD	2.10	1.46	1.41
3	B	313	CLA	CMD-C2D	-2.10	1.46	1.50
4	C	311	KC2	C1D-CHD	2.10	1.46	1.41
4	A	310	KC2	C1C-C2C	-2.09	1.40	1.44
4	A	312	KC2	C1D-CHD	2.09	1.46	1.41
4	C	313	KC2	C1C-C2C	-2.08	1.40	1.44
6	A	318	SQD	O4-C4	-2.08	1.38	1.43
6	A	318	SQD	O3-C3	-2.07	1.38	1.43
6	C	319	SQD	O4-C4	-2.07	1.38	1.43
3	C	314	CLA	CMD-C2D	-2.07	1.46	1.50
6	B	318	SQD	O4-C4	-2.06	1.38	1.43
3	C	310	CLA	CMD-C2D	-2.06	1.46	1.50
3	A	316	CLA	CMD-C2D	-2.06	1.46	1.50
6	C	319	SQD	O3-C3	-2.06	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	312	CLA	CMD-C2D	-2.06	1.46	1.50
3	B	309	CLA	CMC-C2C	-2.05	1.46	1.50
3	B	316	CLA	CMD-C2D	-2.05	1.46	1.50
6	B	318	SQD	O3-C3	-2.04	1.38	1.43
3	A	309	CLA	CMD-C2D	-2.04	1.46	1.50
3	C	315	CLA	CMD-C2D	-2.04	1.46	1.50
3	C	317	CLA	CMD-C2D	-2.04	1.46	1.50
3	C	309	CLA	CMD-C2D	-2.03	1.46	1.50
3	A	319	CLA	CMD-C2D	-2.03	1.46	1.50
4	B	310	KC2	C1C-C2C	-2.03	1.40	1.44
3	B	319	CLA	CMD-C2D	-2.03	1.46	1.50
4	C	311	KC2	C1C-C2C	-2.03	1.40	1.44
3	B	308	CLA	CMD-C2D	-2.02	1.46	1.50
3	B	311	CLA	CMD-C2D	-2.02	1.46	1.50
3	B	309	CLA	CMD-C2D	-2.02	1.46	1.50
3	A	309	CLA	CMC-C2C	-2.02	1.46	1.50
3	A	311	CLA	CMD-C2D	-2.02	1.46	1.50
3	A	317	CLA	CMD-C2D	-2.01	1.46	1.50
3	A	308	CLA	CMD-C2D	-2.01	1.46	1.50

All (675) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	A86	O1-C20-C19	41.67	144.69	113.38
2	B	302	A86	O1-C20-C19	39.26	142.88	113.38
2	C	303	A86	O1-C20-C19	36.82	141.04	113.38
2	B	305	A86	O1-C20-C19	34.63	139.40	113.38
2	B	306	A86	O1-C20-C19	34.49	139.29	113.38
2	C	307	A86	O1-C20-C19	34.42	139.24	113.38
2	A	306	A86	O1-C20-C19	34.36	139.19	113.38
2	A	303	A86	O1-C20-C19	33.55	138.58	113.38
2	C	308	A86	O1-C20-C19	33.25	138.36	113.38
2	C	304	A86	O1-C20-C19	33.11	138.25	113.38
2	C	306	A86	O1-C20-C19	32.63	137.89	113.38
2	B	304	A86	O1-C20-C19	32.58	137.86	113.38
2	B	301	A86	O1-C20-C19	32.58	137.85	113.38
2	B	307	A86	O1-C20-C19	32.26	137.62	113.38
2	A	307	A86	O1-C20-C19	32.20	137.57	113.38
2	B	303	A86	O1-C20-C19	32.19	137.57	113.38
2	A	304	A86	O1-C20-C19	31.93	137.37	113.38
2	A	305	A86	O1-C20-C19	31.70	137.20	113.38
2	A	301	A86	O1-C20-C19	31.47	137.02	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	304	A86	C34-O4-C38	30.81	175.31	117.90
2	C	305	A86	O1-C20-C19	30.66	136.41	113.38
2	A	303	A86	C34-O4-C38	30.53	174.79	117.90
2	C	302	A86	O1-C20-C19	29.80	135.77	113.38
2	A	302	A86	O1-C15-C14	-29.22	54.57	113.21
2	B	302	A86	O1-C15-C14	-27.16	58.71	113.21
2	A	307	A86	O1-C15-C14	-26.22	60.59	113.21
2	C	303	A86	O1-C15-C14	-26.18	60.68	113.21
2	C	308	A86	O1-C15-C14	-26.11	60.81	113.21
2	B	307	A86	O1-C15-C14	-23.63	65.80	113.21
2	C	302	A86	O1-C15-C14	-23.51	66.04	113.21
2	B	306	A86	O1-C15-C14	-22.85	67.36	113.21
2	B	301	A86	O1-C15-C14	-22.68	67.69	113.21
2	A	301	A86	O1-C15-C14	-22.25	68.56	113.21
2	A	306	A86	O1-C15-C14	-21.89	69.28	113.21
2	C	306	A86	O1-C15-C14	-21.79	69.48	113.21
2	C	307	A86	O1-C15-C14	-21.39	70.28	113.21
2	B	305	A86	O1-C15-C14	-21.08	70.91	113.21
2	C	304	A86	O1-C15-C14	-20.09	72.89	113.21
2	A	305	A86	O1-C15-C14	-20.08	72.91	113.21
2	B	307	A86	C34-O4-C38	19.84	154.87	117.90
2	B	303	A86	O1-C15-C14	-18.85	75.39	113.21
2	A	303	A86	O1-C15-C14	-18.78	75.51	113.21
2	A	307	A86	C34-O4-C38	18.59	152.54	117.90
2	B	304	A86	O1-C15-C14	-17.79	77.51	113.21
2	C	308	A86	C34-O4-C38	17.78	151.03	117.90
2	A	304	A86	O1-C15-C14	-16.79	79.52	113.21
2	C	305	A86	O1-C15-C14	-14.61	83.89	113.21
2	C	305	A86	C34-O4-C38	10.61	137.67	117.90
2	A	306	A86	C34-O4-C38	-10.35	98.60	117.90
2	C	307	A86	C34-O4-C38	-10.08	99.12	117.90
2	A	301	A86	C34-O4-C38	9.89	136.32	117.90
2	B	306	A86	C34-O4-C38	-9.05	101.03	117.90
2	A	302	A86	C34-O4-C38	-8.34	102.36	117.90
2	C	302	A86	C34-O4-C38	8.32	133.41	117.90
2	C	306	A86	C34-O4-C38	7.57	132.01	117.90
2	A	305	A86	C34-O4-C38	7.48	131.84	117.90
4	B	310	KC2	CHB-C1B-NB	7.37	131.22	124.45
4	A	310	KC2	CHB-C1B-NB	7.35	131.21	124.45
4	C	311	KC2	CHB-C1B-NB	7.34	131.20	124.45
2	C	303	A86	C34-O4-C38	-7.29	104.31	117.90
2	B	305	A86	C34-O4-C38	7.29	131.47	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	312	KC2	CHB-C1B-NB	7.22	131.09	124.45
4	C	313	KC2	CHB-C1B-NB	7.19	131.06	124.45
2	A	302	A86	O1-C20-C21	-7.18	106.46	115.06
4	A	312	KC2	CHB-C1B-NB	7.18	131.05	124.45
2	B	302	A86	C34-O4-C38	-7.10	104.67	117.90
2	B	302	A86	O-C13-C14	-7.05	107.33	121.66
2	B	301	A86	C34-O4-C38	6.87	130.70	117.90
3	B	309	CLA	C4A-NA-C1A	6.69	109.72	106.71
2	C	303	A86	O-C13-C14	-6.66	108.13	121.66
3	A	314	CLA	C4A-NA-C1A	6.65	109.69	106.71
3	B	314	CLA	C4A-NA-C1A	6.63	109.69	106.71
3	C	310	CLA	C4A-NA-C1A	6.62	109.68	106.71
3	B	316	CLA	C4A-NA-C1A	6.62	109.68	106.71
3	A	316	CLA	C4A-NA-C1A	6.60	109.67	106.71
3	C	309	CLA	C4A-NA-C1A	6.60	109.67	106.71
3	A	308	CLA	C4A-NA-C1A	6.58	109.67	106.71
3	C	315	CLA	C4A-NA-C1A	6.55	109.65	106.71
3	A	313	CLA	C4A-NA-C1A	6.55	109.65	106.71
3	A	309	CLA	C4A-NA-C1A	6.54	109.65	106.71
3	C	317	CLA	C4A-NA-C1A	6.54	109.65	106.71
3	B	311	CLA	C4A-NA-C1A	6.54	109.65	106.71
3	B	319	CLA	C4A-NA-C1A	6.54	109.64	106.71
3	B	308	CLA	C4A-NA-C1A	6.48	109.62	106.71
3	A	319	CLA	C4A-NA-C1A	6.46	109.61	106.71
3	C	312	CLA	C4A-NA-C1A	6.45	109.61	106.71
3	A	317	CLA	C4A-NA-C1A	6.43	109.60	106.71
3	A	311	CLA	C4A-NA-C1A	6.43	109.60	106.71
3	B	313	CLA	C4A-NA-C1A	6.38	109.57	106.71
3	B	317	CLA	C4A-NA-C1A	6.37	109.57	106.71
4	A	310	KC2	CHC-C4B-NB	6.37	130.31	124.45
3	C	318	CLA	C4A-NA-C1A	6.36	109.56	106.71
4	A	312	KC2	CHC-C4B-NB	6.35	130.29	124.45
4	C	311	KC2	CHC-C4B-NB	6.34	130.28	124.45
4	B	310	KC2	CHC-C4B-NB	6.33	130.27	124.45
3	C	301	CLA	C4A-NA-C1A	6.29	109.53	106.71
4	B	312	KC2	CHC-C4B-NB	6.29	130.23	124.45
4	C	313	KC2	CHC-C4B-NB	6.28	130.22	124.45
2	A	307	A86	O-C13-C14	-6.27	108.91	121.66
3	C	314	CLA	C4A-NA-C1A	6.24	109.51	106.71
5	A	315	KC1	CHB-C1B-NB	6.24	130.19	124.45
5	B	315	KC1	CHB-C1B-NB	6.20	130.15	124.45
2	B	301	A86	O1-C20-C21	-6.20	107.63	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	A86	O1-C20-C21	-6.19	107.64	115.06
5	C	316	KC1	CHC-C4B-NB	6.17	130.12	124.45
5	C	316	KC1	CHB-C1B-NB	6.15	130.11	124.45
2	B	302	A86	O1-C20-C21	-6.13	107.71	115.06
5	A	315	KC1	CHC-C4B-NB	6.12	130.08	124.45
2	C	307	A86	O1-C20-C21	-6.11	107.74	115.06
2	C	302	A86	O-C13-C14	-6.10	109.26	121.66
5	B	315	KC1	CHC-C4B-NB	6.10	130.06	124.45
2	B	306	A86	O1-C20-C21	-6.04	107.82	115.06
2	A	302	A86	O-C13-C14	-6.00	109.47	121.66
2	C	302	A86	O1-C20-C21	-5.89	108.00	115.06
2	C	306	A86	O1-C20-C21	-5.83	108.07	115.06
2	C	308	A86	O-C13-C14	-5.81	109.84	121.66
2	A	304	A86	C34-O4-C38	5.81	128.73	117.90
2	B	305	A86	O1-C20-C21	-5.81	108.09	115.06
2	A	306	A86	O1-C20-C21	-5.79	108.12	115.06
2	B	307	A86	O1-C20-C21	-5.76	108.16	115.06
2	C	308	A86	O1-C20-C21	-5.72	108.20	115.06
2	A	307	A86	O1-C20-C21	-5.71	108.22	115.06
2	A	305	A86	O1-C20-C21	-5.68	108.25	115.06
2	A	302	A86	C21-C20-C19	-5.66	107.91	114.28
2	C	305	A86	O1-C20-C21	-5.64	108.30	115.06
2	B	304	A86	O1-C20-C21	-5.55	108.40	115.06
2	A	304	A86	O1-C20-C21	-5.53	108.43	115.06
2	C	303	A86	O1-C20-C21	-5.45	108.52	115.06
2	B	301	A86	C4-C5-C6	-5.45	119.54	127.31
2	A	303	A86	O1-C20-C21	-5.35	108.65	115.06
2	C	303	A86	C4-C5-C6	-5.27	119.78	127.31
2	B	303	A86	O1-C20-C21	-5.26	108.75	115.06
2	B	302	A86	C4-C5-C6	-5.21	119.87	127.31
2	A	301	A86	C4-C5-C6	-5.19	119.91	127.31
2	A	302	A86	C4-C5-C6	-5.15	119.96	127.31
2	A	307	A86	C25-C26-C27	-5.15	119.97	127.31
2	C	304	A86	O1-C20-C21	-5.15	108.89	115.06
2	C	302	A86	C4-C5-C6	-5.11	120.02	127.31
2	C	308	A86	C4-C5-C6	-5.03	120.13	127.31
2	A	304	A86	C25-C26-C27	-5.02	120.15	127.31
2	C	308	A86	C25-C26-C27	-5.02	120.15	127.31
2	A	307	A86	C3-C2-C1	-5.01	120.16	127.31
2	C	308	A86	C3-C2-C1	-5.00	120.17	127.31
2	B	303	A86	C3-C2-C1	-4.99	120.18	127.31
2	B	307	A86	C4-C5-C6	-4.98	120.20	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	307	A86	C25-C26-C27	-4.98	120.21	127.31
2	B	307	A86	O-C13-C14	-4.98	111.55	121.66
2	A	307	A86	C4-C5-C6	-4.97	120.21	127.31
2	B	302	A86	C21-C20-C19	-4.97	108.69	114.28
2	B	301	A86	C21-C20-C19	-4.93	108.73	114.28
2	B	304	A86	C25-C26-C27	-4.91	120.31	127.31
2	B	305	A86	C3-C2-C1	-4.89	120.33	127.31
2	A	305	A86	C3-C2-C1	-4.88	120.34	127.31
2	A	306	A86	C4-C5-C6	-4.85	120.39	127.31
2	B	307	A86	C3-C2-C1	-4.84	120.40	127.31
2	B	306	A86	C4-C5-C6	-4.83	120.41	127.31
2	C	305	A86	C25-C26-C27	-4.80	120.45	127.31
2	A	303	A86	C3-C2-C1	-4.79	120.47	127.31
2	C	306	A86	C3-C2-C1	-4.79	120.47	127.31
5	A	315	KC1	O2D-CGD-CBD	4.77	119.74	111.27
2	A	301	A86	C21-C20-C19	-4.75	108.94	114.28
2	C	307	A86	C4-C5-C6	-4.74	120.54	127.31
2	A	306	A86	C3-C2-C1	-4.73	120.57	127.31
5	B	315	KC1	O2D-CGD-CBD	4.71	119.63	111.27
2	C	303	A86	C25-C26-C27	-4.70	120.60	127.31
5	C	316	KC1	O2D-CGD-CBD	4.70	119.62	111.27
2	B	304	A86	C3-C2-C1	-4.68	120.63	127.31
2	A	302	A86	C25-C26-C27	-4.67	120.64	127.31
2	C	302	A86	C21-C20-C19	-4.67	109.03	114.28
2	A	304	A86	C3-C2-C1	-4.66	120.65	127.31
4	C	313	KC2	O2D-CGD-CBD	4.66	119.55	111.27
2	B	302	A86	C25-C26-C27	-4.64	120.69	127.31
2	B	306	A86	C3-C2-C1	-4.64	120.69	127.31
2	B	304	A86	O4-C38-C39	4.63	119.60	111.09
2	C	305	A86	C3-C2-C1	-4.62	120.72	127.31
2	A	305	A86	C25-C26-C27	-4.61	120.73	127.31
2	B	301	A86	O-C13-C14	-4.61	112.29	121.66
2	C	307	A86	C3-C2-C1	-4.60	120.74	127.31
2	C	306	A86	C25-C26-C27	-4.60	120.74	127.31
2	A	303	A86	C25-C26-C27	-4.59	120.76	127.31
2	A	304	A86	O4-C38-C39	4.59	119.53	111.09
2	B	305	A86	C4-C5-C6	-4.58	120.77	127.31
2	C	304	A86	C25-C26-C27	-4.57	120.78	127.31
4	B	312	KC2	O2D-CGD-CBD	4.57	119.40	111.27
4	A	312	KC2	O2D-CGD-CBD	4.57	119.39	111.27
2	C	304	A86	C4-C5-C6	-4.57	120.79	127.31
2	B	305	A86	C25-C26-C27	-4.56	120.80	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	305	A86	O4-C38-C39	4.55	119.46	111.09
2	C	306	A86	C4-C5-C6	-4.53	120.84	127.31
2	B	305	A86	O4-C38-C39	4.52	119.41	111.09
4	C	311	KC2	O2D-CGD-CBD	4.52	119.30	111.27
2	C	307	A86	C21-C20-C19	-4.52	109.19	114.28
2	C	304	A86	C3-C2-C1	-4.52	120.86	127.31
2	B	306	A86	C21-C20-C19	-4.51	109.20	114.28
2	A	305	A86	O4-C38-C39	4.51	119.38	111.09
2	C	306	A86	O4-C38-C39	4.51	119.38	111.09
2	A	304	A86	C4-C5-C6	-4.50	120.89	127.31
2	B	304	A86	C34-O4-C38	4.50	126.28	117.90
2	A	303	A86	O4-C38-C39	4.49	119.35	111.09
2	C	305	A86	C4-C5-C6	-4.48	120.91	127.31
2	B	303	A86	C4-C5-C6	-4.48	120.92	127.31
4	B	310	KC2	O2D-CGD-CBD	4.47	119.21	111.27
2	B	307	A86	O4-C38-C39	4.47	119.31	111.09
2	C	303	A86	O4-C38-C39	4.47	119.31	111.09
2	A	302	A86	O4-C38-C39	4.47	119.31	111.09
2	B	302	A86	O4-C38-C39	4.46	119.30	111.09
2	A	305	A86	C4-C5-C6	-4.46	120.94	127.31
2	B	304	A86	C4-C5-C6	-4.46	120.94	127.31
2	A	301	A86	O4-C38-C39	4.45	119.28	111.09
2	B	301	A86	O4-C38-C39	4.45	119.28	111.09
2	C	304	A86	O4-C38-C39	4.45	119.28	111.09
2	A	303	A86	C21-C20-C19	-4.45	109.28	114.28
2	B	305	A86	O-C13-C14	4.45	130.69	121.66
2	A	303	A86	C4-C5-C6	-4.45	120.97	127.31
2	C	302	A86	O4-C38-C39	4.44	119.27	111.09
2	C	308	A86	O4-C38-C39	4.44	119.27	111.09
2	A	307	A86	O4-C38-C39	4.44	119.27	111.09
2	B	301	A86	C25-C26-C27	-4.40	121.03	127.31
2	A	301	A86	C25-C26-C27	-4.39	121.05	127.31
2	C	307	A86	O4-C38-C39	4.38	119.14	111.09
2	C	303	A86	C21-C20-C19	-4.37	109.36	114.28
4	A	310	KC2	O2D-CGD-CBD	4.37	119.03	111.27
2	B	303	A86	C21-C20-C19	-4.37	109.37	114.28
2	A	306	A86	O4-C38-C39	4.37	119.12	111.09
6	C	319	SQD	O7-S-C6	4.36	112.11	106.94
2	B	306	A86	O4-C38-C39	4.34	119.08	111.09
2	C	302	A86	C25-C26-C27	-4.34	121.12	127.31
2	B	305	A86	C21-C20-C19	-4.34	109.40	114.28
3	A	319	CLA	CMB-C2B-C1B	-4.33	121.80	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	304	A86	C21-C20-C19	-4.32	109.42	114.28
2	B	303	A86	O4-C38-C39	4.32	119.03	111.09
2	C	303	A86	C3-C2-C1	-4.29	121.19	127.31
2	B	306	A86	C25-C26-C27	-4.29	121.19	127.31
2	A	306	A86	C25-C26-C27	-4.28	121.20	127.31
3	B	319	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
2	A	302	A86	C3-C2-C1	-4.27	121.22	127.31
2	A	301	A86	C3-C2-C1	-4.25	121.25	127.31
2	C	306	A86	C21-C20-C19	-4.24	109.51	114.28
2	C	308	A86	C21-C20-C19	-4.23	109.52	114.28
2	C	306	A86	O-C13-C14	4.23	130.25	121.66
6	A	318	SQD	O7-S-C6	4.22	111.95	106.94
2	B	302	A86	C3-C2-C1	-4.21	121.30	127.31
2	A	306	A86	C21-C20-C19	-4.20	109.55	114.28
2	C	307	A86	C25-C26-C27	-4.19	121.33	127.31
2	A	307	A86	C21-C20-C19	-4.17	109.59	114.28
2	C	302	A86	C3-C2-C1	-4.16	121.37	127.31
6	B	318	SQD	O7-S-C6	4.16	111.88	106.94
2	A	305	A86	C21-C20-C19	-4.14	109.62	114.28
2	C	305	A86	C21-C20-C19	-4.13	109.64	114.28
2	B	307	A86	C21-C20-C19	-4.13	109.64	114.28
2	B	301	A86	C3-C2-C1	-4.09	121.47	127.31
3	C	315	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
2	A	304	A86	C21-C20-C19	-4.03	109.75	114.28
3	B	314	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
2	B	304	A86	C21-C20-C19	-4.01	109.77	114.28
3	C	301	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
2	A	301	A86	O-C13-C14	-3.99	113.55	121.66
3	A	314	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
3	C	312	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
3	B	311	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
4	B	310	KC2	C4B-CHC-C1C	-3.87	117.71	126.06
3	A	311	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
3	C	310	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
4	C	311	KC2	C4B-CHC-C1C	-3.87	117.72	126.06
4	A	310	KC2	C4B-CHC-C1C	-3.86	117.73	126.06
3	C	314	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
3	B	313	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
3	A	313	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
4	B	312	KC2	C4B-CHC-C1C	-3.81	117.83	126.06
4	A	312	KC2	C4B-CHC-C1C	-3.80	117.87	126.06
4	C	313	KC2	C4B-CHC-C1C	-3.79	117.88	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	303	A86	C25-C26-C27	-3.76	121.94	127.31
2	A	305	A86	O-C13-C14	3.76	129.30	121.66
3	B	309	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
3	A	309	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
6	C	319	SQD	O9-S-O7	-3.73	101.04	113.95
3	B	308	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
6	A	318	SQD	O9-S-O7	-3.73	101.05	113.95
6	B	318	SQD	O9-S-O7	-3.72	101.06	113.95
3	A	308	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
3	C	317	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
3	A	316	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
3	C	309	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
3	B	316	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
3	A	319	CLA	CMB-C2B-C3B	3.61	131.44	124.68
3	B	319	CLA	CMB-C2B-C3B	3.58	131.38	124.68
2	A	306	A86	O-C13-C14	3.57	128.92	121.66
6	B	318	SQD	O47-C7-C8	3.52	119.09	111.50
6	C	319	SQD	O47-C7-C8	3.50	119.04	111.50
4	B	310	KC2	CHB-C1B-C2B	-3.50	118.15	125.48
4	A	310	KC2	CHB-C1B-C2B	-3.49	118.16	125.48
4	C	311	KC2	CHB-C1B-C2B	-3.48	118.18	125.48
6	A	318	SQD	O47-C7-C8	3.48	119.00	111.50
3	C	318	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
4	C	313	KC2	CHB-C1B-C2B	-3.42	118.31	125.48
4	A	312	KC2	CHB-C1B-C2B	-3.41	118.32	125.48
3	A	317	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
3	B	317	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
4	B	312	KC2	CHB-C1B-C2B	-3.40	118.36	125.48
3	C	315	CLA	CMB-C2B-C3B	3.37	130.99	124.68
3	C	301	CLA	CMB-C2B-C3B	3.35	130.95	124.68
2	C	305	A86	C40-C32-C31	-3.33	107.49	110.47
6	C	319	SQD	C44-O6-C1	3.33	120.24	113.74
4	A	312	KC2	CHC-C4B-C3B	-3.30	119.61	125.26
3	A	314	CLA	CMB-C2B-C3B	3.30	130.85	124.68
3	B	314	CLA	CMB-C2B-C3B	3.29	130.84	124.68
4	C	313	KC2	CHC-C4B-C3B	-3.28	119.65	125.26
4	B	310	KC2	CHC-C4B-C3B	-3.27	119.67	125.26
4	C	311	KC2	CHC-C4B-C3B	-3.26	119.69	125.26
3	A	311	CLA	CMB-C2B-C3B	3.25	130.76	124.68
3	C	312	CLA	CMB-C2B-C3B	3.25	130.76	124.68
4	B	312	KC2	CHC-C4B-C3B	-3.24	119.71	125.26
3	C	310	CLA	CMB-C2B-C3B	3.24	130.75	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	307	A86	C40-C32-C31	-3.24	107.58	110.47
3	B	311	CLA	CMB-C2B-C3B	3.23	130.73	124.68
4	A	310	KC2	CHC-C4B-C3B	-3.23	119.73	125.26
6	B	318	SQD	O9-S-C6	3.23	110.78	106.94
6	A	318	SQD	O9-S-C6	3.21	110.75	106.94
6	A	318	SQD	C44-O6-C1	3.20	120.00	113.74
2	C	308	A86	C40-C32-C31	-3.20	107.61	110.47
6	C	319	SQD	O6-C1-C2	3.15	113.22	108.30
2	B	304	A86	C40-C32-C31	-3.15	107.65	110.47
3	B	313	CLA	CMB-C2B-C3B	3.15	130.57	124.68
2	C	307	A86	O-C13-C14	3.15	128.05	121.66
3	A	309	CLA	CMB-C2B-C3B	3.14	130.56	124.68
6	B	318	SQD	C44-O6-C1	3.14	119.88	113.74
2	A	307	A86	C40-C32-C31	-3.14	107.66	110.47
3	C	314	CLA	CMB-C2B-C3B	3.14	130.55	124.68
3	A	313	CLA	CMB-C2B-C3B	3.13	130.54	124.68
3	B	309	CLA	CMB-C2B-C3B	3.13	130.54	124.68
3	B	308	CLA	CMB-C2B-C3B	3.10	130.48	124.68
3	A	308	CLA	CMB-C2B-C3B	3.09	130.46	124.68
6	C	319	SQD	O9-S-C6	3.08	110.60	106.94
3	C	309	CLA	CMB-C2B-C3B	3.08	130.44	124.68
3	A	316	CLA	CMB-C2B-C3B	3.06	130.40	124.68
2	A	304	A86	C40-C32-C31	-3.06	107.74	110.47
3	C	317	CLA	CMB-C2B-C3B	3.06	130.40	124.68
6	A	318	SQD	O6-C1-C2	3.05	113.06	108.30
6	B	318	SQD	O6-C1-C2	3.02	113.02	108.30
3	B	316	CLA	CMB-C2B-C3B	3.01	130.30	124.68
6	A	318	SQD	O8-S-C6	2.97	110.48	105.74
3	B	311	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
3	C	312	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
3	A	317	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
3	B	317	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
3	A	311	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
2	B	307	A86	C35-C34-C33	-2.94	104.75	109.88
6	B	318	SQD	O8-S-C6	2.94	110.42	105.74
3	C	309	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
6	C	319	SQD	O8-S-C6	2.93	110.41	105.74
3	C	318	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
3	C	310	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
3	B	309	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
3	A	309	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
2	C	304	A86	C40-C32-C31	-2.92	107.86	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	316	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
3	A	308	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
4	B	312	KC2	CBD-CHA-C1A	2.90	134.29	128.88
4	C	313	KC2	CBD-CHA-C1A	2.90	134.28	128.88
2	C	308	A86	C35-C34-C33	-2.90	104.82	109.88
3	A	316	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
4	A	312	KC2	CBD-CHA-C1A	2.89	134.27	128.88
2	A	307	A86	C35-C34-C33	-2.89	104.84	109.88
3	C	317	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
3	C	301	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
4	B	310	KC2	C1A-NA-C4A	-2.85	105.42	106.71
2	B	303	A86	C34-O4-C38	2.85	123.20	117.90
2	A	303	A86	C40-C32-C31	-2.85	107.92	110.47
5	A	315	KC1	CHC-C4B-C3B	-2.84	120.39	125.26
3	A	319	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
3	B	319	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
4	B	312	KC2	C1A-NA-C4A	-2.83	105.43	106.71
3	A	313	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
3	B	313	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
5	B	315	KC1	CHC-C4B-C3B	-2.81	120.44	125.26
5	C	316	KC1	CHC-C4B-C3B	-2.81	120.44	125.26
4	C	313	KC2	C1A-NA-C4A	-2.81	105.44	106.71
4	A	312	KC2	C3D-CAD-CBD	-2.81	103.91	107.61
3	C	318	CLA	CMB-C2B-C3B	2.78	129.88	124.68
4	C	311	KC2	C1A-NA-C4A	-2.77	105.46	106.71
3	B	317	CLA	CMB-C2B-C3B	2.77	129.85	124.68
4	A	310	KC2	C1A-NA-C4A	-2.76	105.47	106.71
3	B	308	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
2	C	305	A86	C35-C34-C33	-2.75	105.08	109.88
4	C	311	KC2	CBD-CHA-C1A	2.75	134.00	128.88
3	C	315	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
3	A	317	CLA	CMB-C2B-C3B	2.74	129.81	124.68
4	A	312	KC2	C1A-NA-C4A	-2.73	105.48	106.71
3	A	314	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
3	B	314	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
4	A	310	KC2	C3D-CAD-CBD	-2.72	104.02	107.61
6	A	318	SQD	O5-C5-C4	2.72	114.64	109.69
3	C	314	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
4	A	310	KC2	CBD-CHA-C1A	2.71	133.94	128.88
4	C	313	KC2	C3D-CAD-CBD	-2.71	104.04	107.61
4	B	310	KC2	C3D-CAD-CBD	-2.71	104.04	107.61
6	C	319	SQD	O5-C5-C4	2.71	114.61	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	304	A86	C35-C34-C33	-2.71	105.15	109.88
6	B	318	SQD	O5-C5-C4	2.70	114.60	109.69
4	C	311	KC2	C3D-CAD-CBD	-2.70	104.05	107.61
5	A	315	KC1	CHB-C1B-C2B	-2.69	119.84	125.48
2	B	304	A86	C35-C34-C33	-2.69	105.18	109.88
3	B	316	CLA	CAA-C2A-C3A	-2.69	109.83	116.10
2	A	304	A86	C35-C34-C33	-2.69	105.19	109.88
2	C	302	A86	C40-C32-C31	-2.68	108.08	110.47
4	B	310	KC2	CBD-CHA-C1A	2.68	133.87	128.88
2	A	303	A86	C35-C34-C33	-2.68	105.21	109.88
2	C	303	A86	C40-C32-C31	-2.67	108.08	110.47
4	B	310	KC2	CHD-C4C-NC	2.67	128.25	124.20
4	A	310	KC2	CHD-C4C-NC	2.66	128.24	124.20
5	B	315	KC1	CHB-C1B-C2B	-2.66	119.90	125.48
4	C	311	KC2	CHD-C4C-NC	2.66	128.24	124.20
4	B	312	KC2	C3D-CAD-CBD	-2.65	104.11	107.61
2	C	303	A86	C35-C34-C33	-2.65	105.26	109.88
5	C	316	KC1	CHB-C1B-C2B	-2.64	119.93	125.48
2	B	306	A86	C35-C34-C33	-2.63	105.29	109.88
3	A	316	CLA	CAA-C2A-C3A	-2.62	109.98	116.10
2	B	302	A86	C35-C34-C33	-2.61	105.32	109.88
3	C	317	CLA	CAA-C2A-C3A	-2.61	110.02	116.10
2	A	302	A86	C35-C34-C33	-2.60	105.34	109.88
2	B	301	A86	C40-C32-C31	-2.59	108.15	110.47
2	C	307	A86	C35-C34-C33	-2.59	105.36	109.88
2	C	302	A86	C35-C34-C33	-2.59	105.36	109.88
2	A	306	A86	C35-C34-C33	-2.58	105.38	109.88
2	B	301	A86	C35-C34-C33	-2.57	105.39	109.88
2	A	301	A86	C40-C32-C31	-2.57	108.17	110.47
5	A	315	KC1	CBD-CHA-C1A	2.56	133.66	128.88
2	A	301	A86	C9-C10-C11	-2.56	119.08	126.61
2	A	301	A86	C35-C34-C33	-2.55	105.42	109.88
5	B	315	KC1	CBD-CHA-C1A	2.55	133.64	128.88
5	C	316	KC1	CBD-CHA-C1A	2.54	133.62	128.88
6	A	318	SQD	O48-C23-C24	2.52	119.83	111.91
3	B	311	CLA	CHB-C4A-NA	2.52	127.99	124.51
2	A	302	A86	C40-C32-C31	-2.51	108.23	110.47
3	C	309	CLA	CHB-C4A-NA	2.51	127.98	124.51
3	A	316	CLA	CHB-C4A-NA	2.50	127.97	124.51
2	A	303	A86	C12-C11-C13	2.50	120.23	116.02
3	A	311	CLA	CHB-C4A-NA	2.50	127.97	124.51
3	A	314	CLA	C1-C2-C3	-2.50	121.73	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	319	SQD	O48-C23-C24	2.49	119.73	111.91
3	C	312	CLA	CHB-C4A-NA	2.49	127.96	124.51
2	A	306	A86	C12-C11-C13	2.49	120.20	116.02
6	B	318	SQD	O48-C23-C24	2.49	119.71	111.91
3	C	301	CLA	C1-C2-C3	-2.48	121.75	126.04
3	B	316	CLA	CHB-C4A-NA	2.48	127.95	124.51
2	B	301	A86	C4-C3-C2	-2.48	118.39	123.47
5	C	316	KC1	C4B-CHC-C1C	-2.48	120.72	126.06
3	A	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
3	B	319	CLA	CHB-C4A-NA	2.47	127.93	124.51
2	C	304	A86	C12-C11-C13	2.47	120.17	116.02
3	A	308	CLA	CHB-C4A-NA	2.47	127.93	124.51
3	B	313	CLA	CHB-C4A-NA	2.47	127.92	124.51
3	B	314	CLA	CHB-C4A-NA	2.47	127.92	124.51
3	B	317	CLA	CHB-C4A-NA	2.47	127.92	124.51
2	C	302	A86	C9-C10-C11	-2.47	119.36	126.61
2	B	303	A86	C12-C11-C13	2.46	120.16	116.02
5	A	315	KC1	C4B-CHC-C1C	-2.46	120.74	126.06
3	C	314	CLA	CHB-C4A-NA	2.46	127.92	124.51
3	A	314	CLA	CHB-C4A-NA	2.46	127.91	124.51
3	B	308	CLA	CHB-C4A-NA	2.46	127.91	124.51
3	C	317	CLA	CHB-C4A-NA	2.46	127.91	124.51
3	C	315	CLA	CHB-C4A-NA	2.45	127.91	124.51
4	A	310	KC2	O1D-CGD-CBD	-2.45	119.48	124.48
3	B	309	CLA	CHB-C4A-NA	2.44	127.89	124.51
3	A	319	CLA	CHB-C4A-NA	2.44	127.89	124.51
3	A	317	CLA	CHB-C4A-NA	2.44	127.88	124.51
2	A	301	A86	C9-C8-C6	-2.44	119.57	126.42
5	B	315	KC1	C4B-CHC-C1C	-2.44	120.80	126.06
2	C	307	A86	C12-C11-C13	2.44	120.11	116.02
3	C	318	CLA	CHB-C4A-NA	2.44	127.88	124.51
3	A	309	CLA	CHB-C4A-NA	2.43	127.87	124.51
3	C	310	CLA	CHB-C4A-NA	2.43	127.87	124.51
2	B	307	A86	C12-C11-C13	2.43	120.10	116.02
2	B	306	A86	C12-C11-C13	2.42	120.09	116.02
3	C	301	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
2	C	306	A86	C35-C34-C33	-2.42	105.65	109.88
2	A	305	A86	O4-C38-O5	-2.41	118.18	122.96
2	B	302	A86	C40-C32-C31	-2.40	108.32	110.47
2	C	306	A86	O4-C38-O5	-2.40	118.19	122.96
2	A	305	A86	C35-C34-C33	-2.40	105.68	109.88
2	B	305	A86	C35-C34-C33	-2.40	105.69	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	312	KC2	CHD-C4C-NC	2.40	127.84	124.20
3	A	309	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
3	C	310	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
2	C	302	A86	C9-C8-C6	-2.38	119.72	126.42
2	C	308	A86	C12-C11-C13	2.38	120.03	116.02
2	B	305	A86	O4-C38-O5	-2.38	118.23	122.96
3	B	309	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
4	C	313	KC2	CHD-C4C-NC	2.37	127.80	124.20
4	B	310	KC2	O1D-CGD-CBD	-2.37	119.63	124.48
4	A	312	KC2	CHD-C4C-NC	2.37	127.80	124.20
3	C	314	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
2	C	305	A86	O4-C38-O5	-2.37	118.26	122.96
4	B	312	KC2	O1D-CGD-CBD	-2.37	119.64	124.48
3	C	312	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
3	C	301	CLA	CHB-C4A-NA	2.36	127.78	124.51
3	A	311	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
2	A	302	A86	O4-C38-O5	-2.36	118.28	122.96
3	A	311	CLA	C1-C2-C3	-2.36	121.97	126.04
2	C	302	A86	C4-C3-C2	-2.36	118.65	123.47
3	B	313	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
2	C	303	A86	O4-C38-O5	-2.35	118.28	122.96
2	A	307	A86	C12-C11-C13	2.35	119.98	116.02
3	C	312	CLA	C1-C2-C3	-2.35	121.97	126.04
3	A	319	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
2	A	305	A86	C12-C11-C13	2.35	119.97	116.02
3	B	319	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
3	C	315	CLA	C1-C2-C3	-2.35	121.98	126.04
2	B	301	A86	C9-C10-C11	-2.35	119.71	126.61
3	B	311	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
4	C	311	KC2	O1D-CGD-CBD	-2.34	119.69	124.48
2	A	303	A86	O4-C38-O5	-2.34	118.31	122.96
2	A	304	A86	O4-C38-O5	-2.34	118.31	122.96
3	B	311	CLA	C1-C2-C3	-2.34	122.00	126.04
2	B	304	A86	O4-C38-O5	-2.34	118.32	122.96
2	C	304	A86	O4-C38-O5	-2.34	118.32	122.96
2	B	305	A86	C12-C11-C13	2.34	119.95	116.02
2	B	302	A86	O4-C38-O5	-2.34	118.32	122.96
2	B	302	A86	C4-C3-C2	-2.33	118.69	123.47
2	B	303	A86	C35-C34-C33	-2.33	105.81	109.88
2	C	308	A86	O4-C38-O5	-2.33	118.33	122.96
2	A	307	A86	O4-C38-O5	-2.33	118.33	122.96
3	B	317	CLA	C1B-CHB-C4A	-2.32	125.51	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	A86	O4-C38-O5	-2.32	118.35	122.96
2	B	307	A86	O4-C38-O5	-2.32	118.36	122.96
2	B	301	A86	C9-C8-C6	-2.31	119.92	126.42
3	A	308	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
2	C	306	A86	C12-C11-C13	2.31	119.90	116.02
2	A	307	A86	C9-C8-C6	-2.31	119.93	126.42
2	A	302	A86	C12-C11-C13	2.31	119.90	116.02
3	C	309	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
3	B	308	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
2	C	302	A86	O4-C38-O5	-2.30	118.38	122.96
2	C	303	A86	C9-C8-C6	-2.30	119.94	126.42
2	A	301	A86	C4-C3-C2	-2.30	118.76	123.47
3	A	313	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
2	C	303	A86	C4-C3-C2	-2.30	118.76	123.47
3	A	317	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
3	B	314	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
2	C	307	A86	O4-C38-O5	-2.30	118.40	122.96
2	A	307	A86	C9-C10-C11	-2.29	119.86	126.61
3	A	319	CLA	C1-C2-C3	-2.29	122.08	126.04
2	B	306	A86	O4-C38-O5	-2.29	118.41	122.96
2	A	303	A86	C3-C4-C5	-2.29	118.78	123.47
2	B	301	A86	O4-C38-O5	-2.29	118.41	122.96
3	C	315	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
2	B	303	A86	C3-C4-C5	-2.29	118.79	123.47
2	C	308	A86	C9-C10-C11	-2.28	119.89	126.61
2	C	308	A86	C9-C8-C6	-2.28	120.00	126.42
3	C	318	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
2	B	307	A86	C9-C8-C6	-2.28	120.01	126.42
3	A	314	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
2	A	302	A86	C4-C3-C2	-2.28	118.81	123.47
4	A	310	KC2	O2D-CGD-O1D	-2.28	119.39	123.84
2	A	304	A86	C28-C27-C26	-2.27	119.74	122.92
2	B	301	A86	C12-C11-C13	2.27	119.83	116.02
4	C	313	KC2	O1D-CGD-CBD	-2.27	119.84	124.48
2	A	306	A86	O4-C38-O5	-2.27	118.46	122.96
4	A	312	KC2	O1D-CGD-CBD	-2.27	119.85	124.48
2	B	303	A86	O4-C38-O5	-2.27	118.46	122.96
2	B	307	A86	C9-C10-C11	-2.26	119.96	126.61
3	B	316	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
2	C	303	A86	C9-C10-C11	-2.25	119.99	126.61
2	A	307	A86	C25-C24-C1	-2.25	120.10	126.42
4	C	313	KC2	C1B-CHB-C4A	-2.24	121.22	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	316	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
5	C	316	KC1	O1D-CGD-CBD	-2.24	119.89	124.48
2	B	302	A86	C9-C8-C6	-2.24	120.12	126.42
4	B	312	KC2	C1B-CHB-C4A	-2.23	121.24	126.06
3	C	317	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
5	C	316	KC1	C2A-C3A-C4A	2.23	108.14	106.49
5	A	315	KC1	O1D-CGD-CBD	-2.23	119.92	124.48
4	A	312	KC2	C1B-CHB-C4A	-2.23	121.25	126.06
4	C	311	KC2	C1B-CHB-C4A	-2.22	121.26	126.06
2	A	306	A86	C33-C32-C31	-2.22	107.05	109.21
2	C	308	A86	C25-C24-C1	-2.22	120.18	126.42
6	C	319	SQD	C1-O5-C5	2.22	118.04	113.69
4	A	310	KC2	C1B-CHB-C4A	-2.22	121.28	126.06
4	B	310	KC2	C1B-CHB-C4A	-2.22	121.28	126.06
2	C	305	A86	C12-C11-C13	2.21	119.74	116.02
2	B	302	A86	C12-C11-C13	2.21	119.73	116.02
2	C	303	A86	C12-C11-C13	2.21	119.73	116.02
4	B	310	KC2	O2D-CGD-O1D	-2.21	119.52	123.84
5	A	315	KC1	C3D-CAD-CBD	-2.20	104.70	107.61
5	B	315	KC1	O1D-CGD-CBD	-2.20	119.97	124.48
4	A	312	KC2	CHB-C4A-C3A	-2.20	121.53	124.98
2	A	301	A86	C12-C11-C13	2.20	119.72	116.02
2	B	302	A86	C9-C10-C11	-2.20	120.15	126.61
4	C	313	KC2	CHB-C4A-C3A	-2.19	121.55	124.98
2	C	304	A86	C3-C4-C5	-2.19	118.98	123.47
2	C	302	A86	C12-C11-C13	2.18	119.69	116.02
2	A	302	A86	C9-C8-C6	-2.18	120.30	126.42
3	C	315	CLA	CHD-C1D-ND	-2.18	122.45	124.45
2	C	304	A86	C4-C3-C2	-2.17	119.03	123.47
2	C	305	A86	C9-C10-C11	-2.16	120.26	126.61
4	C	311	KC2	O2D-CGD-O1D	-2.16	119.62	123.84
2	B	306	A86	C33-C32-C31	-2.15	107.12	109.21
5	B	315	KC1	C3D-CAD-CBD	-2.15	104.78	107.61
4	C	311	KC2	CHB-C4A-C3A	-2.14	121.64	124.98
5	C	316	KC1	C3D-CAD-CBD	-2.14	104.79	107.61
3	C	315	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
3	A	314	CLA	CHD-C1D-ND	-2.13	122.49	124.45
3	A	314	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
3	B	314	CLA	C1-C2-C3	-2.13	122.36	126.04
2	B	307	A86	C25-C24-C1	-2.13	120.43	126.42
2	A	302	A86	C9-C10-C11	-2.13	120.36	126.61
2	C	307	A86	C33-C32-C31	-2.12	107.15	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	314	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
2	B	306	A86	C4-C3-C2	-2.11	119.14	123.47
3	C	310	CLA	CHD-C1D-ND	-2.11	122.51	124.45
3	B	311	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
4	B	312	KC2	CHB-C4A-C3A	-2.11	121.68	124.98
2	A	306	A86	C9-C8-C6	-2.11	120.50	126.42
6	B	318	SQD	C1-O5-C5	2.11	117.82	113.69
3	B	314	CLA	CHD-C1D-ND	-2.10	122.52	124.45
3	A	311	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
6	A	318	SQD	C1-O5-C5	2.10	117.81	113.69
4	A	310	KC2	CHB-C4A-C3A	-2.10	121.70	124.98
3	C	312	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
2	C	307	A86	C40-C32-C31	-2.10	108.60	110.47
3	A	319	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
5	B	315	KC1	C2A-C3A-C4A	2.09	108.04	106.49
2	B	304	A86	O-C13-C14	-2.09	117.41	121.66
3	B	309	CLA	CHD-C1D-ND	-2.09	122.53	124.45
4	B	312	KC2	O2D-CGD-O1D	-2.09	119.75	123.84
5	A	315	KC1	C2A-C3A-C4A	2.09	108.03	106.49
2	A	306	A86	C4-C3-C2	-2.09	119.20	123.47
3	A	309	CLA	CHD-C1D-ND	-2.08	122.54	124.45
2	B	306	A86	C9-C8-C6	-2.08	120.57	126.42
3	A	319	CLA	CHD-C1D-ND	-2.08	122.54	124.45
2	B	305	A86	C3-C4-C5	-2.08	119.21	123.47
2	B	304	A86	C12-C11-C13	2.08	119.51	116.02
4	B	310	KC2	CHB-C4A-C3A	-2.08	121.73	124.98
3	C	301	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
3	B	317	CLA	CHD-C1D-ND	-2.07	122.55	124.45
3	B	319	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
2	A	305	A86	C3-C4-C5	-2.07	119.24	123.47
2	B	303	A86	C40-C32-C31	-2.06	108.63	110.47
3	B	319	CLA	CHD-C1D-ND	-2.06	122.56	124.45
3	B	319	CLA	C1-C2-C3	-2.06	122.48	126.04
2	C	307	A86	C9-C8-C6	-2.06	120.63	126.42
2	C	306	A86	C3-C4-C5	-2.05	119.27	123.47
2	B	306	A86	C40-C32-C31	-2.05	108.64	110.47
3	C	309	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
2	B	307	A86	C4-C3-C2	-2.05	119.28	123.47
2	C	305	A86	C28-C27-C26	-2.05	120.05	122.92
3	B	309	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
2	C	307	A86	C14-C15-C16	2.04	126.58	118.75
3	A	308	CLA	O2A-CGA-O1A	-2.04	118.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	304	A86	C12-C11-C13	2.04	119.45	116.02
2	C	307	A86	C3-C4-C5	-2.04	119.30	123.47
3	A	311	CLA	CHD-C1D-ND	-2.03	122.58	124.45
3	C	301	CLA	CHD-C1D-ND	-2.03	122.58	124.45
3	A	309	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
2	A	306	A86	C40-C32-C31	-2.03	108.65	110.47
2	C	304	A86	C9-C10-C11	-2.03	120.64	126.61
3	B	313	CLA	CHD-C1D-ND	-2.03	122.59	124.45
2	A	304	A86	C9-C10-C11	-2.03	120.65	126.61
2	C	307	A86	C4-C3-C2	-2.02	119.33	123.47
2	B	306	A86	C9-C10-C11	-2.02	120.66	126.61
3	B	308	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
2	B	304	A86	C9-C10-C11	-2.02	120.67	126.61
3	A	317	CLA	CHD-C1D-ND	-2.02	122.60	124.45
2	C	305	A86	C3-C4-C5	-2.02	119.34	123.47
2	B	303	A86	C-C1-C2	-2.02	120.10	122.92
3	C	310	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
4	A	312	KC2	O2D-CGD-O1D	-2.01	119.90	123.84
5	C	316	KC1	O2D-CGD-O1D	-2.01	119.91	123.84
3	B	317	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
2	A	306	A86	C3-C4-C5	-2.01	119.36	123.47
3	C	318	CLA	CHD-C1D-ND	-2.01	122.61	124.45
2	B	304	A86	C25-C24-C1	-2.00	120.78	126.42
2	B	304	A86	C28-C27-C26	-2.00	120.12	122.92
3	A	317	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
2	A	303	A86	C9-C10-C11	-2.00	120.73	126.61

