



## Full wwPDB EM Validation Report ⓘ

Nov 17, 2024 – 12:34 AM JST

PDB ID : 8WCK  
EMDB ID : EMD-37441  
Title : FCP tetramer in Chaetoceros gracilis  
Authors : Feng, Y.; Li, Z.; Zhou, C.; Shen, J.-R.; Liu, C.; Wang, W.  
Deposited on : 2023-09-12  
Resolution : 2.71 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

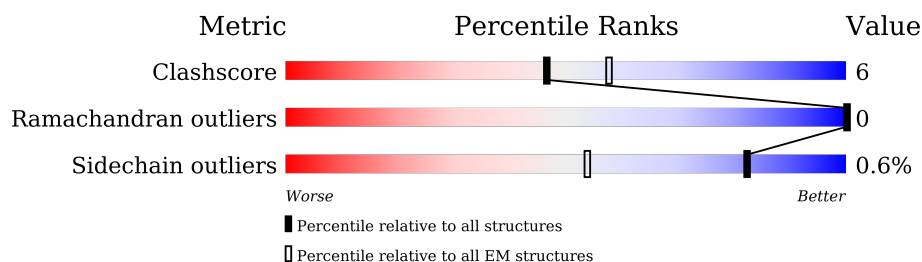
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.71 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	1	207	
1	2	207	
1	3	207	
1	4	207	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	1	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	1	309	X	-	-	-
3	CLA	1	312	X	-	-	-
3	CLA	1	314	X	-	-	-
3	CLA	1	315	X	-	-	-
3	CLA	1	318	X	-	-	-
3	CLA	2	401	X	-	-	-
3	CLA	2	408	X	-	-	-
3	CLA	2	409	X	-	-	-
3	CLA	2	411	X	-	-	-
3	CLA	2	414	X	-	-	-
3	CLA	2	416	X	-	-	-
3	CLA	2	417	X	-	-	-
3	CLA	3	307	X	-	-	-
3	CLA	3	308	X	-	-	-
3	CLA	3	310	X	-	-	-
3	CLA	3	313	X	-	-	-
3	CLA	3	315	X	-	-	-
3	CLA	3	316	X	-	-	-
3	CLA	4	307	X	-	-	-
3	CLA	4	309	X	-	-	-
3	CLA	4	312	X	-	-	-
3	CLA	4	314	X	-	-	-
3	CLA	4	315	X	-	-	-

## 2 Entry composition i

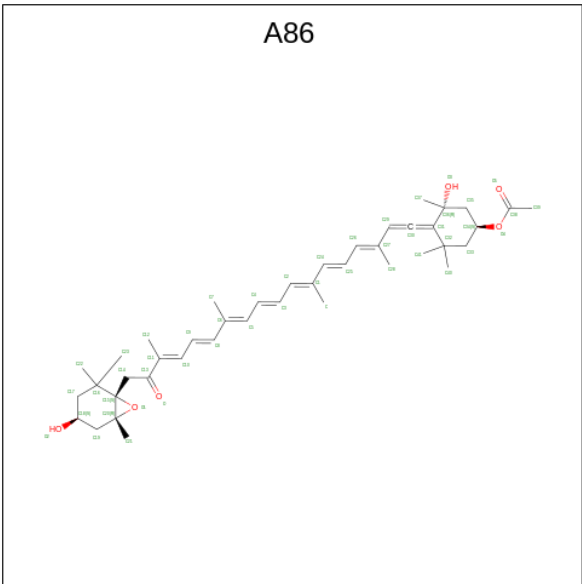
There are 6 unique types of molecules in this entry. The entry contains 8612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
1	2	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
1	3	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
1	4	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		

- Molecule 2 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (three-letter code: A86) (formula: C<sub>42</sub>H<sub>58</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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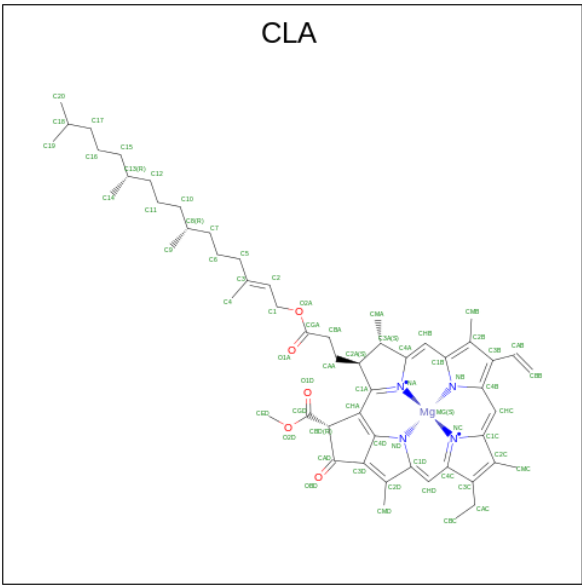
Mol	Chain	Residues	Atoms			AltConf
2	1	1	Total	C	O	0
			48	42	6	
2	1	1	Total	C	O	0
			48	42	6	
2	1	1	Total	C	O	0
			48	42	6	
2	1	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
2	4	1	Total	C	O	0
			48	42	6	

- Molecule 3 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



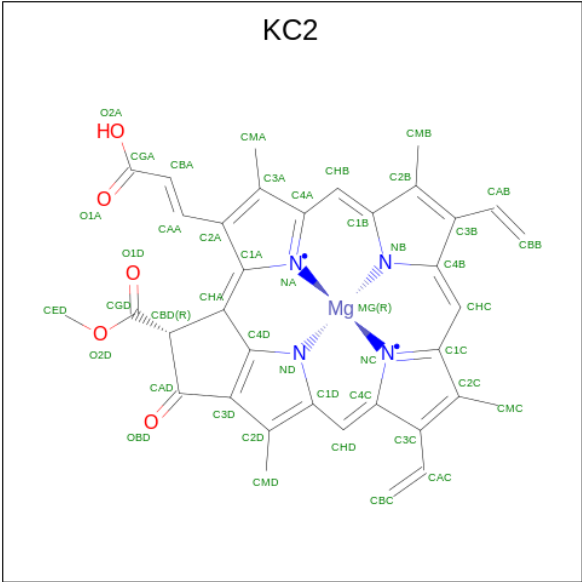
Mol	Chain	Residues	Atoms					AltConf
3	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
3	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

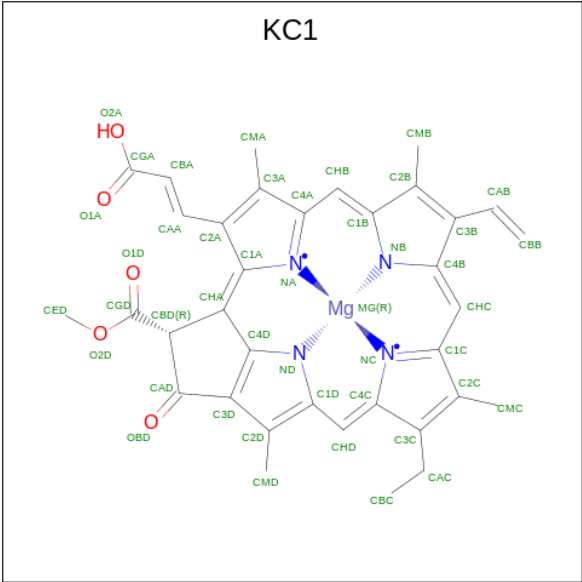
- Molecule 4 is Chlorophyll c2 (three-letter code: KC2) (formula:  $C_{35}H_{28}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

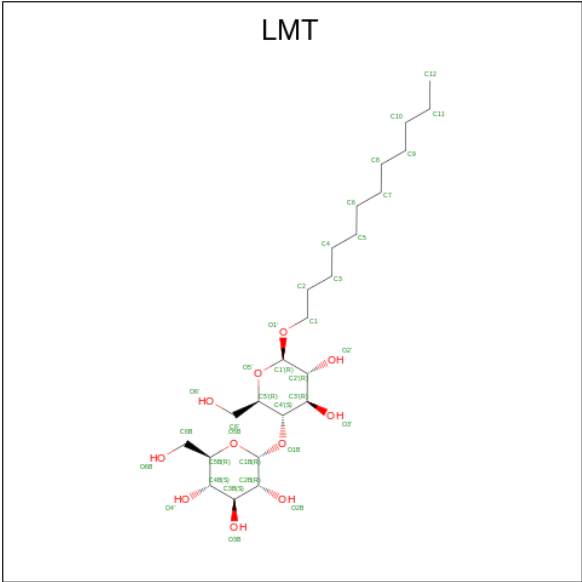
- Molecule 5 is Chlorophyll c1 (three-letter code: KC1) (formula: C<sub>35</sub>H<sub>30</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
5	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 6 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).

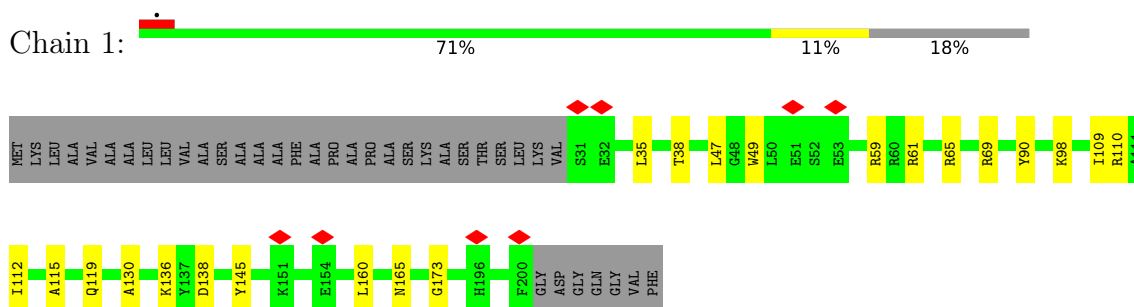


Mol	Chain	Residues	Atoms			AltConf
6	1	1	Total	C	O	0
			28	17	11	
6	1	1	Total	C	O	0
			32	21	11	
6	2	1	Total	C	O	0
			28	17	11	
6	2	1	Total	C	O	0
			32	21	11	
6	3	1	Total	C	O	0
			28	17	11	
6	3	1	Total	C	O	0
			32	21	11	
6	4	1	Total	C	O	0
			28	17	11	
6	4	1	Total	C	O	0
			32	21	11	

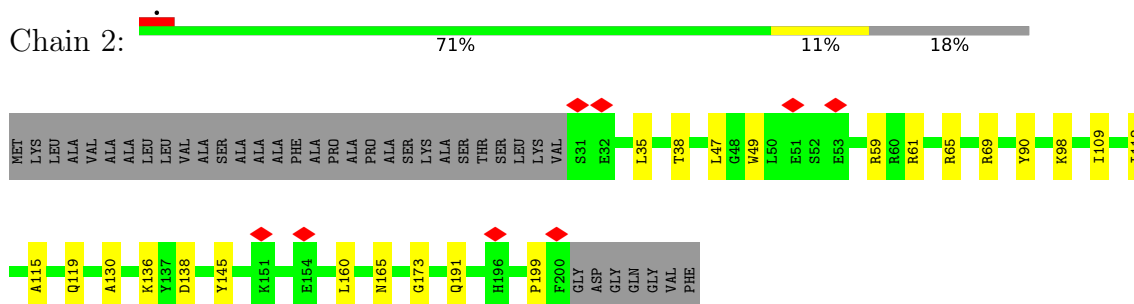
### 3 Residue-property plots [i](#)

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.

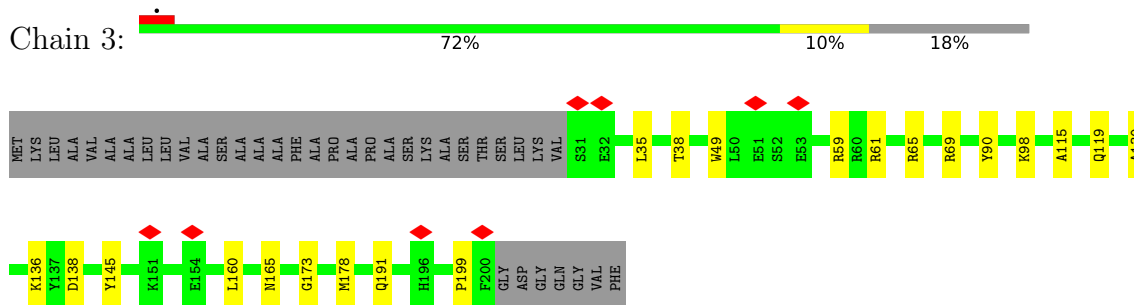
- Molecule 1: Chlorophyll a/b-binding protein



- Molecule 1: Chlorophyll a/b-binding protein

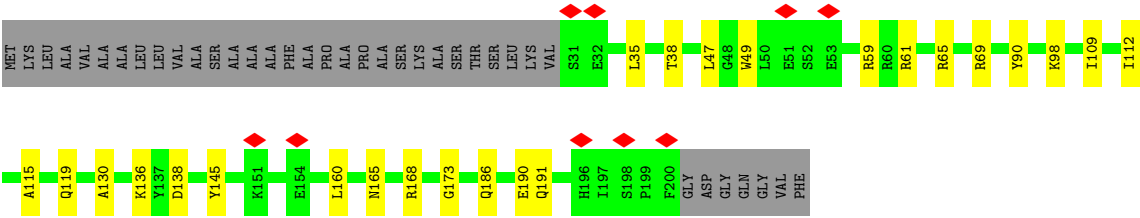


- Molecule 1: Chlorophyll a/b-binding protein



- Molecule 1: Chlorophyll a/b-binding protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	946436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.174	Depositor
Minimum map value	-0.373	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: CLA, KC2, KC1, A86, LMT

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	1	0.31	0/1337	0.47	0/1813
1	2	0.31	0/1337	0.47	0/1813
1	3	0.31	0/1337	0.47	0/1813
1	4	0.31	0/1337	0.47	0/1813
All	All	0.31	0/5348	0.47	0/7252

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1307	0	1276	18	0
1	2	1307	0	1276	20	0
1	3	1307	0	1276	18	0
1	4	1307	0	1276	19	0
2	1	288	0	0	3	0
2	2	288	0	0	4	0
2	3	288	0	0	3	0
2	4	288	0	0	2	0
3	1	318	0	280	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	383	0	352	19	0
3	3	318	0	280	14	0
3	4	253	0	208	9	0
4	1	90	0	0	1	0
4	2	90	0	0	1	0
4	3	90	0	0	1	0
4	4	90	0	0	1	0
5	1	90	0	0	0	0
5	2	90	0	0	0	0
5	3	90	0	0	0	0
5	4	90	0	0	0	0
6	1	60	0	64	1	0
6	2	60	0	64	1	0
6	3	60	0	64	1	0
6	4	60	0	64	1	0
All	All	8612	0	6480	89	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 6.

All (89) 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)
1:1:165:ASN:ND2	3:2:401:CLA:O1D	2.34	0.61
3:1:318:CLA:O1D	1:4:165:ASN:ND2	2.34	0.60
1:2:165:ASN:ND2	3:2:408:CLA:O1D	2.34	0.60
1:3:165:ASN:ND2	3:3:307:CLA:O1D	2.34	0.58
2:2:405:A86:C24	3:2:414:CLA:HAB	2.34	0.58
2:3:304:A86:C24	3:3:313:CLA:HAB	2.34	0.58
2:4:304:A86:C24	3:4:312:CLA:HAB	2.34	0.58
2:1:304:A86:C24	3:1:312:CLA:HAB	2.34	0.57
1:1:110:ARG:NH2	3:1:315:CLA:O1D	2.38	0.56
1:2:145:TYR:HB2	3:2:414:CLA:HAA1	1.91	0.53
1:1:145:TYR:HB2	3:1:312:CLA:HAA1	1.91	0.52
1:3:145:TYR:HB2	3:3:313:CLA:H3A	1.92	0.52
1:4:115:ALA:O	1:4:119:GLN:HG3	2.10	0.51
1:3:115:ALA:O	1:3:119:GLN:HG3	2.10	0.51
1:2:112:ILE:HD11	3:2:411:CLA:H3A	1.93	0.51
1:3:145:TYR:HB2	3:3:313:CLA:HAA1	1.91	0.51
1:1:115:ALA:O	1:1:119:GLN:HG3	2.10	0.51
1:1:112:ILE:HD11	3:1:309:CLA:H3A	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:115:ALA:O	1:2:119:GLN:HG3	2.11	0.50
1:4:145:TYR:HB2	3:4:312:CLA:HAA1	1.93	0.50
1:1:145:TYR:HB2	3:1:312:CLA:H3A	1.93	0.49
1:2:145:TYR:HB2	3:2:414:CLA:H3A	1.95	0.49
1:4:112:ILE:HD11	3:4:309:CLA:H3A	1.94	0.49
1:1:109:ILE:HD12	1:1:112:ILE:HD12	1.96	0.47
1:4:90:TYR:HA	1:4:98:LYS:HA	1.97	0.47
1:2:90:TYR:HA	1:2:98:LYS:HA	1.98	0.46
1:3:59:ARG:NH1	4:3:309:KC2:O2A	2.48	0.46
1:1:173:GLY:HA2	3:1:314:CLA:HBB1	1.97	0.46
1:2:173:GLY:HA2	3:2:416:CLA:HBB1	1.98	0.46
1:3:173:GLY:HA2	3:3:315:CLA:HBB1	1.98	0.46
1:1:59:ARG:NH1	4:1:308:KC2:O2A	2.48	0.46
1:4:173:GLY:HA2	3:4:314:CLA:HBB1	1.98	0.45
3:1:318:CLA:H93	3:1:318:CLA:H111	1.72	0.45
1:2:59:ARG:NH1	4:2:410:KC2:O2A	2.49	0.45
1:4:191:GLN:NE2	3:4:314:CLA:O1D	2.50	0.45
1:1:90:TYR:HA	1:1:98:LYS:HA	1.99	0.45
3:1:318:CLA:HMA3	1:4:38:THR:HG22	1.98	0.45
1:4:59:ARG:NH1	4:4:308:KC2:O2A	2.49	0.44
1:3:35:LEU:HD11	1:3:160:LEU:HD13	1.99	0.44
1:3:38:THR:HG22	3:3:307:CLA:HMA3	1.99	0.44
1:1:136:LYS:HG2	1:1:138:ASP:OD1	2.18	0.44
1:2:38:THR:HG22	3:2:408:CLA:HMA3	1.99	0.44
1:4:61:ARG:NH2	3:4:307:CLA:O1D	2.51	0.44
1:2:109:ILE:HD12	1:2:112:ILE:HD12	1.99	0.44
1:3:90:TYR:HA	1:3:98:LYS:HA	2.00	0.44
1:4:109:ILE:HD12	1:4:112:ILE:HD12	1.99	0.44
1:1:61:ARG:NH2	3:1:307:CLA:O1D	2.51	0.43
1:1:35:LEU:HD11	1:1:160:LEU:HD13	2.00	0.43
1:1:38:THR:HG22	3:2:401:CLA:HMA3	1.98	0.43
1:4:35:LEU:HD11	1:4:160:LEU:HD13	1.99	0.43
1:2:35:LEU:HD11	1:2:160:LEU:HD13	1.99	0.43
1:4:65:ARG:HD3	1:4:69:ARG:NH2	2.34	0.43
1:2:136:LYS:HG2	1:2:138:ASP:OD1	2.19	0.43
1:3:65:ARG:HD3	1:3:69:ARG:NH2	2.33	0.43
1:1:65:ARG:HD3	1:1:69:ARG:NH2	2.33	0.43
1:3:136:LYS:HG2	1:3:138:ASP:OD1	2.19	0.43
2:1:303:A86:C25	3:1:307:CLA:HMC2	2.49	0.43
2:2:404:A86:C25	3:2:409:CLA:HMC2	2.49	0.43
3:2:408:CLA:H93	3:2:408:CLA:H111	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:61:ARG:NH2	3:2:409:CLA:O1D	2.51	0.42
1:2:65:ARG:HD3	1:2:69:ARG:NH2	2.33	0.42
2:3:303:A86:C25	3:3:308:CLA:HMC2	2.49	0.42
1:1:49:TRP:HZ3	3:1:307:CLA:H42	1.84	0.42
1:3:49:TRP:HZ3	3:3:308:CLA:H42	1.84	0.42
2:4:303:A86:C25	3:4:307:CLA:HMC2	2.49	0.42
2:1:305:A86:O	3:1:315:CLA:HAA2	2.19	0.42
1:4:49:TRP:HZ3	3:4:307:CLA:H42	1.84	0.42
1:4:136:LYS:HG2	1:4:138:ASP:OD1	2.19	0.42
1:2:49:TRP:HZ3	3:2:409:CLA:H42	1.84	0.42
1:3:61:ARG:NH2	3:3:308:CLA:O1D	2.53	0.41
1:1:59:ARG:HD2	6:1:317:LMT:H3B	2.02	0.41
3:2:408:CLA:C2B	1:3:130:ALA:HB1	2.50	0.41
2:3:305:A86:O	3:3:316:CLA:HAA2	2.20	0.41
1:4:186:GLN:HB3	1:4:190:GLU:HB2	2.02	0.41
1:2:130:ALA:HB1	3:2:401:CLA:C2B	2.51	0.41
1:1:130:ALA:HB1	3:1:318:CLA:C2B	2.50	0.41
1:2:90:TYR:O	2:2:403:A86:O3	2.37	0.41
1:3:199:PRO:HD3	3:3:315:CLA:HAA1	2.01	0.41
1:2:199:PRO:HD3	3:2:416:CLA:HAA1	2.02	0.41
1:3:191:GLN:NE2	3:3:315:CLA:O1D	2.51	0.41
1:2:59:ARG:HD2	6:2:419:LMT:H3B	2.02	0.41
3:2:401:CLA:H93	3:2:401:CLA:H111	1.72	0.41
1:2:191:GLN:NE2	3:2:416:CLA:O1D	2.51	0.40
1:4:59:ARG:HD2	6:4:317:LMT:H3B	2.02	0.40
1:4:168:ARG:HB3	3:4:307:CLA:CAC	2.52	0.40
2:2:402:A86:O	3:2:408:CLA:HAC2	2.22	0.40
1:3:59:ARG:HD2	6:3:318:LMT:H3B	2.02	0.40
1:3:178:MET:HE3	3:3:316:CLA:HHB	2.03	0.40
3:3:307:CLA:C2B	1:4:130:ALA:HB1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	1	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
1	2	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
1	3	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
1	4	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
All	All	672/828 (81%)	660 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1	135/158 (85%)	134 (99%)	1 (1%)	81	92
1	2	135/158 (85%)	134 (99%)	1 (1%)	81	92
1	3	135/158 (85%)	135 (100%)	0	100	100
1	4	135/158 (85%)	134 (99%)	1 (1%)	81	92
All	All	540/632 (85%)	537 (99%)	3 (1%)	82	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	47	LEU
1	2	47	LEU
1	4	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

72 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	A86	4	302	-	44,50,50	1.26	5 (11%)	51,76,76	3.20	13 (25%)
3	CLA	4	312	1	47,55,73	1.71	6 (12%)	54,91,113	1.60	7 (12%)
6	LMT	1	316	-	29,29,36	1.31	5 (17%)	40,40,47	1.05	3 (7%)
5	KC1	2	413	1	48,53,53	1.56	7 (14%)	55,89,89	1.85	11 (20%)
5	KC1	3	314	-	48,53,53	1.59	7 (14%)	55,89,89	1.88	10 (18%)
4	KC2	2	412	-	48,53,53	1.88	10 (20%)	54,89,89	2.11	14 (25%)
2	A86	2	405	-	44,50,50	1.24	3 (6%)	51,76,76	3.48	19 (37%)
4	KC2	4	310	-	48,53,53	1.88	10 (20%)	54,89,89	2.12	14 (25%)
3	CLA	4	315	-	46,54,73	1.78	6 (13%)	53,90,113	1.51	7 (13%)
3	CLA	2	414	1	47,55,73	1.73	6 (12%)	54,91,113	1.60	8 (14%)
2	A86	1	304	-	44,50,50	1.25	3 (6%)	51,76,76	3.47	19 (37%)
3	CLA	3	307	-	65,73,73	1.45	6 (9%)	76,113,113	1.45	7 (9%)
5	KC1	1	313	-	48,53,53	1.59	7 (14%)	55,89,89	1.88	10 (18%)
2	A86	4	303	-	44,50,50	1.28	4 (9%)	51,76,76	4.97	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CLA	4	314	-	46,54,73	1.72	6 (13%)	53,90,113	1.53	6 (11%)
4	KC2	3	311	-	48,53,53	1.88	10 (20%)	54,89,89	2.11	14 (25%)
5	KC1	4	311	1	48,53,53	1.55	7 (14%)	55,89,89	1.85	11 (20%)
3	CLA	1	318	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
3	CLA	4	309	-	55,63,73	1.59	6 (10%)	64,101,113	1.46	8 (12%)
2	A86	3	305	-	44,50,50	1.22	3 (6%)	51,76,76	3.73	15 (29%)
3	CLA	2	408	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	8 (10%)
2	A86	1	302	-	44,50,50	1.27	5 (11%)	51,76,76	3.20	13 (25%)
5	KC1	3	312	1	48,53,53	1.56	7 (14%)	55,89,89	1.84	11 (20%)
3	CLA	1	312	1	47,55,73	1.72	6 (12%)	54,91,113	1.60	7 (12%)
2	A86	2	406	-	44,50,50	1.21	3 (6%)	51,76,76	3.74	14 (27%)
6	LMT	1	317	-	33,33,36	1.23	5 (15%)	44,44,47	1.00	2 (4%)
2	A86	3	306	-	44,50,50	1.24	3 (6%)	51,76,76	3.49	15 (29%)
3	CLA	3	316	-	46,54,73	1.79	6 (13%)	53,90,113	1.52	7 (13%)
6	LMT	3	317	-	29,29,36	1.32	6 (20%)	40,40,47	1.04	3 (7%)
2	A86	1	301	-	44,50,50	1.25	4 (9%)	51,76,76	4.15	16 (31%)
2	A86	2	402	-	44,50,50	1.25	4 (9%)	51,76,76	4.14	16 (31%)
2	A86	3	301	-	44,50,50	1.25	4 (9%)	51,76,76	4.15	16 (31%)
2	A86	4	306	-	44,50,50	1.24	3 (6%)	51,76,76	3.03	15 (29%)
3	CLA	4	307	1	59,67,73	1.51	7 (11%)	68,105,113	1.48	7 (10%)
3	CLA	1	315	-	46,54,73	1.78	5 (10%)	53,90,113	1.52	7 (13%)
3	CLA	3	313	1	47,55,73	1.72	6 (12%)	54,91,113	1.59	7 (12%)
2	A86	4	301	-	44,50,50	1.26	4 (9%)	51,76,76	4.14	16 (31%)
2	A86	3	302	-	44,50,50	1.27	5 (11%)	51,76,76	3.20	13 (25%)
2	A86	4	305	-	44,50,50	1.22	3 (6%)	51,76,76	3.74	14 (27%)
3	CLA	3	315	-	46,54,73	1.71	6 (13%)	53,90,113	1.53	6 (11%)
3	CLA	1	314	-	46,54,73	1.71	6 (13%)	53,90,113	1.53	6 (11%)
5	KC1	2	415	1	48,53,53	1.59	7 (14%)	55,89,89	1.89	10 (18%)
2	A86	2	404	-	44,50,50	1.28	4 (9%)	51,76,76	4.92	13 (25%)
6	LMT	3	318	-	33,33,36	1.22	5 (15%)	44,44,47	0.99	2 (4%)
3	CLA	1	309	-	55,63,73	1.59	6 (10%)	64,101,113	1.46	9 (14%)
4	KC2	3	309	-	48,53,53	1.88	11 (22%)	54,89,89	2.17	15 (27%)
3	CLA	3	310	-	55,63,73	1.60	6 (10%)	64,101,113	1.46	9 (14%)
3	CLA	2	417	-	46,54,73	1.78	6 (13%)	53,90,113	1.52	7 (13%)
3	CLA	2	409	1	59,67,73	1.50	7 (11%)	68,105,113	1.48	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A86	3	304	-	44,50,50	1.24	3 (6%)	51,76,76	3.46	19 (37%)
3	CLA	1	307	1	59,67,73	1.50	7 (11%)	68,105,113	1.48	7 (10%)
4	KC2	4	308	-	48,53,53	1.88	10 (20%)	54,89,89	2.17	15 (27%)
5	KC1	1	311	1	48,53,53	1.55	7 (14%)	55,89,89	1.86	11 (20%)
2	A86	1	305	-	44,50,50	1.23	3 (6%)	51,76,76	3.73	15 (29%)
6	LMT	2	419	-	33,33,36	1.23	5 (15%)	44,44,47	0.99	2 (4%)
2	A86	2	403	-	44,50,50	1.26	5 (11%)	51,76,76	3.20	12 (23%)
6	LMT	2	418	-	29,29,36	1.32	6 (20%)	40,40,47	1.04	2 (5%)
2	A86	1	303	-	44,50,50	1.28	4 (9%)	51,76,76	4.98	13 (25%)
4	KC2	1	308	-	48,53,53	1.88	10 (20%)	54,89,89	2.17	15 (27%)
3	CLA	2	411	-	55,63,73	1.59	6 (10%)	64,101,113	1.46	9 (14%)
2	A86	1	306	-	44,50,50	1.28	4 (9%)	51,76,76	4.38	18 (35%)
2	A86	4	304	-	44,50,50	1.24	3 (6%)	51,76,76	3.46	19 (37%)
4	KC2	1	310	-	48,53,53	1.87	10 (20%)	54,89,89	2.13	14 (25%)
3	CLA	3	308	1	59,67,73	1.50	7 (11%)	68,105,113	1.49	7 (10%)
5	KC1	4	313	-	48,53,53	1.58	7 (14%)	55,89,89	1.87	11 (20%)
6	LMT	4	317	-	33,33,36	1.22	5 (15%)	44,44,47	0.99	2 (4%)
3	CLA	2	401	-	65,73,73	1.45	6 (9%)	76,113,113	1.45	7 (9%)
2	A86	3	303	-	44,50,50	1.28	3 (6%)	51,76,76	5.09	13 (25%)
6	LMT	4	316	-	29,29,36	1.32	5 (17%)	40,40,47	1.06	3 (7%)
2	A86	2	407	-	44,50,50	1.24	3 (6%)	51,76,76	3.16	15 (29%)
3	CLA	2	416	-	46,54,73	1.71	6 (13%)	53,90,113	1.54	6 (11%)
4	KC2	2	410	-	48,53,53	1.88	11 (22%)	54,89,89	2.17	15 (27%)

