



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 01:58 PM JST

PDB ID : 8HG3  
EMDB ID : EMD-34733  
Title : Cryo-EM structure of the Lhcp complex from *Ostreococcus tauri*  
Authors : Shan, J.; Sheng, X.; Ishii, A.; Watanabe, A.; Song, C.; Murata, K.; Minagawa, J.; Liu, Z.  
Deposited on : 2022-11-13  
Resolution : 2.94 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

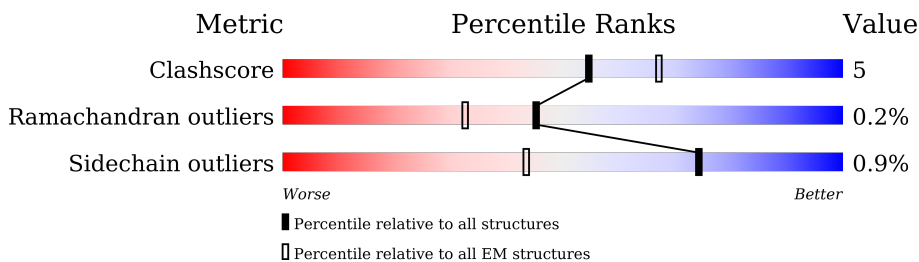
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.94 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ . 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	S	233	
1	T	233	
1	U	233	

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
2	CLA	S	301	X	-	-	-
2	CLA	S	302	X	-	-	-
2	CLA	S	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	S	309	X	-	-	-
2	CLA	S	310	X	-	-	-
2	CLA	S	311	X	-	-	-
2	CLA	S	312	X	-	-	-
2	CLA	S	313	X	-	-	-
2	CLA	T	301	X	-	-	-
2	CLA	T	302	X	-	-	-
2	CLA	T	303	X	-	-	-
2	CLA	T	309	X	-	-	-
2	CLA	T	310	X	-	-	-
2	CLA	T	311	X	-	-	-
2	CLA	T	312	X	-	-	-
2	CLA	T	313	X	-	-	-
2	CLA	U	301	X	-	-	-
2	CLA	U	302	X	-	-	-
2	CLA	U	303	X	-	-	-
2	CLA	U	308	X	-	-	-
2	CLA	U	309	X	-	-	-
2	CLA	U	310	X	-	-	-
2	CLA	U	311	X	-	-	-
2	CLA	U	312	X	-	-	-
3	CHL	S	304	X	-	-	-
3	CHL	S	305	X	-	-	-
3	CHL	S	306	X	-	-	-
3	CHL	S	307	X	-	-	-
3	CHL	S	314	X	-	-	-
3	CHL	T	304	X	-	-	-
3	CHL	T	305	X	-	-	-
3	CHL	T	306	X	-	-	-
3	CHL	T	307	X	-	-	-
3	CHL	T	314	X	-	-	-
3	CHL	T	320	X	-	-	-
3	CHL	U	304	X	-	-	-
3	CHL	U	305	X	-	-	-
3	CHL	U	306	X	-	-	-
3	CHL	U	313	X	-	-	-

## 2 Entry composition [i](#)

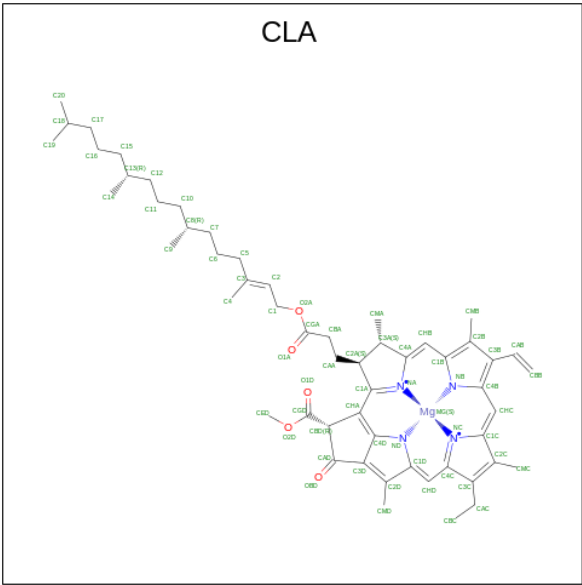
There are 7 unique types of molecules in this entry. The entry contains 7456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	202	Total	C	N	O	S	0	0
			1512	971	247	288	6		
1	T	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
1	U	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



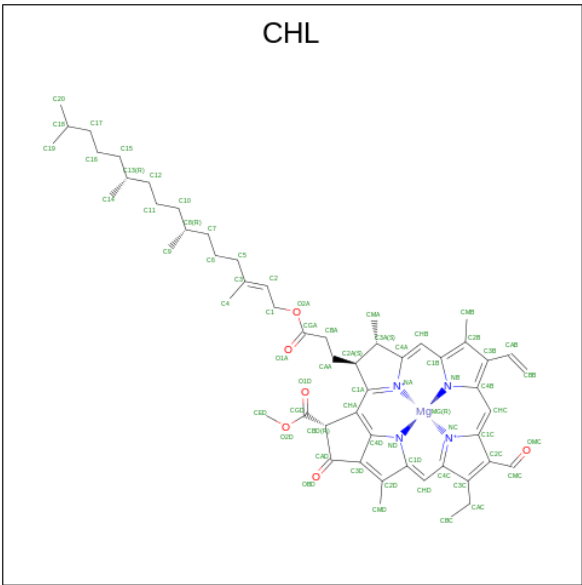
Mol	Chain	Residues	Atoms					AltConf
2	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
2	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
2	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
2	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
2	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
2	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
2	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
2	T	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
2	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
2	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
2	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
2	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
2	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
2	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
2	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
2	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
2	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
2	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
2	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 3 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



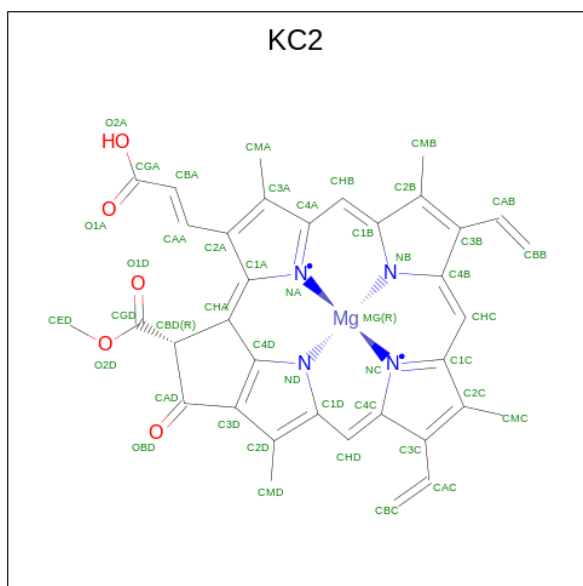
Mol	Chain	Residues	Atoms					AltConf
3	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
3	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
3	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
3	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
3	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	T	1	Total 43	C 34	Mg 1	N 4	O 4	0
3	T	1	Total 49	C 38	Mg 1	N 4	O 6	0
3	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
3	T	1	Total 44	C 35	Mg 1	N 4	O 4	0
3	T	1	Total 42	C 33	Mg 1	N 4	O 4	0
3	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
3	U	1	Total 42	C 33	Mg 1	N 4	O 4	0
3	U	1	Total 46	C 35	Mg 1	N 4	O 6	0
3	U	1	Total 44	C 35	Mg 1	N 4	O 4	0

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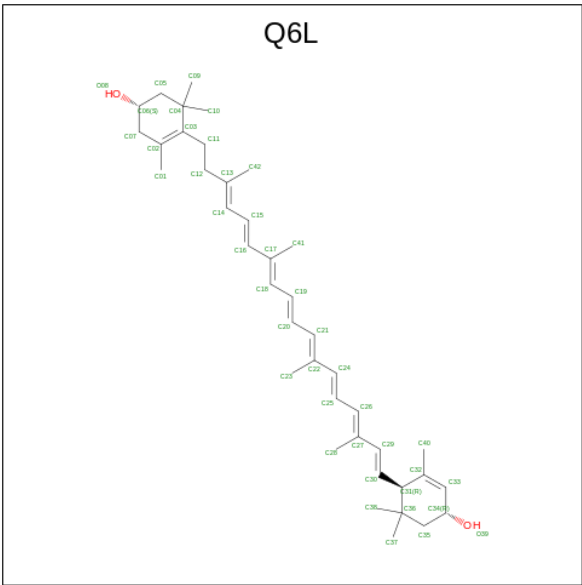
Mol	Chain	Residues	Atoms					AltConf
3	U	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 4 is Chlorophyll c2 (three-letter code: KC2) (formula:  $C_{35}H_{28}MgN_4O_5$ ).



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

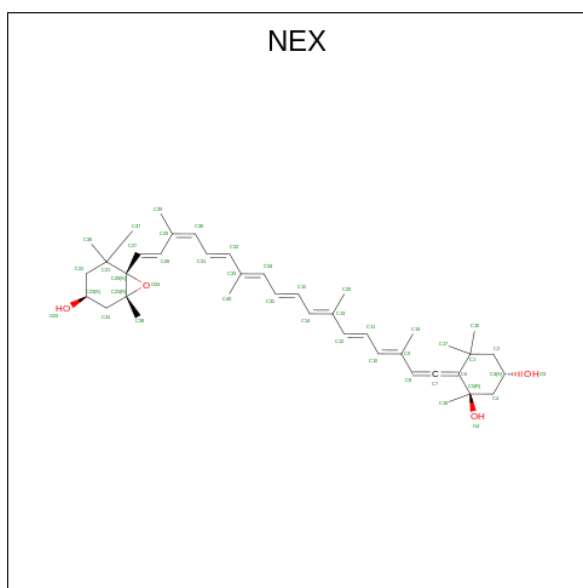
- Molecule 5 is (1 {S})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl] octadeca-3,5,7,9,11,13,15,17-octaenyl]cyclohex-3-en-1-ol (three-letter code: Q6L) (formula:  $C_{40}H_{58}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	S	1	Total	C	O	0
			42	40	2	
5	S	1	Total	C	O	0
			42	40	2	
5	S	1	Total	C	O	0
			42	40	2	
5	S	1	Total	C	O	0
			42	40	2	
5	S	1	Total	C	O	0
			42	40	2	
5	T	1	Total	C	O	0
			42	40	2	
5	T	1	Total	C	O	0
			42	40	2	
5	T	1	Total	C	O	0
			42	40	2	
5	T	1	Total	C	O	0
			42	40	2	
5	U	1	Total	C	O	0
			42	40	2	
5	U	1	Total	C	O	0
			42	40	2	
5	U	1	Total	C	O	0
			42	40	2	

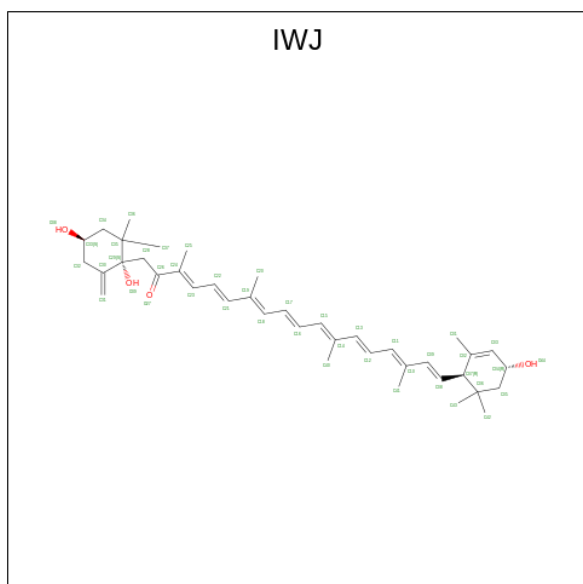
- Molecule 6 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,

3-DIOL (three-letter code: NEX) (formula:  $C_{40}H_{56}O_4$ ).



Mol	Chain	Residues	Atoms			AltConf
6	S	1	Total	C	O	0
			44	40	4	
6	T	1	Total	C	O	0
			44	40	4	

- Molecule 7 is (3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-1-[(1 {S},4 {S})-2,2-dimethyl-6-methyldene-1,4-bis(oxidanyl)cyclohexyl]-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-2-one (three-letter code: IWJ) (formula:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).

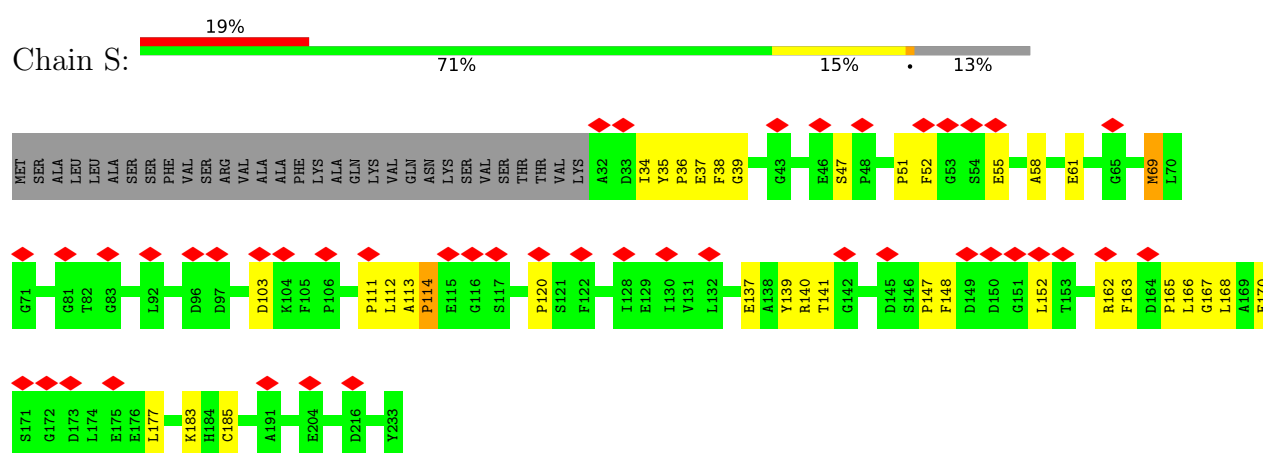


Mol	Chain	Residues	Atoms			AltConf
7	S	1	Total 44	C 40	O 4	0
7	S	1	Total 44	C 40	O 4	0
7	S	1	Total 44	C 40	O 4	0
7	T	1	Total 44	C 40	O 4	0
7	T	1	Total 44	C 40	O 4	0
7	U	1	Total 44	C 40	O 4	0

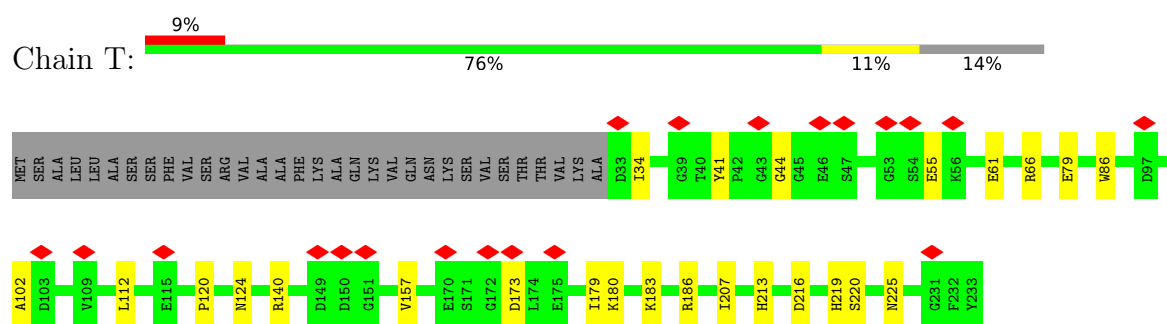
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

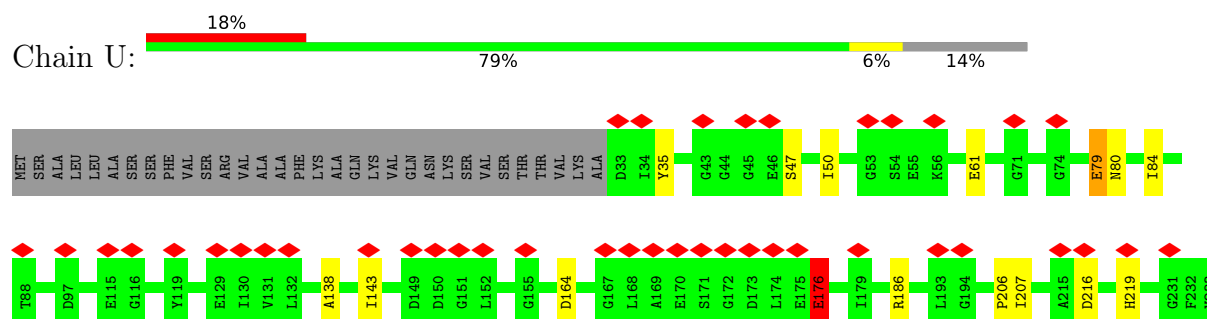
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, Q6L, IWJ, NEX, KC2, CLA

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	S	0.52	0/1558	0.72	3/2129 (0.1%)
1	T	0.48	0/1553	0.68	1/2122 (0.0%)
1	U	0.57	2/1553 (0.1%)	0.69	1/2122 (0.0%)
All	All	0.53	2/4664 (0.0%)	0.70	5/6373 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	79	GLU	CG-CD	-9.89	1.37	1.51
1	U	176	GLU	CD-OE1	5.11	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	176	GLU	CG-CD-OE1	6.91	132.12	118.30
1	S	114	PRO	CA-N-CD	-6.88	101.88	111.50
1	S	103	ASP	CB-CG-OD1	-6.82	112.17	118.30
1	T	55	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	S	69	MET	CG-SD-CE	-5.58	91.27	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	176	GLU	Mainchain

## 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	S	1512	0	1434	33	0
1	T	1507	0	1429	16	0
1	U	1507	0	1429	11	0
2	S	443	0	414	11	0
2	T	438	0	411	3	0
2	U	378	0	296	1	0
3	S	223	0	151	7	0
3	T	282	0	199	1	0
3	U	175	0	118	0	0
4	S	45	0	0	1	0
4	T	45	0	0	1	0
4	U	45	0	0	0	0
5	S	210	0	0	1	0
5	T	168	0	0	1	0
5	U	126	0	0	2	0
6	S	44	0	56	0	0
6	T	44	0	56	0	0
7	S	132	0	0	2	0
7	T	88	0	0	2	0
7	U	44	0	0	0	0
All	All	7456	0	5993	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:S:39:GLY:HA3	2:S:301:CLA:HMD1	1.34	1.07
1:U:47:SER:OG	1:U:50:ILE:O	1.99	0.76
1:S:52:PHE:HZ	1:S:55:GLU:HA	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:52:PHE:CD1	2:S:301:CLA:HMA2	2.24	0.72
1:U:84:ILE:O	1:U:84:ILE:HD12	1.94	0.68
1:S:52:PHE:HD1	2:S:301:CLA:HMA2	1.60	0.65
1:S:34:ILE:O	1:S:36:PRO:HD3	1.98	0.64
1:S:168:LEU:HD13	2:S:309:CLA:H42	1.81	0.61
1:U:35:TYR:OH	1:U:186:ARG:NH1	2.34	0.61
7:T:318:IWJ:O39	7:T:318:IWJ:O27	2.16	0.60
1:S:52:PHE:CZ	1:S:55:GLU:HA	2.34	0.60
1:S:167:GLY:O	1:S:170:GLU:HG2	2.02	0.59
1:T:41:TYR:CE1	1:T:44:GLY:N	2.71	0.59
1:U:206:PRO:O	5:U:314:Q6L:O08	2.24	0.56
1:T:61:GLU:OE2	1:T:186:ARG:NH2	2.39	0.55
7:S:322:IWJ:O27	7:S:322:IWJ:O39	2.26	0.53
1:S:139:TYR:CD2	1:S:147:PRO:HD3	2.43	0.53
1:S:112:LEU:O	3:S:304:CHL:C4D	2.56	0.53
1:U:216:ASP:OD2	1:U:219:HIS:CD2	2.61	0.53
1:U:79:GLU:HB2	1:U:207:ILE:HD13	1.92	0.52
1:T:140:ARG:NH1	4:T:308:KC2:O1D	2.39	0.51
1:T:216:ASP:OD1	1:T:219:HIS:ND1	2.45	0.50
1:S:137:GLU:OE1	4:S:308:KC2:NB	2.45	0.49
1:U:61:GLU:OE1	2:U:301:CLA:C4A	2.56	0.49
1:T:66:ARG:NH2	1:T:157:VAL:O	2.45	0.49
1:T:225:ASN:ND2	2:T:312:CLA:OBD	2.45	0.49
1:T:79:GLU:HG2	1:T:207:ILE:HB	1.95	0.48
1:T:102:ALA:HA	1:T:112:LEU:HD23	1.95	0.48
1:U:138:ALA:HA	1:U:143:ILE:HD12	1.95	0.48
1:S:147:PRO:CD	1:S:148:PHE:H	2.27	0.48
1:T:66:ARG:NH1	3:T:307:CHL:OBD	2.44	0.47
1:S:47:SER:OG	1:S:51:PRO:HA	2.13	0.47
1:S:114:PRO:HD2	3:S:304:CHL:C1B	2.45	0.47
1:T:86:TRP:O	5:T:316:Q6L:O39	2.32	0.47
1:S:137:GLU:O	1:S:141:THR:HG22	2.15	0.47
1:U:164:ASP:OD1	5:U:314:Q6L:O39	2.33	0.47
1:S:163:PHE:HZ	3:S:307:CHL:NB	2.13	0.47
1:T:180:LYS:HD3	2:T:311:CLA:HBD	1.96	0.47
1:S:52:PHE:CE1	2:S:301:CLA:HMA2	2.51	0.46
1:S:61:GLU:OE1	2:S:301:CLA:C4A	2.63	0.46
1:S:177:LEU:HG	2:S:309:CLA:H3A	1.98	0.46
1:S:168:LEU:CD1	2:S:309:CLA:H42	2.46	0.45
1:S:168:LEU:HD22	2:S:309:CLA:H11	1.99	0.45
7:T:321:IWJ:O27	7:T:321:IWJ:O39	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:213:HIS:HA	1:T:220:SER:HB2	1.99	0.45
1:S:162:ARG:O	1:S:165:PRO:HD3	2.17	0.44
1:S:37:GLU:OE2	1:S:183:LYS:HD3	2.17	0.44
1:S:163:PHE:CZ	3:S:307:CHL:NC	2.86	0.43
1:T:34:ILE:HD11	1:T:179:ILE:HG13	2.01	0.43
1:S:166:LEU:HD22	5:S:315:Q6L:C35	2.48	0.43
1:U:176:GLU:OE1	1:U:176:GLU:C	2.57	0.42
1:S:52:PHE:CE1	1:S:58:ALA:HB2	2.54	0.42
1:S:69:MET:HE2	1:S:185:CYS:HA	2.00	0.42
1:S:111:PRO:HB2	1:S:113:ALA:O	2.20	0.42
1:S:140:ARG:HA	3:S:307:CHL:C4C	2.50	0.42
1:S:35:TYR:CE1	1:S:37:GLU:HB2	2.54	0.42
1:T:102:ALA:HB2	1:T:120:PRO:HG2	2.00	0.42
1:U:79:GLU:CB	1:U:207:ILE:HD13	2.49	0.42
1:S:47:SER:HB3	2:S:301:CLA:OBD	2.19	0.42
1:S:152:LEU:HB3	3:S:307:CHL:HBC3	2.01	0.42
2:S:310:CLA:H2A	2:S:310:CLA:O2D	2.20	0.41
1:T:41:TYR:CD1	1:T:44:GLY:N	2.88	0.41
7:S:319:IWJ:O27	7:S:319:IWJ:O39	2.38	0.41
1:S:163:PHE:HE1	3:S:307:CHL:NA	2.19	0.41
1:T:183:LYS:HD2	2:T:310:CLA:C3D	2.52	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	S	200/233 (86%)	190 (95%)	9 (4%)	1 (0%)	25	50
1	T	199/233 (85%)	189 (95%)	10 (5%)	0	100	100
1	U	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
All	All	598/699 (86%)	570 (95%)	27 (4%)	1 (0%)	45	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	120	PRO

### 5.3.2 Protein sidechains ⓘ

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	S	153/179 (86%)	152 (99%)	1 (1%)	81	89
1	T	153/179 (86%)	151 (99%)	2 (1%)	65	80
1	U	153/179 (86%)	152 (99%)	1 (1%)	81	89
All	All	459/537 (86%)	455 (99%)	4 (1%)	74	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	38	PHE
1	T	124	ASN
1	T	173	ASP
1	U	80	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	219	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

62 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
2	CLA	T	311	-	60,68,73	1.52	6 (10%)	70,107,113	1.55	9 (12%)
7	IWJ	U	316	-	43,45,45	1.15	4 (9%)	43,65,65	1.35	5 (11%)
2	CLA	T	313	-	42,50,73	1.87	8 (19%)	48,85,113	1.35	6 (12%)
5	Q6L	U	314	-	42,43,43	1.85	7 (16%)	47,60,60	1.65	6 (12%)
2	CLA	T	310	1	42,50,73	1.89	7 (16%)	48,85,113	1.36	6 (12%)
4	KC2	S	308	1	48,53,53	2.58	15 (31%)	54,89,89	2.42	18 (33%)
3	CHL	U	305	-	46,54,74	1.75	6 (13%)	49,90,114	1.73	8 (16%)
2	CLA	U	308	1	41,49,73	1.90	10 (24%)	47,84,113	1.92	13 (27%)
4	KC2	T	308	1	48,53,53	2.57	14 (29%)	54,89,89	2.41	19 (35%)
5	Q6L	T	315	-	42,43,43	1.86	7 (16%)	47,60,60	1.39	6 (12%)
2	CLA	U	309	1	46,54,73	1.75	7 (15%)	53,90,113	1.46	8 (15%)
5	Q6L	U	315	-	42,43,43	1.90	8 (19%)	47,60,60	1.73	9 (19%)
2	CLA	U	311	1	55,63,73	1.64	8 (14%)	64,101,113	1.67	10 (15%)
5	Q6L	S	320	-	42,43,43	1.92	7 (16%)	47,60,60	1.65	9 (19%)
2	CLA	S	309	1	60,68,73	1.58	8 (13%)	70,107,113	1.36	10 (14%)
2	CLA	T	312	1	55,63,73	1.63	7 (12%)	64,101,113	1.48	10 (15%)
5	Q6L	S	315	-	42,43,43	1.76	5 (11%)	47,60,60	1.65	9 (19%)
3	CHL	T	307	-	44,52,74	1.76	6 (13%)	46,87,114	1.75	6 (13%)
7	IWJ	T	321	-	43,45,45	1.20	5 (11%)	43,65,65	1.10	3 (6%)
2	CLA	T	303	-	50,58,73	1.72	8 (16%)	58,95,113	1.51	6 (10%)
2	CLA	U	301	1	45,53,73	1.76	10 (22%)	52,89,113	1.67	9 (17%)
2	CLA	S	301	1	65,73,73	1.55	9 (13%)	76,113,113	1.41	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CLA	U	303	-	50,58,73	1.76	8 (16%)	58,95,113	1.49	9 (15%)
3	CHL	U	306	-	44,52,74	1.76	7 (15%)	46,87,114	1.34	5 (10%)
7	IWJ	S	322	-	43,45,45	1.18	5 (11%)	43,65,65	1.18	3 (6%)
2	CLA	T	309	1	59,67,73	1.63	10 (16%)	68,105,113	1.46	12 (17%)
3	CHL	S	306	-	52,60,74	1.67	11 (21%)	56,97,114	2.21	17 (30%)
3	CHL	U	313	1	43,51,74	1.81	6 (13%)	45,86,114	1.55	8 (17%)
5	Q6L	T	316	-	42,43,43	1.86	7 (16%)	47,60,60	1.62	10 (21%)
2	CLA	S	303	-	50,58,73	1.73	7 (14%)	58,95,113	1.66	10 (17%)
2	CLA	U	302	-	56,64,73	1.63	11 (19%)	65,102,113	1.53	8 (12%)
3	CHL	T	304	1	43,51,74	1.76	5 (11%)	45,86,114	1.94	7 (15%)
3	CHL	T	320	-	52,60,74	1.66	7 (13%)	56,97,114	1.65	12 (21%)
3	CHL	T	305	-	49,57,74	1.68	6 (12%)	52,93,114	1.88	11 (21%)
6	NEX	T	317	-	38,46,46	1.26	4 (10%)	50,70,70	2.54	15 (30%)
5	Q6L	S	323	-	42,43,43	1.86	6 (14%)	47,60,60	1.81	11 (23%)
3	CHL	U	304	1	42,50,74	1.82	9 (21%)	44,85,114	1.74	11 (25%)
5	Q6L	S	316	-	42,43,43	1.87	7 (16%)	47,60,60	1.56	5 (10%)
7	IWJ	T	318	-	43,45,45	1.17	5 (11%)	43,65,65	1.18	4 (9%)
2	CLA	S	302	-	65,73,73	1.53	10 (15%)	76,113,113	1.38	10 (13%)
5	Q6L	S	321	-	42,43,43	1.96	8 (19%)	47,60,60	1.41	6 (12%)
3	CHL	S	304	1	42,50,74	1.94	8 (19%)	44,85,114	1.77	9 (20%)
3	CHL	S	314	1	45,53,74	1.76	5 (11%)	46,88,114	1.62	6 (13%)
3	CHL	S	305	1	42,50,74	1.77	8 (19%)	44,85,114	1.79	8 (18%)
5	Q6L	T	322	-	42,43,43	1.91	8 (19%)	47,60,60	1.45	4 (8%)
6	NEX	S	317	-	38,46,46	1.32	4 (10%)	50,70,70	2.71	16 (32%)
2	CLA	U	310	-	44,52,73	1.83	7 (15%)	49,87,113	1.46	10 (20%)
2	CLA	S	313	-	41,49,73	1.88	6 (14%)	47,84,113	1.43	8 (17%)
7	IWJ	S	318	-	43,45,45	1.16	5 (11%)	43,65,65	1.38	6 (13%)
3	CHL	S	307	-	42,50,74	1.85	6 (14%)	44,85,114	1.80	7 (15%)
2	CLA	S	310	1	60,68,73	1.59	9 (15%)	70,107,113	1.41	11 (15%)
2	CLA	S	311	-	47,55,73	1.69	6 (12%)	54,91,113	1.71	9 (16%)
2	CLA	T	301	1	65,73,73	1.54	8 (12%)	76,113,113	1.67	14 (18%)
3	CHL	T	314	1	42,50,74	1.79	6 (14%)	44,85,114	1.69	8 (18%)
3	CHL	T	306	-	52,60,74	1.60	7 (13%)	56,97,114	1.63	11 (19%)
2	CLA	U	312	-	41,49,73	1.86	6 (14%)	47,84,113	1.41	6 (12%)
5	Q6L	T	319	-	42,43,43	1.85	7 (16%)	47,60,60	1.46	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	KC2	U	307	1	48,53,53	2.57	14 (29%)	54,89,89	2.35	18 (33%)
5	Q6L	U	317	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	5 (10%)
2	CLA	S	312	1	55,63,73	1.63	8 (14%)	64,101,113	1.37	9 (14%)
7	IWJ	S	319	-	43,45,45	1.19	7 (16%)	43,65,65	1.26	6 (13%)
2	CLA	T	302	-	65,73,73	1.54	8 (12%)	76,113,113	1.34	9 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	T	311	-	1/1/14/20	15/31/109/115	-
7	IWJ	U	316	-	-	2/33/76/76	0/2/2/2
2	CLA	T	313	-	1/1/10/20	4/10/88/115	-
5	Q6L	U	314	-	-	7/29/67/67	0/2/2/2
2	CLA	T	310	1	1/1/10/20	3/10/88/115	-
4	KC2	S	308	1	-	7/15/71/71	-
3	CHL	U	305	-	3/3/16/26	6/15/113/137	-
2	CLA	U	308	1	1/1/10/20	1/8/86/115	-
4	KC2	T	308	1	-	8/15/71/71	-
5	Q6L	T	315	-	-	6/29/67/67	0/2/2/2
2	CLA	U	309	1	1/1/11/20	9/15/93/115	-
5	Q6L	U	315	-	-	2/29/67/67	0/2/2/2
2	CLA	U	311	1	1/1/13/20	6/25/103/115	-
5	Q6L	S	320	-	-	7/29/67/67	0/2/2/2
2	CLA	S	309	1	1/1/14/20	12/31/109/115	-
2	CLA	T	312	1	1/1/13/20	12/25/103/115	-
5	Q6L	S	315	-	-	5/29/67/67	0/2/2/2
3	CHL	T	307	-	3/3/15/26	3/13/111/137	-
7	IWJ	T	321	-	-	4/33/76/76	1/2/2/2
2	CLA	T	303	-	1/1/12/20	6/19/97/115	-
2	CLA	U	301	1	1/1/11/20	7/13/91/115	-
2	CLA	S	301	1	1/1/15/20	9/37/115/115	-
2	CLA	U	303	-	1/1/12/20	6/19/97/115	-
3	CHL	U	306	-	3/3/15/26	5/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IWJ	S	322	-	-	5/33/76/76	0/2/2/2
2	CLA	T	309	1	1/1/13/20	10/30/108/115	-
3	CHL	S	306	-	3/3/17/26	7/23/121/137	-
3	CHL	U	313	1	3/3/15/26	3/12/110/137	-
5	Q6L	T	316	-	-	1/29/67/67	0/2/2/2
2	CLA	S	303	-	1/1/12/20	5/19/97/115	-
2	CLA	U	302	-	1/1/13/20	11/27/105/115	-
3	CHL	T	304	1	3/3/15/26	5/12/110/137	-
3	CHL	T	320	-	3/3/17/26	8/23/121/137	-
3	CHL	T	305	-	3/3/16/26	5/19/117/137	-
6	NEX	T	317	-	-	3/27/83/83	0/3/3/3
5	Q6L	S	323	-	-	9/29/67/67	0/2/2/2
3	CHL	U	304	1	3/3/15/26	5/10/108/137	-
5	Q6L	S	316	-	-	3/29/67/67	0/2/2/2
7	IWJ	T	318	-	-	6/33/76/76	0/2/2/2
2	CLA	S	302	-	1/1/15/20	11/37/115/115	-
5	Q6L	S	321	-	-	11/29/67/67	0/2/2/2
3	CHL	S	304	1	3/3/15/26	3/10/108/137	-
3	CHL	S	314	1	3/3/15/26	5/13/112/137	-
3	CHL	S	305	1	3/3/15/26	4/10/108/137	-
5	Q6L	T	322	-	-	8/29/67/67	0/2/2/2
6	NEX	S	317	-	-	3/27/83/83	0/3/3/3
2	CLA	U	310	-	1/1/10/20	5/11/90/115	-
2	CLA	S	313	-	1/1/10/20	1/8/86/115	-
7	IWJ	S	318	-	-	4/33/76/76	0/2/2/2
3	CHL	S	307	-	3/3/15/26	5/10/108/137	-
2	CLA	S	310	1	1/1/14/20	11/31/109/115	-
2	CLA	S	311	-	1/1/11/20	6/16/94/115	-
2	CLA	T	301	1	1/1/15/20	13/37/115/115	-
3	CHL	T	314	1	3/3/15/26	3/10/108/137	-
3	CHL	T	306	-	3/3/17/26	6/23/121/137	-
2	CLA	U	312	-	1/1/10/20	1/8/86/115	-
5	Q6L	T	319	-	-	8/29/67/67	0/2/2/2
4	KC2	U	307	1	-	11/15/71/71	-
5	Q6L	U	317	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	S	312	1	1/1/13/20	7/25/103/115	-
7	IWJ	S	319	-	-	7/33/76/76	1/2/2/2
2	CLA	T	302	-	1/1/15/20	14/37/115/115	-