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	308	CLA	ND
3	A	309	CLA	ND
3	A	311	CLA	ND
3	A	313	CLA	ND
3	A	314	CLA	ND
3	A	316	CLA	ND
3	A	317	CLA	ND
3	A	319	CLA	ND
3	B	308	CLA	ND
3	B	309	CLA	ND
3	B	311	CLA	ND
3	B	313	CLA	ND

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Mol	Chain	Res	Type	Atom
3	B	314	CLA	ND
3	B	316	CLA	ND
3	B	317	CLA	ND
3	B	319	CLA	ND
3	C	301	CLA	ND
3	C	309	CLA	ND
3	C	310	CLA	ND
3	C	312	CLA	ND
3	C	314	CLA	ND
3	C	315	CLA	ND
3	C	317	CLA	ND
3	C	318	CLA	ND

All (332) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	304	A86	C35-C34-O4-C38
2	A	307	A86	C33-C34-O4-C38
2	B	304	A86	C35-C34-O4-C38
2	B	307	A86	C33-C34-O4-C38
2	C	305	A86	C35-C34-O4-C38
2	C	308	A86	C33-C34-O4-C38
3	A	308	CLA	CHA-CBD-CGD-O1D
3	A	308	CLA	CHA-CBD-CGD-O2D
3	A	309	CLA	C2-C3-C5-C6
3	A	309	CLA	C4-C3-C5-C6
3	A	314	CLA	C1A-C2A-CAA-CBA
3	A	314	CLA	C3A-C2A-CAA-CBA
3	B	308	CLA	CHA-CBD-CGD-O1D
3	B	314	CLA	C1A-C2A-CAA-CBA
3	B	314	CLA	C3A-C2A-CAA-CBA
3	B	319	CLA	C2-C3-C5-C6
3	B	319	CLA	C4-C3-C5-C6
3	C	310	CLA	C2-C3-C5-C6
3	C	310	CLA	C4-C3-C5-C6
3	C	315	CLA	C1A-C2A-CAA-CBA
3	C	315	CLA	C3A-C2A-CAA-CBA
4	A	310	KC2	C1A-C2A-CAA-CBA
4	A	310	KC2	C2B-C3B-CAB-CBB
4	A	310	KC2	C4B-C3B-CAB-CBB
4	A	310	KC2	C2C-C3C-CAC-CBC
4	A	312	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	A	312	KC2	C2B-C3B-CAB-CBB
4	A	312	KC2	C4B-C3B-CAB-CBB
4	B	310	KC2	C1A-C2A-CAA-CBA
4	B	310	KC2	C2B-C3B-CAB-CBB
4	B	310	KC2	C4B-C3B-CAB-CBB
4	B	310	KC2	C2C-C3C-CAC-CBC
4	B	312	KC2	C1A-C2A-CAA-CBA
4	B	312	KC2	C2B-C3B-CAB-CBB
4	B	312	KC2	C4B-C3B-CAB-CBB
4	C	311	KC2	C1A-C2A-CAA-CBA
4	C	311	KC2	C2B-C3B-CAB-CBB
4	C	311	KC2	C4B-C3B-CAB-CBB
4	C	311	KC2	C2C-C3C-CAC-CBC
4	C	313	KC2	C1A-C2A-CAA-CBA
4	C	313	KC2	C2B-C3B-CAB-CBB
4	C	313	KC2	C4B-C3B-CAB-CBB
5	A	315	KC1	C1A-C2A-CAA-CBA
5	B	315	KC1	C1A-C2A-CAA-CBA
5	C	316	KC1	C1A-C2A-CAA-CBA
6	A	318	SQD	O5-C1-O6-C44
6	A	318	SQD	O49-C7-O47-C45
6	B	318	SQD	O5-C1-O6-C44
6	B	318	SQD	O49-C7-O47-C45
6	C	319	SQD	O5-C1-O6-C44
6	C	319	SQD	O49-C7-O47-C45
2	A	301	A86	C39-C38-O4-C34
2	A	302	A86	C39-C38-O4-C34
2	A	304	A86	C39-C38-O4-C34
2	A	306	A86	C39-C38-O4-C34
2	A	307	A86	C39-C38-O4-C34
2	B	301	A86	C39-C38-O4-C34
2	B	302	A86	C39-C38-O4-C34
2	B	304	A86	C39-C38-O4-C34
2	B	306	A86	C39-C38-O4-C34
2	B	307	A86	C39-C38-O4-C34
2	C	302	A86	C39-C38-O4-C34
2	C	303	A86	C39-C38-O4-C34
2	C	305	A86	C39-C38-O4-C34
2	C	307	A86	C39-C38-O4-C34
2	C	308	A86	C39-C38-O4-C34
3	A	314	CLA	CBD-CGD-O2D-CED
3	B	314	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	C	315	CLA	CBD-CGD-O2D-CED
3	C	309	CLA	O1A-CGA-O2A-C1
6	A	318	SQD	O10-C23-O48-C46
6	B	318	SQD	O10-C23-O48-C46
6	C	319	SQD	O10-C23-O48-C46
2	A	301	A86	O5-C38-O4-C34
2	A	302	A86	O5-C38-O4-C34
2	A	304	A86	O5-C38-O4-C34
2	A	306	A86	O5-C38-O4-C34
2	A	307	A86	O5-C38-O4-C34
2	B	301	A86	O5-C38-O4-C34
2	B	302	A86	O5-C38-O4-C34
2	B	304	A86	O5-C38-O4-C34
2	B	306	A86	O5-C38-O4-C34
2	B	307	A86	O5-C38-O4-C34
2	C	302	A86	O5-C38-O4-C34
2	C	303	A86	O5-C38-O4-C34
2	C	305	A86	O5-C38-O4-C34
2	C	307	A86	O5-C38-O4-C34
2	C	308	A86	O5-C38-O4-C34
3	C	309	CLA	C3-C5-C6-C7
3	B	313	CLA	CBA-CGA-O2A-C1
6	C	319	SQD	C24-C23-O48-C46
6	A	318	SQD	C8-C7-O47-C45
6	B	318	SQD	C8-C7-O47-C45
6	C	319	SQD	C8-C7-O47-C45
3	B	309	CLA	C4-C3-C5-C6
3	B	309	CLA	C2-C3-C5-C6
3	C	309	CLA	CBA-CGA-O2A-C1
6	A	318	SQD	C24-C23-O48-C46
6	B	318	SQD	C24-C23-O48-C46
3	A	309	CLA	O1A-CGA-O2A-C1
3	B	309	CLA	O1A-CGA-O2A-C1
3	B	313	CLA	O1A-CGA-O2A-C1
3	C	310	CLA	O1A-CGA-O2A-C1
2	A	303	A86	C39-C38-O4-C34
2	A	305	A86	C39-C38-O4-C34
2	B	303	A86	C39-C38-O4-C34
2	B	305	A86	C39-C38-O4-C34
2	C	304	A86	C39-C38-O4-C34
2	C	306	A86	C39-C38-O4-C34
3	A	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	B	313	CLA	CBD-CGD-O2D-CED
3	C	315	CLA	O1D-CGD-O2D-CED
3	A	309	CLA	CBA-CGA-O2A-C1
3	B	308	CLA	CBA-CGA-O2A-C1
3	B	309	CLA	CBA-CGA-O2A-C1
3	C	310	CLA	CBA-CGA-O2A-C1
2	A	303	A86	O5-C38-O4-C34
2	A	305	A86	O5-C38-O4-C34
2	B	303	A86	O5-C38-O4-C34
2	B	305	A86	O5-C38-O4-C34
2	C	304	A86	O5-C38-O4-C34
2	C	306	A86	O5-C38-O4-C34
3	A	313	CLA	O1A-CGA-O2A-C1
3	C	314	CLA	O1A-CGA-O2A-C1
3	B	314	CLA	O1D-CGD-O2D-CED
3	B	316	CLA	CBD-CGD-O2D-CED
3	A	314	CLA	O1D-CGD-O2D-CED
3	A	313	CLA	CBA-CGA-O2A-C1
3	C	314	CLA	CBA-CGA-O2A-C1
3	B	308	CLA	O1A-CGA-O2A-C1
3	A	308	CLA	CBA-CGA-O2A-C1
3	A	314	CLA	CBA-CGA-O2A-C1
3	C	315	CLA	CBA-CGA-O2A-C1
6	A	318	SQD	C2-C1-O6-C44
6	B	318	SQD	C2-C1-O6-C44
6	C	319	SQD	C2-C1-O6-C44
3	A	314	CLA	O1A-CGA-O2A-C1
3	C	310	CLA	C14-C13-C15-C16
3	C	312	CLA	CBD-CGD-O2D-CED
3	A	308	CLA	O1A-CGA-O2A-C1
3	C	315	CLA	O1A-CGA-O2A-C1
3	B	309	CLA	C11-C12-C13-C15
4	A	310	KC2	CBD-CGD-O2D-CED
3	C	309	CLA	C5-C6-C7-C8
3	B	309	CLA	C13-C15-C16-C17
3	C	317	CLA	CBD-CGD-O2D-CED
3	A	313	CLA	O1D-CGD-O2D-CED
3	A	309	CLA	C6-C7-C8-C9
3	B	313	CLA	O1D-CGD-O2D-CED
3	B	317	CLA	CBA-CGA-O2A-C1
3	A	319	CLA	CBA-CGA-O2A-C1
3	B	316	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	A	317	CLA	CBA-CGA-O2A-C1
6	B	318	SQD	C28-C29-C30-C31
3	A	309	CLA	C6-C7-C8-C10
3	C	310	CLA	C6-C7-C8-C10
3	C	310	CLA	C12-C13-C15-C16
3	A	319	CLA	O1A-CGA-O2A-C1
3	B	317	CLA	O1A-CGA-O2A-C1
6	A	318	SQD	C28-C29-C30-C31
6	C	319	SQD	C28-C29-C30-C31
3	C	312	CLA	C8-C10-C11-C12
3	B	314	CLA	CBA-CGA-O2A-C1
3	B	319	CLA	CBA-CGA-O2A-C1
3	C	301	CLA	CBA-CGA-O2A-C1
3	C	318	CLA	CBA-CGA-O2A-C1
4	B	312	KC2	C2C-C3C-CAC-CBC
5	A	315	KC1	C2B-C3B-CAB-CBB
5	B	315	KC1	C2B-C3B-CAB-CBB
5	C	316	KC1	C2B-C3B-CAB-CBB
4	A	310	KC2	C4C-C3C-CAC-CBC
4	B	310	KC2	C4C-C3C-CAC-CBC
4	C	311	KC2	C4C-C3C-CAC-CBC
5	C	316	KC1	C4B-C3B-CAB-CBB
3	A	317	CLA	O1A-CGA-O2A-C1
3	A	311	CLA	C8-C10-C11-C12
3	A	311	CLA	C11-C12-C13-C14
3	B	311	CLA	C11-C12-C13-C14
3	C	310	CLA	C6-C7-C8-C9
3	C	312	CLA	C11-C12-C13-C14
3	A	316	CLA	CBD-CGD-O2D-CED
3	C	301	CLA	O1A-CGA-O2A-C1
3	A	309	CLA	C1A-C2A-CAA-CBA
3	B	309	CLA	C1A-C2A-CAA-CBA
3	C	310	CLA	C1A-C2A-CAA-CBA
4	A	310	KC2	CAA-CBA-CGA-O2A
3	B	319	CLA	O1A-CGA-O2A-C1
6	C	319	SQD	C27-C28-C29-C30
3	C	310	CLA	C13-C15-C16-C17
6	B	318	SQD	C10-C11-C12-C13
3	A	309	CLA	C13-C15-C16-C17
6	C	319	SQD	C30-C31-C32-C33
3	C	318	CLA	O1A-CGA-O2A-C1
3	B	314	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
6	A	318	SQD	C30-C31-C32-C33
6	B	318	SQD	C30-C31-C32-C33
3	B	311	CLA	C4-C3-C5-C6
6	B	318	SQD	C27-C28-C29-C30
3	C	312	CLA	O1D-CGD-O2D-CED
3	B	309	CLA	C3-C5-C6-C7
3	A	309	CLA	C8-C10-C11-C12
3	A	311	CLA	C11-C12-C13-C15
3	B	309	CLA	C6-C7-C8-C10
3	B	311	CLA	C11-C12-C13-C15
3	C	312	CLA	C11-C12-C13-C15
3	A	309	CLA	C14-C13-C15-C16
3	B	309	CLA	C6-C7-C8-C9
3	B	309	CLA	C11-C12-C13-C14
3	B	311	CLA	C11-C10-C8-C9
3	B	311	CLA	C8-C10-C11-C12
3	C	310	CLA	C8-C10-C11-C12
2	A	301	A86	C33-C34-O4-C38
3	C	317	CLA	O1D-CGD-O2D-CED
2	C	304	A86	C11-C10-C9-C8
2	A	305	A86	O-C13-C14-C15
2	A	306	A86	O-C13-C14-C15
2	B	301	A86	O-C13-C14-C15
2	B	305	A86	O-C13-C14-C15
2	C	302	A86	O-C13-C14-C15
2	C	306	A86	O-C13-C14-C15
2	C	307	A86	O-C13-C14-C15
6	A	318	SQD	C10-C11-C12-C13
4	C	311	KC2	CAA-CBA-CGA-O2A
3	A	311	CLA	C11-C10-C8-C9
3	C	312	CLA	C11-C10-C8-C9
2	A	303	A86	C11-C10-C9-C8
2	B	303	A86	C11-C10-C9-C8
3	A	311	CLA	C2A-CAA-CBA-CGA
3	C	310	CLA	C3-C5-C6-C7
4	B	312	KC2	CBD-CGD-O2D-CED
3	A	313	CLA	CAD-CBD-CGD-O2D
2	A	302	A86	C12-C11-C13-O
5	A	315	KC1	C4B-C3B-CAB-CBB
5	B	315	KC1	C4B-C3B-CAB-CBB
3	C	312	CLA	C2A-CAA-CBA-CGA
6	A	318	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
3	B	308	CLA	CHA-CBD-CGD-O2D
2	A	302	A86	C10-C11-C13-O
3	A	311	CLA	C4-C3-C5-C6
3	B	311	CLA	C2-C3-C5-C6
3	A	316	CLA	O1D-CGD-O2D-CED
3	B	317	CLA	C6-C7-C8-C9
3	B	311	CLA	CBD-CGD-O2D-CED
3	A	309	CLA	C3-C5-C6-C7
3	C	301	CLA	C5-C6-C7-C8
3	B	311	CLA	C6-C7-C8-C10
6	C	319	SQD	C9-C10-C11-C12
3	A	317	CLA	C2A-CAA-CBA-CGA
3	B	311	CLA	C2A-CAA-CBA-CGA
3	B	317	CLA	C2A-CAA-CBA-CGA
3	A	319	CLA	C6-C7-C8-C10
2	B	302	A86	C13-C14-C15-C20
2	C	303	A86	C13-C14-C15-C20
3	B	313	CLA	C6-C7-C8-C9
3	C	314	CLA	C6-C7-C8-C9
3	A	317	CLA	C6-C7-C8-C9
3	C	301	CLA	C2A-CAA-CBA-CGA
3	C	318	CLA	C2A-CAA-CBA-CGA
3	C	318	CLA	C6-C7-C8-C9
3	A	309	CLA	C12-C13-C15-C16
3	A	311	CLA	C2-C3-C5-C6
3	B	313	CLA	C10-C11-C12-C13
3	B	313	CLA	C16-C17-C18-C20
4	C	313	KC2	C2C-C3C-CAC-CBC
3	B	311	CLA	O1D-CGD-O2D-CED
3	A	319	CLA	C2A-CAA-CBA-CGA
4	B	312	KC2	C4C-C3C-CAC-CBC
3	C	312	CLA	C2-C3-C5-C6
3	A	319	CLA	C6-C7-C8-C9
3	B	319	CLA	C2A-CAA-CBA-CGA
2	A	301	A86	O-C13-C14-C15
2	B	306	A86	O-C13-C14-C15
3	C	312	CLA	C4-C3-C5-C6
3	A	311	CLA	CBD-CGD-O2D-CED
3	A	313	CLA	C6-C7-C8-C9
3	B	309	CLA	C11-C10-C8-C9
3	C	301	CLA	C3-C5-C6-C7
3	C	314	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
3	A	311	CLA	C6-C7-C8-C10
4	B	310	KC2	C3A-C2A-CAA-CBA
3	A	311	CLA	O1D-CGD-O2D-CED
6	B	318	SQD	C9-C10-C11-C12
2	A	301	A86	C11-C10-C9-C8
2	A	304	A86	C11-C10-C9-C8
2	C	305	A86	C11-C10-C9-C8
3	B	314	CLA	C4-C3-C5-C6
3	C	315	CLA	C5-C6-C7-C8
3	A	309	CLA	C11-C12-C13-C15
2	B	304	A86	C11-C10-C9-C8
6	C	319	SQD	C10-C11-C12-C13
3	A	313	CLA	C10-C11-C12-C13
3	A	311	CLA	C6-C7-C8-C9
3	B	311	CLA	C6-C7-C8-C9
3	B	311	CLA	CAD-CBD-CGD-O2D
3	C	301	CLA	CAD-CBD-CGD-O2D
3	C	312	CLA	CAD-CBD-CGD-O2D
6	A	318	SQD	C46-C45-O47-C7
6	B	318	SQD	C46-C45-O47-C7
6	C	319	SQD	C11-C10-C9-C8
6	C	319	SQD	C26-C27-C28-C29
3	A	309	CLA	O2A-C1-C2-C3
3	B	309	CLA	O2A-C1-C2-C3
3	C	310	CLA	O2A-C1-C2-C3
3	A	317	CLA	CHA-CBD-CGD-O1D
3	A	317	CLA	CHA-CBD-CGD-O2D
3	B	316	CLA	CHA-CBD-CGD-O1D
3	B	316	CLA	CHA-CBD-CGD-O2D
3	B	319	CLA	CHA-CBD-CGD-O1D
3	C	309	CLA	CHA-CBD-CGD-O1D
3	C	309	CLA	CHA-CBD-CGD-O2D
3	C	318	CLA	CHA-CBD-CGD-O1D
3	C	318	CLA	CHA-CBD-CGD-O2D
6	A	318	SQD	O6-C44-C45-O47
6	B	318	SQD	O6-C44-C45-O47
4	B	310	KC2	CAA-CBA-CGA-O2A
2	C	302	A86	C33-C34-O4-C38
3	A	313	CLA	C16-C17-C18-C20
3	A	308	CLA	C4-C3-C5-C6
3	C	301	CLA	C4-C3-C5-C6
3	C	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	A	318	SQD	O6-C44-C45-C46
6	B	318	SQD	O6-C44-C45-C46
3	A	319	CLA	CAA-CBA-CGA-O2A
3	B	319	CLA	CAA-CBA-CGA-O2A
3	A	319	CLA	CAD-CBD-CGD-O1D
3	B	319	CLA	CAD-CBD-CGD-O1D
6	C	319	SQD	C46-C45-O47-C7
3	C	314	CLA	C10-C11-C12-C13
3	C	309	CLA	C6-C7-C8-C9
3	C	301	CLA	CAA-CBA-CGA-O2A
3	C	310	CLA	C11-C12-C13-C15
2	A	302	A86	O-C13-C14-C15

There are no ring outliers.