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	A86	4	302	-	-	11/34/90/90	0/3/3/3
3	CLA	4	312	1	1/1/11/20	7/16/94/115	-
6	LMT	1	316	-	-	6/14/54/61	0/2/2/2
5	KC1	2	413	1	-	4/15/71/71	-
5	KC1	3	314	-	-	6/15/71/71	-
4	KC2	2	412	-	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A86	2	405	-	-	8/34/90/90	0/3/3/3
4	KC2	4	310	-	-	8/15/71/71	-
3	CLA	4	315	-	1/1/11/20	7/15/93/115	-
3	CLA	2	414	1	1/1/11/20	7/16/94/115	-
2	A86	1	304	-	-	8/34/90/90	0/3/3/3
3	CLA	3	307	-	1/1/15/20	10/37/115/115	-
5	KC1	1	313	-	-	5/15/71/71	-
3	CLA	4	314	-	1/1/11/20	7/15/93/115	-
2	A86	4	303	-	-	9/34/90/90	0/3/3/3
4	KC2	3	311	-	-	8/15/71/71	-
5	KC1	4	311	1	-	4/15/71/71	-
3	CLA	1	318	-	1/1/15/20	10/37/115/115	-
3	CLA	4	309	-	1/1/13/20	11/25/103/115	-
2	A86	3	305	-	-	15/34/90/90	0/3/3/3
3	CLA	2	408	-	1/1/15/20	10/37/115/115	-
2	A86	1	302	-	-	11/34/90/90	0/3/3/3
5	KC1	3	312	1	-	4/15/71/71	-
3	CLA	1	312	1	1/1/11/20	7/16/94/115	-
2	A86	2	406	-	-	15/34/90/90	0/3/3/3
6	LMT	1	317	-	-	9/18/58/61	0/2/2/2
2	A86	3	306	-	-	10/34/90/90	0/3/3/3
3	CLA	3	316	-	1/1/11/20	5/15/93/115	-
6	LMT	3	317	-	-	5/14/54/61	0/2/2/2
2	A86	1	301	-	-	9/34/90/90	0/3/3/3
3	CLA	4	307	1	1/1/13/20	6/30/108/115	-
2	A86	2	402	-	-	9/34/90/90	0/3/3/3
2	A86	3	301	-	-	9/34/90/90	0/3/3/3
2	A86	4	306	-	-	10/34/90/90	0/3/3/3
3	CLA	1	315	-	1/1/11/20	8/15/93/115	-
3	CLA	3	313	1	1/1/11/20	7/16/94/115	-
2	A86	4	301	-	-	9/34/90/90	0/3/3/3
2	A86	3	302	-	-	11/34/90/90	0/3/3/3
2	A86	4	305	-	-	15/34/90/90	0/3/3/3
3	CLA	3	315	-	1/1/11/20	7/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	1	314	-	1/1/11/20	9/15/93/115	-
5	KC1	2	415	1	-	6/15/71/71	-
2	A86	2	404	-	-	9/34/90/90	0/3/3/3
6	LMT	3	318	-	-	9/18/58/61	0/2/2/2
3	CLA	1	309	-	1/1/13/20	11/25/103/115	-
4	KC2	3	309	-	-	9/15/71/71	-
3	CLA	3	310	-	1/1/13/20	11/25/103/115	-
3	CLA	2	417	-	1/1/11/20	5/15/93/115	-
3	CLA	2	409	1	1/1/13/20	6/30/108/115	-
3	CLA	1	307	1	1/1/13/20	6/30/108/115	-
2	A86	3	304	-	-	8/34/90/90	0/3/3/3
4	KC2	4	308	-	-	9/15/71/71	-
5	KC1	1	311	1	-	4/15/71/71	-
2	A86	1	305	-	-	15/34/90/90	0/3/3/3
6	LMT	2	419	-	-	9/18/58/61	0/2/2/2
2	A86	2	403	-	-	11/34/90/90	0/3/3/3
6	LMT	2	418	-	-	6/14/54/61	0/2/2/2
2	A86	1	303	-	-	9/34/90/90	0/3/3/3
4	KC2	1	308	-	-	10/15/71/71	-
3	CLA	2	411	-	1/1/13/20	11/25/103/115	-
2	A86	1	306	-	-	8/34/90/90	0/3/3/3
2	A86	4	304	-	-	8/34/90/90	0/3/3/3
4	KC2	1	310	-	-	8/15/71/71	-
3	CLA	3	308	1	1/1/13/20	6/30/108/115	-
5	KC1	4	313	-	-	6/15/71/71	-
6	LMT	4	317	-	-	9/18/58/61	0/2/2/2
3	CLA	2	401	-	1/1/15/20	10/37/115/115	-
2	A86	3	303	-	-	9/34/90/90	0/3/3/3
6	LMT	4	316	-	-	6/14/54/61	0/2/2/2
2	A86	2	407	-	-	10/34/90/90	0/3/3/3
3	CLA	2	416	-	1/1/11/20	7/15/93/115	-
4	KC2	2	410	-	-	9/15/71/71	-

All (416) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	316	CLA	C4B-NB	7.71	1.42	1.35
3	4	315	CLA	C4B-NB	7.71	1.42	1.35
3	1	315	CLA	C4B-NB	7.62	1.42	1.35
3	2	417	CLA	C4B-NB	7.60	1.42	1.35
3	3	310	CLA	C4B-NB	7.28	1.41	1.35
3	1	309	CLA	C4B-NB	7.25	1.41	1.35
3	2	411	CLA	C4B-NB	7.25	1.41	1.35
3	2	414	CLA	C4B-NB	7.23	1.41	1.35
3	4	309	CLA	C4B-NB	7.15	1.41	1.35
3	1	312	CLA	C4B-NB	7.13	1.41	1.35
3	3	313	CLA	C4B-NB	7.13	1.41	1.35
5	3	314	KC1	C4D-CHA	-7.10	1.36	1.45
3	4	312	CLA	C4B-NB	7.09	1.41	1.35
5	1	313	KC1	C4D-CHA	-7.05	1.36	1.45
5	2	415	KC1	C4D-CHA	-7.03	1.36	1.45
5	4	313	KC1	C4D-CHA	-7.03	1.36	1.45
3	4	314	CLA	C4B-NB	7.02	1.41	1.35
3	2	401	CLA	C4B-NB	7.01	1.41	1.35
3	3	315	CLA	C4B-NB	7.00	1.41	1.35
3	2	416	CLA	C4B-NB	6.99	1.41	1.35
3	1	314	CLA	C4B-NB	6.97	1.41	1.35
3	3	307	CLA	C4B-NB	6.96	1.41	1.35
3	4	307	CLA	C4B-NB	6.92	1.41	1.35
3	1	318	CLA	C4B-NB	6.92	1.41	1.35
3	2	408	CLA	C4B-NB	6.92	1.41	1.35
3	1	307	CLA	C4B-NB	6.91	1.41	1.35
3	2	409	CLA	C4B-NB	6.83	1.41	1.35
3	3	308	CLA	C4B-NB	6.81	1.41	1.35
4	3	311	KC2	C4D-CHA	-6.74	1.36	1.45
4	1	308	KC2	C4D-CHA	-6.71	1.36	1.45
4	4	308	KC2	C4D-CHA	-6.70	1.36	1.45
4	1	310	KC2	C4D-CHA	-6.69	1.36	1.45
4	2	412	KC2	C4D-CHA	-6.69	1.36	1.45
4	3	309	KC2	C4D-CHA	-6.69	1.36	1.45
4	2	410	KC2	C4D-CHA	-6.68	1.36	1.45
4	4	310	KC2	C4D-CHA	-6.68	1.36	1.45
5	2	413	KC1	C4D-CHA	-6.57	1.36	1.45
5	3	312	KC1	C4D-CHA	-6.55	1.36	1.45
5	1	311	KC1	C4D-CHA	-6.51	1.36	1.45
5	4	311	KC1	C4D-CHA	-6.51	1.36	1.45
4	4	308	KC2	CHD-C4C	5.42	1.48	1.35
4	2	412	KC2	CHD-C4C	5.41	1.48	1.35
4	3	311	KC2	CHD-C4C	5.40	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1	310	KC2	CHD-C4C	5.40	1.48	1.35
4	1	308	KC2	CHD-C4C	5.39	1.48	1.35
4	2	410	KC2	CHD-C4C	5.38	1.48	1.35
4	4	310	KC2	CHD-C4C	5.37	1.48	1.35
4	3	309	KC2	CHD-C4C	5.37	1.48	1.35
5	4	311	KC1	MG-NB	-4.86	1.96	2.05
5	4	313	KC1	MG-NB	-4.85	1.96	2.05
5	3	314	KC1	MG-NB	-4.83	1.96	2.05
5	2	415	KC1	MG-NB	-4.82	1.96	2.05
5	1	311	KC1	MG-NB	-4.82	1.96	2.05
5	1	313	KC1	MG-NB	-4.82	1.96	2.05
5	3	312	KC1	MG-NB	-4.81	1.96	2.05
5	2	413	KC1	MG-NB	-4.79	1.96	2.05
2	2	402	A86	O4-C38	4.76	1.46	1.35
2	4	301	A86	O4-C38	4.75	1.45	1.35
2	4	305	A86	O4-C38	4.75	1.45	1.35
2	3	305	A86	O4-C38	4.74	1.45	1.35
2	1	301	A86	O4-C38	4.74	1.45	1.35
2	1	305	A86	O4-C38	4.73	1.45	1.35
2	2	406	A86	O4-C38	4.71	1.45	1.35
2	3	301	A86	O4-C38	4.70	1.45	1.35
2	2	407	A86	O4-C38	4.65	1.45	1.35
2	1	303	A86	O4-C38	4.64	1.45	1.35
2	2	404	A86	O4-C38	4.63	1.45	1.35
2	3	303	A86	O4-C38	4.63	1.45	1.35
2	1	304	A86	O4-C38	4.63	1.45	1.35
2	4	303	A86	O4-C38	4.61	1.45	1.35
2	1	306	A86	O4-C38	4.61	1.45	1.35
2	4	306	A86	O4-C38	4.60	1.45	1.35
2	4	304	A86	O4-C38	4.59	1.45	1.35
2	3	304	A86	O4-C38	4.59	1.45	1.35
2	2	405	A86	O4-C38	4.58	1.45	1.35
2	1	302	A86	O4-C38	4.57	1.45	1.35
2	3	302	A86	O4-C38	4.56	1.45	1.35
2	2	403	A86	O4-C38	4.56	1.45	1.35
2	3	306	A86	O4-C38	4.55	1.45	1.35
2	4	302	A86	O4-C38	4.53	1.45	1.35
4	3	309	KC2	MG-NB	-4.23	1.97	2.05
4	1	308	KC2	MG-NB	-4.22	1.97	2.05
4	4	308	KC2	MG-NB	-4.21	1.97	2.05
4	2	410	KC2	MG-NB	-4.18	1.97	2.05
4	2	412	KC2	MG-NB	-4.14	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	310	KC2	MG-NB	-4.13	1.97	2.05
4	1	310	KC2	MG-NB	-4.13	1.97	2.05
4	3	311	KC2	MG-NB	-4.11	1.97	2.05
4	4	310	KC2	CHC-C1C	4.06	1.48	1.39
4	2	412	KC2	CHC-C1C	4.05	1.48	1.39
4	3	311	KC2	CHC-C1C	4.03	1.48	1.39
4	2	410	KC2	CHC-C1C	4.00	1.48	1.39
4	4	308	KC2	CHC-C1C	4.00	1.48	1.39
4	1	308	KC2	CHC-C1C	3.99	1.48	1.39
4	1	310	KC2	CHC-C1C	3.98	1.48	1.39
4	3	309	KC2	CHC-C1C	3.97	1.48	1.39
4	3	311	KC2	CHC-C4B	3.94	1.46	1.38
4	4	310	KC2	CHC-C4B	3.92	1.46	1.38
4	1	310	KC2	CHC-C4B	3.92	1.46	1.38
4	2	412	KC2	CHC-C4B	3.89	1.45	1.38
4	1	308	KC2	CHC-C4B	3.87	1.45	1.38
4	2	410	KC2	CHC-C4B	3.83	1.45	1.38
4	3	309	KC2	CHC-C4B	3.83	1.45	1.38
3	1	315	CLA	C1D-ND	3.82	1.42	1.37
3	3	316	CLA	C1D-ND	3.82	1.42	1.37
4	4	308	KC2	CHC-C4B	3.82	1.45	1.38
3	2	417	CLA	C1D-ND	3.80	1.42	1.37
3	4	315	CLA	C1D-ND	3.78	1.42	1.37
3	1	318	CLA	C1D-ND	3.77	1.42	1.37
3	3	307	CLA	C1D-ND	3.74	1.42	1.37
3	1	312	CLA	C1D-ND	3.72	1.42	1.37
3	2	408	CLA	C1D-ND	3.71	1.42	1.37
3	3	313	CLA	C1D-ND	3.69	1.42	1.37
2	3	302	A86	C30-C29	-3.69	1.25	1.32
3	2	401	CLA	C1D-ND	3.69	1.42	1.37
2	1	306	A86	C30-C29	-3.68	1.25	1.32
3	2	416	CLA	C1D-ND	3.67	1.42	1.37
2	4	302	A86	C30-C29	-3.66	1.25	1.32
3	4	312	CLA	C1D-ND	3.66	1.42	1.37
3	2	414	CLA	C1D-ND	3.65	1.42	1.37
2	1	302	A86	C30-C29	-3.65	1.25	1.32
3	1	314	CLA	C1D-ND	3.64	1.42	1.37
3	4	314	CLA	C1D-ND	3.64	1.42	1.37
3	3	315	CLA	C1D-ND	3.63	1.42	1.37
2	2	403	A86	C30-C29	-3.62	1.25	1.32
2	2	404	A86	C30-C29	-3.62	1.25	1.32
2	1	303	A86	C30-C29	-3.61	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	303	A86	C30-C29	-3.60	1.26	1.32
2	4	306	A86	C30-C29	-3.57	1.26	1.32
2	2	407	A86	C30-C29	-3.57	1.26	1.32
3	3	310	CLA	C1D-ND	3.57	1.42	1.37
2	4	303	A86	C30-C29	-3.56	1.26	1.32
2	3	306	A86	C30-C29	-3.56	1.26	1.32
3	4	309	CLA	C1D-ND	3.52	1.42	1.37
2	3	301	A86	C30-C29	-3.50	1.26	1.32
2	1	301	A86	C30-C29	-3.50	1.26	1.32
2	2	402	A86	C30-C29	-3.50	1.26	1.32
2	4	301	A86	C30-C29	-3.49	1.26	1.32
3	2	411	CLA	C1D-ND	3.48	1.42	1.37
2	3	305	A86	C30-C29	-3.47	1.26	1.32
3	1	309	CLA	C1D-ND	3.45	1.42	1.37
3	3	308	CLA	C1D-ND	3.45	1.42	1.37
2	2	406	A86	C30-C29	-3.44	1.26	1.32
3	1	307	CLA	C1D-ND	3.44	1.42	1.37
3	4	307	CLA	C1D-ND	3.44	1.42	1.37
2	4	304	A86	C30-C29	-3.43	1.26	1.32
2	4	305	A86	C30-C29	-3.42	1.26	1.32
2	1	305	A86	C30-C29	-3.42	1.26	1.32
3	2	409	CLA	C1D-ND	3.42	1.42	1.37
2	1	304	A86	C30-C29	-3.39	1.26	1.32
2	2	405	A86	C30-C29	-3.39	1.26	1.32
2	3	304	A86	C30-C29	-3.36	1.26	1.32
3	2	409	CLA	C4D-ND	-3.18	1.33	1.37
3	3	308	CLA	C4D-ND	-3.18	1.33	1.37
3	1	315	CLA	CHC-C1C	3.17	1.43	1.35
3	3	316	CLA	CHC-C1C	3.16	1.43	1.35
3	2	417	CLA	CHC-C1C	3.15	1.43	1.35
3	4	315	CLA	CHC-C1C	3.15	1.43	1.35
3	1	314	CLA	C4D-ND	-3.15	1.33	1.37
5	2	415	KC1	C4B-NB	-3.14	1.33	1.37
3	4	309	CLA	C4D-ND	-3.11	1.33	1.37
5	1	311	KC1	C4B-NB	-3.11	1.34	1.37
5	2	413	KC1	C4B-NB	-3.11	1.34	1.37
3	1	309	CLA	CHC-C1C	3.11	1.42	1.35
3	2	401	CLA	C4D-ND	-3.10	1.33	1.37
3	1	307	CLA	CHC-C1C	3.10	1.42	1.35
3	2	409	CLA	CHC-C1C	3.10	1.42	1.35
3	1	307	CLA	C4D-ND	-3.10	1.33	1.37
3	4	307	CLA	C4D-ND	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	313	KC1	C4B-NB	-3.10	1.34	1.37
3	2	411	CLA	CHC-C1C	3.10	1.42	1.35
3	4	314	CLA	C4D-ND	-3.09	1.33	1.37
3	3	308	CLA	CHC-C1C	3.09	1.42	1.35
3	2	416	CLA	C4D-ND	-3.09	1.33	1.37
5	3	312	KC1	C4B-NB	-3.09	1.34	1.37
3	4	309	CLA	CHC-C1C	3.09	1.42	1.35
3	2	408	CLA	C4D-ND	-3.09	1.33	1.37
3	3	310	CLA	C4D-ND	-3.08	1.33	1.37
3	3	310	CLA	CHC-C1C	3.08	1.42	1.35
3	2	411	CLA	C4D-ND	-3.08	1.33	1.37
5	3	314	KC1	C4B-NB	-3.07	1.34	1.37
5	4	313	KC1	C4B-NB	-3.07	1.34	1.37
3	4	312	CLA	CHC-C1C	3.06	1.42	1.35
3	4	307	CLA	CHC-C1C	3.06	1.42	1.35
5	4	311	KC1	C4B-NB	-3.06	1.34	1.37
5	3	312	KC1	CBA-CGA	-3.05	1.41	1.48
3	1	318	CLA	C4D-ND	-3.05	1.33	1.37
3	3	307	CLA	C4D-ND	-3.05	1.33	1.37
3	1	309	CLA	C4D-ND	-3.05	1.33	1.37
5	1	311	KC1	CBA-CGA	-3.03	1.41	1.48
3	3	313	CLA	CHC-C1C	3.03	1.42	1.35
3	1	312	CLA	CHC-C1C	3.03	1.42	1.35
3	2	414	CLA	CHC-C1C	3.03	1.42	1.35
5	2	413	KC1	CBA-CGA	-3.02	1.41	1.48
3	3	315	CLA	C4D-ND	-3.01	1.33	1.37
3	1	312	CLA	C4D-ND	-3.00	1.33	1.37
5	4	311	KC1	CBA-CGA	-2.97	1.41	1.48
3	2	408	CLA	CHC-C1C	2.96	1.42	1.35
3	3	315	CLA	CHC-C1C	2.95	1.42	1.35
4	3	311	KC2	CBA-CGA	-2.95	1.41	1.48
3	4	312	CLA	C4D-ND	-2.94	1.33	1.37
5	1	313	KC1	CBA-CGA	-2.94	1.41	1.48
3	2	414	CLA	C4D-ND	-2.94	1.33	1.37
3	2	416	CLA	CHC-C1C	2.94	1.42	1.35
3	3	313	CLA	C4D-ND	-2.94	1.33	1.37
4	2	412	KC2	CBA-CGA	-2.93	1.41	1.48
3	2	401	CLA	CHC-C1C	2.92	1.42	1.35
4	1	308	KC2	CBA-CGA	-2.92	1.41	1.48
5	2	415	KC1	CBA-CGA	-2.92	1.41	1.48
5	4	313	KC1	CBA-CGA	-2.92	1.41	1.48
3	4	314	CLA	CHC-C1C	2.91	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	307	CLA	CHC-C1C	2.91	1.42	1.35
3	1	314	CLA	CHC-C1C	2.91	1.42	1.35
3	3	316	CLA	C4D-ND	-2.90	1.33	1.37
3	1	318	CLA	CHC-C1C	2.90	1.42	1.35
4	2	410	KC2	CBA-CGA	-2.89	1.41	1.48
4	4	308	KC2	CBA-CGA	-2.89	1.41	1.48
3	2	417	CLA	C4D-ND	-2.89	1.33	1.37
3	1	315	CLA	C4D-ND	-2.89	1.33	1.37
4	4	310	KC2	CBA-CGA	-2.88	1.41	1.48
4	3	309	KC2	CBA-CGA	-2.88	1.41	1.48
5	3	314	KC1	CBA-CGA	-2.88	1.41	1.48
3	4	315	CLA	C4D-ND	-2.87	1.33	1.37
4	1	310	KC2	CBA-CGA	-2.86	1.41	1.48
2	3	303	A86	O1-C20	-2.83	1.42	1.46
2	2	404	A86	O1-C20	-2.82	1.42	1.46
2	4	303	A86	O1-C20	-2.78	1.42	1.46
6	2	419	LMT	O3'-C3'	-2.78	1.36	1.43
2	1	303	A86	O1-C20	-2.77	1.42	1.46
6	1	317	LMT	O3'-C3'	-2.75	1.36	1.43
6	4	317	LMT	O3'-C3'	-2.75	1.36	1.43
6	3	318	LMT	O3'-C3'	-2.75	1.36	1.43
6	2	418	LMT	O3'-C3'	-2.68	1.36	1.43
6	1	316	LMT	O3'-C3'	-2.67	1.36	1.43
6	4	316	LMT	O3'-C3'	-2.67	1.36	1.43
6	3	317	LMT	O3'-C3'	-2.65	1.36	1.43
4	1	308	KC2	C4B-NB	-2.65	1.34	1.37
4	3	309	KC2	C4B-NB	-2.65	1.34	1.37
4	4	310	KC2	C4B-NB	-2.65	1.34	1.37
4	2	412	KC2	C4B-NB	-2.61	1.34	1.37
4	3	311	KC2	C4B-NB	-2.61	1.34	1.37
4	2	410	KC2	C4B-NB	-2.61	1.34	1.37
5	1	311	KC1	C1B-NB	-2.61	1.34	1.37
2	1	306	A86	O1-C20	-2.59	1.42	1.46
4	1	310	KC2	C4B-NB	-2.59	1.34	1.37
4	4	308	KC2	C4B-NB	-2.58	1.34	1.37
5	3	312	KC1	C1B-NB	-2.58	1.34	1.37
3	2	414	CLA	CMB-C2B	-2.57	1.46	1.51
5	4	311	KC1	C1B-NB	-2.56	1.34	1.37
3	1	312	CLA	CMB-C2B	-2.56	1.46	1.51
3	3	313	CLA	CMB-C2B	-2.56	1.46	1.51
3	4	312	CLA	CMB-C2B	-2.56	1.46	1.51
5	2	413	KC1	C1B-NB	-2.56	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	415	KC1	C1B-NB	-2.56	1.34	1.37
5	4	313	KC1	C1B-NB	-2.56	1.34	1.37
5	1	313	KC1	C1B-NB	-2.56	1.34	1.37
5	3	314	KC1	C1B-NB	-2.55	1.34	1.37
3	4	314	CLA	CMB-C2B	-2.55	1.46	1.51
3	3	310	CLA	CMB-C2B	-2.53	1.46	1.51
3	1	309	CLA	CMB-C2B	-2.52	1.46	1.51
3	2	411	CLA	CMB-C2B	-2.52	1.46	1.51
3	4	309	CLA	CMB-C2B	-2.52	1.46	1.51
3	3	307	CLA	CMB-C2B	-2.50	1.46	1.51
3	3	315	CLA	CMB-C2B	-2.50	1.46	1.51
3	1	314	CLA	CMB-C2B	-2.50	1.46	1.51
3	4	307	CLA	CMB-C2B	-2.49	1.46	1.51
2	1	304	A86	O1-C20	-2.49	1.42	1.46
3	2	416	CLA	CMB-C2B	-2.49	1.46	1.51
2	1	305	A86	O1-C20	-2.48	1.42	1.46
3	2	409	CLA	CMB-C2B	-2.47	1.46	1.51
3	3	316	CLA	CMB-C2B	-2.46	1.46	1.51
2	2	405	A86	O1-C20	-2.46	1.42	1.46
3	2	417	CLA	CMB-C2B	-2.46	1.46	1.51
5	3	312	KC1	C4A-C3A	-2.46	1.39	1.44
3	3	308	CLA	CMB-C2B	-2.46	1.46	1.51
2	3	304	A86	O1-C20	-2.46	1.42	1.46
3	2	401	CLA	CMB-C2B	-2.46	1.46	1.51
3	2	408	CLA	CMB-C2B	-2.46	1.46	1.51
3	1	318	CLA	CMB-C2B	-2.45	1.46	1.51
3	1	315	CLA	CMB-C2B	-2.45	1.46	1.51
4	4	308	KC2	C4A-C3A	-2.44	1.39	1.44
2	4	304	A86	O1-C20	-2.44	1.42	1.46
5	2	413	KC1	C4A-C3A	-2.44	1.39	1.44
3	1	307	CLA	CMB-C2B	-2.44	1.46	1.51
4	2	410	KC2	C4A-C3A	-2.43	1.39	1.44
4	1	308	KC2	C4A-C3A	-2.43	1.39	1.44
4	3	309	KC2	C4A-C3A	-2.43	1.39	1.44
3	4	315	CLA	CMB-C2B	-2.42	1.46	1.51
6	3	317	LMT	O2'-C2'	-2.40	1.37	1.43
5	1	311	KC1	C4A-C3A	-2.39	1.39	1.44
5	4	311	KC1	C4A-C3A	-2.39	1.39	1.44
2	3	305	A86	O1-C20	-2.39	1.42	1.46
6	3	318	LMT	O2'-C2'	-2.39	1.37	1.43
6	1	316	LMT	O3B-C3B	-2.38	1.37	1.43
6	4	316	LMT	O3B-C3B	-2.37	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	419	LMT	O2'-C2'	-2.37	1.37	1.43
6	1	317	LMT	O2'-C2'	-2.37	1.37	1.43
6	4	317	LMT	O2'-C2'	-2.37	1.37	1.43
6	1	317	LMT	O2B-C2B	-2.37	1.37	1.43
6	3	317	LMT	O3B-C3B	-2.37	1.37	1.43
6	4	317	LMT	O2B-C2B	-2.36	1.37	1.43
4	2	412	KC2	C4A-C3A	-2.36	1.40	1.44
6	2	418	LMT	O3B-C3B	-2.36	1.37	1.43
4	1	310	KC2	C4A-C3A	-2.36	1.40	1.44
6	2	419	LMT	O2B-C2B	-2.35	1.37	1.43
4	4	310	KC2	C4A-C3A	-2.35	1.40	1.44
6	4	317	LMT	O3B-C3B	-2.34	1.37	1.43
4	3	311	KC2	C4A-C3A	-2.34	1.40	1.44
6	3	318	LMT	O2B-C2B	-2.34	1.37	1.43
6	4	316	LMT	O2'-C2'	-2.34	1.37	1.43
6	3	318	LMT	O3B-C3B	-2.33	1.37	1.43
6	2	419	LMT	O3B-C3B	-2.33	1.37	1.43
6	1	316	LMT	O2'-C2'	-2.33	1.37	1.43
6	2	418	LMT	O2'-C2'	-2.33	1.37	1.43
6	2	418	LMT	O2B-C2B	-2.32	1.37	1.43
2	3	301	A86	C13-C11	-2.32	1.45	1.49
6	1	316	LMT	O2B-C2B	-2.31	1.37	1.43
6	4	316	LMT	O2B-C2B	-2.31	1.37	1.43
2	4	301	A86	C13-C11	-2.31	1.45	1.49
2	4	302	A86	O1-C20	-2.31	1.42	1.46
6	1	317	LMT	O3B-C3B	-2.31	1.37	1.43
2	1	302	A86	O1-C20	-2.31	1.42	1.46
6	3	317	LMT	O2B-C2B	-2.31	1.37	1.43
2	2	403	A86	O1-C20	-2.30	1.42	1.46
2	3	306	A86	O1-C20	-2.29	1.42	1.46
2	2	407	A86	O1-C20	-2.28	1.42	1.46
2	2	402	A86	C13-C11	-2.28	1.45	1.49
2	3	302	A86	O1-C20	-2.28	1.43	1.46
2	3	301	A86	O1-C20	-2.26	1.43	1.46
2	4	301	A86	O1-C20	-2.26	1.43	1.46
5	2	415	KC1	CHD-C4C	2.26	1.40	1.35
2	1	301	A86	C13-C11	-2.26	1.45	1.49
5	3	314	KC1	CHD-C4C	2.25	1.40	1.35
2	4	306	A86	O1-C20	-2.25	1.43	1.46
2	1	302	A86	C32-C31	-2.25	1.50	1.54
2	1	301	A86	O1-C20	-2.25	1.43	1.46
5	1	313	KC1	CHD-C4C	2.24	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	403	A86	C32-C31	-2.23	1.50	1.54
2	3	302	A86	C32-C31	-2.23	1.50	1.54
2	2	402	A86	O1-C20	-2.23	1.43	1.46
5	2	413	KC1	CHD-C4C	2.22	1.40	1.35
5	4	313	KC1	CHD-C4C	2.22	1.40	1.35
4	4	308	KC2	C1C-C2C	-2.22	1.40	1.44
4	4	310	KC2	C1C-C2C	-2.21	1.40	1.44
5	3	312	KC1	CHD-C4C	2.21	1.40	1.35
4	1	308	KC2	C1C-C2C	-2.20	1.40	1.44
4	3	309	KC2	C1C-C2C	-2.20	1.40	1.44
5	1	311	KC1	CHD-C4C	2.20	1.40	1.35
5	4	311	KC1	CHD-C4C	2.20	1.40	1.35
4	2	410	KC2	C1C-C2C	-2.20	1.40	1.44
2	4	302	A86	C32-C31	-2.20	1.50	1.54
3	3	315	CLA	CMD-C2D	-2.19	1.46	1.50
6	3	318	LMT	O4'-C4B	-2.17	1.37	1.43
4	2	412	KC2	C1C-C2C	-2.17	1.40	1.44
2	4	305	A86	O1-C20	-2.17	1.43	1.46
3	2	416	CLA	CMD-C2D	-2.17	1.46	1.50
3	1	314	CLA	CMD-C2D	-2.17	1.46	1.50
2	2	406	A86	O1-C20	-2.16	1.43	1.46
4	1	310	KC2	C1C-C2C	-2.16	1.40	1.44
6	2	419	LMT	O4'-C4B	-2.16	1.37	1.43
6	4	317	LMT	O4'-C4B	-2.16	1.37	1.43
2	1	302	A86	C13-C11	-2.16	1.45	1.49
6	1	317	LMT	O4'-C4B	-2.14	1.37	1.43
3	4	314	CLA	CMD-C2D	-2.14	1.46	1.50
4	3	311	KC2	C1C-C2C	-2.14	1.40	1.44
4	2	412	KC2	C1D-CHD	2.14	1.46	1.41
3	3	307	CLA	CMD-C2D	-2.14	1.46	1.50
3	2	408	CLA	CMD-C2D	-2.12	1.46	1.50
3	2	409	CLA	CMD-C2D	-2.12	1.46	1.50
3	4	307	CLA	CMD-C2D	-2.12	1.46	1.50
3	1	318	CLA	CMD-C2D	-2.12	1.46	1.50
3	2	401	CLA	CMD-C2D	-2.12	1.46	1.50
5	1	313	KC1	C4A-C3A	-2.12	1.40	1.44
5	3	314	KC1	C4A-C3A	-2.12	1.40	1.44
3	1	307	CLA	CMD-C2D	-2.11	1.46	1.50
4	3	309	KC2	C1B-NB	-2.11	1.35	1.37
6	4	316	LMT	O4'-C4B	-2.11	1.38	1.43
2	3	302	A86	C13-C11	-2.11	1.45	1.49
2	4	302	A86	C13-C11	-2.11	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	308	KC2	C1B-NB	-2.11	1.35	1.37
4	4	310	KC2	C1D-CHD	2.11	1.46	1.41
3	3	313	CLA	CMD-C2D	-2.11	1.46	1.50
4	1	310	KC2	C1D-CHD	2.10	1.46	1.41
4	1	308	KC2	C1B-NB	-2.10	1.35	1.37
3	3	310	CLA	CMD-C2D	-2.10	1.46	1.50
4	2	410	KC2	C1B-NB	-2.10	1.35	1.37
3	1	312	CLA	CMD-C2D	-2.10	1.46	1.50
3	4	312	CLA	CMD-C2D	-2.10	1.46	1.50
4	3	311	KC2	C1D-CHD	2.10	1.46	1.41
5	4	313	KC1	C4A-C3A	-2.09	1.40	1.44
3	2	414	CLA	CMD-C2D	-2.09	1.46	1.50
5	2	415	KC1	C4A-C3A	-2.09	1.40	1.44
3	2	411	CLA	CMD-C2D	-2.08	1.46	1.50
3	3	308	CLA	CMD-C2D	-2.08	1.46	1.50
6	3	317	LMT	O4'-C4B	-2.08	1.38	1.43
3	1	309	CLA	CMD-C2D	-2.07	1.46	1.50
3	2	409	CLA	CMC-C2C	-2.07	1.46	1.50
2	1	306	A86	C13-C11	-2.07	1.45	1.49
6	2	418	LMT	O4'-C4B	-2.07	1.38	1.43
2	2	403	A86	C13-C11	-2.06	1.45	1.49
3	4	309	CLA	CMD-C2D	-2.05	1.46	1.50
2	2	404	A86	C13-C11	-2.05	1.45	1.49
6	1	316	LMT	O4'-C4B	-2.05	1.38	1.43
2	4	303	A86	C13-C11	-2.04	1.45	1.49
3	4	307	CLA	CMC-C2C	-2.04	1.46	1.50
3	3	308	CLA	CMC-C2C	-2.03	1.46	1.50
3	1	307	CLA	CMC-C2C	-2.03	1.46	1.50
4	3	309	KC2	C1D-CHD	2.02	1.46	1.41
3	4	315	CLA	CMD-C2D	-2.01	1.46	1.50
6	2	418	LMT	O1'-C1'	-2.01	1.36	1.40
6	3	317	LMT	O1'-C1'	-2.01	1.36	1.40
3	3	316	CLA	CMD-C2D	-2.00	1.46	1.50
4	2	410	KC2	C1D-CHD	2.00	1.46	1.41
3	1	318	CLA	CMC-C2C	-2.00	1.46	1.50
3	2	417	CLA	CMD-C2D	-2.00	1.46	1.50
2	1	303	A86	C13-C11	-2.00	1.45	1.49