All (461) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	321	Q6L	C29-C30	8.59	1.52	1.32
4	S	308	KC2	C2A-C3A	8.56	1.54	1.37
3	S	304	CHL	C4B-NB	8.54	1.42	1.35
5	U	315	Q6L	C29-C30	8.45	1.52	1.32
5	S	316	Q6L	C29-C30	8.45	1.52	1.32
5	T	322	Q6L	C29-C30	8.43	1.52	1.32
5	U	317	Q6L	C29-C30	8.41	1.52	1.32
5	T	319	Q6L	C29-C30	8.40	1.52	1.32
5	T	316	Q6L	C29-C30	8.33	1.51	1.32
5	S	320	Q6L	C29-C30	8.32	1.51	1.32
4	T	308	KC2	C2A-C3A	8.28	1.54	1.37
5	T	315	Q6L	C29-C30	8.24	1.51	1.32
5	S	323	Q6L	C29-C30	8.24	1.51	1.32
5	U	314	Q6L	C29-C30	8.17	1.51	1.32
4	U	307	KC2	C2A-C3A	8.12	1.53	1.37
2	T	310	CLA	C4B-NB	7.99	1.42	1.35
3	S	307	CHL	C4B-NB	7.93	1.42	1.35
5	S	315	Q6L	C29-C30	7.92	1.51	1.32
3	S	314	CHL	C4B-NB	7.78	1.42	1.35
3	T	307	CHL	C4B-NB	7.74	1.42	1.35
2	U	308	CLA	C4B-NB	7.67	1.42	1.35
3	U	313	CHL	C4B-NB	7.66	1.42	1.35
2	S	309	CLA	C4B-NB	7.65	1.42	1.35
2	T	302	CLA	C4B-NB	7.64	1.42	1.35
3	T	304	CHL	C4B-NB	7.63	1.42	1.35
3	T	314	CHL	C4B-NB	7.61	1.42	1.35
3	T	305	CHL	C4B-NB	7.59	1.42	1.35
2	S	313	CLA	C4B-NB	7.59	1.42	1.35
2	S	303	CLA	C4B-NB	7.58	1.42	1.35
2	T	312	CLA	C4B-NB	7.57	1.42	1.35
2	T	313	CLA	C4B-NB	7.51	1.41	1.35
2	U	310	CLA	C4B-NB	7.50	1.41	1.35
2	T	303	CLA	C4B-NB	7.50	1.41	1.35
2	U	312	CLA	C4B-NB	7.48	1.41	1.35
4	S	308	KC2	C1D-ND	7.47	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	310	CLA	C4B-NB	7.42	1.41	1.35
2	T	301	CLA	C4B-NB	7.41	1.41	1.35
2	S	312	CLA	C4B-NB	7.38	1.41	1.35
2	U	309	CLA	C4B-NB	7.38	1.41	1.35
2	U	303	CLA	C4B-NB	7.36	1.41	1.35
4	U	307	KC2	C1D-ND	7.35	1.41	1.35
3	U	305	CHL	C4B-NB	7.34	1.41	1.35
4	T	308	KC2	C1D-ND	7.33	1.41	1.35
2	T	311	CLA	C4B-NB	7.33	1.41	1.35
2	U	311	CLA	C4B-NB	7.33	1.41	1.35
2	S	311	CLA	C4B-NB	7.32	1.41	1.35
2	T	309	CLA	C4B-NB	7.31	1.41	1.35
2	S	301	CLA	C4B-NB	7.21	1.41	1.35
3	U	304	CHL	C4B-NB	7.20	1.41	1.35
3	U	306	CHL	C4B-NB	7.13	1.41	1.35
2	S	302	CLA	C4B-NB	6.96	1.41	1.35
2	U	302	CLA	C4B-NB	6.93	1.41	1.35
3	T	320	CHL	C4B-NB	6.91	1.41	1.35
3	S	306	CHL	C4B-NB	6.79	1.41	1.35
3	T	306	CHL	C4B-NB	6.71	1.41	1.35
3	S	305	CHL	C4B-NB	6.70	1.41	1.35
4	T	308	KC2	C3D-C4D	6.64	1.46	1.40
4	U	307	KC2	C3D-C4D	6.41	1.46	1.40
4	S	308	KC2	C3D-C4D	6.36	1.46	1.40
4	U	307	KC2	CBA-CAA	6.08	1.51	1.33
4	T	308	KC2	CBA-CAA	5.97	1.51	1.33
4	S	308	KC2	CBA-CAA	5.90	1.50	1.33
2	U	301	CLA	C4B-NB	5.88	1.40	1.35
5	S	320	Q6L	C12-C11	-5.50	1.34	1.52
5	S	321	Q6L	C12-C11	-5.47	1.34	1.52
5	T	315	Q6L	C12-C11	-5.47	1.34	1.52
5	U	314	Q6L	C12-C11	-5.47	1.34	1.52
5	T	322	Q6L	C12-C11	-5.39	1.34	1.52
5	S	323	Q6L	C12-C11	-5.38	1.34	1.52
5	S	315	Q6L	C12-C11	-5.32	1.35	1.52
5	U	317	Q6L	C12-C11	-5.27	1.35	1.52
5	U	315	Q6L	C12-C11	-5.27	1.35	1.52
5	T	319	Q6L	C12-C11	-5.23	1.35	1.52
5	S	316	Q6L	C12-C11	-5.17	1.35	1.52
5	T	316	Q6L	C12-C11	-5.12	1.35	1.52
4	S	308	KC2	C4A-C3A	4.12	1.52	1.44
2	U	308	CLA	C4D-ND	-3.99	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	301	CLA	C4D-ND	-3.97	1.32	1.37
2	S	302	CLA	C1D-ND	3.94	1.42	1.37
4	T	308	KC2	C4A-C3A	3.92	1.52	1.44
4	U	307	KC2	C4A-C3A	3.92	1.52	1.44
2	T	301	CLA	C4D-ND	-3.88	1.32	1.37
6	S	317	NEX	C7-C8	-3.85	1.25	1.32
3	U	313	CHL	C1D-ND	3.85	1.42	1.37
2	T	302	CLA	C1D-ND	3.83	1.42	1.37
3	S	314	CHL	C1D-ND	3.81	1.42	1.37
2	S	301	CLA	C4D-ND	-3.81	1.32	1.37
2	U	311	CLA	C1D-ND	3.73	1.42	1.37
2	U	302	CLA	C1D-ND	3.68	1.42	1.37
2	U	310	CLA	C1D-ND	3.67	1.42	1.37
2	U	310	CLA	C4D-ND	-3.66	1.32	1.37
2	U	303	CLA	C1D-ND	3.65	1.42	1.37
3	S	304	CHL	C4D-ND	-3.64	1.32	1.37
3	T	320	CHL	C1D-ND	3.61	1.42	1.37
2	T	309	CLA	C1D-ND	3.59	1.42	1.37
3	T	304	CHL	C1D-ND	3.57	1.42	1.37
2	T	313	CLA	C4D-ND	-3.57	1.32	1.37
2	T	310	CLA	C1D-ND	3.57	1.42	1.37
2	U	309	CLA	C1D-ND	3.54	1.42	1.37
3	U	305	CHL	C1D-ND	3.54	1.42	1.37
3	T	314	CHL	C1D-ND	3.53	1.42	1.37
2	U	312	CLA	C1D-ND	3.51	1.42	1.37
3	U	304	CHL	C1D-ND	3.51	1.42	1.37
3	U	306	CHL	C1D-ND	3.51	1.42	1.37
3	T	304	CHL	CHC-C1C	3.50	1.43	1.35
2	S	313	CLA	C1D-ND	3.50	1.42	1.37
6	T	317	NEX	C7-C8	-3.49	1.26	1.32
2	T	311	CLA	C1D-ND	3.48	1.42	1.37
2	S	312	CLA	C1D-ND	3.45	1.42	1.37
7	T	321	IWJ	C09-C10	3.44	1.53	1.45
2	S	301	CLA	CMC-C2C	-3.40	1.43	1.50
2	T	312	CLA	C1D-ND	3.38	1.41	1.37
7	T	318	IWJ	C09-C10	3.38	1.53	1.45
2	S	310	CLA	C1D-ND	3.37	1.41	1.37
3	S	307	CHL	CHC-C1C	3.37	1.43	1.35
2	S	303	CLA	C1D-ND	3.37	1.41	1.37
3	T	307	CHL	C4D-ND	-3.37	1.33	1.37
2	S	311	CLA	C1D-ND	3.37	1.41	1.37
7	S	322	IWJ	C09-C10	3.37	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	305	CHL	C1D-ND	3.36	1.41	1.37
7	S	319	IWJ	C09-C10	3.36	1.53	1.45
3	S	306	CHL	C4C-C3C	3.34	1.50	1.45
5	S	320	Q6L	C34-C33	3.34	1.54	1.50
7	U	316	IWJ	C09-C10	3.32	1.53	1.45
3	U	304	CHL	C4D-ND	-3.31	1.33	1.37
7	S	318	IWJ	C09-C10	3.30	1.53	1.45
3	T	306	CHL	C4D-ND	-3.30	1.33	1.37
2	S	310	CLA	C4D-ND	-3.29	1.33	1.37
3	T	307	CHL	C1D-ND	3.28	1.41	1.37
2	U	301	CLA	CHC-C1C	3.27	1.43	1.35
3	T	305	CHL	CHC-C1C	3.27	1.43	1.35
2	T	301	CLA	C1D-ND	3.26	1.41	1.37
2	T	313	CLA	C1D-ND	3.25	1.41	1.37
3	T	306	CHL	C1D-ND	3.25	1.41	1.37
2	U	309	CLA	C4D-ND	-3.23	1.33	1.37
3	U	304	CHL	CHC-C1C	3.22	1.43	1.35
3	S	305	CHL	CHC-C1C	3.22	1.43	1.35
3	S	305	CHL	C4D-ND	-3.19	1.33	1.37
2	S	313	CLA	CHC-C1C	3.19	1.43	1.35
2	U	303	CLA	C3B-C2B	-3.18	1.36	1.40
2	T	301	CLA	CHC-C1C	3.18	1.43	1.35
2	U	302	CLA	C4D-ND	-3.16	1.33	1.37
2	T	303	CLA	C4D-ND	-3.16	1.33	1.37
3	U	306	CHL	C4D-ND	-3.16	1.33	1.37
2	S	301	CLA	CHC-C1C	3.14	1.43	1.35
2	T	311	CLA	C4D-ND	-3.14	1.33	1.37
2	U	301	CLA	C1D-ND	3.14	1.41	1.37
2	U	303	CLA	CMB-C2B	-3.13	1.45	1.51
3	T	305	CHL	C1D-ND	3.12	1.41	1.37
4	U	307	KC2	C4D-ND	-3.11	1.32	1.35
2	S	311	CLA	C4D-ND	-3.10	1.33	1.37
2	S	309	CLA	CHC-C1C	3.10	1.42	1.35
2	T	309	CLA	CHC-C1C	3.09	1.42	1.35
2	S	302	CLA	C4D-ND	-3.08	1.33	1.37
2	U	301	CLA	CMD-C2D	-3.08	1.44	1.50
3	T	307	CHL	CHC-C1C	3.08	1.42	1.35
2	T	302	CLA	C4D-ND	-3.08	1.33	1.37
2	S	309	CLA	CMD-C2D	-3.07	1.44	1.50
2	U	311	CLA	CHC-C1C	3.07	1.42	1.35
3	U	306	CHL	CHC-C1C	3.06	1.42	1.35
7	S	322	IWJ	C04-C03	3.05	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	312	CLA	C4D-ND	-3.04	1.33	1.37
2	T	312	CLA	C4D-ND	-3.04	1.33	1.37
2	T	313	CLA	CHC-C1C	3.04	1.42	1.35
2	S	312	CLA	CHC-C1C	3.04	1.42	1.35
3	U	305	CHL	CHC-C1C	3.04	1.42	1.35
3	T	305	CHL	CMD-C2D	-3.03	1.44	1.50
2	S	303	CLA	CHC-C1C	3.03	1.42	1.35
2	U	310	CLA	CHC-C1C	3.02	1.42	1.35
3	U	305	CHL	C4D-ND	-3.02	1.33	1.37
2	T	303	CLA	C1D-ND	3.02	1.41	1.37
3	S	304	CHL	CHC-C1C	3.02	1.42	1.35
2	S	313	CLA	C4D-ND	-3.01	1.33	1.37
2	U	312	CLA	CHC-C1C	3.01	1.42	1.35
2	U	312	CLA	C4D-ND	-2.99	1.33	1.37
2	T	310	CLA	CHC-C1C	2.99	1.42	1.35
2	U	303	CLA	C4D-ND	-2.98	1.33	1.37
2	T	312	CLA	CHC-C1C	2.97	1.42	1.35
7	T	321	IWJ	C04-C03	2.97	1.54	1.50
4	S	308	KC2	CMD-C2D	-2.96	1.45	1.51
2	S	309	CLA	C1D-ND	2.96	1.41	1.37
3	T	320	CHL	C4D-ND	-2.96	1.33	1.37
7	U	316	IWJ	C04-C03	2.94	1.54	1.50
3	S	307	CHL	C4D-ND	-2.94	1.33	1.37
5	T	322	Q6L	C34-C33	2.93	1.54	1.50
7	T	318	IWJ	C04-C03	2.93	1.54	1.50
2	U	311	CLA	C4D-ND	-2.93	1.33	1.37
2	U	303	CLA	CHC-C1C	2.92	1.42	1.35
4	T	308	KC2	C4D-ND	-2.92	1.32	1.35
2	T	303	CLA	CHC-C1C	2.91	1.42	1.35
7	S	319	IWJ	C04-C03	2.91	1.54	1.50
2	S	311	CLA	CHC-C1C	2.90	1.42	1.35
7	S	318	IWJ	C04-C03	2.90	1.54	1.50
5	U	317	Q6L	C02-C03	2.88	1.38	1.34
2	T	311	CLA	CHC-C1C	2.87	1.42	1.35
5	S	320	Q6L	C33-C32	2.86	1.36	1.33
3	T	320	CHL	CHC-C1C	2.86	1.42	1.35
2	U	309	CLA	CHC-C1C	2.86	1.42	1.35
2	T	310	CLA	C4D-ND	-2.86	1.33	1.37
3	S	314	CHL	C4D-ND	-2.85	1.33	1.37
2	S	302	CLA	CHC-C1C	2.85	1.42	1.35
2	S	309	CLA	C4D-ND	-2.84	1.33	1.37
4	S	308	KC2	C4B-NB	2.84	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	321	Q6L	C34-C33	2.84	1.54	1.50
2	S	303	CLA	CMB-C2B	-2.84	1.45	1.51
5	S	323	Q6L	C12-C13	-2.83	1.45	1.51
4	U	307	KC2	C2A-C1A	2.83	1.53	1.44
3	T	314	CHL	CHC-C1C	2.83	1.42	1.35
3	T	314	CHL	C4D-ND	-2.82	1.33	1.37
2	U	308	CLA	MG-NC	2.82	2.13	2.06
4	T	308	KC2	CMD-C2D	-2.82	1.45	1.51
3	S	307	CHL	CMB-C2B	-2.81	1.45	1.51
2	T	303	CLA	CMB-C2B	-2.81	1.45	1.51
3	T	306	CHL	CHC-C1C	2.80	1.42	1.35
5	U	315	Q6L	C34-C33	2.80	1.54	1.50
3	T	304	CHL	C4D-ND	-2.80	1.33	1.37
5	T	316	Q6L	C02-C03	2.80	1.38	1.34
4	U	307	KC2	CMD-C2D	-2.80	1.45	1.51
3	U	313	CHL	C4D-ND	-2.80	1.33	1.37
6	T	317	NEX	C22-C21	-2.80	1.50	1.54
4	T	308	KC2	C2A-C1A	2.80	1.53	1.44
5	T	319	Q6L	C34-C33	2.80	1.54	1.50
3	U	313	CHL	CHC-C1C	2.79	1.42	1.35
5	S	321	Q6L	C12-C13	-2.79	1.45	1.51
5	S	320	Q6L	C12-C13	-2.79	1.45	1.51
2	S	310	CLA	CHC-C1C	2.78	1.42	1.35
2	S	301	CLA	C1D-ND	2.78	1.41	1.37
5	T	315	Q6L	C34-C33	2.78	1.54	1.50
3	S	314	CHL	CHC-C1C	2.77	1.42	1.35
2	U	302	CLA	CHC-C1C	2.76	1.42	1.35
2	S	313	CLA	CMD-C2D	-2.75	1.45	1.50
3	T	307	CHL	CMB-C2B	-2.75	1.45	1.51
5	T	316	Q6L	C34-C33	2.73	1.54	1.50
2	S	303	CLA	C4D-ND	-2.73	1.33	1.37
2	T	313	CLA	CMB-C2B	-2.73	1.46	1.51
5	T	322	Q6L	C12-C13	-2.72	1.45	1.51
3	S	307	CHL	C1D-ND	2.72	1.41	1.37
5	T	315	Q6L	C12-C13	-2.71	1.45	1.51
7	T	321	IWJ	C03-C02	2.71	1.36	1.33
2	S	310	CLA	C3B-C2B	-2.71	1.36	1.40
3	T	305	CHL	C4D-ND	-2.69	1.34	1.37
7	S	319	IWJ	C03-C02	2.69	1.36	1.33
2	S	302	CLA	CMB-C2B	-2.68	1.46	1.51
5	S	321	Q6L	C33-C32	2.68	1.36	1.33
2	U	312	CLA	CMD-C2D	-2.68	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	317	NEX	C22-C21	-2.68	1.50	1.54
5	U	314	Q6L	C34-C33	2.68	1.54	1.50
3	S	306	CHL	C1D-ND	2.67	1.41	1.37
5	U	314	Q6L	C12-C13	-2.67	1.45	1.51
3	S	304	CHL	CMB-C2B	-2.66	1.46	1.51
5	S	316	Q6L	C34-C33	2.65	1.53	1.50
7	U	316	IWJ	C03-C02	2.64	1.36	1.33
2	S	310	CLA	CMB-C2B	-2.64	1.46	1.51
4	T	308	KC2	C4B-NB	2.63	1.41	1.37
4	U	307	KC2	C4B-NB	2.63	1.41	1.37
7	S	322	IWJ	C03-C02	2.63	1.36	1.33
5	S	323	Q6L	C02-C03	2.63	1.37	1.34
4	S	308	KC2	C2A-C1A	2.63	1.52	1.44
2	T	309	CLA	C3B-C2B	-2.62	1.36	1.40
2	S	301	CLA	CMD-C2D	-2.62	1.45	1.50
3	S	306	CHL	CMB-C2B	-2.62	1.46	1.51
5	U	314	Q6L	C02-C03	2.61	1.37	1.34
3	S	306	CHL	C4D-ND	-2.61	1.34	1.37
2	S	303	CLA	CMD-C2D	-2.60	1.45	1.50
3	T	320	CHL	C3B-C2B	-2.59	1.36	1.40
2	T	309	CLA	C4D-ND	-2.58	1.34	1.37
3	S	306	CHL	C1D-C2D	2.57	1.50	1.45
5	U	315	Q6L	C02-C03	2.57	1.37	1.34
2	T	303	CLA	CMD-C2D	-2.57	1.45	1.50
7	T	318	IWJ	C03-C02	2.57	1.36	1.33
2	U	311	CLA	CMB-C2B	-2.57	1.46	1.51
2	T	302	CLA	CHC-C1C	2.56	1.41	1.35
2	T	309	CLA	CMB-C2B	-2.56	1.46	1.51
2	U	302	CLA	C3B-CAB	-2.56	1.42	1.47
2	T	301	CLA	CMB-C2B	-2.56	1.46	1.51
2	S	302	CLA	CMD-C2D	-2.55	1.45	1.50
5	S	320	Q6L	C02-C03	2.54	1.37	1.34
3	S	306	CHL	CMC-C2C	2.53	1.50	1.45
2	T	310	CLA	CMD-C2D	-2.53	1.45	1.50
2	U	302	CLA	CMD-C2D	-2.52	1.45	1.50
5	S	316	Q6L	C02-C03	2.52	1.37	1.34
5	S	315	Q6L	C12-C13	-2.51	1.46	1.51
5	U	317	Q6L	C34-C33	2.51	1.53	1.50
2	T	302	CLA	CMB-C2B	-2.50	1.46	1.51
2	U	309	CLA	CMB-C2B	-2.49	1.46	1.51
2	T	312	CLA	CMB-C2B	-2.49	1.46	1.51
4	U	307	KC2	CMC-C2C	-2.48	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	322	Q6L	C02-C03	2.48	1.37	1.34
3	T	306	CHL	CMB-C2B	-2.48	1.46	1.51
7	S	318	IWJ	C03-C02	2.47	1.36	1.33
2	U	303	CLA	C3B-CAB	-2.47	1.42	1.47
2	T	301	CLA	CMC-C2C	-2.47	1.45	1.50
3	T	320	CHL	CMB-C2B	-2.47	1.46	1.51
2	U	302	CLA	CMB-C2B	-2.46	1.46	1.51
4	S	308	KC2	CMB-C2B	-2.46	1.45	1.50
5	T	322	Q6L	C33-C32	2.46	1.36	1.33
3	S	304	CHL	C3B-C2B	-2.46	1.37	1.40
4	U	307	KC2	CMB-C2B	-2.45	1.45	1.50
2	T	310	CLA	CMB-C2B	-2.44	1.46	1.51
2	T	309	CLA	CMD-C2D	-2.44	1.45	1.50
2	S	312	CLA	CMB-C2B	-2.44	1.46	1.51
4	T	308	KC2	CMC-C2C	-2.42	1.45	1.50
4	U	307	KC2	O2A-CGA	2.42	1.36	1.30
3	S	304	CHL	MG-ND	-2.42	2.01	2.05
2	U	301	CLA	CMC-C2C	-2.42	1.45	1.50
5	S	315	Q6L	C02-C03	2.42	1.37	1.34
2	T	309	CLA	C1B-NB	2.41	1.37	1.35
2	S	302	CLA	C3B-C2B	-2.41	1.37	1.40
4	T	308	KC2	CMB-C2B	-2.41	1.45	1.50
5	S	316	Q6L	C12-C13	-2.41	1.46	1.51
2	S	309	CLA	CMB-C2B	-2.41	1.46	1.51
4	S	308	KC2	CMC-C2C	-2.40	1.45	1.50
3	T	314	CHL	CMB-C2B	-2.40	1.46	1.51
3	S	305	CHL	CMD-C2D	-2.40	1.45	1.50
2	U	308	CLA	C4B-CHC	-2.39	1.34	1.41
4	T	308	KC2	CHD-C4C	2.39	1.41	1.35
5	U	315	Q6L	C12-C13	-2.39	1.46	1.51
2	T	312	CLA	CMD-C2D	-2.39	1.45	1.50
5	S	321	Q6L	C02-C03	2.39	1.37	1.34
2	S	303	CLA	C3B-C2B	-2.39	1.37	1.40
2	S	312	CLA	CMC-C2C	-2.38	1.45	1.50
2	S	310	CLA	MG-NA	2.38	2.11	2.06
2	T	309	CLA	C3B-CAB	-2.37	1.43	1.47
3	U	304	CHL	CMB-C2B	-2.37	1.46	1.51
5	T	319	Q6L	C02-C03	2.37	1.37	1.34
5	U	317	Q6L	C12-C13	-2.37	1.46	1.51
2	S	302	CLA	C3B-CAB	-2.37	1.43	1.47
4	S	308	KC2	O2A-CGA	2.37	1.36	1.30
6	S	317	NEX	C35-C15	-2.36	1.29	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	310	CLA	CMB-C2B	-2.35	1.46	1.51
5	U	315	Q6L	C33-C32	2.35	1.36	1.33
7	T	318	IWJ	C29-C35	-2.35	1.52	1.56
3	U	304	CHL	C3B-C2B	-2.35	1.37	1.40
4	S	308	KC2	C4D-ND	-2.35	1.33	1.35
2	T	301	CLA	CMD-C2D	-2.34	1.45	1.50
2	T	313	CLA	C3B-C2B	-2.33	1.37	1.40
5	S	321	Q6L	C29-C27	2.33	1.50	1.45
2	T	303	CLA	C3B-C2B	-2.33	1.37	1.40
5	T	319	Q6L	C12-C13	-2.32	1.46	1.51
2	U	302	CLA	C3B-C2B	-2.32	1.37	1.40
2	U	308	CLA	C1D-ND	2.32	1.40	1.37
2	U	312	CLA	CMB-C2B	-2.31	1.46	1.51
3	U	306	CHL	C3B-C2B	-2.31	1.37	1.40
5	T	316	Q6L	C33-C32	2.31	1.36	1.33
2	S	302	CLA	CMC-C2C	-2.31	1.45	1.50
2	U	308	CLA	CHC-C1C	2.31	1.40	1.35
2	S	313	CLA	CMB-C2B	-2.30	1.46	1.51
2	U	308	CLA	C3B-C2B	-2.30	1.37	1.40
3	T	306	CHL	C3B-CAB	-2.30	1.43	1.47
2	S	301	CLA	CMB-C2B	-2.30	1.46	1.51
4	T	308	KC2	O2A-CGA	2.29	1.36	1.30
5	T	319	Q6L	C33-C32	2.29	1.35	1.33
4	U	307	KC2	MG-NB	-2.28	2.01	2.05
3	S	305	CHL	MG-ND	-2.28	2.01	2.05
5	S	320	Q6L	C01-C02	2.28	1.54	1.50
2	S	311	CLA	CMB-C2B	-2.28	1.46	1.51
2	T	311	CLA	CMB-C2B	-2.27	1.46	1.51
3	U	306	CHL	CMD-C2D	-2.27	1.46	1.50
3	U	313	CHL	CMB-C2B	-2.27	1.46	1.51
3	T	314	CHL	CMD-C2D	-2.27	1.46	1.50
5	T	315	Q6L	C33-C32	2.26	1.35	1.33
3	S	307	CHL	CMD-C2D	-2.26	1.46	1.50
4	U	307	KC2	CHD-C4C	2.26	1.40	1.35
2	U	301	CLA	CMB-C2B	-2.26	1.46	1.51
2	T	313	CLA	CMD-C2D	-2.26	1.46	1.50
5	S	323	Q6L	C34-C33	2.25	1.53	1.50
2	U	302	CLA	CMC-C2C	-2.24	1.46	1.50
3	S	305	CHL	CMB-C2B	-2.24	1.47	1.51
3	S	304	CHL	CMD-C2D	-2.24	1.46	1.50
2	S	301	CLA	MG-ND	-2.24	2.01	2.05
3	U	313	CHL	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	314	Q6L	C01-C02	2.24	1.54	1.50
7	S	319	IWJ	C29-C35	-2.23	1.53	1.56
5	T	322	Q6L	C01-C02	2.23	1.54	1.50
5	T	315	Q6L	C02-C03	2.23	1.37	1.34
5	S	316	Q6L	C33-C32	2.23	1.35	1.33
2	S	311	CLA	CMD-C2D	-2.23	1.46	1.50
6	T	317	NEX	C35-C15	-2.23	1.30	1.36
3	U	305	CHL	CMD-C2D	-2.23	1.46	1.50
3	U	306	CHL	CMB-C2B	-2.23	1.47	1.51
3	U	305	CHL	CMB-C2B	-2.22	1.47	1.51
5	T	319	Q6L	C01-C02	2.22	1.54	1.50
2	T	302	CLA	CMD-C2D	-2.22	1.46	1.50
2	T	312	CLA	CMC-C2C	-2.22	1.46	1.50
4	S	308	KC2	CHD-C4C	2.21	1.40	1.35
3	S	306	CHL	C4B-CHC	-2.21	1.34	1.41
5	T	315	Q6L	C01-C02	2.21	1.54	1.50
3	S	314	CHL	CMB-C2B	-2.21	1.47	1.51
5	T	316	Q6L	C12-C13	-2.21	1.46	1.51
5	U	317	Q6L	C01-C02	2.20	1.54	1.50
5	U	314	Q6L	C33-C32	2.20	1.35	1.33
2	S	312	CLA	CMD-C2D	-2.20	1.46	1.50
5	S	316	Q6L	C01-C02	2.20	1.54	1.50
5	S	321	Q6L	C01-C02	2.20	1.54	1.50
4	S	308	KC2	MG-NB	-2.19	2.01	2.05
2	S	312	CLA	C3B-C2B	-2.19	1.37	1.40
7	T	321	IWJ	C29-C35	-2.18	1.53	1.56
7	T	321	IWJ	O39-C29	-2.18	1.39	1.43
7	S	322	IWJ	C29-C35	-2.16	1.53	1.56
5	U	315	Q6L	C01-C02	2.16	1.54	1.50
2	U	308	CLA	CMB-C2B	-2.15	1.47	1.51
2	S	301	CLA	C3B-CAB	-2.15	1.43	1.47
7	S	322	IWJ	C26-C24	-2.15	1.45	1.49
5	T	316	Q6L	C01-C02	2.15	1.54	1.50
5	S	315	Q6L	C01-C02	2.14	1.54	1.50
4	T	308	KC2	MG-NB	-2.14	2.01	2.05
3	U	304	CHL	CMD-C2D	-2.14	1.46	1.50
2	T	302	CLA	CMC-C2C	-2.13	1.46	1.50
7	S	318	IWJ	C29-C35	-2.13	1.53	1.56
2	U	311	CLA	C3B-C2B	-2.13	1.37	1.40
2	S	309	CLA	C1A-CHA	-2.13	1.34	1.43
6	S	317	NEX	O24-C25	-2.13	1.43	1.46
2	U	303	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	311	CLA	CMD-C2D	-2.12	1.46	1.50
3	T	306	CHL	CMD-C2D	-2.12	1.46	1.50
7	S	319	IWJ	C26-C24	-2.11	1.45	1.49
3	T	320	CHL	C3B-CAB	-2.11	1.43	1.47
2	U	310	CLA	C3B-C2B	-2.11	1.37	1.40
7	S	318	IWJ	C32-C30	2.11	1.55	1.51
3	U	304	CHL	C3B-CAB	-2.11	1.43	1.47
3	S	306	CHL	CMD-C2D	-2.10	1.46	1.50
3	T	307	CHL	CMD-C2D	-2.10	1.46	1.50
2	U	301	CLA	MG-ND	-2.10	2.01	2.05
6	T	317	NEX	O24-C25	-2.10	1.43	1.46
2	T	302	CLA	C3B-C2B	-2.10	1.37	1.40
2	T	301	CLA	CMA-C3A	-2.09	1.48	1.53
2	U	309	CLA	CMD-C2D	-2.09	1.46	1.50
2	U	308	CLA	CMD-C2D	-2.09	1.46	1.50
5	U	317	Q6L	C33-C32	2.08	1.35	1.33
2	U	309	CLA	C3B-C2B	-2.08	1.37	1.40
2	S	309	CLA	CMC-C2C	-2.08	1.46	1.50
2	T	310	CLA	C3B-C2B	-2.08	1.37	1.40
3	S	304	CHL	C1D-ND	2.08	1.40	1.37
3	S	305	CHL	C3B-CAB	-2.07	1.43	1.47
2	U	310	CLA	CMC-C2C	-2.07	1.46	1.50
2	U	301	CLA	C3B-CAB	-2.07	1.43	1.47
2	S	302	CLA	C4B-CHC	-2.07	1.35	1.41
2	S	310	CLA	CMD-C2D	-2.06	1.46	1.50
5	S	323	Q6L	C01-C02	2.06	1.54	1.50
2	U	311	CLA	CMD-C2D	-2.06	1.46	1.50
3	T	305	CHL	CMB-C2B	-2.06	1.47	1.51
7	S	319	IWJ	O39-C29	-2.05	1.40	1.43
2	U	301	CLA	C3B-C2B	-2.05	1.37	1.40
3	S	306	CHL	CHC-C1C	2.05	1.40	1.35
2	U	311	CLA	CMC-C2C	-2.05	1.46	1.50
2	T	303	CLA	MG-ND	-2.04	2.01	2.05
2	S	310	CLA	C4B-CHC	-2.04	1.35	1.41
5	T	322	Q6L	C29-C27	2.04	1.50	1.45
3	T	304	CHL	CMB-C2B	-2.04	1.47	1.51
7	T	318	IWJ	O39-C29	-2.04	1.40	1.43
3	U	304	CHL	MG-ND	-2.03	2.01	2.05
5	U	315	Q6L	C29-C27	2.03	1.50	1.45
4	S	308	KC2	MG-NC	2.03	2.11	2.06
2	U	302	CLA	C4B-CHC	-2.03	1.35	1.41
2	T	309	CLA	C1A-CHA	-2.02	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	319	IWJ	C32-C30	2.02	1.55	1.51
7	U	316	IWJ	C32-C30	2.02	1.55	1.51
2	U	308	CLA	C1A-CHA	-2.02	1.34	1.43
2	U	302	CLA	MG-ND	-2.02	2.01	2.05
3	S	306	CHL	MG-ND	-2.02	2.01	2.05
2	T	313	CLA	CMC-C2C	-2.01	1.46	1.50