29 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	311	CLA	2	0
3	A	308	CLA	2	0
5	B	315	KC1	1	0
3	A	309	CLA	5	0
3	B	314	CLA	1	0
3	A	316	CLA	1	0
3	C	314	CLA	2	0
3	C	301	CLA	2	0
3	A	313	CLA	2	0
2	B	304	A86	1	0
2	C	305	A86	1	0
3	C	310	CLA	2	0
3	C	312	CLA	1	0
3	C	317	CLA	1	0
2	A	304	A86	1	0
3	B	316	CLA	1	0
6	C	319	SQD	1	0
3	B	313	CLA	1	0
5	A	315	KC1	1	0
3	A	319	CLA	3	0
3	B	308	CLA	1	0
3	B	311	CLA	1	0
3	C	315	CLA	2	0
5	C	316	KC1	1	0
6	A	318	SQD	2	0

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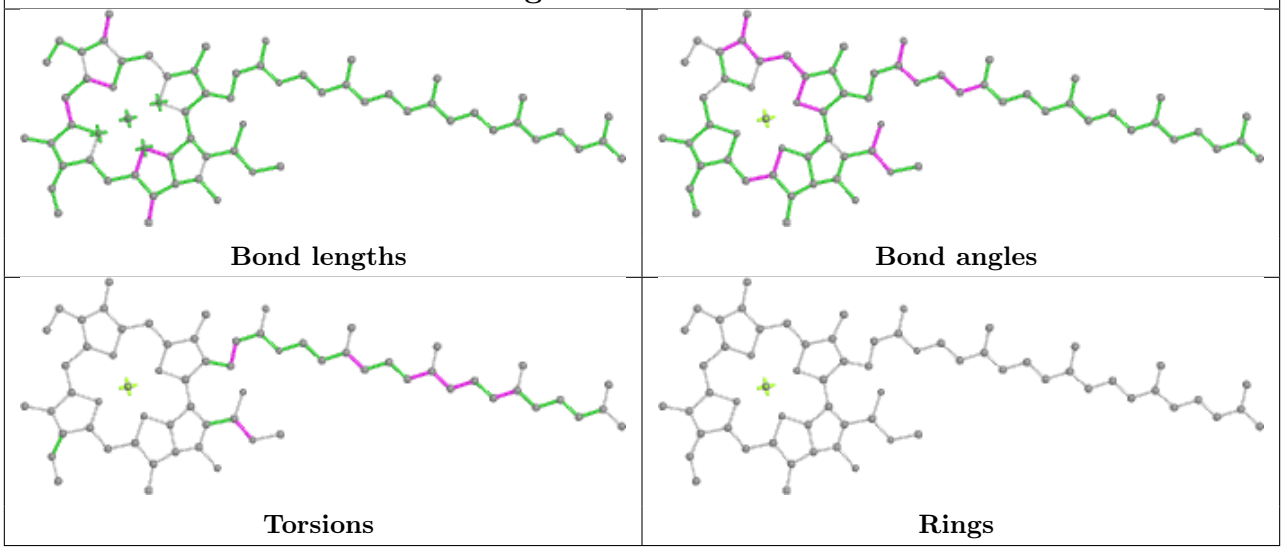
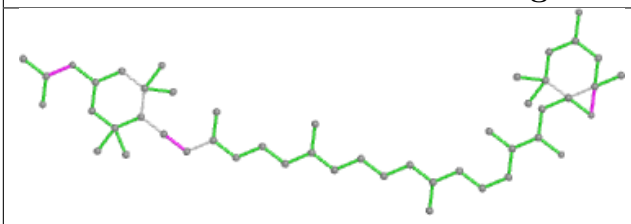
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	314	CLA	2	0
3	B	319	CLA	3	0
3	B	309	CLA	2	0
3	C	309	CLA	2	0

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.

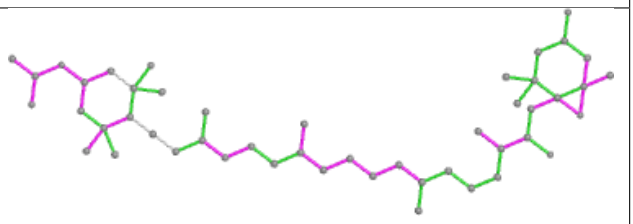
Ligand CLA A 311



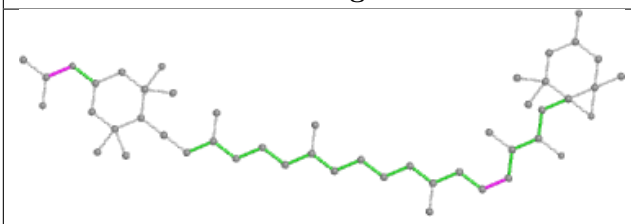
Ligand A86 B 303



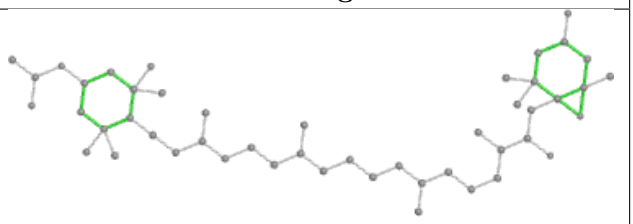
Bond lengths



Bond angles

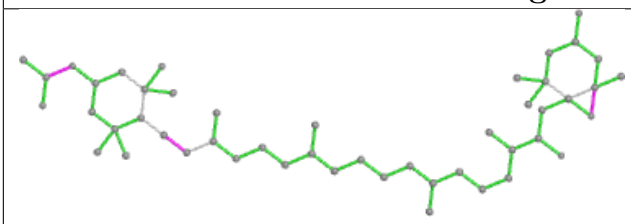


Torsions

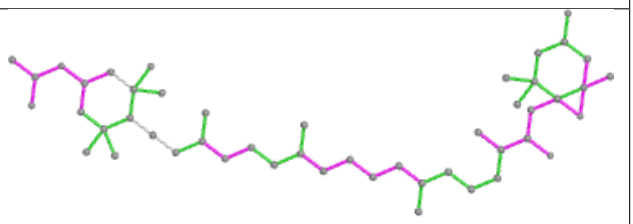


Rings

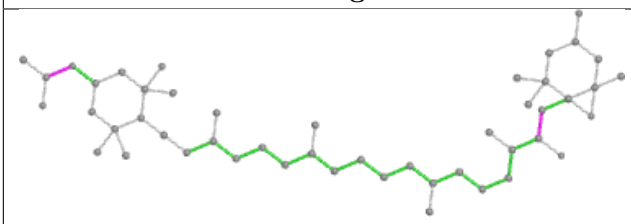
Ligand A86 A 305



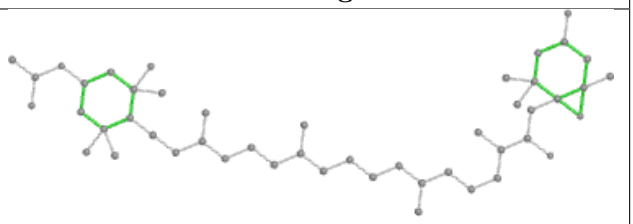
Bond lengths



Bond angles

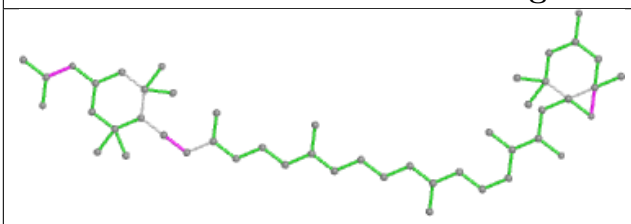


Torsions

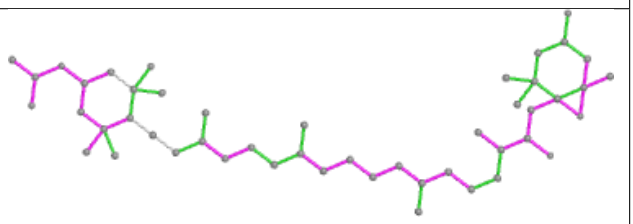


Rings

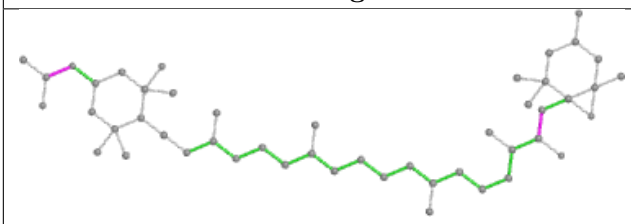
Ligand A86 A 306



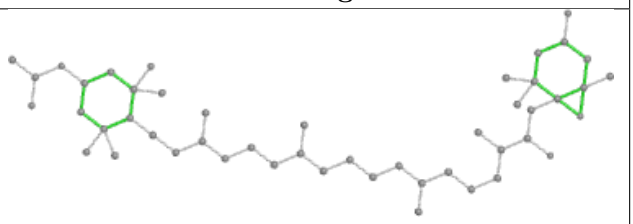
Bond lengths



Bond angles

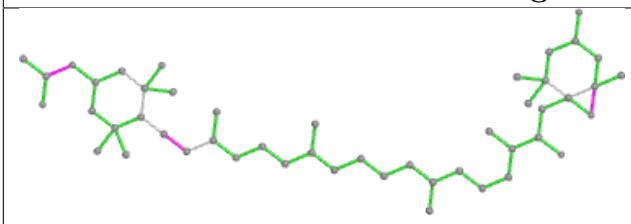


Torsions

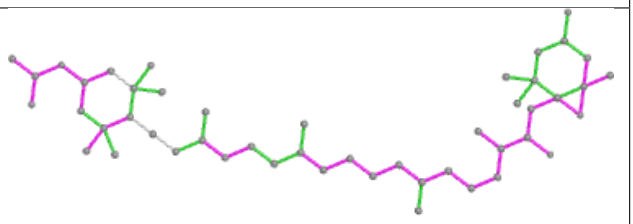


Rings

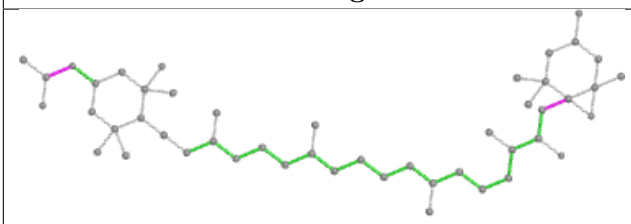
Ligand A86 B 302



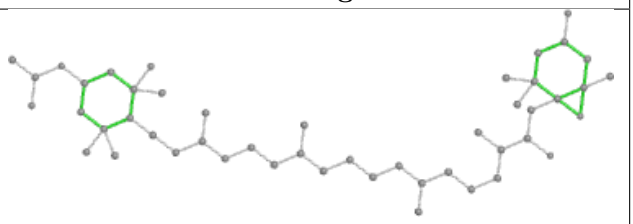
Bond lengths



Bond angles

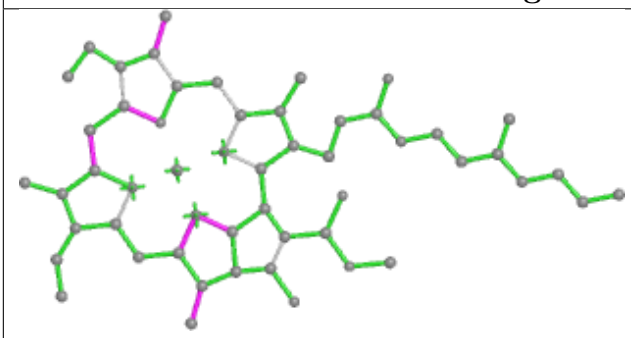


Torsions

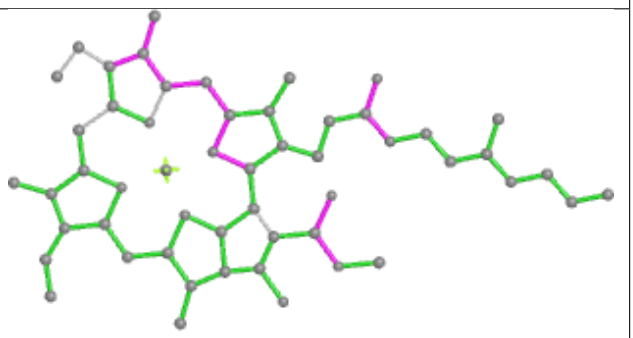


Rings

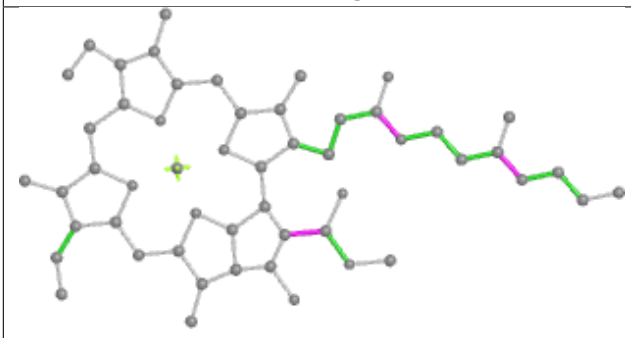
Ligand CLA A 308



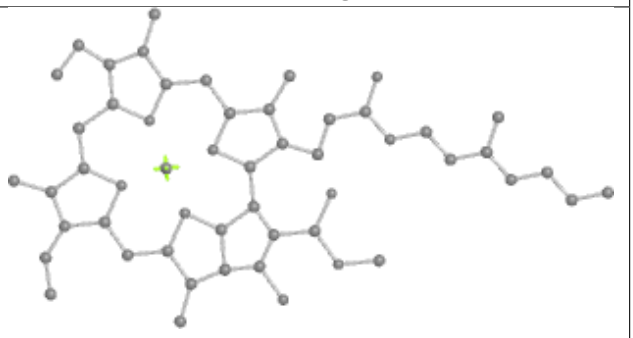
Bond lengths



Bond angles

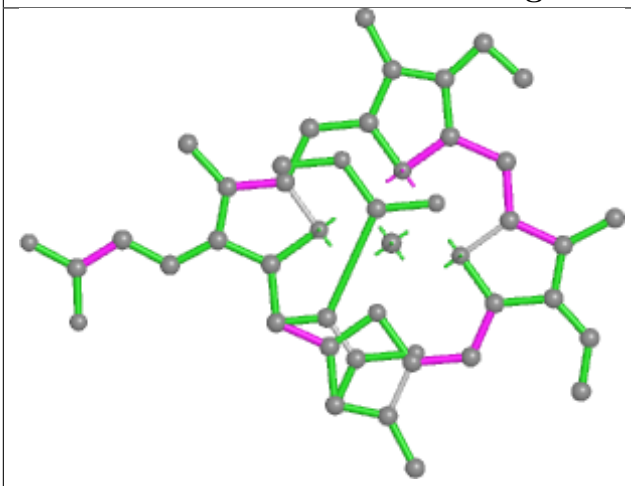


Torsions

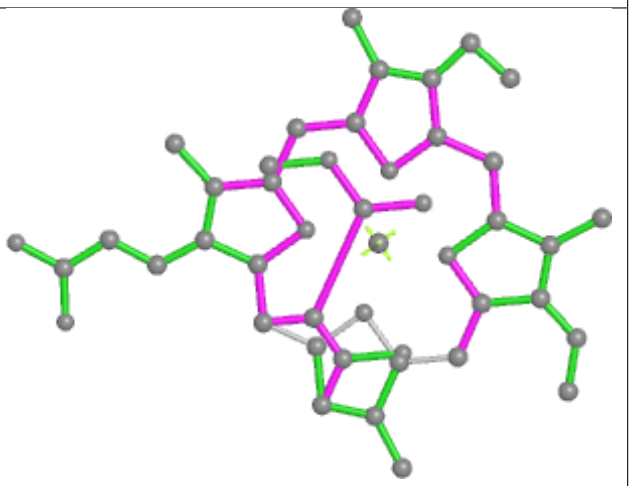


Rings

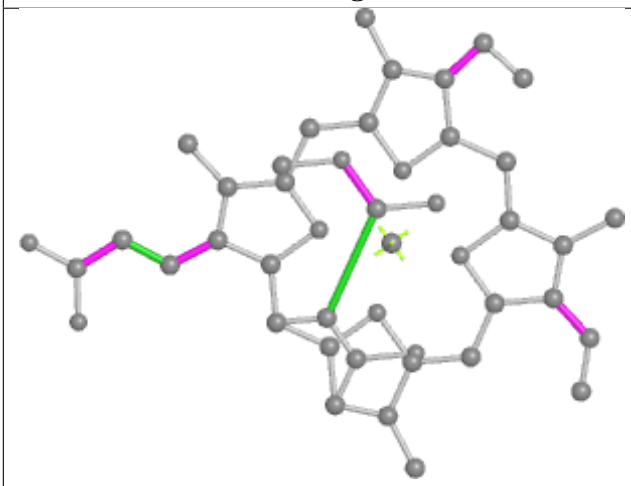
Ligand KC2 A 310



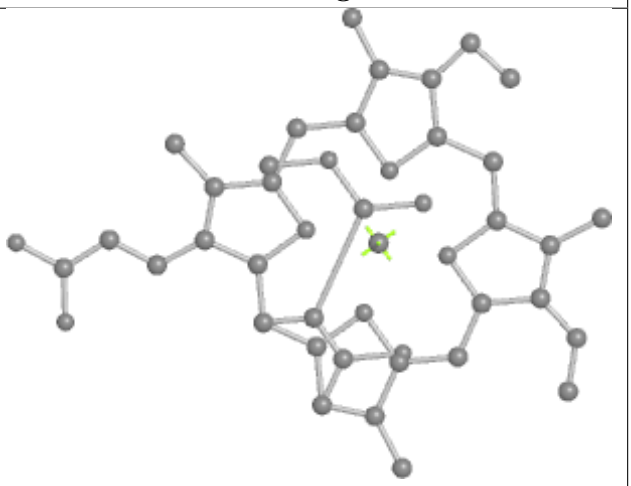
Bond lengths



Bond angles

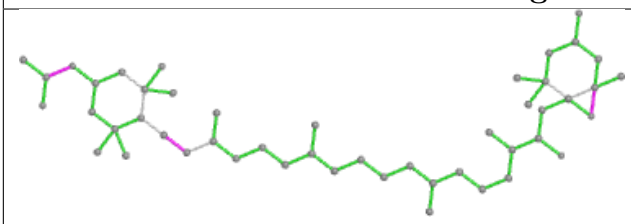


Torsions

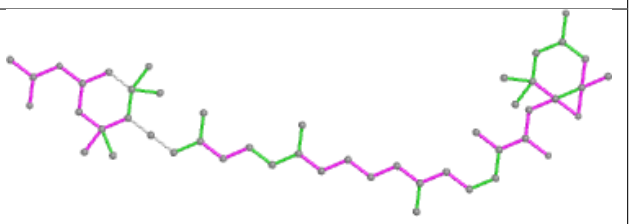


Rings

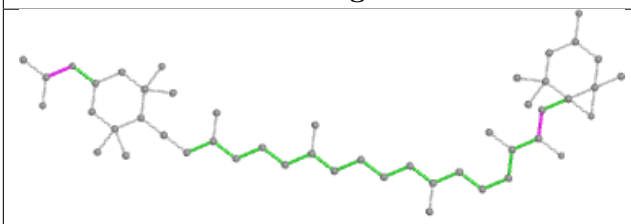
Ligand A86 C 307



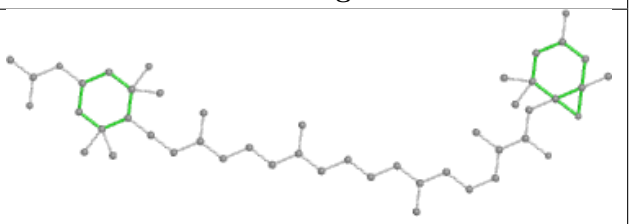
Bond lengths



Bond angles

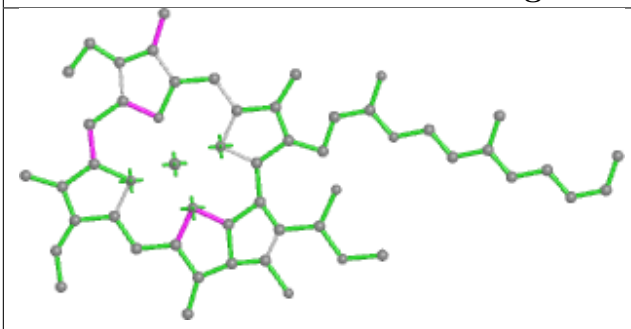


Torsions

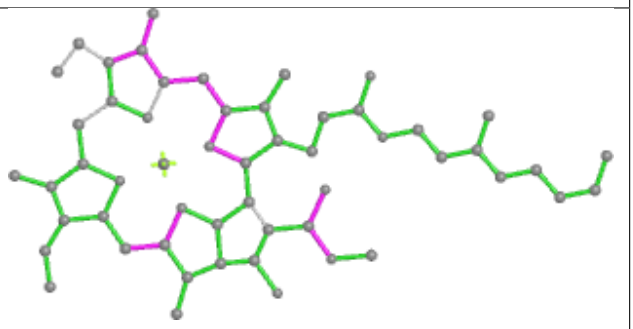


Rings

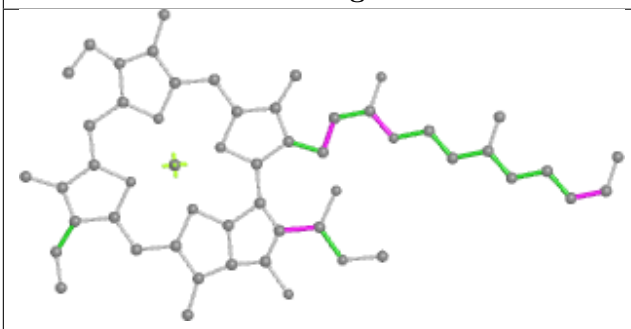
Ligand CLA C 318



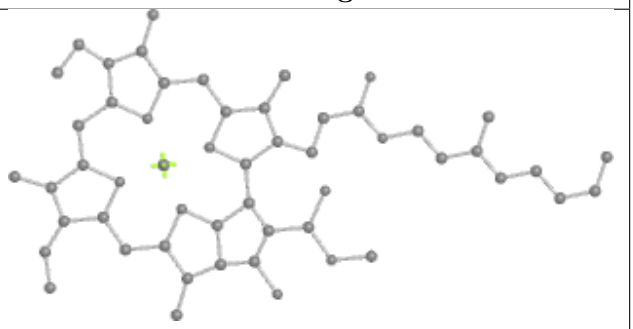
Bond lengths



Bond angles

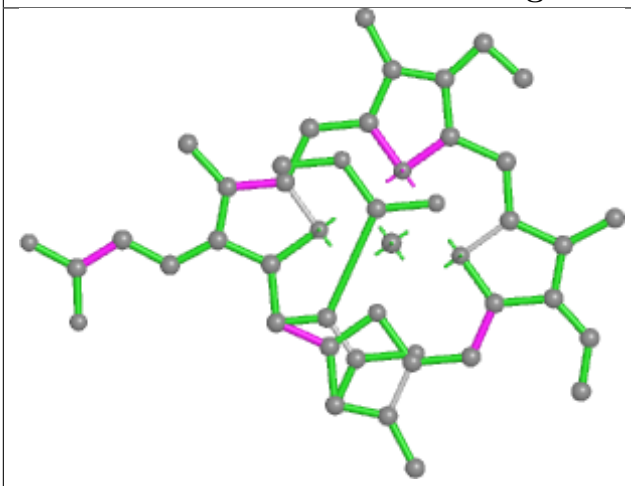


Torsions

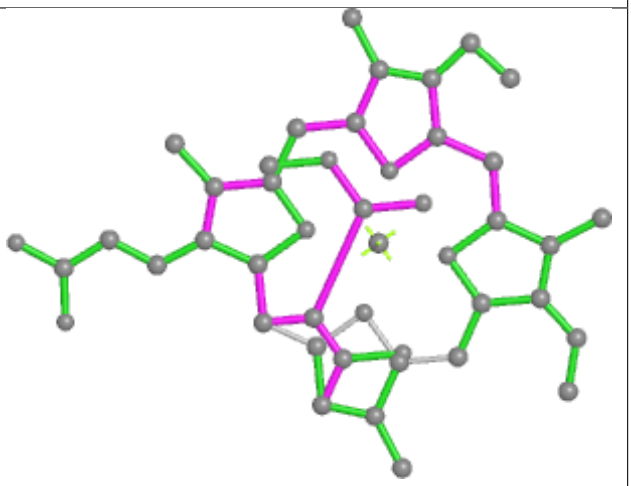


Rings

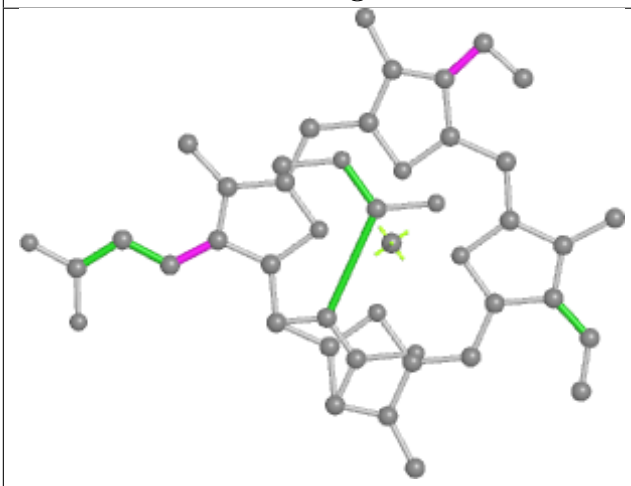
Ligand KC1 B 315



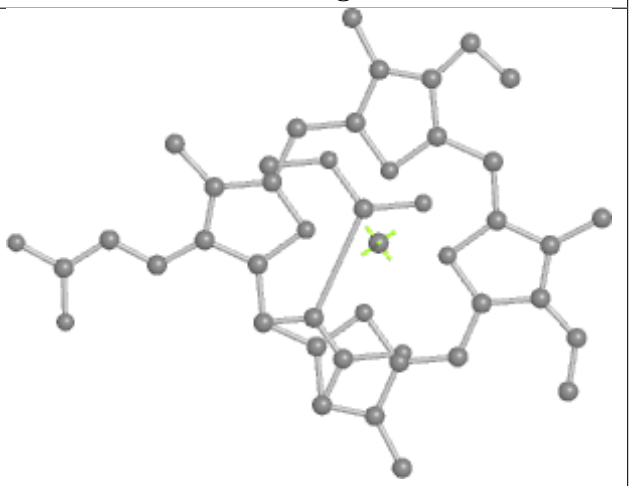
Bond lengths



Bond angles

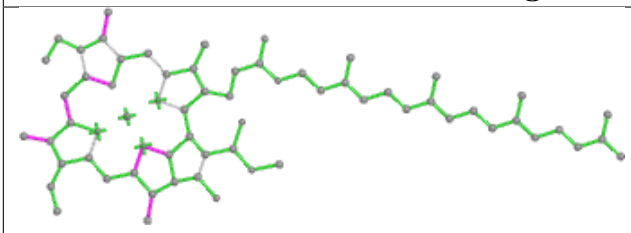


Torsions

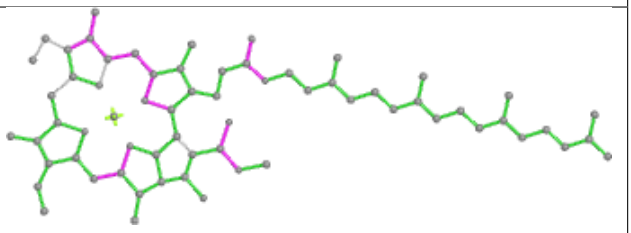


Rings

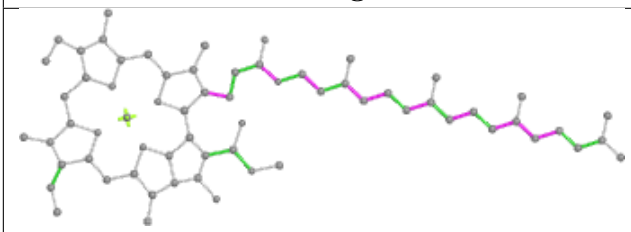
Ligand CLA A 309



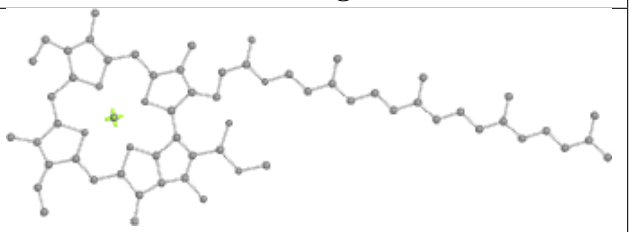
Bond lengths



Bond angles

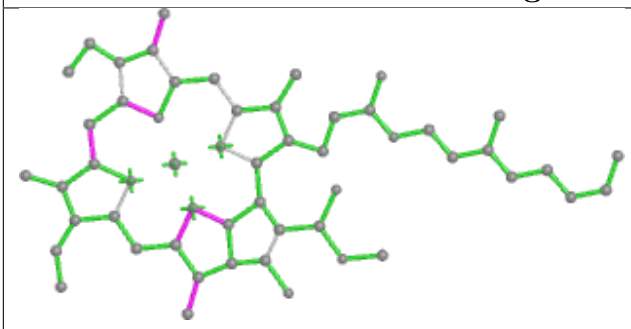


Torsions



Rings

Ligand CLA A 317



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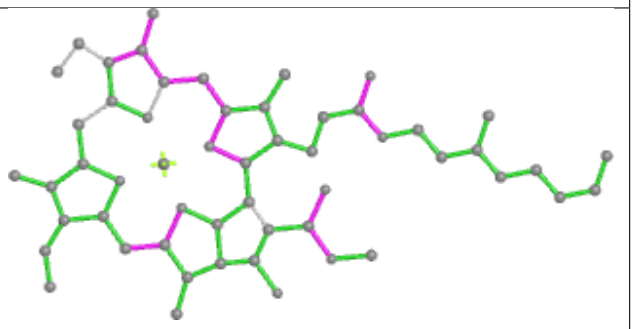
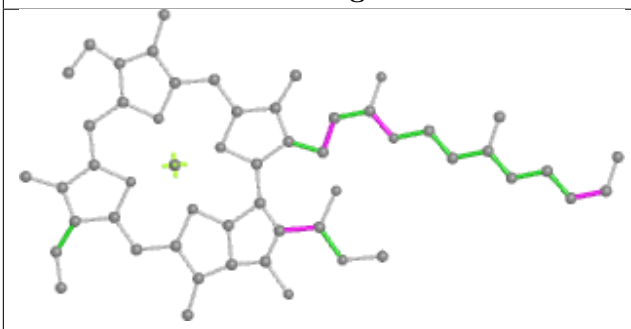
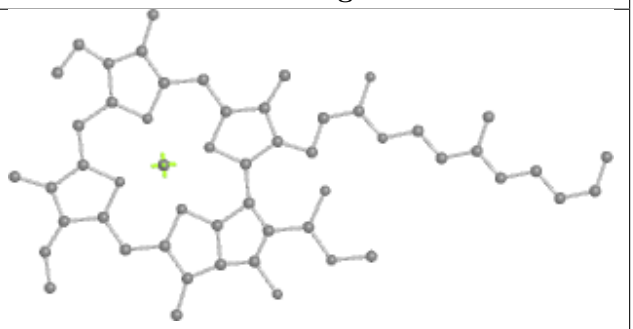