All (759) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	303	A86	C34-O4-C38	29.55	172.97	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	303	A86	C34-O4-C38	28.49	171.00	117.90
2	4	303	A86	C34-O4-C38	28.43	170.88	117.90
2	2	404	A86	C34-O4-C38	28.02	170.12	117.90
2	1	306	A86	O1-C15-C14	-23.79	65.46	113.21
2	1	301	A86	O1-C15-C14	-17.71	77.66	113.21
2	2	402	A86	O1-C15-C14	-17.71	77.66	113.21
2	3	301	A86	O1-C15-C14	-17.70	77.68	113.21
2	4	301	A86	O1-C15-C14	-17.66	77.77	113.21
2	1	302	A86	O1-C15-C14	-17.61	77.88	113.21
2	4	302	A86	O1-C15-C14	-17.60	77.89	113.21
2	3	302	A86	O1-C15-C14	-17.59	77.90	113.21
2	2	403	A86	O1-C15-C14	-17.59	77.92	113.21
2	4	301	A86	C34-O4-C38	17.27	150.07	117.90
2	3	301	A86	C34-O4-C38	17.21	149.97	117.90
2	1	301	A86	C34-O4-C38	17.21	149.97	117.90
2	2	402	A86	C34-O4-C38	17.19	149.92	117.90
2	1	305	A86	O1-C15-C14	-17.13	78.83	113.21
2	3	305	A86	O1-C15-C14	-17.12	78.86	113.21
2	2	406	A86	C34-O4-C38	16.83	149.26	117.90
2	4	305	A86	C34-O4-C38	16.73	149.07	117.90
2	3	306	A86	C34-O4-C38	16.53	148.70	117.90
2	2	406	A86	O1-C15-C14	-16.26	80.58	113.21
2	4	305	A86	O1-C15-C14	-16.20	80.70	113.21
2	3	303	A86	O1-C15-C14	-16.12	80.86	113.21
2	1	303	A86	O1-C15-C14	-16.12	80.87	113.21
2	2	404	A86	O1-C15-C14	-16.11	80.87	113.21
2	4	303	A86	O1-C15-C14	-16.11	80.88	113.21
2	3	305	A86	C34-O4-C38	16.03	147.77	117.90
2	1	305	A86	C34-O4-C38	16.03	147.76	117.90
2	3	304	A86	O1-C15-C14	-16.00	81.09	113.21
2	4	304	A86	O1-C15-C14	-16.00	81.10	113.21
2	1	304	A86	O1-C15-C14	-15.96	81.19	113.21
2	2	405	A86	O1-C15-C14	-15.94	81.22	113.21
2	2	407	A86	C34-O4-C38	12.35	140.92	117.90
2	2	405	A86	C34-O4-C38	11.75	139.78	117.90
2	1	304	A86	C34-O4-C38	11.65	139.60	117.90
2	3	304	A86	C34-O4-C38	11.43	139.20	117.90
2	4	304	A86	C34-O4-C38	11.41	139.16	117.90
2	4	306	A86	C34-O4-C38	10.82	138.05	117.90
2	1	306	A86	C34-O4-C38	10.63	137.71	117.90
2	2	407	A86	C23-C16-C22	-8.52	94.81	107.37
2	3	306	A86	C23-C16-C22	-8.50	94.84	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	306	A86	C23-C16-C22	-8.50	94.84	107.37
2	1	306	A86	C20-C19-C18	-8.32	96.28	112.75
2	4	306	A86	O1-C15-C14	-7.29	98.59	113.21
2	2	407	A86	O1-C15-C14	-7.28	98.60	113.21
2	3	306	A86	O1-C15-C14	-7.23	98.70	113.21
4	1	310	KC2	CHB-C1B-NB	7.19	131.06	124.45
4	2	412	KC2	CHB-C1B-NB	7.11	130.99	124.45
4	2	410	KC2	CHB-C1B-NB	7.10	130.98	124.45
4	4	308	KC2	CHB-C1B-NB	7.10	130.98	124.45
4	4	310	KC2	CHB-C1B-NB	7.10	130.97	124.45
4	1	308	KC2	CHB-C1B-NB	7.09	130.97	124.45
4	3	309	KC2	CHB-C1B-NB	7.07	130.96	124.45
4	3	311	KC2	CHB-C1B-NB	7.07	130.96	124.45
3	2	401	CLA	C4A-NA-C1A	6.96	109.83	106.71
3	3	307	CLA	C4A-NA-C1A	6.92	109.81	106.71
3	2	408	CLA	C4A-NA-C1A	6.88	109.80	106.71
3	1	318	CLA	C4A-NA-C1A	6.85	109.79	106.71
5	1	313	KC1	CHC-C4B-NB	6.81	130.71	124.45
5	2	415	KC1	CHC-C4B-NB	6.80	130.70	124.45
5	1	311	KC1	CHC-C4B-NB	6.79	130.69	124.45
5	2	413	KC1	CHC-C4B-NB	6.79	130.69	124.45
5	3	314	KC1	CHC-C4B-NB	6.76	130.67	124.45
5	4	311	KC1	CHC-C4B-NB	6.76	130.67	124.45
2	2	402	A86	C4-C5-C6	-6.75	117.67	127.31
2	4	301	A86	C4-C5-C6	-6.75	117.68	127.31
5	4	313	KC1	CHC-C4B-NB	6.75	130.66	124.45
3	3	308	CLA	C4A-NA-C1A	6.75	109.74	106.71
2	3	301	A86	C4-C5-C6	-6.75	117.68	127.31
5	3	312	KC1	CHC-C4B-NB	6.71	130.62	124.45
2	1	301	A86	C4-C5-C6	-6.71	117.74	127.31
3	1	307	CLA	C4A-NA-C1A	6.70	109.72	106.71
3	4	307	CLA	C4A-NA-C1A	6.70	109.72	106.71
3	2	409	CLA	C4A-NA-C1A	6.68	109.71	106.71
4	1	308	KC2	CHC-C4B-NB	6.66	130.57	124.45
4	2	410	KC2	CHC-C4B-NB	6.65	130.57	124.45
4	3	309	KC2	CHC-C4B-NB	6.64	130.55	124.45
3	4	312	CLA	C4A-NA-C1A	6.63	109.69	106.71
4	4	308	KC2	CHC-C4B-NB	6.63	130.54	124.45
3	1	314	CLA	C4A-NA-C1A	6.60	109.67	106.71
3	2	414	CLA	C4A-NA-C1A	6.60	109.67	106.71
3	1	312	CLA	C4A-NA-C1A	6.58	109.67	106.71
3	2	417	CLA	C4A-NA-C1A	6.58	109.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	416	CLA	C4A-NA-C1A	6.51	109.63	106.71
3	3	313	CLA	C4A-NA-C1A	6.48	109.62	106.71
3	3	316	CLA	C4A-NA-C1A	6.48	109.62	106.71
4	4	310	KC2	CHC-C4B-NB	6.47	130.40	124.45
4	2	412	KC2	CHC-C4B-NB	6.47	130.40	124.45
3	3	315	CLA	C4A-NA-C1A	6.47	109.61	106.71
3	1	315	CLA	C4A-NA-C1A	6.46	109.61	106.71
4	3	311	KC2	CHC-C4B-NB	6.46	130.39	124.45
4	1	310	KC2	CHC-C4B-NB	6.45	130.38	124.45
3	4	315	CLA	C4A-NA-C1A	6.45	109.61	106.71
2	1	304	A86	C33-C32-C31	-6.43	102.96	109.21
2	3	304	A86	C33-C32-C31	-6.43	102.96	109.21
2	4	304	A86	C33-C32-C31	-6.41	102.98	109.21
2	2	405	A86	C33-C32-C31	-6.39	103.00	109.21
3	4	314	CLA	C4A-NA-C1A	6.39	109.58	106.71
2	1	303	A86	O1-C20-C21	-6.36	107.44	115.06
2	3	303	A86	O1-C20-C21	-6.35	107.44	115.06
2	4	303	A86	O1-C20-C21	-6.35	107.45	115.06
5	3	314	KC1	CHB-C1B-NB	6.35	130.29	124.45
5	2	415	KC1	CHB-C1B-NB	6.35	130.29	124.45
2	2	404	A86	O1-C20-C21	-6.32	107.48	115.06
5	1	313	KC1	CHB-C1B-NB	6.29	130.23	124.45
5	4	313	KC1	CHB-C1B-NB	6.29	130.23	124.45
3	4	309	CLA	C4A-NA-C1A	6.28	109.53	106.71
3	3	310	CLA	C4A-NA-C1A	6.27	109.53	106.71
3	2	411	CLA	C4A-NA-C1A	6.27	109.52	106.71
3	1	309	CLA	C4A-NA-C1A	6.19	109.49	106.71
5	1	311	KC1	CHB-C1B-NB	6.02	129.98	124.45
5	4	311	KC1	CHB-C1B-NB	5.98	129.95	124.45
5	3	312	KC1	CHB-C1B-NB	5.96	129.94	124.45
5	2	413	KC1	CHB-C1B-NB	5.95	129.93	124.45
2	2	402	A86	O1-C20-C19	-5.91	108.94	113.38
2	3	301	A86	O1-C20-C19	-5.91	108.95	113.38
2	4	301	A86	O1-C20-C19	-5.83	109.00	113.38
2	1	301	A86	O1-C20-C19	-5.81	109.02	113.38
2	1	305	A86	C3-C2-C1	-5.54	119.40	127.31
2	3	305	A86	C3-C2-C1	-5.47	119.51	127.31
2	2	402	A86	O1-C20-C21	-5.32	108.68	115.06
2	1	301	A86	O1-C20-C21	-5.31	108.69	115.06
2	3	301	A86	O1-C20-C21	-5.30	108.71	115.06
2	4	301	A86	O1-C20-C21	-5.27	108.74	115.06
2	1	304	A86	C25-C26-C27	-5.26	119.80	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	304	A86	C25-C26-C27	-5.26	119.81	127.31
2	3	304	A86	C25-C26-C27	-5.25	119.81	127.31
2	2	405	A86	C25-C26-C27	-5.25	119.81	127.31
2	2	406	A86	C3-C2-C1	-5.16	119.94	127.31
2	4	305	A86	C3-C2-C1	-5.16	119.95	127.31
4	3	309	KC2	O2D-CGD-CBD	5.13	120.38	111.27
4	1	308	KC2	O2D-CGD-CBD	5.12	120.36	111.27
4	4	308	KC2	O2D-CGD-CBD	5.09	120.32	111.27
2	3	301	A86	C25-C26-C27	-5.07	120.07	127.31
2	2	402	A86	C25-C26-C27	-5.06	120.08	127.31
2	4	301	A86	C25-C26-C27	-5.06	120.09	127.31
4	2	410	KC2	O2D-CGD-CBD	5.05	120.24	111.27
2	1	301	A86	C25-C26-C27	-5.05	120.11	127.31
2	2	403	A86	O4-C38-C39	4.98	120.25	111.09
2	2	407	A86	O4-C38-C39	4.98	120.25	111.09
5	1	313	KC1	O2D-CGD-CBD	4.97	120.10	111.27
5	2	415	KC1	O2D-CGD-CBD	4.93	120.03	111.27
5	4	313	KC1	O2D-CGD-CBD	4.92	120.02	111.27
2	4	306	A86	O4-C38-C39	4.91	120.12	111.09
5	3	314	KC1	O2D-CGD-CBD	4.91	119.99	111.27
2	1	306	A86	O4-C38-C39	4.84	119.99	111.09
2	2	407	A86	C20-C19-C18	-4.82	103.22	112.75
2	3	306	A86	C20-C19-C18	-4.81	103.24	112.75
2	3	302	A86	O4-C38-C39	4.80	119.91	111.09
2	3	305	A86	O1-C20-C21	-4.79	109.31	115.06
2	1	302	A86	O4-C38-C39	4.79	119.91	111.09
2	1	306	A86	C3-C2-C1	-4.79	120.47	127.31
2	4	306	A86	C20-C19-C18	-4.79	103.27	112.75
2	4	302	A86	O4-C38-C39	4.78	119.88	111.09
2	3	302	A86	C25-C26-C27	-4.76	120.52	127.31
2	4	302	A86	C25-C26-C27	-4.76	120.52	127.31
2	1	305	A86	O1-C20-C21	-4.76	109.36	115.06
2	3	306	A86	O1-C20-C21	-4.75	109.37	115.06
2	4	306	A86	O1-C20-C21	-4.74	109.38	115.06
2	1	302	A86	C25-C26-C27	-4.71	120.59	127.31
2	2	407	A86	O1-C20-C21	-4.70	109.43	115.06
2	2	403	A86	C25-C26-C27	-4.68	120.63	127.31
2	1	302	A86	C40-C32-C31	-4.67	106.30	110.47
2	2	403	A86	C40-C32-C31	-4.67	106.30	110.47
2	3	306	A86	C3-C2-C1	-4.66	120.67	127.31
2	1	303	A86	O4-C38-C39	4.65	119.64	111.09
2	3	303	A86	O4-C38-C39	4.64	119.63	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	303	A86	O4-C38-C39	4.63	119.61	111.09
2	2	404	A86	O4-C38-C39	4.62	119.58	111.09
2	1	304	A86	O1-C20-C21	-4.61	109.53	115.06
2	1	303	A86	C3-C2-C1	-4.61	120.73	127.31
2	3	304	A86	O1-C20-C21	-4.61	109.53	115.06
2	2	407	A86	C3-C2-C1	-4.60	120.74	127.31
2	4	306	A86	C3-C2-C1	-4.60	120.75	127.31
2	4	304	A86	O1-C20-C21	-4.60	109.55	115.06
2	4	302	A86	C40-C32-C31	-4.59	106.36	110.47
2	2	404	A86	C3-C2-C1	-4.59	120.76	127.31
2	4	303	A86	C3-C2-C1	-4.59	120.76	127.31
2	3	302	A86	C40-C32-C31	-4.59	106.37	110.47
2	2	406	A86	O4-C38-C39	4.59	119.53	111.09
2	2	405	A86	O1-C20-C21	-4.59	109.56	115.06
2	1	305	A86	O4-C38-C39	4.59	119.53	111.09
2	3	305	A86	O4-C38-C39	4.59	119.53	111.09
2	3	303	A86	C3-C2-C1	-4.58	120.77	127.31
2	3	301	A86	O4-C38-C39	4.58	119.51	111.09
4	1	310	KC2	O2D-CGD-CBD	4.57	119.40	111.27
2	1	301	A86	O4-C38-C39	4.57	119.50	111.09
2	2	402	A86	O4-C38-C39	4.56	119.49	111.09
2	4	305	A86	O4-C38-C39	4.56	119.49	111.09
2	4	301	A86	O4-C38-C39	4.55	119.46	111.09
2	2	406	A86	O1-C20-C21	-4.55	109.61	115.06
2	1	302	A86	C4-C5-C6	-4.54	120.83	127.31
4	4	310	KC2	O2D-CGD-CBD	4.54	119.33	111.27
2	4	302	A86	C4-C5-C6	-4.52	120.86	127.31
2	3	302	A86	C4-C5-C6	-4.51	120.88	127.31
4	2	412	KC2	O2D-CGD-CBD	4.50	119.27	111.27
2	4	305	A86	O1-C20-C21	-4.50	109.66	115.06
4	3	311	KC2	O2D-CGD-CBD	4.49	119.24	111.27
2	1	301	A86	C3-C2-C1	-4.48	120.91	127.31
2	2	403	A86	C4-C5-C6	-4.48	120.92	127.31
2	4	306	A86	O1-C20-C19	-4.48	110.02	113.38
2	2	407	A86	O1-C20-C19	-4.46	110.03	113.38
2	4	304	A86	O4-C38-C39	4.46	119.29	111.09
2	2	405	A86	O4-C38-C39	4.45	119.28	111.09
2	1	306	A86	C25-C26-C27	-4.44	120.97	127.31
2	1	304	A86	O4-C38-C39	4.44	119.25	111.09
2	3	304	A86	O4-C38-C39	4.43	119.24	111.09
2	3	306	A86	O4-C38-C39	4.43	119.24	111.09
2	3	306	A86	O1-C20-C19	-4.41	110.07	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	301	A86	C3-C2-C1	-4.41	121.02	127.31
2	3	301	A86	C3-C2-C1	-4.40	121.04	127.31
2	4	305	A86	O1-C20-C19	-4.39	110.08	113.38
2	2	402	A86	C3-C2-C1	-4.38	121.05	127.31
5	1	311	KC1	O2D-CGD-CBD	4.24	118.81	111.27
2	2	403	A86	O1-C20-C21	-4.24	109.98	115.06
2	3	306	A86	C25-C26-C27	-4.22	121.28	127.31
2	4	302	A86	O1-C20-C21	-4.22	110.00	115.06
2	1	306	A86	C4-C5-C6	-4.22	121.29	127.31
2	2	407	A86	C25-C26-C27	-4.21	121.30	127.31
2	1	302	A86	O1-C20-C21	-4.21	110.02	115.06
5	3	312	KC1	O2D-CGD-CBD	4.21	118.74	111.27
5	2	413	KC1	O2D-CGD-CBD	4.20	118.74	111.27
2	3	302	A86	O1-C20-C21	-4.20	110.02	115.06
2	3	302	A86	O1-C20-C19	-4.20	110.23	113.38
5	4	311	KC1	O2D-CGD-CBD	4.20	118.72	111.27
3	2	409	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
2	4	306	A86	C25-C26-C27	-4.19	121.32	127.31
2	2	403	A86	O1-C20-C19	-4.18	110.24	113.38
2	4	302	A86	O1-C20-C19	-4.18	110.24	113.38
3	3	308	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
2	1	302	A86	O1-C20-C19	-4.17	110.25	113.38
3	1	307	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
3	4	307	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
2	2	407	A86	C4-C5-C6	-4.12	121.42	127.31
2	4	306	A86	C4-C5-C6	-4.11	121.44	127.31
2	3	306	A86	C4-C5-C6	-4.11	121.45	127.31
2	2	406	A86	C4-C5-C6	-4.09	121.47	127.31
4	2	410	KC2	C4B-CHC-C1C	-4.05	117.31	126.06
4	1	308	KC2	C4B-CHC-C1C	-4.05	117.32	126.06
4	3	309	KC2	C4B-CHC-C1C	-4.05	117.33	126.06
4	4	308	KC2	C4B-CHC-C1C	-4.05	117.33	126.06
2	4	305	A86	C4-C5-C6	-4.04	121.54	127.31
2	4	304	A86	C3-C2-C1	-3.99	121.61	127.31
2	1	304	A86	C3-C2-C1	-3.99	121.62	127.31
2	2	405	A86	C3-C2-C1	-3.98	121.63	127.31
2	1	303	A86	C4-C5-C6	-3.95	121.67	127.31
2	3	304	A86	C3-C2-C1	-3.94	121.69	127.31
2	2	404	A86	C4-C5-C6	-3.93	121.71	127.31
2	4	303	A86	C4-C5-C6	-3.91	121.73	127.31
4	2	412	KC2	C4B-CHC-C1C	-3.89	117.66	126.06
2	3	303	A86	C4-C5-C6	-3.88	121.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	311	KC2	C4B-CHC-C1C	-3.88	117.68	126.06
3	4	312	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
4	4	310	KC2	C4B-CHC-C1C	-3.88	117.69	126.06
3	2	414	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
4	1	310	KC2	C4B-CHC-C1C	-3.87	117.71	126.06
3	3	313	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
3	1	312	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
2	1	306	A86	O1-C20-C21	-3.81	110.48	115.06
2	2	406	A86	O1-C20-C19	-3.80	110.53	113.38
2	3	302	A86	C3-C2-C1	-3.79	121.89	127.31
2	1	302	A86	C3-C2-C1	-3.77	121.92	127.31
2	4	302	A86	C3-C2-C1	-3.76	121.94	127.31
2	2	403	A86	C3-C2-C1	-3.76	121.94	127.31
2	1	306	A86	C17-C16-C15	-3.69	105.39	109.16
3	1	318	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
3	4	307	CLA	CMB-C2B-C3B	3.56	131.35	124.68
4	1	308	KC2	CHC-C4B-C3B	-3.56	119.16	125.26
3	3	307	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
2	1	306	A86	C33-C32-C31	-3.56	105.75	109.21
2	2	407	A86	C33-C32-C31	-3.56	105.75	109.21
3	2	408	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
3	2	409	CLA	CMB-C2B-C3B	3.56	131.33	124.68
4	3	309	KC2	CHC-C4B-C3B	-3.56	119.17	125.26
3	1	307	CLA	CMB-C2B-C3B	3.55	131.32	124.68
3	3	308	CLA	CMB-C2B-C3B	3.54	131.30	124.68
3	2	401	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
2	2	405	A86	C4-C5-C6	-3.53	122.27	127.31
4	4	308	KC2	CHC-C4B-C3B	-3.51	119.25	125.26
3	3	310	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
4	2	410	KC2	CHC-C4B-C3B	-3.51	119.25	125.26
3	4	309	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
2	3	304	A86	C4-C5-C6	-3.51	122.30	127.31
2	3	305	A86	C4-C5-C6	-3.51	122.30	127.31
2	2	402	A86	C12-C11-C13	3.51	121.91	116.02
2	4	304	A86	C4-C5-C6	-3.50	122.31	127.31
3	2	411	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
2	1	305	A86	C4-C5-C6	-3.50	122.32	127.31
2	1	301	A86	C12-C11-C13	3.49	121.89	116.02
3	1	309	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
2	3	301	A86	C12-C11-C13	3.49	121.88	116.02
2	1	304	A86	C4-C5-C6	-3.48	122.34	127.31
2	3	306	A86	C33-C32-C31	-3.47	105.84	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	301	A86	C12-C11-C13	3.47	121.85	116.02
2	4	303	A86	C25-C26-C27	-3.47	122.36	127.31
2	3	303	A86	C25-C26-C27	-3.46	122.37	127.31
2	2	404	A86	C25-C26-C27	-3.46	122.38	127.31
2	1	303	A86	C25-C26-C27	-3.45	122.38	127.31
3	2	416	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
3	1	314	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
3	4	314	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
4	1	310	KC2	CHB-C1B-C2B	-3.42	118.31	125.48
3	3	315	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
4	4	310	KC2	CHC-C4B-C3B	-3.40	119.44	125.26
2	1	301	A86	C9-C8-C6	-3.39	116.89	126.42
4	3	309	KC2	CHB-C1B-C2B	-3.38	118.38	125.48
4	1	310	KC2	CHC-C4B-C3B	-3.38	119.48	125.26
2	1	306	A86	C22-C16-C17	3.37	114.84	108.98
4	4	308	KC2	CHB-C1B-C2B	-3.37	118.41	125.48
4	3	311	KC2	CHB-C1B-C2B	-3.36	118.43	125.48
4	2	412	KC2	CHC-C4B-C3B	-3.36	119.51	125.26
4	1	308	KC2	CHB-C1B-C2B	-3.36	118.43	125.48
4	3	311	KC2	CHC-C4B-C3B	-3.36	119.51	125.26
4	4	310	KC2	CHB-C1B-C2B	-3.36	118.44	125.48
4	2	410	KC2	CHB-C1B-C2B	-3.36	118.44	125.48
4	2	412	KC2	CHB-C1B-C2B	-3.36	118.44	125.48
2	4	301	A86	C9-C8-C6	-3.36	116.99	126.42
2	2	402	A86	C9-C8-C6	-3.35	117.01	126.42
2	3	301	A86	C9-C8-C6	-3.35	117.02	126.42
3	1	315	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
3	3	316	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
3	4	315	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
3	2	417	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
3	4	312	CLA	CMB-C2B-C3B	3.25	130.76	124.68
2	4	306	A86	C33-C32-C31	-3.25	106.05	109.21
3	2	414	CLA	CMB-C2B-C3B	3.25	130.76	124.68
5	3	314	KC1	CHC-C4B-C3B	-3.25	119.70	125.26
2	1	306	A86	O1-C20-C19	3.25	115.82	113.38
5	2	415	KC1	CHC-C4B-C3B	-3.25	119.71	125.26
5	1	313	KC1	CHC-C4B-C3B	-3.24	119.71	125.26
3	1	312	CLA	CMB-C2B-C3B	3.22	130.71	124.68
3	3	313	CLA	CMB-C2B-C3B	3.22	130.70	124.68
5	4	313	KC1	CHC-C4B-C3B	-3.21	119.76	125.26
5	1	311	KC1	CHC-C4B-C3B	-3.20	119.78	125.26
5	4	311	KC1	CHC-C4B-C3B	-3.19	119.80	125.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	413	KC1	CHC-C4B-C3B	-3.19	119.80	125.26
5	3	312	KC1	CHC-C4B-C3B	-3.19	119.81	125.26
2	4	304	A86	C12-C11-C13	3.15	121.31	116.02
2	3	304	A86	C12-C11-C13	3.14	121.30	116.02
2	1	304	A86	C12-C11-C13	3.14	121.30	116.02
2	2	405	A86	C12-C11-C13	3.13	121.29	116.02
2	2	406	A86	C40-C32-C31	-3.13	107.67	110.47
2	1	306	A86	C23-C16-C22	3.10	111.95	107.37
3	1	318	CLA	CMB-C2B-C3B	3.09	130.47	124.68
2	4	305	A86	C40-C32-C31	-3.09	107.70	110.47
4	2	410	KC2	CBD-CHA-C1A	3.09	134.65	128.88
4	3	309	KC2	CBD-CHA-C1A	3.08	134.62	128.88
4	4	308	KC2	CBD-CHA-C1A	3.08	134.62	128.88
3	2	401	CLA	CMB-C2B-C3B	3.07	130.42	124.68
3	3	307	CLA	CMB-C2B-C3B	3.07	130.41	124.68
3	2	408	CLA	CMB-C2B-C3B	3.06	130.40	124.68
4	1	308	KC2	CBD-CHA-C1A	3.06	134.59	128.88
3	1	309	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
3	2	411	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
3	3	310	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
3	4	309	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
3	2	414	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
2	1	301	A86	C40-C32-C31	-2.99	107.80	110.47
3	4	312	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
3	3	313	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
3	1	312	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
3	4	314	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
3	2	401	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
3	2	408	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
3	1	318	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
3	3	307	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
2	3	301	A86	C40-C32-C31	-2.92	107.86	110.47
2	2	405	A86	O1-C20-C19	-2.92	111.19	113.38
2	1	304	A86	O1-C20-C19	-2.91	111.20	113.38
3	3	308	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
3	2	416	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
2	2	402	A86	C40-C32-C31	-2.90	107.87	110.47
4	1	310	KC2	CBD-CHA-C1A	2.90	134.29	128.88
3	3	315	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
3	2	411	CLA	CMB-C2B-C3B	2.90	130.10	124.68
2	3	304	A86	O1-C20-C19	-2.89	111.21	113.38