All (557) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	317	NEX	O24-C25-C24	13.84	123.78	113.38
6	T	317	NEX	O24-C25-C24	11.34	121.90	113.38
4	T	308	KC2	CMA-C3A-C4A	-7.80	113.16	125.04
4	S	308	KC2	CMA-C3A-C4A	-7.60	113.47	125.04
4	U	307	KC2	CMA-C3A-C4A	-7.45	113.70	125.04
3	S	307	CHL	CMB-C2B-C1B	-7.31	117.22	128.46
3	T	304	CHL	CMB-C2B-C1B	-7.19	117.41	128.46
3	T	307	CHL	CMB-C2B-C1B	-6.92	117.82	128.46
4	T	308	KC2	C1A-NA-C4A	6.69	109.71	106.71
5	U	317	Q6L	C11-C12-C13	6.66	131.61	112.69
2	S	303	CLA	CMB-C2B-C1B	-6.56	118.38	128.46
5	U	314	Q6L	C11-C12-C13	6.45	131.02	112.69
4	S	308	KC2	CMA-C3A-C2A	-6.38	112.68	128.30
5	S	320	Q6L	C11-C12-C13	6.28	130.52	112.69
5	S	323	Q6L	C11-C12-C13	6.24	130.41	112.69
4	U	307	KC2	C1A-NA-C4A	6.23	109.51	106.71
5	T	319	Q6L	C11-C12-C13	6.22	130.37	112.69
4	S	308	KC2	C1A-NA-C4A	6.21	109.50	106.71
3	T	305	CHL	CMB-C2B-C1B	-6.16	119.00	128.46
4	U	307	KC2	CMA-C3A-C2A	-6.07	113.43	128.30
3	S	314	CHL	CMB-C2B-C1B	-6.00	119.24	128.46
3	U	305	CHL	CMB-C2B-C1B	-5.94	119.33	128.46
5	T	315	Q6L	C11-C12-C13	5.90	129.46	112.69
2	T	301	CLA	C4-C3-C5	5.89	125.18	115.27
3	T	304	CHL	CMB-C2B-C3B	5.87	135.66	124.68
2	T	303	CLA	CMB-C2B-C1B	-5.86	119.46	128.46
2	T	311	CLA	C4A-NA-C1A	5.86	109.34	106.71
3	T	305	CHL	C4A-NA-C1A	5.84	109.33	106.71
2	U	311	CLA	C4A-NA-C1A	5.73	109.28	106.71
4	T	308	KC2	CMA-C3A-C2A	-5.71	114.33	128.30
5	T	316	Q6L	C11-C12-C13	5.70	128.89	112.69
5	U	315	Q6L	C11-C12-C13	5.68	128.82	112.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	304	CHL	C4A-NA-C1A	5.63	109.24	106.71
2	S	312	CLA	C4A-NA-C1A	5.63	109.23	106.71
4	U	307	KC2	C1A-C2A-C3A	-5.62	102.66	107.11
2	S	303	CLA	CMB-C2B-C3B	5.44	134.86	124.68
5	S	321	Q6L	C11-C12-C13	5.41	128.07	112.69
2	T	311	CLA	CMB-C2B-C1B	-5.39	120.18	128.46
5	T	322	Q6L	C11-C12-C13	5.36	127.92	112.69
3	S	305	CHL	CMB-C2B-C1B	-5.33	120.27	128.46
5	S	315	Q6L	C11-C12-C13	5.24	127.58	112.69
2	T	302	CLA	C4A-NA-C1A	5.21	109.05	106.71
3	T	320	CHL	C4A-NA-C1A	5.21	109.05	106.71
2	T	301	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
5	S	316	Q6L	C11-C12-C13	5.20	127.46	112.69
2	U	308	CLA	C1D-ND-C4D	-5.14	102.68	106.33
6	T	317	NEX	C26-C27-C28	-5.03	115.35	125.99
3	T	314	CHL	CMB-C2B-C1B	-4.98	120.81	128.46
2	S	311	CLA	C4A-NA-C1A	4.95	108.93	106.71
3	T	305	CHL	CMB-C2B-C3B	4.92	133.89	124.68
3	S	304	CHL	C4A-NA-C1A	-4.90	104.50	106.71
3	S	306	CHL	CMB-C2B-C1B	-4.90	120.94	128.46
3	S	307	CHL	CMB-C2B-C3B	4.89	133.83	124.68
2	U	310	CLA	C4A-NA-C1A	4.86	108.89	106.71
2	U	309	CLA	C4A-NA-C1A	4.83	108.88	106.71
2	T	303	CLA	CMB-C2B-C3B	4.83	133.71	124.68
2	S	311	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
2	T	310	CLA	C4A-NA-C1A	4.79	108.86	106.71
6	S	317	NEX	C26-C27-C28	-4.77	115.92	125.99
3	T	307	CHL	CMB-C2B-C3B	4.72	133.51	124.68
5	U	315	Q6L	C40-C32-C33	-4.68	113.55	123.56
4	S	308	KC2	C2A-C3A-C4A	-4.67	103.02	106.49
6	T	317	NEX	C28-C29-C30	4.67	126.11	118.94
5	U	314	Q6L	C40-C32-C33	-4.66	113.58	123.56
2	U	302	CLA	C4A-NA-C1A	4.65	108.80	106.71
3	U	305	CHL	CMB-C2B-C3B	4.64	133.36	124.68
4	T	308	KC2	C1A-C2A-C3A	-4.64	103.43	107.11
3	S	306	CHL	C1C-C2C-C3C	-4.63	103.44	107.11
2	T	311	CLA	CMB-C2B-C3B	4.63	133.33	124.68
3	T	306	CHL	C4A-NA-C1A	4.62	108.78	106.71
7	U	316	IWJ	C33-C32-C30	4.60	119.90	112.04
2	S	302	CLA	C4A-NA-C1A	4.60	108.77	106.71
3	U	313	CHL	CMB-C2B-C1B	-4.60	121.40	128.46
2	T	312	CLA	C4A-NA-C1A	4.58	108.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	306	CHL	CAC-C3C-C4C	4.55	130.72	124.81
3	S	305	CHL	CMB-C2B-C3B	4.53	133.16	124.68
4	S	308	KC2	CBA-CAA-C2A	-4.53	107.99	125.27
5	S	315	Q6L	C40-C32-C33	-4.53	113.86	123.56
2	U	311	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
2	T	301	CLA	CMB-C2B-C3B	4.47	133.04	124.68
2	U	301	CLA	CMB-C2B-C3B	4.45	133.01	124.68
2	U	301	CLA	CMB-C2B-C1B	-4.44	121.65	128.46
3	S	314	CHL	CMB-C2B-C3B	4.43	132.96	124.68
3	S	306	CHL	CHD-C1D-ND	-4.43	120.39	124.45
5	S	323	Q6L	C40-C32-C33	-4.42	114.10	123.56
7	U	316	IWJ	C01-C02-C03	-4.41	114.13	123.56
2	T	309	CLA	C4-C3-C5	4.35	122.60	115.27
4	T	308	KC2	C2A-C3A-C4A	-4.34	103.26	106.49
3	S	305	CHL	C4A-NA-C1A	4.33	108.65	106.71
5	T	322	Q6L	C40-C32-C33	-4.32	114.31	123.56
3	S	306	CHL	O2D-CGD-O1D	-4.30	115.42	123.84
2	U	303	CLA	C4A-NA-C1A	4.29	108.64	106.71
2	U	302	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
2	S	311	CLA	CMB-C2B-C3B	4.26	132.65	124.68
3	S	306	CHL	CHD-C4C-C3C	4.25	131.09	124.84
2	T	312	CLA	C4-C3-C5	4.19	122.32	115.27
2	U	303	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
2	U	301	CLA	C1B-CHB-C4A	-4.16	121.88	130.12
5	S	316	Q6L	C40-C32-C33	-4.16	114.67	123.56
2	U	311	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
5	U	317	Q6L	C40-C32-C33	-4.14	114.70	123.56
2	U	308	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
2	S	301	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
6	S	317	NEX	C28-C29-C30	4.11	125.25	118.94
7	T	318	IWJ	C01-C02-C03	-4.11	114.78	123.56
5	S	321	Q6L	C40-C32-C33	-4.10	114.78	123.56
7	S	318	IWJ	C01-C02-C03	-4.08	114.82	123.56
7	S	322	IWJ	C01-C02-C03	-4.07	114.84	123.56
7	T	321	IWJ	C01-C02-C03	-4.07	114.86	123.56
2	U	311	CLA	CMB-C2B-C3B	4.05	132.25	124.68
2	U	308	CLA	C4A-NA-C1A	-4.03	104.89	106.71
7	S	319	IWJ	C01-C02-C03	-4.03	114.95	123.56
6	S	317	NEX	C39-C29-C30	-4.02	117.30	122.92
2	U	302	CLA	CMB-C2B-C3B	3.96	132.08	124.68
4	T	308	KC2	CBA-CAA-C2A	-3.95	110.20	125.27
2	S	301	CLA	CMB-C2B-C3B	3.94	132.05	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	316	Q6L	C40-C32-C33	-3.94	115.13	123.56
3	U	304	CHL	C1B-CHB-C4A	-3.92	122.35	130.12
2	U	312	CLA	C4A-NA-C1A	3.91	108.46	106.71
2	S	313	CLA	C4A-NA-C1A	3.90	108.46	106.71
6	T	317	NEX	C39-C29-C30	-3.90	117.47	122.92
3	S	304	CHL	C2A-C3A-C4A	-3.89	96.82	101.78
5	T	319	Q6L	C40-C32-C33	-3.88	115.26	123.56
7	S	318	IWJ	C33-C32-C30	3.87	118.65	112.04
3	T	306	CHL	CMB-C2B-C1B	-3.84	122.56	128.46
2	S	310	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
2	S	309	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
2	S	311	CLA	CHB-C4A-NA	3.75	129.70	124.51
4	S	308	KC2	O2D-CGD-O1D	-3.74	116.53	123.84
4	S	308	KC2	C1A-C2A-C3A	-3.74	104.15	107.11
2	T	312	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
2	S	310	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
2	U	308	CLA	C1B-CHB-C4A	-3.70	122.79	130.12
3	S	306	CHL	CHB-C4A-NA	3.70	129.63	124.51
6	S	317	NEX	C38-C25-C26	-3.70	116.06	122.26
3	T	306	CHL	CHB-C4A-NA	3.68	129.60	124.51
5	T	315	Q6L	C40-C32-C33	-3.67	115.70	123.56
2	S	302	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
2	T	301	CLA	C4A-NA-C1A	3.65	108.35	106.71
3	S	306	CHL	C1B-CHB-C4A	-3.63	122.94	130.12
2	T	302	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
2	T	313	CLA	C4A-NA-C1A	3.59	108.32	106.71
3	T	320	CHL	O2D-CGD-CBD	3.59	117.66	111.27
5	S	323	Q6L	C38-C36-C35	-3.59	102.63	109.44
3	T	314	CHL	CMB-C2B-C3B	3.58	131.38	124.68
3	U	305	CHL	C4A-NA-C1A	3.57	108.31	106.71
3	S	306	CHL	CMB-C2B-C3B	3.55	131.31	124.68
3	T	306	CHL	C1B-CHB-C4A	-3.55	123.09	130.12
2	U	309	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
3	U	306	CHL	CMB-C2B-C1B	-3.52	123.06	128.46
3	S	304	CHL	C1B-CHB-C4A	-3.51	123.16	130.12
6	T	317	NEX	C38-C25-C26	-3.50	116.40	122.26
3	S	304	CHL	CMB-C2B-C1B	-3.49	123.10	128.46
3	S	305	CHL	CHB-C4A-NA	3.49	129.34	124.51
2	U	303	CLA	CMB-C2B-C3B	3.47	131.16	124.68
2	S	309	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
2	U	311	CLA	CHB-C4A-NA	3.45	129.29	124.51
3	T	320	CHL	C1B-CHB-C4A	-3.44	123.30	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	310	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
3	S	304	CHL	OMC-CMC-C2C	-3.40	117.99	125.69
4	S	308	KC2	CAA-CBA-CGA	-3.37	109.93	127.26
5	S	316	Q6L	C05-C06-C07	3.37	114.92	110.30
3	U	306	CHL	C1B-CHB-C4A	-3.37	123.44	130.12
2	U	308	CLA	CMB-C2B-C3B	3.36	130.96	124.68
2	U	301	CLA	CHB-C4A-NA	3.35	129.15	124.51
2	S	309	CLA	CMB-C2B-C3B	3.34	130.94	124.68
3	U	313	CHL	CMB-C2B-C3B	3.34	130.93	124.68
3	T	320	CHL	CHB-C4A-NA	3.33	129.12	124.51
5	U	315	Q6L	C05-C06-C07	3.33	114.86	110.30
5	S	315	Q6L	C35-C34-C33	3.32	115.52	111.74
2	T	313	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
3	T	305	CHL	CHB-C4A-NA	3.32	129.10	124.51
3	T	304	CHL	C1B-CHB-C4A	-3.31	123.56	130.12
5	S	315	Q6L	C05-C06-C07	3.30	114.82	110.30
6	T	317	NEX	O24-C25-C38	3.30	119.01	115.06
6	T	317	NEX	C15-C35-C34	-3.29	116.73	123.47
3	U	313	CHL	C1B-CHB-C4A	-3.29	123.61	130.12
6	S	317	NEX	C17-C1-C6	3.29	113.41	110.47
3	U	304	CHL	CMB-C2B-C1B	-3.28	123.42	128.46
3	S	314	CHL	C1B-CHB-C4A	-3.28	123.62	130.12
3	U	305	CHL	CBC-CAC-C3C	3.27	121.45	112.43
4	U	307	KC2	CBA-CAA-C2A	-3.27	112.81	125.27
2	U	301	CLA	C4A-NA-C1A	3.26	108.17	106.71
3	S	304	CHL	CMA-C3A-C4A	3.26	120.53	111.77
4	U	307	KC2	O2D-CGD-O1D	-3.26	117.47	123.84
3	T	314	CHL	C1B-CHB-C4A	-3.24	123.69	130.12
2	U	309	CLA	CMB-C2B-C3B	3.24	130.74	124.68
2	S	302	CLA	CMB-C2B-C3B	3.23	130.71	124.68
2	S	309	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
2	T	301	CLA	O1D-CGD-CBD	3.21	131.05	124.48
3	T	314	CHL	O2D-CGD-O1D	-3.20	117.57	123.84
2	U	311	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
3	S	306	CHL	C2D-C1D-ND	-3.20	107.75	110.10
3	S	306	CHL	O2D-CGD-CBD	3.20	116.95	111.27
7	S	318	IWJ	C17-C18-C19	-3.20	122.75	127.31
2	T	312	CLA	CMB-C2B-C3B	3.19	130.65	124.68
6	T	317	NEX	C19-C9-C10	3.19	127.39	122.92
3	T	307	CHL	C4A-NA-C1A	3.18	108.14	106.71
4	T	308	KC2	O2D-CGD-O1D	-3.16	117.67	123.84
2	S	310	CLA	CMB-C2B-C3B	3.15	130.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	303	CLA	C4A-NA-C1A	3.15	108.12	106.71
5	T	322	Q6L	C19-C18-C17	-3.13	122.84	127.31
2	U	309	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
6	S	317	NEX	C15-C35-C34	-3.12	117.08	123.47
2	U	308	CLA	C2C-C1C-NC	3.11	112.89	109.97
3	T	306	CHL	CMB-C2B-C3B	3.11	130.50	124.68
2	T	301	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
2	U	312	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
2	S	313	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
4	T	308	KC2	CAA-CBA-CGA	-3.07	111.48	127.26
3	T	304	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
6	T	317	NEX	C31-C30-C29	-3.04	122.97	127.31
6	T	317	NEX	C5-C4-C3	3.04	115.34	111.75
3	S	305	CHL	C1B-CHB-C4A	-3.04	124.10	130.12
2	S	310	CLA	C4-C3-C5	3.03	120.37	115.27
4	S	308	KC2	CHB-C4A-C3A	-3.03	120.25	124.98
2	T	311	CLA	CHB-C4A-NA	3.01	128.68	124.51
2	T	313	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
6	S	317	NEX	C31-C30-C29	-3.01	123.02	127.31
2	S	312	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
3	U	305	CHL	CHB-C4A-NA	2.99	128.65	124.51
4	U	307	KC2	C2A-C3A-C4A	-2.99	104.27	106.49
2	T	309	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
2	U	302	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
3	T	320	CHL	O2D-CGD-O1D	-2.98	118.01	123.84
2	T	302	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
3	S	306	CHL	C4-C3-C5	2.98	119.39	115.98
4	T	308	KC2	CHB-C4A-C3A	-2.98	120.33	124.98
3	T	307	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
2	S	303	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
3	S	306	CHL	CHD-C1D-C2D	2.96	131.69	125.48
7	S	318	IWJ	C36-C35-C34	-2.96	103.84	108.98
5	S	315	Q6L	C06-C07-C02	2.93	117.70	111.85
2	U	303	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
2	S	301	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
2	T	309	CLA	CMB-C2B-C3B	2.92	130.14	124.68
3	U	305	CHL	C1B-CHB-C4A	-2.92	124.34	130.12
2	T	303	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
2	T	303	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
2	S	302	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
3	T	314	CHL	O2D-CGD-CBD	2.88	116.39	111.27
4	S	308	KC2	CAA-C2A-C1A	-2.87	111.53	124.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	301	CLA	C1-C2-C3	-2.87	121.07	126.04
2	U	310	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
4	U	307	KC2	CMD-C2D-C3D	2.87	130.04	124.68
3	T	305	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
2	T	301	CLA	CHB-C4A-NA	2.87	128.47	124.51
2	U	302	CLA	C2D-C1D-ND	-2.86	107.99	110.10
7	U	316	IWJ	C36-C35-C34	-2.84	104.05	108.98
3	S	306	CHL	CBC-CAC-C3C	2.84	120.26	112.43
2	S	301	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
2	U	312	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
3	T	320	CHL	CMB-C2B-C1B	-2.83	124.11	128.46
3	S	307	CHL	C1B-CHB-C4A	-2.82	124.52	130.12
3	S	314	CHL	O2D-CGD-O1D	-2.82	118.32	123.84
2	T	313	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
2	U	309	CLA	CHB-C4A-NA	2.82	128.41	124.51
3	S	304	CHL	CAA-C2A-C3A	-2.82	109.52	116.10
5	U	315	Q6L	C19-C20-C21	-2.82	117.70	123.47
5	S	320	Q6L	C35-C34-C33	2.81	114.94	111.74
4	U	307	KC2	CMD-C2D-C1D	-2.81	124.15	128.46
2	T	312	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
2	S	313	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
5	U	317	Q6L	C42-C13-C12	2.80	119.98	115.27
2	S	309	CLA	CHB-C4A-NA	2.80	128.38	124.51
5	S	320	Q6L	C40-C32-C33	-2.80	117.57	123.56
3	U	313	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
2	U	308	CLA	CMC-C2C-C1C	2.80	129.30	125.04
3	S	307	CHL	CHB-C4A-NA	2.79	128.37	124.51
2	U	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
4	T	308	KC2	CAA-C2A-C1A	-2.79	111.93	124.75
2	U	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
2	T	310	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
2	T	310	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
3	U	306	CHL	CHB-C4A-NA	2.77	128.34	124.51
2	S	311	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
5	T	316	Q6L	C29-C27-C26	-2.77	114.69	118.94
5	S	323	Q6L	C20-C21-C22	2.76	131.25	127.31
3	T	304	CHL	CHB-C4A-NA	2.76	128.33	124.51
2	S	303	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
4	U	307	KC2	CHB-C4A-C3A	-2.75	120.68	124.98
5	S	323	Q6L	C09-C04-C03	2.75	113.63	109.71
2	U	301	CLA	C2A-C1A-CHA	2.74	128.66	123.86
2	S	309	CLA	CBA-CAA-C2A	2.73	121.93	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	312	CLA	CMB-C2B-C3B	2.73	129.78	124.68
6	T	317	NEX	C11-C10-C9	-2.73	123.42	127.31
2	S	310	CLA	O2D-CGD-CBD	2.72	116.10	111.27
3	S	314	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
2	S	301	CLA	CMD-C2D-C3D	2.71	133.86	127.61
3	T	307	CHL	CHB-C4A-NA	2.71	128.26	124.51
2	S	311	CLA	CED-O2D-CGD	2.70	122.05	115.94
2	T	302	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
2	S	311	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
2	T	310	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
3	U	304	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
7	S	318	IWJ	C17-C16-C15	-2.68	117.97	123.47
6	S	317	NEX	C25-C24-C23	2.67	118.04	112.75
4	T	308	KC2	O1A-CGA-CBA	2.67	129.34	120.99
2	U	312	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
2	S	310	CLA	CHD-C1D-ND	-2.66	122.01	124.45
2	S	312	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
3	T	305	CHL	C2A-C1A-CHA	2.65	128.49	123.86
2	T	301	CLA	C5-C3-C2	-2.64	115.77	121.12
5	S	320	Q6L	C37-C36-C35	-2.63	104.45	109.44
5	T	316	Q6L	C01-C02-C07	-2.63	109.48	114.36
3	T	306	CHL	C3A-C2A-C1A	2.63	105.28	101.34
3	U	313	CHL	CHB-C4A-NA	2.63	128.14	124.51
2	T	312	CLA	CHB-C4A-NA	2.62	128.14	124.51
3	S	305	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
5	S	323	Q6L	C04-C05-C06	-2.62	107.73	113.64
2	S	313	CLA	CMB-C2B-C3B	2.62	129.58	124.68
2	T	302	CLA	CMB-C2B-C3B	2.62	129.57	124.68
3	S	306	CHL	CMD-C2D-C1D	2.61	129.31	124.71
3	U	313	CHL	C1C-C2C-C3C	-2.61	105.05	107.11
2	T	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
7	T	318	IWJ	C16-C17-C18	-2.60	118.16	123.47
3	U	306	CHL	CMB-C2B-C3B	2.60	129.53	124.68
3	T	314	CHL	CHB-C4A-NA	2.59	128.10	124.51
2	T	313	CLA	CMB-C2B-C3B	2.59	129.53	124.68
2	U	302	CLA	CHB-C4A-NA	2.59	128.09	124.51
3	S	306	CHL	CHD-C4C-NC	-2.59	120.13	124.20
3	T	314	CHL	C4A-NA-C1A	2.58	107.87	106.71
4	U	307	KC2	CAA-CBA-CGA	-2.58	114.01	127.26
3	U	304	CHL	CHB-C4A-NA	2.58	128.08	124.51
2	U	301	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
6	S	317	NEX	C15-C14-C13	-2.58	123.63	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	310	CLA	C1-C2-C3	-2.58	121.59	126.04
2	S	313	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
5	S	316	Q6L	C19-C20-C21	-2.57	118.21	123.47
2	U	302	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
2	S	312	CLA	CHB-C4A-NA	2.56	128.05	124.51
5	S	323	Q6L	C19-C18-C17	-2.55	123.67	127.31
3	T	305	CHL	CAA-C2A-C1A	2.55	120.33	111.97
2	T	303	CLA	CHB-C4A-NA	2.55	128.03	124.51
2	T	309	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
2	S	303	CLA	CHB-C4A-NA	2.54	128.03	124.51
2	S	310	CLA	CHB-C4A-NA	2.54	128.03	124.51
2	S	309	CLA	O2D-CGD-CBD	2.53	115.77	111.27
3	S	307	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
5	T	316	Q6L	C26-C25-C24	-2.53	115.32	123.22
5	U	314	Q6L	C12-C13-C14	-2.53	114.33	121.98
5	S	320	Q6L	C42-C13-C12	2.53	119.52	115.27
3	T	306	CHL	O2D-CGD-O1D	-2.52	118.90	123.84
2	T	309	CLA	C4A-NA-C1A	2.52	107.84	106.71
5	U	314	Q6L	C42-C13-C12	2.52	119.51	115.27
2	U	311	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
4	U	307	KC2	CAA-C2A-C1A	-2.51	113.19	124.75
2	S	312	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
5	T	316	Q6L	C24-C22-C21	-2.51	115.09	118.94
2	U	301	CLA	CAA-C2A-C1A	-2.51	103.76	111.97
2	U	302	CLA	C4-C3-C5	2.51	119.49	115.27
3	T	305	CHL	CMA-C3A-C4A	2.51	118.51	111.77
2	S	302	CLA	C2D-C1D-ND	-2.50	108.26	110.10
3	S	304	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
6	S	317	NEX	C19-C9-C10	2.48	126.40	122.92
7	T	321	IWJ	C25-C24-C26	2.48	120.18	116.02
2	U	310	CLA	CMB-C2B-C3B	2.48	129.31	124.68
2	U	303	CLA	CHB-C4A-NA	2.47	127.93	124.51
5	U	314	Q6L	C16-C17-C18	-2.47	115.16	118.94
2	T	309	CLA	CHD-C1D-ND	-2.47	122.19	124.45
2	U	308	CLA	CMA-C3A-C2A	-2.46	110.35	116.10
5	S	320	Q6L	C12-C13-C14	-2.46	114.54	121.98
4	T	308	KC2	CAC-C3C-C2C	-2.44	120.55	128.60
5	S	323	Q6L	C36-C31-C32	2.44	115.80	111.42
5	T	322	Q6L	C38-C36-C35	-2.44	104.81	109.44
3	T	320	CHL	C3A-C2A-C1A	2.44	104.99	101.34
2	U	303	CLA	CHD-C1D-ND	-2.44	122.22	124.45
7	T	318	IWJ	C05-C04-C03	2.43	114.51	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	303	CLA	C2D-C1D-ND	-2.43	108.31	110.10
5	S	320	Q6L	C01-C02-C07	-2.42	109.87	114.36
2	U	311	CLA	O1D-CGD-CBD	2.42	129.43	124.48
4	T	308	KC2	CHB-C4A-NA	2.41	128.00	124.20
2	T	311	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
5	S	320	Q6L	O39-C34-C35	-2.40	104.66	110.74
2	U	308	CLA	CHD-C4C-C3C	-2.40	121.31	124.84
2	T	309	CLA	CBA-CAA-C2A	2.40	120.94	113.86
4	S	308	KC2	CAC-C3C-C2C	-2.39	120.72	128.60
2	S	303	CLA	O2D-CGD-CBD	2.39	115.52	111.27
4	U	307	KC2	CHC-C4B-NB	2.39	126.65	124.45
2	S	301	CLA	CMD-C2D-C1D	-2.39	120.50	124.71
2	S	301	CLA	C5-C3-C2	2.39	125.95	121.12
2	U	310	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
6	T	317	NEX	C32-C33-C34	-2.38	115.28	118.94
2	U	309	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
3	S	307	CHL	C1C-C2C-C3C	-2.38	105.22	107.11
3	S	314	CHL	CHB-C4A-NA	2.38	127.80	124.51
2	T	312	CLA	O2A-CGA-O1A	-2.38	117.60	123.59
4	T	308	KC2	CMD-C2D-C1D	-2.37	124.81	128.46
2	T	312	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
6	T	317	NEX	C15-C14-C13	-2.37	123.92	127.31
5	T	315	Q6L	C01-C02-C07	-2.37	109.96	114.36
2	U	310	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
6	S	317	NEX	C32-C33-C34	-2.36	115.31	118.94
3	S	306	CHL	C4A-NA-C1A	2.36	107.77	106.71
3	U	304	CHL	CMB-C2B-C3B	2.36	129.10	124.68
4	S	308	KC2	O1A-CGA-CBA	2.36	128.36	120.99
2	T	309	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
2	T	312	CLA	CBA-CAA-C2A	2.35	120.79	113.86
7	S	319	IWJ	C21-C19-C18	-2.34	115.35	118.94
2	S	303	CLA	C4A-NA-C1A	2.34	107.76	106.71
2	S	310	CLA	CED-O2D-CGD	2.34	121.23	115.94
2	S	301	CLA	CAC-C3C-C4C	2.34	127.85	124.81
3	U	304	CHL	CED-O2D-CGD	2.34	121.23	115.94
4	U	307	KC2	O2A-CGA-O1A	-2.34	117.81	122.67
4	U	307	KC2	CHB-C4A-NA	2.34	127.89	124.20
2	S	301	CLA	CHB-C4A-NA	2.34	127.74	124.51
2	U	309	CLA	CED-O2D-CGD	2.34	121.22	115.94
2	U	310	CLA	CHA-C1A-NA	-2.33	121.05	126.40
2	T	310	CLA	CMB-C2B-C3B	2.33	129.04	124.68
2	S	301	CLA	CHA-C1A-NA	-2.32	121.07	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	309	CLA	CHD-C1D-ND	-2.32	122.32	124.45
3	T	304	CHL	CHD-C1D-ND	-2.32	122.33	124.45
2	S	302	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
2	T	301	CLA	CHA-C1A-NA	-2.32	121.09	126.40
2	T	313	CLA	CHD-C1D-ND	-2.31	122.33	124.45
4	S	308	KC2	O2D-CGD-CBD	2.31	115.37	111.27
5	U	315	Q6L	C29-C27-C26	-2.31	115.40	118.94
3	S	307	CHL	CMA-C3A-C2A	-2.31	110.71	116.10
7	S	319	IWJ	C25-C24-C26	2.30	119.89	116.02
4	U	307	KC2	CAC-C3C-C2C	-2.30	121.03	128.60
3	U	305	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
2	U	310	CLA	CHB-C4A-NA	2.29	127.68	124.51
3	T	320	CHL	CMB-C2B-C3B	2.29	128.96	124.68
4	U	307	KC2	O1A-CGA-CBA	2.29	128.13	120.99
4	S	308	KC2	CHC-C4B-NB	2.28	126.55	124.45
5	U	315	Q6L	C35-C34-C33	2.28	114.34	111.74
4	T	308	KC2	O2D-CGD-CBD	2.28	115.32	111.27
5	S	321	Q6L	C19-C18-C17	-2.28	124.06	127.31
5	S	316	Q6L	C24-C22-C21	-2.28	115.44	118.94
2	S	301	CLA	C4A-NA-C1A	2.28	107.73	106.71
7	S	322	IWJ	C36-C35-C34	-2.28	105.02	108.98
2	S	302	CLA	CHB-C4A-NA	2.27	127.65	124.51
2	T	311	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
5	U	315	Q6L	C20-C19-C18	2.27	128.12	123.47
5	S	315	Q6L	C42-C13-C12	2.26	119.08	115.27
3	T	304	CHL	C2D-C1D-ND	-2.26	108.44	110.10
2	T	301	CLA	CBA-CAA-C2A	2.26	120.53	113.86
4	T	308	KC2	CMD-C2D-C3D	2.26	128.90	124.68
3	T	314	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
7	S	322	IWJ	C25-C24-C26	2.25	119.81	116.02
4	T	308	KC2	O2A-CGA-O1A	-2.25	117.99	122.67
2	S	309	CLA	C3A-C2A-C1A	-2.25	97.97	101.34
3	S	305	CHL	CBC-CAC-C3C	2.25	118.63	112.43
5	U	317	Q6L	C12-C13-C14	-2.24	115.19	121.98
2	T	309	CLA	C1D-ND-C4D	-2.24	104.75	106.33
2	U	310	CLA	C2A-C1A-CHA	2.24	127.77	123.86
2	T	301	CLA	C6-C5-C3	2.24	119.32	113.45
2	S	313	CLA	CMA-C3A-C2A	-2.23	110.89	116.10
3	T	306	CHL	CAC-C3C-C4C	2.23	127.70	124.81
2	S	309	CLA	CHD-C1D-ND	-2.23	122.41	124.45
5	T	319	Q6L	C42-C13-C12	2.23	119.02	115.27
4	T	308	KC2	CHC-C4B-NB	2.22	126.49	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	313	CLA	C2D-C1D-ND	-2.22	108.47	110.10
4	S	308	KC2	CMD-C2D-C1D	-2.22	125.05	128.46
2	S	312	CLA	CMB-C2B-C3B	2.22	128.82	124.68
6	T	317	NEX	C16-C1-C6	2.21	112.45	110.47
2	S	303	CLA	CHD-C1D-ND	-2.21	122.42	124.45
2	U	310	CLA	C4D-CHA-C1A	2.21	123.94	121.25
7	U	316	IWJ	C05-C04-C03	2.21	114.26	111.74
3	U	304	CHL	CAC-C3C-C4C	2.21	127.67	124.81
3	U	305	CHL	O2D-CGD-CBD	2.20	115.18	111.27
2	T	312	CLA	O2D-CGD-CBD	2.20	115.17	111.27
5	S	321	Q6L	C19-C20-C21	-2.19	118.98	123.47
5	S	323	Q6L	C24-C22-C21	-2.19	115.58	118.94
2	S	302	CLA	CHD-C1D-ND	-2.19	122.44	124.45
5	T	315	Q6L	C12-C13-C14	-2.19	115.35	121.98
4	S	308	KC2	CHB-C1B-NB	2.19	126.47	124.45
6	S	317	NEX	C35-C34-C33	-2.18	124.19	127.31
2	T	301	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
3	T	306	CHL	O2A-CGA-O1A	-2.18	118.08	123.59
5	S	323	Q6L	C35-C34-C33	2.18	114.22	111.74
3	T	305	CHL	OMC-CMC-C2C	-2.18	120.76	125.69
2	T	301	CLA	C2A-C1A-CHA	2.18	127.67	123.86
3	T	306	CHL	C4-C3-C2	-2.18	118.09	123.68
3	T	320	CHL	C4-C3-C5	-2.17	113.50	115.98
2	T	311	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
5	U	314	Q6L	C01-C02-C03	2.17	127.34	124.49
3	U	306	CHL	CAC-C3C-C4C	2.17	127.62	124.81
3	T	320	CHL	C2A-C1A-CHA	2.17	127.65	123.86
3	T	320	CHL	CAC-C3C-C4C	2.15	127.60	124.81
7	T	318	IWJ	C36-C35-C34	-2.15	105.25	108.98
2	U	303	CLA	C1-C2-C3	-2.14	123.28	126.75
3	T	305	CHL	C1B-CHB-C4A	-2.14	125.87	130.12
6	T	317	NEX	C36-C21-C22	-2.14	105.26	108.98
2	U	308	CLA	CHB-C4A-NA	2.14	127.47	124.51
7	U	316	IWJ	C17-C16-C15	-2.14	119.10	123.47
5	S	323	Q6L	C01-C02-C07	-2.14	110.40	114.36
2	T	310	CLA	CHB-C4A-NA	2.13	127.46	124.51
5	T	315	Q6L	C05-C06-C07	2.13	113.22	110.30
2	T	311	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
7	T	321	IWJ	C36-C35-C34	-2.13	105.28	108.98
3	T	307	CHL	O2D-CGD-O1D	-2.13	119.68	123.84
2	S	310	CLA	CHA-C1A-NA	-2.12	121.53	126.40
5	T	316	Q6L	C25-C26-C27	2.12	130.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	302	CLA	CAC-C3C-C4C	2.12	127.56	124.81
5	U	315	Q6L	C20-C21-C22	2.12	130.33	127.31
2	U	312	CLA	CMA-C3A-C2A	-2.12	111.16	116.10
3	S	304	CHL	CAC-C3C-C4C	2.11	127.55	124.81
2	S	311	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
7	S	319	IWJ	C36-C35-C34	-2.11	105.31	108.98
6	S	317	NEX	C36-C21-C22	-2.11	105.31	108.98
4	T	308	KC2	CBD-CHA-C1A	2.11	132.82	128.88
2	S	302	CLA	C3A-C2A-C1A	2.11	104.50	101.34
5	T	316	Q6L	C19-C20-C21	-2.11	119.16	123.47
5	S	315	Q6L	C01-C02-C07	-2.11	110.45	114.36
2	S	311	CLA	C2A-C3A-C4A	2.11	105.27	101.87
2	S	312	CLA	C4-C3-C5	2.10	118.81	115.27
2	S	303	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
5	T	319	Q6L	C05-C06-C07	2.10	113.18	110.30
3	T	305	CHL	CHA-C4D-ND	2.10	136.90	132.50
3	U	304	CHL	C3C-C4C-NC	-2.10	108.22	110.57
2	S	313	CLA	CAA-C2A-C3A	-2.10	111.20	116.10
2	U	311	CLA	O2A-CGA-CBA	2.09	118.47	111.91
2	S	309	CLA	C2D-C1D-ND	-2.09	108.56	110.10
2	S	301	CLA	O1D-CGD-CBD	2.09	128.76	124.48
5	T	316	Q6L	C23-C22-C21	2.07	125.83	122.92
3	S	305	CHL	CHA-C4D-ND	2.07	136.84	132.50
5	U	317	Q6L	C01-C02-C07	-2.07	110.51	114.36
3	U	313	CHL	C2D-C1D-ND	-2.07	108.58	110.10
7	S	319	IWJ	C23-C22-C21	-2.07	116.75	123.22
2	U	310	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
2	U	303	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
2	U	301	CLA	CHA-C1A-NA	-2.07	121.66	126.40
3	T	306	CHL	C2A-C1A-CHA	2.07	127.47	123.86
4	S	308	KC2	O2A-CGA-O1A	-2.07	118.38	122.67
4	U	307	KC2	CHB-C1B-NB	2.06	126.35	124.45
5	T	315	Q6L	C42-C13-C12	2.06	118.74	115.27
6	S	317	NEX	C40-C33-C32	2.06	121.33	118.08
5	S	320	Q6L	C16-C17-C18	-2.06	115.78	118.94
3	T	320	CHL	CAA-CBA-CGA	-2.06	107.25	113.25
2	U	311	CLA	C1-C2-C3	-2.05	122.50	126.04
2	T	309	CLA	CAA-C2A-C3A	2.04	118.38	112.78
2	T	302	CLA	C5-C3-C2	2.04	125.25	121.12
2	U	308	CLA	CBC-CAC-C3C	2.04	118.06	112.43
5	T	319	Q6L	C19-C20-C21	-2.04	119.30	123.47
7	S	319	IWJ	C33-C32-C30	2.04	115.52	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	321	Q6L	C38-C36-C35	-2.03	105.58	109.44
6	S	317	NEX	C11-C12-C13	-2.03	120.70	126.42
3	U	304	CHL	O2D-CGD-CBD	2.03	114.88	111.27
2	T	302	CLA	CHB-C4A-NA	2.03	127.32	124.51
4	S	308	KC2	CBD-CHA-C1A	2.03	132.67	128.88
5	T	316	Q6L	C35-C34-C33	2.03	114.05	111.74
5	S	315	Q6L	C12-C13-C14	-2.03	115.84	121.98
2	T	311	CLA	CHA-C1A-NA	-2.03	121.76	126.40
7	S	318	IWJ	C05-C04-C03	2.03	114.05	111.74
2	S	302	CLA	CMC-C2C-C1C	-2.02	121.96	125.04
3	U	304	CHL	CHD-C1D-ND	-2.02	122.60	124.45
2	T	302	CLA	O2A-C1-C2	-2.02	103.33	108.64
5	U	315	Q6L	C41-C17-C16	-2.02	114.90	118.08
5	S	321	Q6L	C01-C02-C07	-2.02	110.62	114.36
3	U	313	CHL	C4A-NA-C1A	2.02	107.61	106.71
2	S	312	CLA	CBA-CAA-C2A	2.02	119.81	113.86
5	S	315	Q6L	C19-C20-C21	-2.01	119.35	123.47
2	U	308	CLA	C3C-C4C-NC	2.01	112.83	110.57
2	T	309	CLA	C6-C5-C3	2.01	118.72	113.45
2	S	312	CLA	CHD-C1D-ND	-2.01	122.61	124.45
2	S	301	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	S	301	CLA	ND
2	S	302	CLA	ND
2	S	303	CLA	ND
2	S	309	CLA	ND
2	S	310	CLA	ND
2	S	311	CLA	ND
2	S	312	CLA	ND
2	S	313	CLA	ND
2	T	301	CLA	ND
2	T	302	CLA	ND
2	T	303	CLA	ND
2	T	309	CLA	ND
2	T	310	CLA	ND
2	T	311	CLA	ND
2	T	312	CLA	ND
2	T	313	CLA	ND
2	U	301	CLA	ND

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Mol	Chain	Res	Type	Atom
2	U	302	CLA	ND
2	U	303	CLA	ND
2	U	308	CLA	ND
2	U	309	CLA	ND
2	U	310	CLA	ND
2	U	311	CLA	ND
2	U	312	CLA	ND
3	S	304	CHL	NC
3	S	304	CHL	NA
3	S	304	CHL	ND
3	S	305	CHL	NC
3	S	305	CHL	NA
3	S	305	CHL	ND
3	S	306	CHL	NC
3	S	306	CHL	NA
3	S	306	CHL	ND
3	S	307	CHL	NC
3	S	307	CHL	NA
3	S	307	CHL	ND
3	S	314	CHL	NC
3	S	314	CHL	NA
3	S	314	CHL	ND
3	T	304	CHL	NC
3	T	304	CHL	NA
3	T	304	CHL	ND
3	T	305	CHL	NC
3	T	305	CHL	NA
3	T	305	CHL	ND
3	T	306	CHL	NC
3	T	306	CHL	NA
3	T	306	CHL	ND
3	T	307	CHL	NC
3	T	307	CHL	NA
3	T	307	CHL	ND
3	T	314	CHL	NC
3	T	314	CHL	NA
3	T	314	CHL	ND
3	T	320	CHL	NC
3	T	320	CHL	NA
3	T	320	CHL	ND
3	U	304	CHL	NC
3	U	304	CHL	NA

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Mol	Chain	Res	Type	Atom
3	U	304	CHL	ND
3	U	305	CHL	NC
3	U	305	CHL	NA
3	U	305	CHL	ND
3	U	306	CHL	NC
3	U	306	CHL	NA
3	U	306	CHL	ND
3	U	313	CHL	NC
3	U	313	CHL	NA
3	U	313	CHL	ND

All (390) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	301	CLA	C3A-C2A-CAA-CBA
2	S	302	CLA	C6-C7-C8-C9
2	S	303	CLA	CHA-CBD-CGD-O1D
2	S	303	CLA	CHA-CBD-CGD-O2D
2	S	309	CLA	C1A-C2A-CAA-CBA
2	S	309	CLA	C3A-C2A-CAA-CBA
2	S	310	CLA	C1A-C2A-CAA-CBA
2	S	311	CLA	CBD-CGD-O2D-CED
2	S	312	CLA	CHA-CBD-CGD-O1D
2	S	312	CLA	CHA-CBD-CGD-O2D
2	T	301	CLA	C3A-C2A-CAA-CBA
2	T	301	CLA	C4-C3-C5-C6
2	T	302	CLA	C1A-C2A-CAA-CBA
2	T	302	CLA	C3A-C2A-CAA-CBA
2	T	303	CLA	CHA-CBD-CGD-O1D
2	T	303	CLA	CHA-CBD-CGD-O2D
2	T	303	CLA	CBD-CGD-O2D-CED
2	T	309	CLA	C1A-C2A-CAA-CBA
2	T	309	CLA	C3A-C2A-CAA-CBA
2	T	309	CLA	C2-C3-C5-C6
2	T	309	CLA	C4-C3-C5-C6
2	T	310	CLA	C1A-C2A-CAA-CBA
2	T	310	CLA	CHA-CBD-CGD-O1D
2	T	310	CLA	CHA-CBD-CGD-O2D
2	T	311	CLA	CBD-CGD-O2D-CED
2	T	312	CLA	C1A-C2A-CAA-CBA
2	T	313	CLA	C1A-C2A-CAA-CBA
2	U	301	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	U	301	CLA	C3A-C2A-CAA-CBA
2	U	301	CLA	CBD-CGD-O2D-CED
2	U	303	CLA	CHA-CBD-CGD-O1D
2	U	303	CLA	CHA-CBD-CGD-O2D
2	U	311	CLA	CBD-CGD-O2D-CED
3	S	304	CHL	C3C-C2C-CMC-OMC
3	S	306	CHL	CAD-CBD-CGD-O1D
3	S	306	CHL	CAD-CBD-CGD-O2D
3	S	307	CHL	CBD-CGD-O2D-CED
3	S	314	CHL	CHA-CBD-CGD-O1D
3	S	314	CHL	CHA-CBD-CGD-O2D
3	T	304	CHL	CBD-CGD-O2D-CED
3	T	320	CHL	CHA-CBD-CGD-O2D
3	U	304	CHL	CHA-CBD-CGD-O1D
3	U	304	CHL	CHA-CBD-CGD-O2D
3	U	304	CHL	CBD-CGD-O2D-CED
4	S	308	KC2	C3A-C2A-CAA-CBA
4	S	308	KC2	C2A-CAA-CBA-CGA
4	S	308	KC2	CHA-CBD-CGD-O1D
4	S	308	KC2	CHA-CBD-CGD-O2D
4	T	308	KC2	C3A-C2A-CAA-CBA
4	T	308	KC2	C2A-CAA-CBA-CGA
4	U	307	KC2	C1A-C2A-CAA-CBA
4	U	307	KC2	C3A-C2A-CAA-CBA
4	U	307	KC2	C2A-CAA-CBA-CGA
4	U	307	KC2	CAA-CBA-CGA-O1A
4	U	307	KC2	CAA-CBA-CGA-O2A
5	S	315	Q6L	C28-C27-C29-C30
5	S	315	Q6L	C26-C27-C29-C30
5	S	320	Q6L	C11-C12-C13-C42
5	S	320	Q6L	C21-C22-C24-C25
5	S	320	Q6L	C23-C22-C24-C25
5	S	320	Q6L	C27-C29-C30-C31
5	S	321	Q6L	C02-C03-C11-C12
5	S	321	Q6L	C29-C30-C31-C36
5	S	321	Q6L	C29-C30-C31-C32
5	S	321	Q6L	C15-C16-C17-C18
5	S	321	Q6L	C15-C16-C17-C41
5	S	323	Q6L	C02-C03-C11-C12
5	S	323	Q6L	C29-C30-C31-C36
5	S	323	Q6L	C29-C30-C31-C32
5	T	315	Q6L	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
5	T	315	Q6L	C15-C16-C17-C18
5	T	315	Q6L	C15-C16-C17-C41
5	T	316	Q6L	C13-C14-C15-C16
5	T	319	Q6L	C11-C12-C13-C42
5	T	319	Q6L	C27-C29-C30-C31
5	T	322	Q6L	C02-C03-C11-C12
5	T	322	Q6L	C11-C12-C13-C14
5	T	322	Q6L	C11-C12-C13-C42
5	T	322	Q6L	C28-C27-C29-C30
5	T	322	Q6L	C29-C30-C31-C36
5	T	322	Q6L	C29-C30-C31-C32
5	U	314	Q6L	C11-C12-C13-C14
5	U	314	Q6L	C11-C12-C13-C42
5	U	314	Q6L	C28-C27-C29-C30
5	U	314	Q6L	C26-C27-C29-C30
5	U	314	Q6L	C15-C16-C17-C41
5	U	317	Q6L	C29-C30-C31-C36
5	U	317	Q6L	C29-C30-C31-C32
7	S	319	IWJ	C18-C19-C21-C22
7	S	319	IWJ	C20-C19-C21-C22
7	S	319	IWJ	C26-C28-C29-C30
7	S	319	IWJ	C26-C28-C29-O39
7	S	322	IWJ	C26-C28-C29-C30
7	S	322	IWJ	C26-C28-C29-C35
7	S	322	IWJ	C26-C28-C29-O39
7	T	318	IWJ	C18-C19-C21-C22
7	T	318	IWJ	C20-C19-C21-C22
7	T	318	IWJ	C26-C28-C29-C30
7	T	318	IWJ	C26-C28-C29-O39
7	T	321	IWJ	C26-C28-C29-C30
7	T	321	IWJ	C26-C28-C29-O39
2	U	311	CLA	O1D-CGD-O2D-CED
3	S	307	CHL	O1D-CGD-O2D-CED
3	U	304	CHL	O1D-CGD-O2D-CED
2	S	311	CLA	O1D-CGD-O2D-CED
2	S	309	CLA	CBD-CGD-O2D-CED
2	T	302	CLA	CBD-CGD-O2D-CED
2	T	312	CLA	CBD-CGD-O2D-CED
2	T	313	CLA	CBD-CGD-O2D-CED
2	U	302	CLA	CBD-CGD-O2D-CED
2	U	310	CLA	CBD-CGD-O2D-CED
3	S	305	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	T	305	CHL	CBD-CGD-O2D-CED
4	U	307	KC2	CBD-CGD-O2D-CED
2	U	311	CLA	O1A-CGA-O2A-C1
2	T	302	CLA	O1D-CGD-O2D-CED
2	T	303	CLA	O1D-CGD-O2D-CED
3	T	304	CHL	O1D-CGD-O2D-CED
2	U	311	CLA	CBA-CGA-O2A-C1
3	U	306	CHL	CBD-CGD-O2D-CED
2	S	311	CLA	O1A-CGA-O2A-C1
2	T	309	CLA	O1A-CGA-O2A-C1
3	S	306	CHL	O1A-CGA-O2A-C1
2	T	311	CLA	O1D-CGD-O2D-CED
2	U	301	CLA	O1D-CGD-O2D-CED
2	S	312	CLA	CBD-CGD-O2D-CED
3	U	305	CHL	CBD-CGD-O2D-CED
2	U	302	CLA	O1D-CGD-O2D-CED
3	T	305	CHL	O1D-CGD-O2D-CED
2	S	301	CLA	C3-C5-C6-C7
2	T	309	CLA	C3-C5-C6-C7
2	S	311	CLA	CBA-CGA-O2A-C1
3	S	306	CHL	CBA-CGA-O2A-C1
3	T	307	CHL	CBD-CGD-O2D-CED
5	U	317	Q6L	C11-C12-C13-C42
2	T	301	CLA	C2-C3-C5-C6
5	S	320	Q6L	C11-C12-C13-C14
5	T	319	Q6L	C11-C12-C13-C14
2	T	301	CLA	CBD-CGD-O2D-CED
2	T	301	CLA	C3-C5-C6-C7
2	T	309	CLA	CBA-CGA-O2A-C1
2	T	313	CLA	O1D-CGD-O2D-CED
2	U	310	CLA	O1D-CGD-O2D-CED
3	S	305	CHL	O1D-CGD-O2D-CED
2	T	312	CLA	O1D-CGD-O2D-CED
5	S	320	Q6L	C24-C25-C26-C27
5	U	315	Q6L	C13-C14-C15-C16
4	U	307	KC2	O1D-CGD-O2D-CED
2	S	303	CLA	CBD-CGD-O2D-CED
2	U	309	CLA	CBD-CGD-O2D-CED
3	T	314	CHL	CBD-CGD-O2D-CED
2	S	309	CLA	O1D-CGD-O2D-CED
4	S	308	KC2	CAA-CBA-CGA-O2A
5	S	321	Q6L	C11-C12-C13-C42

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Mol	Chain	Res	Type	Atoms
5	S	323	Q6L	C11-C12-C13-C42
5	S	321	Q6L	C11-C12-C13-C14
5	S	323	Q6L	C11-C12-C13-C14
2	T	312	CLA	CBA-CGA-O2A-C1
3	T	306	CHL	CBA-CGA-O2A-C1
4	S	308	KC2	CAA-CBA-CGA-O1A
2	T	311	CLA	C5-C6-C7-C8
2	T	312	CLA	O1A-CGA-O2A-C1
5	U	317	Q6L	C11-C12-C13-C14
3	T	306	CHL	C2A-CAA-CBA-CGA
5	S	321	Q6L	C28-C27-C29-C30
5	S	323	Q6L	C28-C27-C29-C30
5	T	319	Q6L	C28-C27-C29-C30
7	S	318	IWJ	C20-C19-C21-C22
5	S	321	Q6L	C26-C27-C29-C30
5	S	323	Q6L	C26-C27-C29-C30
5	T	319	Q6L	C26-C27-C29-C30
5	T	322	Q6L	C26-C27-C29-C30
3	U	306	CHL	O1D-CGD-O2D-CED
2	U	309	CLA	CBA-CGA-O2A-C1
4	T	308	KC2	CAA-CBA-CGA-O1A
2	S	309	CLA	CBA-CGA-O2A-C1
2	S	302	CLA	C5-C6-C7-C8
2	T	301	CLA	C8-C10-C11-C12
2	U	303	CLA	CBD-CGD-O2D-CED
2	S	301	CLA	C8-C10-C11-C12
4	T	308	KC2	CAA-CBA-CGA-O2A
2	T	302	CLA	C6-C7-C8-C10
5	S	316	Q6L	C13-C14-C15-C16
2	U	309	CLA	C2A-CAA-CBA-CGA
3	T	306	CHL	O1A-CGA-O2A-C1
2	S	312	CLA	O1D-CGD-O2D-CED
2	S	309	CLA	O1A-CGA-O2A-C1
2	T	301	CLA	O1D-CGD-O2D-CED
3	T	307	CHL	O1D-CGD-O2D-CED
3	U	305	CHL	O1D-CGD-O2D-CED
2	U	302	CLA	C5-C6-C7-C8
3	T	305	CHL	CBA-CGA-O2A-C1
2	T	312	CLA	C6-C7-C8-C9
2	S	309	CLA	C6-C7-C8-C9
2	U	302	CLA	C6-C7-C8-C9
5	T	315	Q6L	C26-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
5	U	314	Q6L	C15-C16-C17-C18
7	S	318	IWJ	C18-C19-C21-C22
2	T	312	CLA	C6-C7-C8-C10
2	S	310	CLA	C3A-C2A-CAA-CBA
2	S	311	CLA	C3A-C2A-CAA-CBA
2	T	312	CLA	C3A-C2A-CAA-CBA
5	S	315	Q6L	C11-C12-C13-C42
5	S	315	Q6L	C11-C12-C13-C14
3	T	305	CHL	O1A-CGA-O2A-C1
3	S	306	CHL	C2-C1-O2A-CGA
2	S	303	CLA	O1D-CGD-O2D-CED
2	T	302	CLA	C8-C10-C11-C12
3	T	314	CHL	O1D-CGD-O2D-CED
2	S	309	CLA	C6-C7-C8-C10
2	S	310	CLA	C6-C7-C8-C10
2	U	302	CLA	C6-C7-C8-C10
2	S	310	CLA	C10-C11-C12-C13
2	U	309	CLA	O1D-CGD-O2D-CED
4	T	308	KC2	C4C-C3C-CAC-CBC
4	U	307	KC2	C4C-C3C-CAC-CBC
2	S	302	CLA	CBD-CGD-O2D-CED
2	S	310	CLA	C6-C7-C8-C9
2	T	311	CLA	C2A-CAA-CBA-CGA
2	S	301	CLA	C1A-C2A-CAA-CBA
2	S	311	CLA	C1A-C2A-CAA-CBA
2	T	301	CLA	C1A-C2A-CAA-CBA
3	U	306	CHL	C1A-C2A-CAA-CBA
2	U	309	CLA	O1A-CGA-O2A-C1
2	U	303	CLA	O1D-CGD-O2D-CED
2	T	301	CLA	O1A-CGA-O2A-C1
3	U	313	CHL	CBD-CGD-O2D-CED
2	S	310	CLA	CBA-CGA-O2A-C1
2	T	301	CLA	CBA-CGA-O2A-C1
3	T	320	CHL	CBA-CGA-O2A-C1
2	U	301	CLA	C2A-CAA-CBA-CGA
2	S	302	CLA	C11-C12-C13-C15
2	T	309	CLA	C11-C10-C8-C7
2	S	301	CLA	C6-C7-C8-C9
2	S	302	CLA	C11-C12-C13-C14
2	S	309	CLA	C11-C10-C8-C9
5	U	314	Q6L	C24-C25-C26-C27
2	S	301	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
3	S	314	CHL	CBD-CGD-O2D-CED
7	S	318	IWJ	O27-C26-C28-C29
7	S	319	IWJ	O27-C26-C28-C29
7	S	322	IWJ	O27-C26-C28-C29
7	T	321	IWJ	O27-C26-C28-C29
7	U	316	IWJ	O27-C26-C28-C29
2	U	302	CLA	C3-C5-C6-C7
2	S	310	CLA	O1A-CGA-O2A-C1
3	U	304	CHL	C3C-C2C-CMC-OMC
3	U	306	CHL	C3C-C2C-CMC-OMC
3	T	320	CHL	O1A-CGA-O2A-C1
2	T	311	CLA	C3-C5-C6-C7
2	T	302	CLA	C5-C6-C7-C8
2	S	302	CLA	C2-C1-O2A-CGA
2	S	310	CLA	C11-C10-C8-C9
2	T	301	CLA	C11-C12-C13-C14
2	T	302	CLA	C6-C7-C8-C9
2	T	311	CLA	C11-C10-C8-C9
2	U	311	CLA	C2A-CAA-CBA-CGA
2	U	302	CLA	C11-C10-C8-C9
2	S	301	CLA	O1A-CGA-O2A-C1
2	S	302	CLA	C6-C7-C8-C10
2	S	309	CLA	C11-C10-C8-C7
2	S	310	CLA	C11-C10-C8-C7
5	S	321	Q6L	C17-C18-C19-C20
5	T	319	Q6L	C24-C25-C26-C27
7	S	318	IWJ	C14-C15-C16-C17
2	S	302	CLA	C10-C11-C12-C13
3	S	314	CHL	O1D-CGD-O2D-CED
2	S	309	CLA	CAD-CBD-CGD-O2D
2	T	301	CLA	CAD-CBD-CGD-O2D
2	T	302	CLA	CAD-CBD-CGD-O2D
2	T	312	CLA	CAD-CBD-CGD-O2D
2	U	308	CLA	CAD-CBD-CGD-O2D
2	U	312	CLA	CAD-CBD-CGD-O2D
3	S	305	CHL	CAD-CBD-CGD-O2D
3	T	305	CHL	CAD-CBD-CGD-O2D
3	T	314	CHL	CAD-CBD-CGD-O2D
3	U	306	CHL	CAD-CBD-CGD-O2D
4	T	308	KC2	C2B-C3B-CAB-CBB
2	T	311	CLA	C8-C10-C11-C12
4	S	308	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	T	320	CHL	C2A-CAA-CBA-CGA
2	S	310	CLA	CHA-CBD-CGD-O1D
2	U	309	CLA	CHA-CBD-CGD-O1D
3	S	307	CHL	CHA-CBD-CGD-O1D
3	T	304	CHL	CHA-CBD-CGD-O1D
3	T	304	CHL	CHA-CBD-CGD-O2D
3	T	320	CHL	CHA-CBD-CGD-O1D
5	T	319	Q6L	C02-C03-C11-C12
5	U	317	Q6L	C02-C03-C11-C12
2	T	309	CLA	C11-C10-C8-C9
5	S	316	Q6L	C04-C03-C11-C12
5	S	323	Q6L	C04-C03-C11-C12
5	T	322	Q6L	C04-C03-C11-C12
2	T	311	CLA	C2-C1-O2A-CGA
2	T	311	CLA	C10-C11-C12-C13
2	T	312	CLA	C3-C5-C6-C7
3	U	305	CHL	C2C-C3C-CAC-CBC
2	S	302	CLA	O1D-CGD-O2D-CED
2	U	310	CLA	CAD-CBD-CGD-O1D
3	S	306	CHL	C2-C3-C5-C6
3	T	304	CHL	CAD-CBD-CGD-O1D
3	T	306	CHL	C2-C3-C5-C6
2	S	312	CLA	CBA-CGA-O2A-C1
2	T	312	CLA	C4-C3-C5-C6
5	S	316	Q6L	C29-C30-C31-C32
5	T	319	Q6L	C29-C30-C31-C32
7	U	316	IWJ	C02-C07-C08-C09
2	T	311	CLA	O1A-CGA-O2A-C1
3	U	305	CHL	C2A-CAA-CBA-CGA
3	S	304	CHL	C1C-C2C-CMC-OMC
7	S	319	IWJ	C26-C28-C29-C35
7	T	318	IWJ	C26-C28-C29-C35
7	T	321	IWJ	C26-C28-C29-C35
3	U	313	CHL	O1D-CGD-O2D-CED
2	S	312	CLA	O1A-CGA-O2A-C1
2	T	311	CLA	CBA-CGA-O2A-C1
2	T	309	CLA	C11-C12-C13-C14
3	S	307	CHL	C2C-C3C-CAC-CBC
2	S	312	CLA	C2A-CAA-CBA-CGA
2	T	312	CLA	C2-C3-C5-C6
5	S	323	Q6L	C17-C18-C19-C20
2	U	302	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
5	S	321	Q6L	C13-C14-C15-C16
7	T	318	IWJ	C16-C17-C18-C19
4	T	308	KC2	C4B-C3B-CAB-CBB
5	T	315	Q6L	C11-C12-C13-C42
3	T	306	CHL	CAA-CBA-CGA-O2A
2	T	302	CLA	C2-C1-O2A-CGA
2	T	311	CLA	C11-C12-C13-C15
2	U	309	CLA	C3A-C2A-CAA-CBA
6	S	317	NEX	C39-C29-C30-C31
6	T	317	NEX	C39-C29-C30-C31
2	U	310	CLA	C1A-C2A-CAA-CBA
3	T	307	CHL	C1A-C2A-CAA-CBA
6	S	317	NEX	C28-C29-C30-C31
6	T	317	NEX	C28-C29-C30-C31
3	U	305	CHL	CAA-CBA-CGA-O1A
3	S	306	CHL	C4-C3-C5-C6
3	T	306	CHL	C4-C3-C5-C6
4	T	308	KC2	C1A-C2A-CAA-CBA
2	S	302	CLA	C13-C15-C16-C17
7	S	319	IWJ	C21-C22-C23-C24
2	T	302	CLA	C2-C3-C5-C6
3	U	305	CHL	CAA-CBA-CGA-O2A
2	T	311	CLA	C11-C10-C8-C7
2	T	303	CLA	C3A-C2A-CAA-CBA
2	S	301	CLA	CAD-CBD-CGD-O2D
2	S	310	CLA	CAD-CBD-CGD-O2D
2	S	313	CLA	CAD-CBD-CGD-O2D
2	T	313	CLA	CAD-CBD-CGD-O2D
2	U	302	CLA	CAD-CBD-CGD-O2D
3	S	304	CHL	CAD-CBD-CGD-O2D
3	U	313	CHL	CAD-CBD-CGD-O2D
4	U	307	KC2	C2B-C3B-CAB-CBB
4	U	307	KC2	CAD-CBD-CGD-O2D
2	U	303	CLA	O1A-CGA-O2A-C1
6	S	317	NEX	O24-C26-C27-C28
6	T	317	NEX	O24-C26-C27-C28
2	U	301	CLA	CAA-CBA-CGA-O2A
2	S	302	CLA	O2A-C1-C2-C3
2	T	311	CLA	O2A-C1-C2-C3
4	U	307	KC2	C4B-C3B-CAB-CBB
2	U	301	CLA	CAA-CBA-CGA-O1A
2	T	311	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	U	309	CLA	CHA-CBD-CGD-O2D
3	S	307	CHL	CHA-CBD-CGD-O2D
7	S	322	IWJ	C16-C17-C18-C19
2	U	303	CLA	CBA-CGA-O2A-C1
2	T	302	CLA	C4-C3-C5-C6
2	U	302	CLA	C4-C3-C5-C6
2	S	303	CLA	C1A-C2A-CAA-CBA
2	T	303	CLA	C1A-C2A-CAA-CBA
2	U	302	CLA	C1A-C2A-CAA-CBA
2	U	309	CLA	C1A-C2A-CAA-CBA
3	S	314	CHL	C1A-C2A-CAA-CBA
5	S	315	Q6L	C04-C03-C11-C12
2	T	302	CLA	C16-C17-C18-C19
2	T	301	CLA	C2A-CAA-CBA-CGA
5	U	315	Q6L	C17-C18-C19-C20
5	T	315	Q6L	C11-C12-C13-C14
2	U	311	CLA	CAD-CBD-CGD-O1D
3	T	320	CHL	CAD-CBD-CGD-O1D
3	T	320	CHL	CAA-CBA-CGA-O2A
2	S	301	CLA	C14-C13-C15-C16
3	S	305	CHL	C4C-C3C-CAC-CBC
2	U	310	CLA	C3A-C2A-CAA-CBA
5	S	320	Q6L	C29-C30-C31-C32
3	T	320	CHL	CAA-CBA-CGA-O1A
2	S	309	CLA	CAA-CBA-CGA-O2A
2	T	302	CLA	C2A-CAA-CBA-CGA