Bond angles

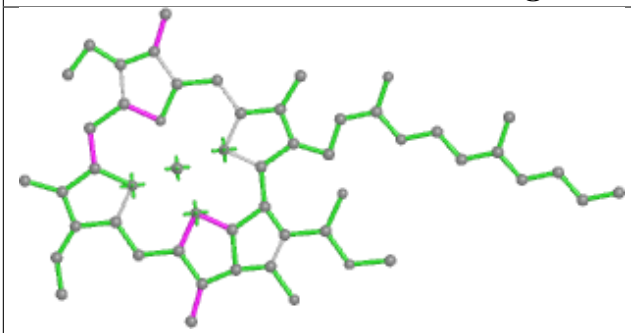


Torsions

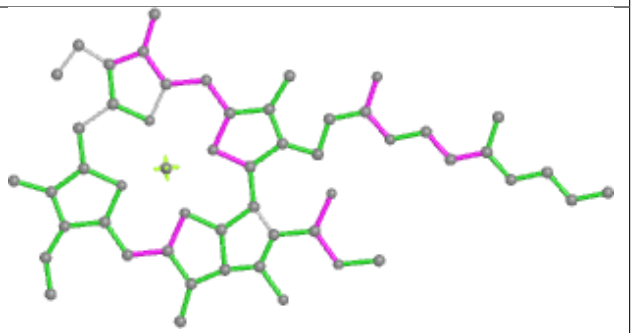


Rings

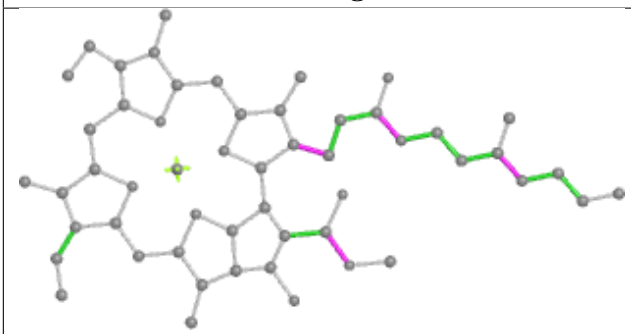
Ligand CLA B 314



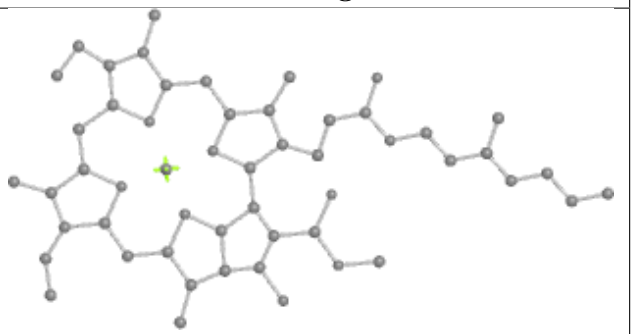
Bond lengths



Bond angles

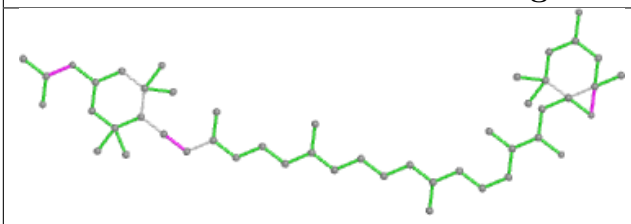


Torsions

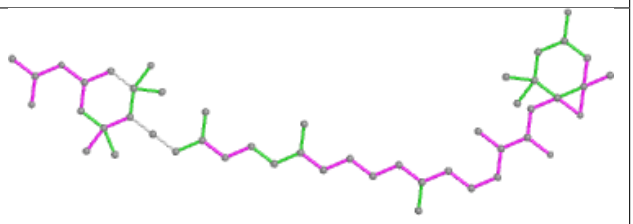


Rings

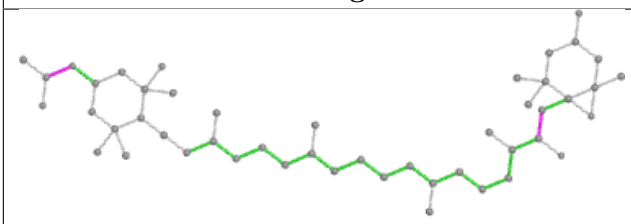
Ligand A86 B 301



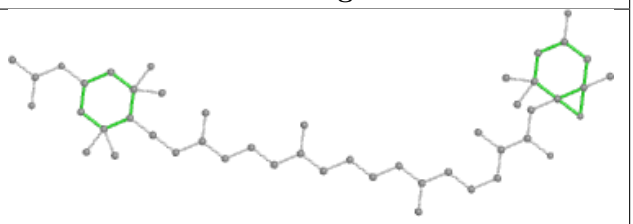
Bond lengths



Bond angles

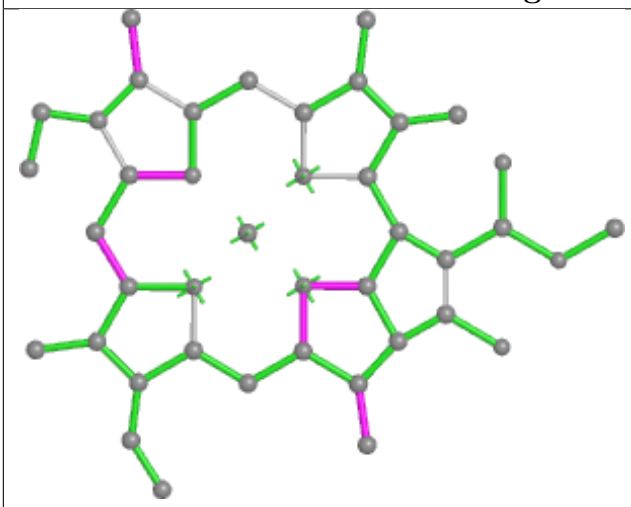


Torsions

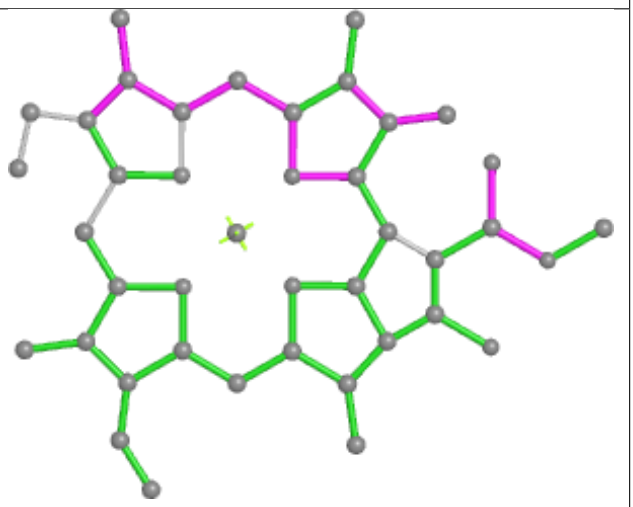


Rings

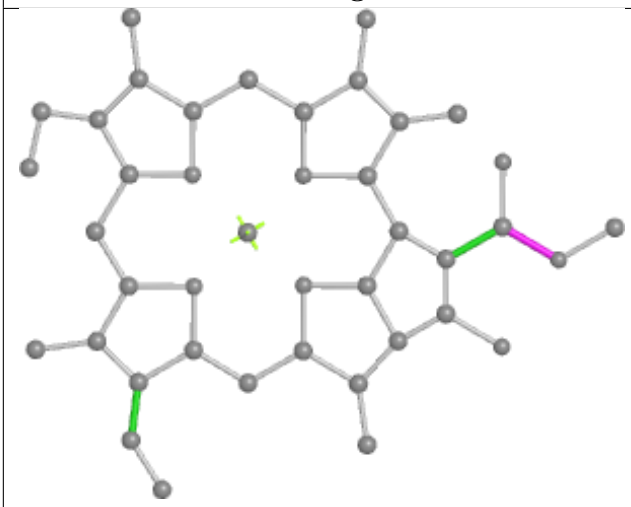
Ligand CLA A 316



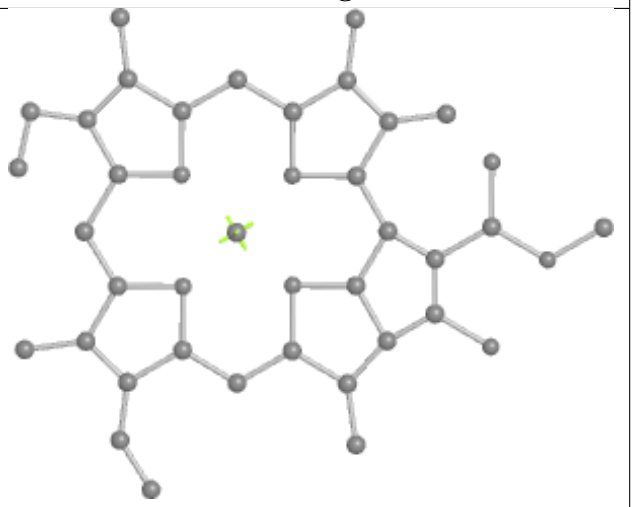
Bond lengths



Bond angles

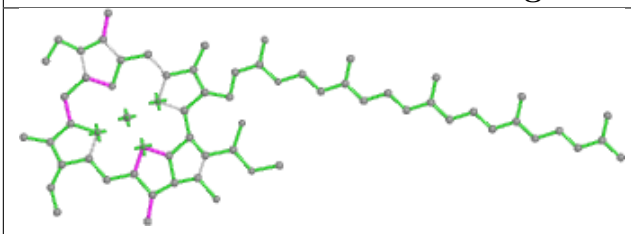


Torsions

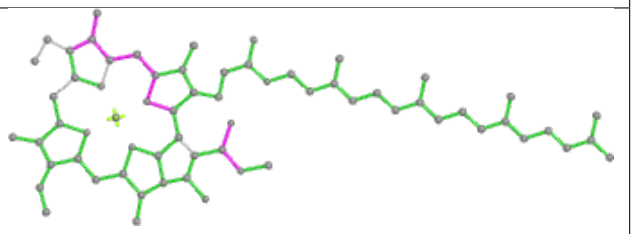


Rings

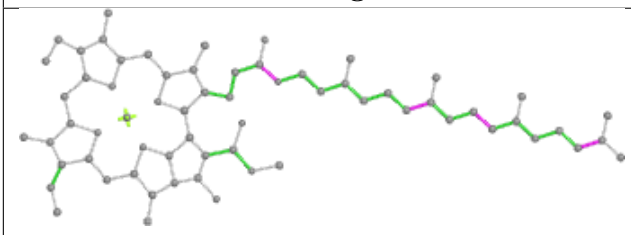
Ligand CLA C 314



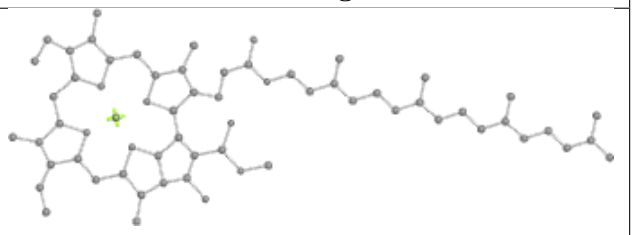
Bond lengths



Bond angles

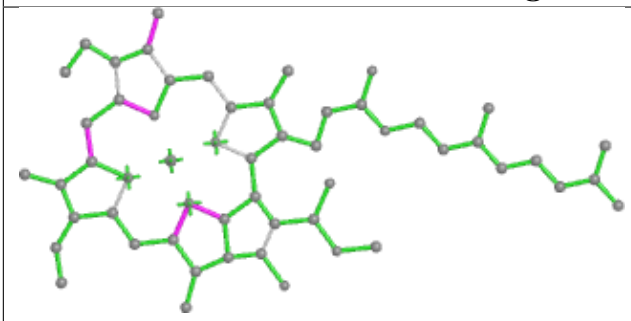


Torsions

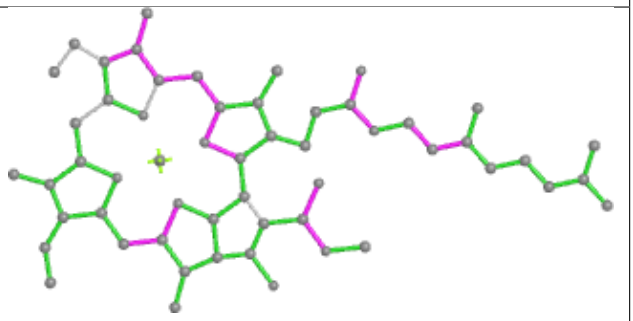


Rings

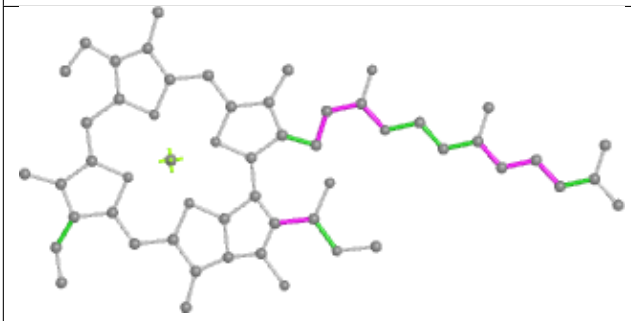
Ligand CLA C 301



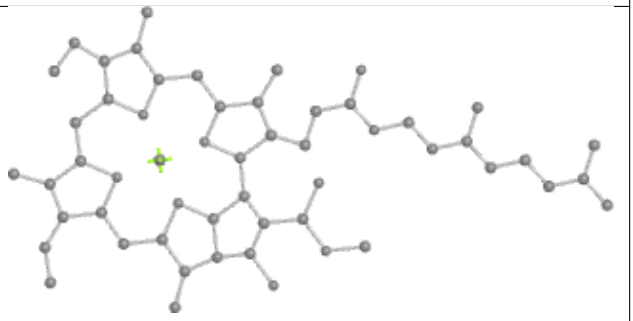
Bond lengths



Bond angles

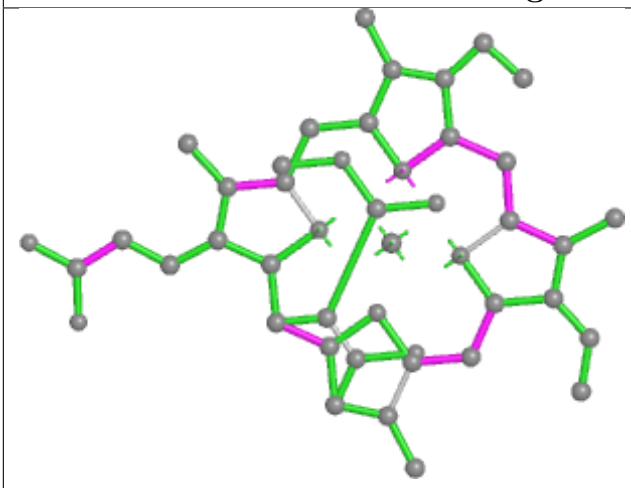


Torsions



Rings

Ligand KC2 B 312



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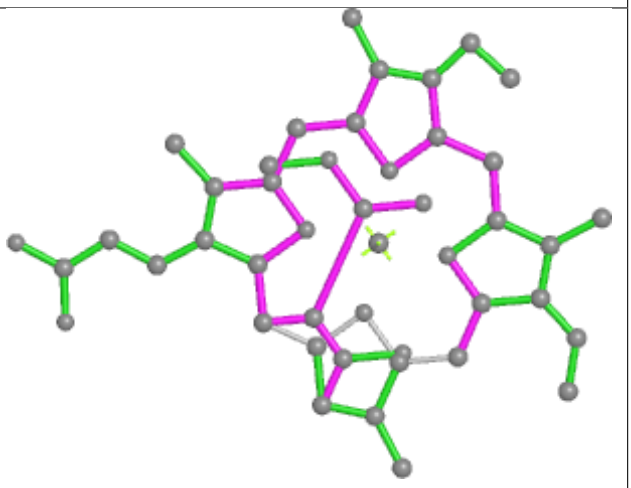
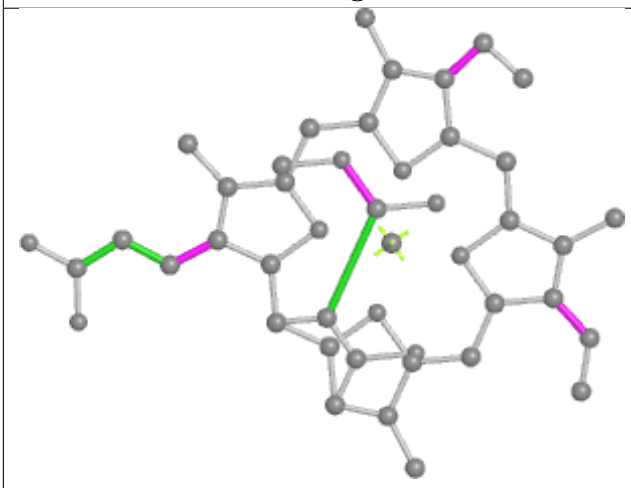
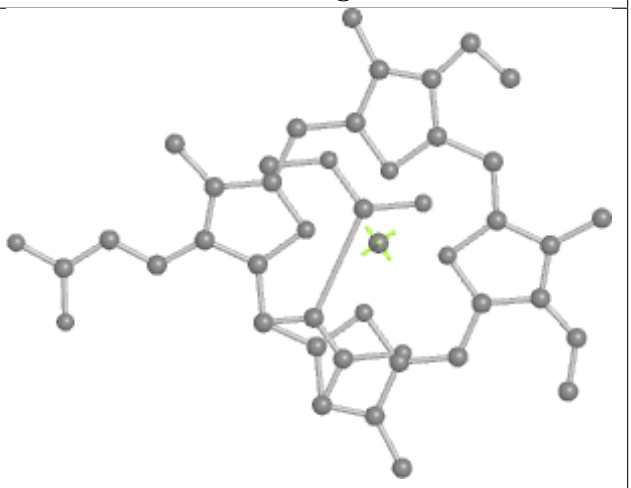


Bond angles

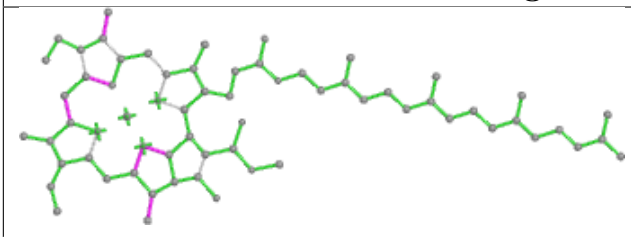


Torsions

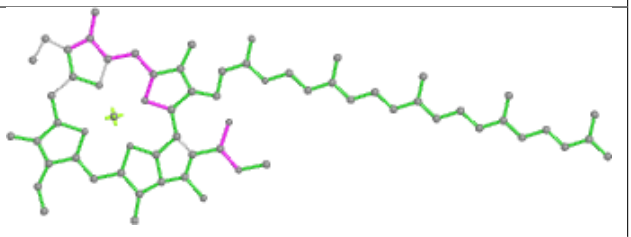


Rings

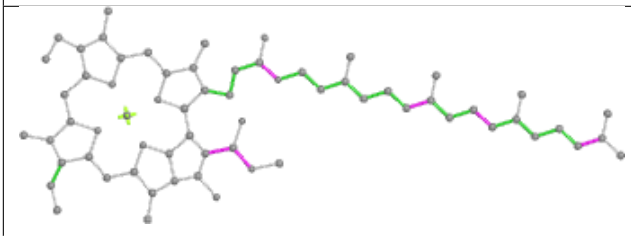
Ligand CLA A 313



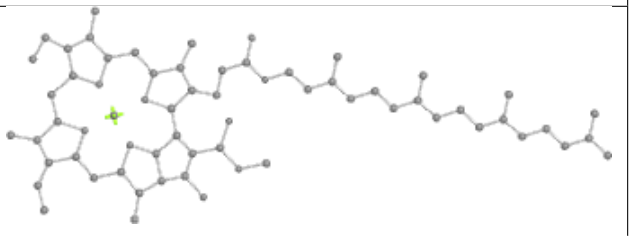
Bond lengths



Bond angles

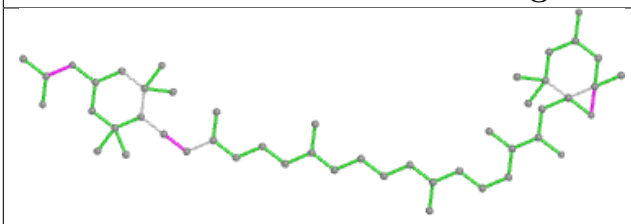


Torsions



Rings

Ligand A86 B 304



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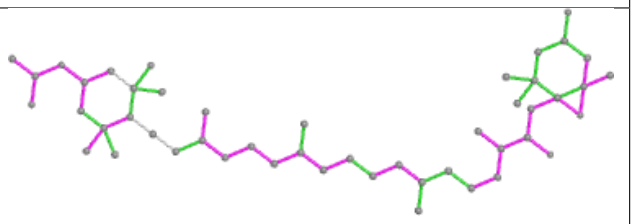
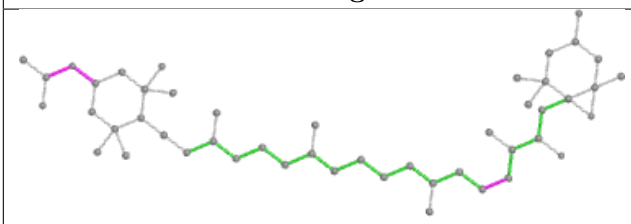
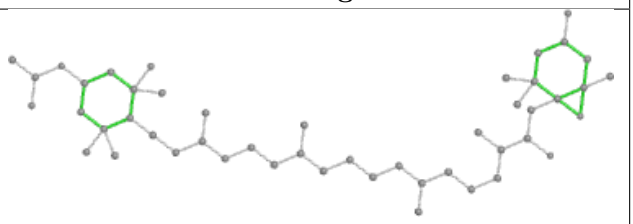


Bond angles

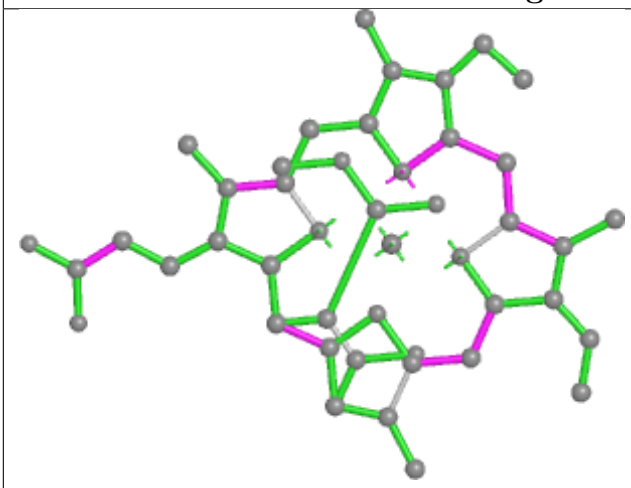


Torsions

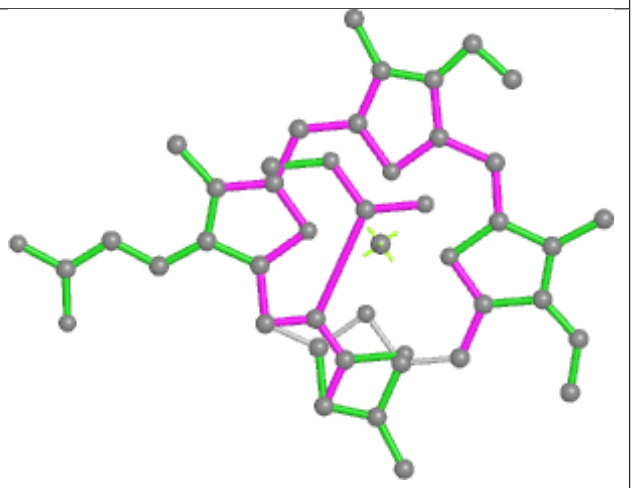


Rings

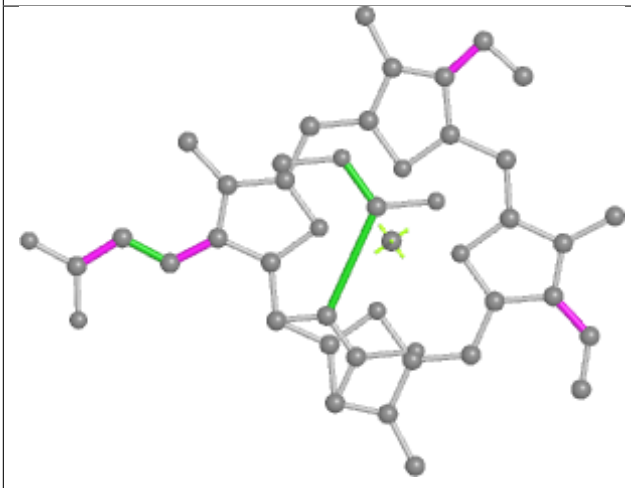
Ligand KC2 C 311



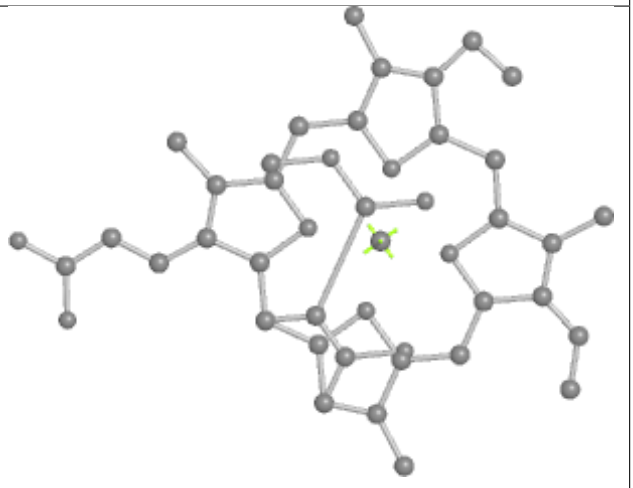
Bond lengths



Bond angles

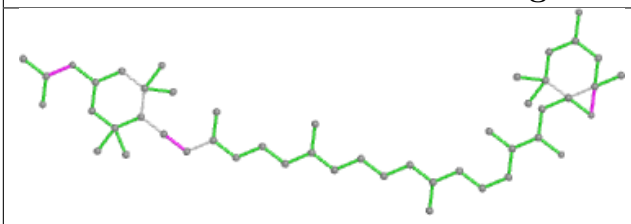


Torsions

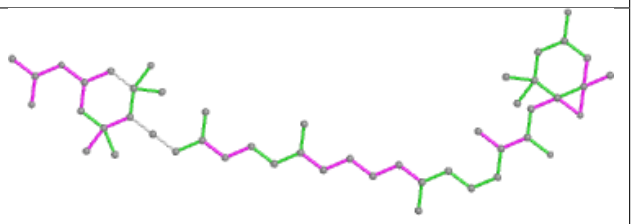


Rings

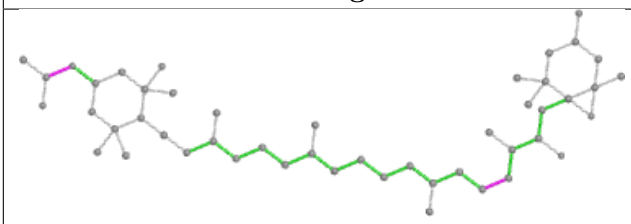
Ligand A86 A 303



Bond lengths



Bond angles



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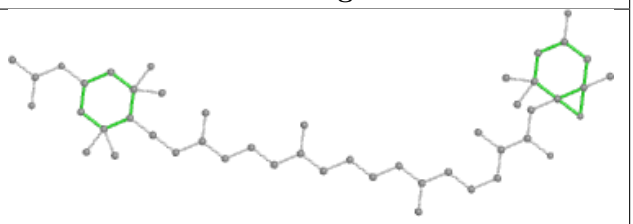
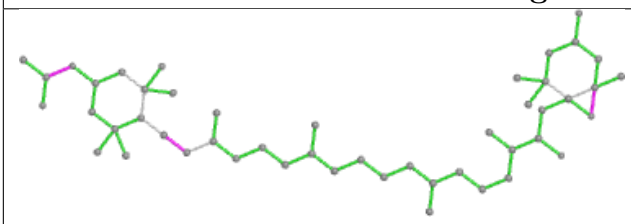
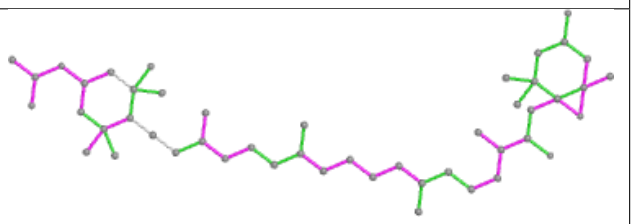