6	4	316	LMT	C3'-C4'-C5'	-2.89	104.30	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	314	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
2	4	304	A86	O1-C20-C19	-2.88	111.22	113.38
3	1	309	CLA	CMB-C2B-C3B	2.88	130.07	124.68
3	1	307	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
3	4	307	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
3	4	309	CLA	CMB-C2B-C3B	2.88	130.07	124.68
3	1	315	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
3	2	409	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
3	3	310	CLA	CMB-C2B-C3B	2.87	130.05	124.68
6	1	316	LMT	C3'-C4'-C5'	-2.87	104.35	110.93
2	4	301	A86	C40-C32-C31	-2.87	107.91	110.47
6	2	418	LMT	C3'-C4'-C5'	-2.87	104.35	110.93
3	4	315	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
3	3	316	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
5	1	311	KC1	O1D-CGD-CBD	-2.84	118.67	124.48
3	2	417	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
5	3	312	KC1	O1D-CGD-CBD	-2.82	118.71	124.48
4	1	310	KC2	C1A-NA-C4A	-2.81	105.44	106.71
4	3	311	KC2	C1A-NA-C4A	-2.81	105.44	106.71
3	2	416	CLA	CMB-C2B-C3B	2.81	129.94	124.68
5	4	311	KC1	O1D-CGD-CBD	-2.81	118.73	124.48
4	3	311	KC2	CBD-CHA-C1A	2.81	134.12	128.88
4	4	310	KC2	CBD-CHA-C1A	2.81	134.12	128.88
2	1	302	A86	C12-C11-C13	2.81	120.74	116.02
3	4	314	CLA	CMB-C2B-C3B	2.81	129.93	124.68
4	4	310	KC2	C1A-NA-C4A	-2.80	105.45	106.71
2	3	302	A86	C12-C11-C13	2.79	120.71	116.02
2	4	302	A86	C12-C11-C13	2.79	120.71	116.02
3	1	314	CLA	CMB-C2B-C3B	2.79	129.90	124.68
5	2	413	KC1	O1D-CGD-CBD	-2.79	118.78	124.48
4	2	412	KC2	CBD-CHA-C1A	2.79	134.08	128.88
6	1	317	LMT	C1'-O5'-C5'	-2.78	108.23	113.69
6	4	317	LMT	C1'-O5'-C5'	-2.78	108.24	113.69
3	3	315	CLA	CMB-C2B-C3B	2.78	129.87	124.68
6	3	318	LMT	C1'-O5'-C5'	-2.77	108.25	113.69
5	1	311	KC1	CBD-CHA-C1A	2.76	134.02	128.88
3	3	316	CLA	CMB-C2B-C3B	2.76	129.84	124.68
6	2	419	LMT	C1'-O5'-C5'	-2.76	108.28	113.69
2	2	403	A86	C12-C11-C13	2.75	120.64	116.02
2	1	305	A86	C40-C32-C31	-2.75	108.01	110.47
5	4	311	KC1	CBD-CHA-C1A	2.75	134.00	128.88
5	2	413	KC1	CBD-CHA-C1A	2.74	134.00	128.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	315	CLA	CMB-C2B-C3B	2.74	129.80	124.68
2	3	302	A86	C4-C3-C2	-2.74	117.87	123.47
2	1	306	A86	O1-C15-C20	-2.73	56.73	59.40
3	2	417	CLA	CMB-C2B-C3B	2.72	129.78	124.68
5	3	312	KC1	CBD-CHA-C1A	2.72	133.95	128.88
3	4	315	CLA	CMB-C2B-C3B	2.72	129.76	124.68
2	1	302	A86	C4-C3-C2	-2.71	117.92	123.47
2	3	301	A86	C4-C3-C2	-2.70	117.95	123.47
2	4	302	A86	C4-C3-C2	-2.70	117.95	123.47
2	3	305	A86	C40-C32-C31	-2.70	108.06	110.47
6	3	317	LMT	C3'-C4'-C5'	-2.69	104.76	110.93
2	2	402	A86	C4-C3-C2	-2.69	117.97	123.47
2	4	301	A86	C4-C3-C2	-2.68	117.98	123.47
3	2	401	CLA	CHB-C4A-NA	2.68	128.22	124.51
3	2	408	CLA	CHB-C4A-NA	2.68	128.22	124.51
3	1	318	CLA	CHB-C4A-NA	2.66	128.18	124.51
2	2	403	A86	C4-C3-C2	-2.66	118.03	123.47
3	1	312	CLA	CHB-C4A-NA	2.65	128.18	124.51
3	4	312	CLA	CHB-C4A-NA	2.65	128.18	124.51
3	3	307	CLA	CHB-C4A-NA	2.65	128.17	124.51
5	2	413	KC1	O2D-CGD-O1D	-2.64	118.67	123.84
4	2	412	KC2	C1A-NA-C4A	-2.64	105.52	106.71
2	2	403	A86	O4-C38-O5	-2.64	117.72	122.96
4	4	308	KC2	C3D-CAD-CBD	-2.64	104.14	107.61
3	2	414	CLA	CHB-C4A-NA	2.64	128.16	124.51
5	2	415	KC1	CHB-C1B-C2B	-2.63	119.95	125.48
5	3	314	KC1	CHB-C1B-C2B	-2.63	119.97	125.48
3	3	310	CLA	CHB-C4A-NA	2.62	128.14	124.51
5	2	415	KC1	C3D-CAD-CBD	-2.62	104.16	107.61
5	4	313	KC1	CHB-C1B-C2B	-2.61	120.00	125.48
3	3	313	CLA	CHB-C4A-NA	2.61	128.12	124.51
5	3	312	KC1	O2D-CGD-O1D	-2.60	118.75	123.84
2	1	301	A86	C4-C3-C2	-2.60	118.14	123.47
4	1	308	KC2	C3D-CAD-CBD	-2.60	104.18	107.61
5	3	314	KC1	C3D-CAD-CBD	-2.60	104.18	107.61
2	1	306	A86	C12-C11-C13	2.60	120.39	116.02
5	1	313	KC1	CHB-C1B-C2B	-2.60	120.03	125.48
4	2	410	KC2	C3D-CAD-CBD	-2.60	104.18	107.61
5	4	311	KC1	O2D-CGD-O1D	-2.60	118.76	123.84
4	3	309	KC2	C3D-CAD-CBD	-2.59	104.19	107.61
5	4	311	KC1	C4B-CHC-C1C	-2.59	120.47	126.06
3	4	309	CLA	CHB-C4A-NA	2.59	128.09	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	313	KC1	C3D-CAD-CBD	-2.59	104.19	107.61
5	1	311	KC1	O2D-CGD-O1D	-2.59	118.78	123.84
5	1	311	KC1	C4B-CHC-C1C	-2.59	120.47	126.06
5	4	313	KC1	C3D-CAD-CBD	-2.58	104.21	107.61
6	3	317	LMT	C1'-O5'-C5'	-2.58	108.63	113.69
3	1	309	CLA	CHB-C4A-NA	2.57	128.07	124.51
3	2	411	CLA	CHB-C4A-NA	2.57	128.07	124.51
4	3	309	KC2	CHD-C4C-NC	2.57	128.10	124.20
5	2	413	KC1	C4B-CHC-C1C	-2.57	120.52	126.06
5	3	312	KC1	C4B-CHC-C1C	-2.56	120.53	126.06
2	1	302	A86	O4-C38-O5	-2.56	117.88	122.96
5	3	314	KC1	C4B-CHC-C1C	-2.55	120.55	126.06
3	3	315	CLA	CHB-C4A-NA	2.55	128.04	124.51
5	2	415	KC1	C4B-CHC-C1C	-2.55	120.56	126.06
5	1	311	KC1	CHB-C1B-C2B	-2.55	120.14	125.48
2	3	302	A86	O4-C38-O5	-2.55	117.91	122.96
5	1	313	KC1	C4B-CHC-C1C	-2.54	120.57	126.06
3	4	314	CLA	CHB-C4A-NA	2.54	128.03	124.51
2	2	407	A86	O4-C38-O5	-2.54	117.92	122.96
4	2	410	KC2	CHD-C4C-NC	2.53	128.05	124.20
5	4	311	KC1	CHB-C1B-C2B	-2.53	120.17	125.48
3	1	307	CLA	CHB-C4A-NA	2.53	128.01	124.51
3	4	307	CLA	CHB-C4A-NA	2.53	128.01	124.51
6	4	316	LMT	C1'-O5'-C5'	-2.53	108.72	113.69
3	1	314	CLA	CHB-C4A-NA	2.52	128.00	124.51
4	1	308	KC2	CHD-C4C-NC	2.52	128.03	124.20
2	4	302	A86	O4-C38-O5	-2.52	117.95	122.96
3	2	416	CLA	CHB-C4A-NA	2.52	128.00	124.51
5	4	313	KC1	C4B-CHC-C1C	-2.52	120.63	126.06
3	2	409	CLA	CHB-C4A-NA	2.51	127.99	124.51
3	3	316	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
3	3	308	CLA	CHB-C4A-NA	2.51	127.98	124.51
3	1	315	CLA	C1B-CHB-C4A	-2.51	125.16	130.12
5	2	413	KC1	CHB-C1B-C2B	-2.50	120.23	125.48
4	2	412	KC2	C3D-CAD-CBD	-2.50	104.31	107.61
5	3	312	KC1	CHB-C1B-C2B	-2.50	120.23	125.48
3	2	417	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
3	4	315	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
4	4	308	KC2	CHD-C4C-NC	2.50	127.99	124.20
3	2	417	CLA	CHB-C4A-NA	2.49	127.95	124.51
4	4	310	KC2	O1D-CGD-CBD	-2.49	119.39	124.48
3	1	315	CLA	CHB-C4A-NA	2.49	127.95	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	304	A86	C3-C4-C5	-2.49	118.38	123.47
3	3	316	CLA	CHB-C4A-NA	2.48	127.95	124.51
2	4	306	A86	O4-C38-O5	-2.48	118.03	122.96
2	1	304	A86	C3-C4-C5	-2.48	118.40	123.47
5	3	314	KC1	CBD-CHA-C1A	2.47	133.50	128.88
2	1	305	A86	C9-C8-C6	-2.47	119.47	126.42
2	2	405	A86	C3-C4-C5	-2.47	118.41	123.47
2	2	407	A86	C12-C11-C13	2.47	120.17	116.02
2	3	306	A86	C12-C11-C13	2.46	120.16	116.02
4	4	310	KC2	C3D-CAD-CBD	-2.46	104.36	107.61
3	4	315	CLA	CHB-C4A-NA	2.46	127.92	124.51
6	1	316	LMT	C1'-O5'-C5'	-2.46	108.86	113.69
2	4	304	A86	C3-C4-C5	-2.46	118.44	123.47
4	2	412	KC2	O1D-CGD-CBD	-2.45	119.46	124.48
2	1	303	A86	C3-C4-C5	-2.45	118.45	123.47
2	1	303	A86	O4-C38-O5	-2.45	118.09	122.96
5	2	415	KC1	CBD-CHA-C1A	2.45	133.45	128.88
4	3	311	KC2	O1D-CGD-CBD	-2.45	119.47	124.48
5	4	313	KC1	CBD-CHA-C1A	2.45	133.44	128.88
2	1	306	A86	O4-C38-O5	-2.45	118.10	122.96
2	3	305	A86	C9-C8-C6	-2.45	119.54	126.42
2	3	305	A86	C3-C4-C5	-2.45	118.46	123.47
5	1	313	KC1	CBD-CHA-C1A	2.44	133.44	128.88
2	4	303	A86	C3-C4-C5	-2.44	118.47	123.47
3	4	314	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
2	2	404	A86	C3-C4-C5	-2.43	118.50	123.47
2	4	303	A86	O4-C38-O5	-2.43	118.14	122.96
4	3	311	KC2	C3D-CAD-CBD	-2.43	104.41	107.61
2	4	306	A86	C12-C11-C13	2.43	120.10	116.02
2	1	305	A86	C3-C4-C5	-2.43	118.50	123.47
2	3	303	A86	C3-C4-C5	-2.42	118.51	123.47
4	1	310	KC2	O1D-CGD-CBD	-2.42	119.53	124.48
2	1	306	A86	C3-C4-C5	-2.42	118.52	123.47
3	1	314	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
3	3	315	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
3	2	416	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
2	3	305	A86	C25-C24-C1	-2.41	119.64	126.42
4	4	310	KC2	CHD-C4C-NC	2.41	127.85	124.20
2	3	303	A86	O4-C38-O5	-2.40	118.19	122.96
3	2	408	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
3	2	401	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
4	1	310	KC2	C3D-CAD-CBD	-2.39	104.45	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	305	A86	C25-C24-C1	-2.39	119.69	126.42
4	1	310	KC2	CHD-C4C-NC	2.39	127.83	124.20
3	1	318	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
4	2	412	KC2	CHD-C4C-NC	2.39	127.83	124.20
2	2	404	A86	O4-C38-O5	-2.39	118.22	122.96
2	1	304	A86	C10-C9-C8	-2.38	115.78	123.22
2	4	304	A86	C10-C9-C8	-2.38	115.79	123.22
2	2	405	A86	C10-C9-C8	-2.38	115.79	123.22
4	3	311	KC2	CHD-C4C-NC	2.38	127.81	124.20
6	2	418	LMT	C1'-O5'-C5'	-2.37	109.03	113.69
2	2	402	A86	O4-C38-O5	-2.37	118.25	122.96
3	3	307	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
2	3	306	A86	O4-C38-O5	-2.37	118.25	122.96
2	3	304	A86	C10-C9-C8	-2.37	115.83	123.22
2	4	305	A86	O4-C38-O5	-2.37	118.26	122.96
2	2	406	A86	O4-C38-O5	-2.37	118.26	122.96
2	2	407	A86	O1-C15-C20	-2.36	57.09	59.40
2	3	306	A86	O1-C15-C20	-2.36	57.09	59.40
4	2	410	KC2	O1D-CGD-CBD	-2.36	119.65	124.48
2	2	404	A86	O1-C15-C20	-2.36	57.09	59.40
2	3	306	A86	C3-C4-C5	-2.36	118.64	123.47
2	1	301	A86	O4-C38-O5	-2.36	118.28	122.96
3	4	309	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
2	3	303	A86	O1-C15-C20	-2.35	57.10	59.40
2	3	301	A86	O4-C38-O5	-2.35	118.29	122.96
2	4	301	A86	O4-C38-O5	-2.35	118.29	122.96
3	3	310	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
2	4	306	A86	O1-C15-C20	-2.35	57.10	59.40
2	1	305	A86	O4-C38-O5	-2.35	118.30	122.96
2	3	305	A86	O4-C38-O5	-2.35	118.30	122.96
4	3	311	KC2	O2D-CGD-O1D	-2.35	119.25	123.84
3	1	309	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
2	3	305	A86	C20-C19-C18	2.34	117.39	112.75
4	1	310	KC2	CHB-C4A-C3A	-2.34	121.33	124.98
4	4	308	KC2	C1A-NA-C4A	-2.34	105.66	106.71
4	4	308	KC2	O1D-CGD-CBD	-2.33	119.72	124.48
3	2	411	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
2	4	303	A86	O1-C15-C20	-2.32	57.13	59.40
4	4	310	KC2	O2D-CGD-O1D	-2.31	119.31	123.84
2	1	303	A86	O1-C15-C20	-2.31	57.14	59.40
4	2	412	KC2	O2D-CGD-O1D	-2.31	119.32	123.84
2	2	406	A86	C3-C4-C5	-2.31	118.75	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	305	A86	C3-C4-C5	-2.30	118.76	123.47
4	1	308	KC2	O1D-CGD-CBD	-2.30	119.78	124.48
4	4	310	KC2	CHB-C4A-C3A	-2.29	121.39	124.98
2	1	305	A86	C20-C19-C18	2.29	117.28	112.75
4	1	310	KC2	O2D-CGD-O1D	-2.28	119.37	123.84
2	4	305	A86	C25-C24-C1	-2.28	120.01	126.42
4	3	309	KC2	O1D-CGD-CBD	-2.28	119.82	124.48
4	2	412	KC2	CHB-C4A-C3A	-2.28	121.42	124.98
4	3	311	KC2	CHB-C4A-C3A	-2.28	121.42	124.98
4	1	308	KC2	C1A-NA-C4A	-2.28	105.68	106.71
4	3	309	KC2	C1A-NA-C4A	-2.28	105.68	106.71
3	1	309	CLA	C1-C2-C3	-2.27	122.11	126.04
5	3	314	KC1	O1D-CGD-CBD	-2.27	119.84	124.48
2	4	305	A86	C20-C19-C18	2.27	117.24	112.75
2	2	406	A86	C20-C19-C18	2.27	117.23	112.75
3	4	309	CLA	C1-C2-C3	-2.27	122.12	126.04
3	1	312	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
3	4	307	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
3	4	312	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
4	2	410	KC2	CHB-C4A-C3A	-2.26	121.45	124.98
2	1	301	A86	C8-C6-C5	2.26	122.41	118.94
3	2	409	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
3	2	411	CLA	C1-C2-C3	-2.26	122.14	126.04
3	2	414	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
3	3	308	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
4	2	410	KC2	O2D-CGD-O1D	-2.25	119.44	123.84
3	1	307	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
2	4	304	A86	O4-C38-O5	-2.24	118.50	122.96
2	1	304	A86	O4-C38-O5	-2.24	118.51	122.96
5	2	415	KC1	O1D-CGD-CBD	-2.24	119.90	124.48
5	4	313	KC1	O1D-CGD-CBD	-2.24	119.91	124.48
3	3	313	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
4	2	412	KC2	C1B-CHB-C4A	-2.24	121.23	126.06
4	1	310	KC2	C1B-CHB-C4A	-2.24	121.24	126.06
3	3	310	CLA	C1-C2-C3	-2.23	122.18	126.04
2	4	306	A86	C3-C4-C5	-2.23	118.90	123.47
2	2	407	A86	C3-C4-C5	-2.23	118.90	123.47
2	2	405	A86	O4-C38-O5	-2.23	118.53	122.96
2	2	406	A86	C25-C24-C1	-2.23	120.15	126.42
2	3	301	A86	C25-C24-C1	-2.23	120.15	126.42
2	3	304	A86	O4-C38-O5	-2.23	118.54	122.96
2	2	402	A86	C25-C24-C1	-2.23	120.16	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	309	KC2	O2D-CGD-O1D	-2.22	119.49	123.84
5	1	313	KC1	O1D-CGD-CBD	-2.22	119.93	124.48
2	2	405	A86	C20-C19-C18	2.22	117.15	112.75
4	4	308	KC2	O2D-CGD-O1D	-2.22	119.49	123.84
4	2	410	KC2	C1A-NA-C4A	-2.22	105.71	106.71
2	4	304	A86	C20-C19-C18	2.21	117.13	112.75
2	1	301	A86	C25-C24-C1	-2.21	120.20	126.42
2	4	301	A86	C25-C24-C1	-2.21	120.20	126.42
4	3	309	KC2	CHB-C4A-C3A	-2.21	121.52	124.98
2	4	305	A86	C17-C16-C15	2.21	111.42	109.16
4	4	308	KC2	CHB-C4A-C3A	-2.21	121.53	124.98
4	4	310	KC2	C1B-CHB-C4A	-2.20	121.30	126.06
2	2	405	A86	C28-C27-C26	-2.20	119.84	122.92
4	1	308	KC2	CHB-C4A-C3A	-2.20	121.54	124.98
4	1	308	KC2	O2D-CGD-O1D	-2.20	119.54	123.84
2	3	304	A86	C20-C19-C18	2.20	117.09	112.75
2	3	305	A86	C12-C11-C13	2.20	119.71	116.02
3	2	409	CLA	C1-C2-C3	-2.20	122.25	126.04
4	3	311	KC2	C1B-CHB-C4A	-2.19	121.32	126.06
2	1	305	A86	C12-C11-C13	2.18	119.69	116.02
3	4	307	CLA	C1-C2-C3	-2.18	122.28	126.04
2	1	304	A86	C20-C19-C18	2.17	117.05	112.75
3	1	307	CLA	C1-C2-C3	-2.17	122.29	126.04
4	1	308	KC2	O2A-CGA-O1A	-2.16	118.18	122.67
2	3	304	A86	C28-C27-C26	-2.16	119.90	122.92
2	3	301	A86	C8-C6-C5	2.15	122.25	118.94
6	3	318	LMT	C3'-C4'-C5'	-2.15	106.00	110.93
2	2	402	A86	C8-C6-C5	2.15	122.24	118.94
6	1	317	LMT	C3'-C4'-C5'	-2.15	106.00	110.93
2	3	305	A86	C-C1-C2	-2.14	119.92	122.92
6	2	419	LMT	C3'-C4'-C5'	-2.14	106.01	110.93
2	4	304	A86	C28-C27-C26	-2.14	119.92	122.92
4	4	308	KC2	C1B-CHB-C4A	-2.14	121.44	126.06
4	2	410	KC2	O2A-CGA-O1A	-2.14	118.22	122.67
4	2	410	KC2	C1B-CHB-C4A	-2.14	121.44	126.06
4	3	309	KC2	C1B-CHB-C4A	-2.14	121.44	126.06
4	3	309	KC2	O2A-CGA-O1A	-2.13	118.24	122.67
6	4	317	LMT	C3'-C4'-C5'	-2.13	106.04	110.93
4	4	308	KC2	O2A-CGA-O1A	-2.13	118.25	122.67
2	1	304	A86	C28-C27-C26	-2.13	119.94	122.92
5	2	415	KC1	O2D-CGD-O1D	-2.13	119.68	123.84
3	1	312	CLA	C2A-C1A-CHA	2.13	127.58	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	308	KC2	C1B-CHB-C4A	-2.12	121.48	126.06
3	3	313	CLA	C2A-C1A-CHA	2.12	127.57	123.86
5	3	314	KC1	O2D-CGD-O1D	-2.12	119.69	123.84
2	2	406	A86	C9-C8-C6	-2.12	120.46	126.42
3	3	308	CLA	C1-C2-C3	-2.12	122.38	126.04
2	4	301	A86	C8-C6-C5	2.12	122.19	118.94
3	1	318	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
3	2	401	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
2	3	303	A86	C26-C25-C24	-2.11	116.62	123.22
3	2	408	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
3	4	312	CLA	C2A-C1A-CHA	2.11	127.55	123.86
3	1	315	CLA	CHD-C1D-ND	-2.11	122.52	124.45
3	3	307	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
2	1	305	A86	C-C1-C2	-2.10	119.98	122.92
2	4	301	A86	C7-C6-C5	-2.10	119.98	122.92
5	4	313	KC1	O2D-CGD-O1D	-2.10	119.73	123.84
2	4	303	A86	C26-C25-C24	-2.10	116.67	123.22
3	2	414	CLA	C2A-C1A-CHA	2.10	127.52	123.86
2	1	301	A86	C7-C6-C5	-2.10	119.99	122.92
2	3	301	A86	C7-C6-C5	-2.10	119.99	122.92
2	2	404	A86	C26-C25-C24	-2.09	116.69	123.22
2	1	302	A86	C28-C27-C26	-2.09	119.99	122.92
5	1	313	KC1	O2D-CGD-O1D	-2.09	119.75	123.84
2	1	305	A86	O1-C15-C20	-2.09	57.36	59.40
2	1	303	A86	C26-C25-C24	-2.09	116.69	123.22
2	4	304	A86	C41-C32-C31	2.09	112.34	110.47
2	3	305	A86	O1-C15-C20	-2.08	57.37	59.40
2	1	304	A86	C41-C32-C31	2.07	112.33	110.47
2	3	304	A86	C41-C32-C31	2.07	112.33	110.47
2	1	304	A86	O1-C15-C20	-2.07	57.38	59.40
5	1	311	KC1	C2A-C3A-C4A	2.07	108.02	106.49
5	2	413	KC1	C2A-C3A-C4A	2.07	108.02	106.49
2	2	405	A86	O1-C15-C20	-2.07	57.38	59.40
2	3	304	A86	O1-C15-C20	-2.06	57.38	59.40
3	1	318	CLA	CHD-C1D-ND	-2.06	122.56	124.45
2	4	302	A86	C28-C27-C26	-2.06	120.04	122.92
2	2	405	A86	C25-C24-C1	-2.05	120.64	126.42
2	4	303	A86	C33-C32-C31	-2.05	107.22	109.21
2	2	402	A86	C7-C6-C5	-2.05	120.05	122.92
2	3	302	A86	C28-C27-C26	-2.05	120.06	122.92
6	4	316	LMT	O5B-C5B-C4B	2.05	113.41	109.69
3	3	310	CLA	O2A-CGA-O1A	-2.04	118.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	315	CLA	CHD-C1D-ND	-2.04	122.58	124.45
2	1	306	A86	C10-C9-C8	-2.04	116.85	123.22
2	2	404	A86	C10-C9-C8	-2.04	116.85	123.22
2	2	405	A86	C41-C32-C31	2.04	112.30	110.47
2	1	303	A86	C10-C9-C8	-2.04	116.85	123.22
2	4	305	A86	C9-C8-C6	-2.04	120.69	126.42
3	3	310	CLA	CHD-C1D-ND	-2.03	122.58	124.45
2	1	303	A86	C12-C11-C13	2.03	119.44	116.02
3	2	408	CLA	CHD-C1D-ND	-2.03	122.58	124.45
2	1	304	A86	C25-C24-C1	-2.03	120.71	126.42
5	2	413	KC1	C3D-CAD-CBD	-2.03	104.93	107.61
3	2	417	CLA	CHD-C1D-ND	-2.03	122.59	124.45
5	3	312	KC1	C2A-C3A-C4A	2.03	107.99	106.49
2	2	404	A86	C12-C11-C13	2.03	119.43	116.02
2	1	302	A86	C10-C9-C8	-2.03	116.88	123.22
2	3	302	A86	C10-C9-C8	-2.03	116.88	123.22
2	4	304	A86	O1-C15-C20	-2.03	57.42	59.40
3	4	309	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
6	3	317	LMT	O5B-C5B-C4B	2.03	113.38	109.69
2	4	304	A86	C25-C24-C1	-2.03	120.72	126.42
5	3	312	KC1	C3D-CAD-CBD	-2.03	104.94	107.61
5	4	313	KC1	CHD-C4C-NC	2.02	127.27	124.20
2	4	303	A86	C10-C9-C8	-2.02	116.90	123.22
5	1	311	KC1	C3D-CAD-CBD	-2.02	104.94	107.61
3	1	309	CLA	CHD-C1D-ND	-2.02	122.60	124.45
2	2	405	A86	C4-C3-C2	-2.02	119.33	123.47
2	3	303	A86	C10-C9-C8	-2.02	116.91	123.22
2	3	304	A86	C25-C24-C1	-2.02	120.74	126.42
2	2	406	A86	C17-C16-C15	2.02	111.22	109.16
5	4	311	KC1	C2A-C3A-C4A	2.02	107.98	106.49
2	4	302	A86	C10-C9-C8	-2.02	116.92	123.22
2	4	303	A86	C12-C11-C13	2.02	119.41	116.02
3	2	411	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
2	3	303	A86	C12-C11-C13	2.02	119.41	116.02
3	3	316	CLA	CHD-C1D-ND	-2.02	122.60	124.45
2	4	304	A86	C4-C3-C2	-2.01	119.35	123.47
2	3	304	A86	C4-C3-C2	-2.01	119.35	123.47
5	4	311	KC1	C3D-CAD-CBD	-2.01	104.96	107.61
2	1	304	A86	C4-C3-C2	-2.01	119.36	123.47
3	2	411	CLA	CHD-C1D-ND	-2.01	122.61	124.45
3	1	309	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
2	2	403	A86	C28-C27-C26	-2.00	120.12	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	414	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
6	1	316	LMT	O5B-C5B-C4B	2.00	113.33	109.69