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	321	IWJ	C29-C30-C32-C33-C34-C35
7	S	319	IWJ	C29-C30-C32-C33-C34-C35

19 monomers are involved in 33 short contacts:

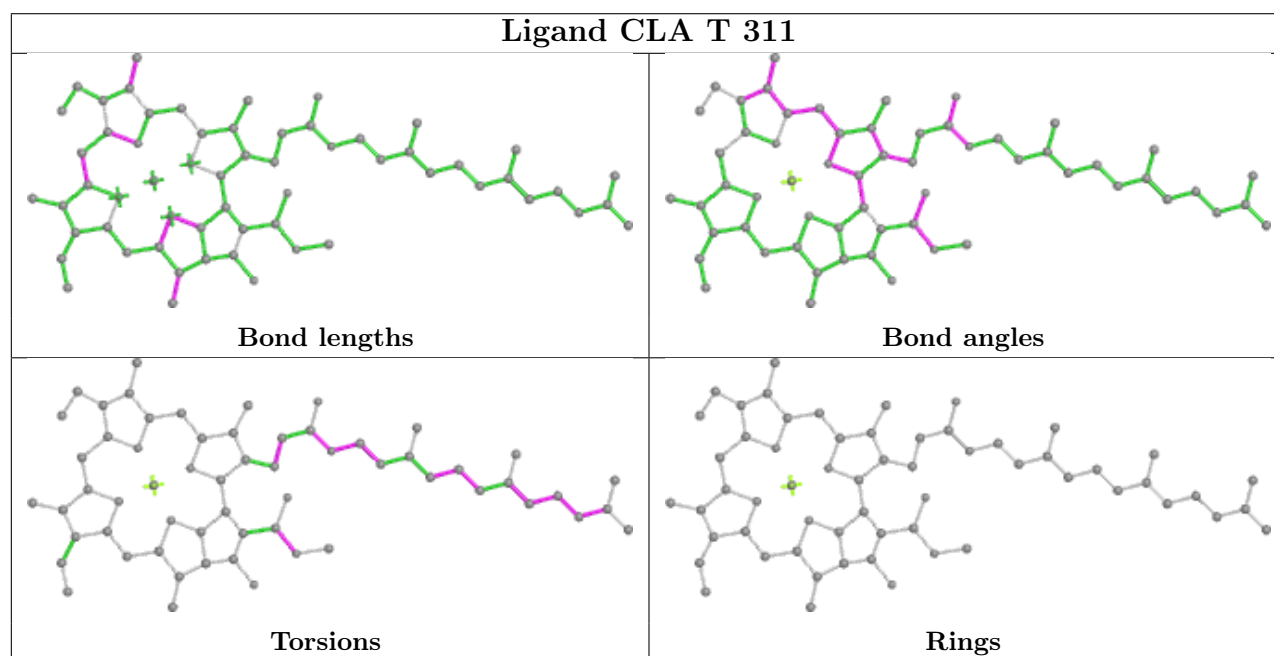
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	311	CLA	1	0
5	U	314	Q6L	2	0
2	T	310	CLA	1	0
4	S	308	KC2	1	0
4	T	308	KC2	1	0
2	S	309	CLA	4	0

*Continued on next page...*

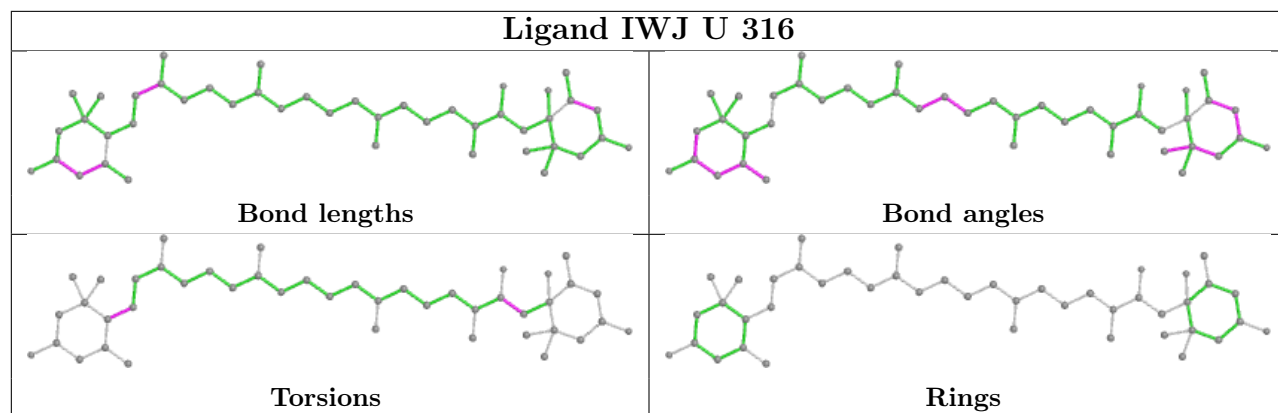
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	312	CLA	1	0
5	S	315	Q6L	1	0
3	T	307	CHL	1	0
7	T	321	IWJ	1	0
2	U	301	CLA	1	0
2	S	301	CLA	6	0
7	S	322	IWJ	1	0
5	T	316	Q6L	1	0
7	T	318	IWJ	1	0
3	S	304	CHL	2	0
3	S	307	CHL	5	0
2	S	310	CLA	1	0
7	S	319	IWJ	1	0

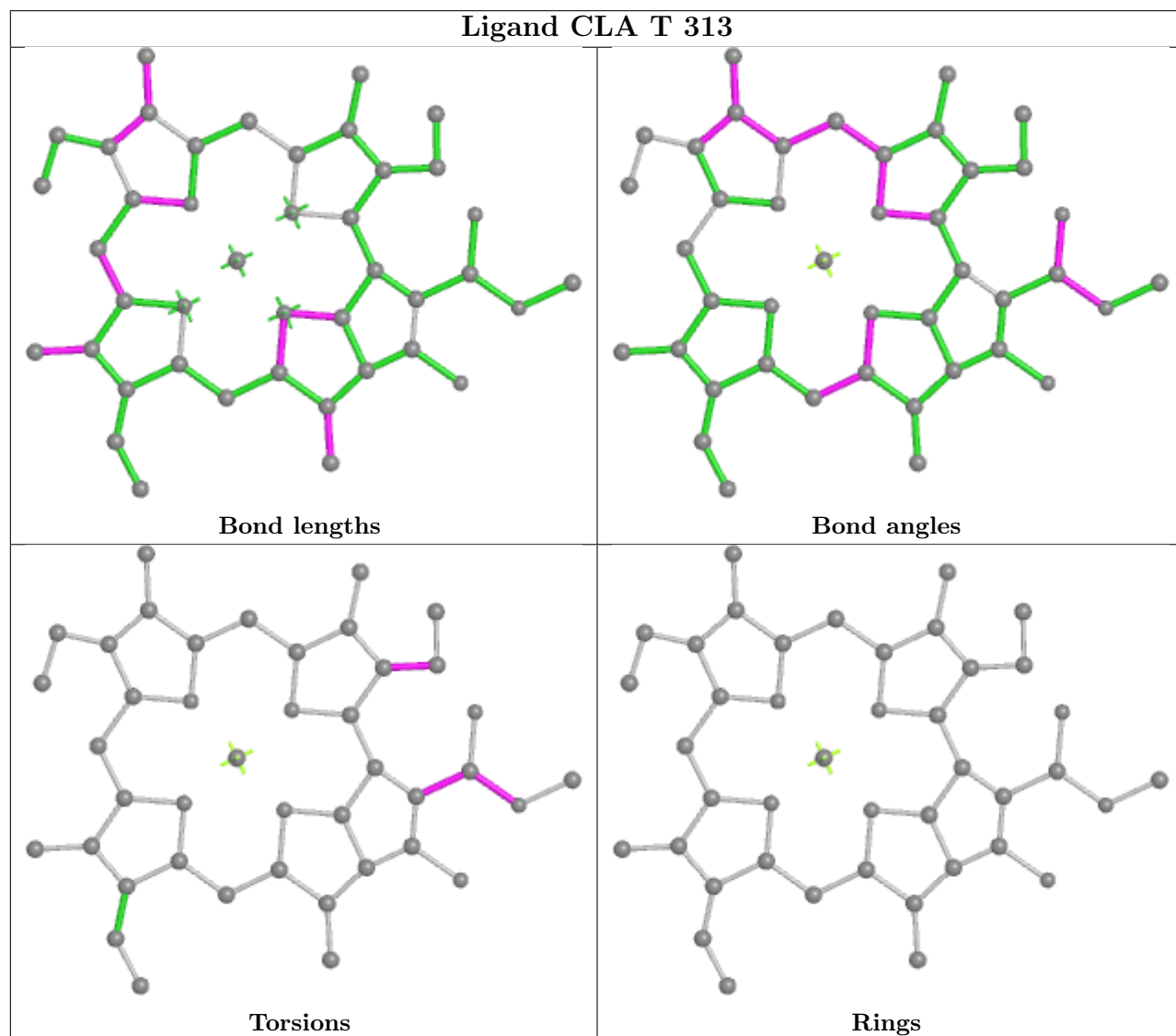
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



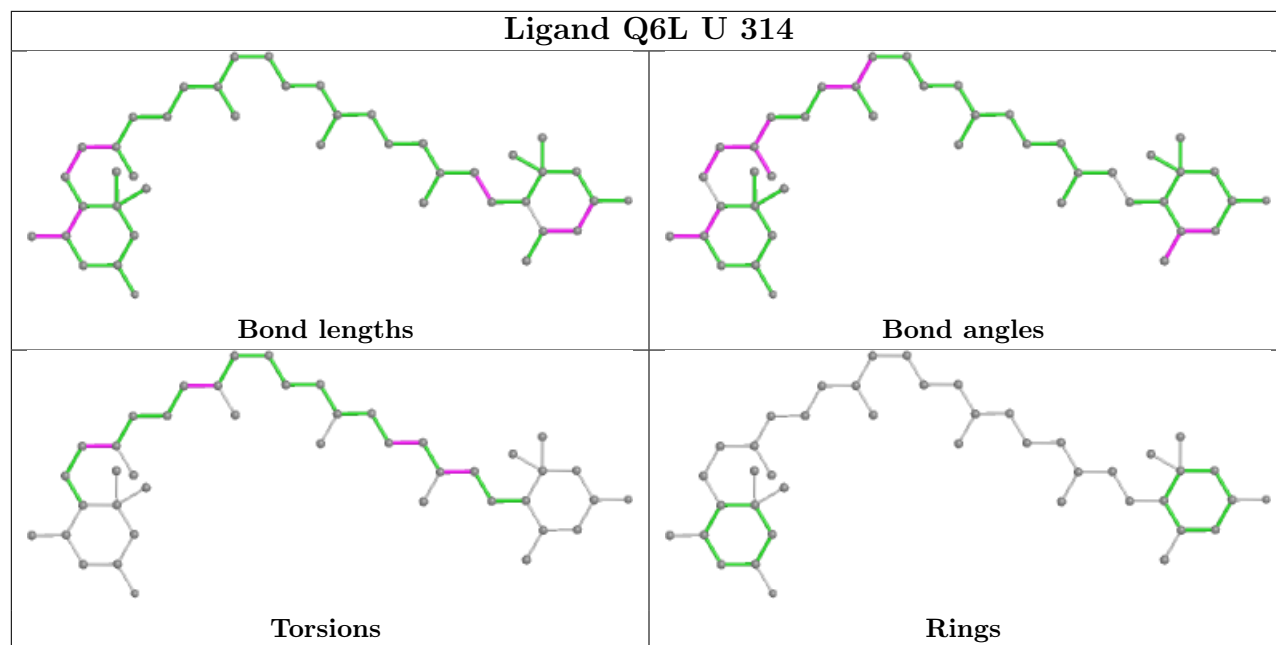
## Ligand IWJ U 316



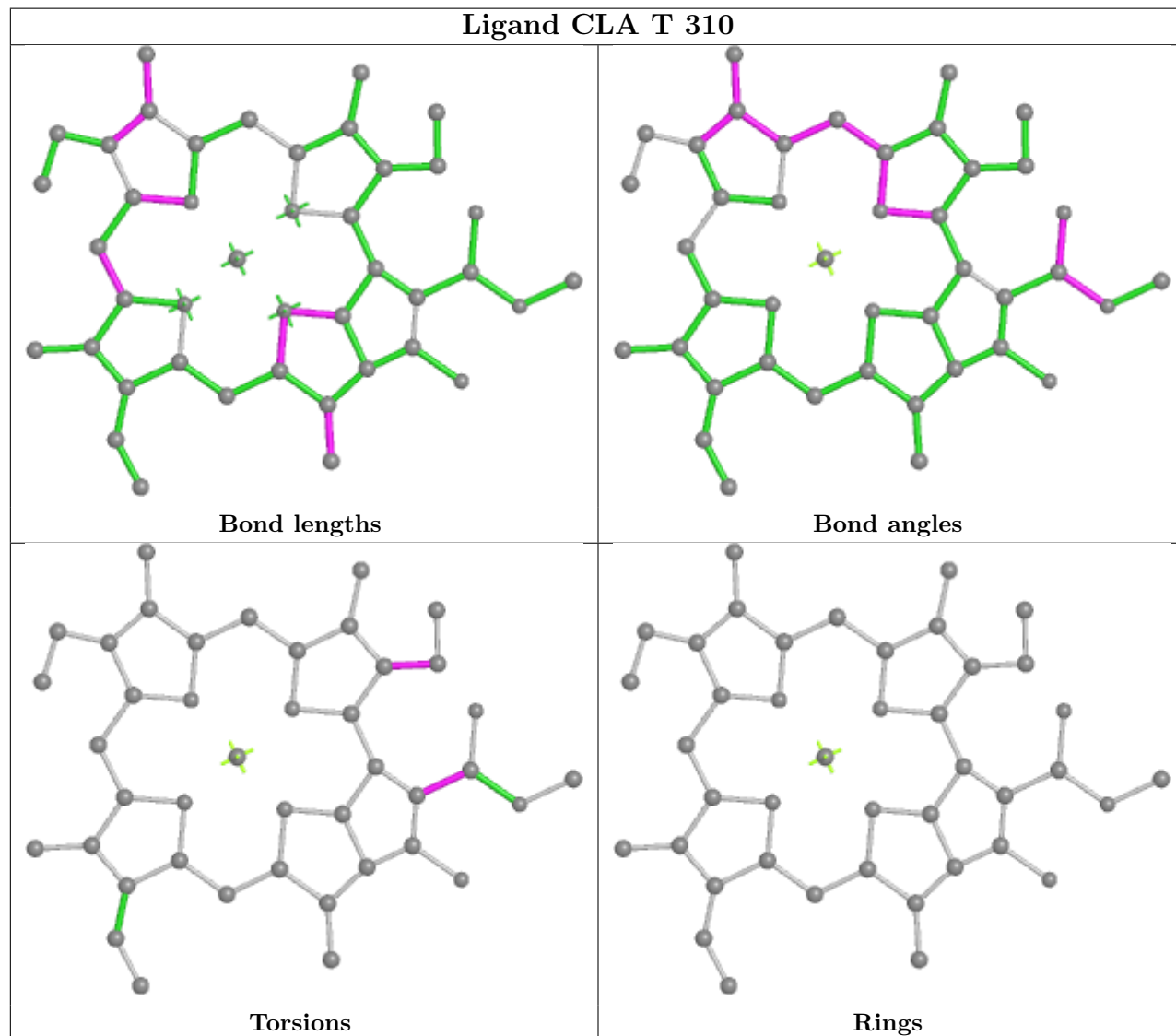
## Ligand CLA T 313



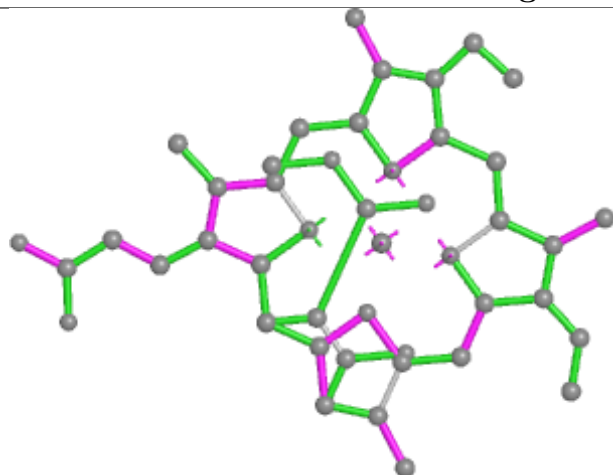
## Ligand Q6L U 314



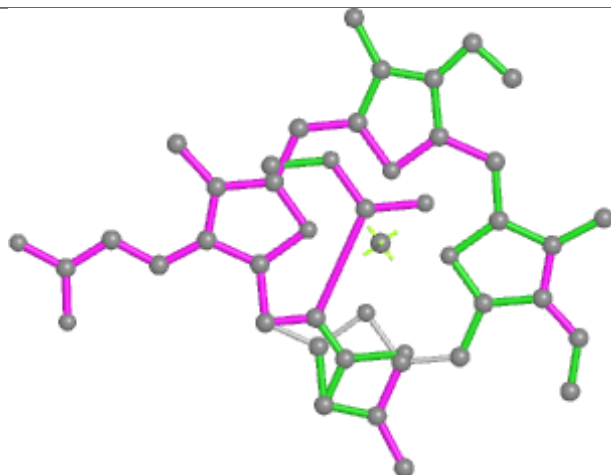
## Ligand CLA T 310



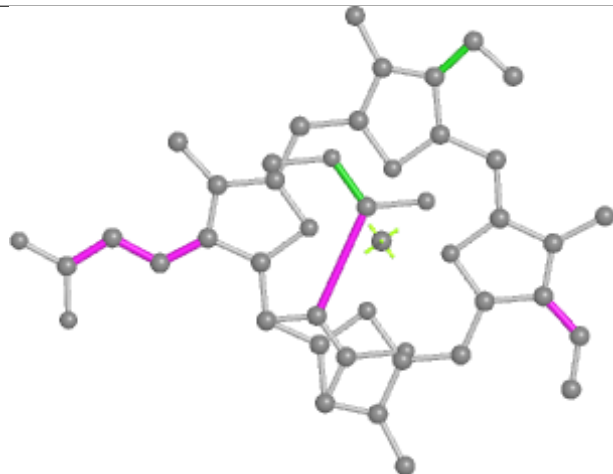
## Ligand KC2 S 308



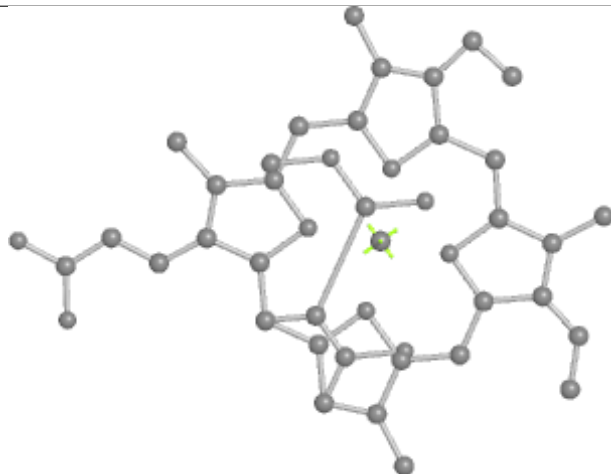
Bond lengths



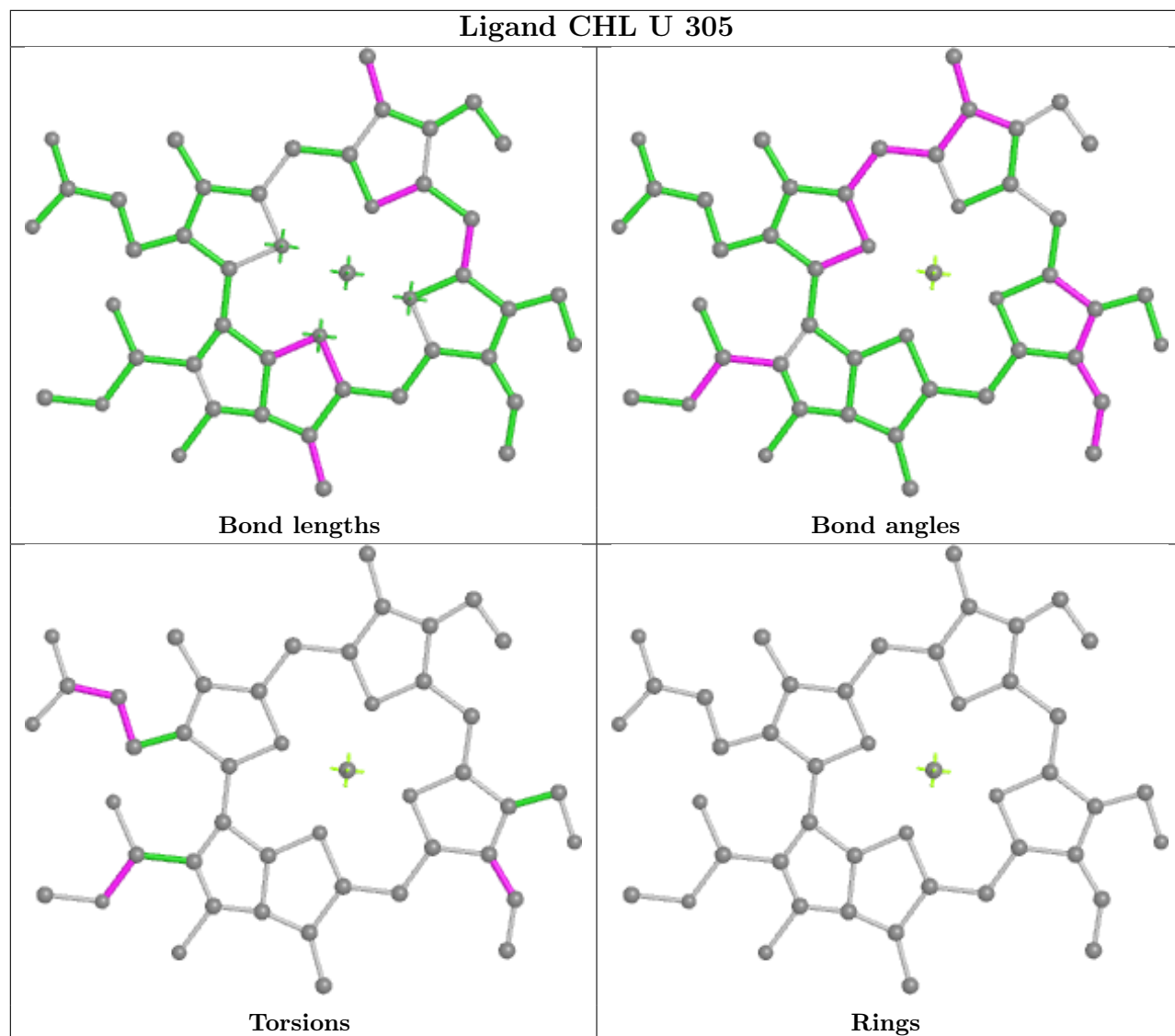
Bond angles



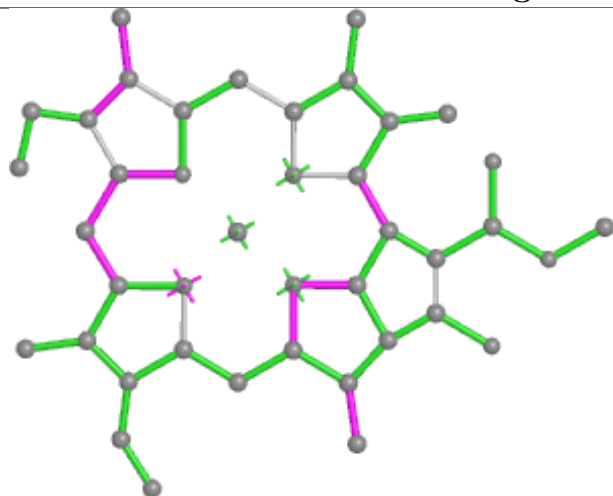
Torsions



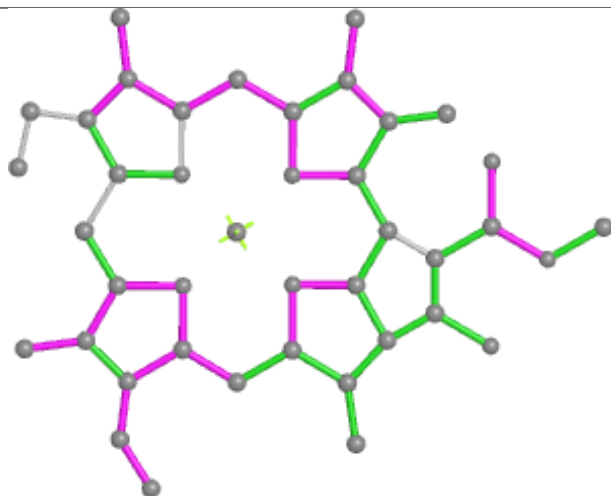
Rings



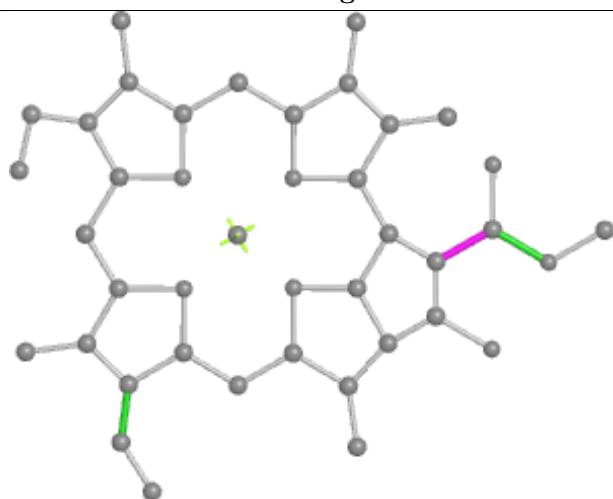
## Ligand CLA U 308



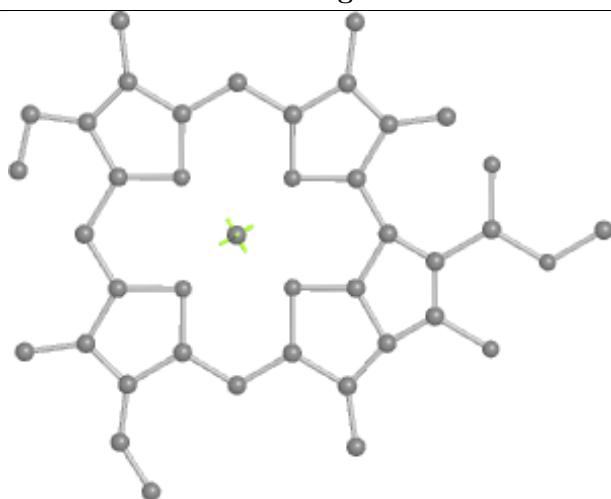
Bond lengths



Bond angles

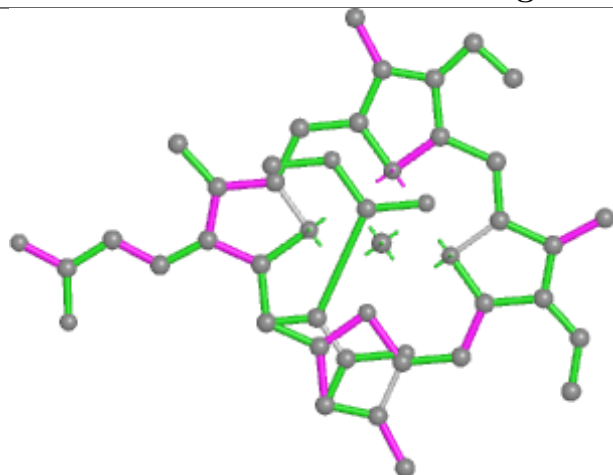


Torsions

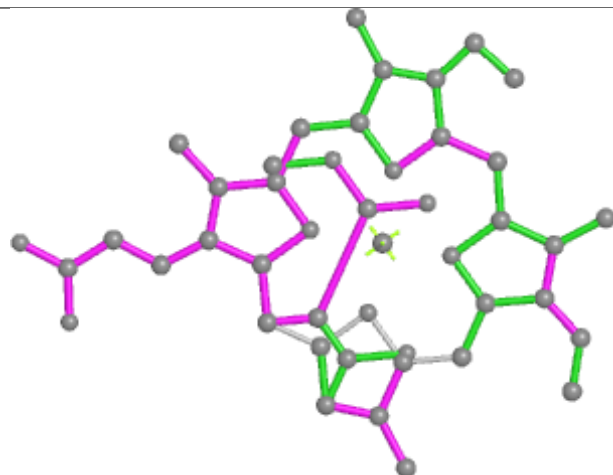


Rings

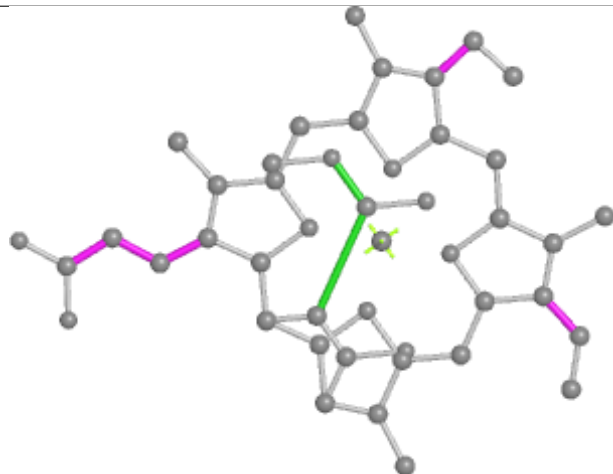
## Ligand KC2 T 308



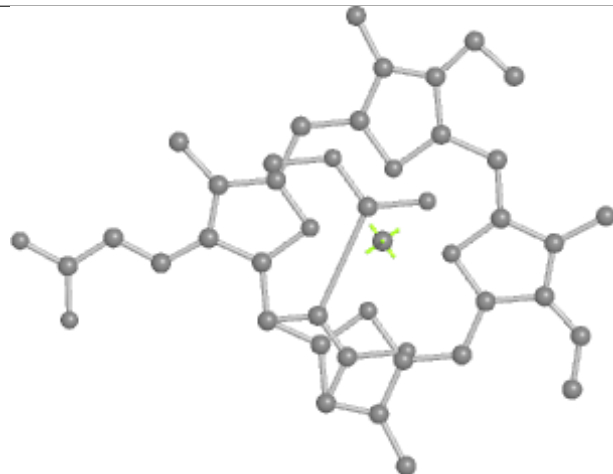
Bond lengths



Bond angles

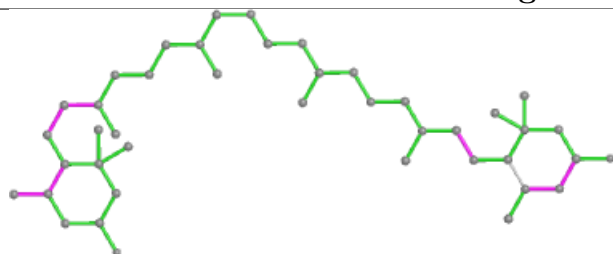


Torsions

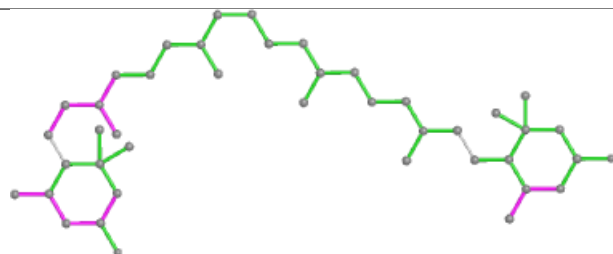


Rings

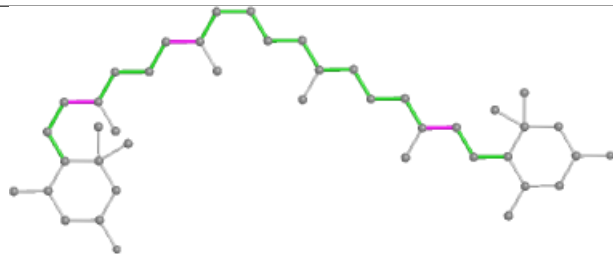
## Ligand Q6L T 315



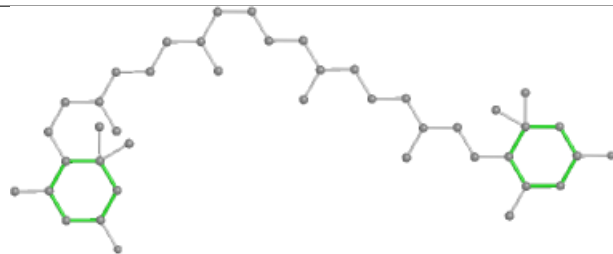
Bond lengths



Bond angles

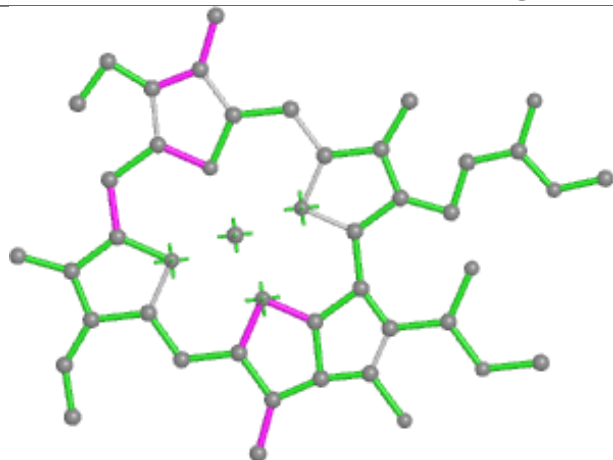


Torsions

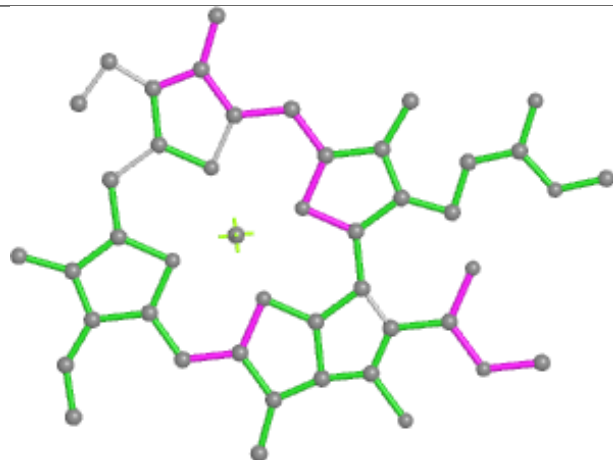


Rings

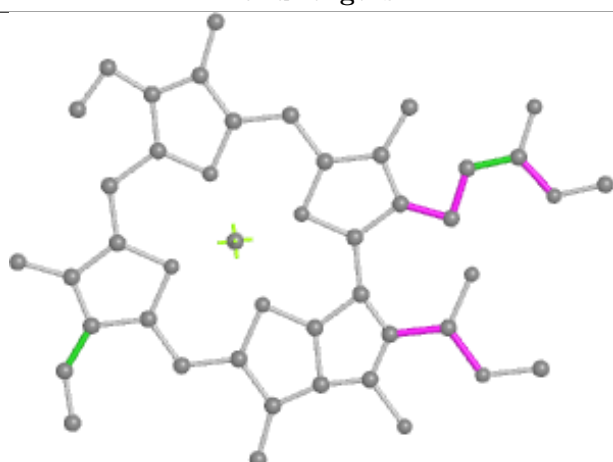
## Ligand CLA U 309



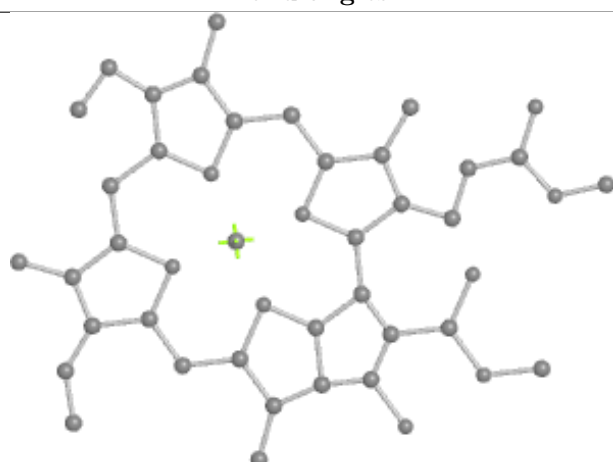
Bond lengths



Bond angles

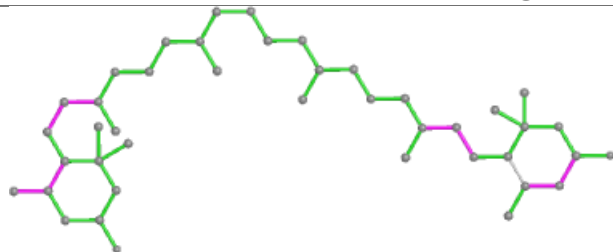


Torsions

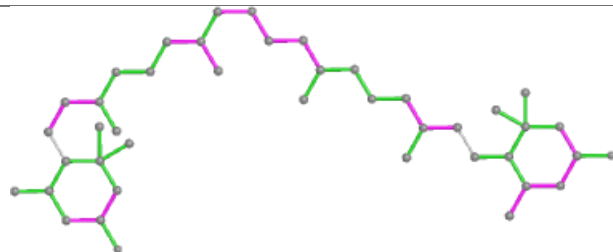


Rings

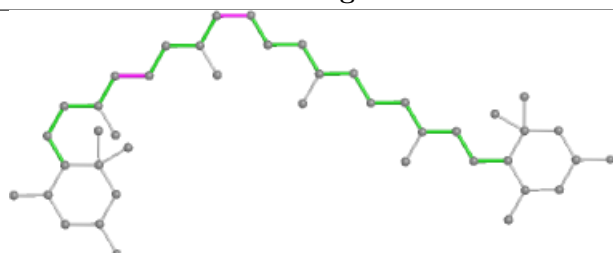
## Ligand Q6L U 315



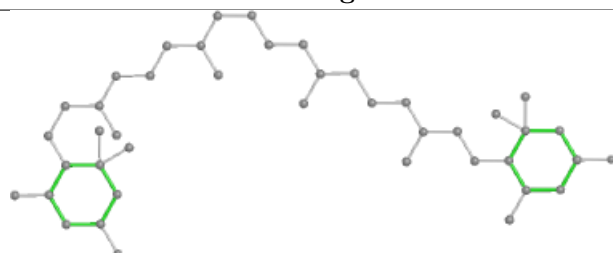
Bond lengths



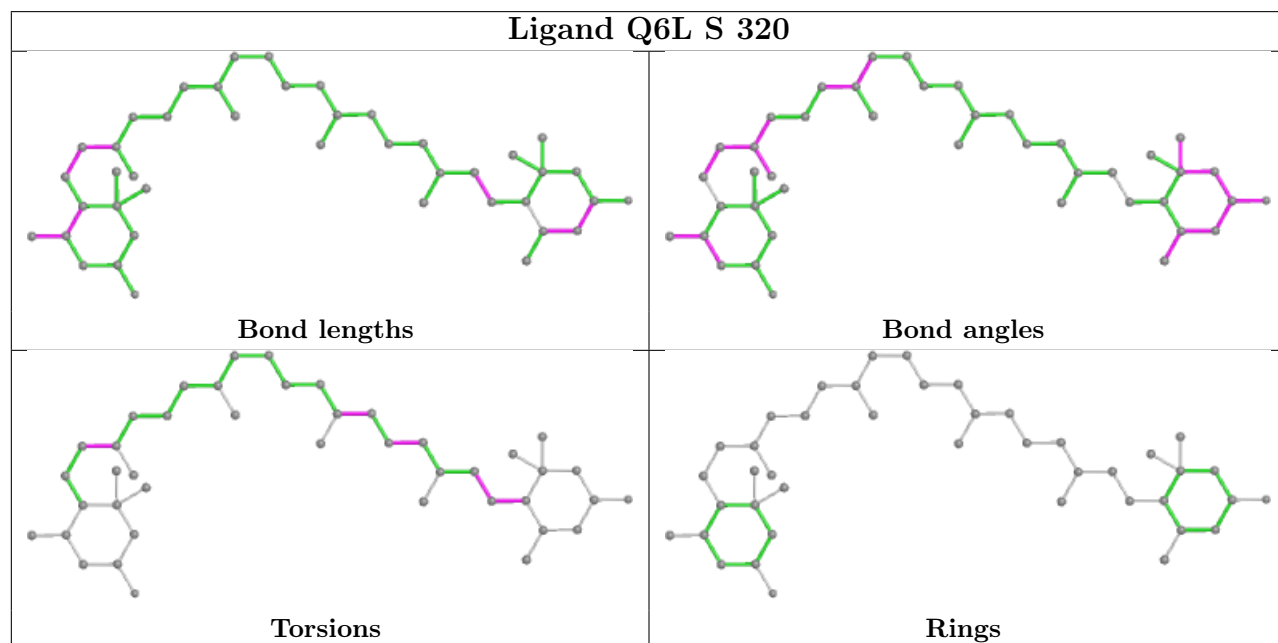
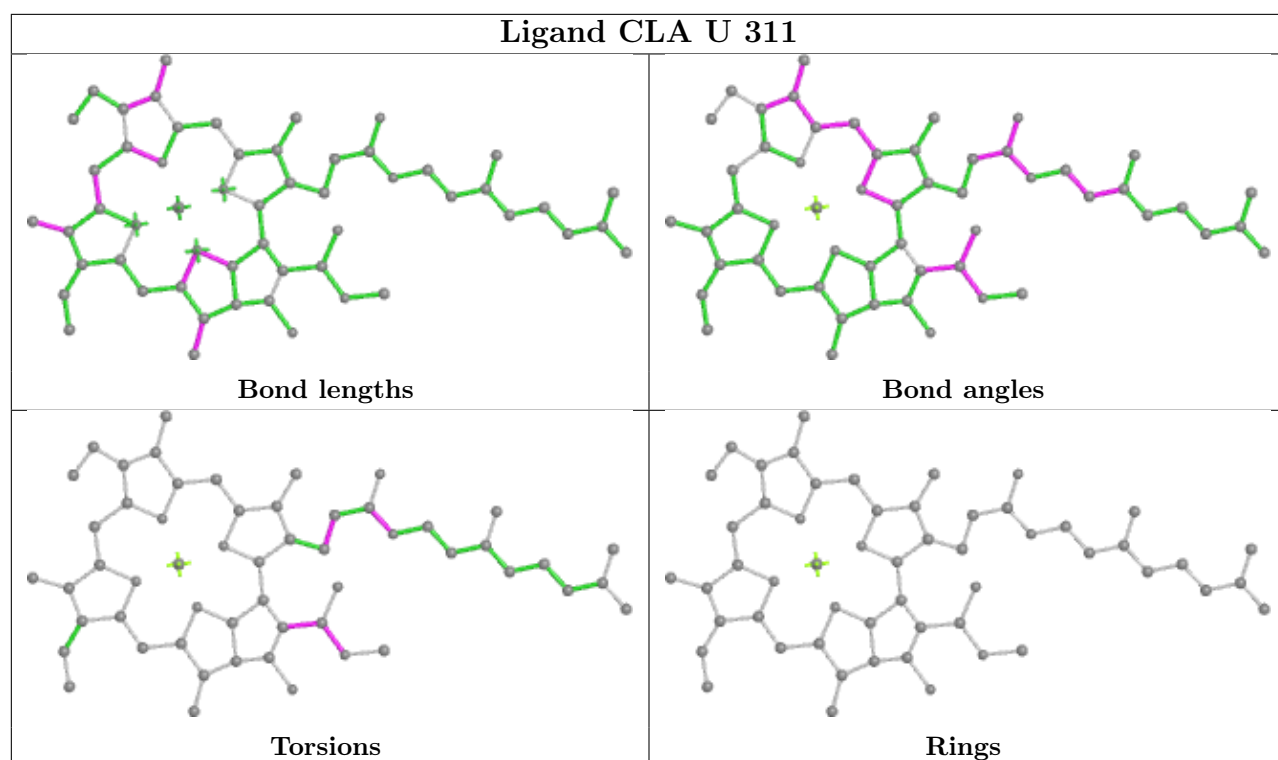
Bond angles