Rings

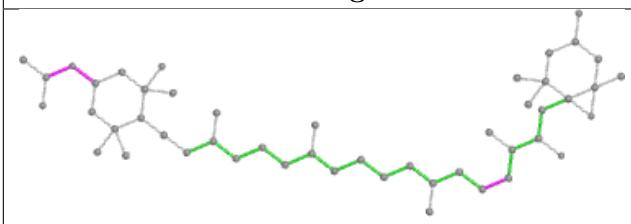
Ligand A86 C 305



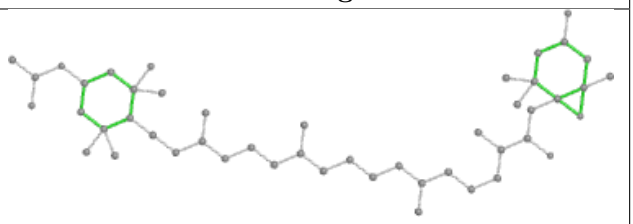
Bond lengths



Bond angles

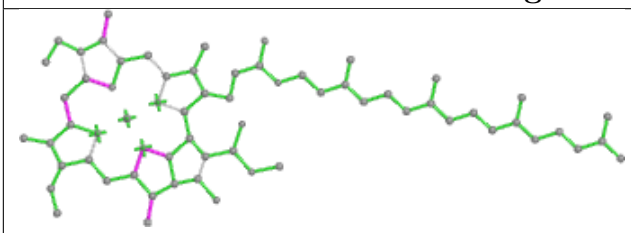


Torsions

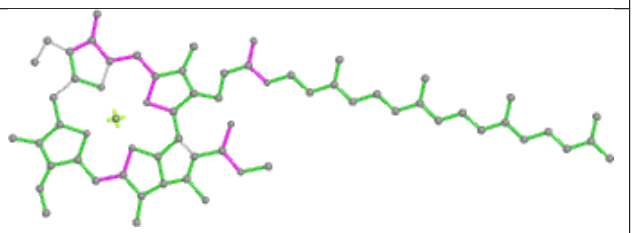


Rings

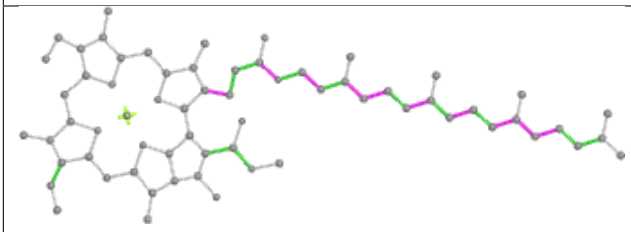
Ligand CLA C 310



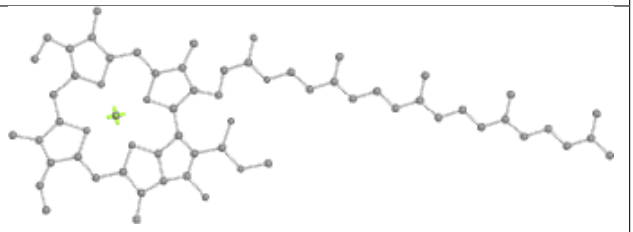
Bond lengths



Bond angles

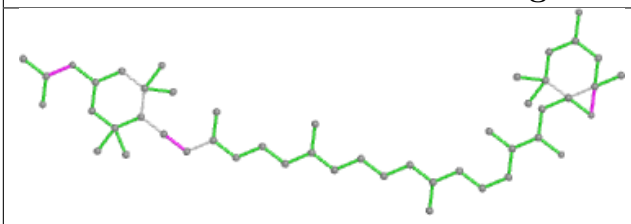


Torsions



Rings

Ligand A86 A 307



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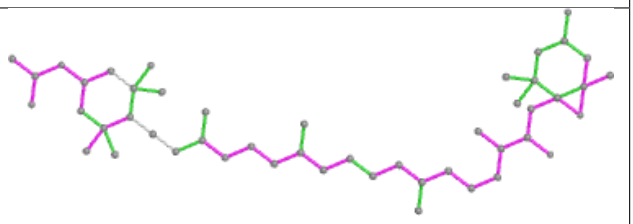
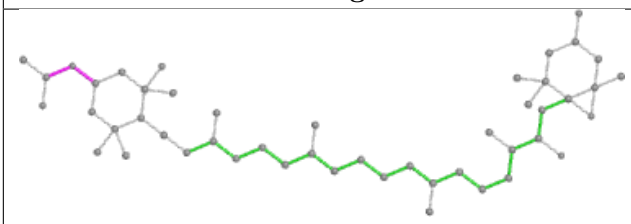
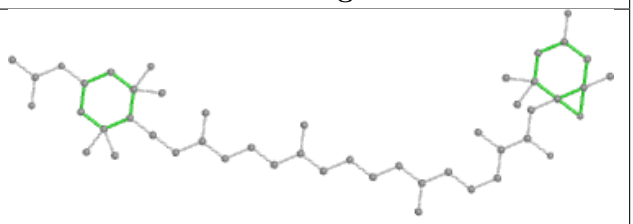


Bond angles

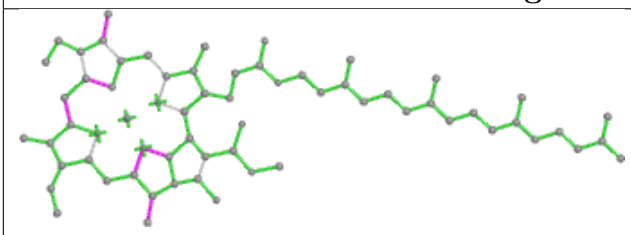


Torsions

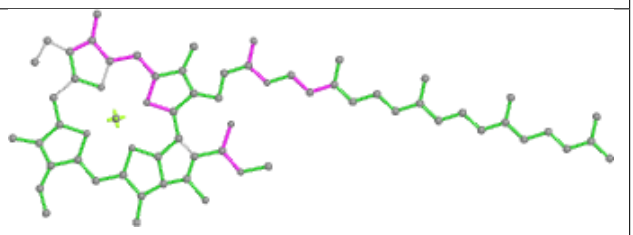


Rings

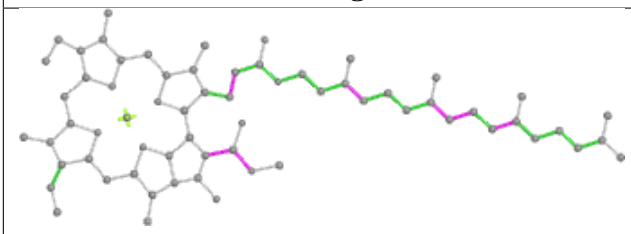
Ligand CLA C 312



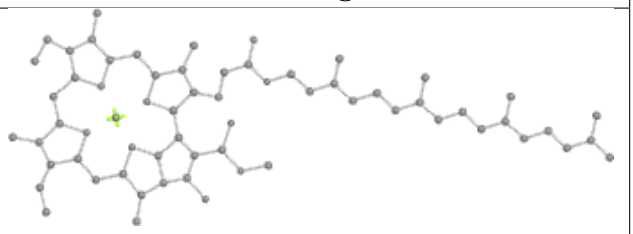
Bond lengths



Bond angles

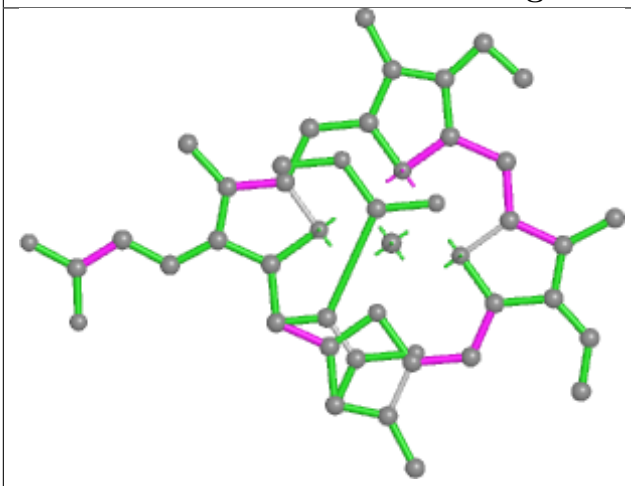


Torsions



Rings

Ligand KC2 B 310



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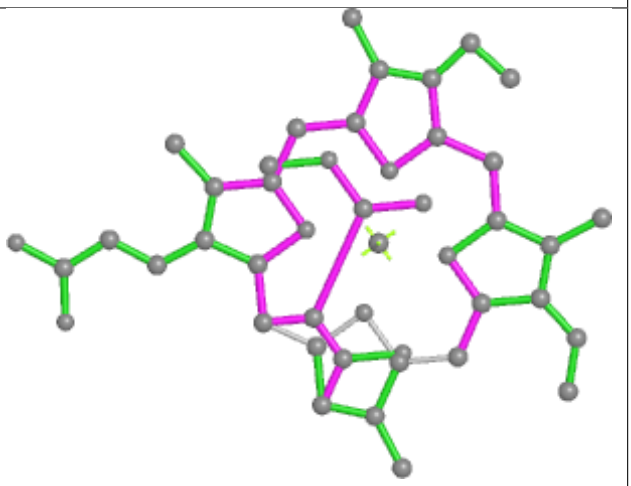
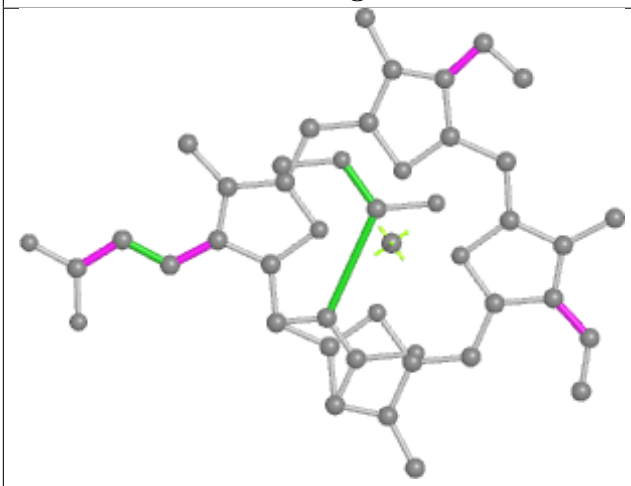
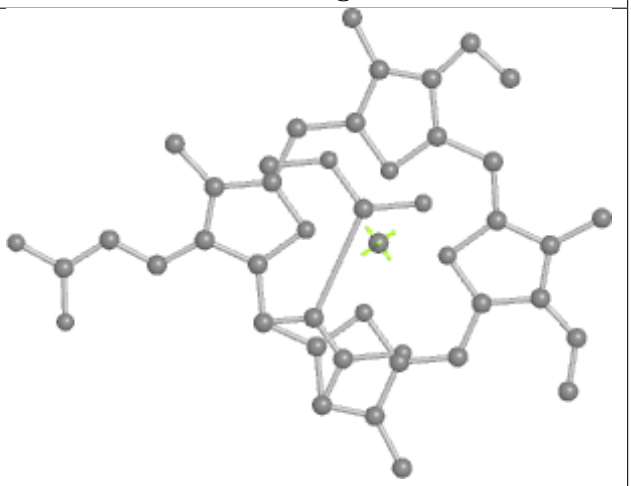


Bond angles

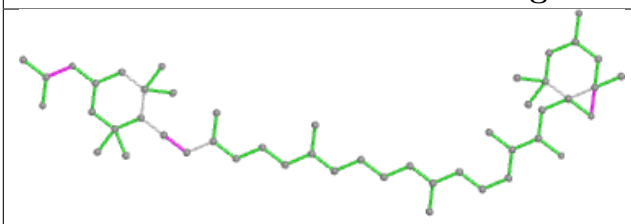


Torsions



Rings

Ligand A86 C 303



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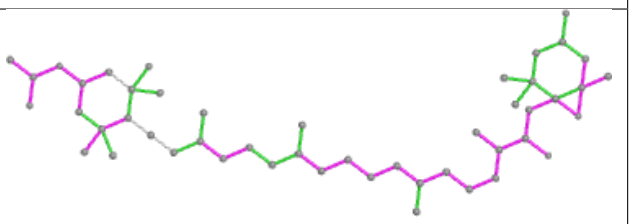
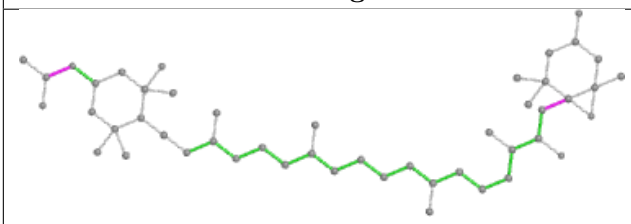
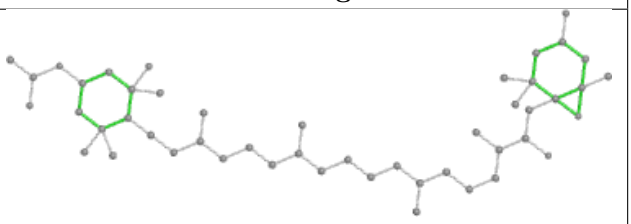


Bond angles

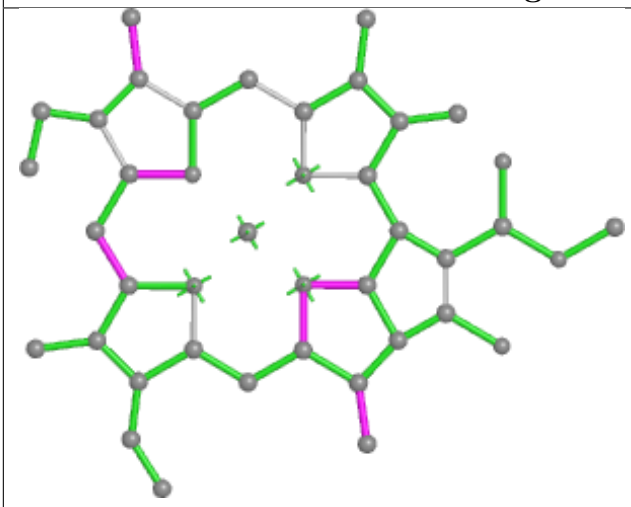


Torsions



Rings

Ligand CLA C 317



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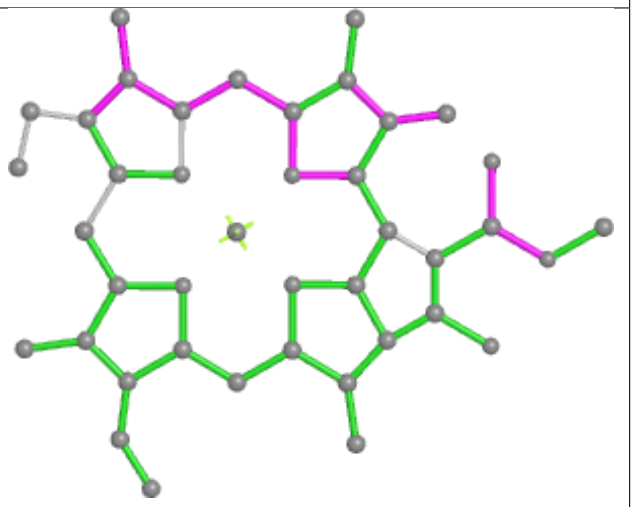
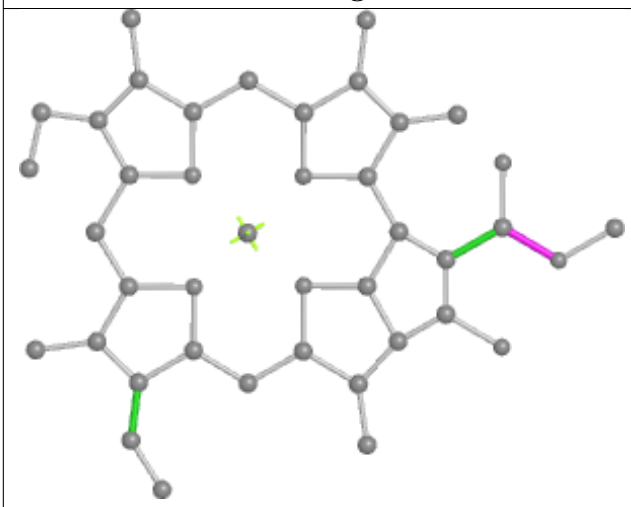
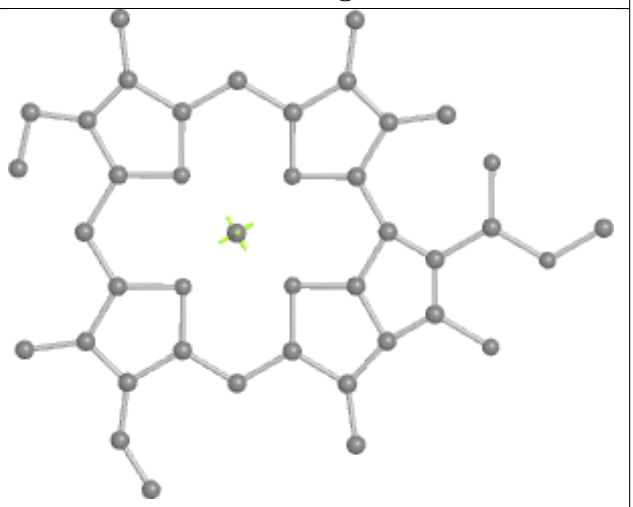


Bond angles

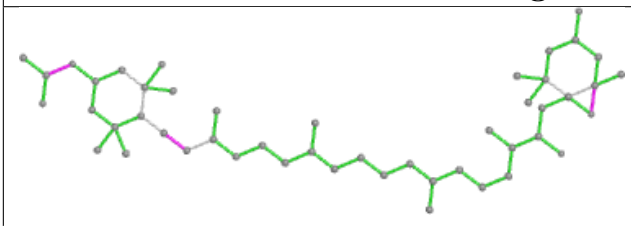


Torsions

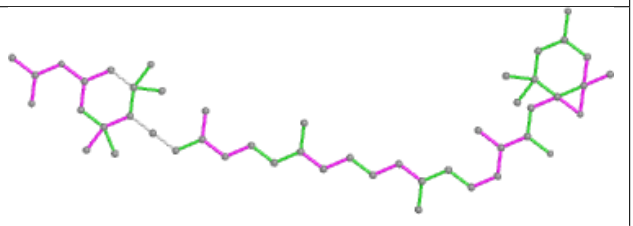


Rings

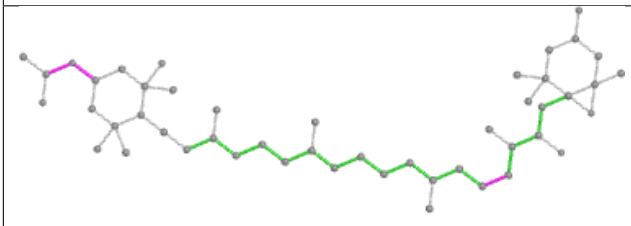
Ligand A86 A 304



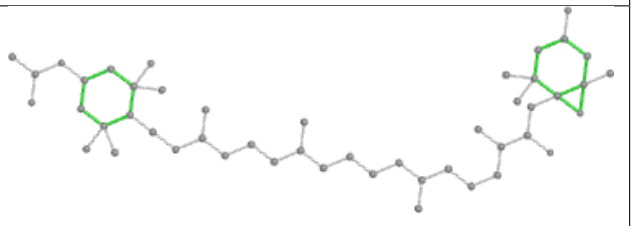
Bond lengths



Bond angles

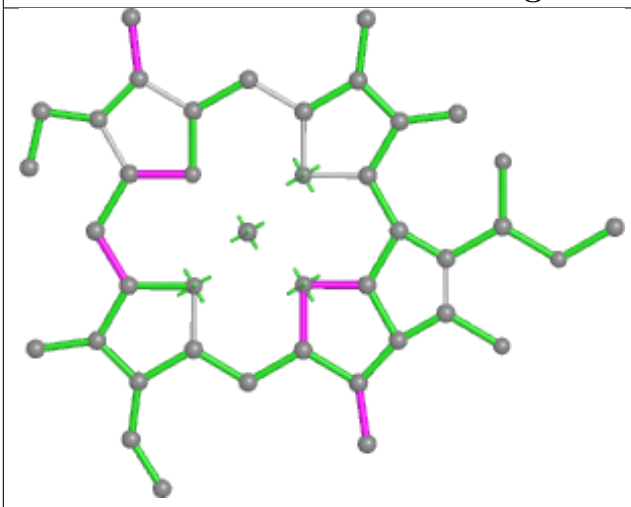


Torsions

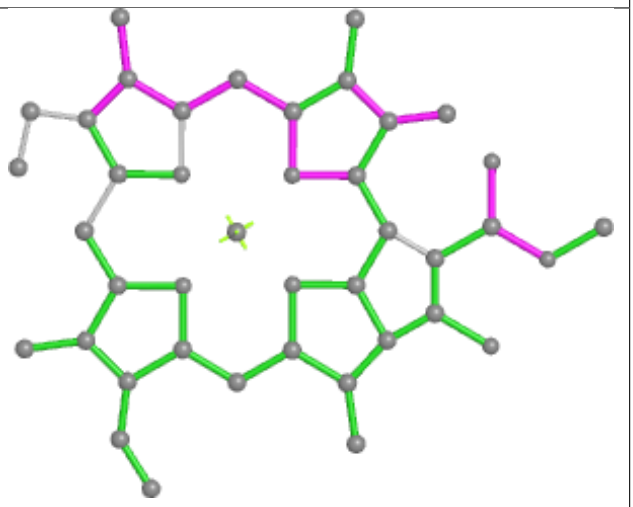


Rings

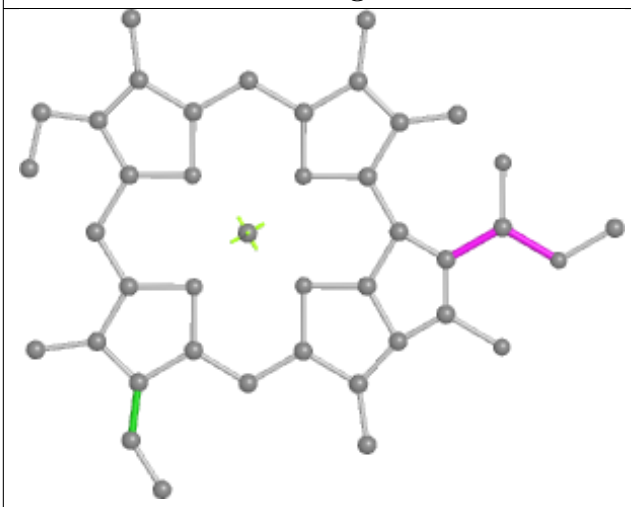
Ligand CLA B 316



Bond lengths



Bond angles



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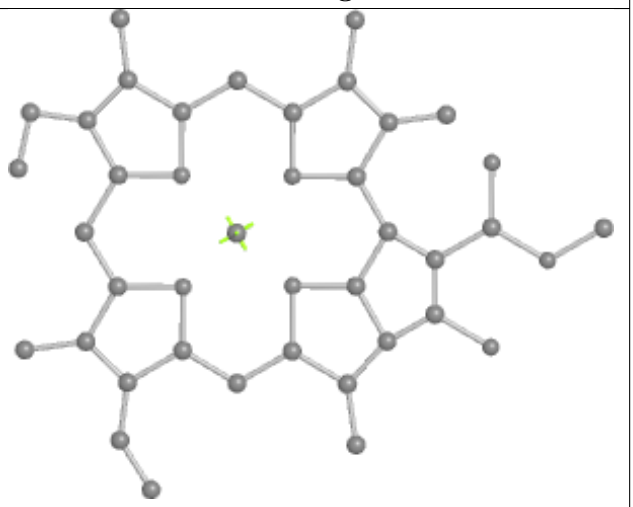
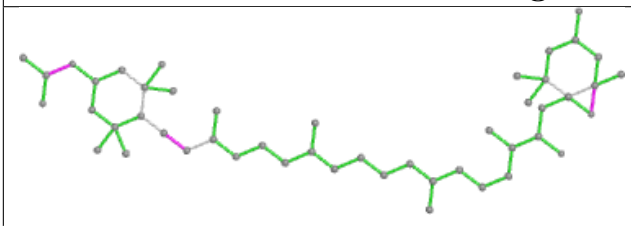
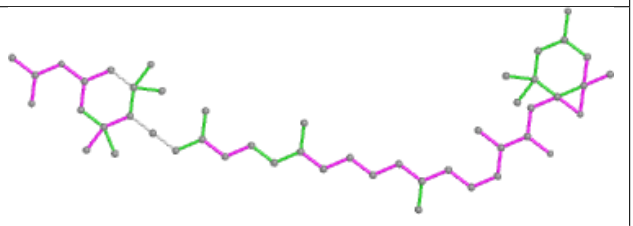


Rings

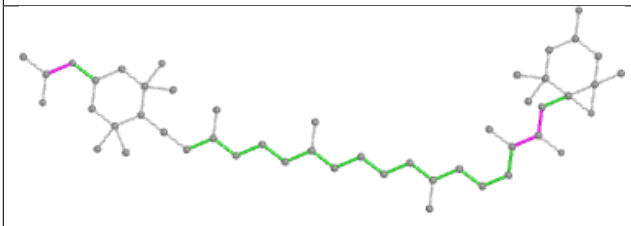
Ligand A86 A 302



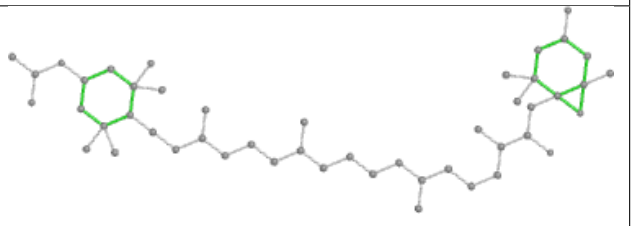
Bond lengths



Bond angles

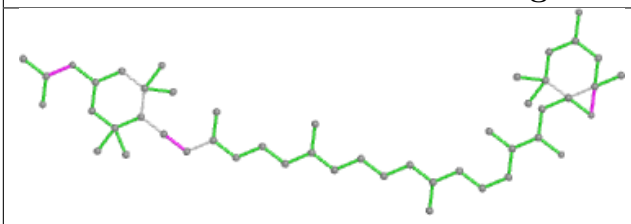


Torsions

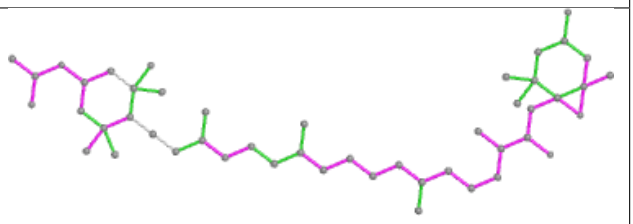


Rings

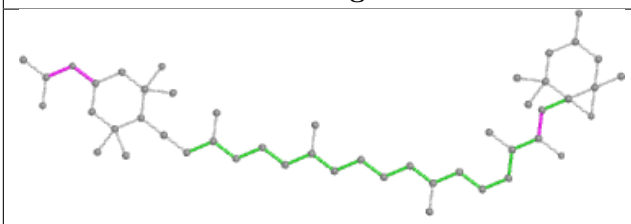
Ligand A86 C 302



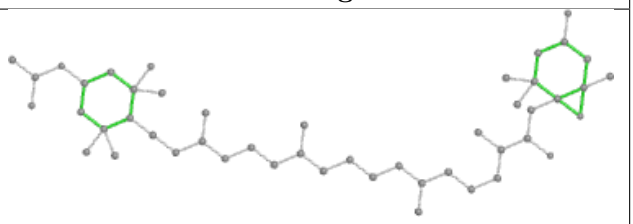
Bond lengths



Bond angles

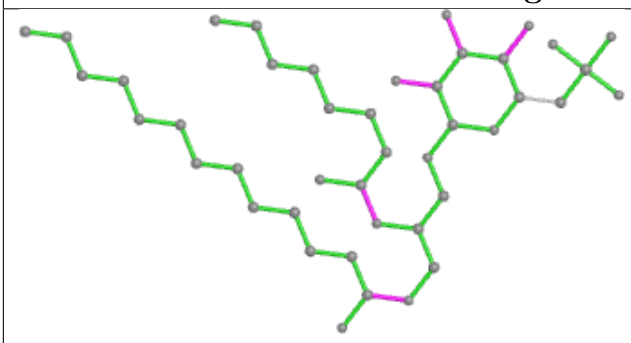


Torsions



Rings

Ligand SQD C 319



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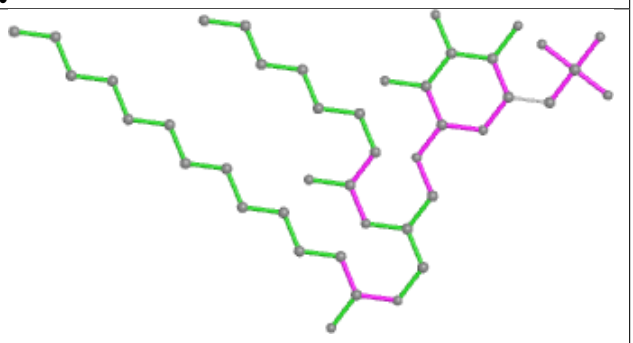
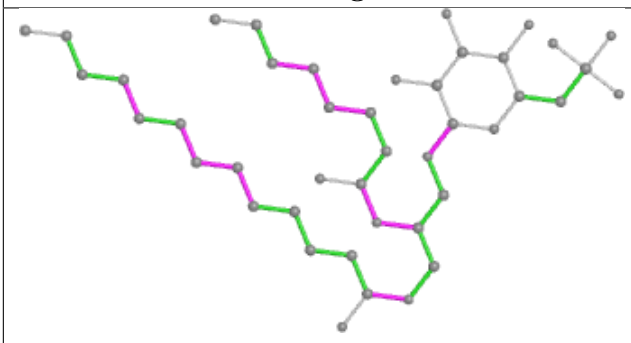


Bond angles



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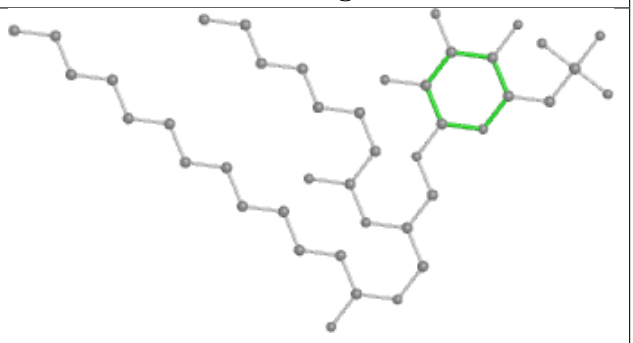
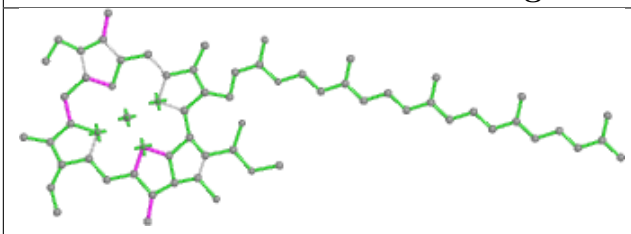
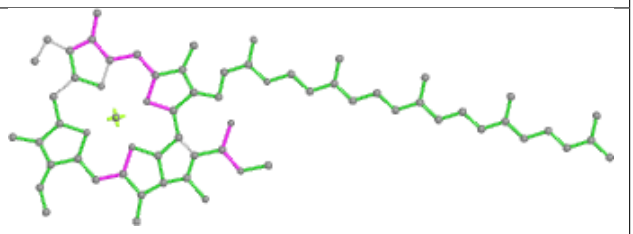