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	1	307	CLA	ND
3	1	309	CLA	ND
3	1	312	CLA	ND
3	1	314	CLA	ND
3	1	315	CLA	ND
3	1	318	CLA	ND
3	2	401	CLA	ND
3	2	408	CLA	ND
3	2	409	CLA	ND
3	2	411	CLA	ND
3	2	414	CLA	ND
3	2	416	CLA	ND
3	2	417	CLA	ND
3	3	307	CLA	ND
3	3	308	CLA	ND
3	3	310	CLA	ND
3	3	313	CLA	ND
3	3	315	CLA	ND
3	3	316	CLA	ND
3	4	307	CLA	ND
3	4	309	CLA	ND
3	4	312	CLA	ND
3	4	314	CLA	ND
3	4	315	CLA	ND

All (604) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	301	A86	C13-C14-C15-O1
2	1	302	A86	C10-C11-C13-O
2	1	302	A86	C12-C11-C13-O
2	1	302	A86	C13-C14-C15-O1
2	1	305	A86	C-C1-C24-C25
2	1	305	A86	C2-C1-C24-C25
2	1	305	A86	C11-C10-C9-C8
2	1	305	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	1	306	A86	C10-C11-C13-O
2	1	306	A86	C12-C11-C13-O
2	2	402	A86	C13-C14-C15-O1
2	2	403	A86	C10-C11-C13-O
2	2	403	A86	C12-C11-C13-O
2	2	403	A86	C13-C14-C15-O1
2	2	406	A86	C11-C10-C9-C8
2	2	406	A86	C12-C11-C13-O
2	2	406	A86	C12-C11-C13-C14
2	2	406	A86	C13-C14-C15-O1
2	2	406	A86	C24-C25-C26-C27
2	2	407	A86	C12-C11-C13-O
2	2	407	A86	C13-C14-C15-O1
2	3	301	A86	C13-C14-C15-O1
2	3	302	A86	C10-C11-C13-O
2	3	302	A86	C12-C11-C13-O
2	3	302	A86	C13-C14-C15-O1
2	3	305	A86	C-C1-C24-C25
2	3	305	A86	C2-C1-C24-C25
2	3	305	A86	C11-C10-C9-C8
2	3	305	A86	C24-C25-C26-C27
2	3	306	A86	C12-C11-C13-O
2	3	306	A86	C13-C14-C15-O1
2	4	301	A86	C13-C14-C15-O1
2	4	302	A86	C10-C11-C13-O
2	4	302	A86	C12-C11-C13-O
2	4	302	A86	C13-C14-C15-O1
2	4	305	A86	C11-C10-C9-C8
2	4	305	A86	C12-C11-C13-O
2	4	305	A86	C12-C11-C13-C14
2	4	305	A86	C13-C14-C15-O1
2	4	305	A86	C24-C25-C26-C27
2	4	306	A86	C12-C11-C13-O
2	4	306	A86	C13-C14-C15-O1
3	1	314	CLA	C1A-C2A-CAA-CBA
3	1	314	CLA	C2A-CAA-CBA-CGA
3	1	315	CLA	CBA-CGA-O2A-C1
3	1	318	CLA	CHA-CBD-CGD-O1D
3	1	318	CLA	CHA-CBD-CGD-O2D
3	2	401	CLA	CHA-CBD-CGD-O1D
3	2	401	CLA	CHA-CBD-CGD-O2D
3	2	408	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	2	408	CLA	CHA-CBD-CGD-O2D
3	2	416	CLA	C2A-CAA-CBA-CGA
3	2	417	CLA	CBA-CGA-O2A-C1
3	2	417	CLA	O1A-CGA-O2A-C1
3	3	307	CLA	CHA-CBD-CGD-O1D
3	3	307	CLA	CHA-CBD-CGD-O2D
3	3	315	CLA	C2A-CAA-CBA-CGA
3	3	316	CLA	CBA-CGA-O2A-C1
3	4	315	CLA	CBA-CGA-O2A-C1
3	4	315	CLA	O1A-CGA-O2A-C1
4	1	308	KC2	C1A-C2A-CAA-CBA
4	1	308	KC2	C3A-C2A-CAA-CBA
4	1	308	KC2	C2B-C3B-CAB-CBB
4	1	310	KC2	C2B-C3B-CAB-CBB
4	1	310	KC2	C4B-C3B-CAB-CBB
4	1	310	KC2	C2C-C3C-CAC-CBC
4	1	310	KC2	C4C-C3C-CAC-CBC
4	2	410	KC2	C1A-C2A-CAA-CBA
4	2	410	KC2	C3A-C2A-CAA-CBA
4	2	410	KC2	C2B-C3B-CAB-CBB
4	2	410	KC2	C4B-C3B-CAB-CBB
4	2	412	KC2	C2B-C3B-CAB-CBB
4	2	412	KC2	C4B-C3B-CAB-CBB
4	2	412	KC2	C2C-C3C-CAC-CBC
4	2	412	KC2	C4C-C3C-CAC-CBC
4	2	412	KC2	C2A-CAA-CBA-CGA
4	3	309	KC2	C1A-C2A-CAA-CBA
4	3	309	KC2	C3A-C2A-CAA-CBA
4	3	309	KC2	C2B-C3B-CAB-CBB
4	3	311	KC2	C2B-C3B-CAB-CBB
4	3	311	KC2	C4B-C3B-CAB-CBB
4	3	311	KC2	C2A-CAA-CBA-CGA
4	4	308	KC2	C1A-C2A-CAA-CBA
4	4	308	KC2	C3A-C2A-CAA-CBA
4	4	308	KC2	C2B-C3B-CAB-CBB
4	4	308	KC2	C4B-C3B-CAB-CBB
4	4	310	KC2	C2B-C3B-CAB-CBB
4	4	310	KC2	C4B-C3B-CAB-CBB
4	4	310	KC2	C4C-C3C-CAC-CBC
4	4	310	KC2	C2A-CAA-CBA-CGA
5	1	311	KC1	C2B-C3B-CAB-CBB
5	1	313	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	2	413	KC1	C2B-C3B-CAB-CBB
5	2	415	KC1	C2B-C3B-CAB-CBB
5	3	312	KC1	C2B-C3B-CAB-CBB
5	3	314	KC1	C2B-C3B-CAB-CBB
5	4	311	KC1	C2B-C3B-CAB-CBB
5	4	313	KC1	C2B-C3B-CAB-CBB
6	1	317	LMT	C2'-C1'-O1'-C1
6	1	317	LMT	O5'-C1'-O1'-C1
6	2	419	LMT	C2'-C1'-O1'-C1
6	2	419	LMT	O5'-C1'-O1'-C1
6	3	318	LMT	C2'-C1'-O1'-C1
6	3	318	LMT	O5'-C1'-O1'-C1
6	4	317	LMT	C2'-C1'-O1'-C1
6	4	317	LMT	O5'-C1'-O1'-C1
2	1	302	A86	C39-C38-O4-C34
2	1	303	A86	C39-C38-O4-C34
2	1	304	A86	C39-C38-O4-C34
2	1	306	A86	C39-C38-O4-C34
2	2	403	A86	C39-C38-O4-C34
2	2	404	A86	C39-C38-O4-C34
2	2	405	A86	C39-C38-O4-C34
2	2	407	A86	C39-C38-O4-C34
2	3	302	A86	C39-C38-O4-C34
2	3	303	A86	C39-C38-O4-C34
2	3	304	A86	C39-C38-O4-C34
2	3	306	A86	C39-C38-O4-C34
2	4	302	A86	C39-C38-O4-C34
2	4	303	A86	C39-C38-O4-C34
2	4	304	A86	C39-C38-O4-C34
2	4	306	A86	C39-C38-O4-C34
3	1	314	CLA	O1D-CGD-O2D-CED
3	1	314	CLA	CBD-CGD-O2D-CED
3	2	416	CLA	CBD-CGD-O2D-CED
3	3	315	CLA	CBD-CGD-O2D-CED
3	4	314	CLA	CBD-CGD-O2D-CED
3	1	315	CLA	O1A-CGA-O2A-C1
3	3	316	CLA	O1A-CGA-O2A-C1
3	2	416	CLA	O1D-CGD-O2D-CED
3	3	315	CLA	O1D-CGD-O2D-CED
3	4	314	CLA	O1D-CGD-O2D-CED
3	4	314	CLA	CBA-CGA-O2A-C1
6	1	316	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
6	2	418	LMT	O5B-C1B-O1B-C4'
6	3	317	LMT	O5B-C1B-O1B-C4'
6	4	316	LMT	O5B-C1B-O1B-C4'
3	1	309	CLA	CBD-CGD-O2D-CED
3	1	315	CLA	CBD-CGD-O2D-CED
3	2	411	CLA	CBD-CGD-O2D-CED
3	3	310	CLA	CBD-CGD-O2D-CED
3	4	309	CLA	CBD-CGD-O2D-CED
3	1	312	CLA	O1A-CGA-O2A-C1
3	2	414	CLA	O1A-CGA-O2A-C1
3	3	313	CLA	O1A-CGA-O2A-C1
3	4	312	CLA	O1A-CGA-O2A-C1
2	1	302	A86	O5-C38-O4-C34
2	1	303	A86	O5-C38-O4-C34
2	1	304	A86	O5-C38-O4-C34
2	1	306	A86	O5-C38-O4-C34
2	2	403	A86	O5-C38-O4-C34
2	2	404	A86	O5-C38-O4-C34
2	2	405	A86	O5-C38-O4-C34
2	2	407	A86	O5-C38-O4-C34
2	3	302	A86	O5-C38-O4-C34
2	3	303	A86	O5-C38-O4-C34
2	3	304	A86	O5-C38-O4-C34
2	3	306	A86	O5-C38-O4-C34
2	4	302	A86	O5-C38-O4-C34
2	4	303	A86	O5-C38-O4-C34
2	4	304	A86	O5-C38-O4-C34
2	4	306	A86	O5-C38-O4-C34
6	1	316	LMT	C2B-C1B-O1B-C4'
6	2	418	LMT	C2B-C1B-O1B-C4'
6	3	317	LMT	C2B-C1B-O1B-C4'
6	4	316	LMT	C2B-C1B-O1B-C4'
3	2	416	CLA	CBA-CGA-O2A-C1
3	3	315	CLA	CBA-CGA-O2A-C1
2	1	306	A86	C35-C34-O4-C38
2	2	407	A86	C35-C34-O4-C38
2	4	306	A86	C35-C34-O4-C38
3	4	315	CLA	CBD-CGD-O2D-CED
3	2	416	CLA	O1A-CGA-O2A-C1
3	3	315	CLA	O1A-CGA-O2A-C1
5	1	313	KC1	CAA-CBA-CGA-O2A
5	2	415	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
5	3	314	KC1	CAA-CBA-CGA-O2A
5	4	313	KC1	CAA-CBA-CGA-O2A
3	1	314	CLA	CBA-CGA-O2A-C1
3	4	314	CLA	C2A-CAA-CBA-CGA
3	4	314	CLA	O1A-CGA-O2A-C1
3	1	312	CLA	CBA-CGA-O2A-C1
3	2	414	CLA	CBA-CGA-O2A-C1
3	3	313	CLA	CBA-CGA-O2A-C1
3	4	312	CLA	CBA-CGA-O2A-C1
2	1	301	A86	C39-C38-O4-C34
2	1	305	A86	C39-C38-O4-C34
2	2	402	A86	C39-C38-O4-C34
2	2	406	A86	C39-C38-O4-C34
2	3	301	A86	C39-C38-O4-C34
2	3	305	A86	C39-C38-O4-C34
2	4	301	A86	C39-C38-O4-C34
2	4	305	A86	C39-C38-O4-C34
2	1	301	A86	O5-C38-O4-C34
2	1	305	A86	O5-C38-O4-C34
2	2	402	A86	O5-C38-O4-C34
2	2	406	A86	O5-C38-O4-C34
2	3	301	A86	O5-C38-O4-C34
2	3	305	A86	O5-C38-O4-C34
2	4	301	A86	O5-C38-O4-C34
2	4	305	A86	O5-C38-O4-C34
5	1	313	KC1	CAA-CBA-CGA-O1A
5	2	415	KC1	CAA-CBA-CGA-O1A
5	4	313	KC1	CAA-CBA-CGA-O1A
3	1	314	CLA	O1A-CGA-O2A-C1
2	1	303	A86	C35-C34-O4-C38
2	2	404	A86	C35-C34-O4-C38
2	3	303	A86	C35-C34-O4-C38
2	4	303	A86	C35-C34-O4-C38
2	1	304	A86	C35-C34-O4-C38
2	2	405	A86	C35-C34-O4-C38
2	3	304	A86	C35-C34-O4-C38
2	4	304	A86	C35-C34-O4-C38
3	3	307	CLA	C11-C12-C13-C14
3	3	310	CLA	O1D-CGD-O2D-CED
2	2	406	A86	C-C1-C24-C25
2	2	406	A86	C7-C6-C8-C9
2	4	305	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
2	4	305	A86	C7-C6-C8-C9
3	1	309	CLA	O1D-CGD-O2D-CED
3	2	411	CLA	O1D-CGD-O2D-CED
6	2	419	LMT	O5B-C5B-C6B-O6B
6	3	318	LMT	O5B-C5B-C6B-O6B
6	4	317	LMT	O5B-C5B-C6B-O6B
3	4	309	CLA	O1D-CGD-O2D-CED
6	1	317	LMT	O5B-C5B-C6B-O6B
4	3	311	KC2	CBD-CGD-O2D-CED
2	2	403	A86	C33-C34-O4-C38
2	3	301	A86	C35-C34-O4-C38
2	3	306	A86	C35-C34-O4-C38
3	3	307	CLA	C8-C10-C11-C12
3	3	308	CLA	C11-C10-C8-C7
2	1	301	A86	C35-C34-O4-C38
2	1	305	A86	C35-C34-O4-C38
2	2	402	A86	C35-C34-O4-C38
2	3	305	A86	C35-C34-O4-C38
2	4	301	A86	C35-C34-O4-C38
3	1	315	CLA	O1D-CGD-O2D-CED
2	2	406	A86	C35-C34-O4-C38
2	4	305	A86	C35-C34-O4-C38
3	1	318	CLA	C10-C11-C12-C13
3	2	408	CLA	C10-C11-C12-C13
3	2	401	CLA	C10-C11-C12-C13
3	4	315	CLA	O1D-CGD-O2D-CED
4	2	412	KC2	CBD-CGD-O2D-CED
4	1	308	KC2	CAA-CBA-CGA-O2A
4	2	410	KC2	CAA-CBA-CGA-O2A
4	3	309	KC2	CAA-CBA-CGA-O2A
4	4	308	KC2	CAA-CBA-CGA-O2A
2	4	302	A86	C33-C34-O4-C38
6	1	316	LMT	O5'-C5'-C6'-O6'
6	3	317	LMT	O5'-C5'-C6'-O6'
6	4	316	LMT	O5'-C5'-C6'-O6'
2	1	302	A86	C33-C34-O4-C38
2	1	302	A86	C35-C34-O4-C38
2	3	302	A86	C33-C34-O4-C38
2	3	302	A86	C35-C34-O4-C38
2	4	302	A86	C35-C34-O4-C38
4	1	310	KC2	C2A-CAA-CBA-CGA
2	2	403	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
6	3	317	LMT	C2'-C1'-O1'-C1
5	3	314	KC1	CAA-CBA-CGA-O1A
2	2	406	A86	C2-C1-C24-C25
2	2	406	A86	C5-C6-C8-C9
2	4	305	A86	C2-C1-C24-C25
2	4	305	A86	C5-C6-C8-C9
6	2	418	LMT	O5'-C5'-C6'-O6'
6	3	317	LMT	O5'-C1'-O1'-C1
2	2	402	A86	C33-C34-O4-C38
2	4	301	A86	C33-C34-O4-C38
3	1	312	CLA	C3A-C2A-CAA-CBA
3	2	414	CLA	C3A-C2A-CAA-CBA
3	3	313	CLA	C3A-C2A-CAA-CBA
3	4	312	CLA	C3A-C2A-CAA-CBA
6	4	316	LMT	C2-C1-O1'-C1'
2	1	301	A86	C33-C34-O4-C38
2	3	301	A86	C33-C34-O4-C38
4	4	310	KC2	CBD-CGD-O2D-CED
3	3	310	CLA	C2-C3-C5-C6
2	1	303	A86	C33-C34-O4-C38
3	1	318	CLA	C8-C10-C11-C12
3	2	401	CLA	C8-C10-C11-C12
3	2	408	CLA	C8-C10-C11-C12
3	1	307	CLA	C11-C10-C8-C7
3	2	409	CLA	C11-C10-C8-C7
3	4	307	CLA	C11-C10-C8-C7
2	1	305	A86	C33-C34-O4-C38
2	2	406	A86	C33-C34-O4-C38
2	4	305	A86	C33-C34-O4-C38
3	1	318	CLA	C5-C6-C7-C8
3	2	408	CLA	C5-C6-C7-C8
3	2	401	CLA	C5-C6-C7-C8
4	1	308	KC2	C2C-C3C-CAC-CBC
4	2	410	KC2	C2C-C3C-CAC-CBC
4	3	309	KC2	C2C-C3C-CAC-CBC
4	3	311	KC2	C2C-C3C-CAC-CBC
4	4	308	KC2	C2C-C3C-CAC-CBC
4	4	310	KC2	C2C-C3C-CAC-CBC
2	3	303	A86	C33-C34-O4-C38
2	3	305	A86	C33-C34-O4-C38
6	4	316	LMT	O5'-C1'-O1'-C1
4	1	308	KC2	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	1	308	KC2	C4C-C3C-CAC-CBC
4	2	410	KC2	C4C-C3C-CAC-CBC
4	3	309	KC2	C4B-C3B-CAB-CBB
4	3	309	KC2	C4C-C3C-CAC-CBC
4	3	311	KC2	C4C-C3C-CAC-CBC
4	4	308	KC2	C4C-C3C-CAC-CBC
5	1	311	KC1	C4B-C3B-CAB-CBB
5	1	313	KC1	C4B-C3B-CAB-CBB
5	2	413	KC1	C4B-C3B-CAB-CBB
5	2	415	KC1	C4B-C3B-CAB-CBB
5	3	312	KC1	C4B-C3B-CAB-CBB
5	3	314	KC1	C4B-C3B-CAB-CBB
5	4	311	KC1	C4B-C3B-CAB-CBB
5	4	313	KC1	C4B-C3B-CAB-CBB
4	1	310	KC2	CBD-CGD-O2D-CED
3	3	307	CLA	C10-C11-C12-C13
3	3	310	CLA	C4-C3-C5-C6
3	1	307	CLA	C11-C10-C8-C9
3	2	401	CLA	C6-C7-C8-C9
3	2	408	CLA	C6-C7-C8-C9
3	3	308	CLA	C11-C10-C8-C9
3	4	307	CLA	C11-C10-C8-C9
2	3	306	A86	C33-C34-O4-C38
2	1	305	A86	C7-C6-C8-C9
2	3	305	A86	C7-C6-C8-C9
2	1	305	A86	C5-C6-C8-C9
2	3	305	A86	C5-C6-C8-C9
3	1	312	CLA	C1A-C2A-CAA-CBA
3	2	414	CLA	C1A-C2A-CAA-CBA
3	3	313	CLA	C1A-C2A-CAA-CBA
3	4	312	CLA	C1A-C2A-CAA-CBA
2	2	404	A86	C33-C34-O4-C38
2	4	303	A86	C33-C34-O4-C38
4	1	310	KC2	CAA-CBA-CGA-O2A
4	2	412	KC2	CAA-CBA-CGA-O2A
4	4	310	KC2	CAA-CBA-CGA-O2A
3	2	411	CLA	C4-C3-C5-C6
3	1	309	CLA	C4-C3-C5-C6
3	4	309	CLA	C4-C3-C5-C6
3	3	316	CLA	CBD-CGD-O2D-CED
2	2	405	A86	C33-C34-O4-C38
2	4	304	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
5	1	311	KC1	CAA-CBA-CGA-O2A
5	2	413	KC1	CAA-CBA-CGA-O2A
5	4	311	KC1	CAA-CBA-CGA-O2A
6	4	316	LMT	C2'-C1'-O1'-C1
2	1	304	A86	C33-C34-O4-C38
2	3	304	A86	C33-C34-O4-C38
3	1	318	CLA	C6-C7-C8-C10
3	2	401	CLA	C6-C7-C8-C10
3	2	408	CLA	C6-C7-C8-C10
3	1	318	CLA	C6-C7-C8-C9
3	2	409	CLA	C11-C10-C8-C9
3	3	307	CLA	C14-C13-C15-C16
5	3	312	KC1	CAA-CBA-CGA-O2A
3	1	307	CLA	C5-C6-C7-C8
3	2	409	CLA	C5-C6-C7-C8
3	1	314	CLA	C3A-C2A-CAA-CBA
6	1	316	LMT	C2-C1-O1'-C1'
6	1	317	LMT	C2-C1-O1'-C1'
6	2	418	LMT	C2-C1-O1'-C1'
6	2	419	LMT	C2-C1-O1'-C1'
6	3	318	LMT	C2-C1-O1'-C1'
6	4	317	LMT	C2-C1-O1'-C1'
3	2	411	CLA	C2-C3-C5-C6
3	4	307	CLA	C5-C6-C7-C8
2	1	303	A86	C10-C11-C13-C14
2	2	404	A86	C10-C11-C13-C14
2	2	406	A86	C10-C11-C13-C14
2	3	303	A86	C10-C11-C13-C14
2	4	303	A86	C10-C11-C13-C14
2	4	305	A86	C10-C11-C13-C14
3	1	318	CLA	C12-C13-C15-C16
3	2	401	CLA	C12-C13-C15-C16
3	2	408	CLA	C12-C13-C15-C16
3	3	307	CLA	C12-C13-C15-C16
3	4	309	CLA	C2-C3-C5-C6
3	3	307	CLA	CBA-CGA-O2A-C1
4	1	310	KC2	CAD-CBD-CGD-O2D
4	2	412	KC2	CAD-CBD-CGD-O2D
4	3	311	KC2	CAD-CBD-CGD-O2D
4	4	310	KC2	CAD-CBD-CGD-O2D
3	2	409	CLA	CBA-CGA-O2A-C1
3	1	309	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
2	1	301	A86	C12-C11-C13-O
2	1	303	A86	C12-C11-C13-O
2	1	304	A86	C12-C11-C13-O
2	1	305	A86	C12-C11-C13-O
2	2	402	A86	C12-C11-C13-O
2	2	404	A86	C12-C11-C13-O
2	2	405	A86	C12-C11-C13-O
2	3	301	A86	C12-C11-C13-O
2	3	303	A86	C12-C11-C13-O
2	3	304	A86	C12-C11-C13-O
2	3	305	A86	C12-C11-C13-O
2	4	301	A86	C12-C11-C13-O
2	4	303	A86	C12-C11-C13-O
2	4	304	A86	C12-C11-C13-O
3	3	308	CLA	C5-C6-C7-C8
3	1	309	CLA	CHA-CBD-CGD-O1D
3	1	314	CLA	CHA-CBD-CGD-O1D
3	1	314	CLA	CHA-CBD-CGD-O2D
3	2	411	CLA	CHA-CBD-CGD-O1D
3	3	310	CLA	CHA-CBD-CGD-O1D
3	4	309	CLA	CHA-CBD-CGD-O1D
4	2	410	KC2	CHA-CBD-CGD-O1D
4	4	308	KC2	CHA-CBD-CGD-O1D
3	1	309	CLA	C6-C7-C8-C10
3	2	411	CLA	C6-C7-C8-C10
3	4	309	CLA	C6-C7-C8-C10
2	1	301	A86	C10-C11-C13-O
2	1	303	A86	C10-C11-C13-O
2	1	304	A86	C10-C11-C13-O
2	1	305	A86	C10-C11-C13-O
2	2	402	A86	C10-C11-C13-O
2	2	404	A86	C10-C11-C13-O
2	2	405	A86	C10-C11-C13-O
2	2	406	A86	C10-C11-C13-O
2	2	407	A86	C10-C11-C13-O
2	3	301	A86	C10-C11-C13-O
2	3	303	A86	C10-C11-C13-O
2	3	304	A86	C10-C11-C13-O
2	3	305	A86	C10-C11-C13-O
2	3	306	A86	C10-C11-C13-O
2	4	301	A86	C10-C11-C13-O
2	4	303	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
2	4	304	A86	C10-C11-C13-O
2	4	305	A86	C10-C11-C13-O
2	4	306	A86	C10-C11-C13-O
3	3	316	CLA	O1D-CGD-O2D-CED
3	3	310	CLA	C6-C7-C8-C10
6	1	317	LMT	O5'-C5'-C6'-O6'
3	3	307	CLA	O1A-CGA-O2A-C1
6	2	419	LMT	O5'-C5'-C6'-O6'
6	3	318	LMT	O5'-C5'-C6'-O6'
3	1	307	CLA	CBA-CGA-O2A-C1
6	4	317	LMT	O5'-C5'-C6'-O6'
6	1	316	LMT	O5'-C1'-O1'-C1
3	1	309	CLA	C6-C7-C8-C9
3	4	309	CLA	C6-C7-C8-C9
3	2	409	CLA	O1A-CGA-O2A-C1
3	4	307	CLA	CBA-CGA-O2A-C1
3	4	314	CLA	C3A-C2A-CAA-CBA
3	1	307	CLA	O1A-CGA-O2A-C1
3	1	309	CLA	C2A-CAA-CBA-CGA
3	2	411	CLA	C2A-CAA-CBA-CGA
3	4	309	CLA	C2A-CAA-CBA-CGA
3	3	310	CLA	C6-C7-C8-C9
3	2	411	CLA	C6-C7-C8-C9
2	1	302	A86	C13-C14-C15-C20
2	1	303	A86	C13-C14-C15-C20
2	1	305	A86	C13-C14-C15-C20
2	2	403	A86	C13-C14-C15-C20
2	2	404	A86	C13-C14-C15-C20
2	3	302	A86	C13-C14-C15-C20
2	3	303	A86	C13-C14-C15-C20
2	3	305	A86	C13-C14-C15-C20
2	4	302	A86	C13-C14-C15-C20
2	4	303	A86	C13-C14-C15-C20
3	1	318	CLA	C14-C13-C15-C16
3	2	401	CLA	C14-C13-C15-C16
3	2	408	CLA	C14-C13-C15-C16
6	2	418	LMT	O5'-C1'-O1'-C1
3	4	307	CLA	O1A-CGA-O2A-C1
3	3	310	CLA	C2A-CAA-CBA-CGA
2	1	301	A86	C12-C11-C13-C14
2	1	302	A86	C12-C11-C13-C14
2	1	303	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
2	1	304	A86	C12-C11-C13-C14
2	1	305	A86	C12-C11-C13-C14
2	1	306	A86	C12-C11-C13-C14
2	2	402	A86	C12-C11-C13-C14
2	2	403	A86	C12-C11-C13-C14
2	2	404	A86	C12-C11-C13-C14
2	2	405	A86	C12-C11-C13-C14
2	2	407	A86	C12-C11-C13-C14
2	3	301	A86	C12-C11-C13-C14
2	3	302	A86	C12-C11-C13-C14
2	3	303	A86	C12-C11-C13-C14
2	3	304	A86	C12-C11-C13-C14
2	3	305	A86	C12-C11-C13-C14
2	3	306	A86	C12-C11-C13-C14
2	4	301	A86	C12-C11-C13-C14
2	4	302	A86	C12-C11-C13-C14
2	4	303	A86	C12-C11-C13-C14
2	4	304	A86	C12-C11-C13-C14
2	4	306	A86	C12-C11-C13-C14
6	1	317	LMT	C4'-C5'-C6'-O6'
6	3	318	LMT	C4B-C5B-C6B-O6B
4	1	308	KC2	CAA-CBA-CGA-O1A
4	3	309	KC2	CAA-CBA-CGA-O1A
6	2	419	LMT	C4B-C5B-C6B-O6B
6	2	419	LMT	C4'-C5'-C6'-O6'
6	3	318	LMT	C4'-C5'-C6'-O6'
6	4	317	LMT	C4B-C5B-C6B-O6B
6	4	317	LMT	C4'-C5'-C6'-O6'
6	1	316	LMT	C2'-C1'-O1'-C1
6	2	418	LMT	C2'-C1'-O1'-C1
3	1	307	CLA	C2A-CAA-CBA-CGA
3	2	409	CLA	C2A-CAA-CBA-CGA
3	1	318	CLA	C11-C10-C8-C9
3	2	401	CLA	C11-C10-C8-C9
3	2	408	CLA	C11-C10-C8-C9
3	4	307	CLA	C2A-CAA-CBA-CGA
6	1	317	LMT	C4B-C5B-C6B-O6B
3	4	314	CLA	C1A-C2A-CAA-CBA
3	3	307	CLA	C11-C12-C13-C15
4	4	308	KC2	CAA-CBA-CGA-O1A
6	2	419	LMT	C3-C4-C5-C6
6	1	317	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	4	317	LMT	C3-C4-C5-C6
6	3	318	LMT	C3-C4-C5-C6
3	3	310	CLA	C3-C5-C6-C7
2	1	302	A86	C13-C14-C15-C16
2	2	403	A86	C13-C14-C15-C16
2	2	407	A86	C13-C14-C15-C16
2	3	302	A86	C13-C14-C15-C16
2	3	306	A86	C13-C14-C15-C16
2	4	302	A86	C13-C14-C15-C16
2	4	306	A86	C13-C14-C15-C16
4	2	410	KC2	CAA-CBA-CGA-O1A
2	1	301	A86	C10-C11-C13-C14
2	1	302	A86	C10-C11-C13-C14
2	1	304	A86	C10-C11-C13-C14
2	1	305	A86	C10-C11-C13-C14
2	1	306	A86	C10-C11-C13-C14
2	2	402	A86	C10-C11-C13-C14
2	2	403	A86	C10-C11-C13-C14
2	2	405	A86	C10-C11-C13-C14
2	2	407	A86	C10-C11-C13-C14
2	3	301	A86	C10-C11-C13-C14
2	3	302	A86	C10-C11-C13-C14
2	3	304	A86	C10-C11-C13-C14
2	3	305	A86	C10-C11-C13-C14
2	3	306	A86	C10-C11-C13-C14
2	4	301	A86	C10-C11-C13-C14
2	4	302	A86	C10-C11-C13-C14
2	4	304	A86	C10-C11-C13-C14
2	4	306	A86	C10-C11-C13-C14
2	1	306	A86	C33-C34-O4-C38
2	2	407	A86	C33-C34-O4-C38
5	1	311	KC1	C1A-C2A-CAA-CBA
5	2	413	KC1	C1A-C2A-CAA-CBA
5	3	312	KC1	C1A-C2A-CAA-CBA
5	4	311	KC1	C1A-C2A-CAA-CBA
3	3	308	CLA	C2A-CAA-CBA-CGA
2	4	306	A86	C33-C34-O4-C38
6	1	317	LMT	O1'-C1-C2-C3
6	2	419	LMT	O1'-C1-C2-C3
6	3	318	LMT	O1'-C1-C2-C3
6	4	317	LMT	O1'-C1-C2-C3
3	2	416	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	3	315	CLA	C3A-C2A-CAA-CBA
3	3	308	CLA	O1A-CGA-O2A-C1
3	3	313	CLA	CAA-CBA-CGA-O2A
3	2	414	CLA	CAA-CBA-CGA-O2A
4	3	311	KC2	CAA-CBA-CGA-O2A
3	1	312	CLA	CAA-CBA-CGA-O2A
3	4	312	CLA	CAA-CBA-CGA-O2A
3	3	308	CLA	CBA-CGA-O2A-C1
3	2	411	CLA	C3-C5-C6-C7
3	1	309	CLA	CHA-CBD-CGD-O2D
3	1	312	CLA	CHA-CBD-CGD-O2D
3	1	315	CLA	CHA-CBD-CGD-O1D
3	1	315	CLA	CHA-CBD-CGD-O2D
3	2	411	CLA	CHA-CBD-CGD-O2D
3	2	414	CLA	CHA-CBD-CGD-O2D
3	2	417	CLA	CHA-CBD-CGD-O1D
3	2	417	CLA	CHA-CBD-CGD-O2D
3	3	310	CLA	CHA-CBD-CGD-O2D
3	3	313	CLA	CHA-CBD-CGD-O2D
3	4	309	CLA	CHA-CBD-CGD-O2D
3	4	312	CLA	CHA-CBD-CGD-O2D
3	4	315	CLA	CHA-CBD-CGD-O1D
3	4	315	CLA	CHA-CBD-CGD-O2D
4	1	308	KC2	CHA-CBD-CGD-O1D
4	3	309	KC2	CHA-CBD-CGD-O1D
5	1	313	KC1	CHA-CBD-CGD-O2D
5	2	415	KC1	CHA-CBD-CGD-O1D
5	2	415	KC1	CHA-CBD-CGD-O2D
5	3	314	KC1	CHA-CBD-CGD-O1D
5	3	314	KC1	CHA-CBD-CGD-O2D
5	4	313	KC1	CHA-CBD-CGD-O1D
5	4	313	KC1	CHA-CBD-CGD-O2D
3	4	309	CLA	C3-C5-C6-C7
3	1	309	CLA	C3-C5-C6-C7
3	2	416	CLA	C1A-C2A-CAA-CBA
3	3	315	CLA	C1A-C2A-CAA-CBA
3	1	312	CLA	CAA-CBA-CGA-O1A
3	2	414	CLA	CAA-CBA-CGA-O1A
3	3	313	CLA	CAA-CBA-CGA-O1A
3	4	312	CLA	CAA-CBA-CGA-O1A
3	4	315	CLA	CAA-CBA-CGA-O2A
4	1	308	KC2	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	1	309	CLA	CAD-CBD-CGD-O1D
3	1	315	CLA	CAD-CBD-CGD-O1D
3	2	411	CLA	CAD-CBD-CGD-O1D
3	3	310	CLA	CAD-CBD-CGD-O1D
3	4	309	CLA	CAD-CBD-CGD-O1D
3	2	417	CLA	CAA-CBA-CGA-O2A
3	1	315	CLA	CAA-CBA-CGA-O2A
3	3	316	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