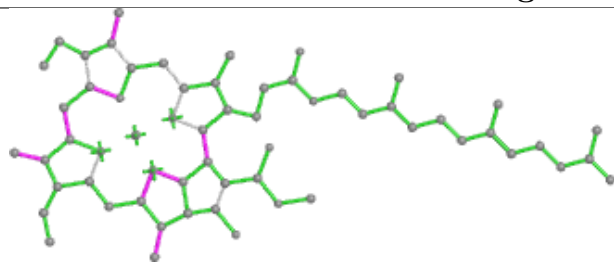
Torsions



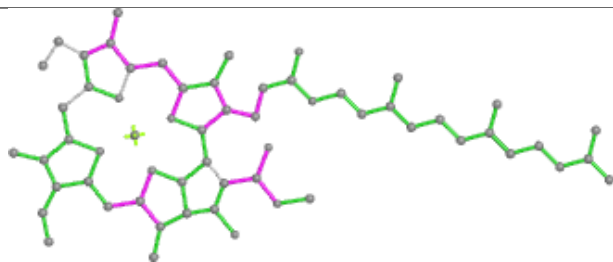
Rings



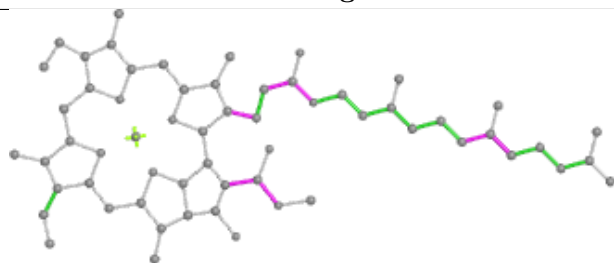
## Ligand CLA S 309



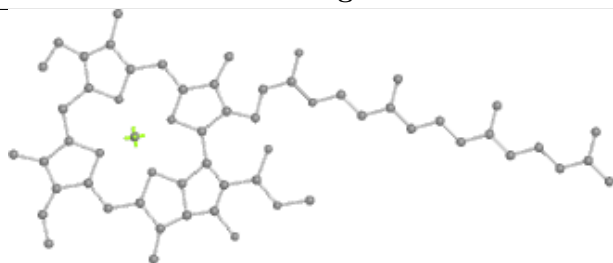
Bond lengths



Bond angles

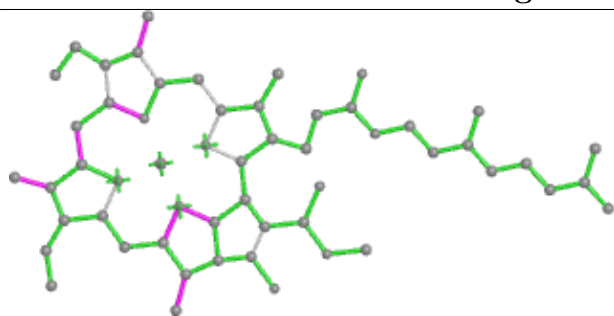


Torsions

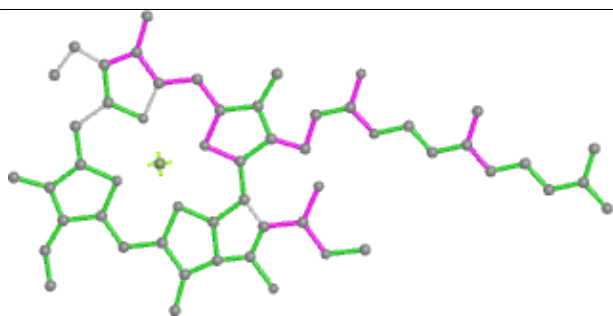


Rings

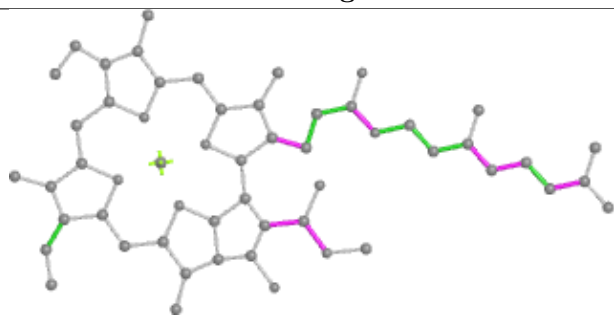
## Ligand CLA T 312



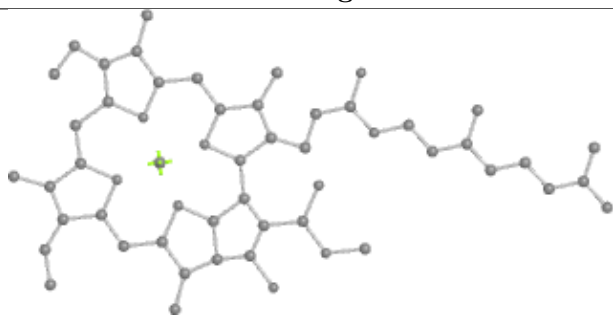
Bond lengths



Bond angles

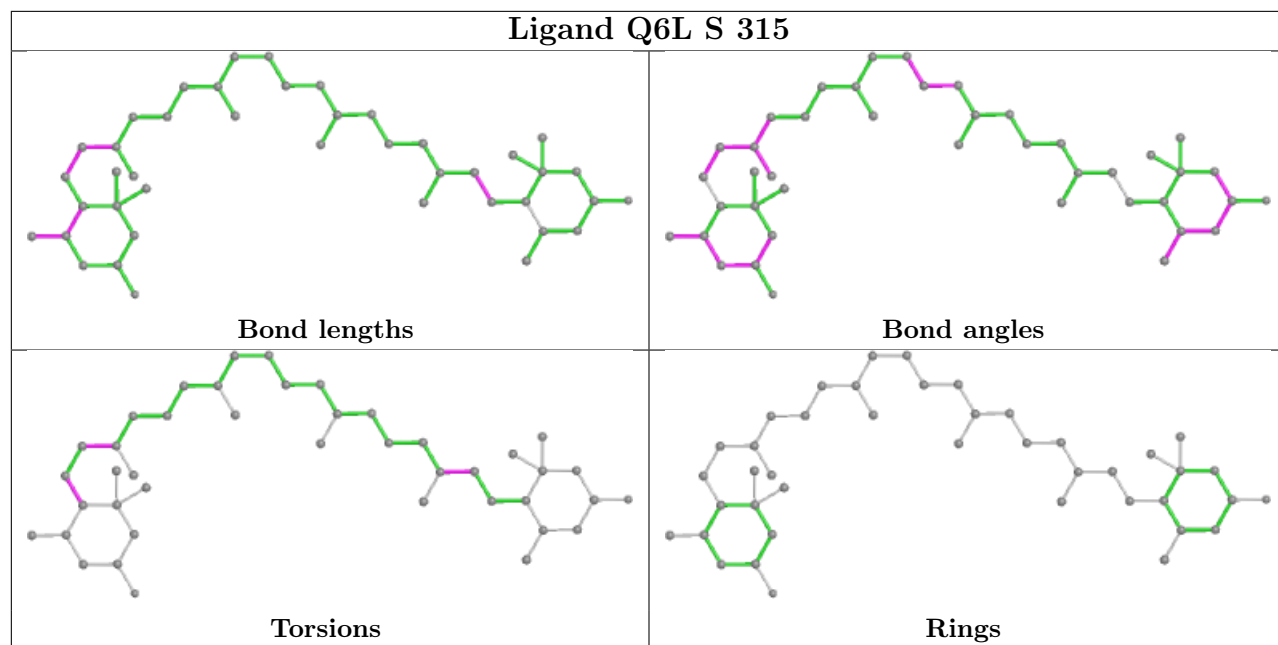


Torsions

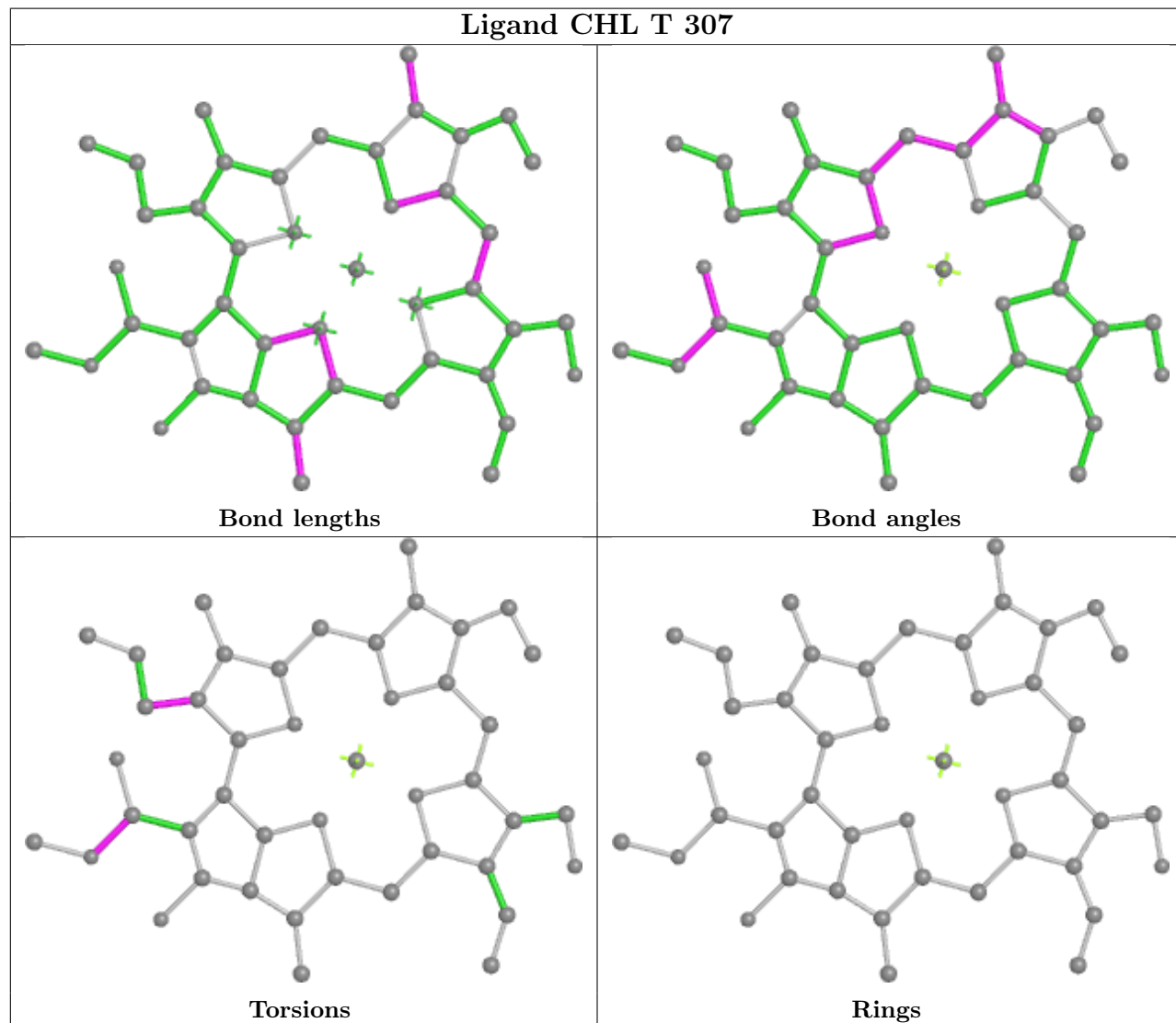


Rings

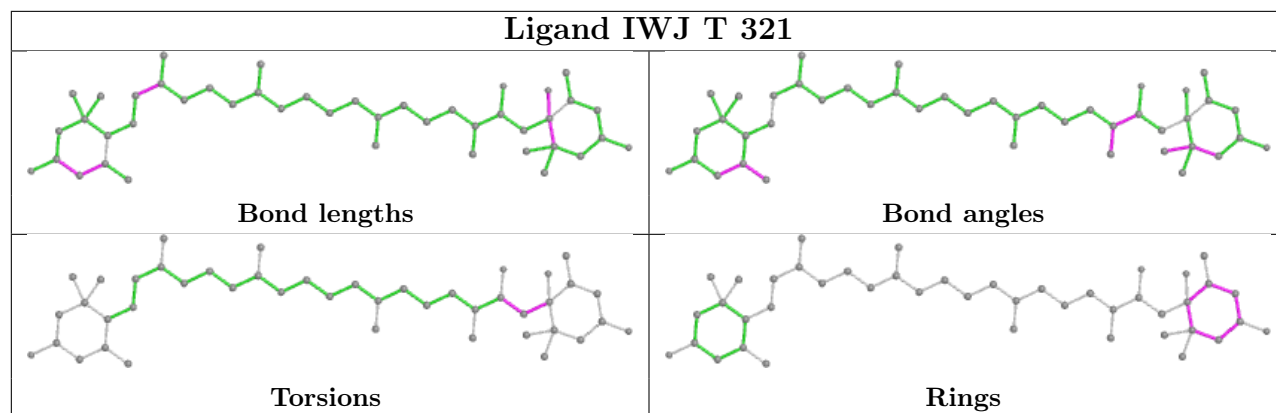
## Ligand Q6L S 315



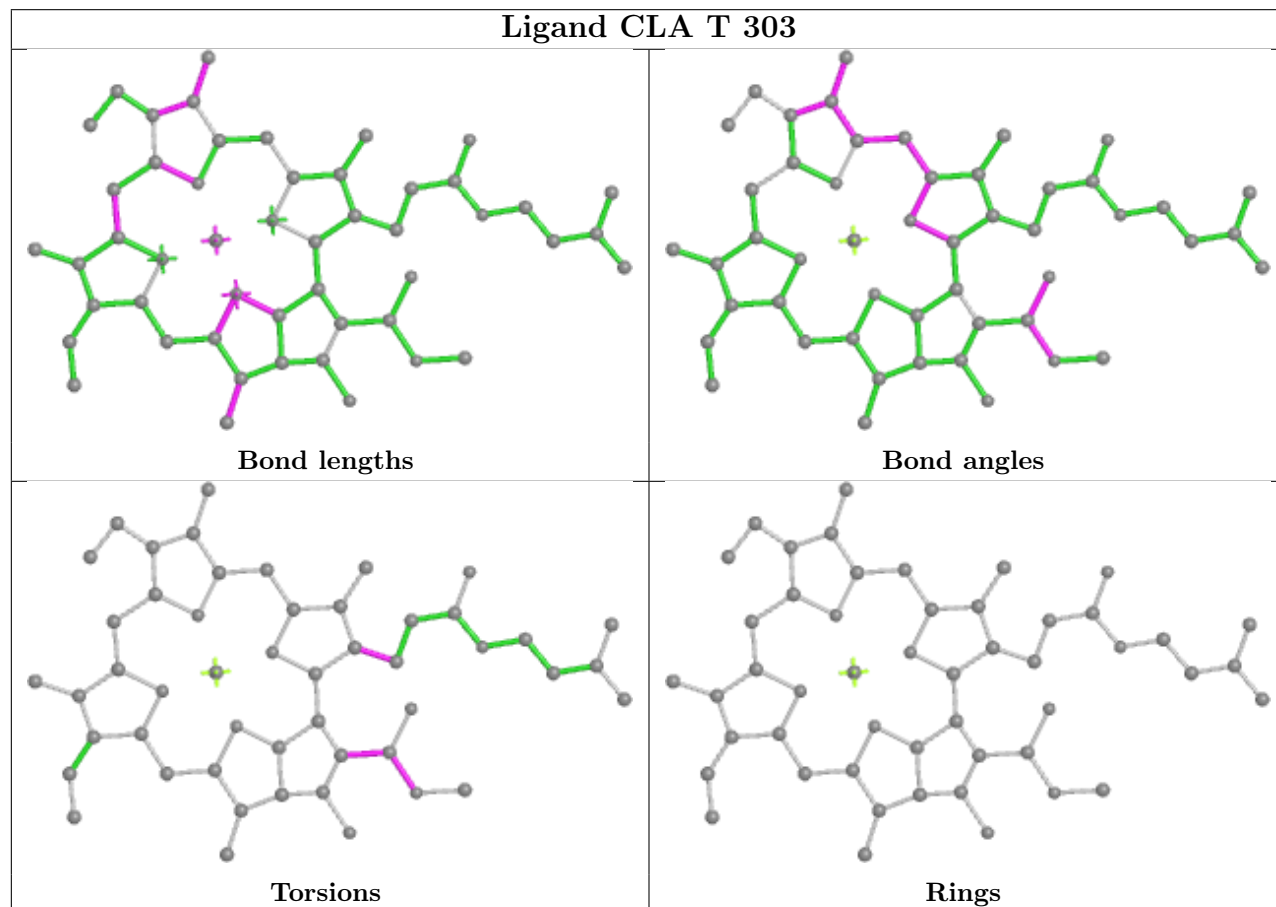
## Ligand CHL T 307



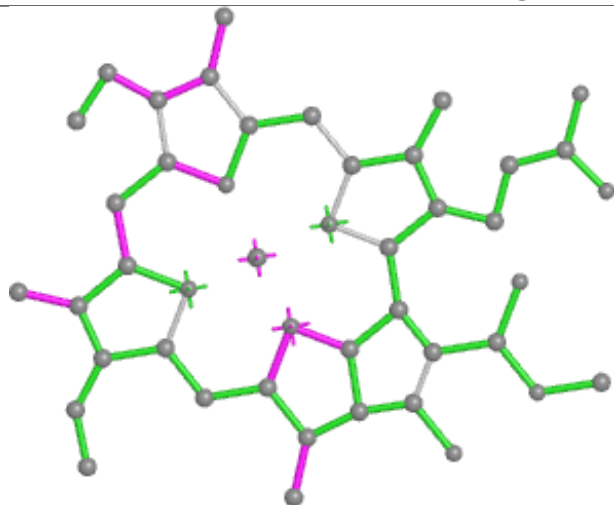
## Ligand IWJ T 321



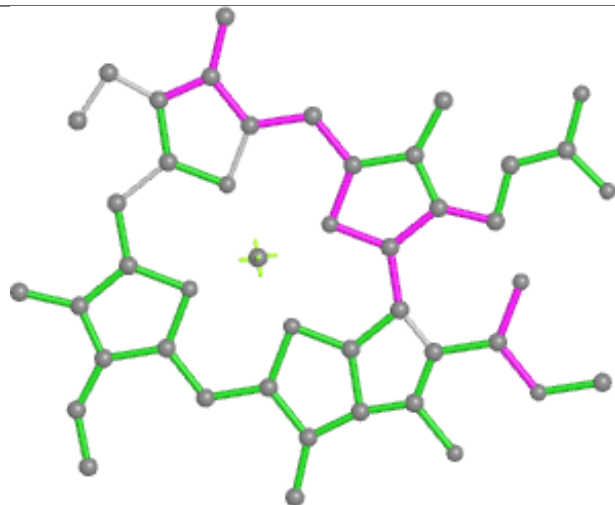
## Ligand CLA T 303



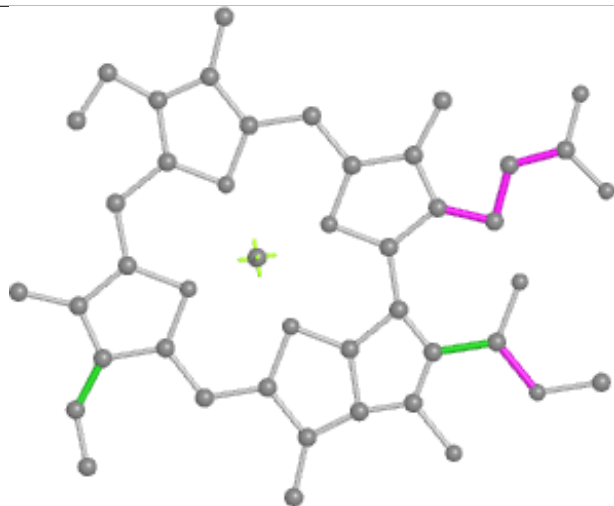
## Ligand CLA U 301



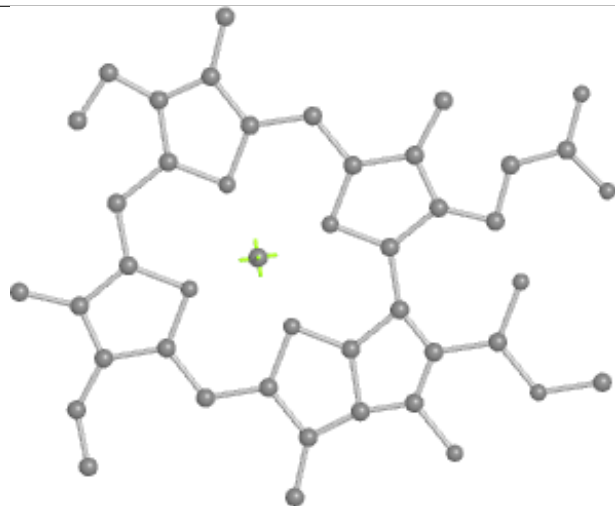
Bond lengths



Bond angles

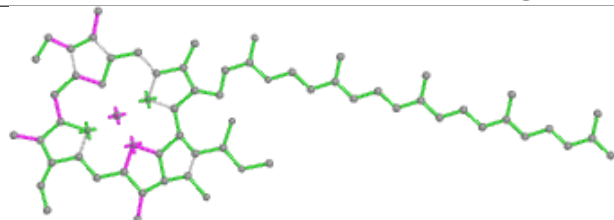


Torsions

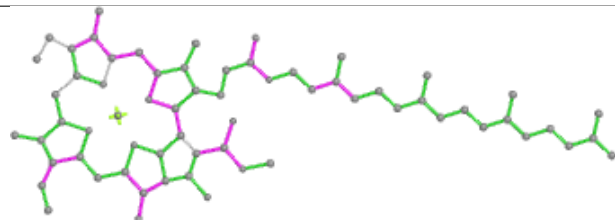


Rings

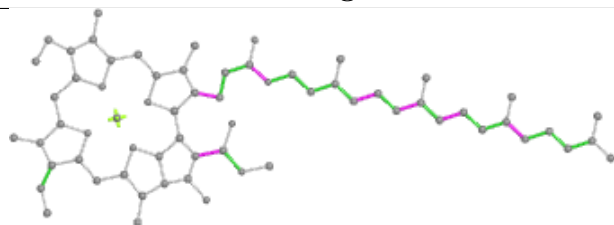
## Ligand CLA S 301



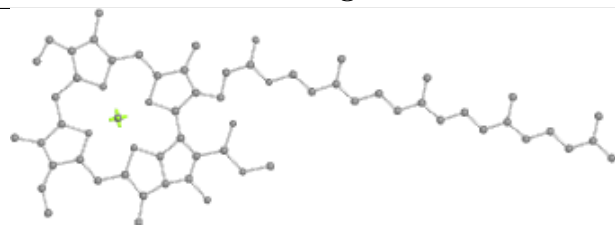
Bond lengths



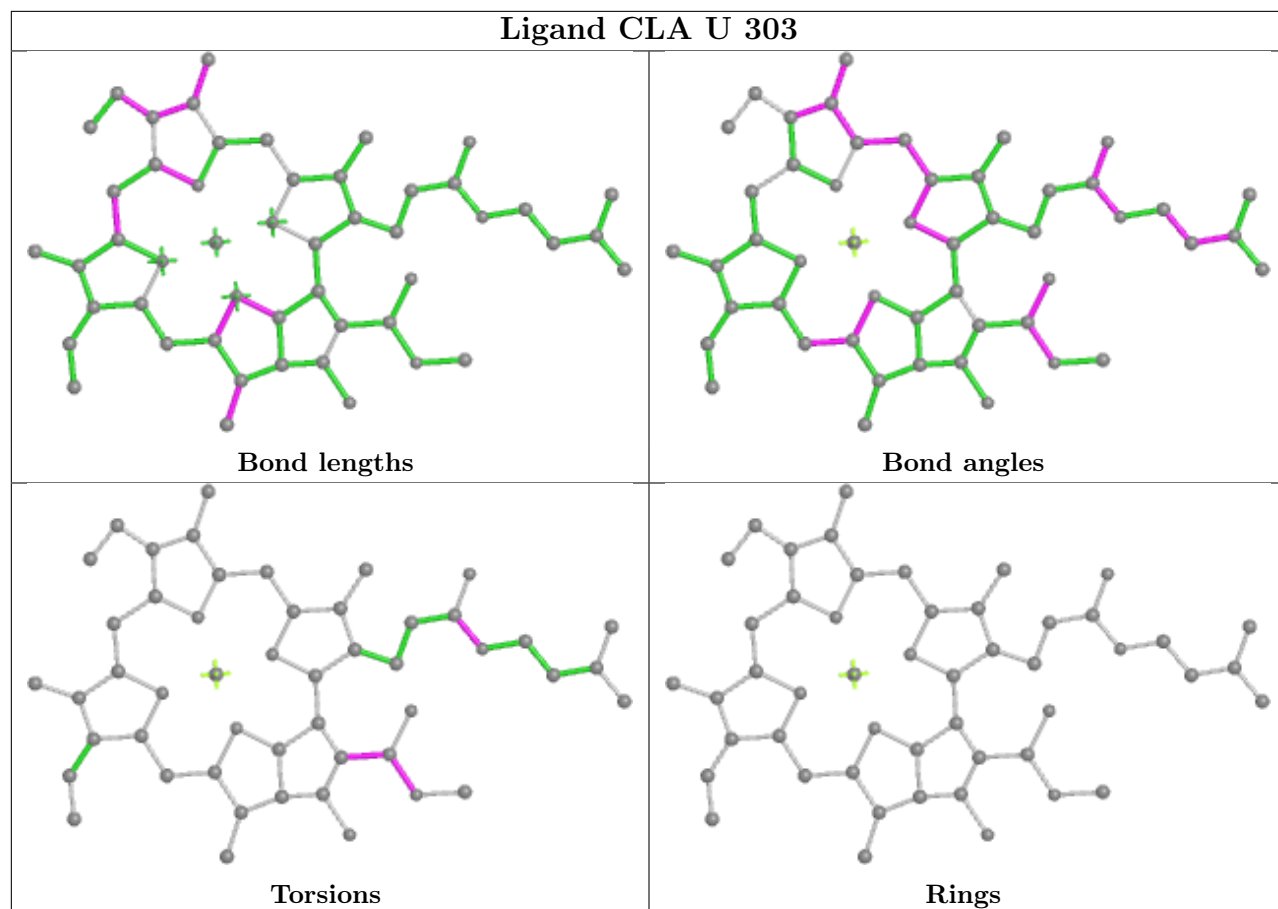
Bond angles



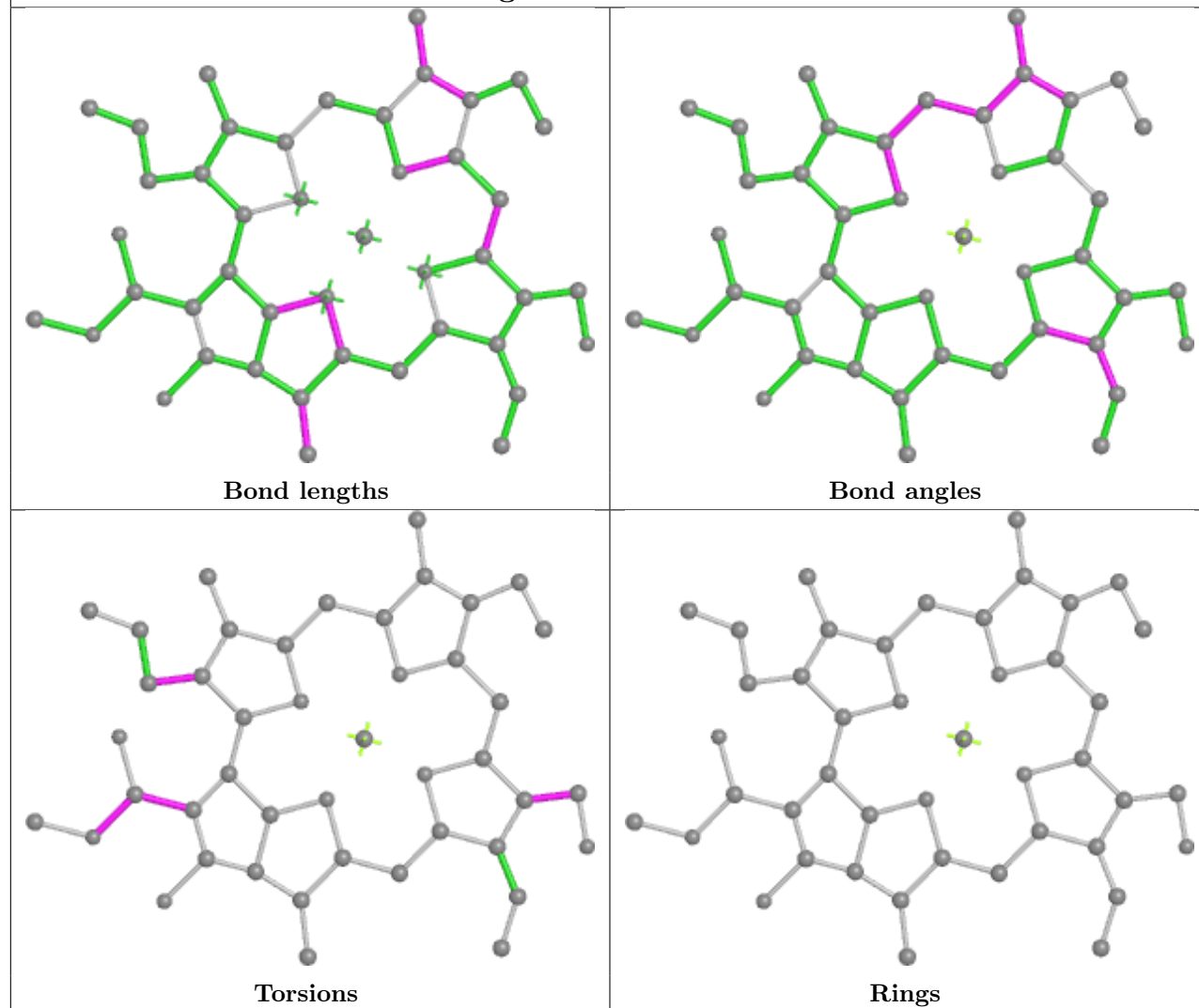
Torsions



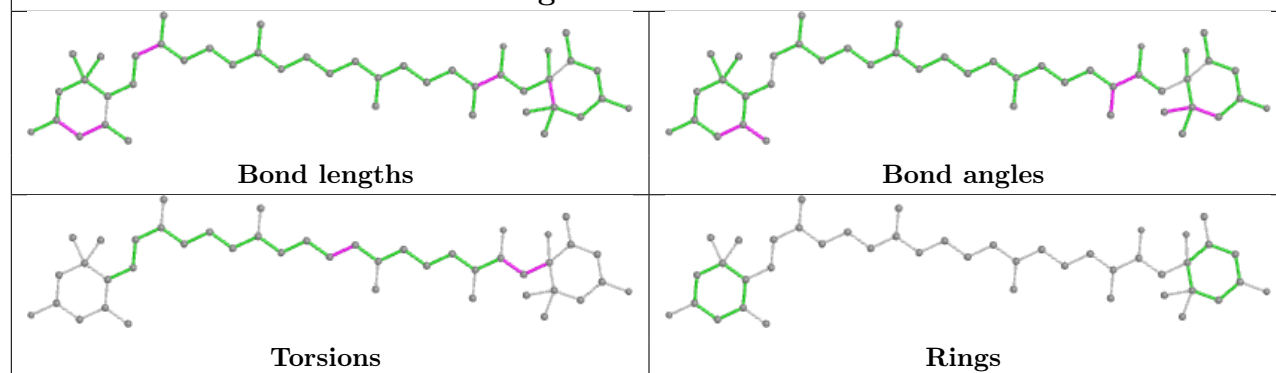
Rings



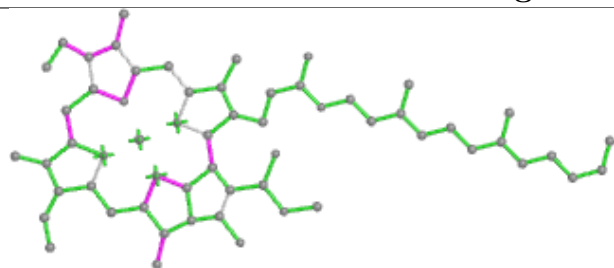
## Ligand CHL U 306



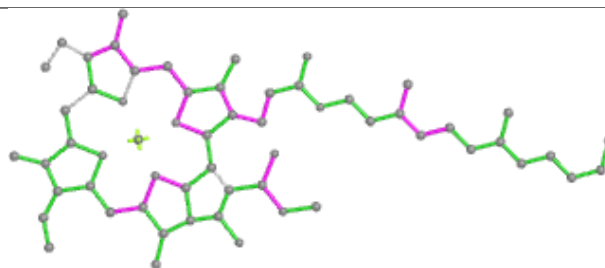
## Ligand IWJ S 322



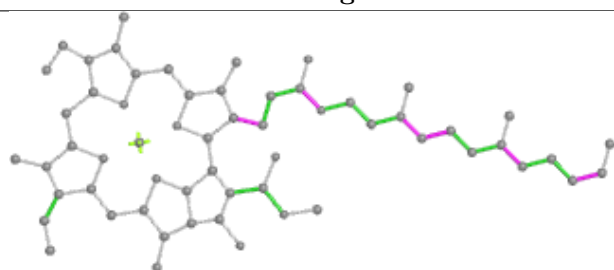
## Ligand CLA T 309



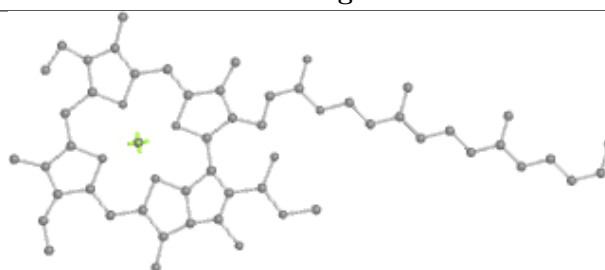
Bond lengths



Bond angles

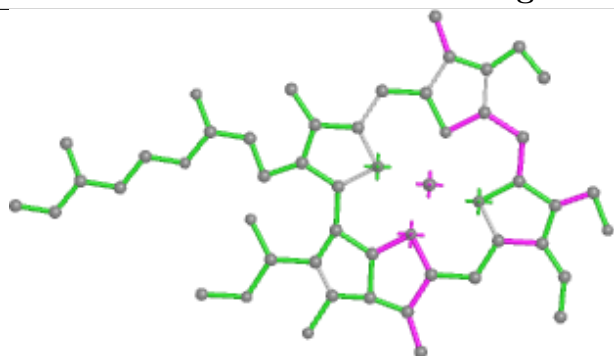


Torsions

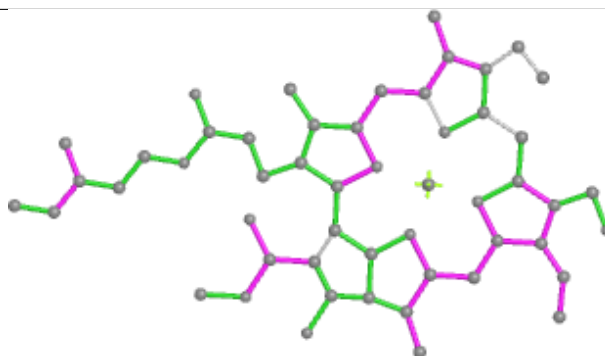


Rings

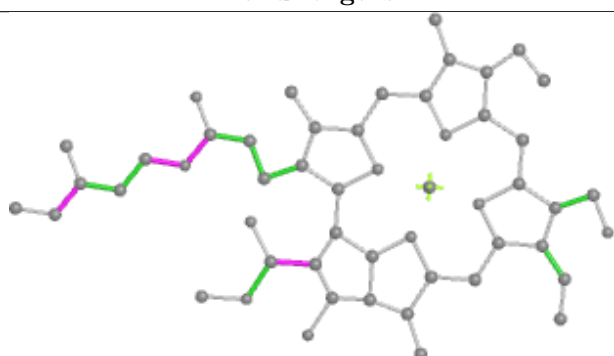
## Ligand CHL S 306



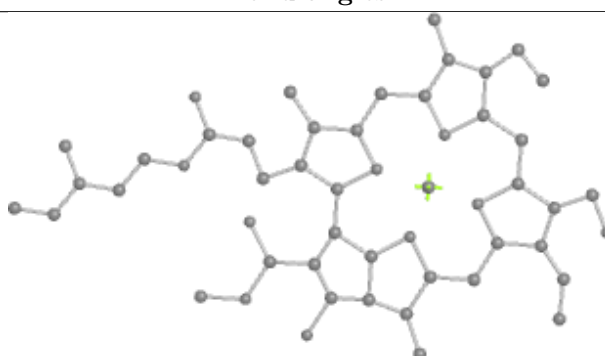
Bond lengths



Bond angles

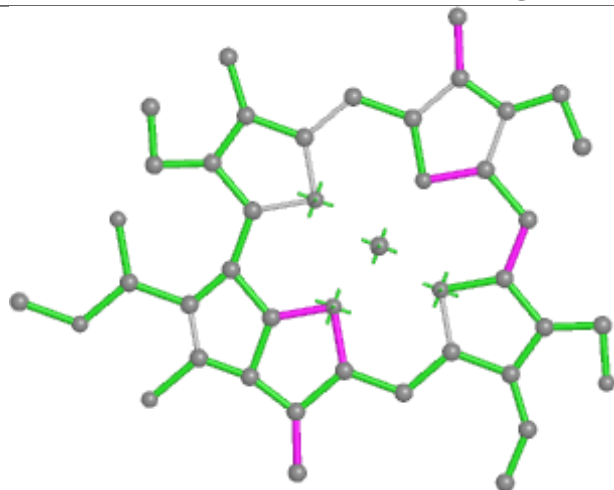


Torsions

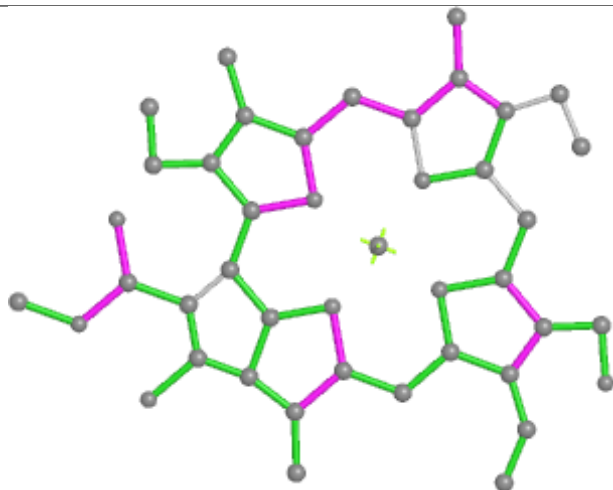


Rings

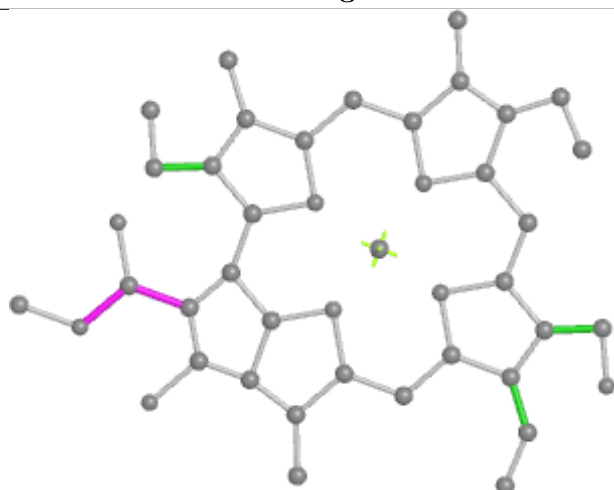
## Ligand CHL U 313



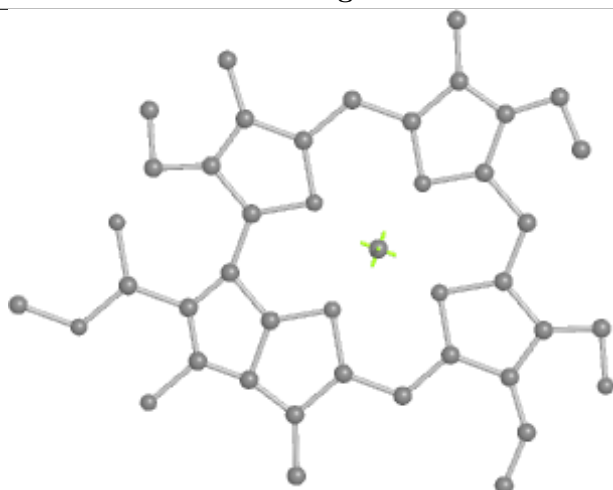
Bond lengths



Bond angles

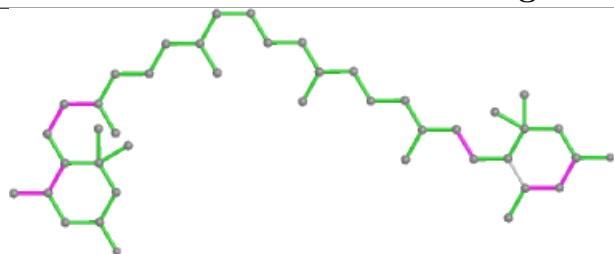


Torsions

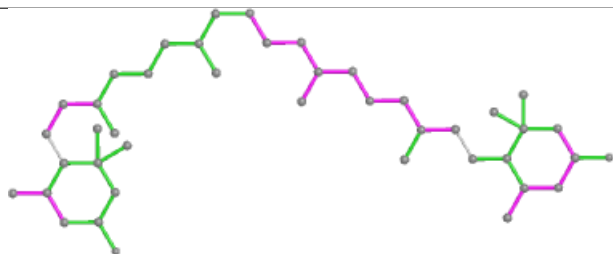


Rings

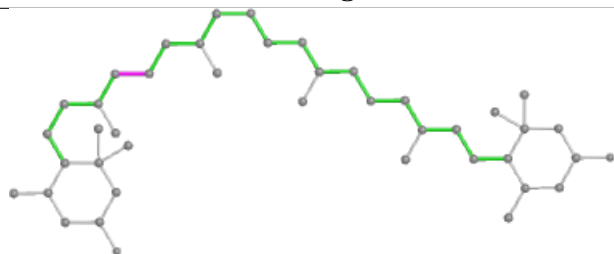
## Ligand Q6L T 316



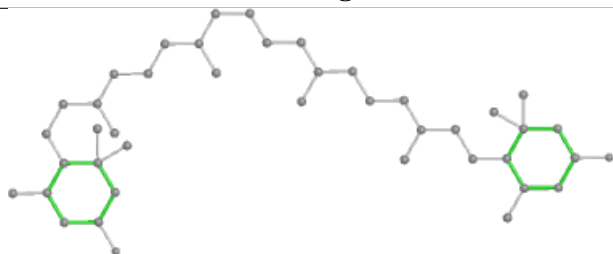
Bond lengths



Bond angles