Rings

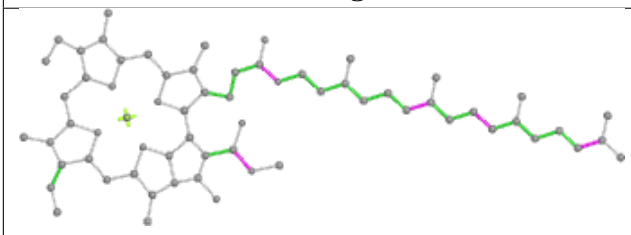
Ligand CLA B 313



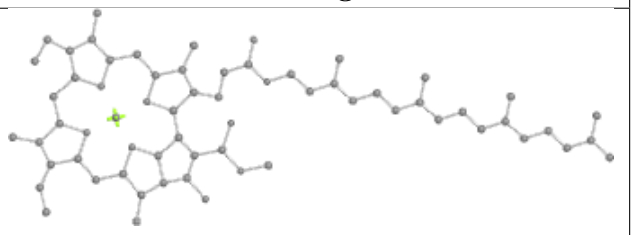
Bond lengths



Bond angles

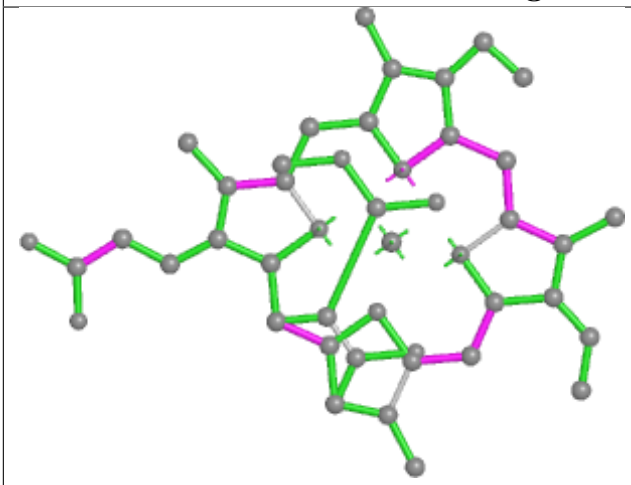


Torsions

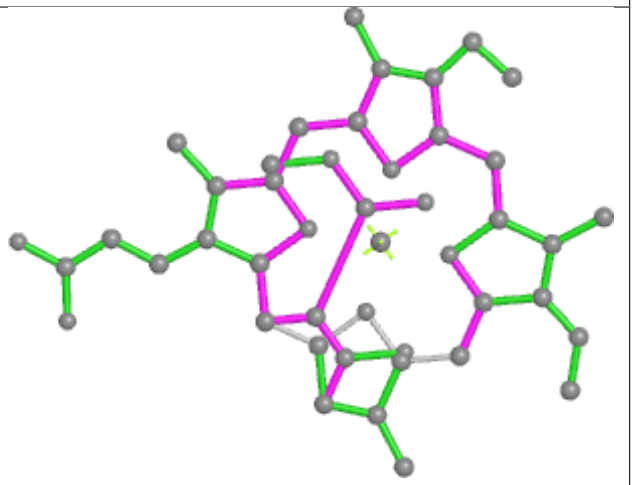


Rings

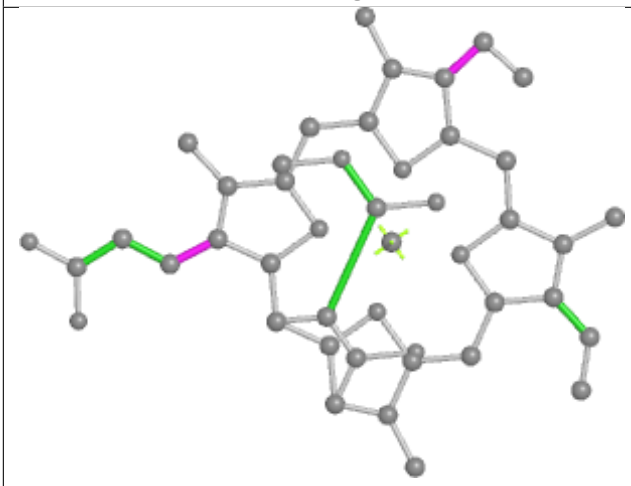
Ligand KC2 A 312



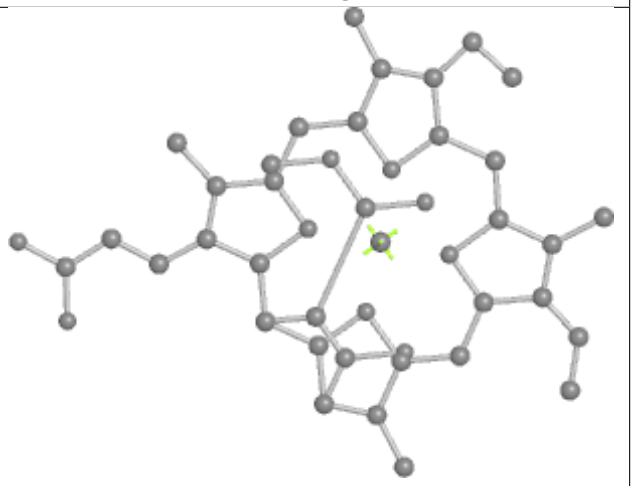
Bond lengths



Bond angles

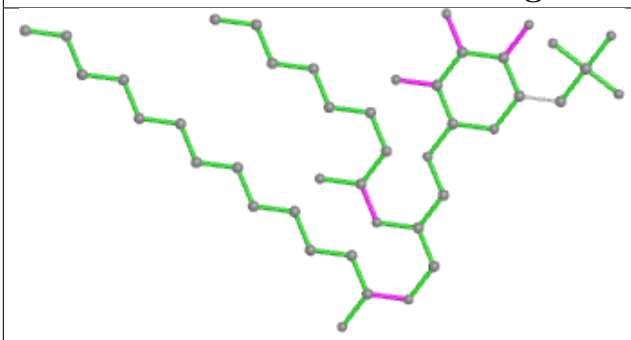


Torsions

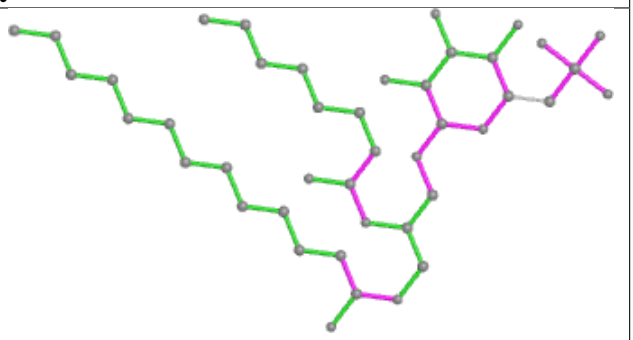


Rings

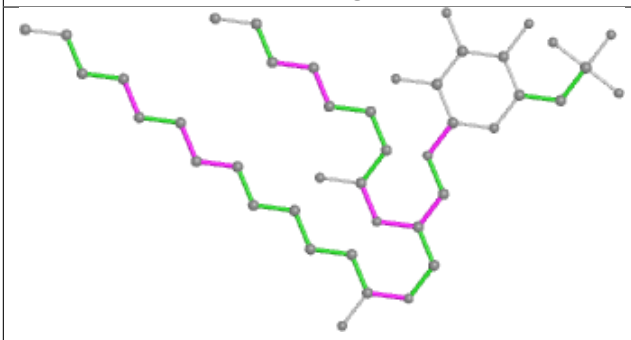
Ligand SQD B 318



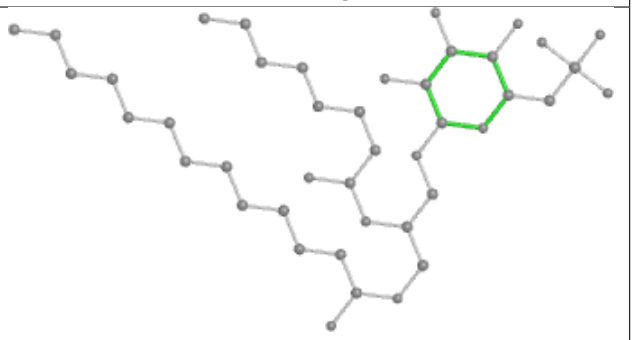
Bond lengths



Bond angles

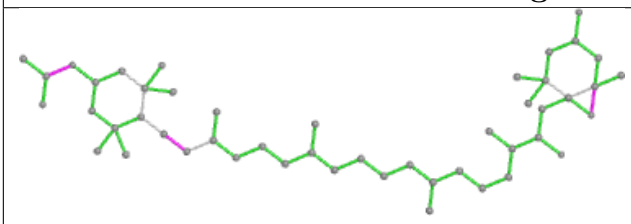


Torsions

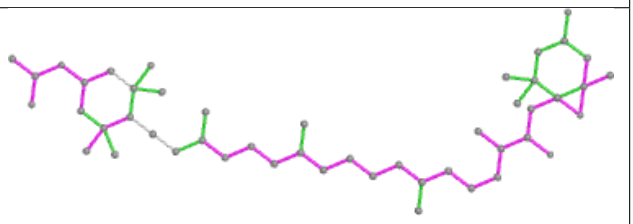


Rings

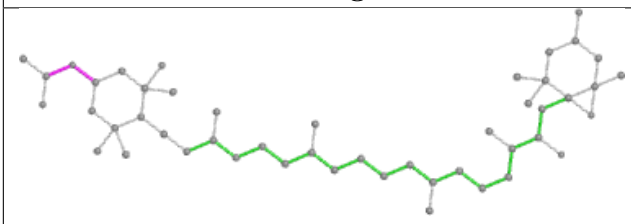
Ligand A86 B 307



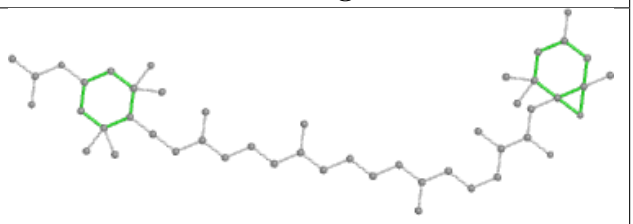
Bond lengths



Bond angles

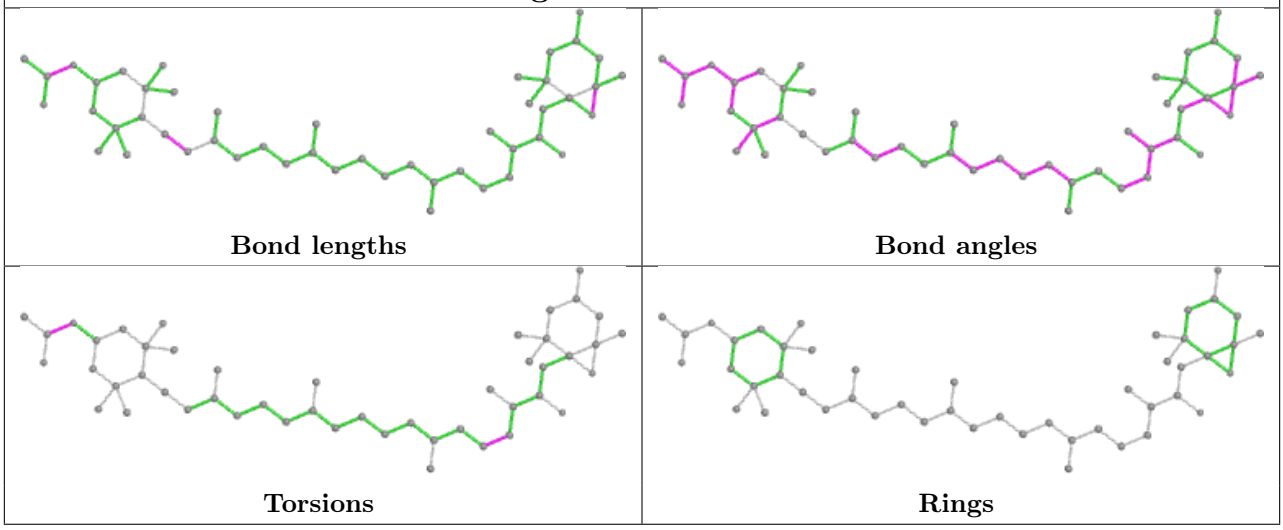


Torsions

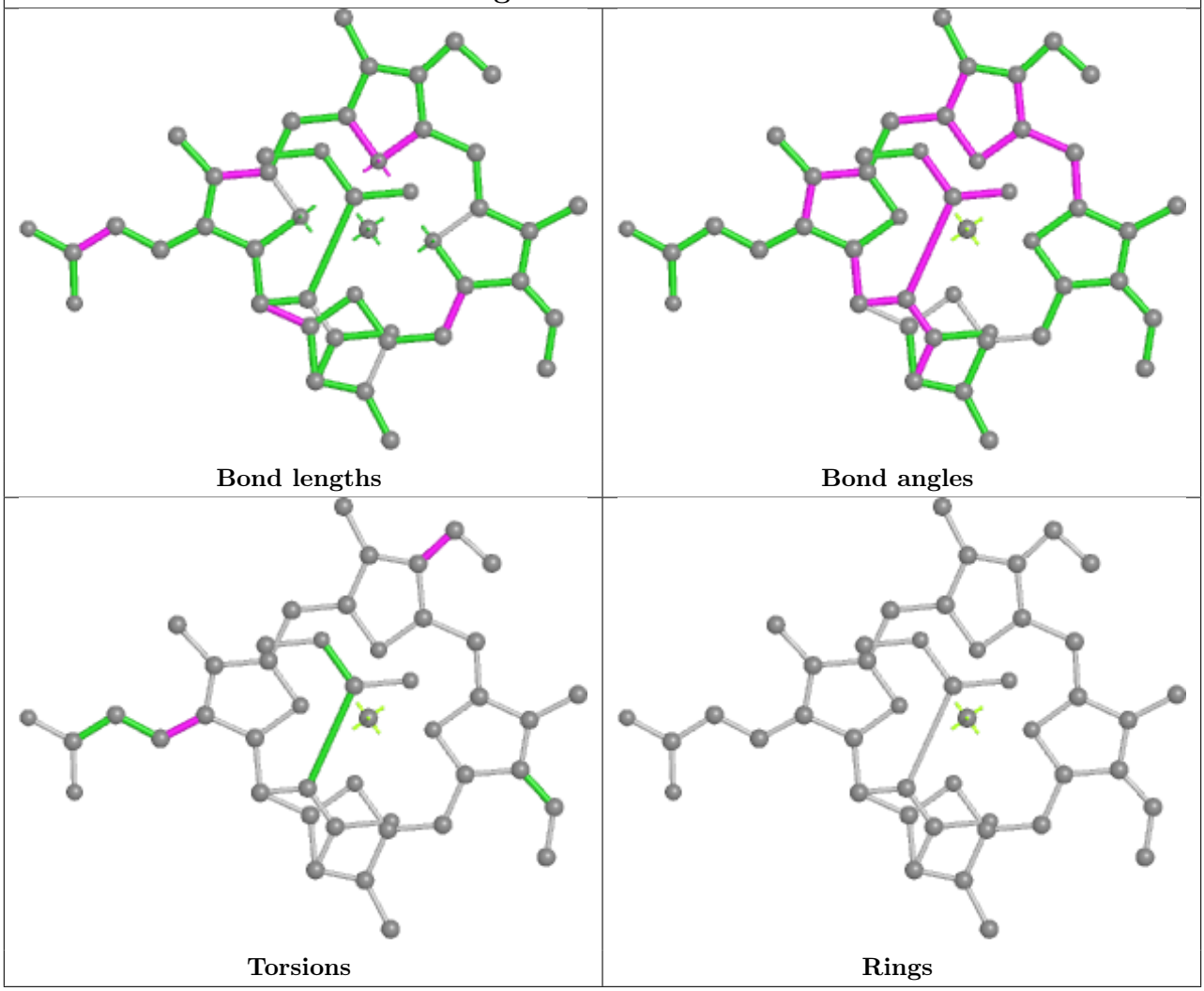


Rings

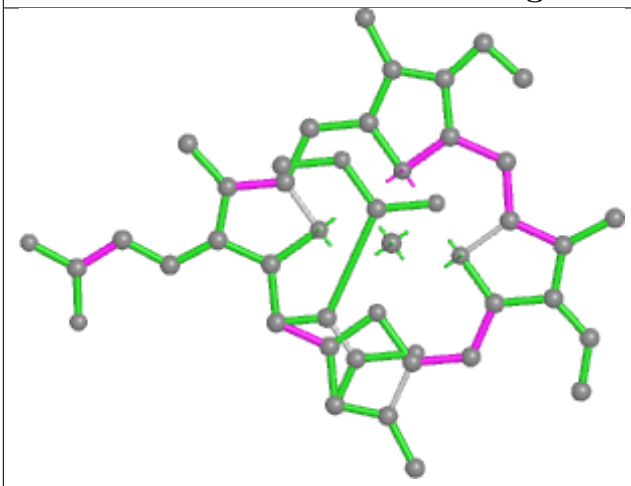
Ligand A86 C 304



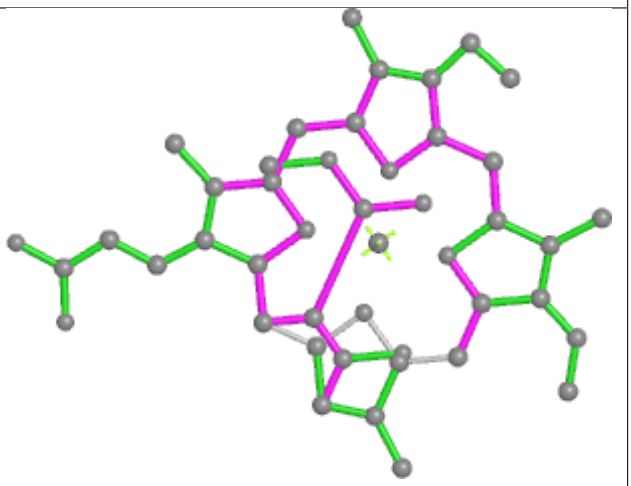
Ligand KC1 A 315



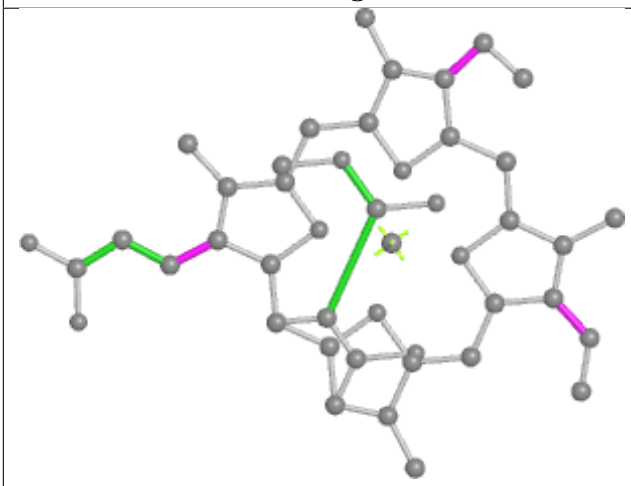
Ligand KC2 C 313



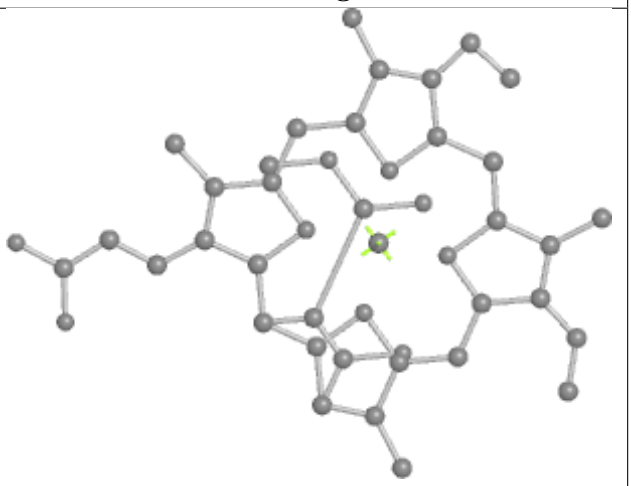
Bond lengths



Bond angles

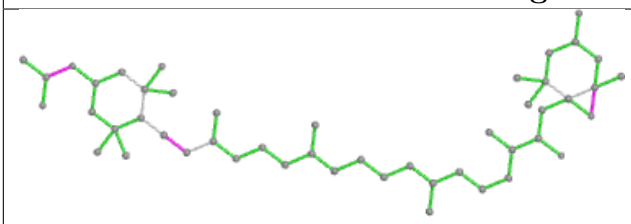


Torsions

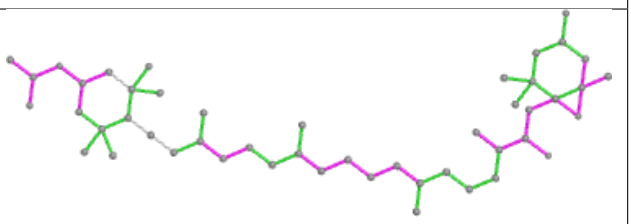


Rings

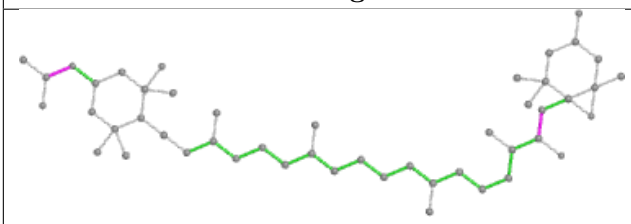
Ligand A86 C 306



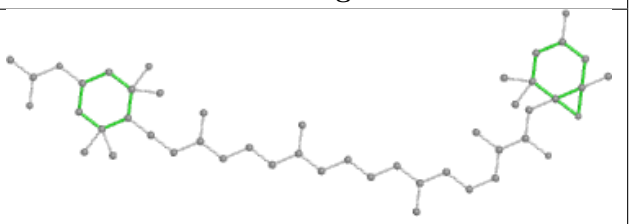
Bond lengths



Bond angles

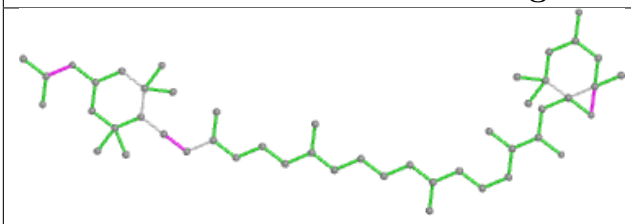


Torsions

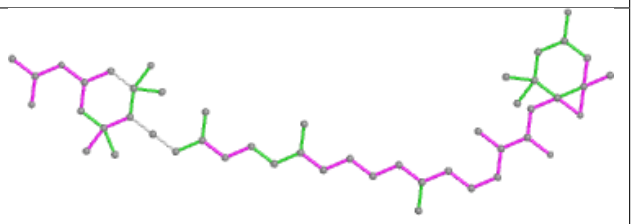


Rings

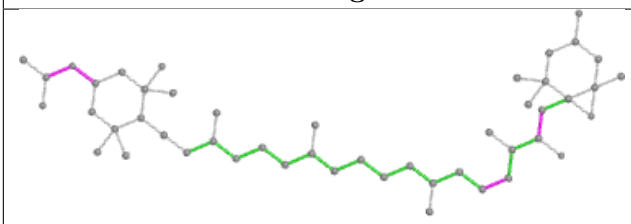
Ligand A86 A 301



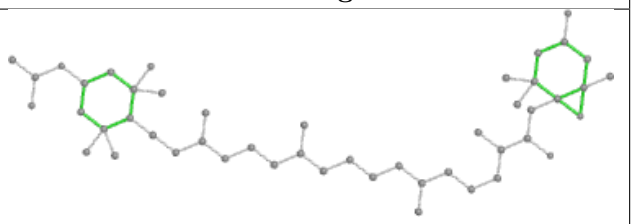
Bond lengths



Bond angles

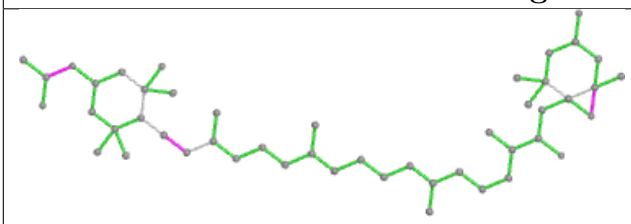


Torsions

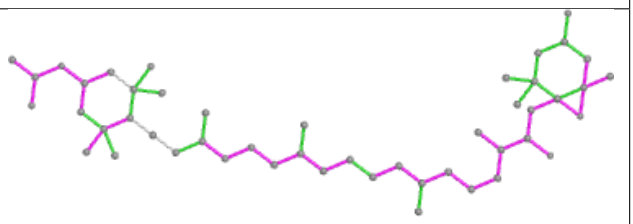


Rings

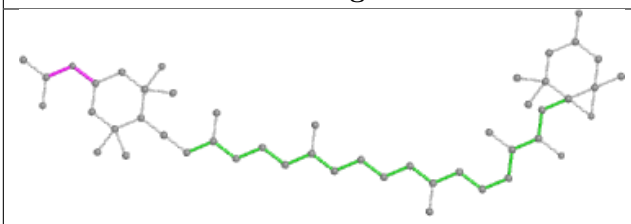
Ligand A86 C 308



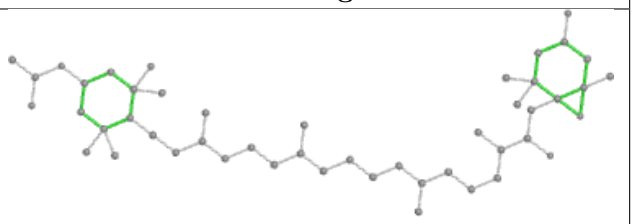
Bond lengths



Bond angles

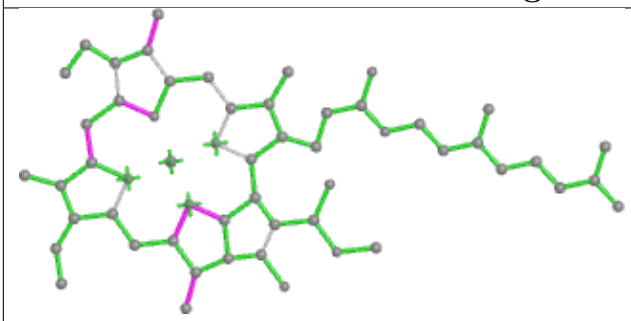


Torsions

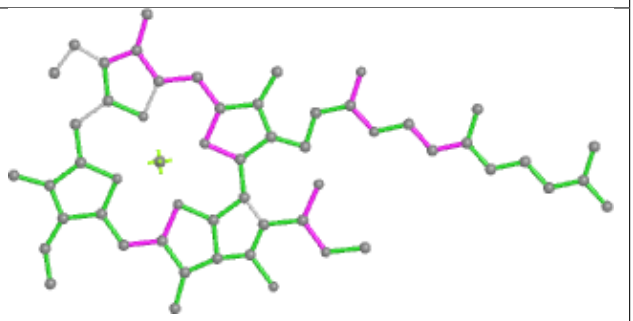


Rings

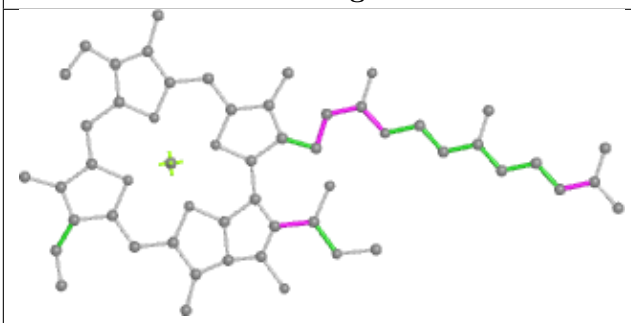
Ligand CLA A 319



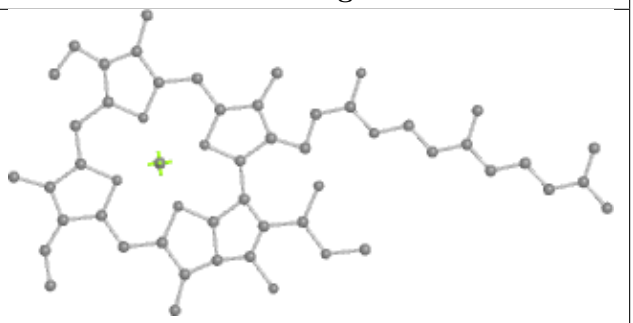
Bond lengths



Bond angles

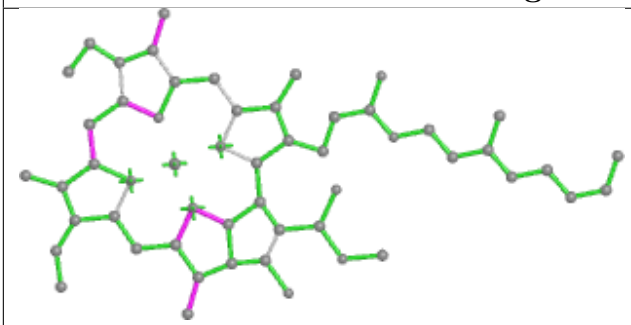


Torsions

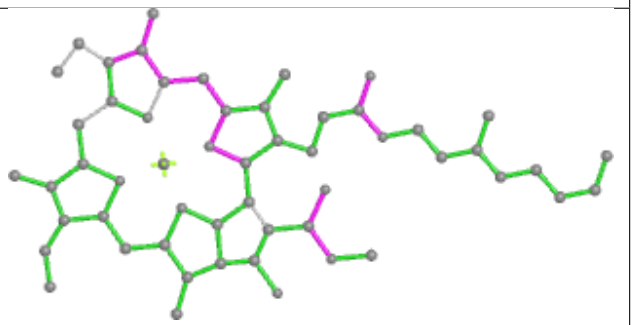


Rings

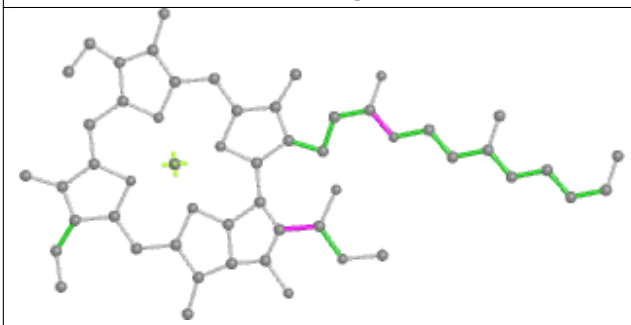
Ligand CLA B 308



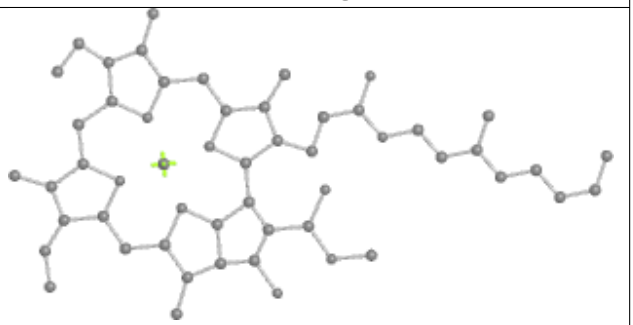
Bond lengths



Bond angles

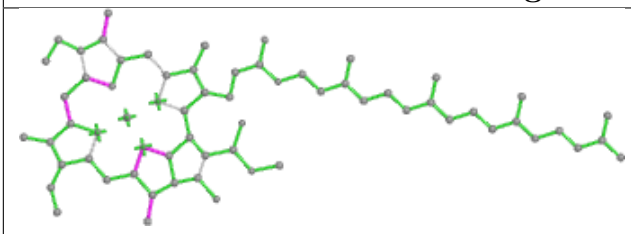


Torsions

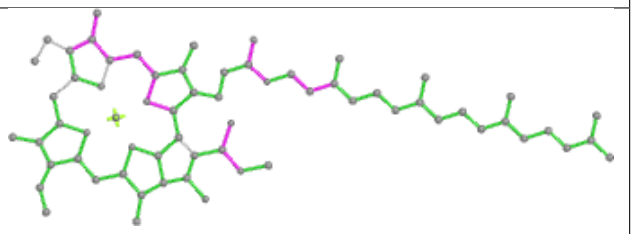


Rings

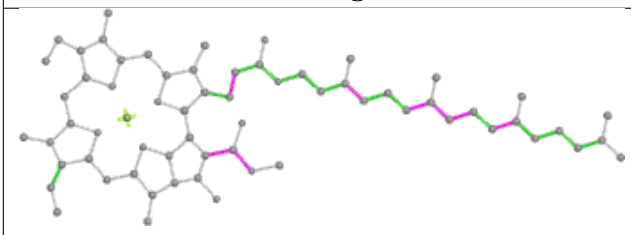
Ligand CLA B 311



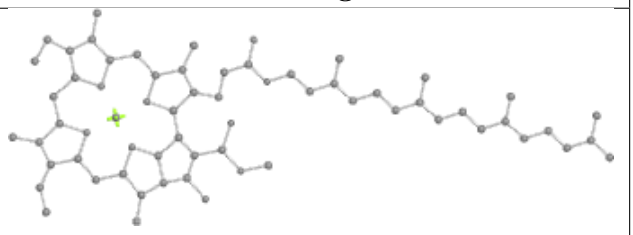
Bond lengths



Bond angles

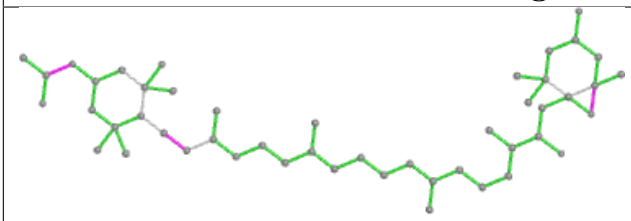


Torsions

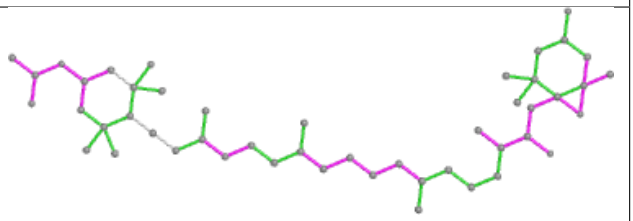


Rings

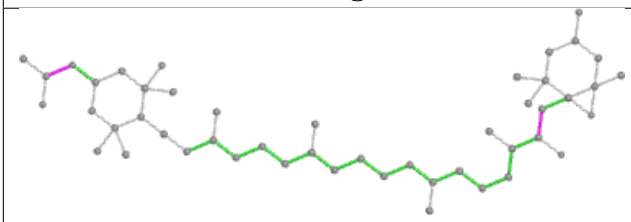
Ligand A86 B 305



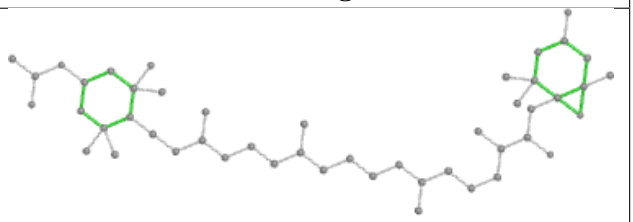
Bond lengths



Bond angles

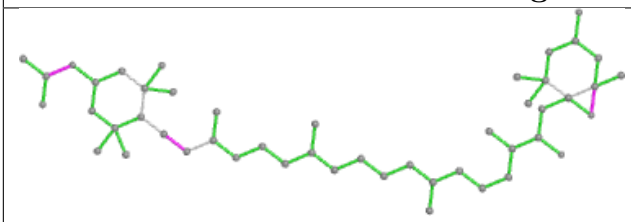


Torsions

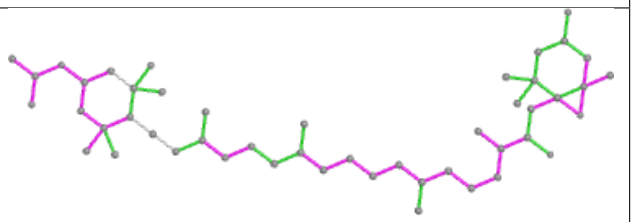


Rings

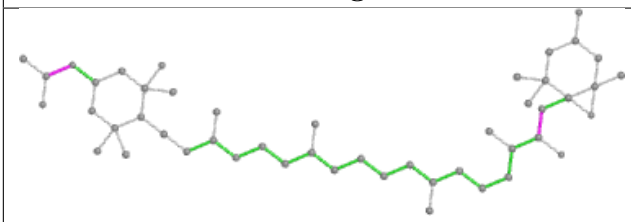
Ligand A86 B 306



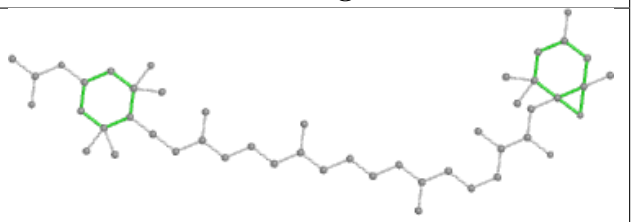
Bond lengths



Bond angles

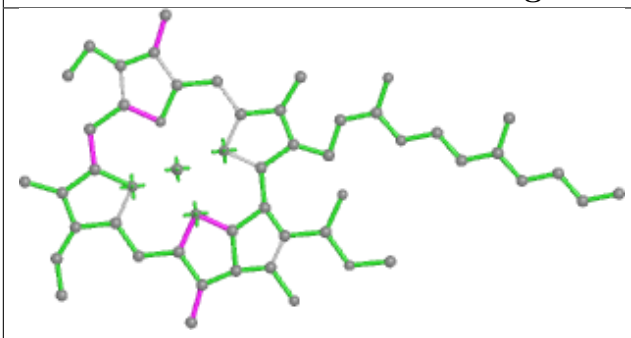


Torsions

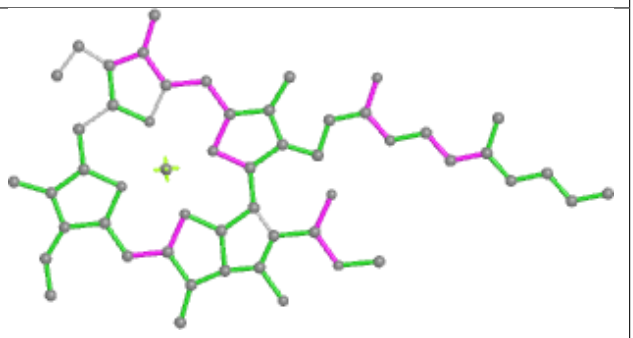


Rings

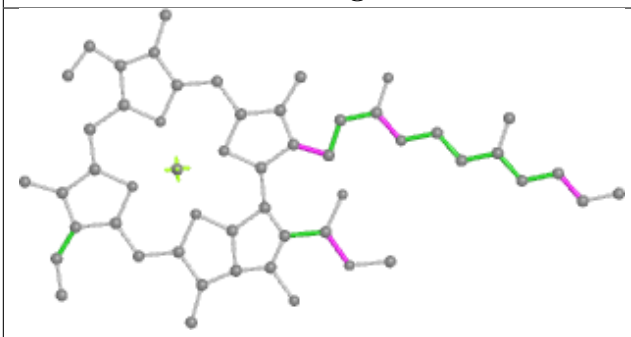
Ligand CLA C 315



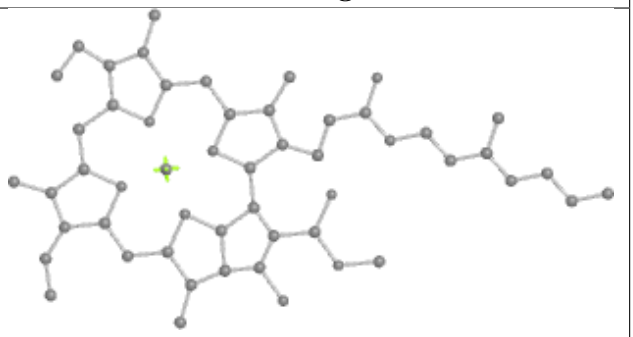