41 monomers are involved in 65 short contacts:

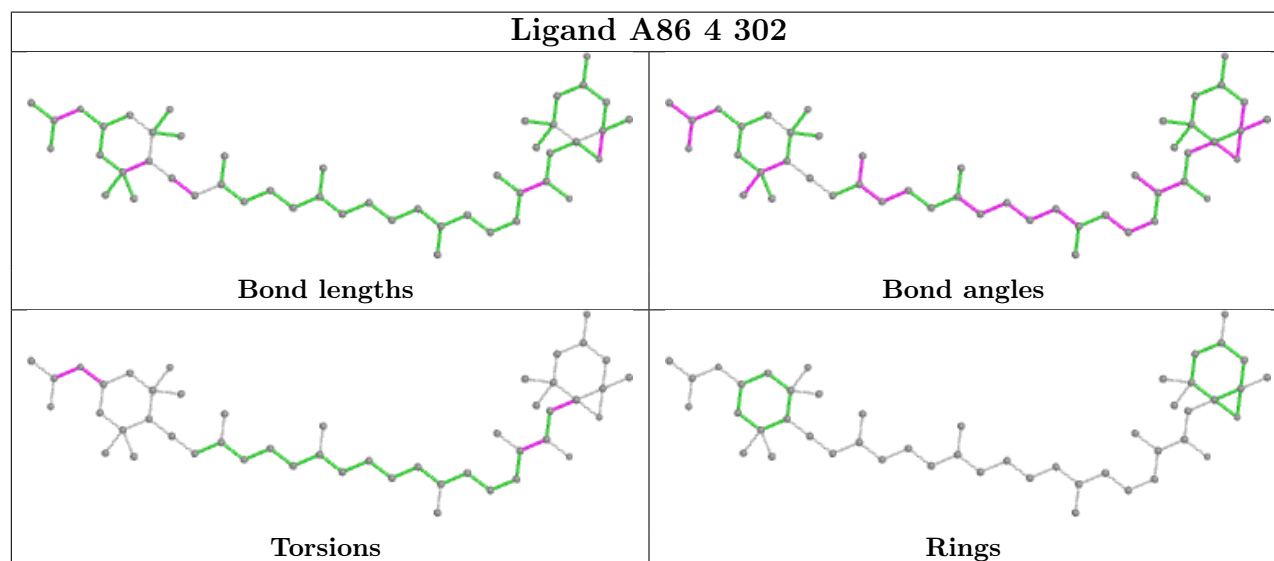
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4	312	CLA	2	0
2	2	405	A86	1	0
3	2	414	CLA	3	0
2	1	304	A86	1	0
3	3	307	CLA	3	0
2	4	303	A86	1	0
3	4	314	CLA	2	0
3	1	318	CLA	4	0
3	4	309	CLA	1	0
2	3	305	A86	1	0
3	2	408	CLA	5	0
3	1	312	CLA	3	0
6	1	317	LMT	1	0
3	3	316	CLA	2	0
2	2	402	A86	1	0
3	4	307	CLA	4	0
3	1	315	CLA	2	0
3	3	313	CLA	3	0
3	3	315	CLA	3	0
3	1	314	CLA	1	0
2	2	404	A86	1	0
6	3	318	LMT	1	0
3	1	309	CLA	1	0
4	3	309	KC2	1	0
3	2	409	CLA	3	0
2	3	304	A86	1	0
3	1	307	CLA	3	0
4	4	308	KC2	1	0
2	1	305	A86	1	0

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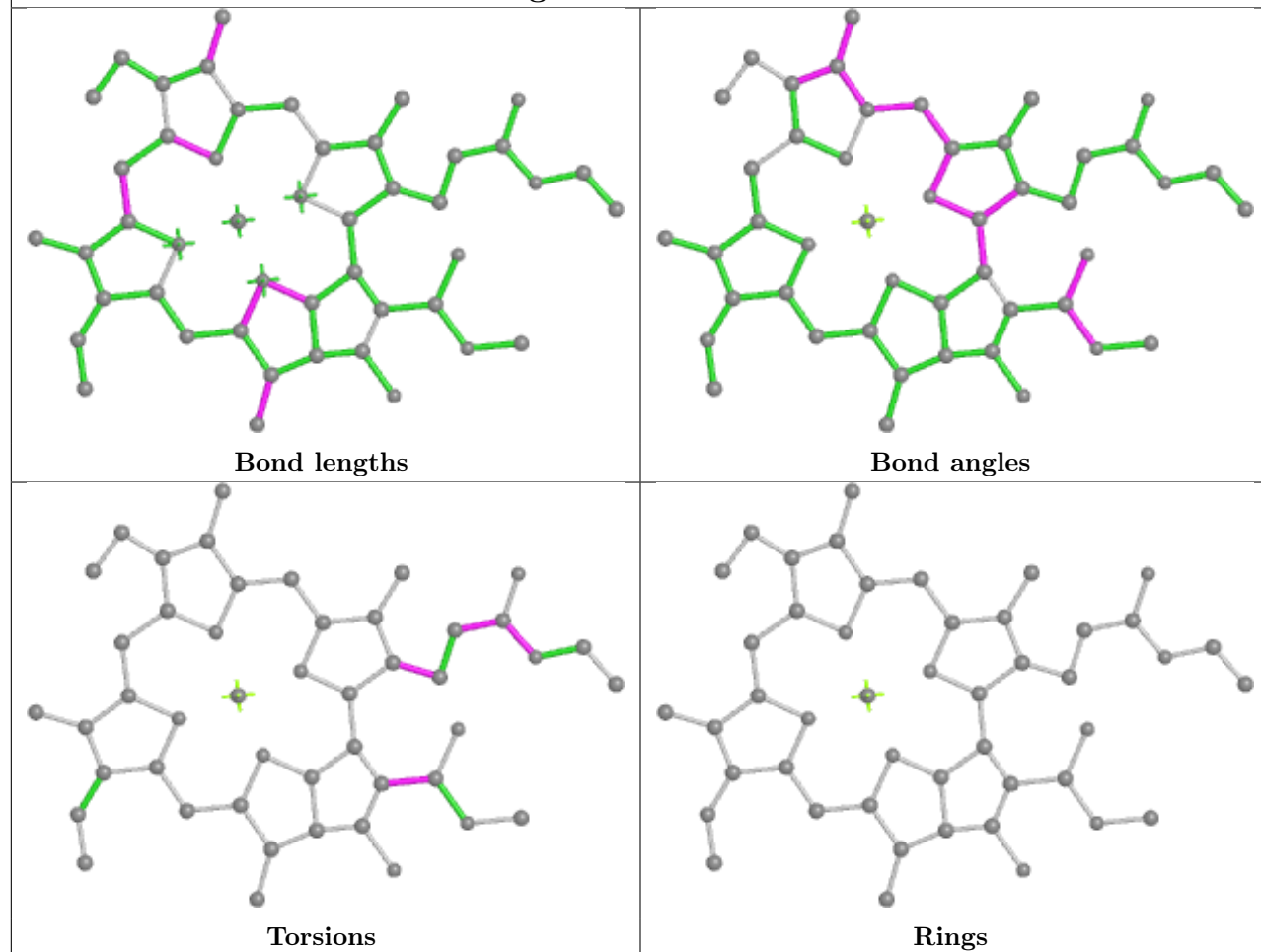
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2	419	LMT	1	0
2	2	403	A86	1	0
2	1	303	A86	1	0
4	1	308	KC2	1	0
3	2	411	CLA	1	0
2	4	304	A86	1	0
3	3	308	CLA	3	0
6	4	317	LMT	1	0
3	2	401	CLA	4	0
2	3	303	A86	1	0
3	2	416	CLA	3	0
4	2	410	KC2	1	0

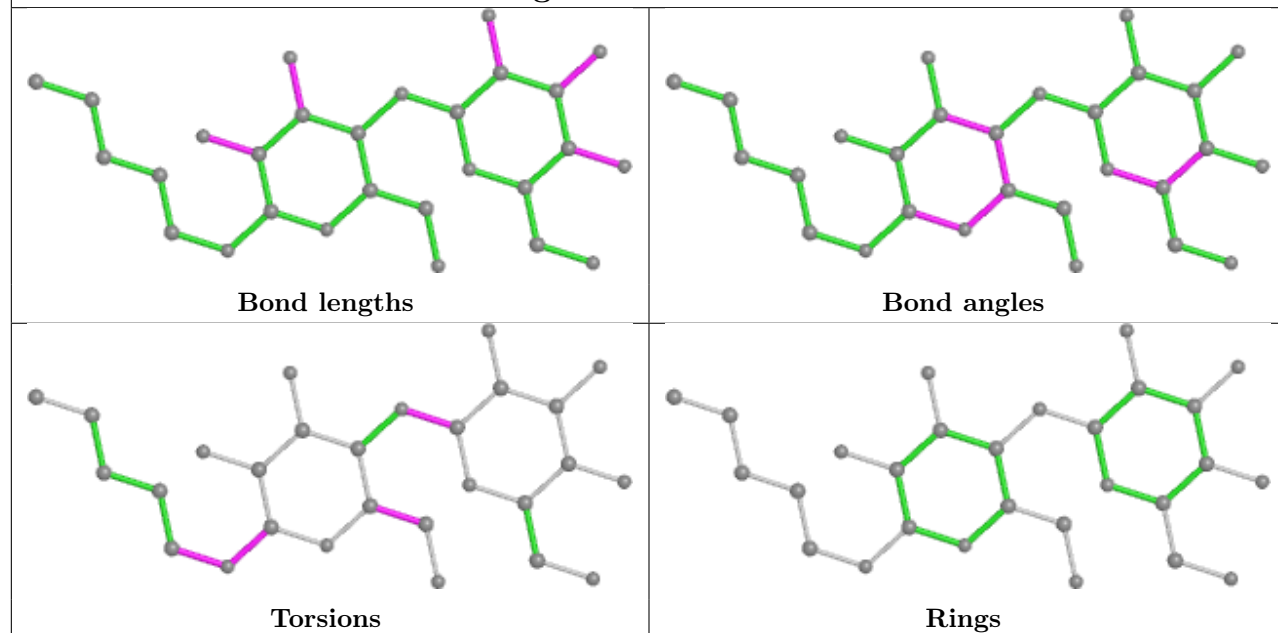
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