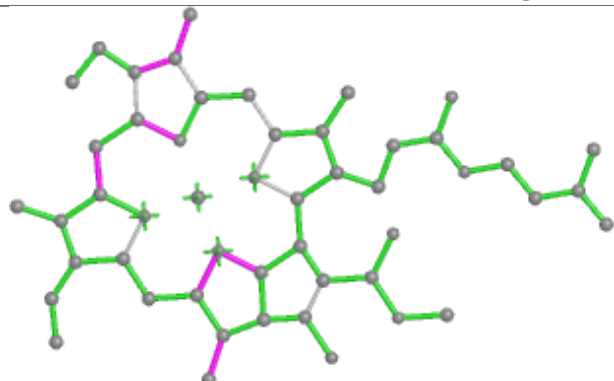


Torsions

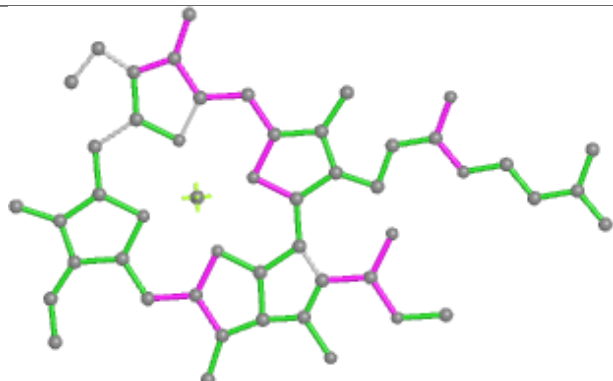


Rings

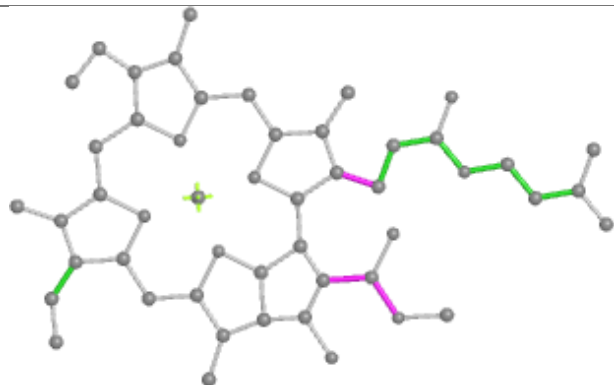
## Ligand CLA S 303



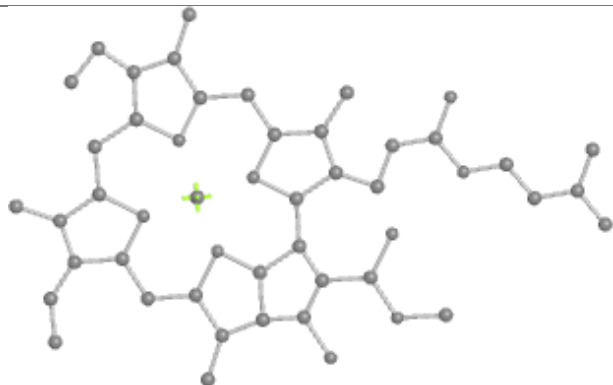
Bond lengths



Bond angles

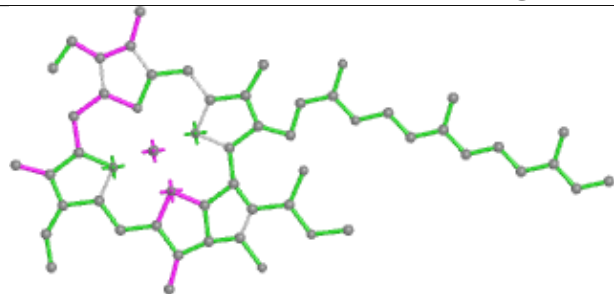


Torsions

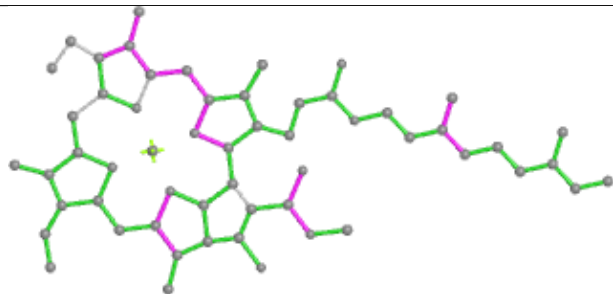


Rings

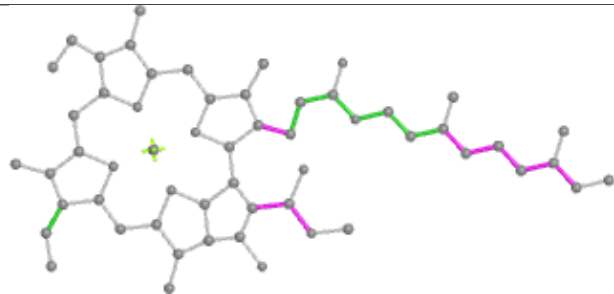
## Ligand CLA U 302



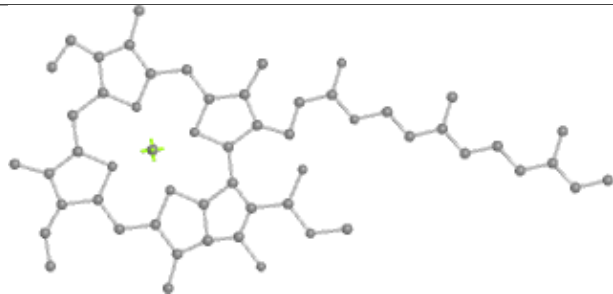
Bond lengths



Bond angles

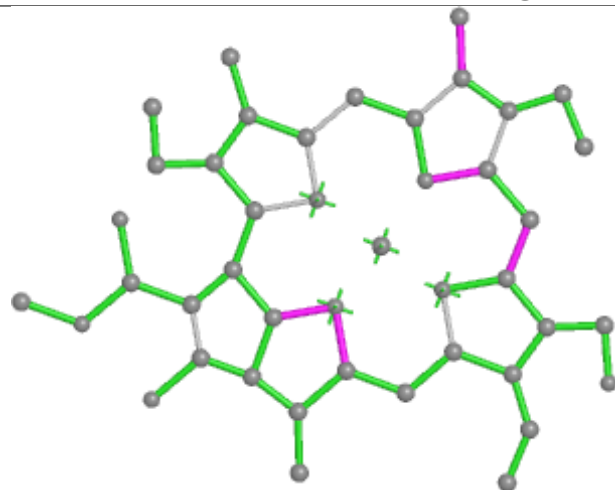


Torsions

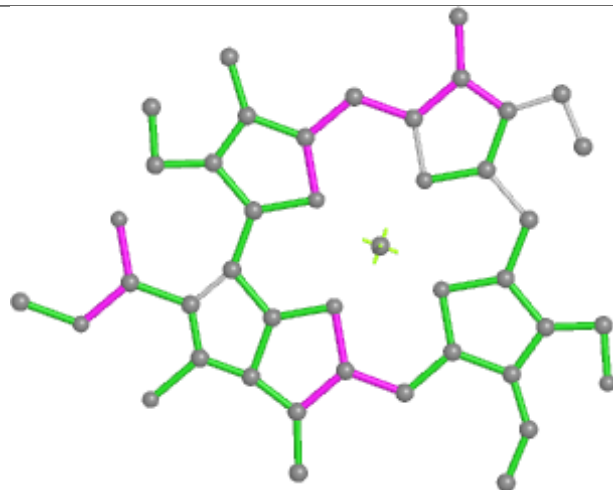


Rings

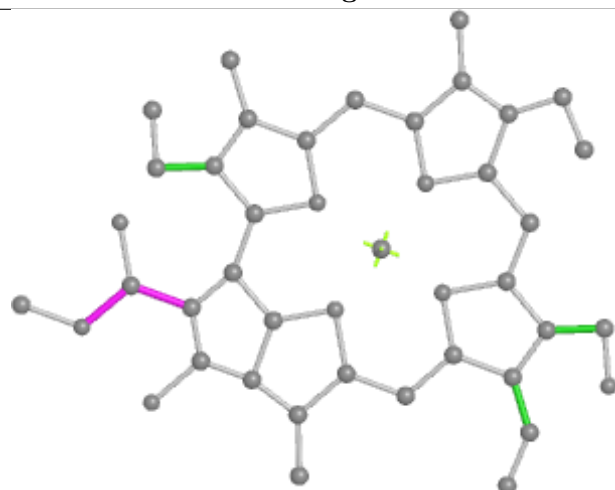
## Ligand CHL T 304



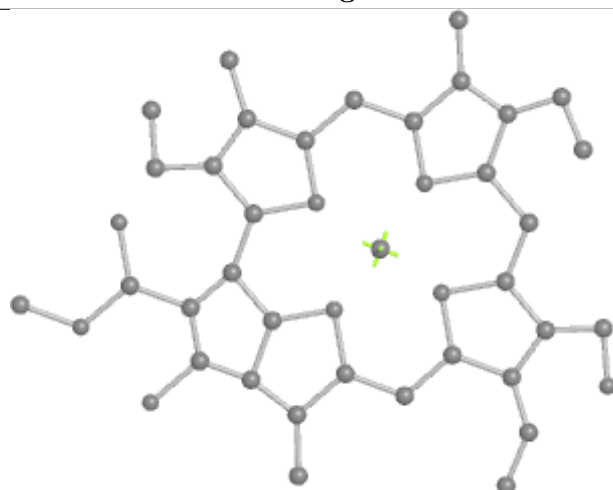
Bond lengths



Bond angles

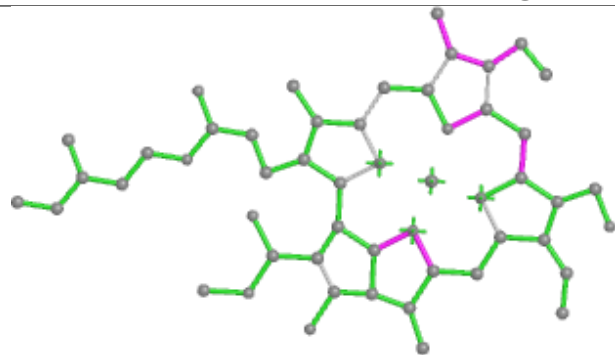


Torsions

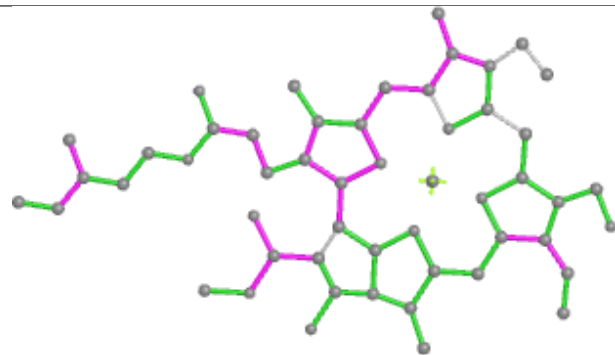


Rings

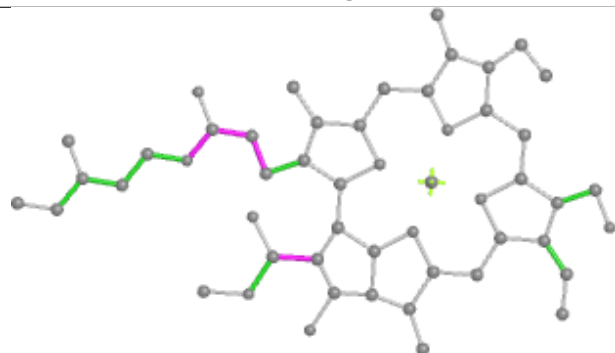
## Ligand CHL T 320



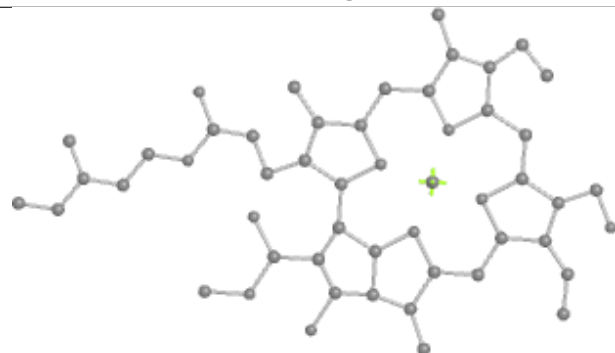
Bond lengths



Bond angles

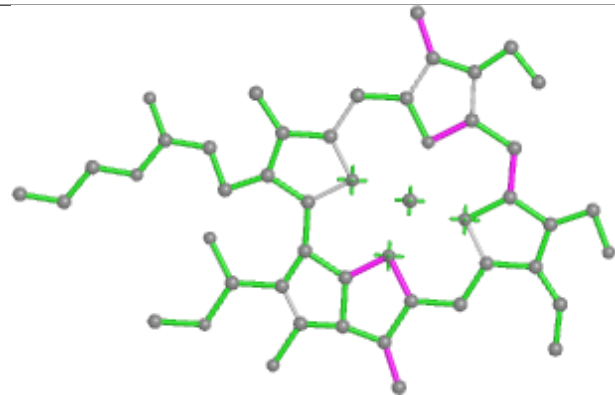


Torsions

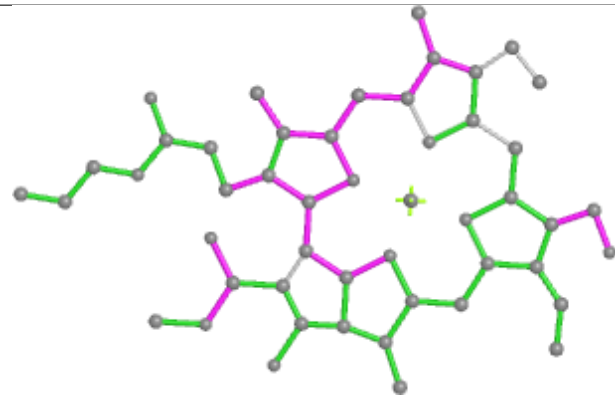


Rings

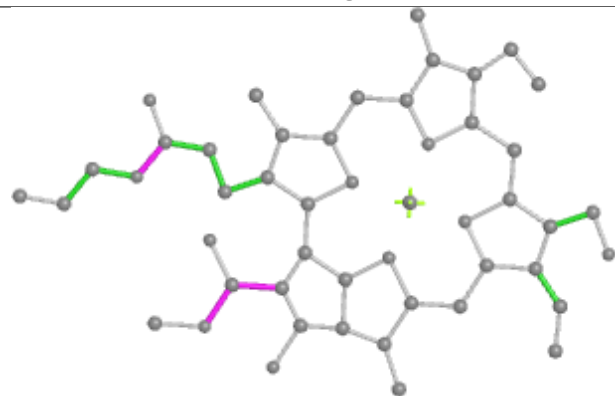
## Ligand CHL T 305



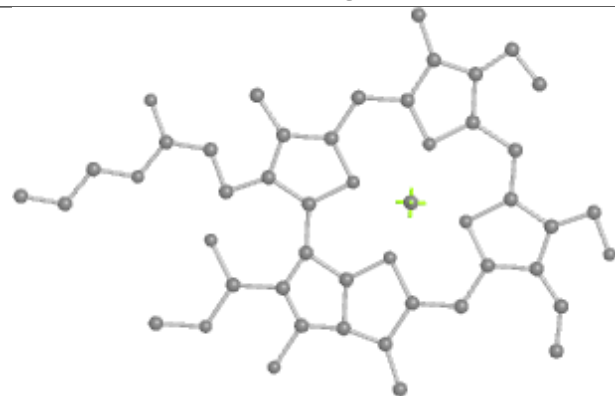
Bond lengths



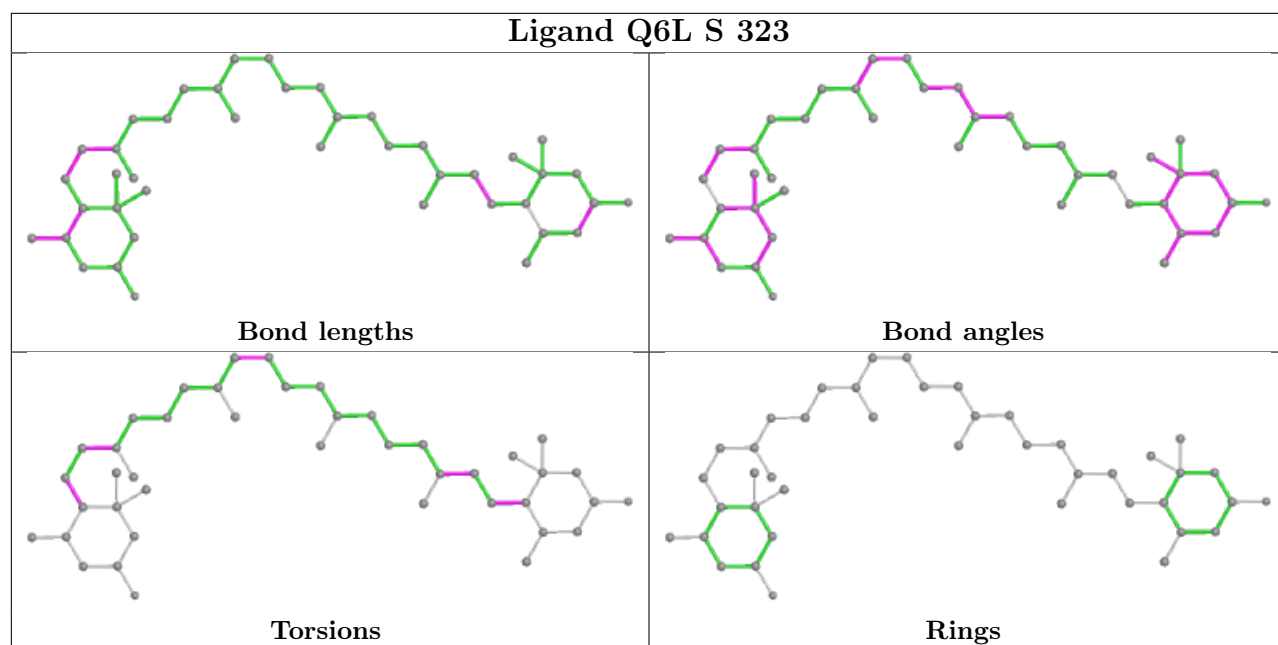
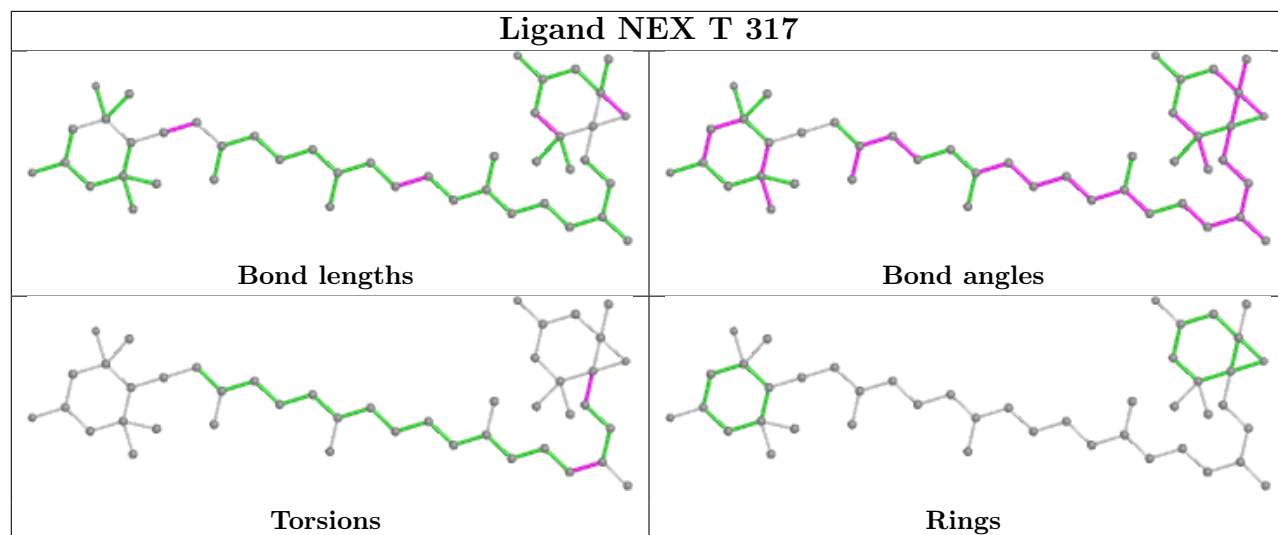
Bond angles

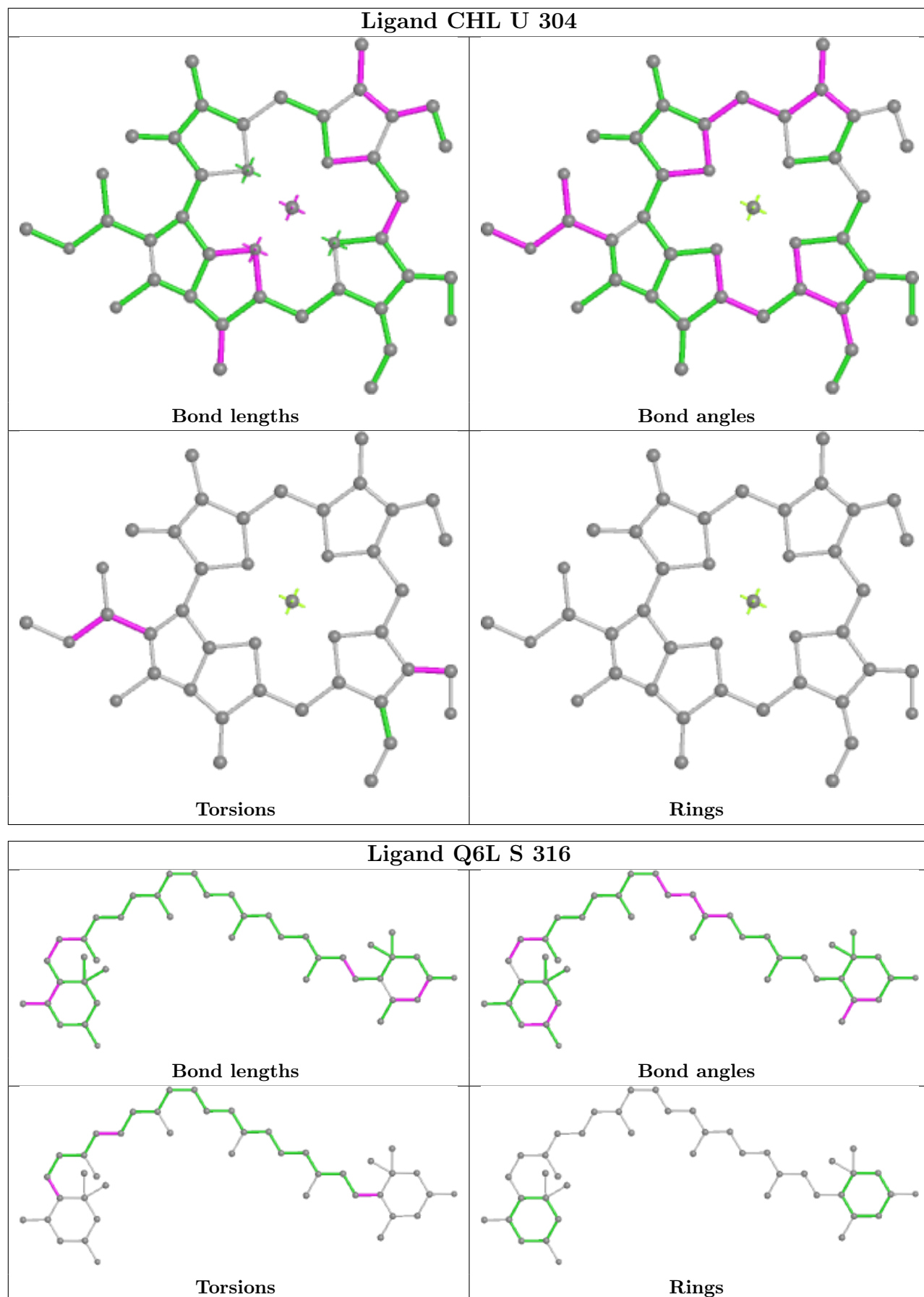


Torsions

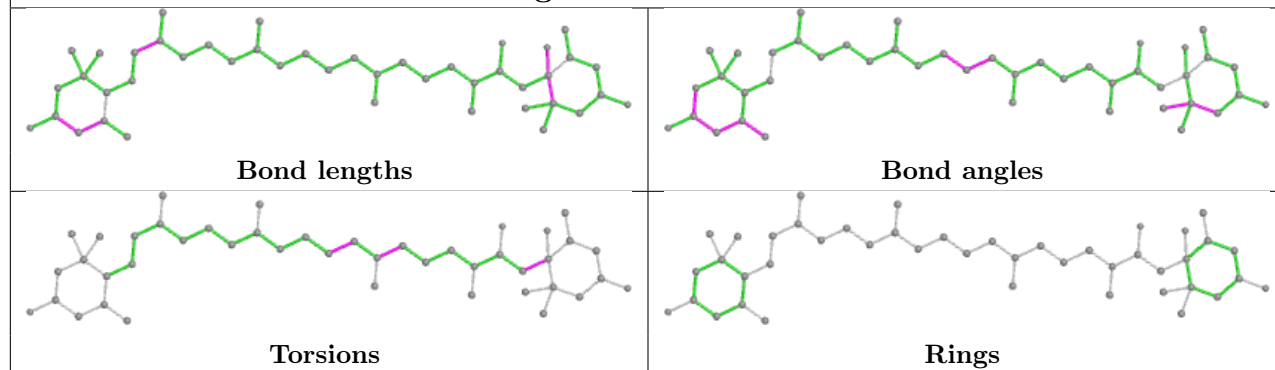


Rings

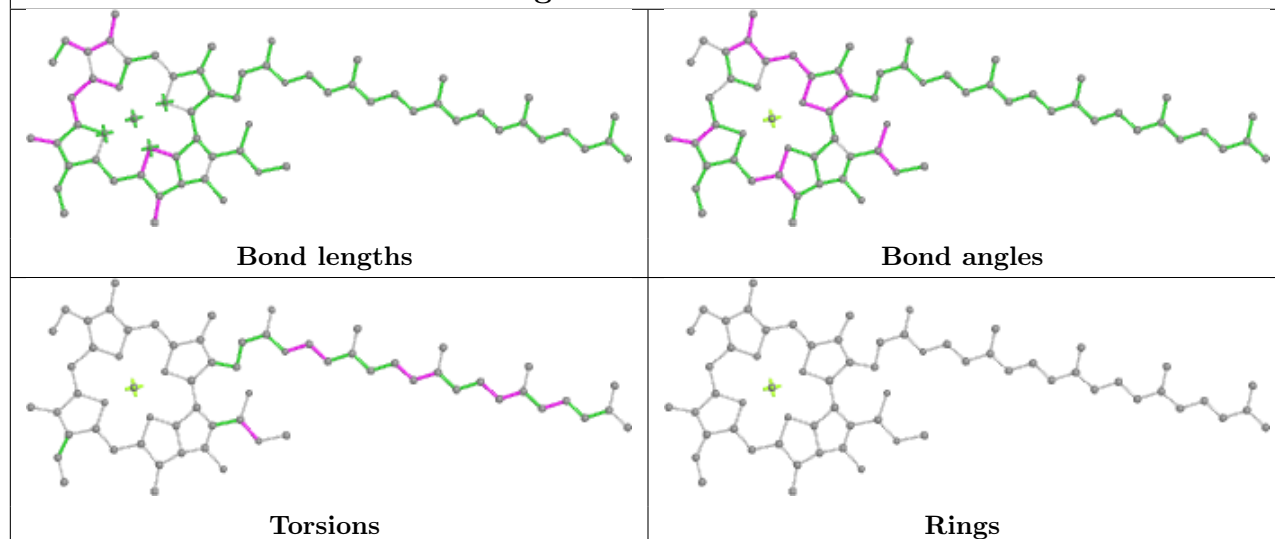




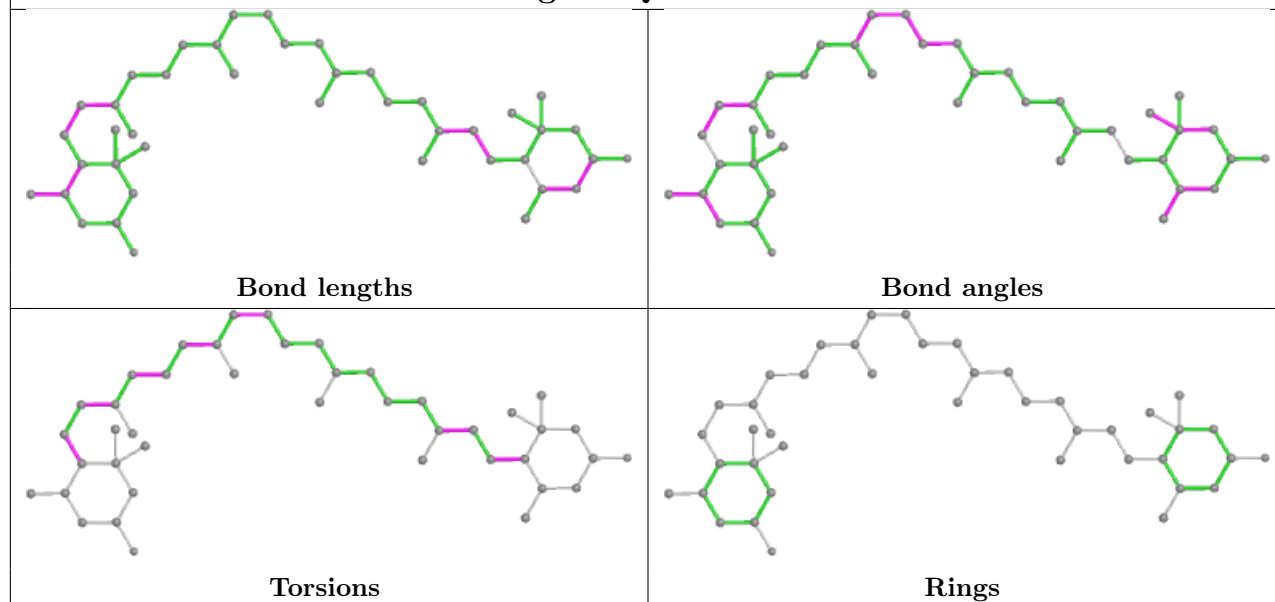
## Ligand IWJ T 318

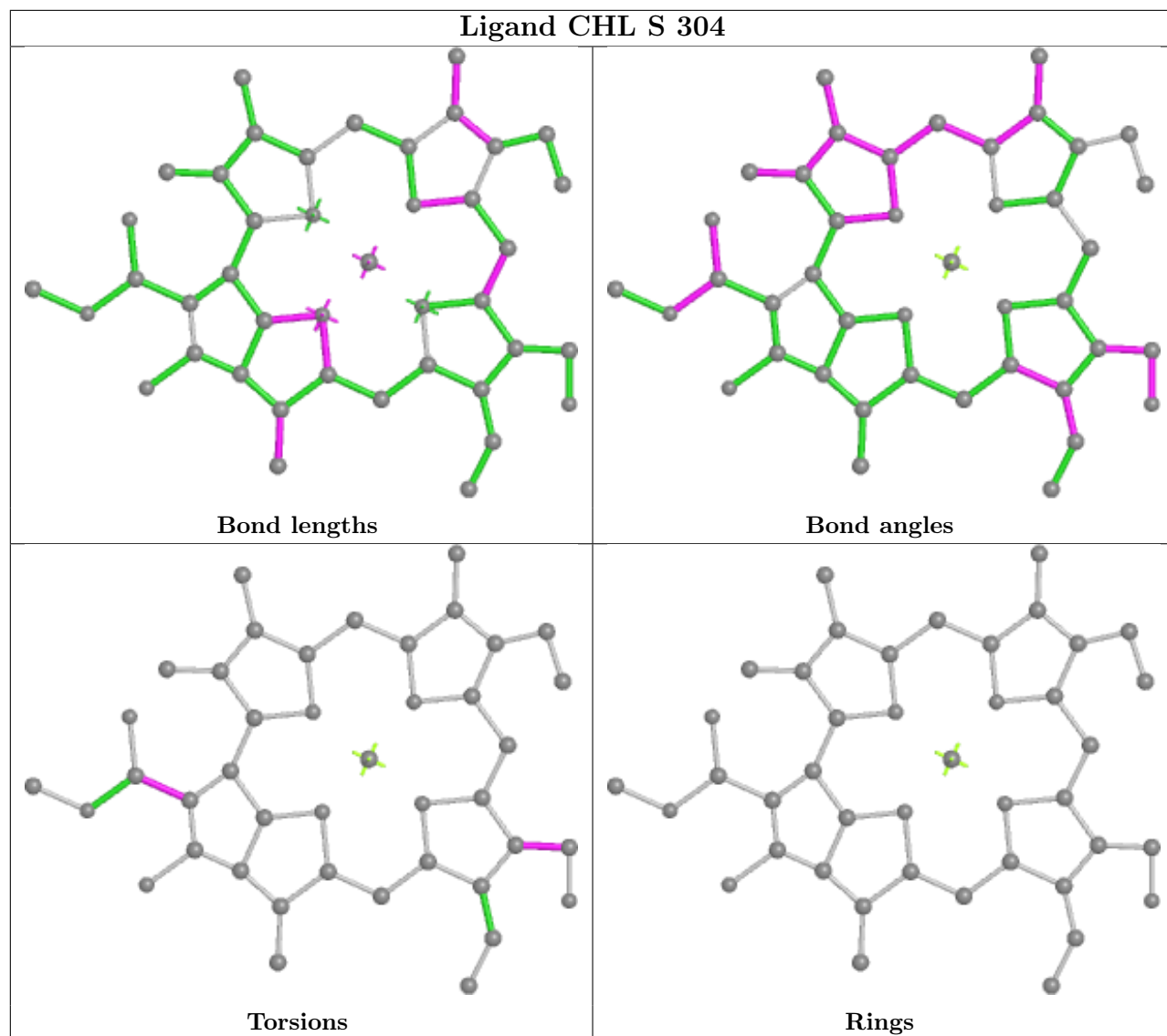


## Ligand CLA S 302

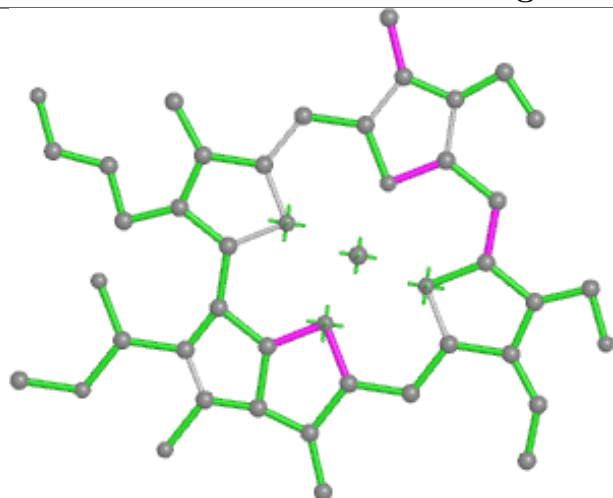


## Ligand Q6L S 321

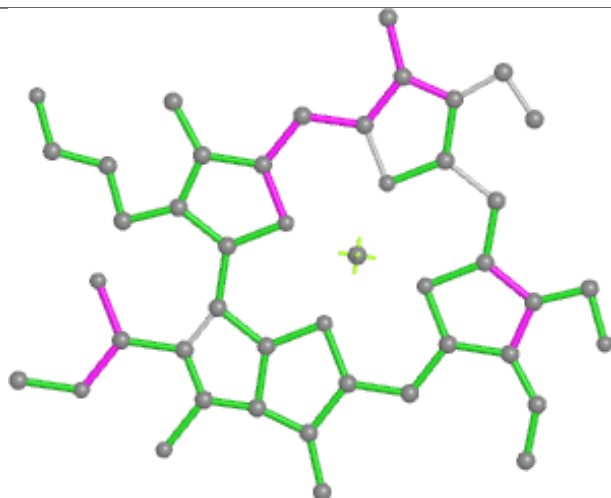




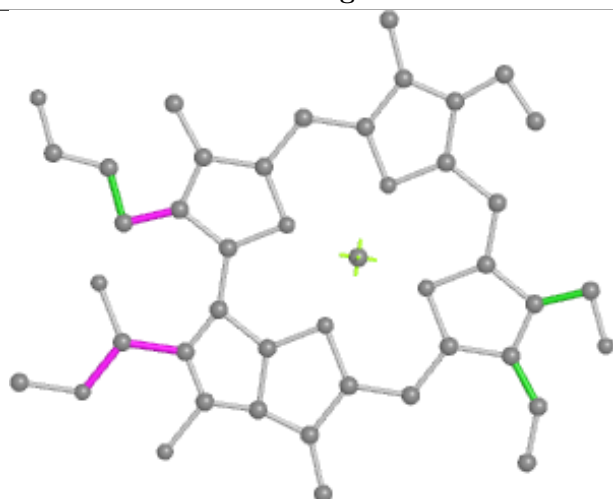
## Ligand CHL S 314



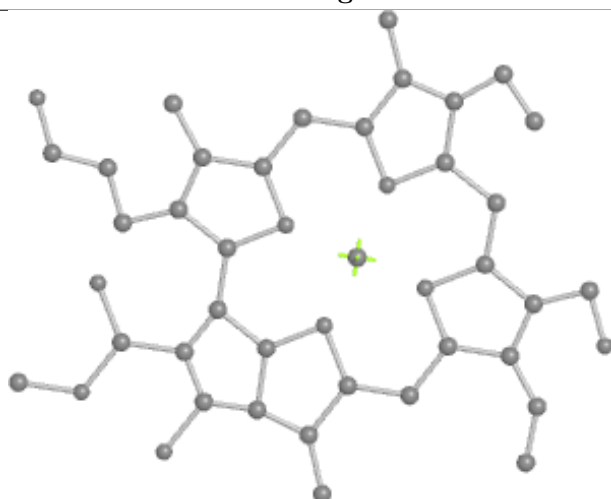
Bond lengths



Bond angles

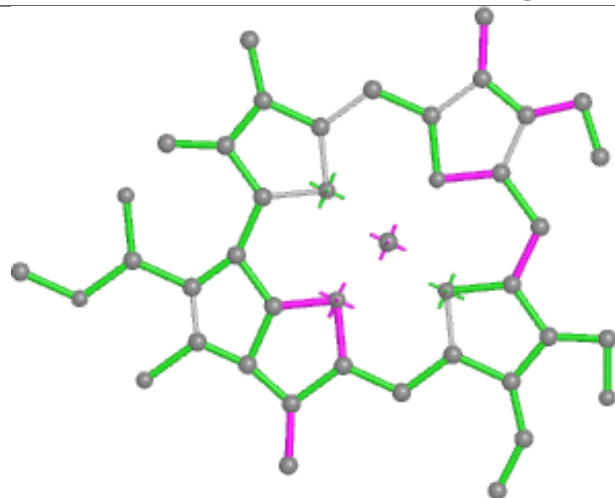


Torsions

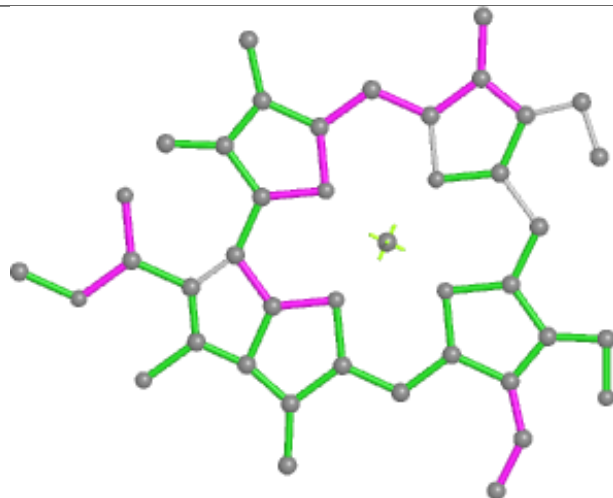


Rings

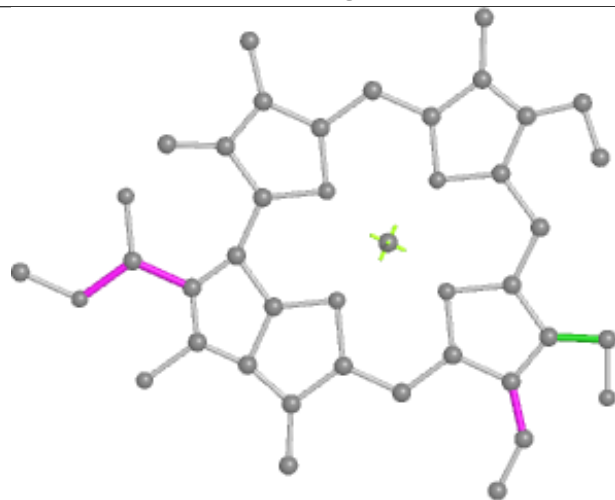
## Ligand CHL S 305



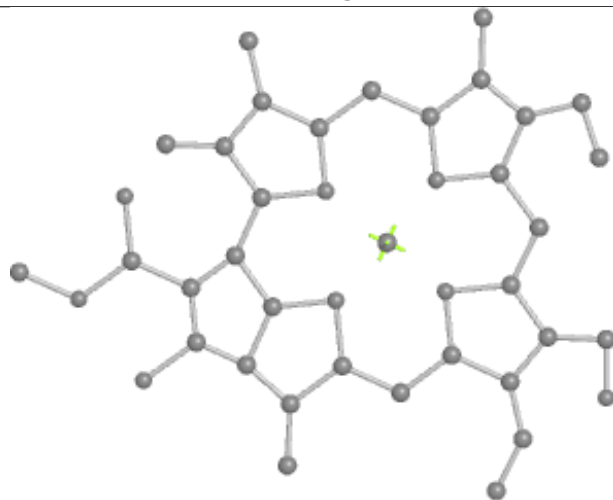
Bond lengths



Bond angles

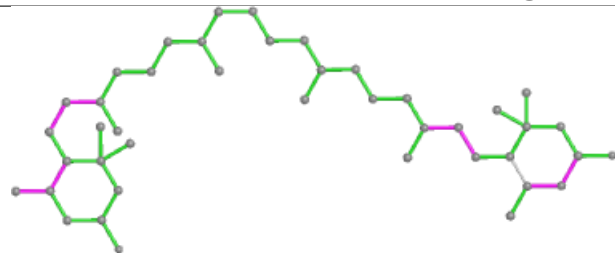


Torsions

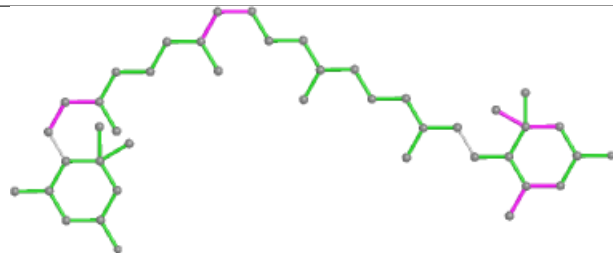


Rings

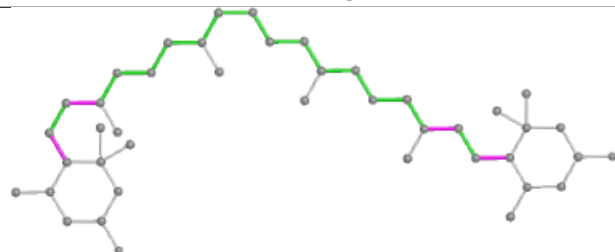
## Ligand Q6L T 322



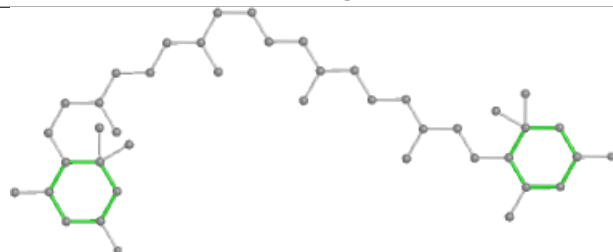
Bond lengths



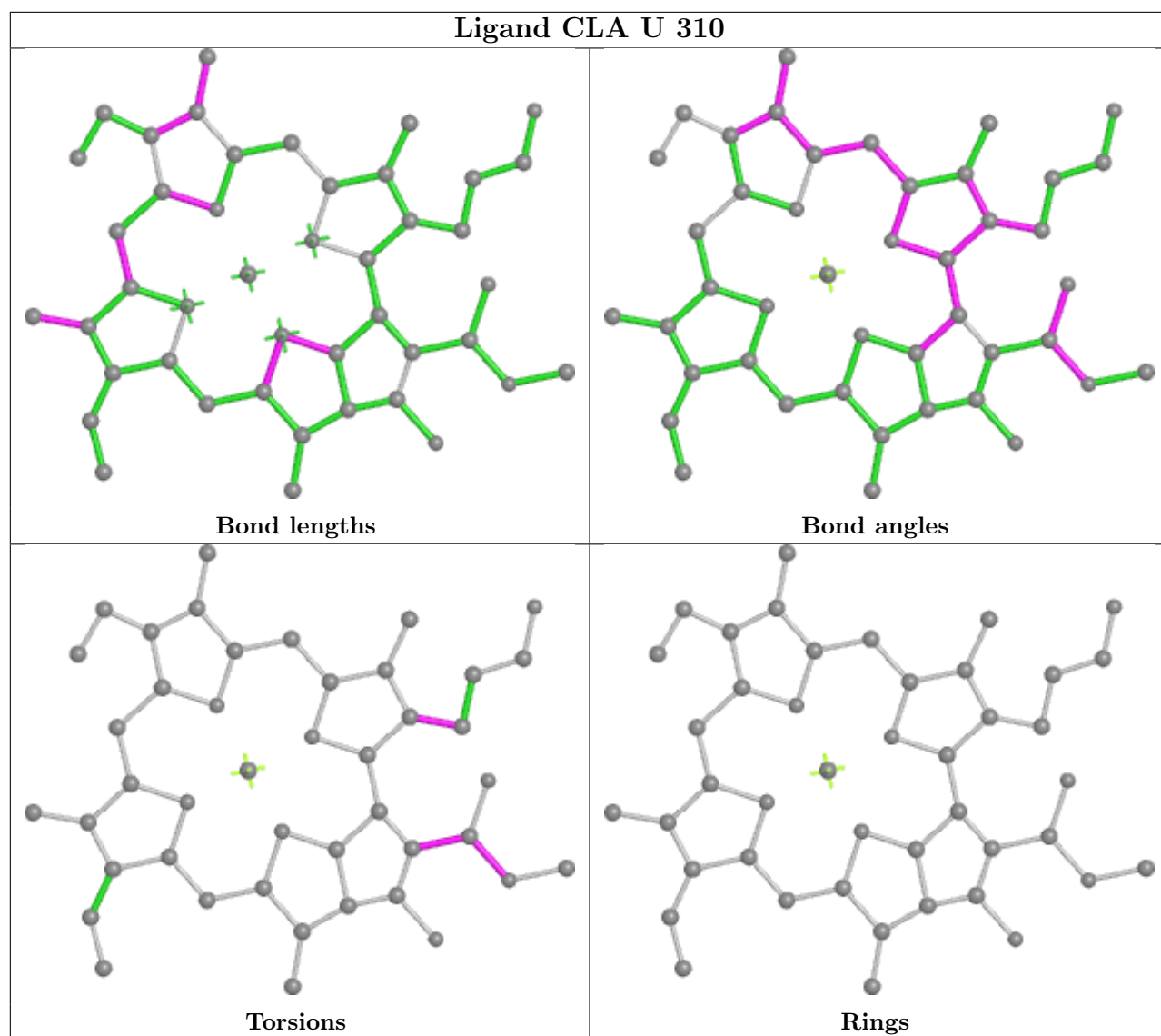
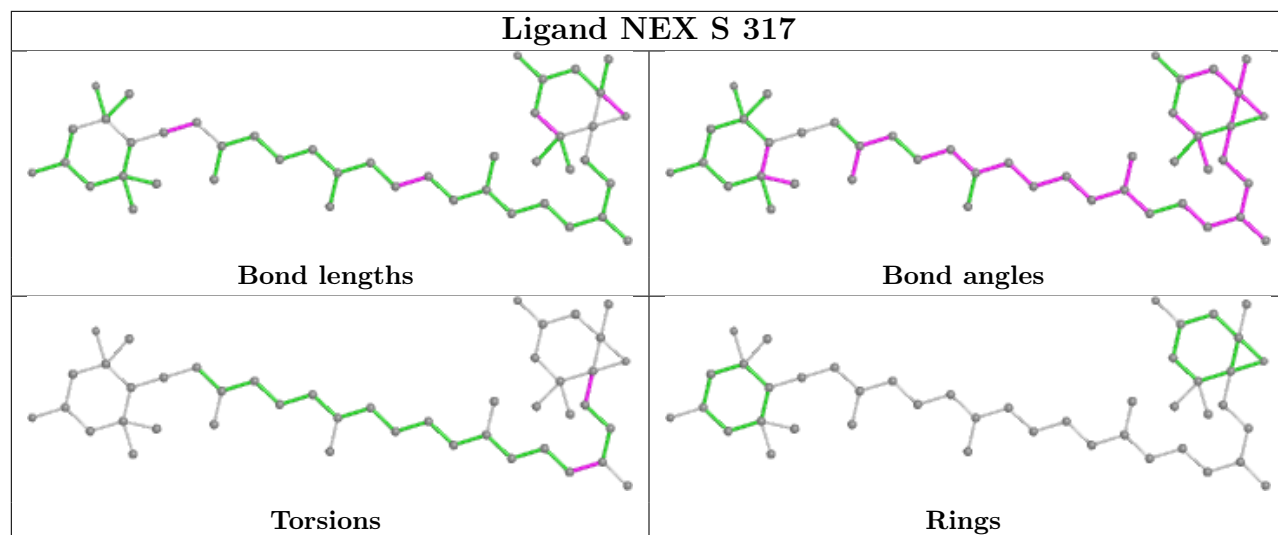
Bond angles