Bond lengths



Bond angles

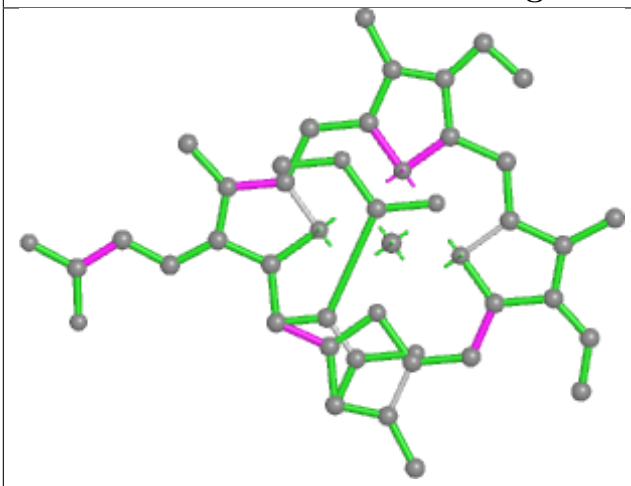


Torsions

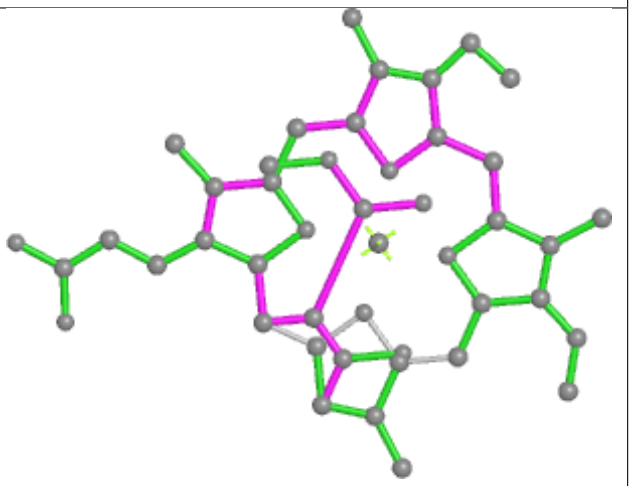


Rings

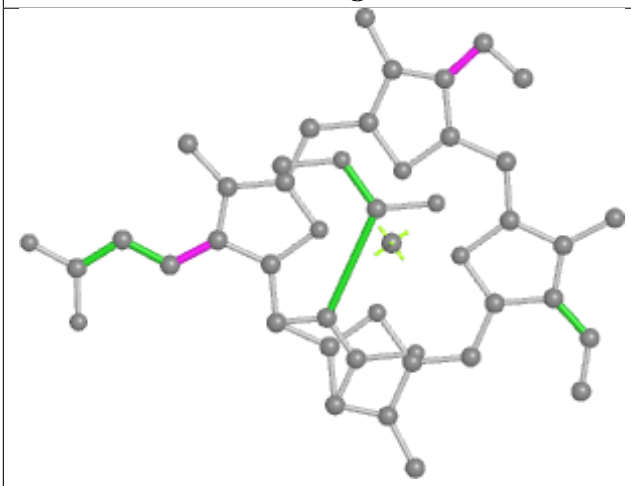
Ligand KC1 C 316



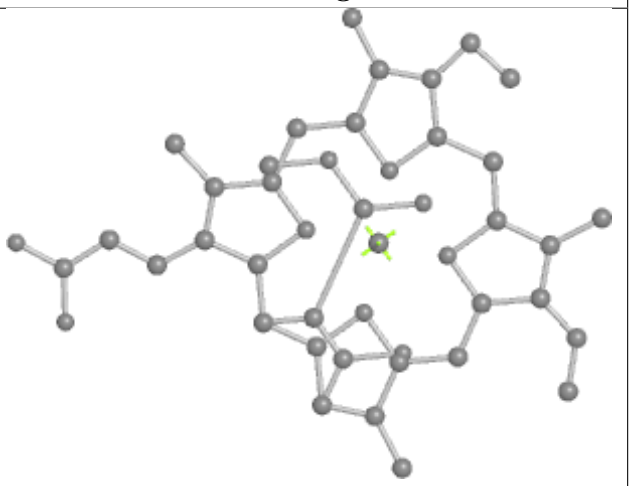
Bond lengths



Bond angles

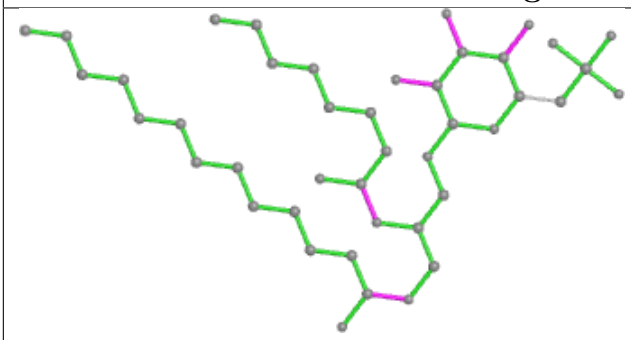


Torsions

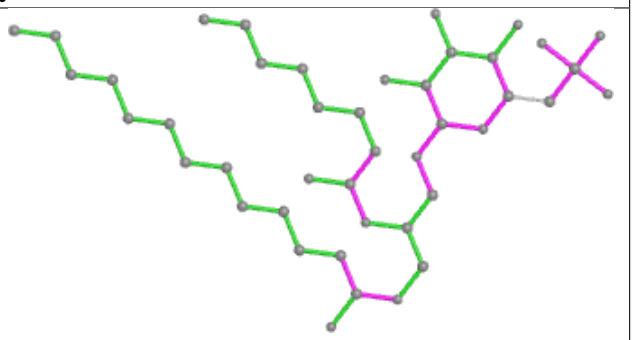


Rings

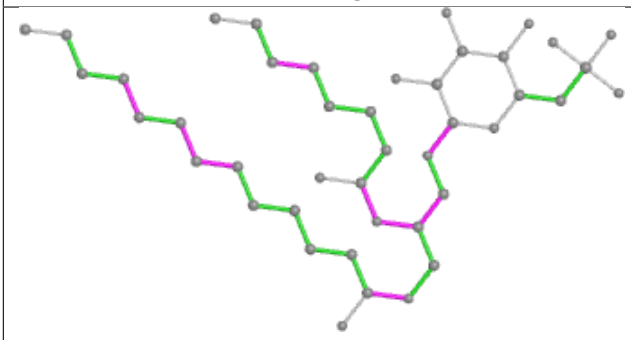
Ligand SQD A 318



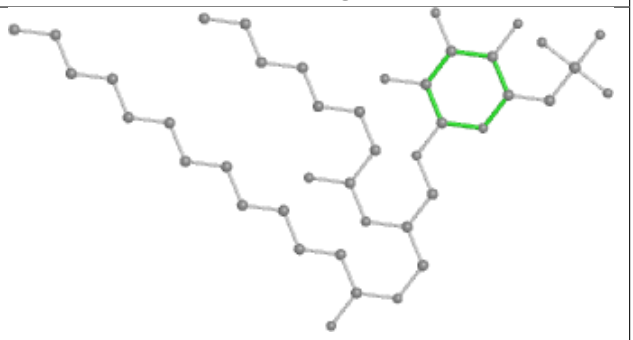
Bond lengths



Bond angles

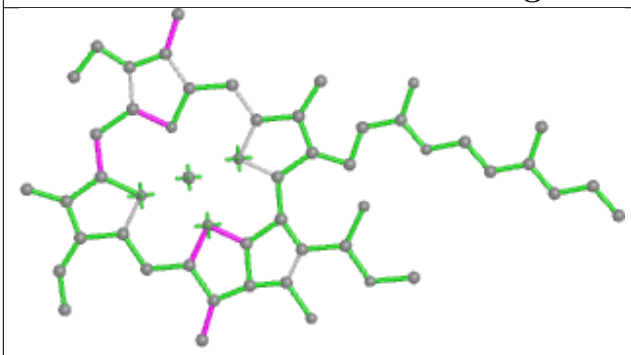


Torsions

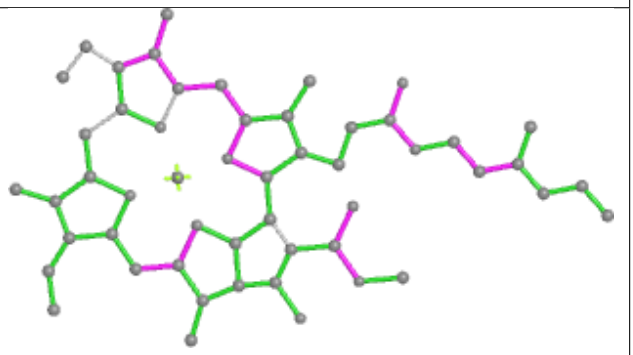


Rings

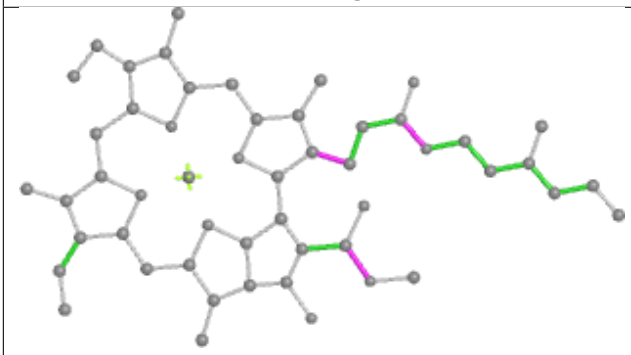
Ligand CLA A 314



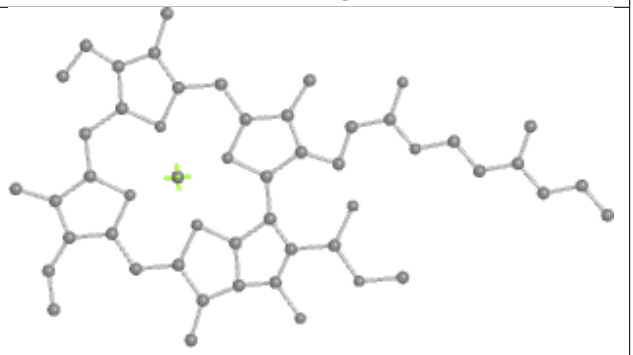
Bond lengths



Bond angles

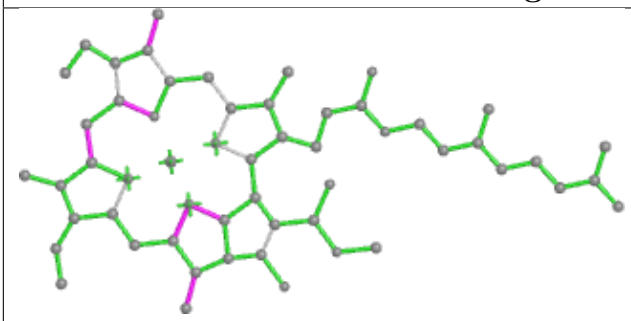


Torsions

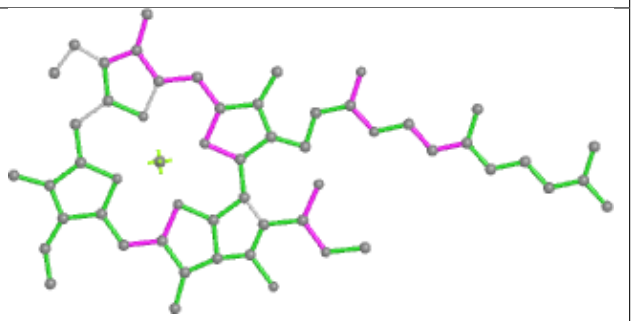


Rings

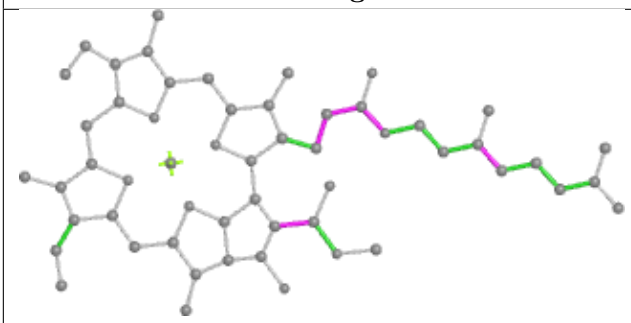
Ligand CLA B 319



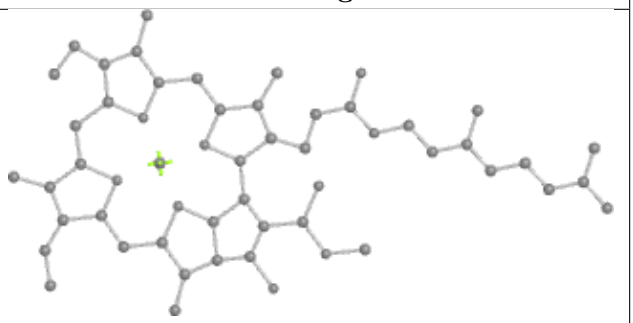
Bond lengths



Bond angles

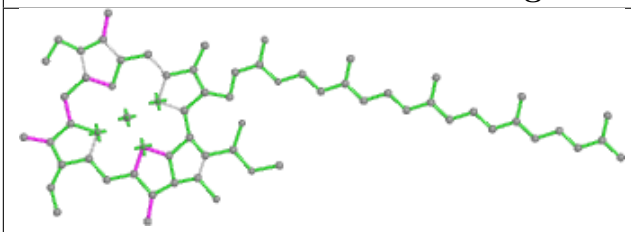


Torsions

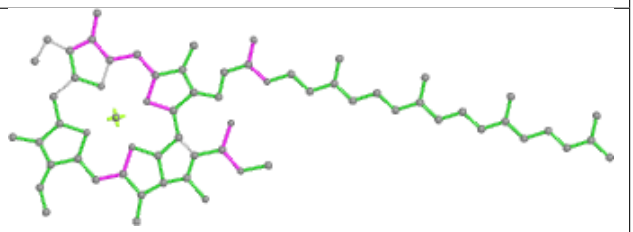


Rings

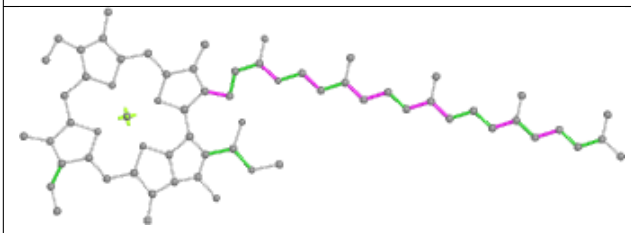
Ligand CLA B 309



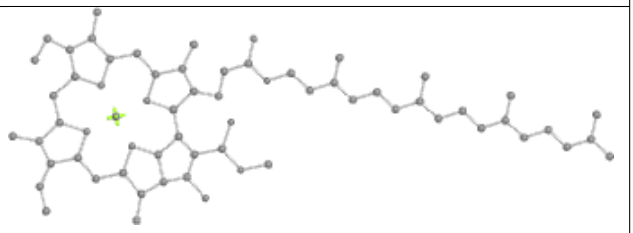
Bond lengths



Bond angles

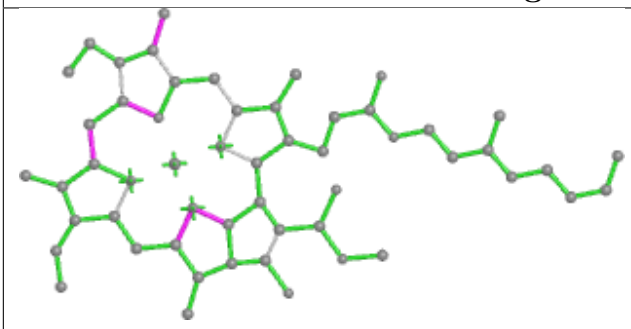


Torsions

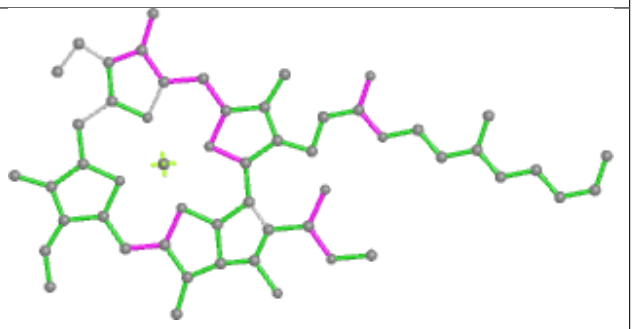


Rings

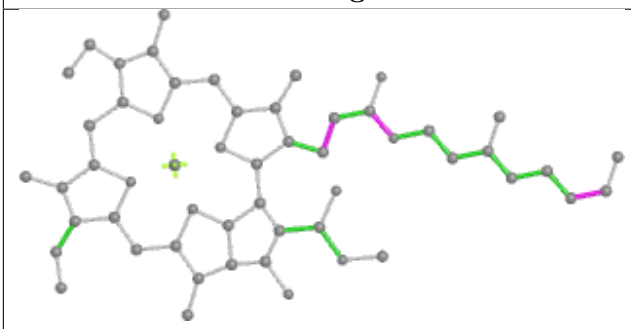
Ligand CLA B 317



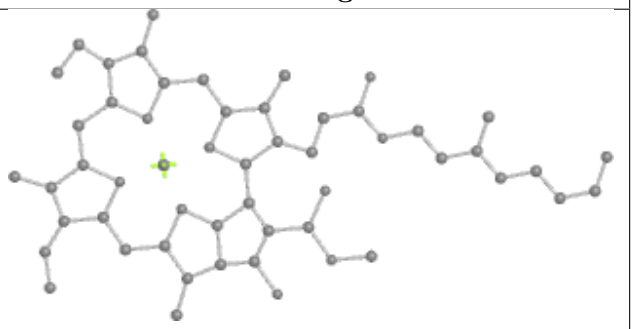
Bond lengths



Bond angles

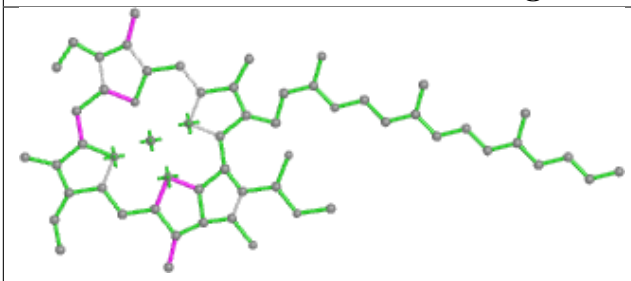


Torsions

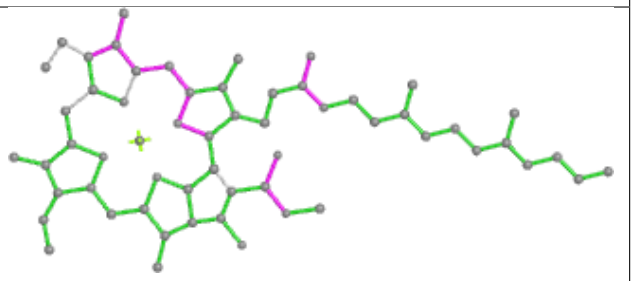


Rings

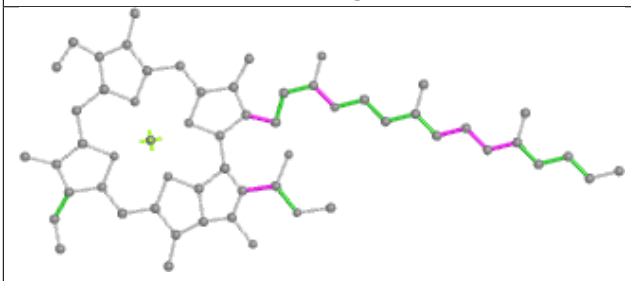
Ligand CLA C 309



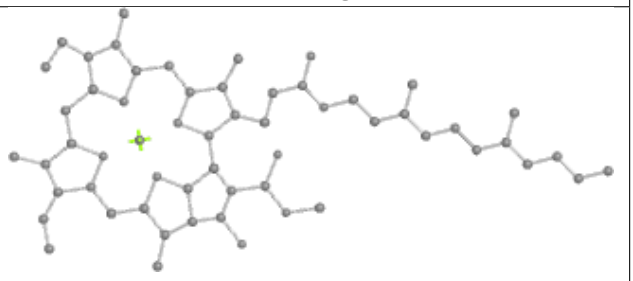
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

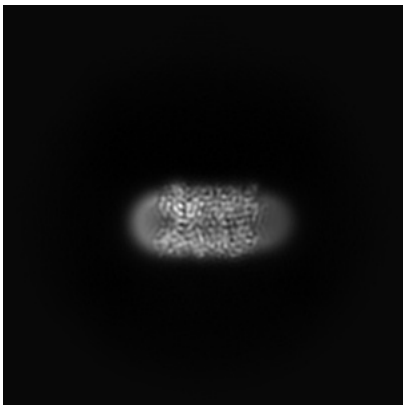
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36054. These allow visual inspection of the internal detail of the map and identification of artifacts.

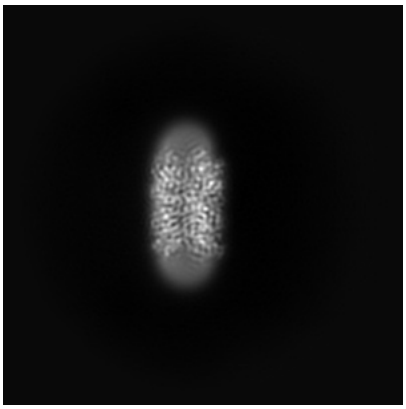
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

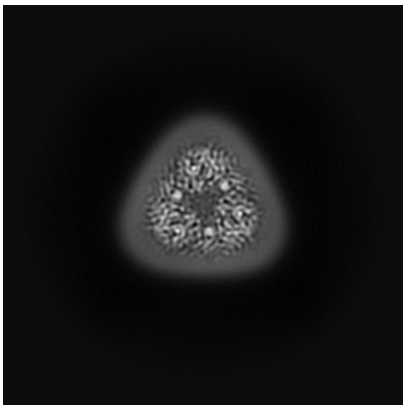
6.1.1 Primary map



X

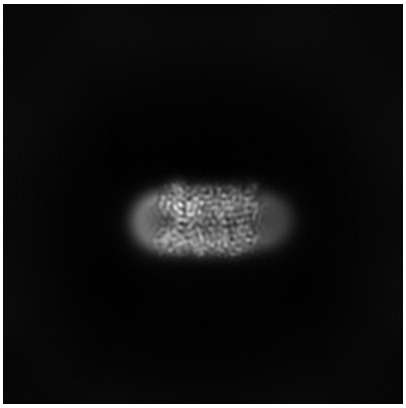


Y

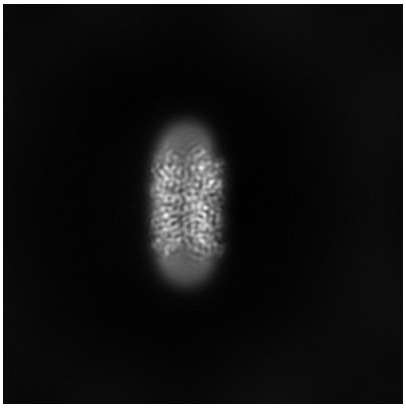


Z

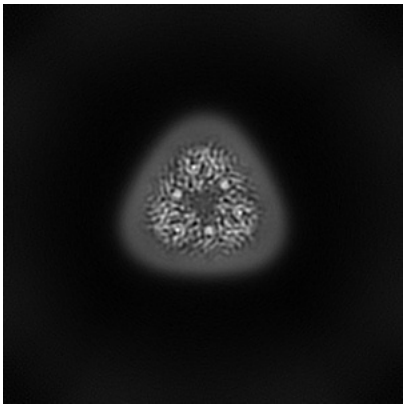
6.1.2 Raw map



X



Y



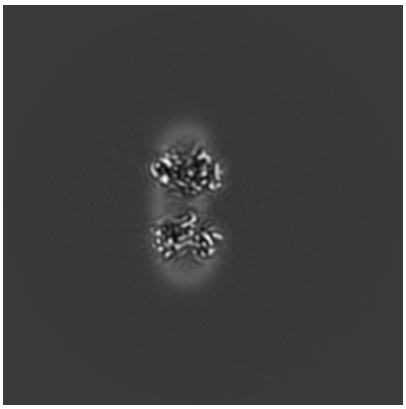
Z

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

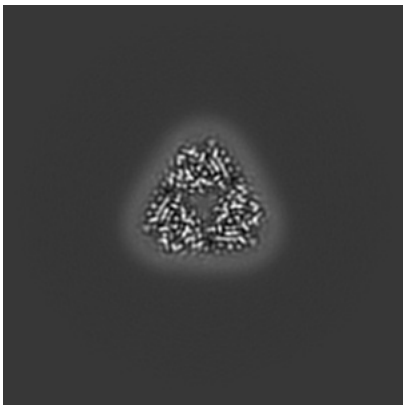
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128

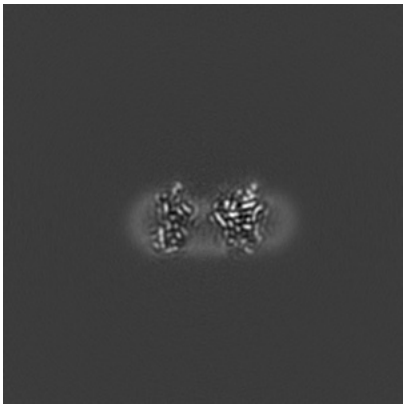


Y Index: 128

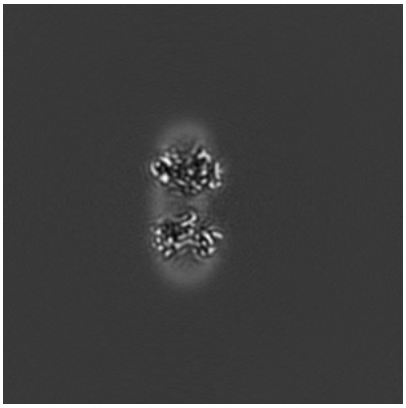


Z Index: 128

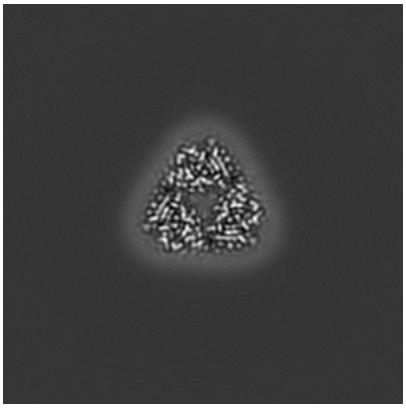
6.2.2 Raw map



X Index: 128



Y Index: 128

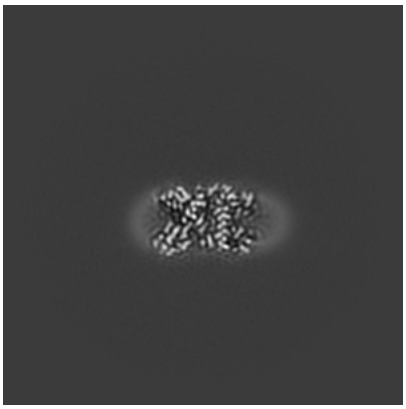


Z Index: 128

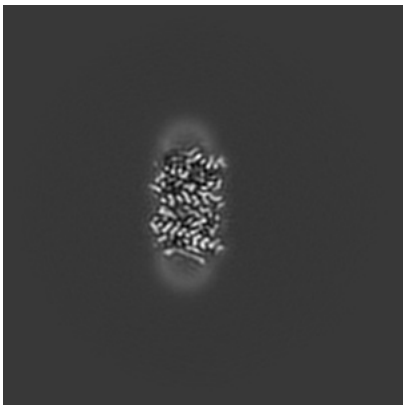
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

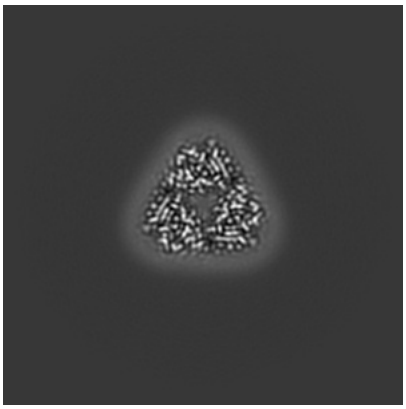
6.3.1 Primary map



X Index: 142

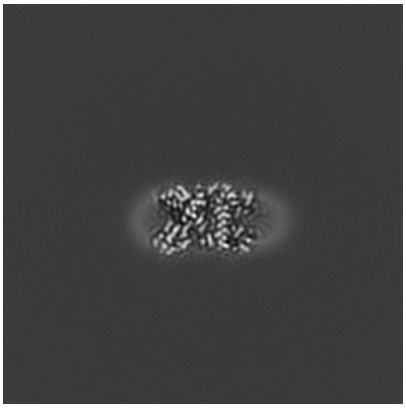


Y Index: 112

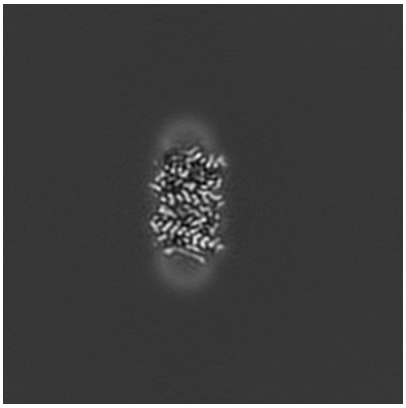


Z Index: 128

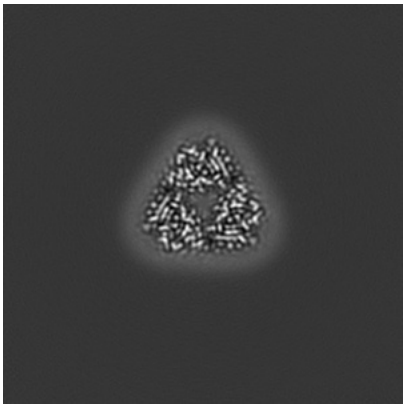
6.3.2 Raw map



X Index: 142



Y Index: 112

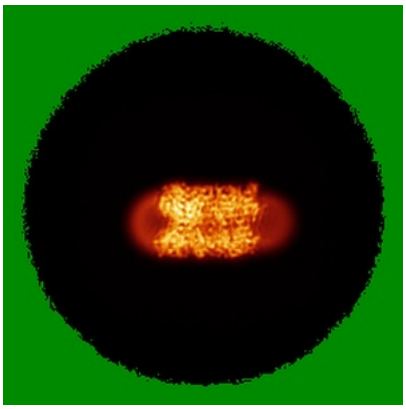


Z Index: 128

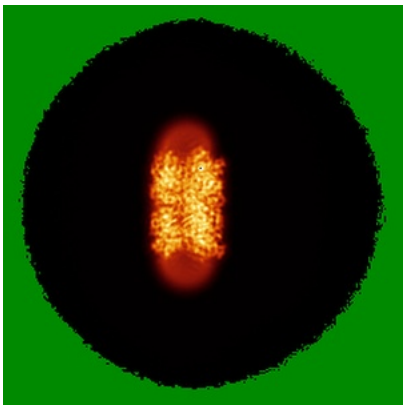
The images above show the largest variance slices of the map in three orthogonal directions.