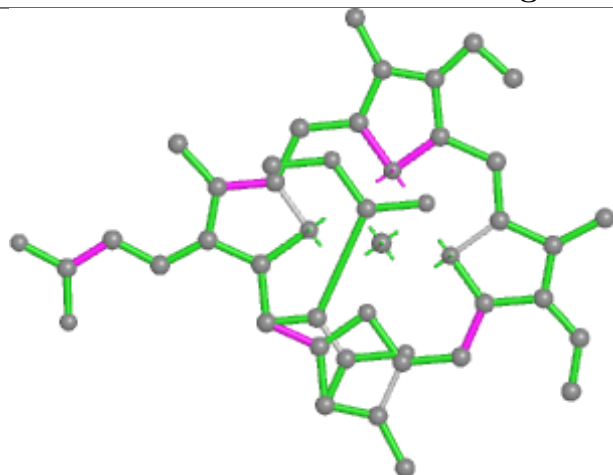
## Ligand CLA 4 312



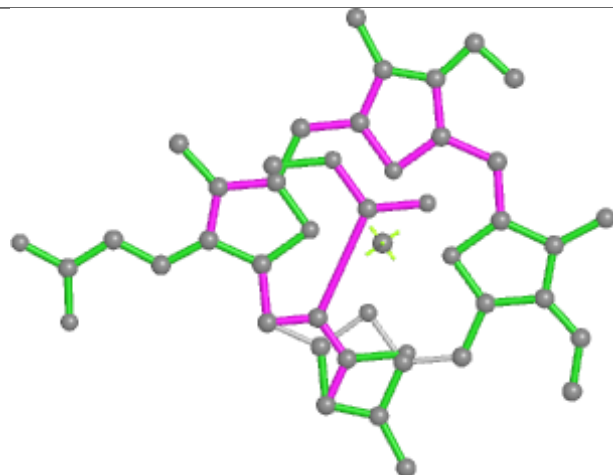
## Ligand LMT 1 316



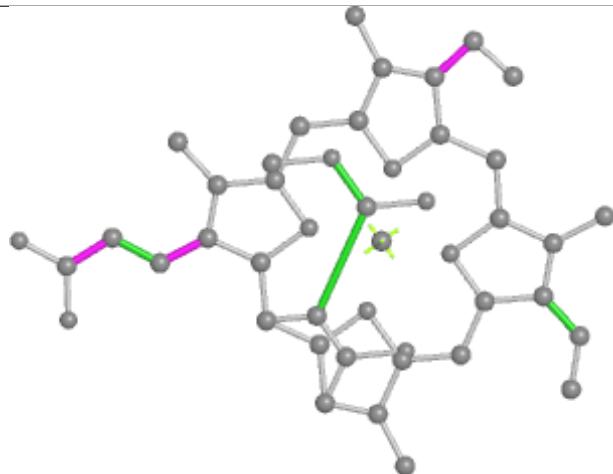
## Ligand KC1 2 413



Bond lengths



Bond angles

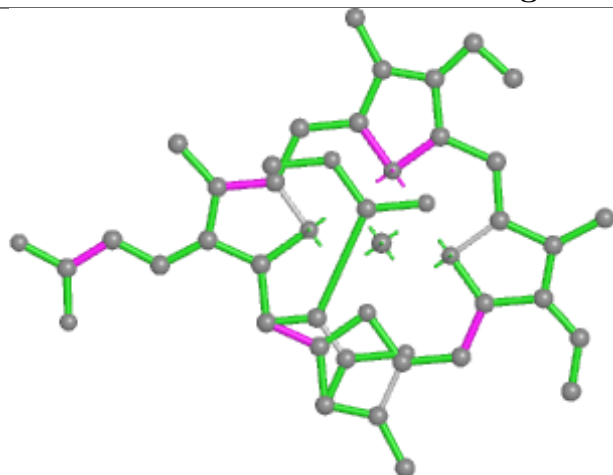


Torsions

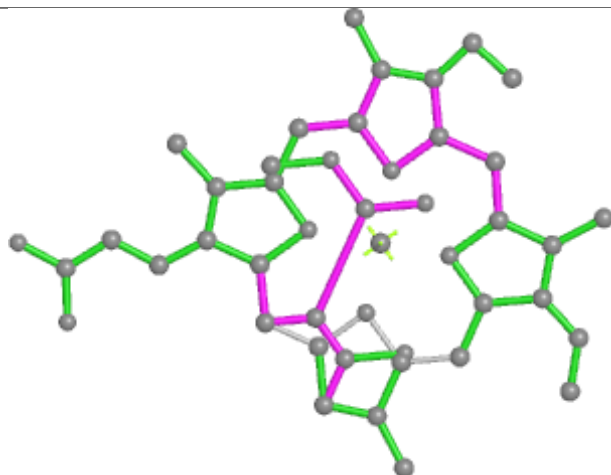


Rings

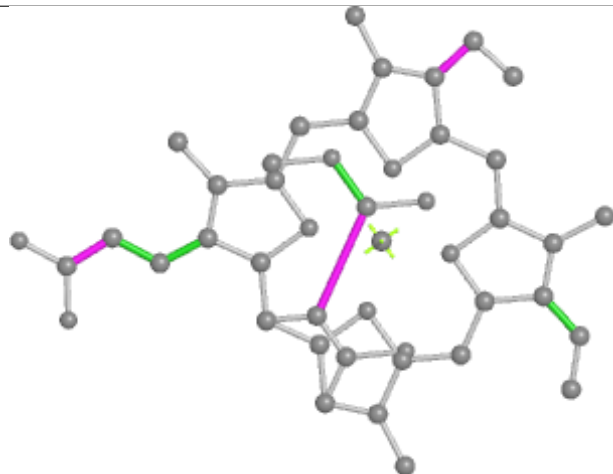
## Ligand KC1 3 314



Bond lengths



Bond angles

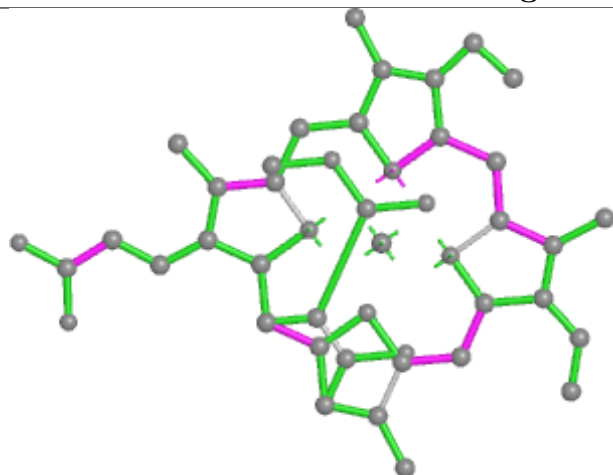


Torsions

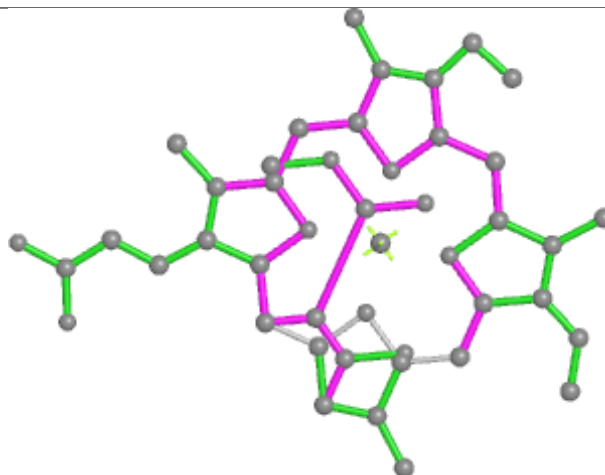


Rings

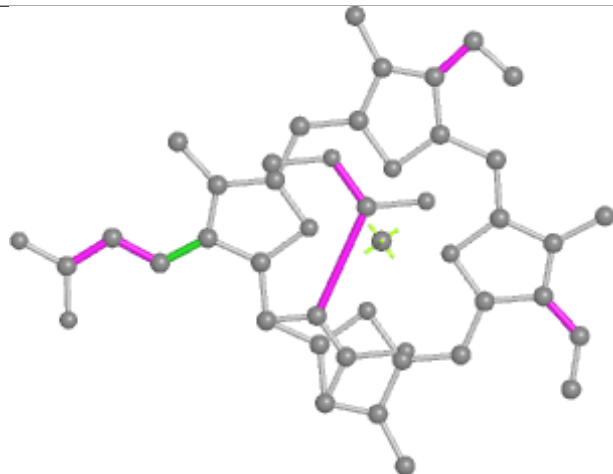
## Ligand KC2 2 412



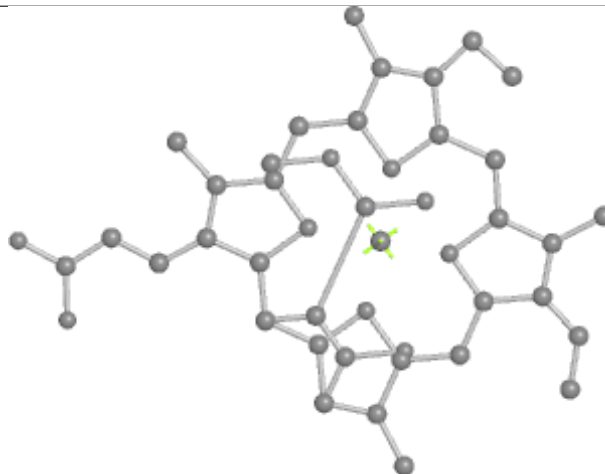
Bond lengths



Bond angles

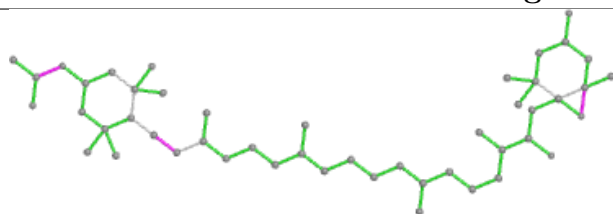


Torsions

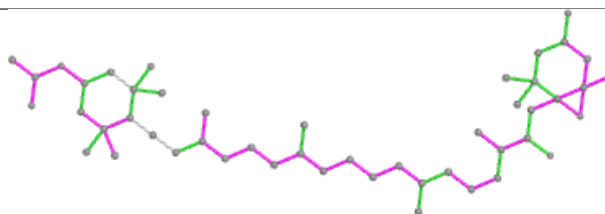


Rings

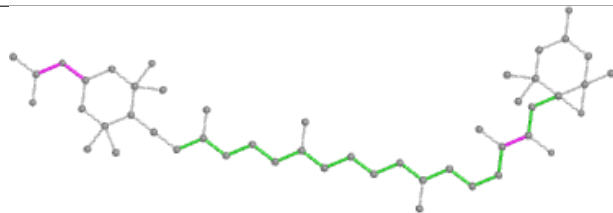
## Ligand A86 2 405



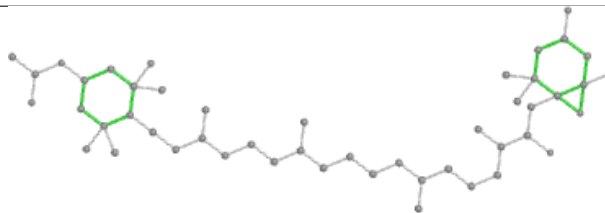
Bond lengths



Bond angles



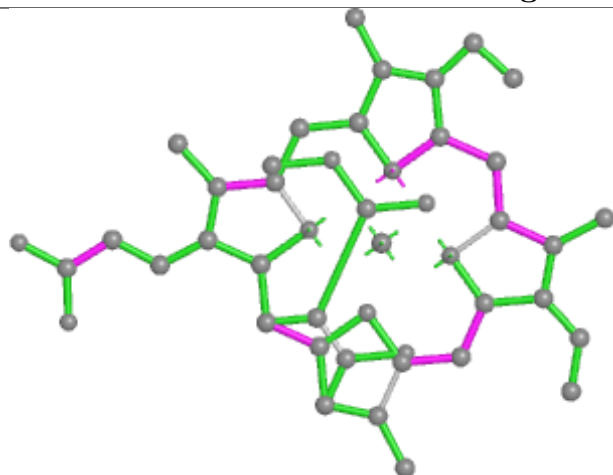
Torsions



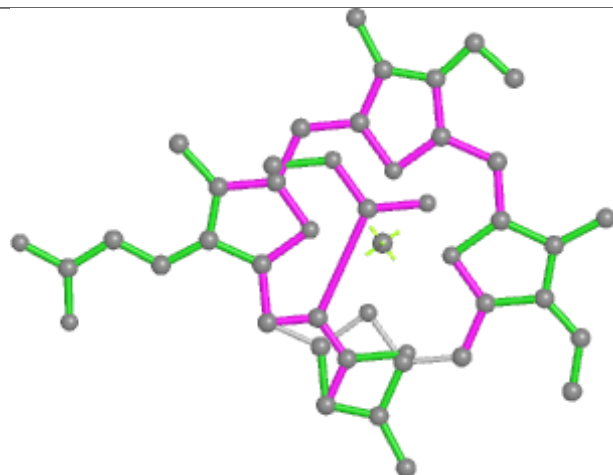
Rings



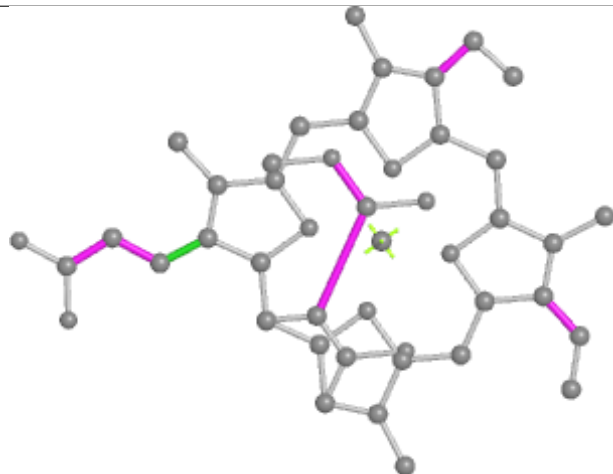
## Ligand KC2 4 310



Bond lengths



Bond angles

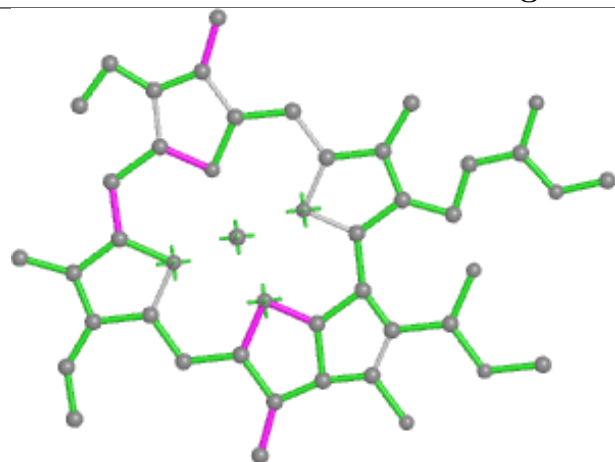


Torsions

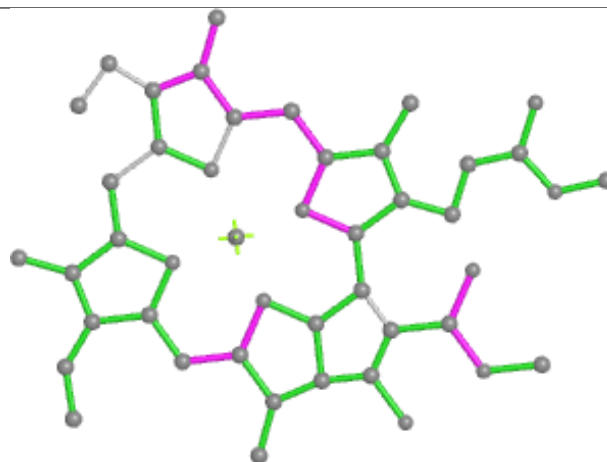


Rings

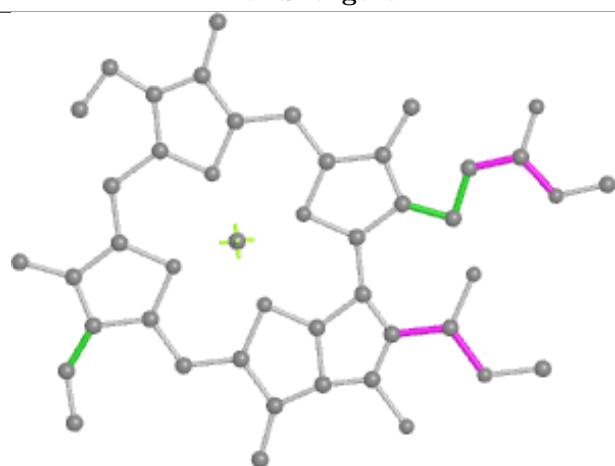
## Ligand CLA 4 315



Bond lengths



Bond angles

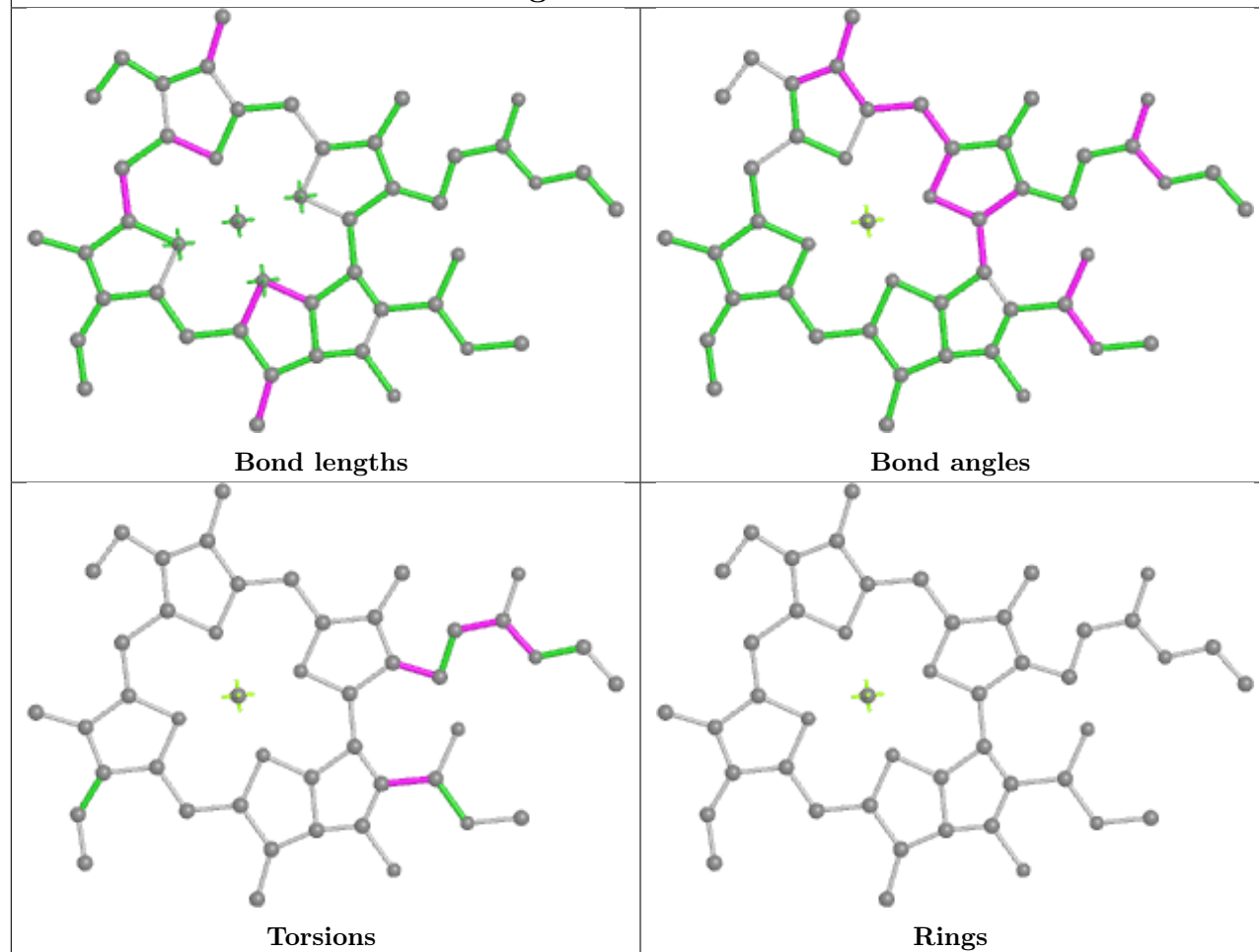


Torsions

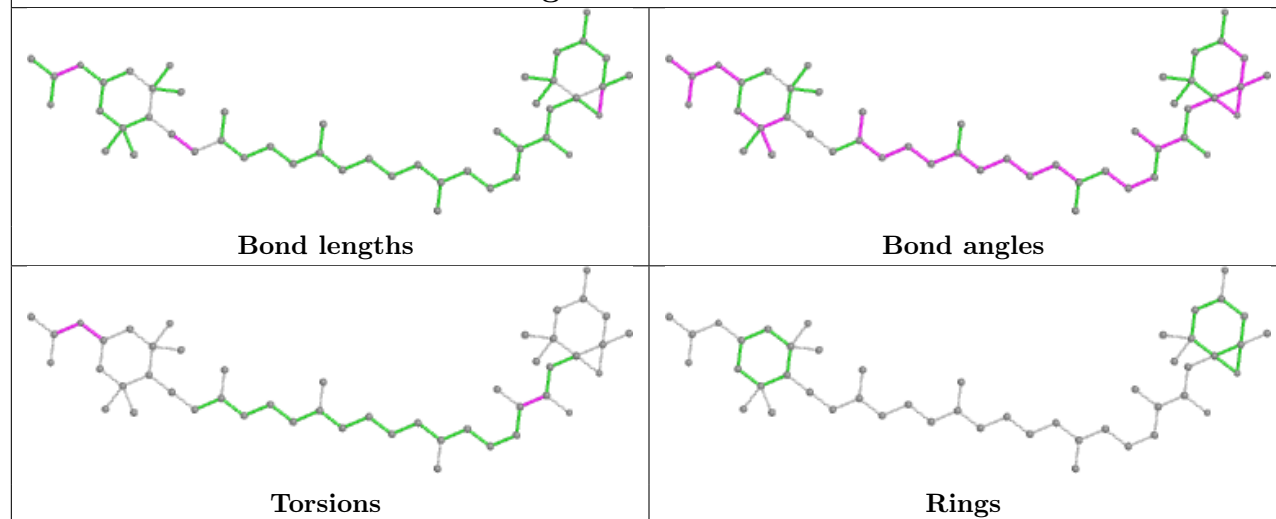


Rings

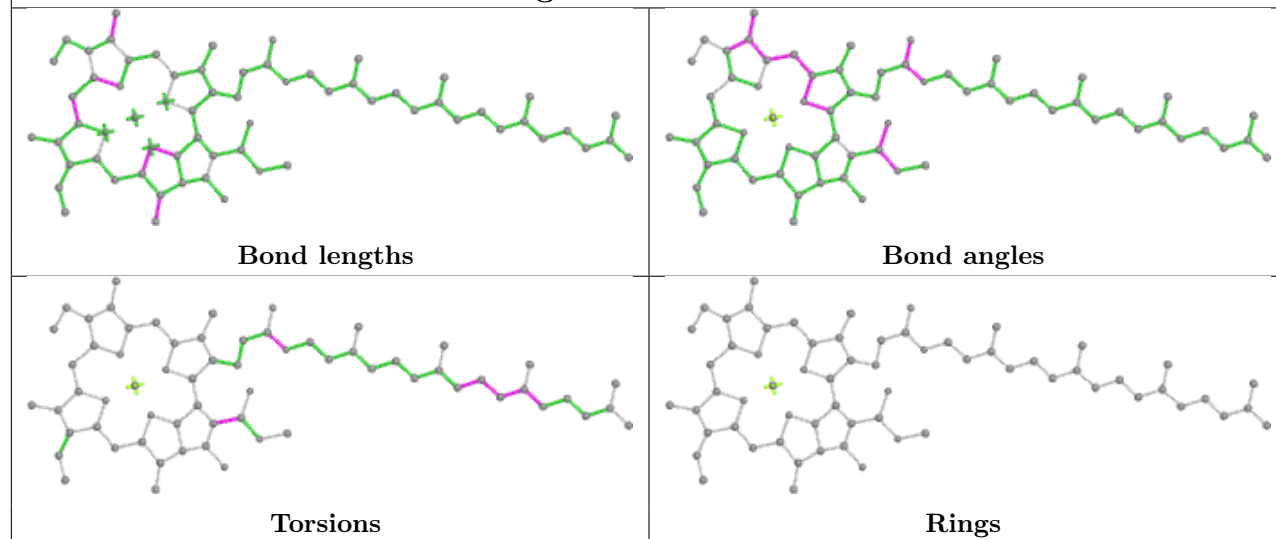
## Ligand CLA 2 414



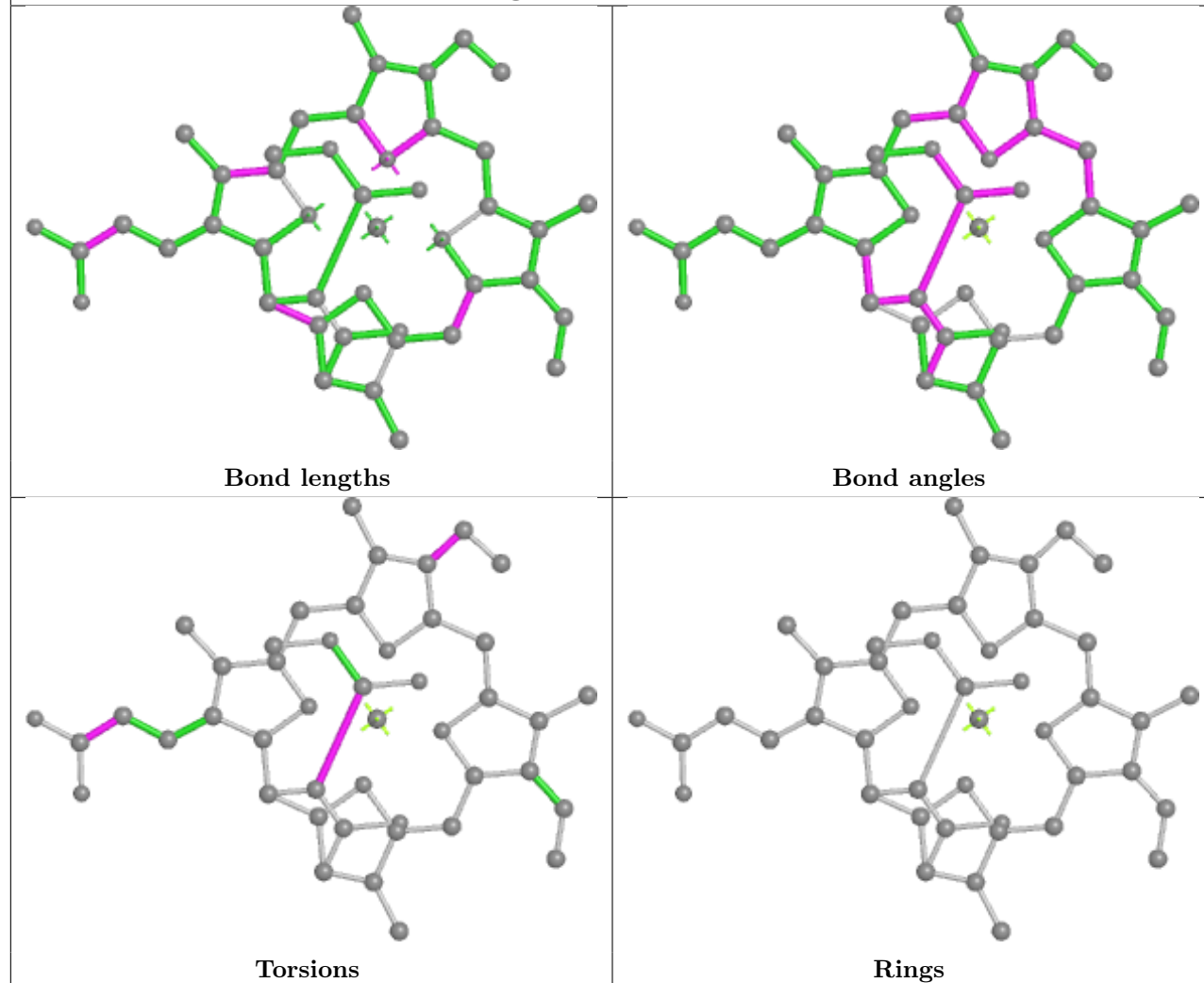
## Ligand A86 1 304



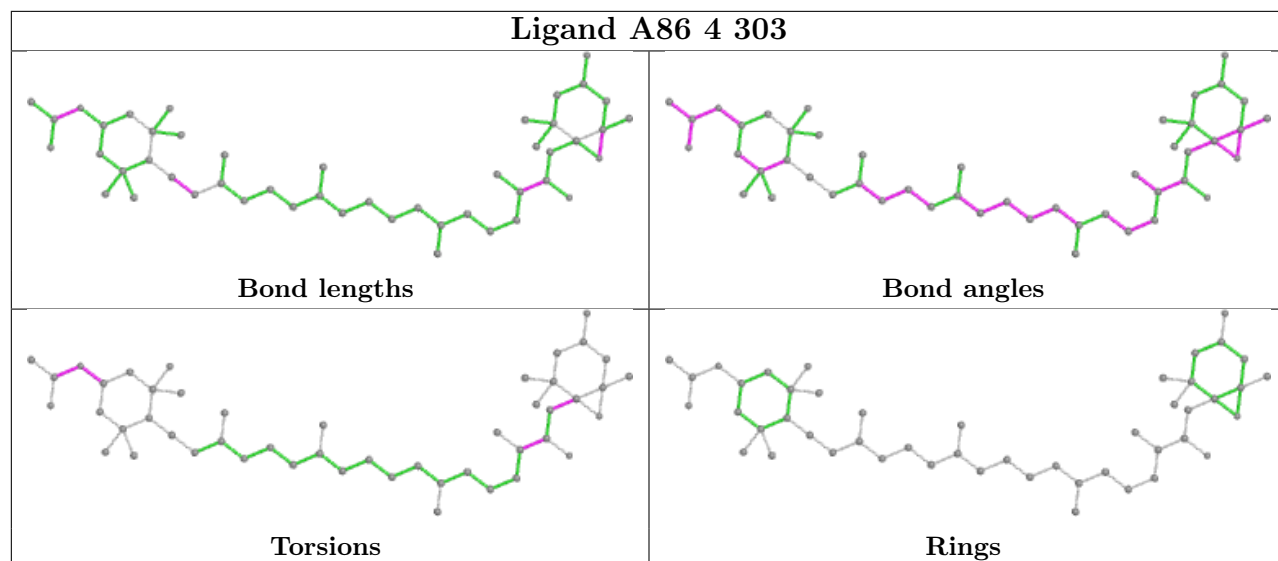