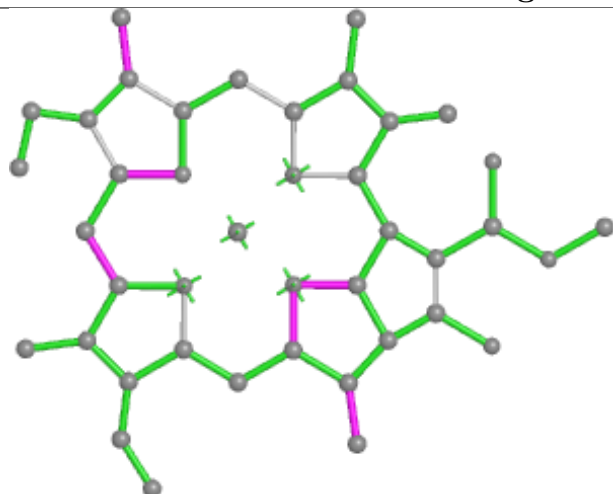
Torsions



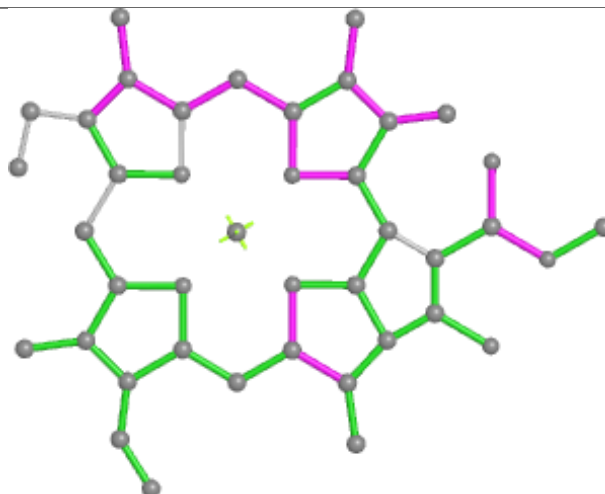
Rings



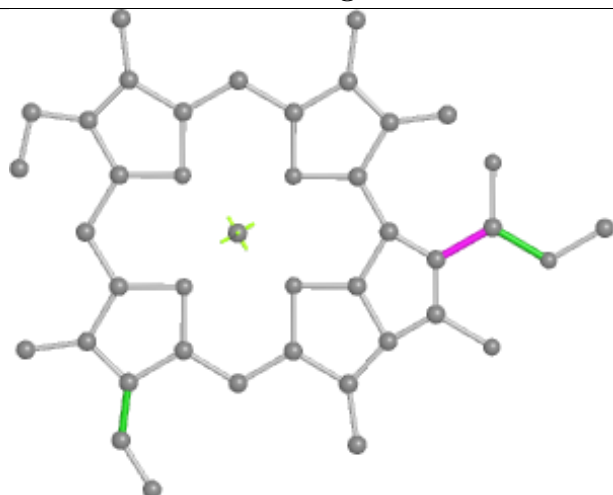
## Ligand CLA S 313



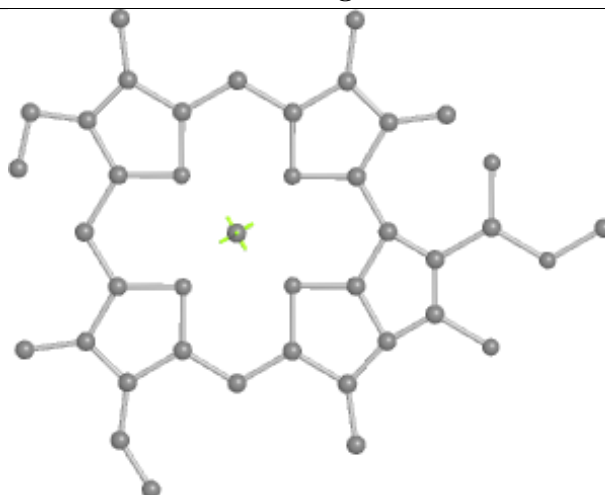
Bond lengths



Bond angles

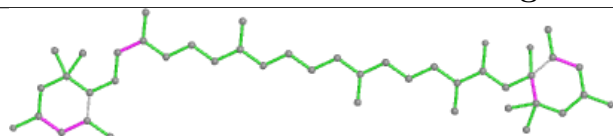


Torsions

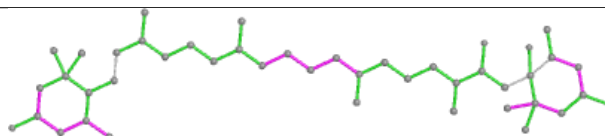


Rings

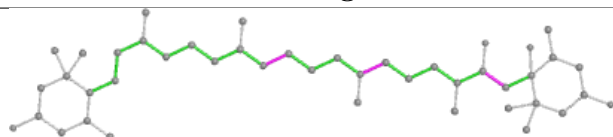
## Ligand IWJ S 318



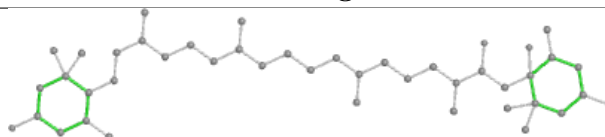
Bond lengths



Bond angles

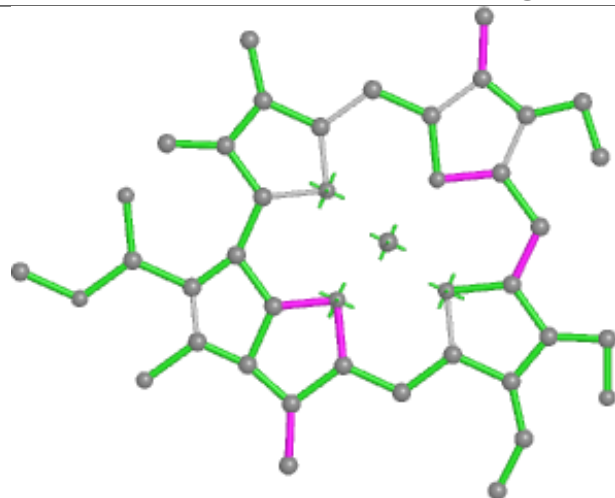


Torsions

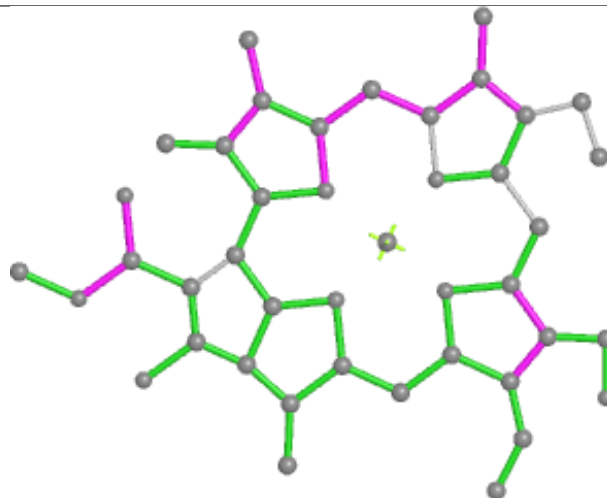


Rings

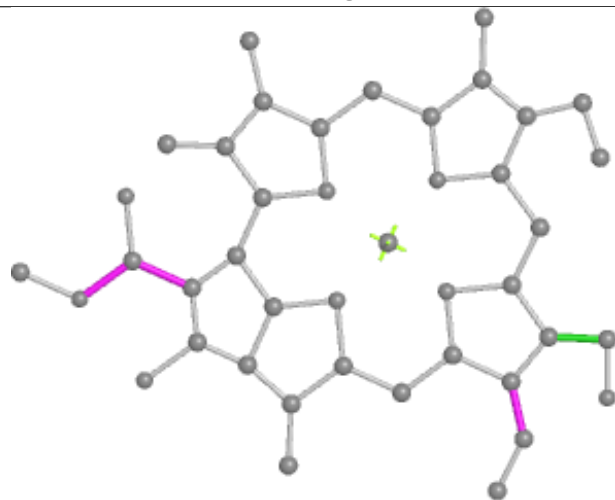
## Ligand CHL S 307



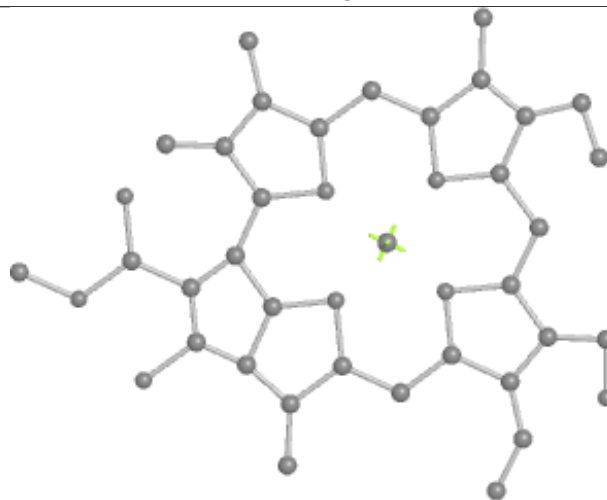
Bond lengths



Bond angles

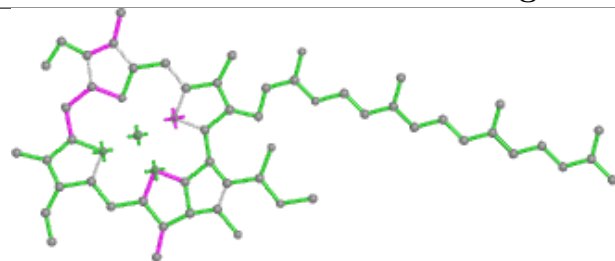


Torsions

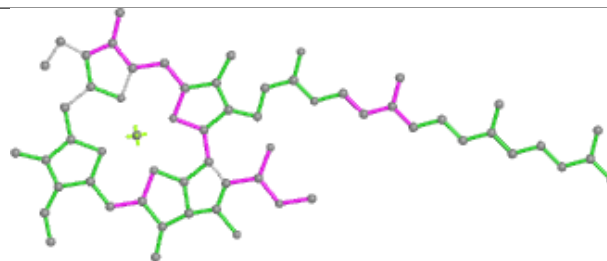


Rings

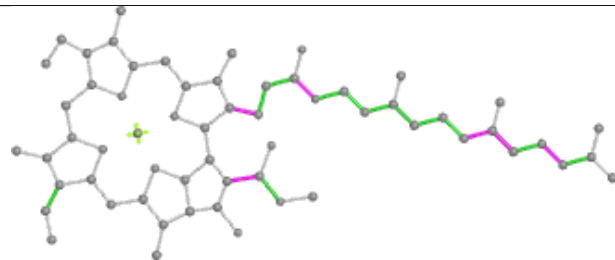
## Ligand CLA S 310



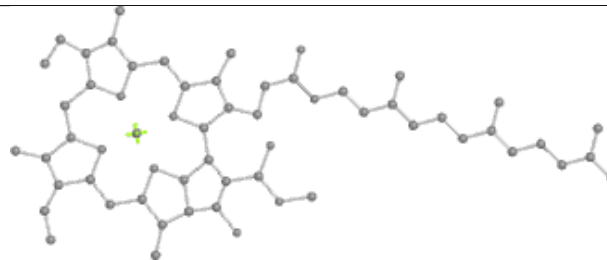
Bond lengths



Bond angles

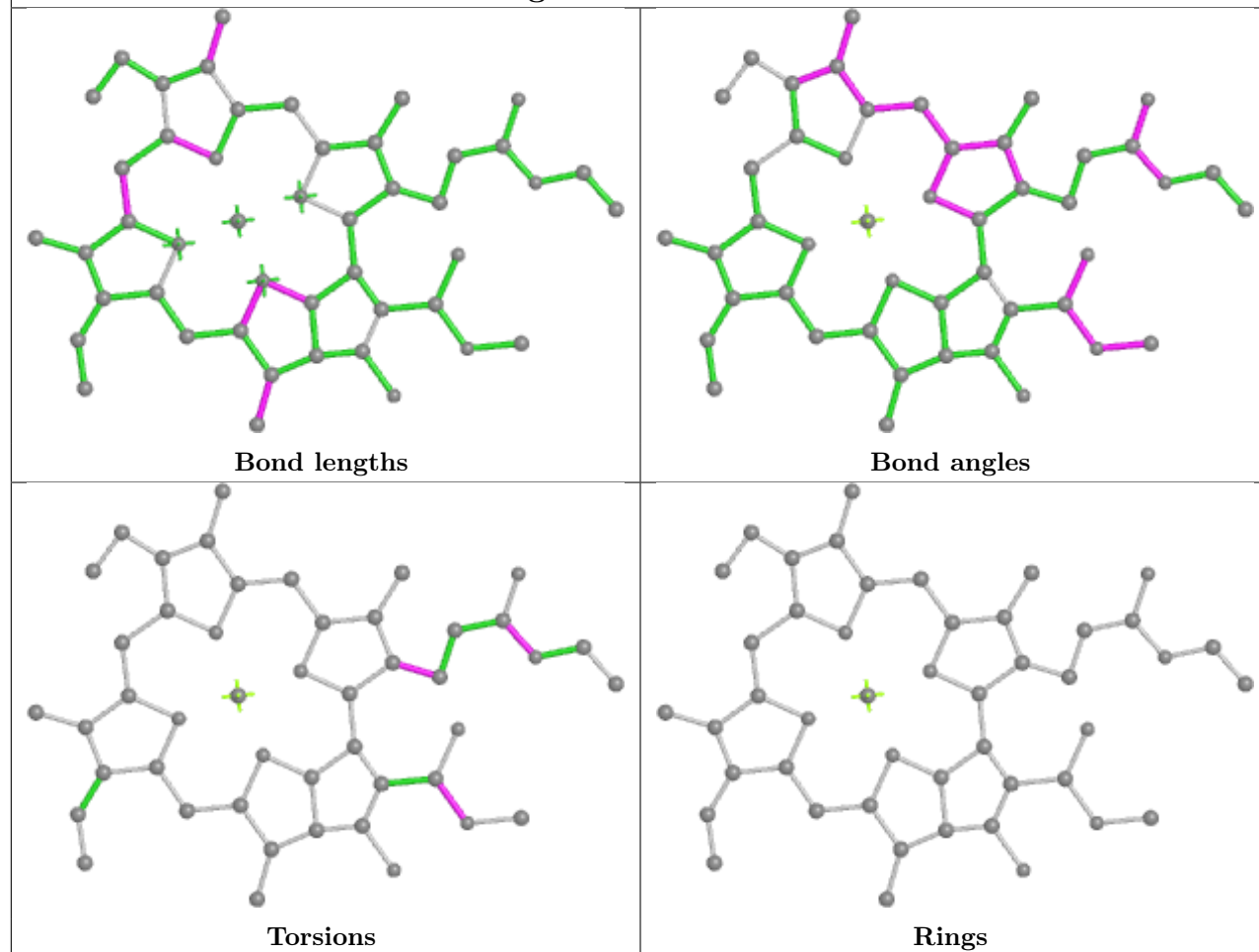


Torsions

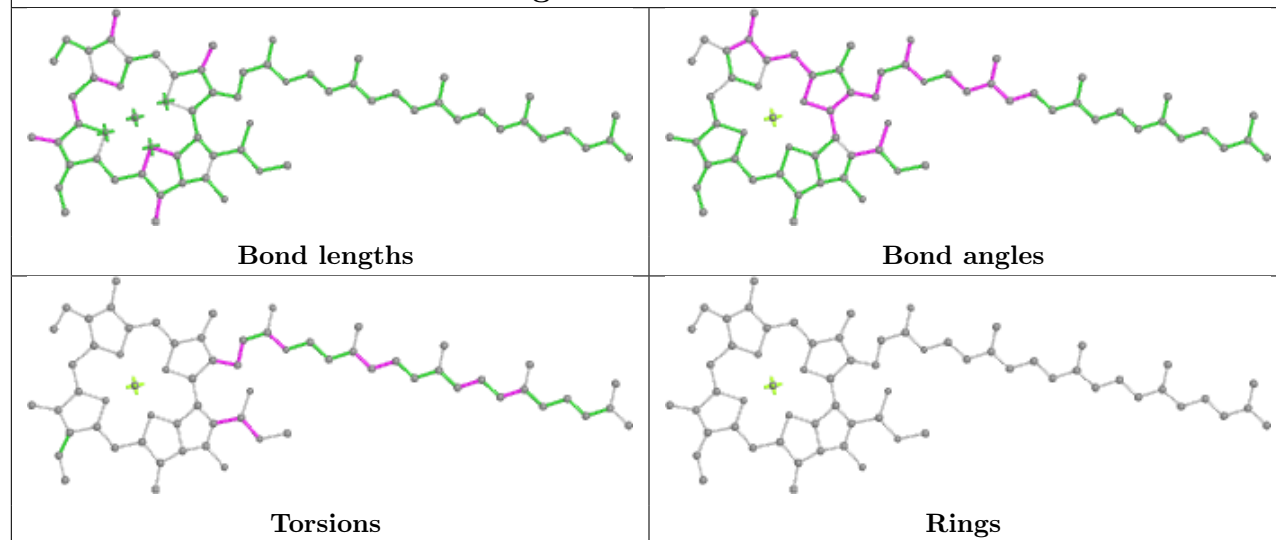


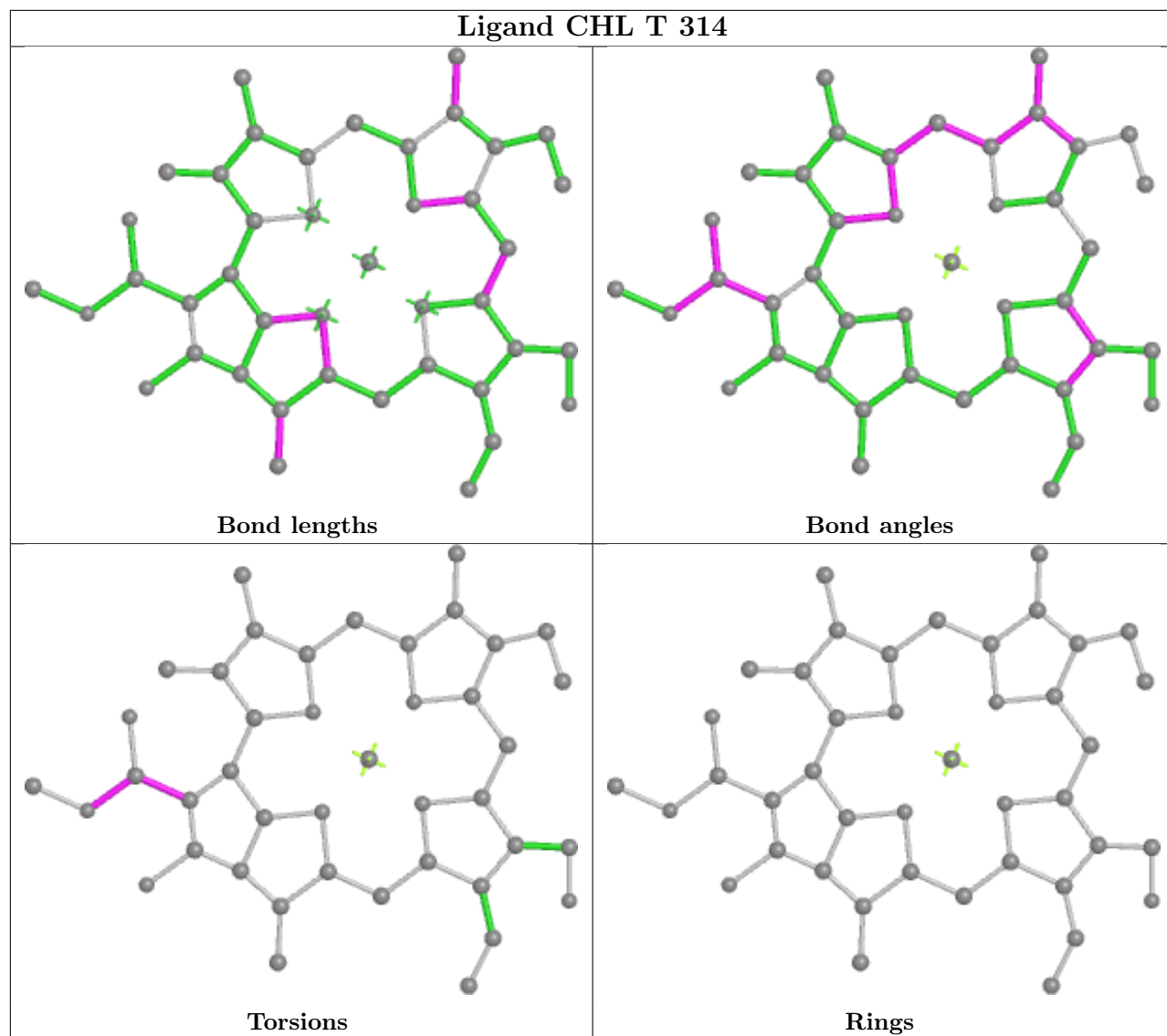
Rings

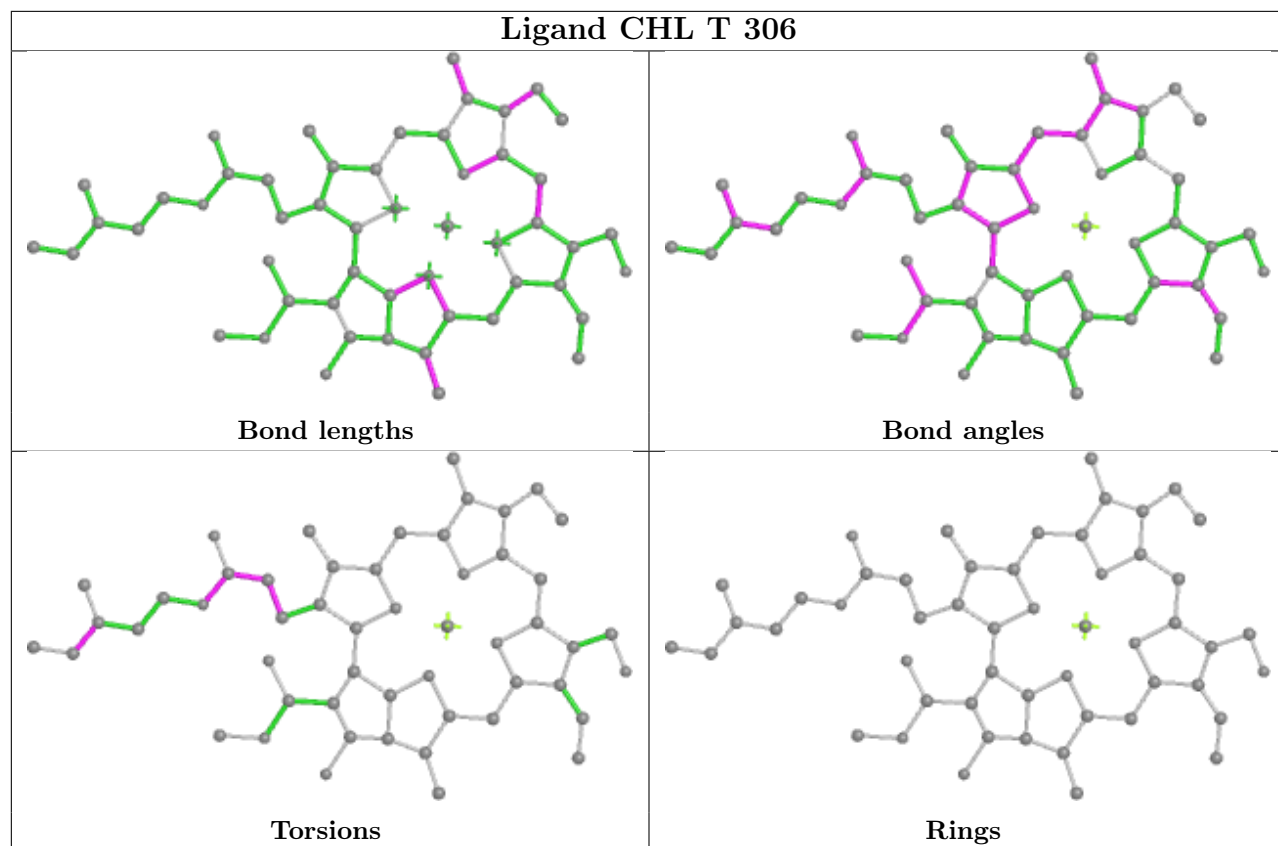
## Ligand CLA S 311



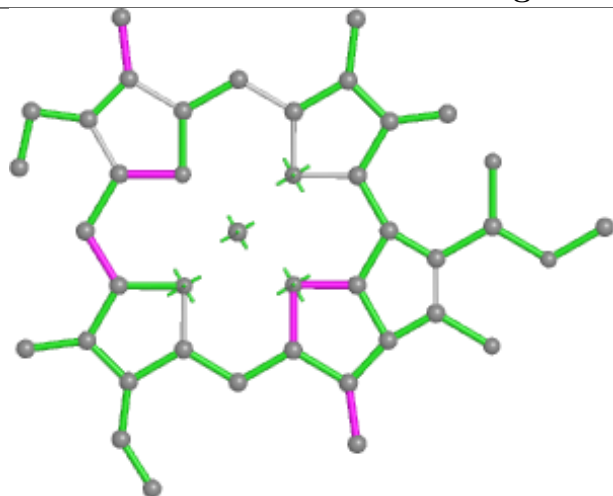
## Ligand CLA T 301



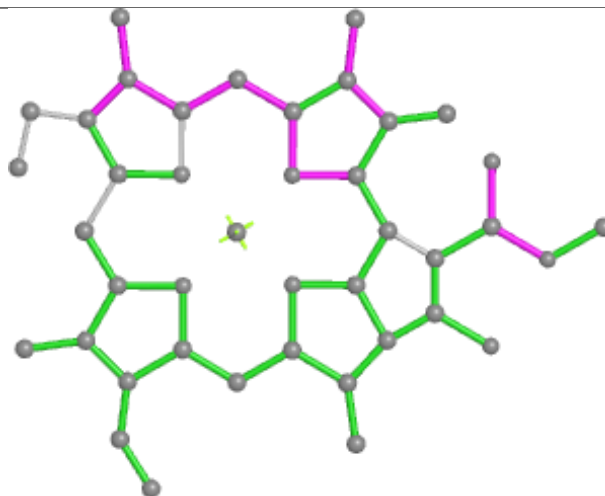




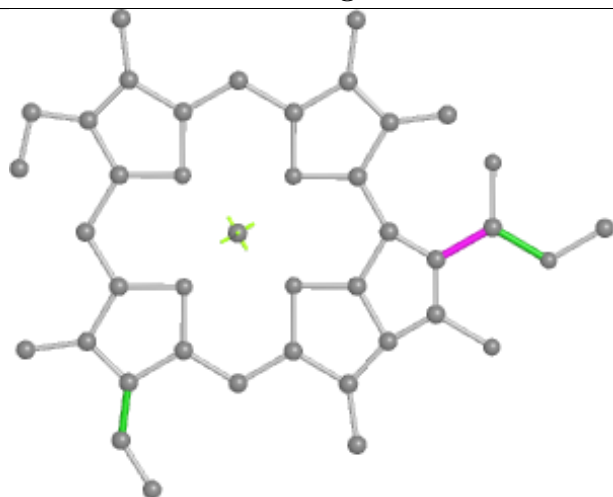
## Ligand CLA U 312



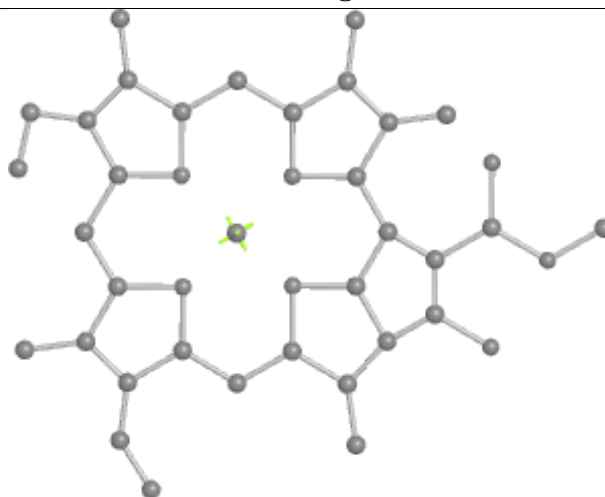
Bond lengths



Bond angles

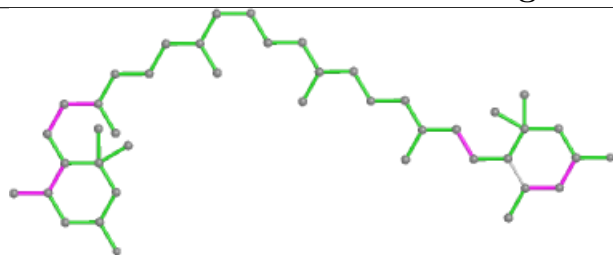


Torsions

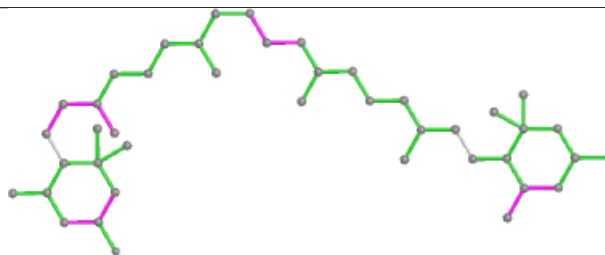


Rings

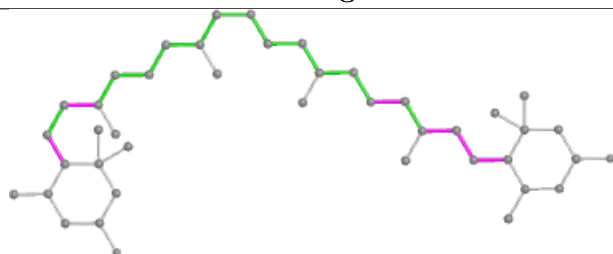
## Ligand Q6L T 319



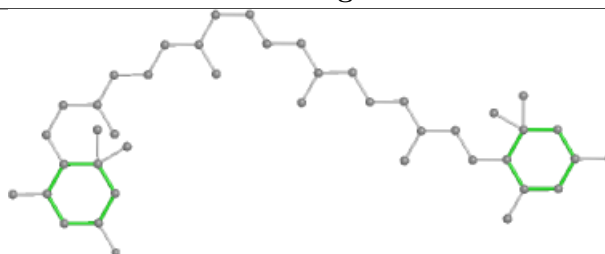
Bond lengths



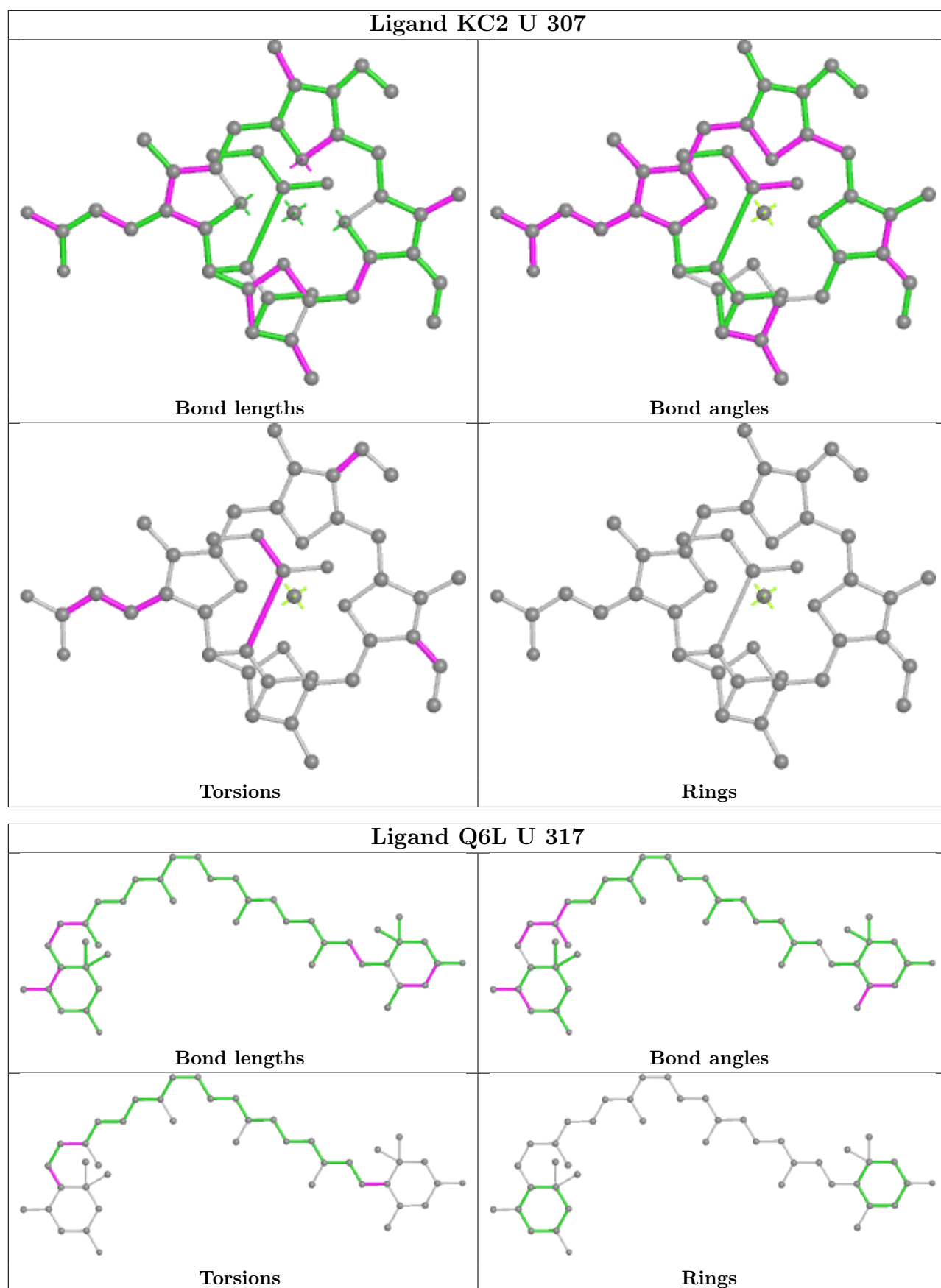
Bond angles



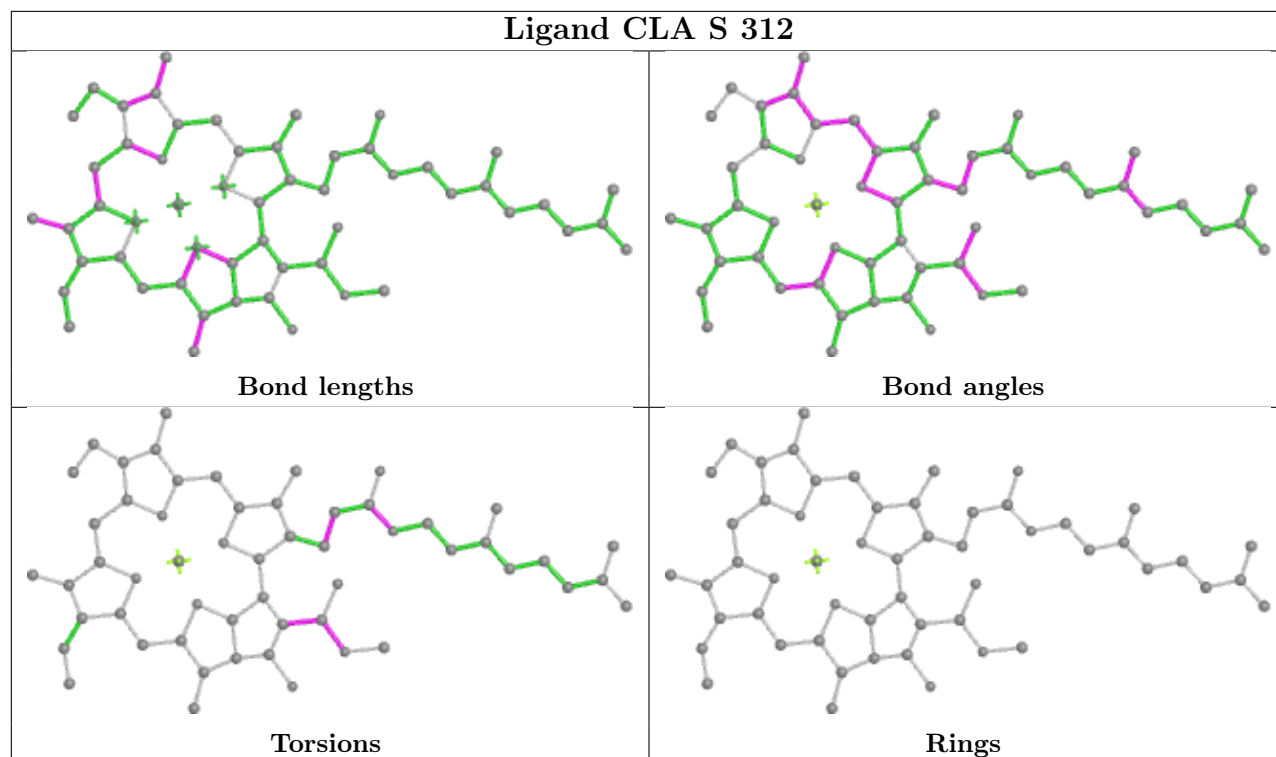
Torsions



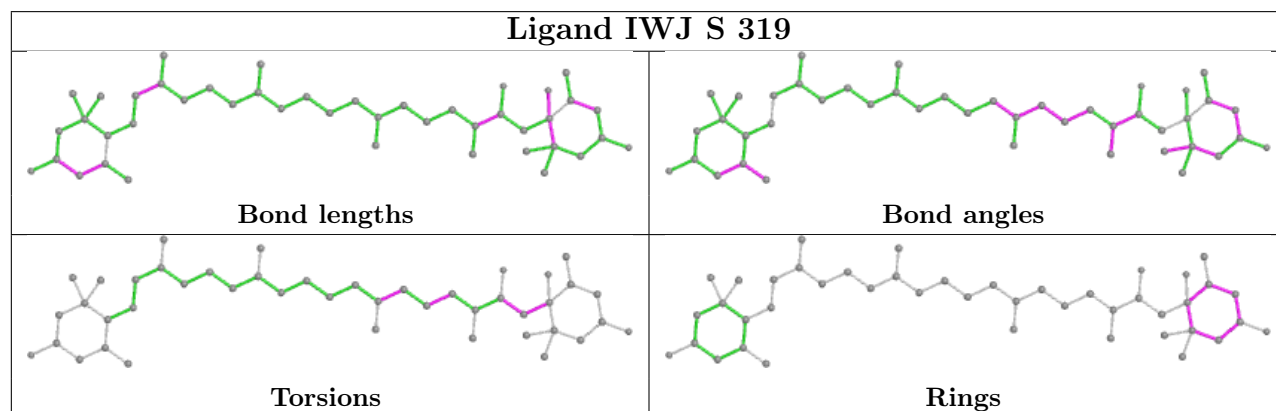
Rings



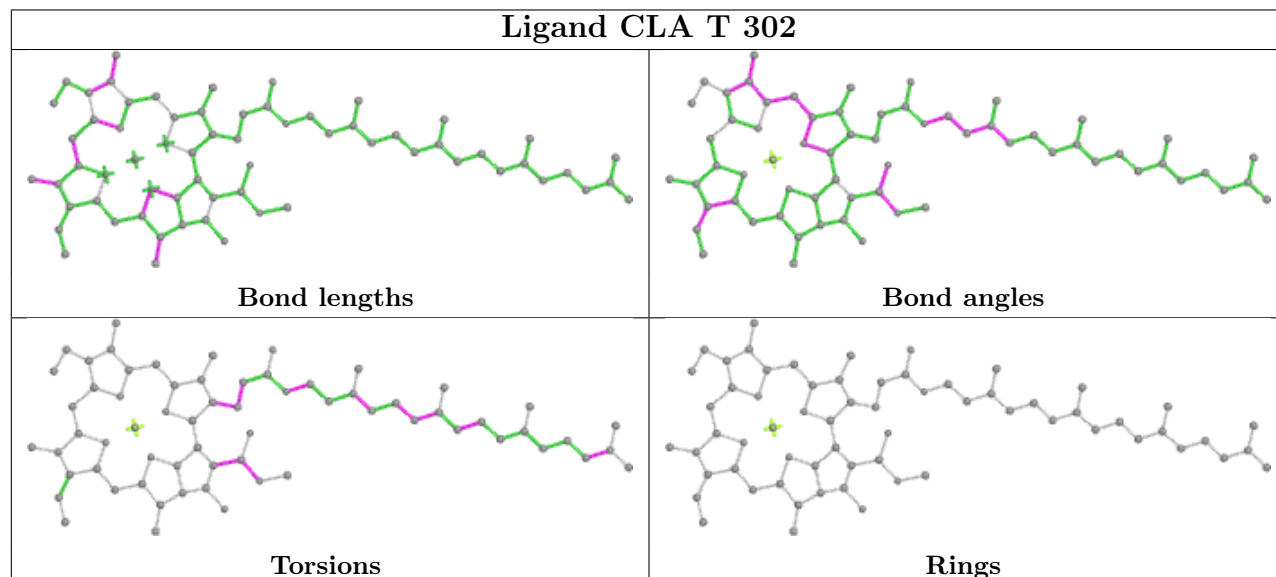
## Ligand CLA S 312



## Ligand IWJ S 319



## Ligand CLA T 302



## 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.

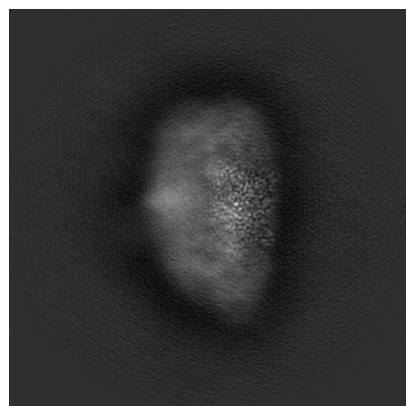
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34733. These allow visual inspection of the internal detail of the map and identification of artifacts.