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

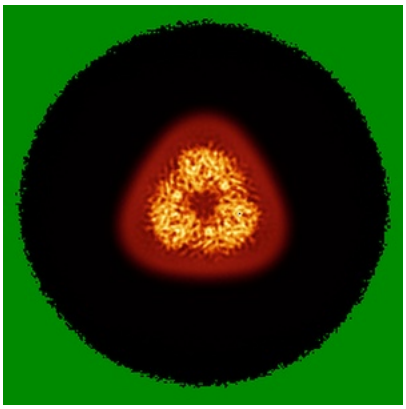
6.4.1 Primary map



X

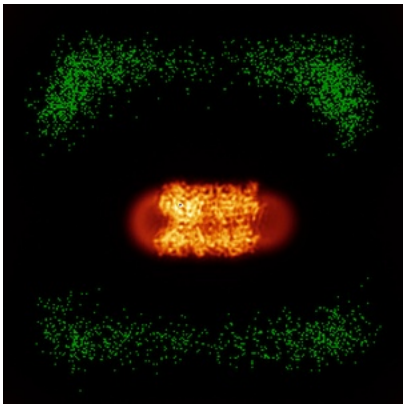


Y

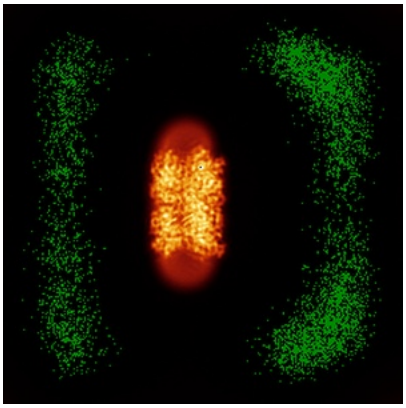


Z

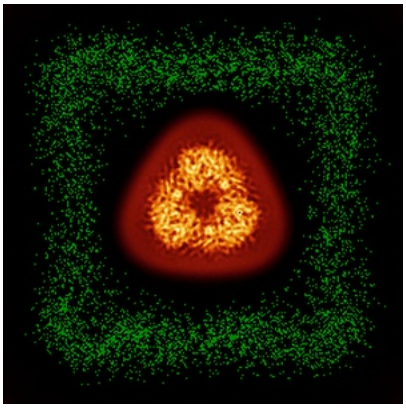
6.4.2 Raw map



X



Y

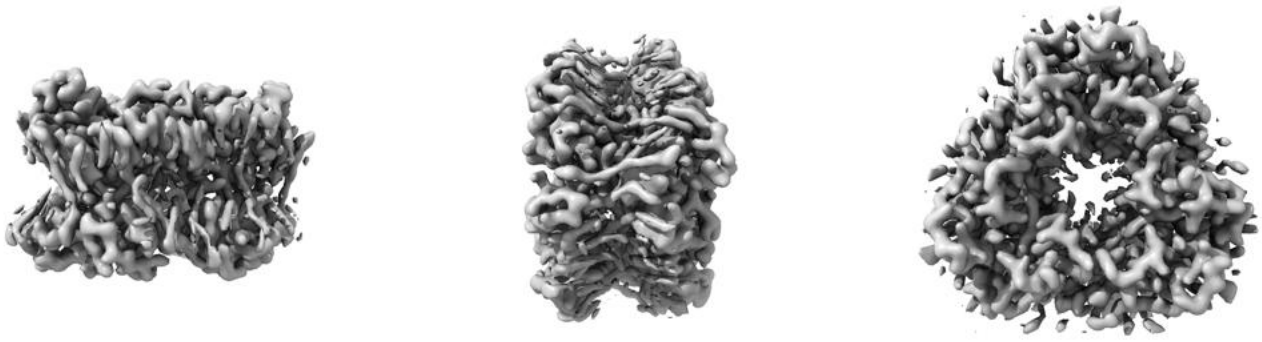


Z

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)

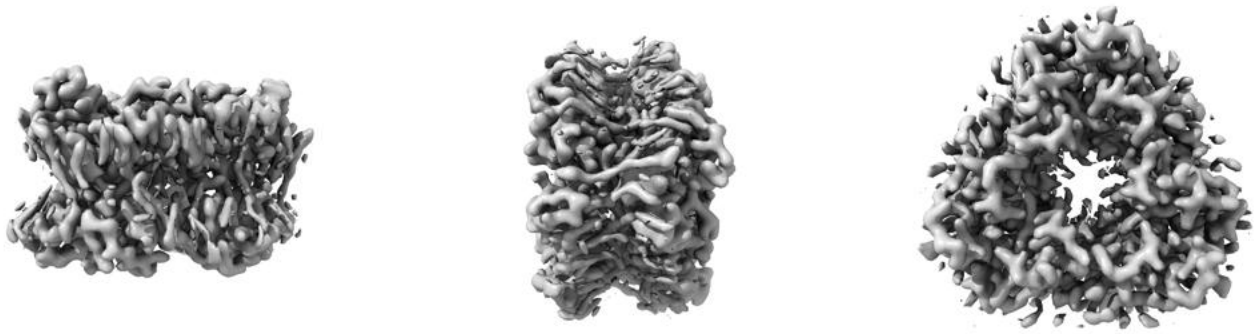
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

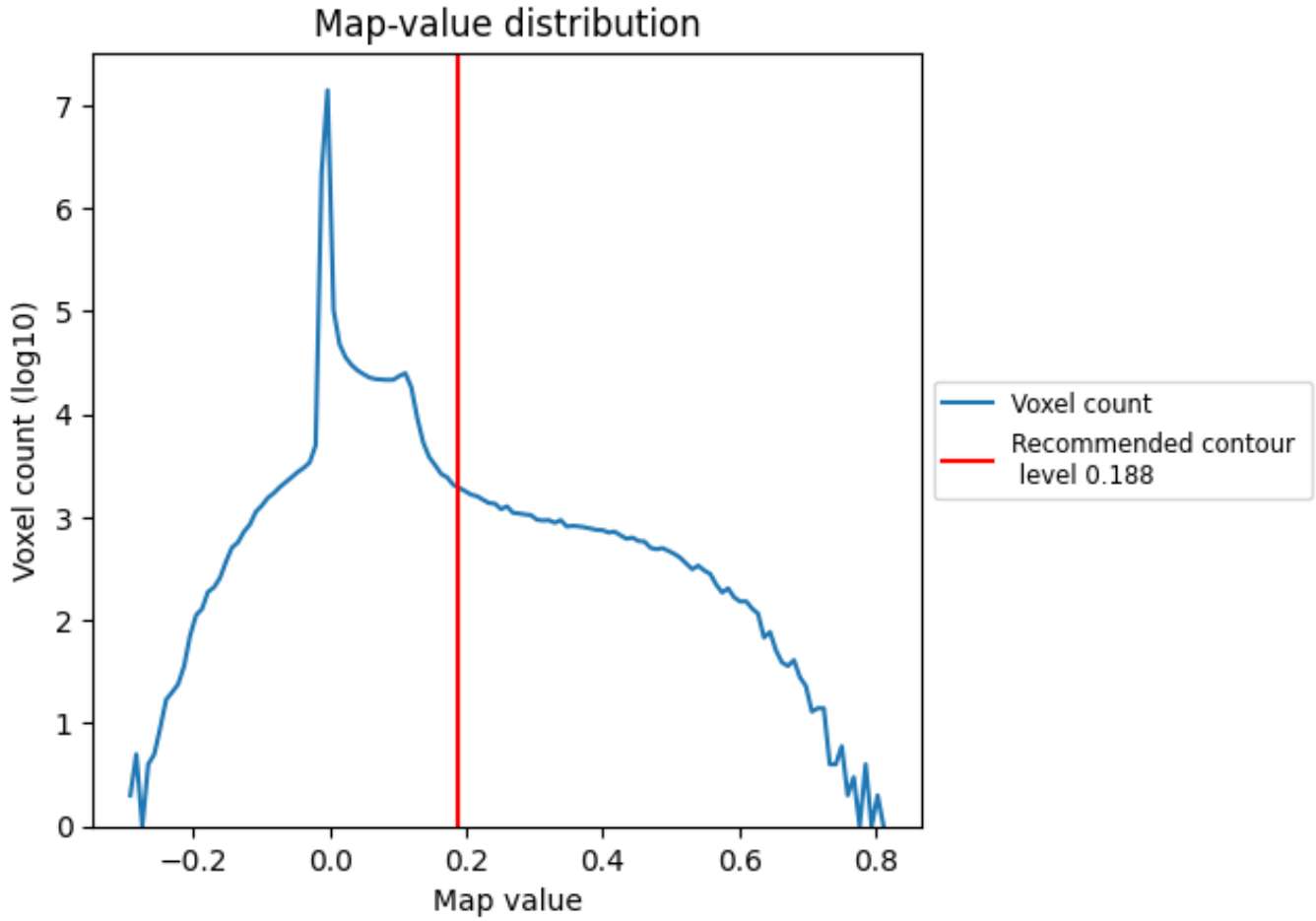
6.6 Mask visualisation (i)

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

7 Map analysis

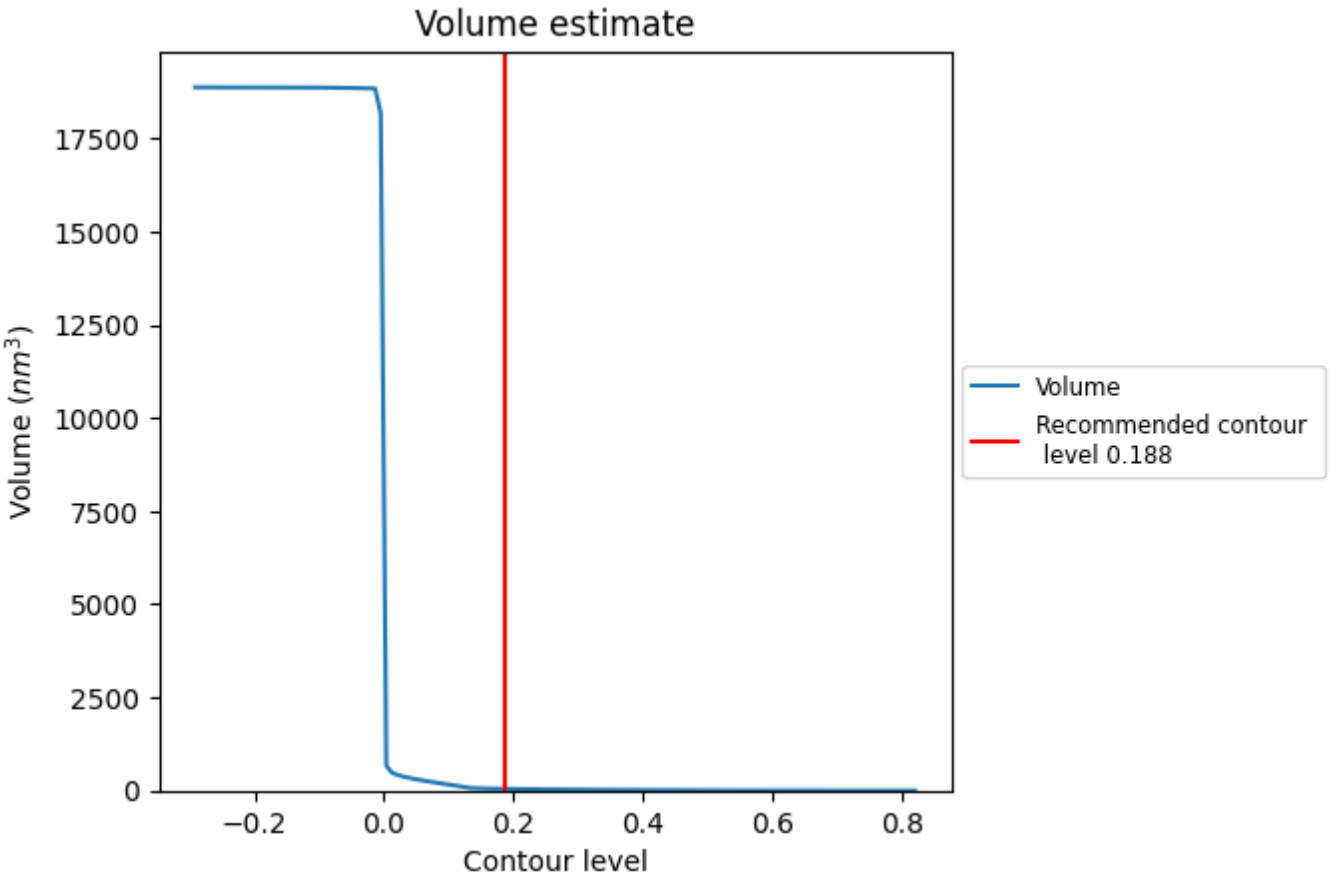
This section contains the results of statistical analysis of the map.

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.

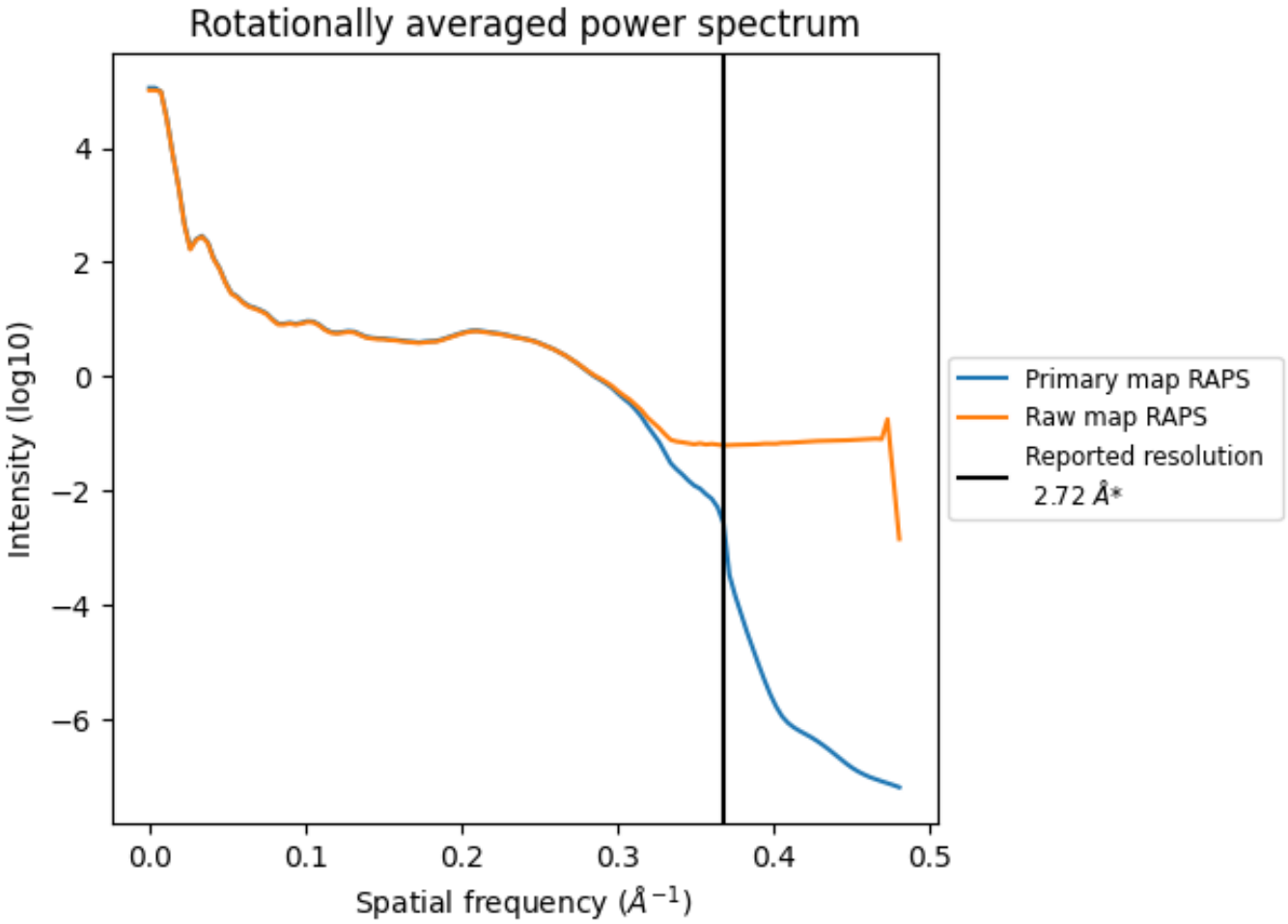
7.2 Volume estimate



The volume at the recommended contour level is 44 nm^3; this corresponds to an approximate mass of 40 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)

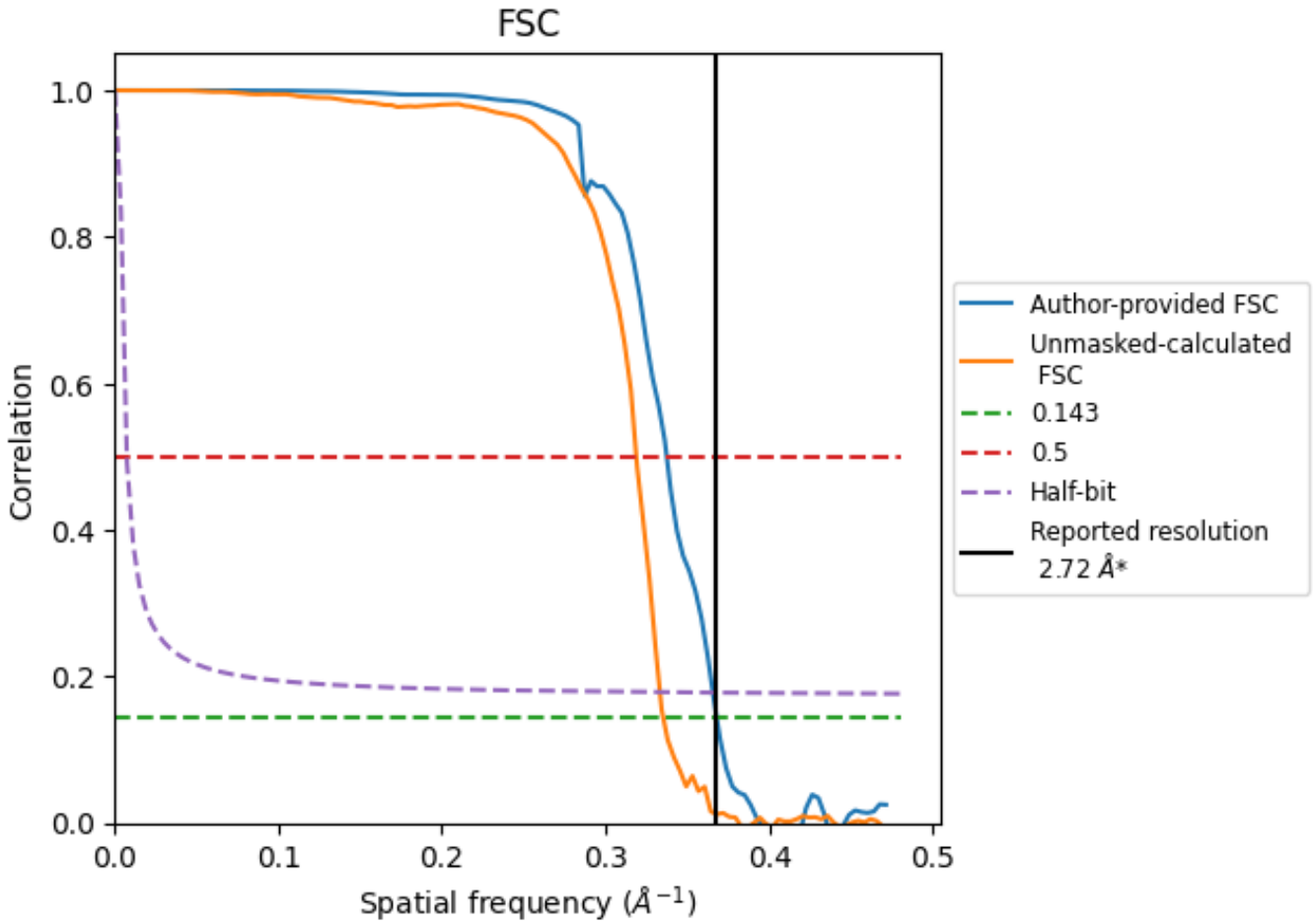


*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8.2 Resolution estimates (i)

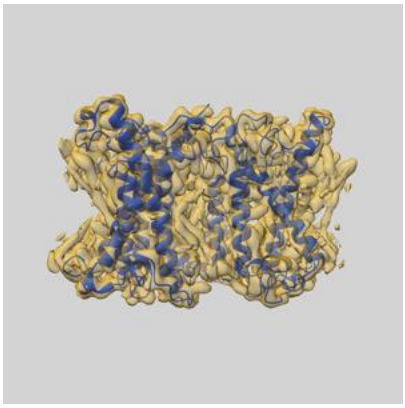
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.72	2.96	2.74
Unmasked-calculated*	2.98	3.14	3.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

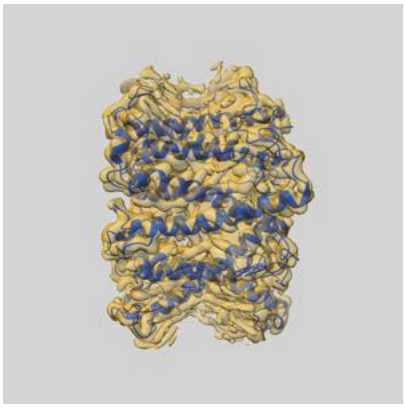
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36054 and PDB model 8J7Z. Per-residue inclusion information can be found in section 3 on page 10.

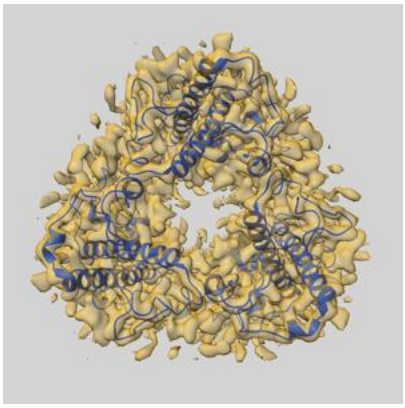
9.1 Map-model overlay



X



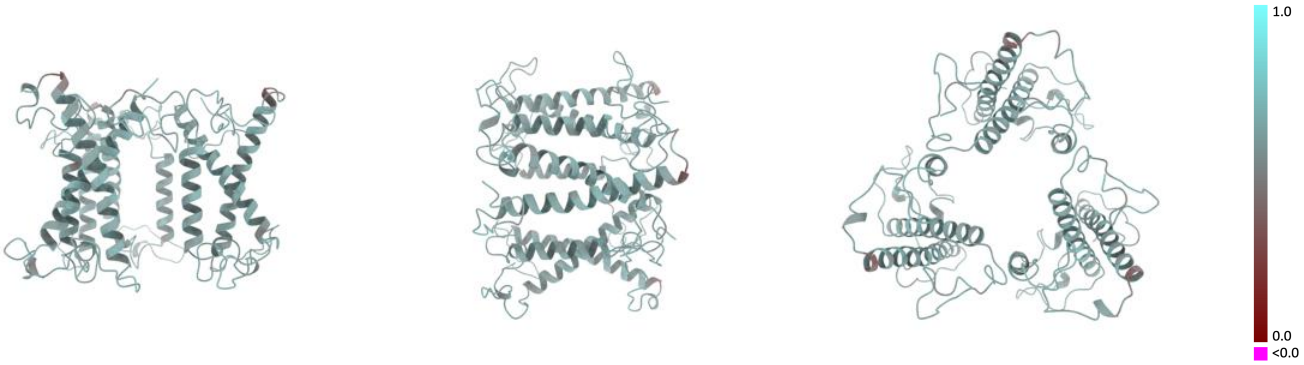
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.188 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.

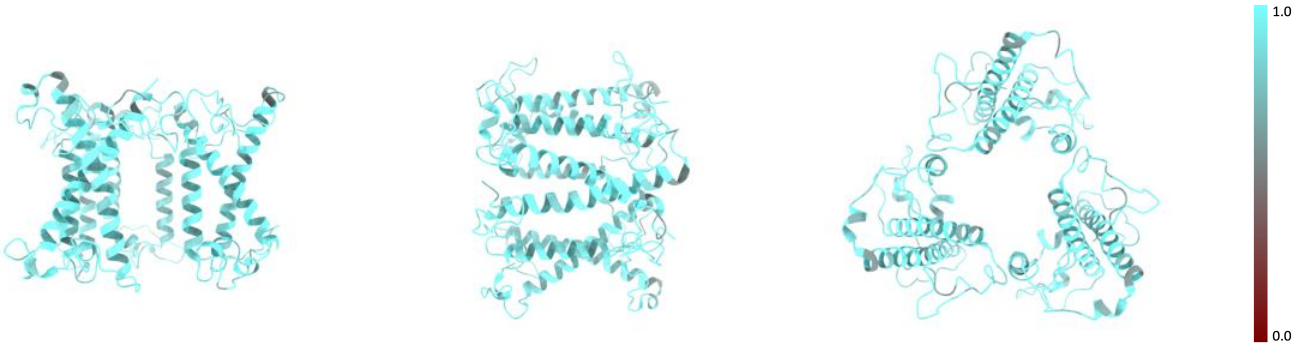
9.2 Q-score mapped to coordinate model (i)



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.

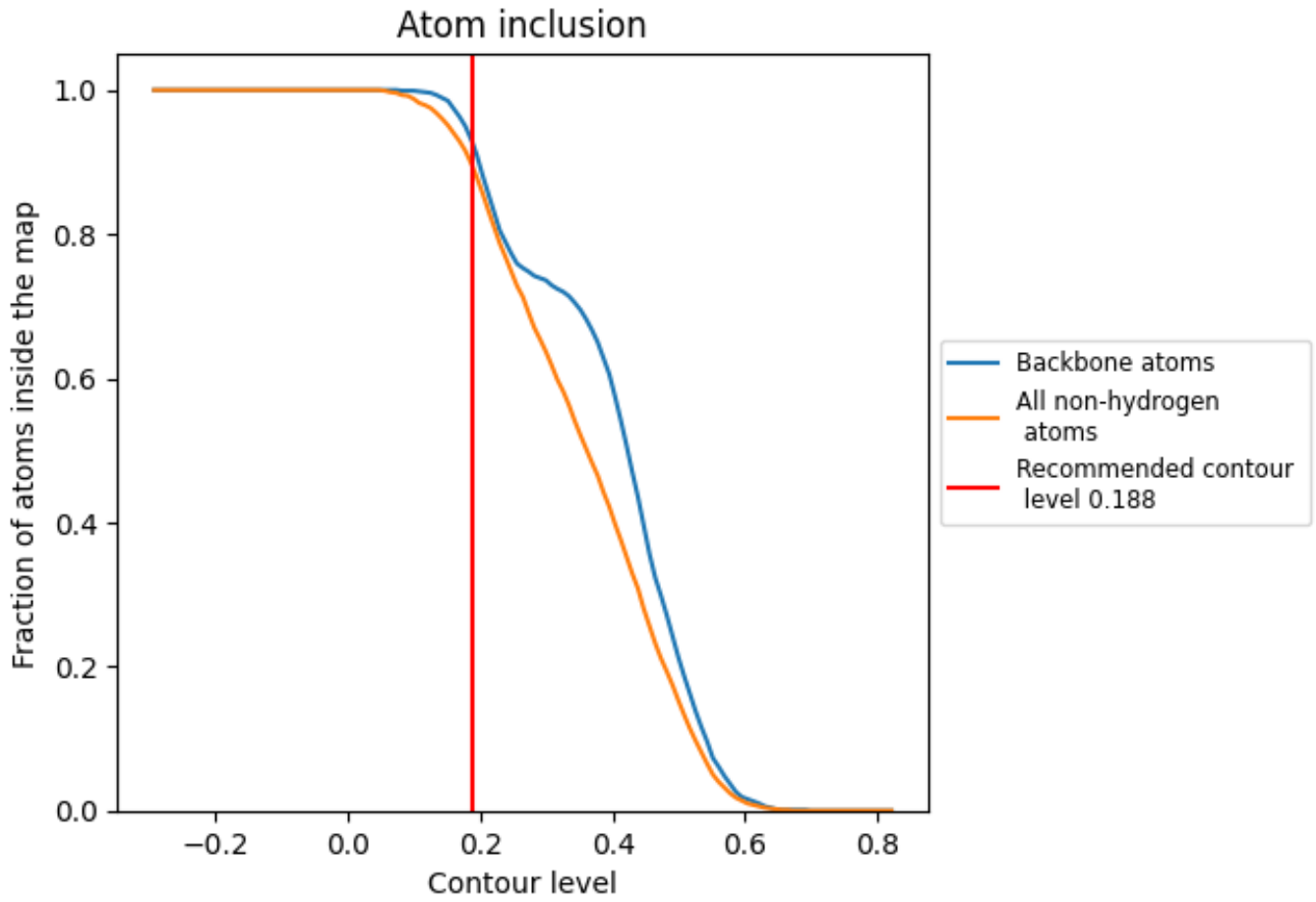
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.188).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.5910
A	0.8970	0.5910
B	0.8970	0.5910
C	0.8930	0.5900