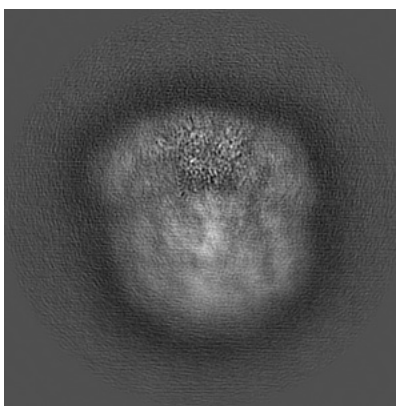
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

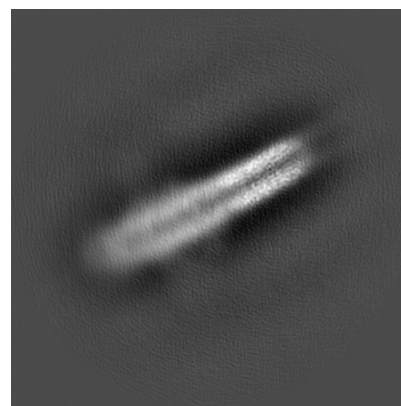
#### 6.1.1 Primary map



X

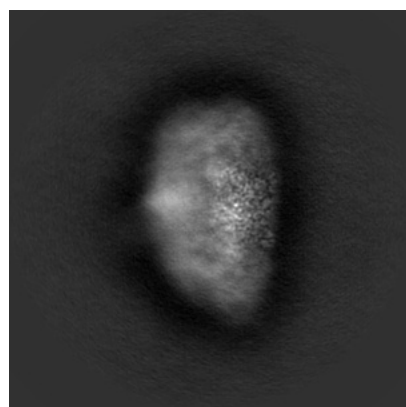


Y

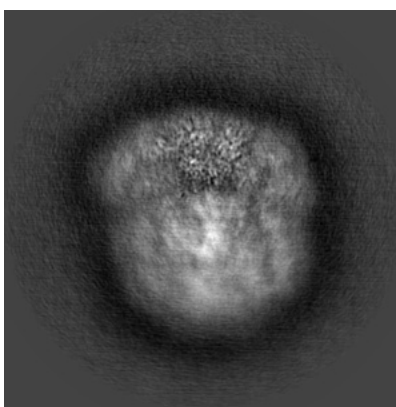


Z

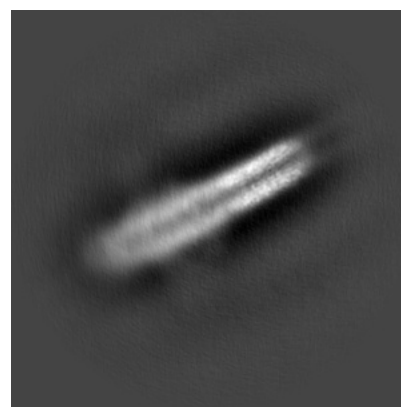
#### 6.1.2 Raw map



X



Y

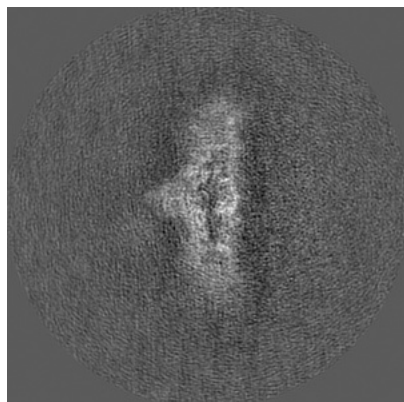


Z

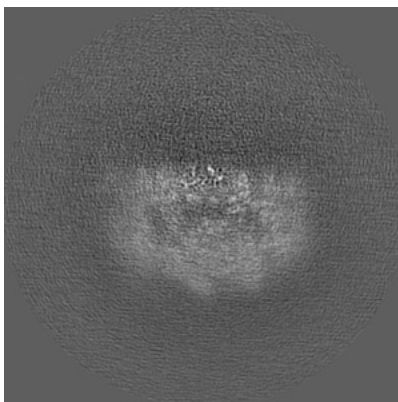
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

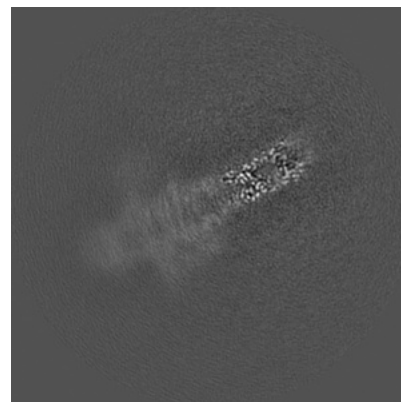
### 6.2.1 Primary map



X Index: 192

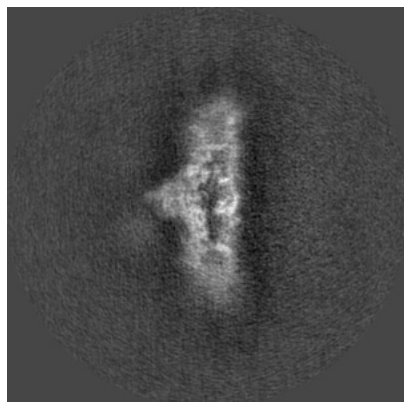


Y Index: 192

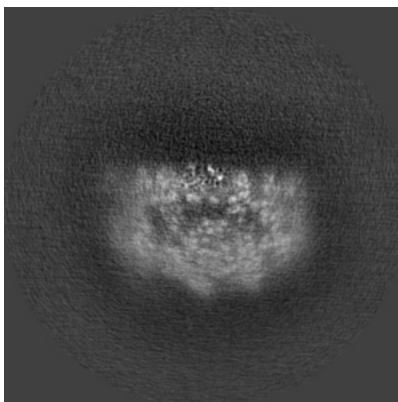


Z Index: 192

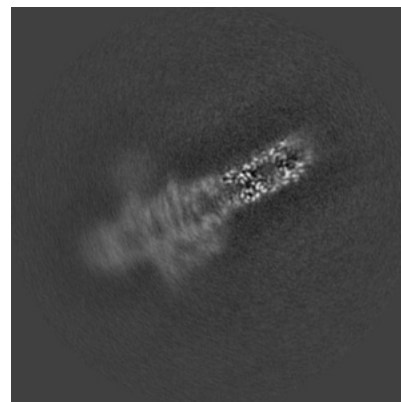
### 6.2.2 Raw map



X Index: 192



Y Index: 192

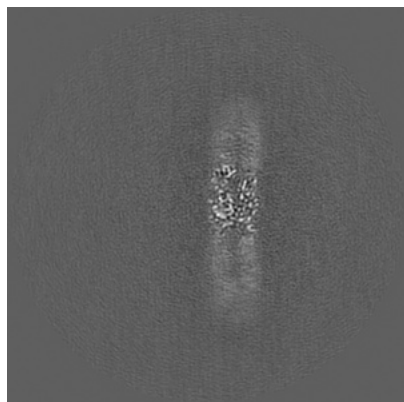


Z Index: 192

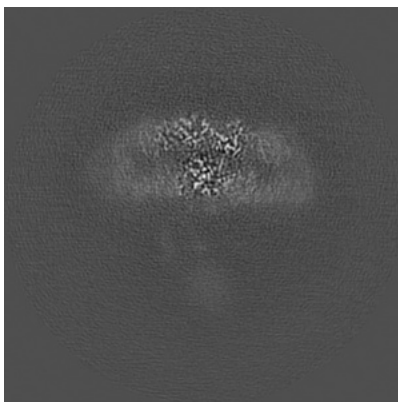
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

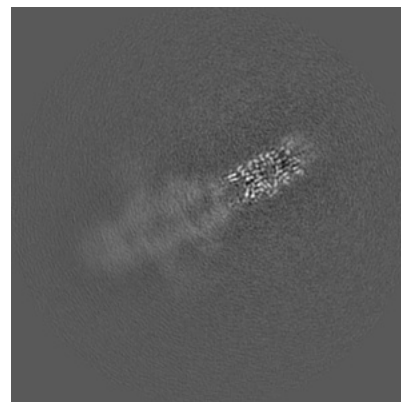
### 6.3.1 Primary map



X Index: 232

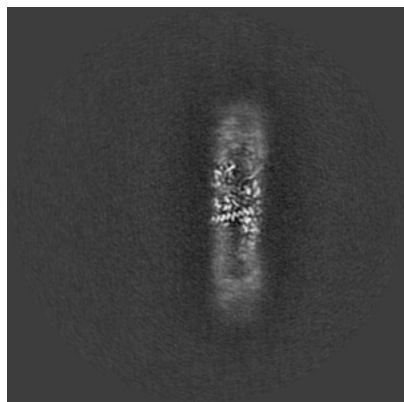


Y Index: 222

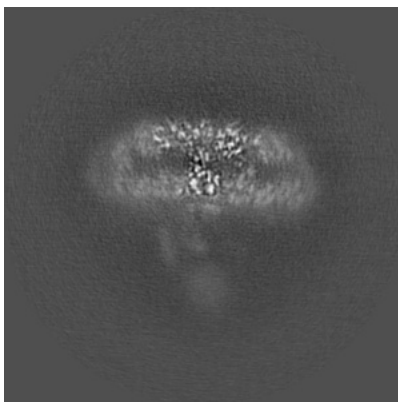


Z Index: 184

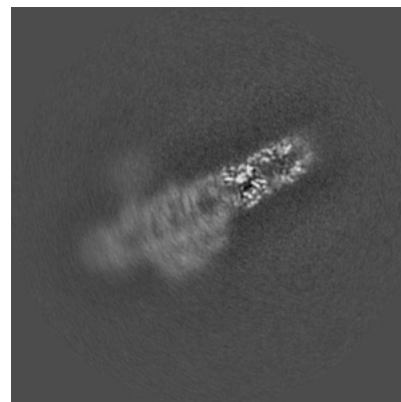
### 6.3.2 Raw map



X Index: 237



Y Index: 219

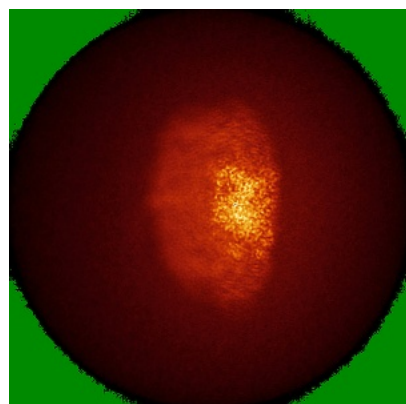


Z Index: 197

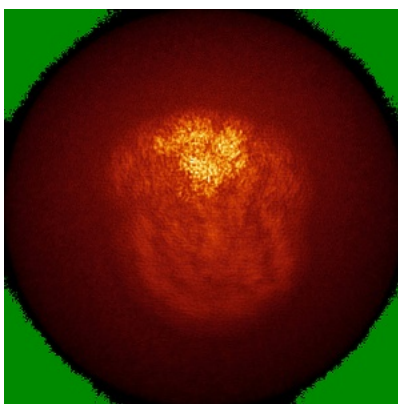
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

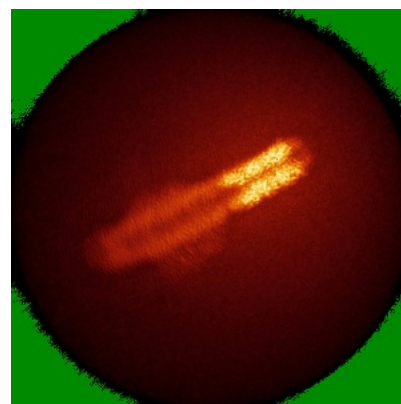
### 6.4.1 Primary map



X

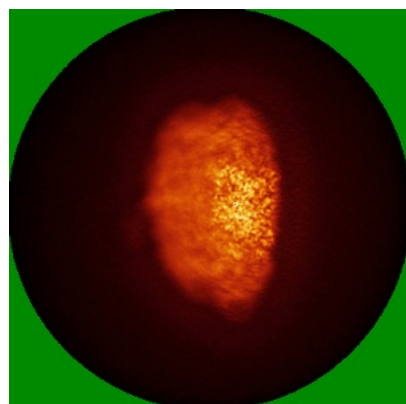


Y

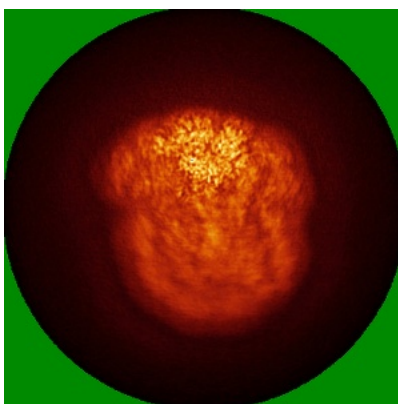


Z

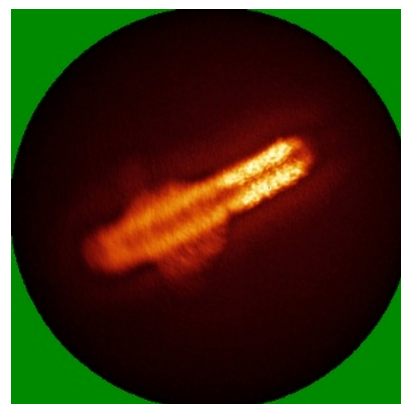
### 6.4.2 Raw map



X



Y

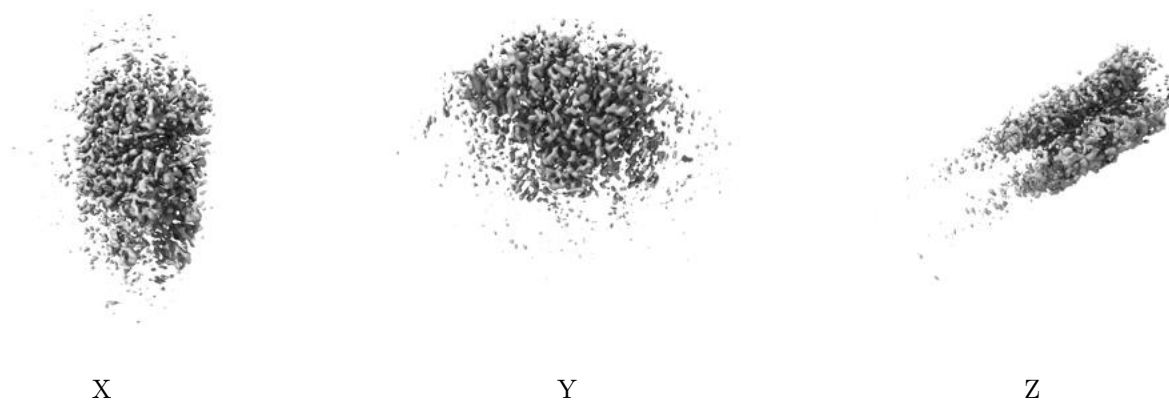


Z

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.

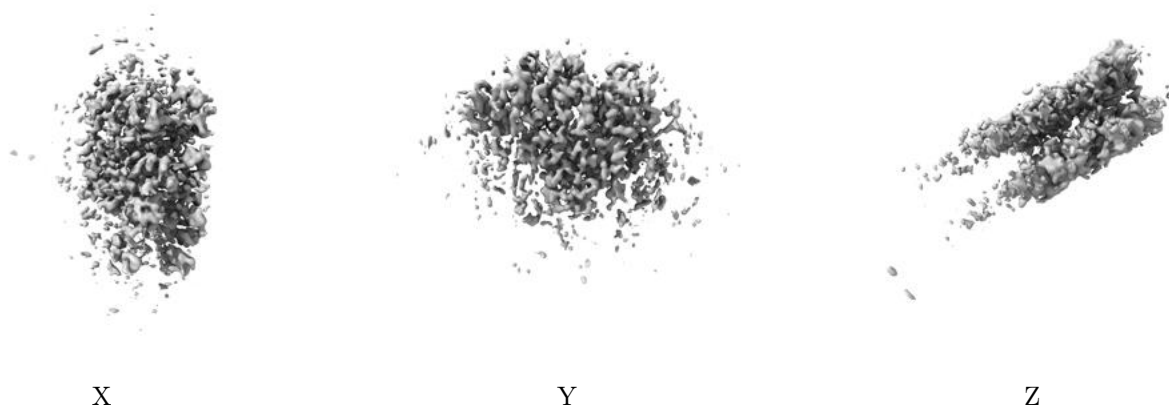
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



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.

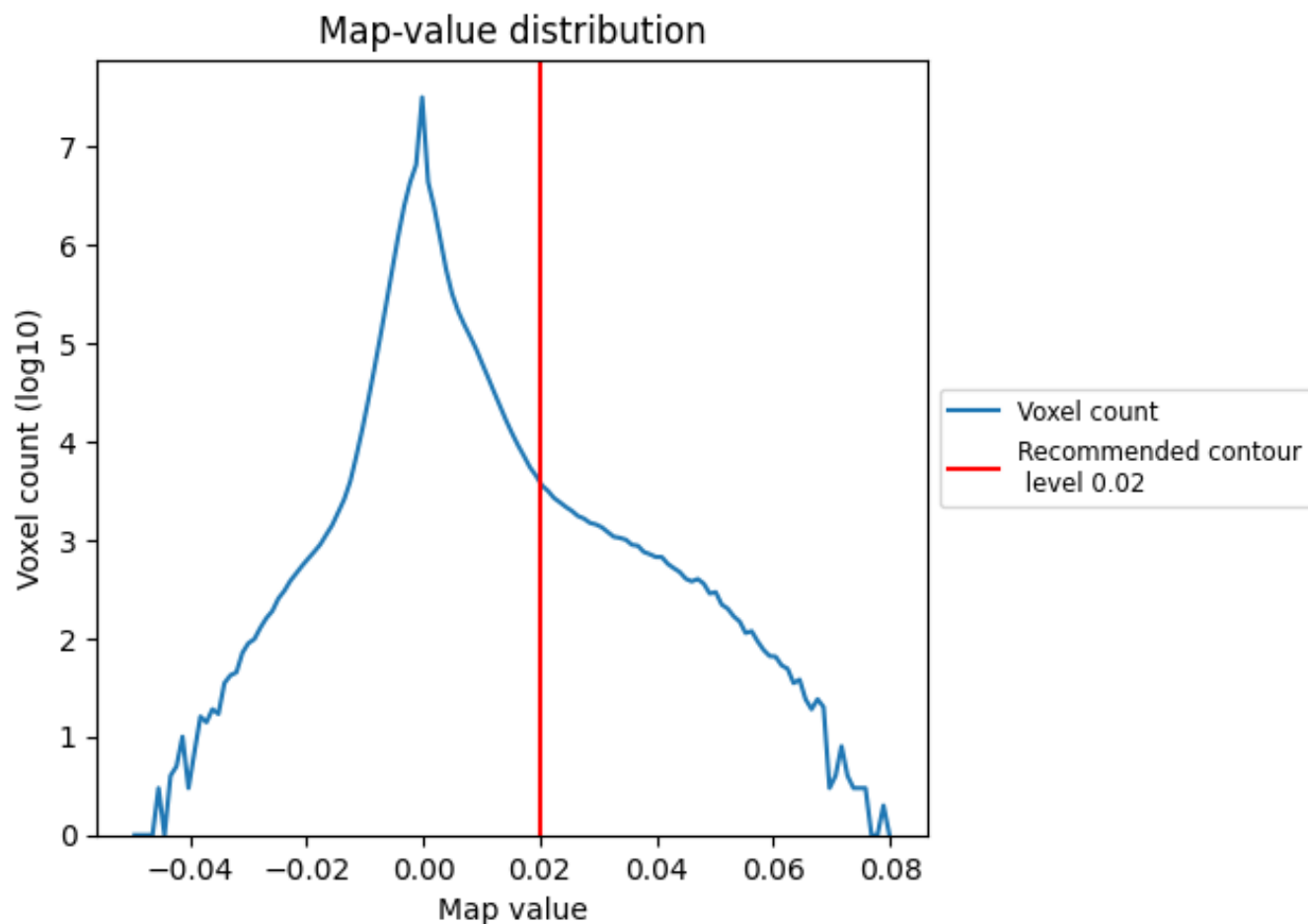
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

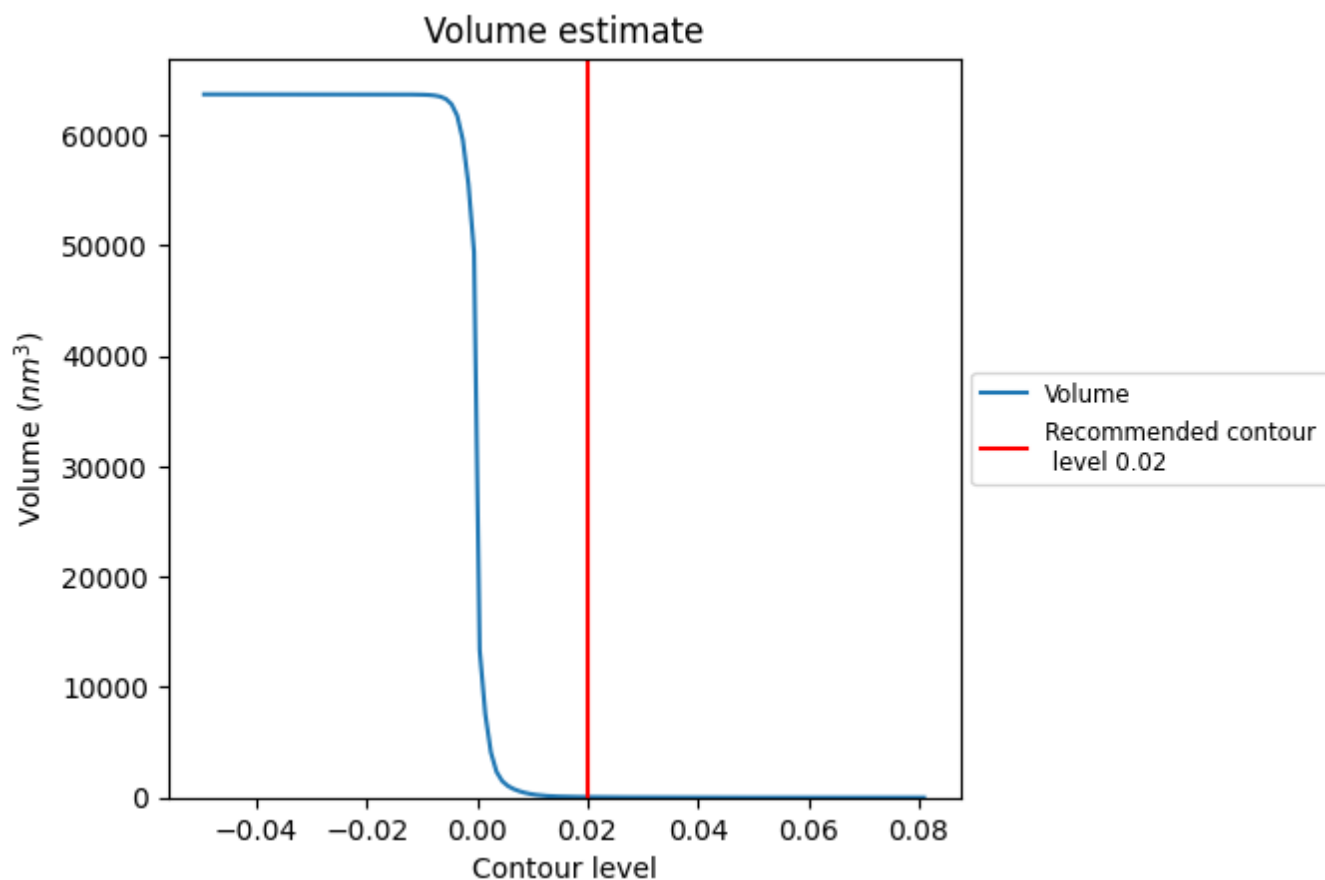
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

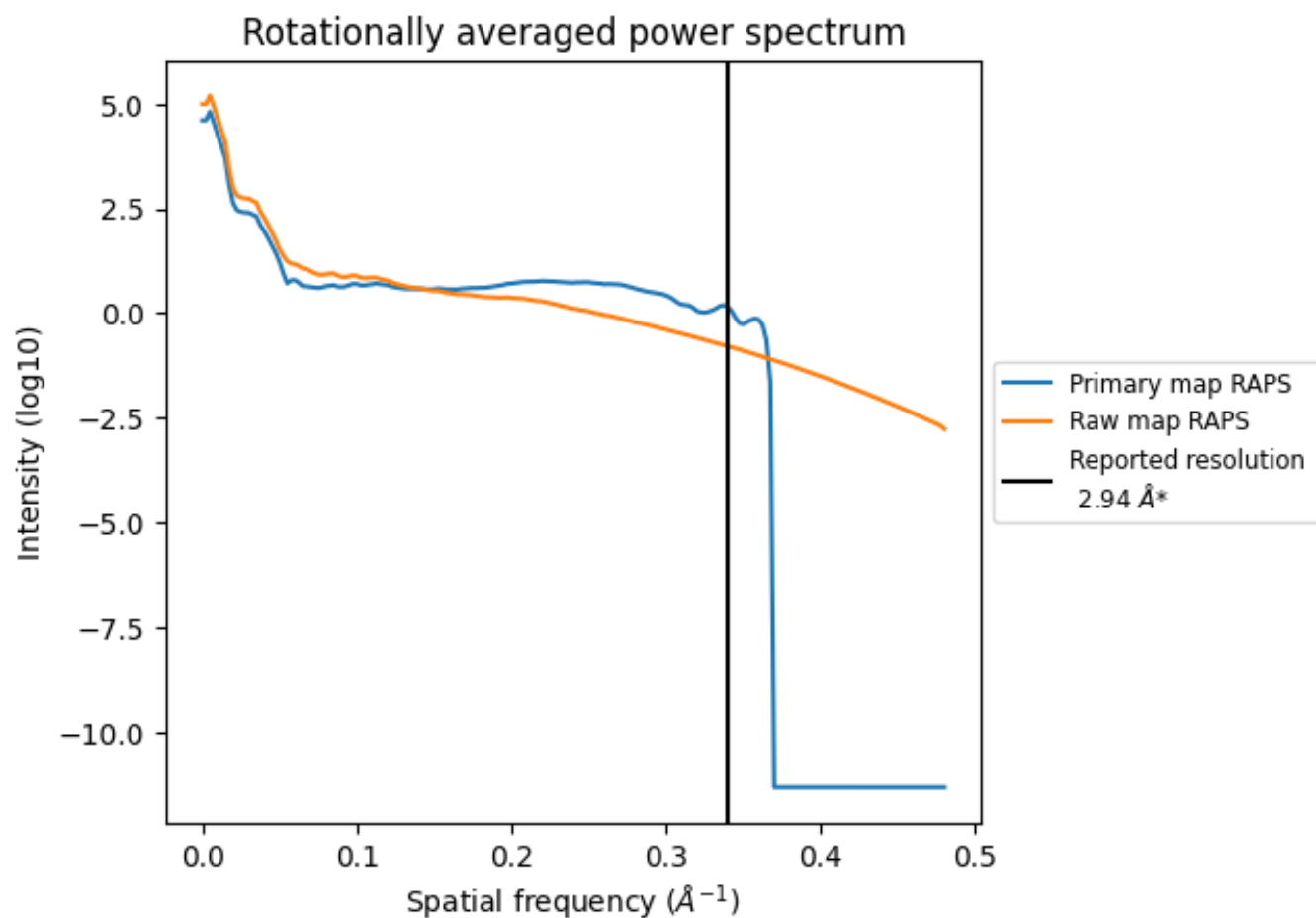
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 44 nm<sup>3</sup>; 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 ⓘ

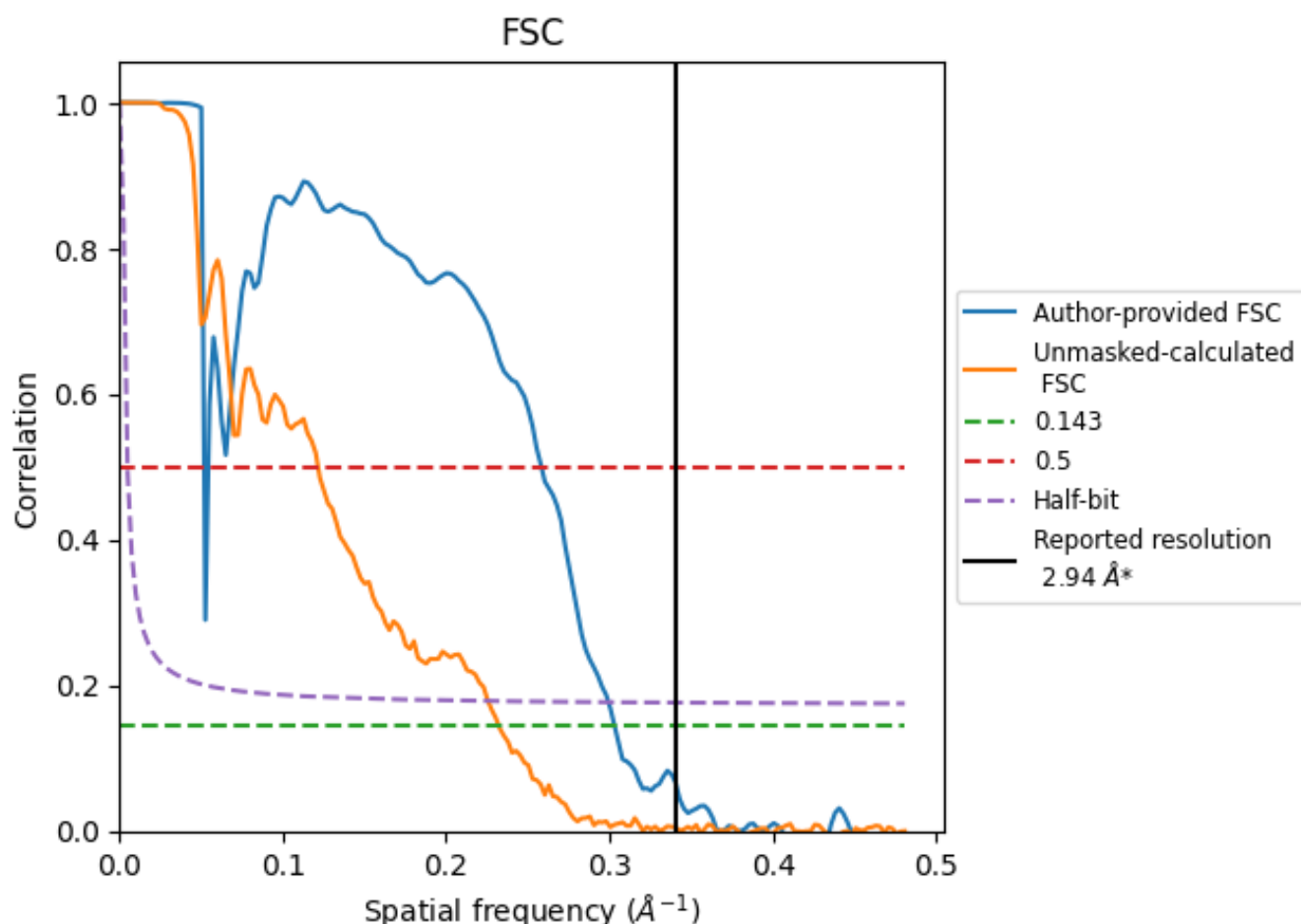


\*Reported resolution corresponds to spatial frequency of 0.340 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.340 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	3.30	19.31	3.34
Unmasked-calculated*	4.30	8.22	4.43

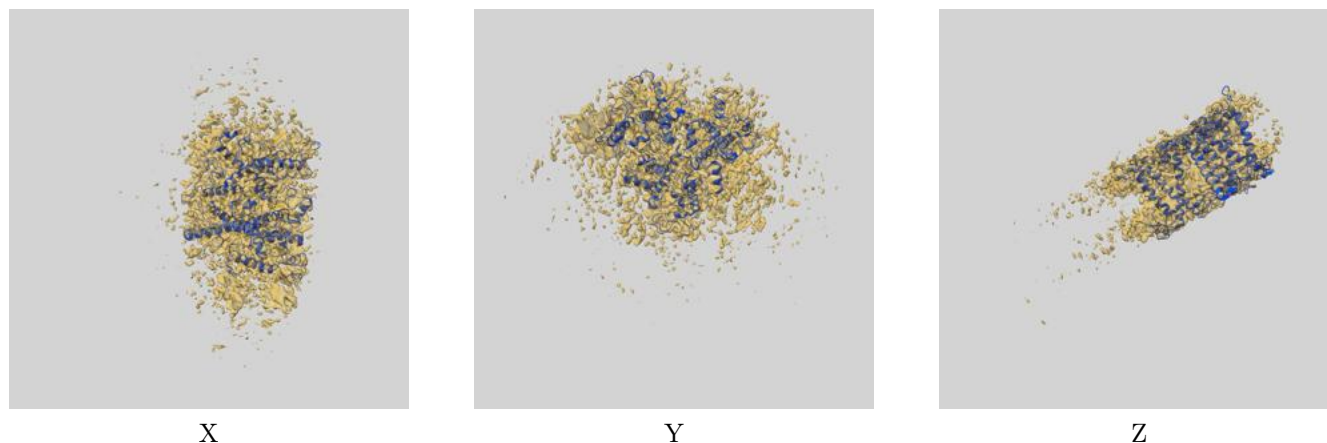
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.94 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 2.94 by more than 10 %

## 9 Map-model fit [i](#)

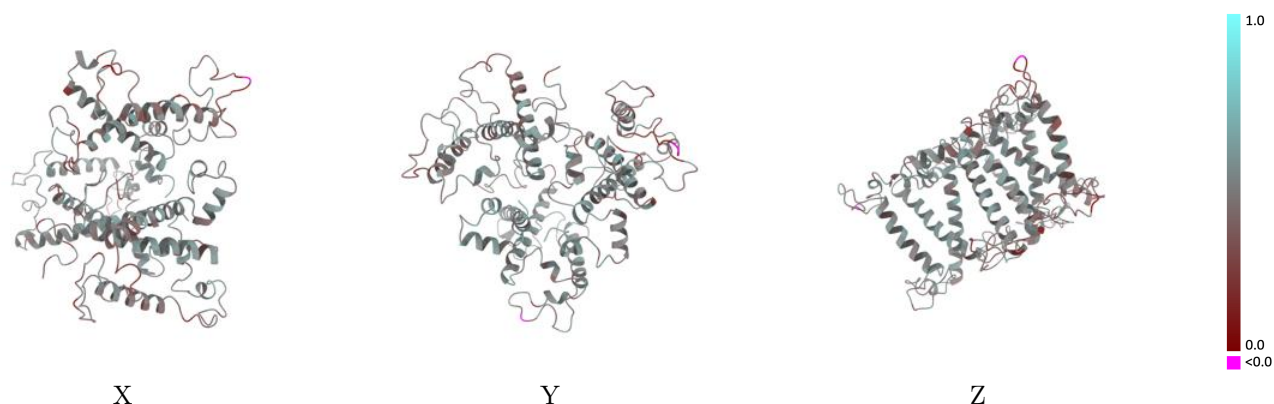
This section contains information regarding the fit between EMDB map EMD-34733 and PDB model 8HG3. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



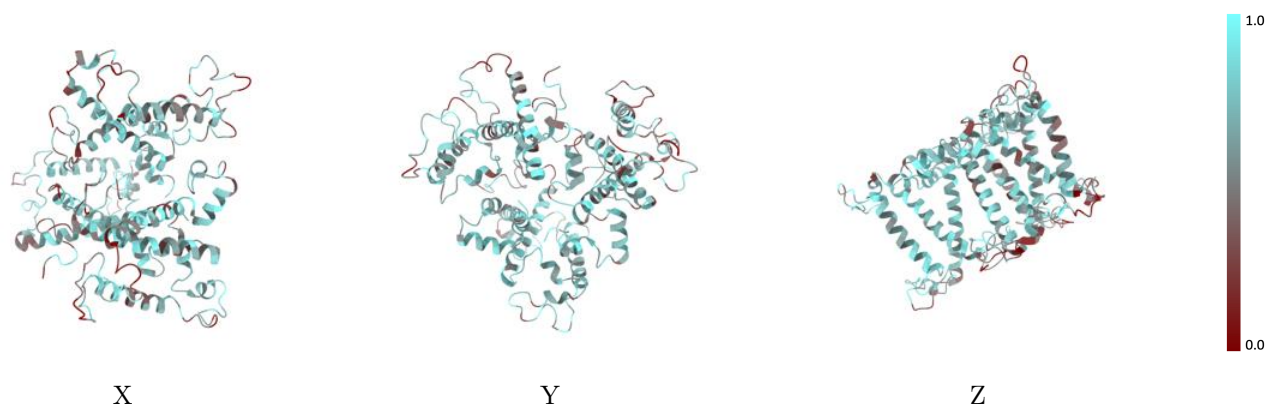
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



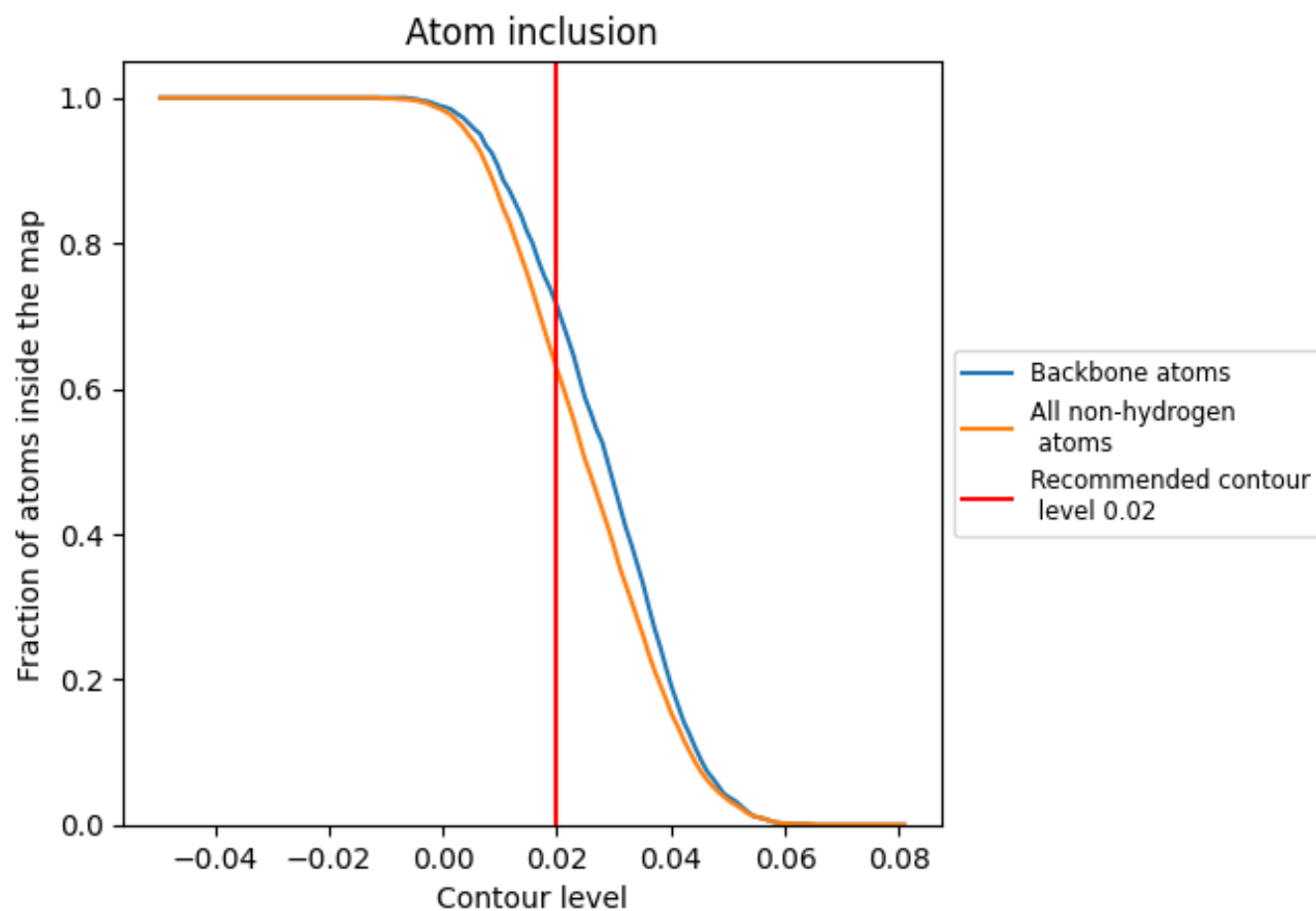
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6270	<div></div> 0.4790
S	<div></div> 0.6010	<div></div> 0.4650
T	<div></div> 0.6680	<div></div> 0.5020
U	<div></div> 0.6120	<div></div> 0.4710