## Ligand CLA 3 307



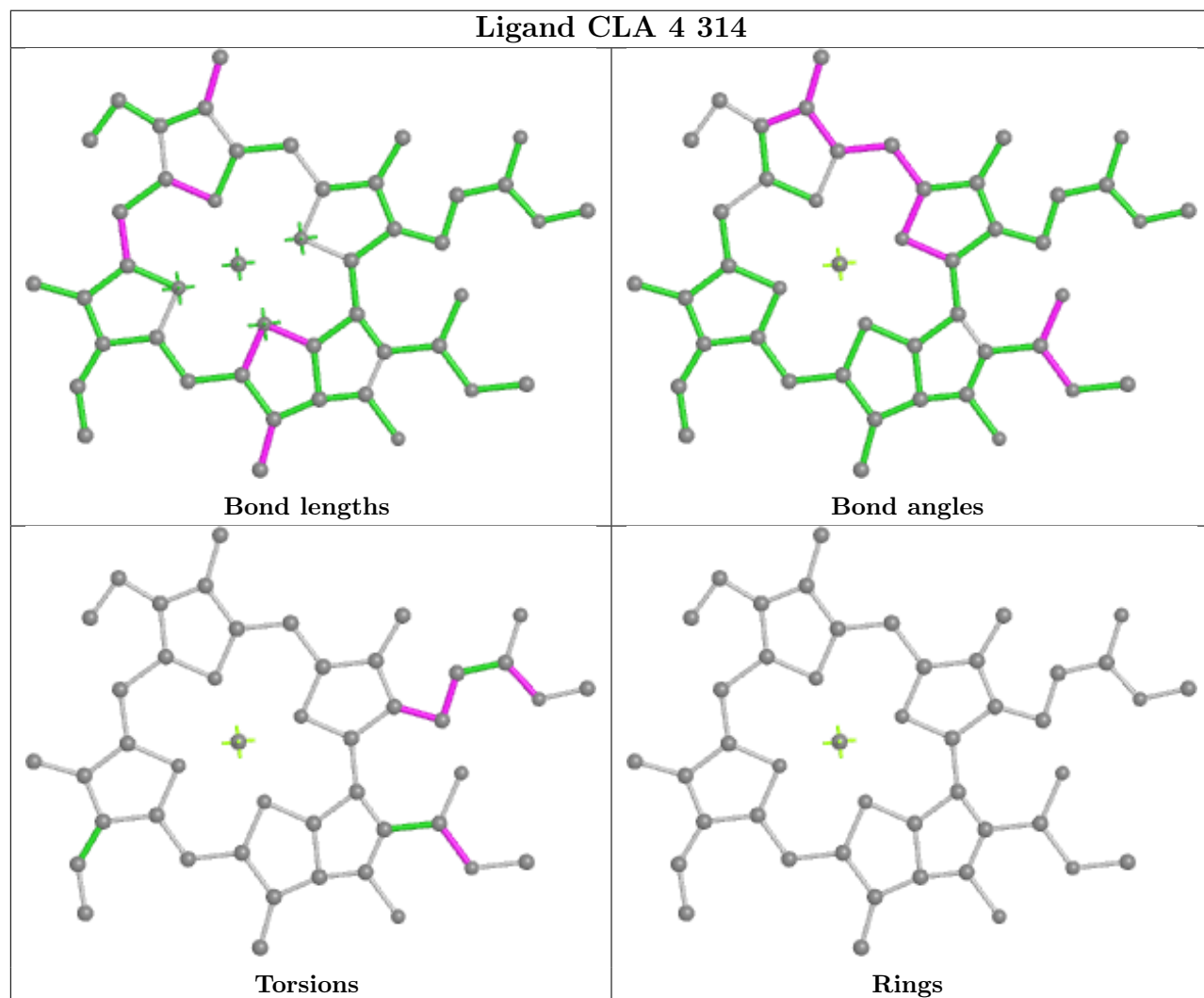
## Ligand KC1 1 313



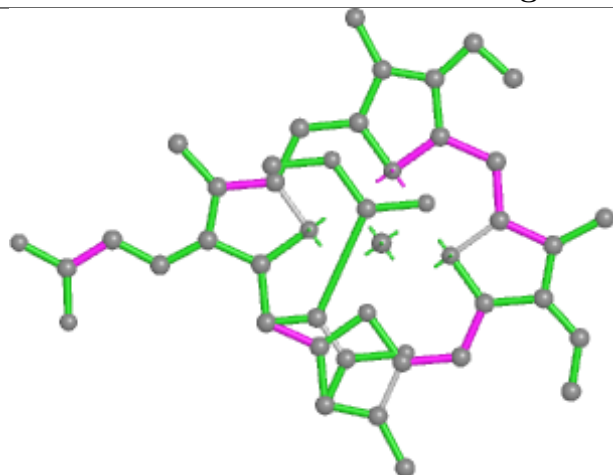
## Ligand A86 4 303



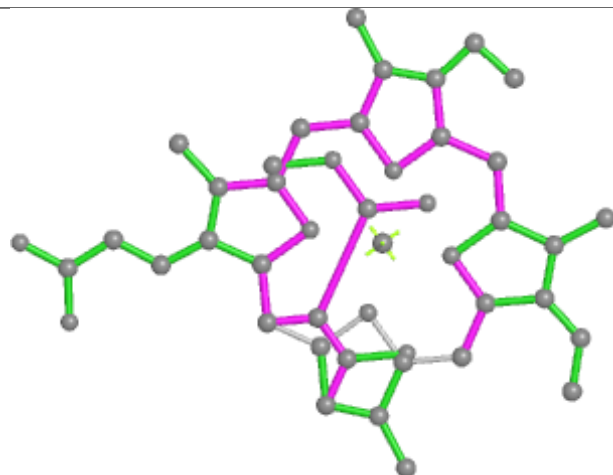
## Ligand CLA 4 314



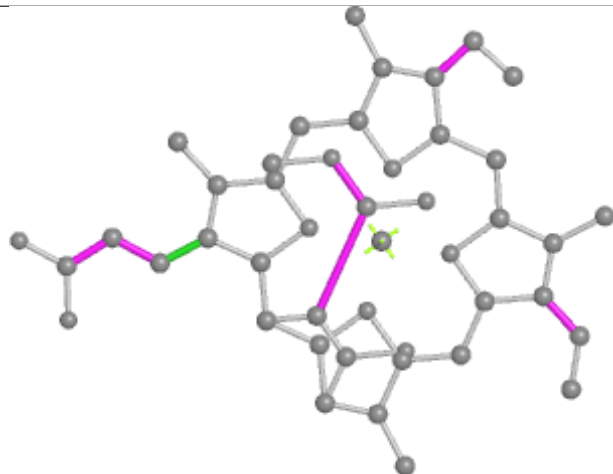
## Ligand KC2 3 311



Bond lengths



Bond angles

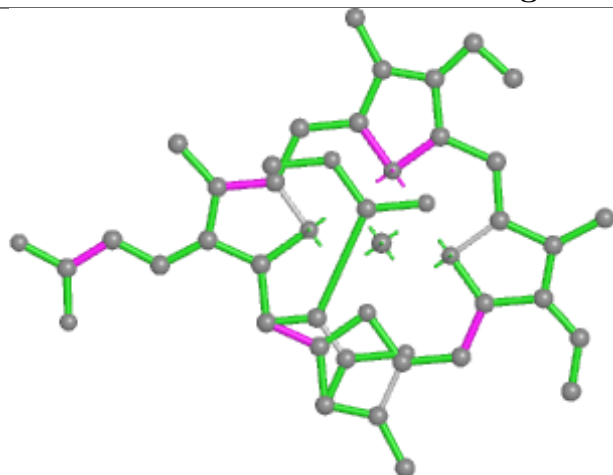


Torsions

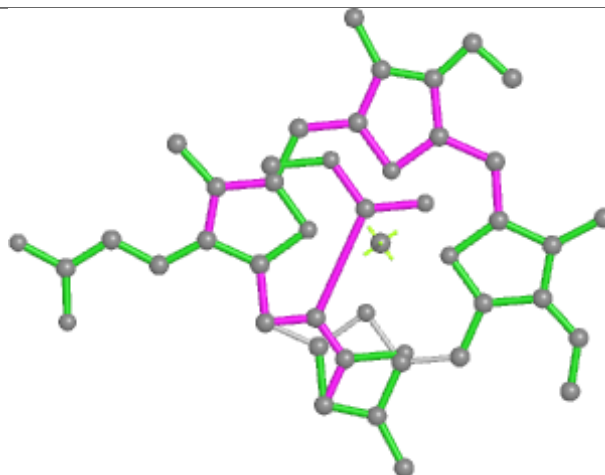


Rings

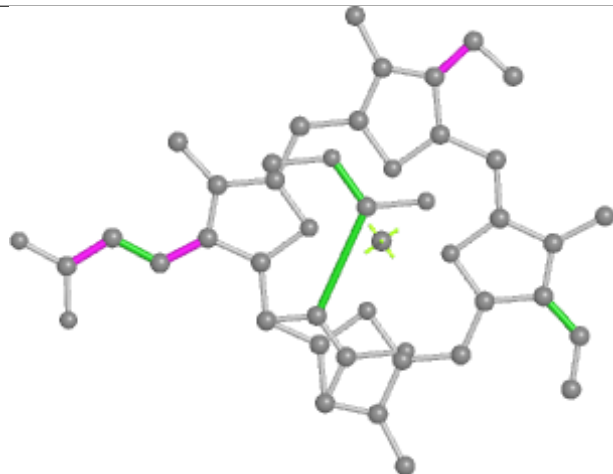
## Ligand KC1 4 311



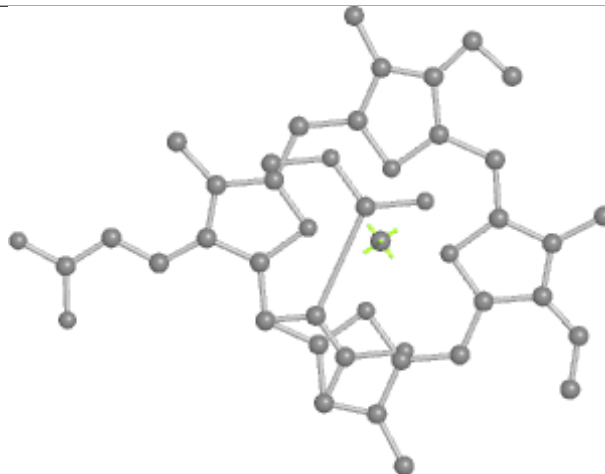
Bond lengths



Bond angles

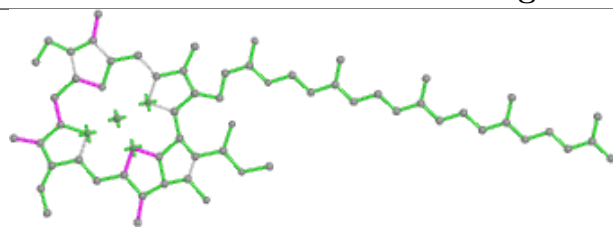


Torsions

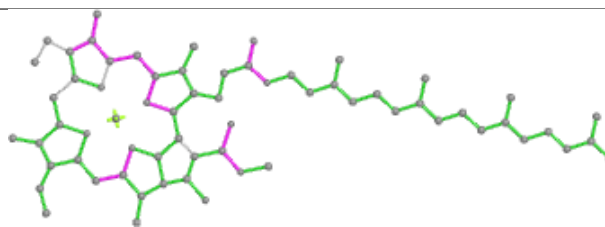


Rings

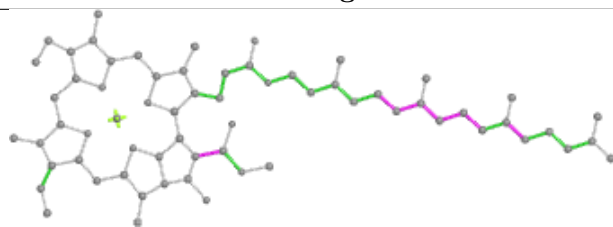
## Ligand CLA 1 318



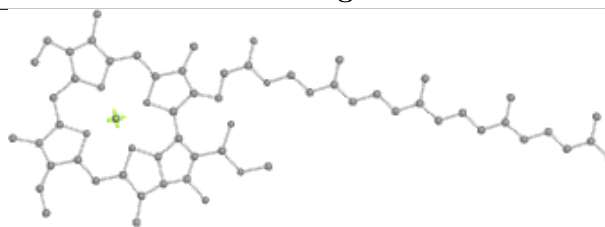
Bond lengths



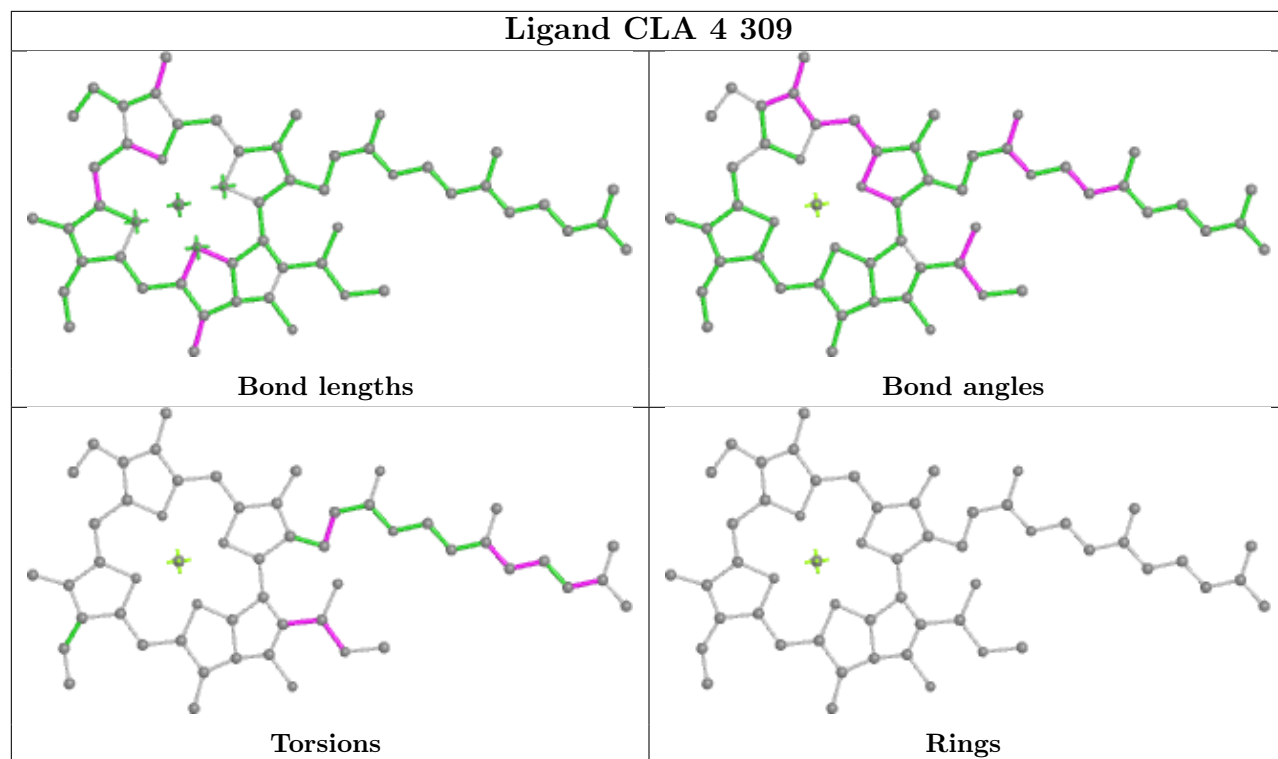
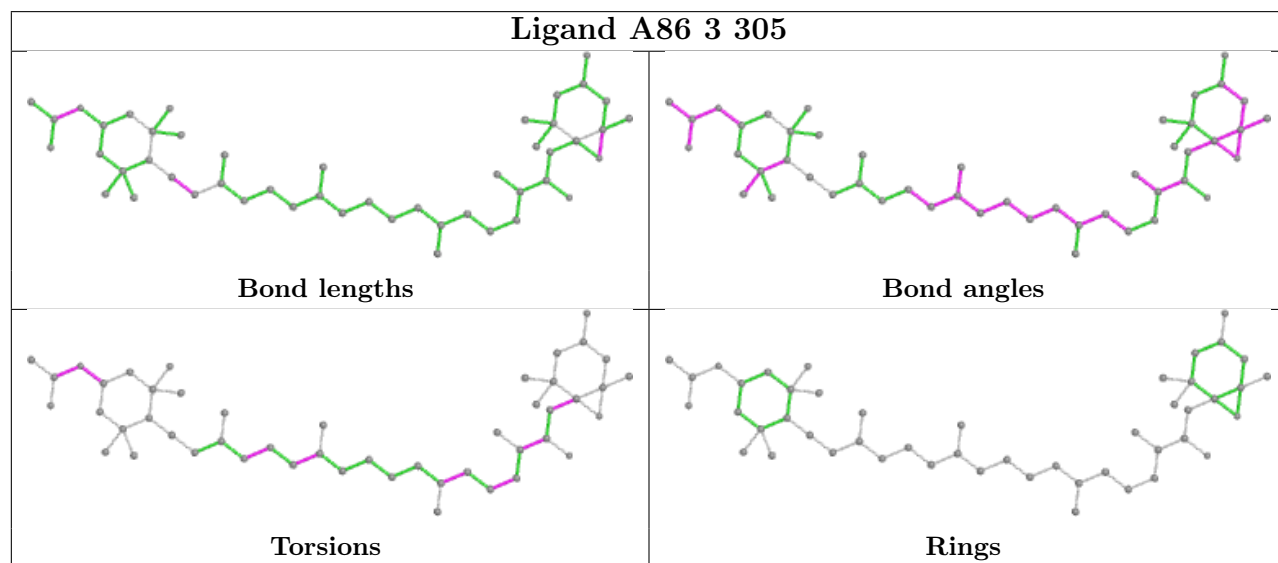
Bond angles



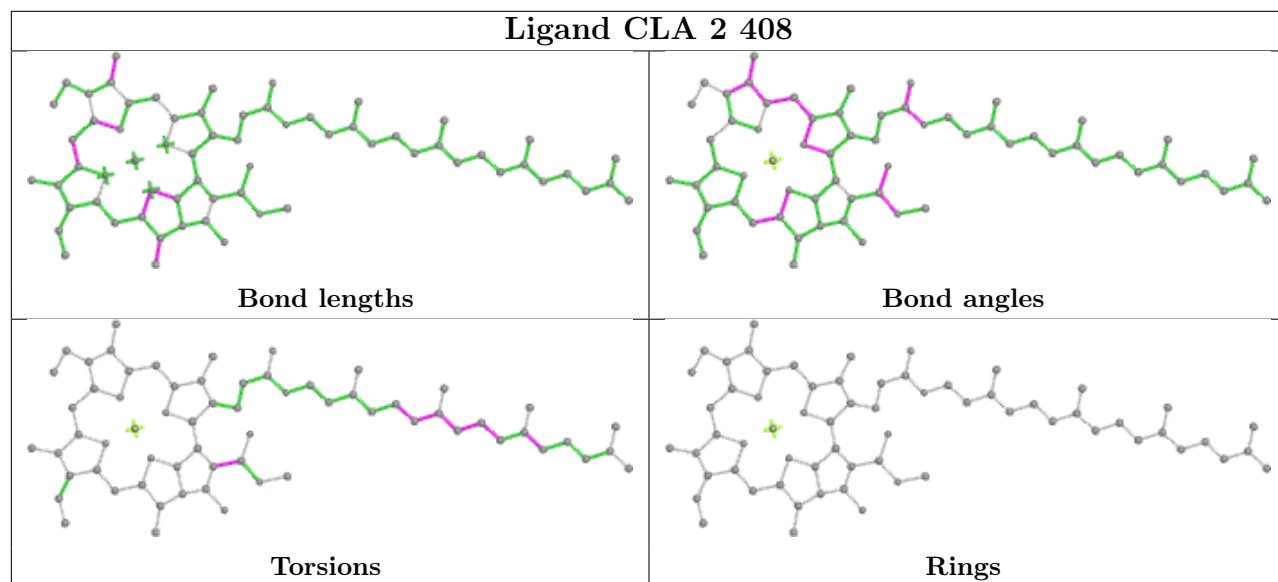
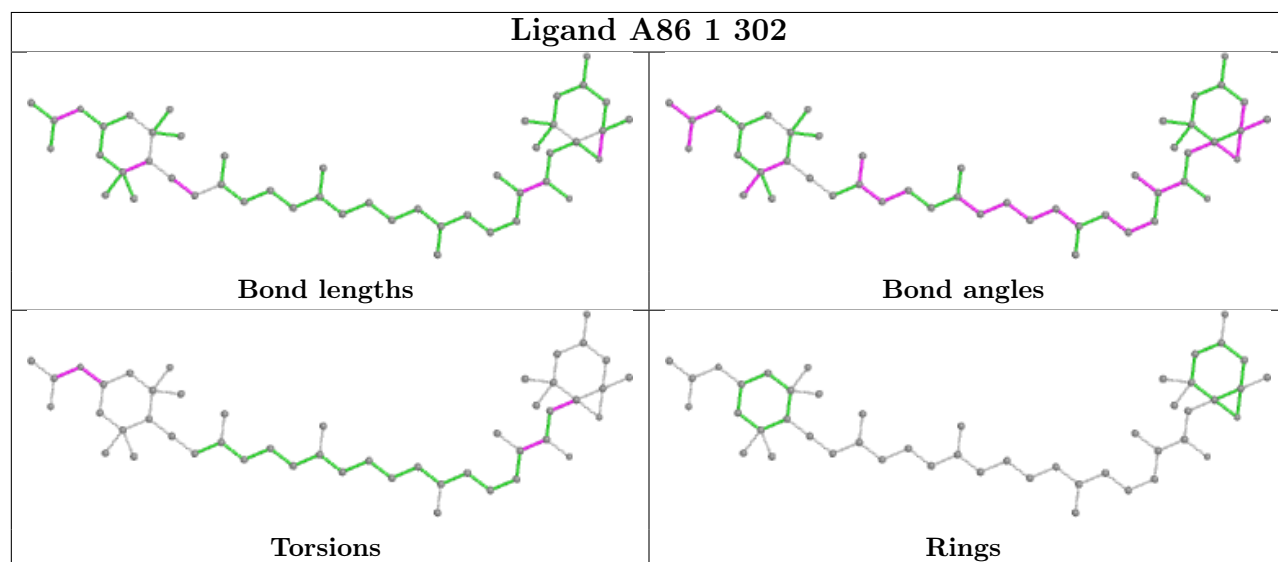
Torsions



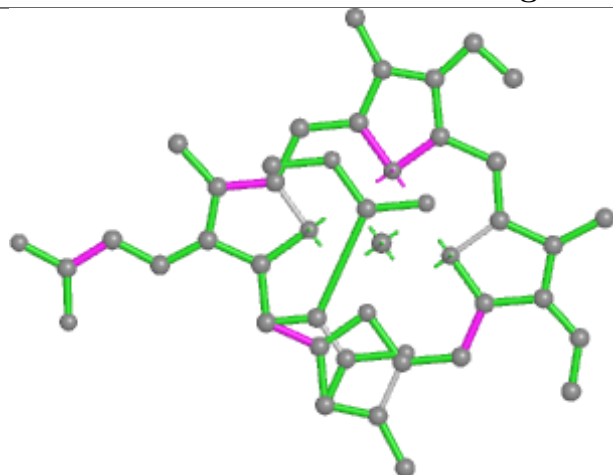
Rings

**Ligand CLA 4 309****Ligand A86 3 305**

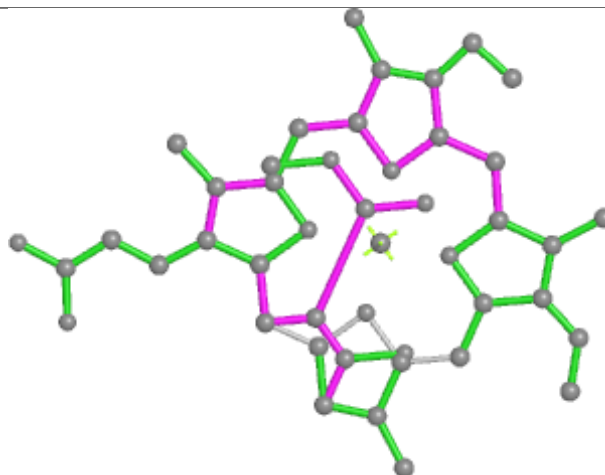


**Ligand CLA 2 408****Ligand A86 1 302**

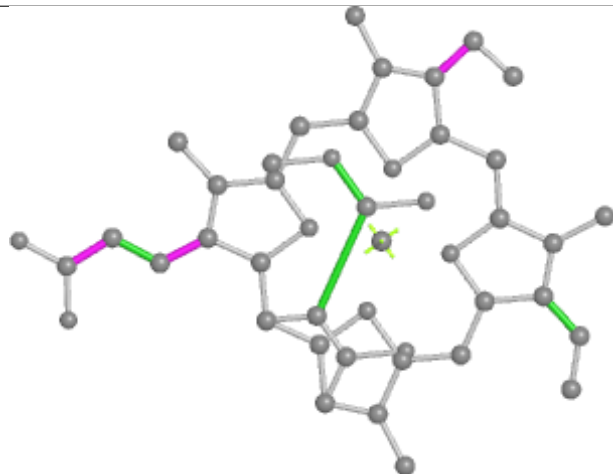
## Ligand KC1 3 312



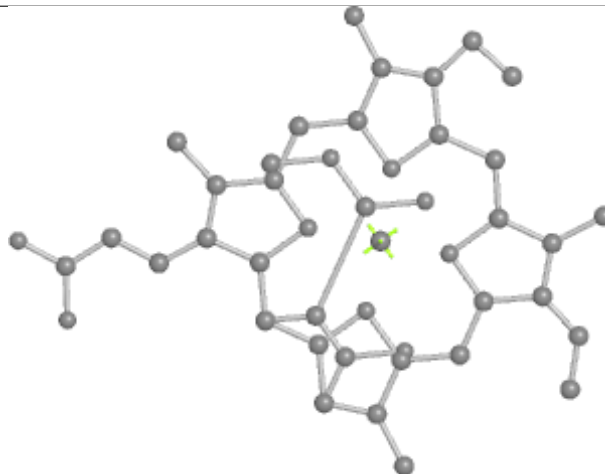
Bond lengths



Bond angles

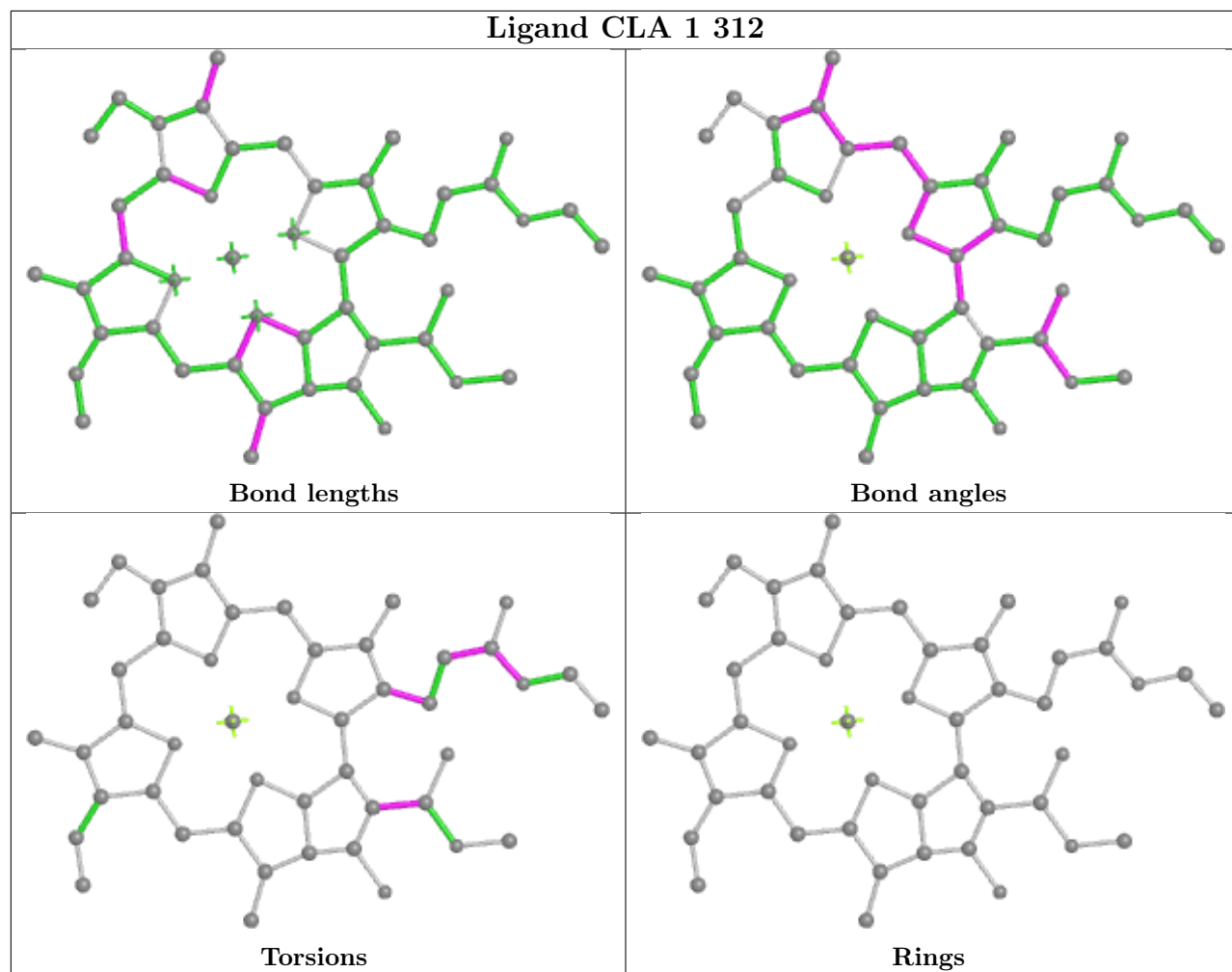


Torsions

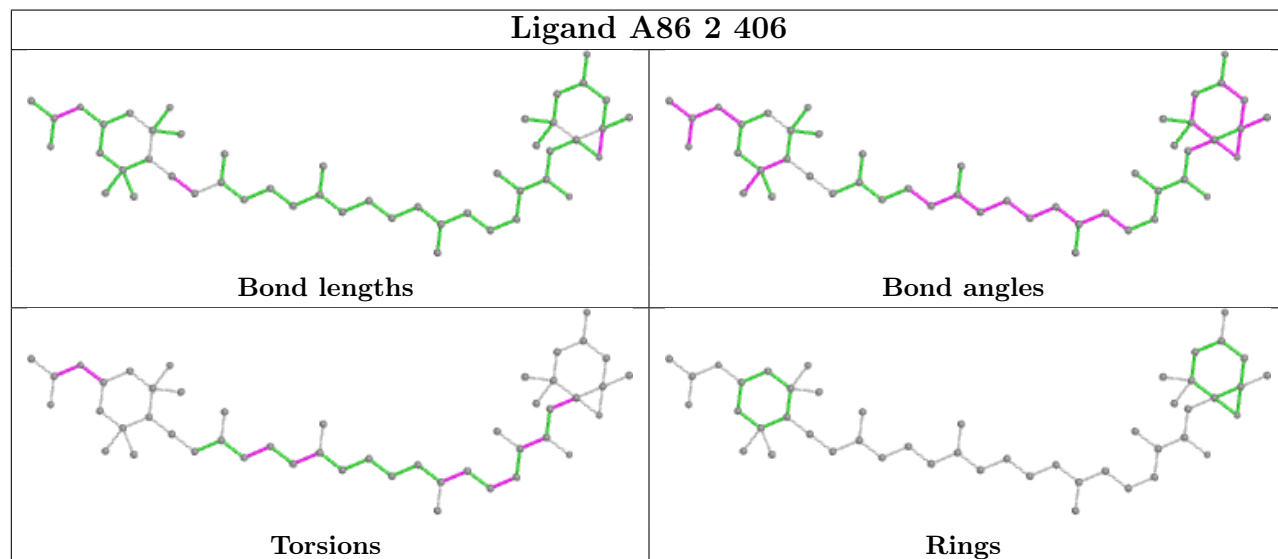


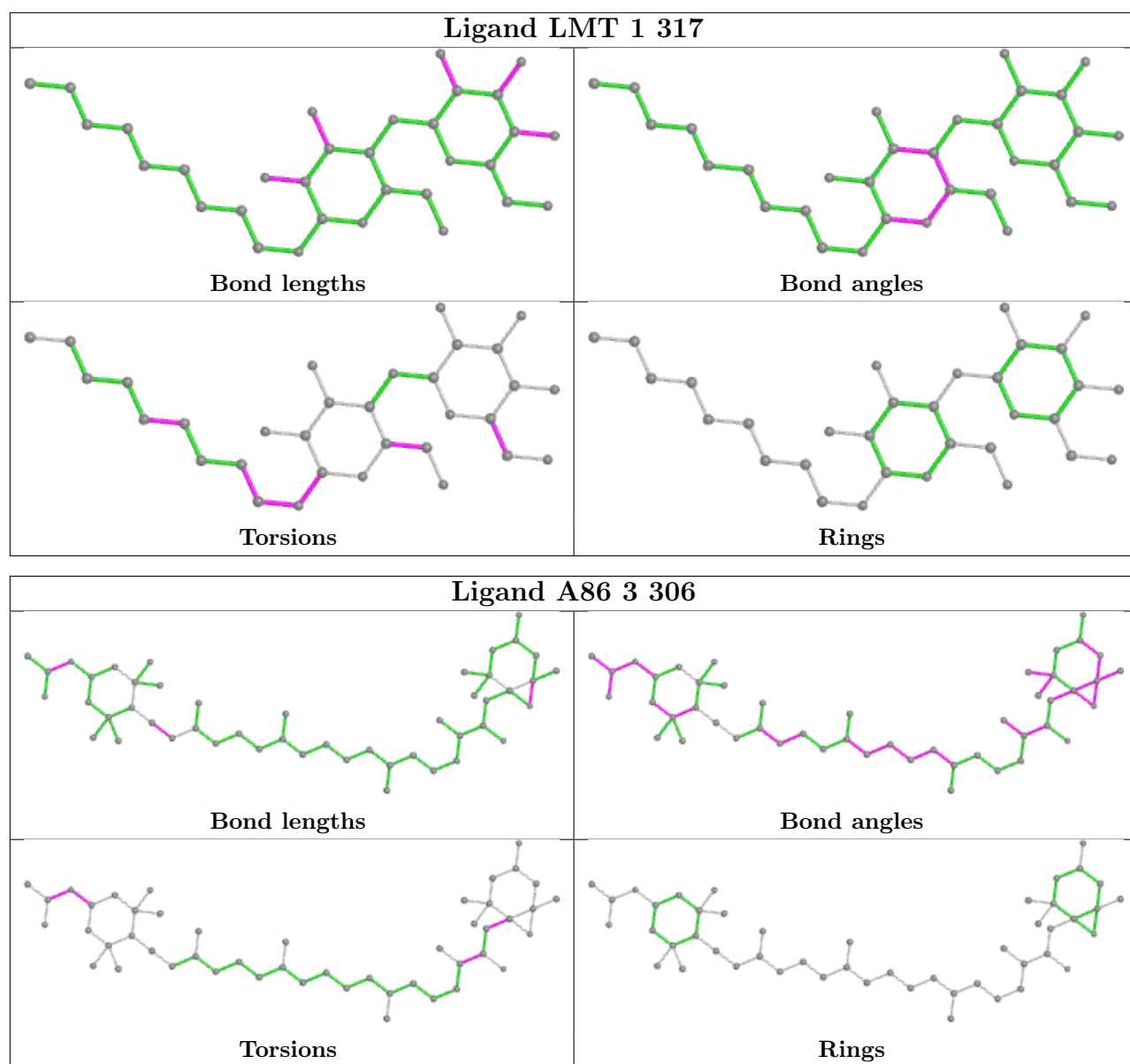
Rings

## Ligand CLA 1 312

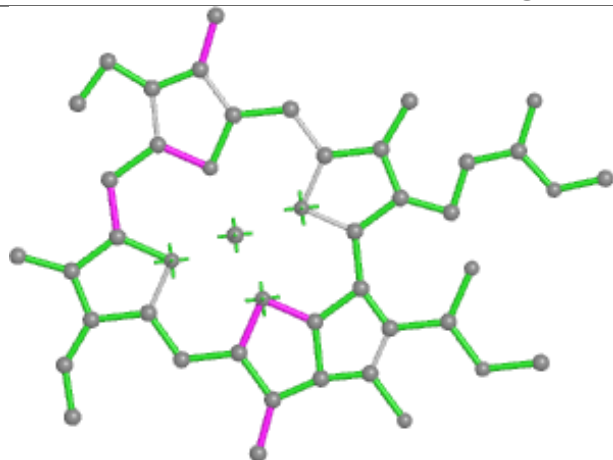


## Ligand A86 2 406

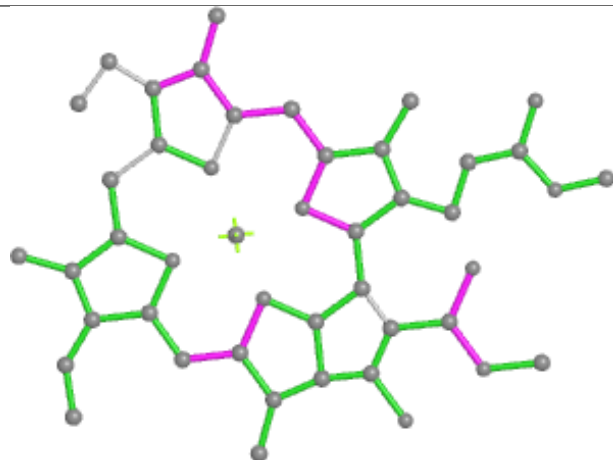




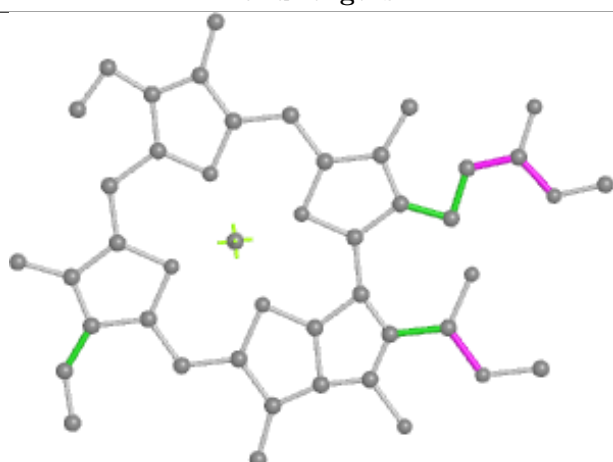
## Ligand CLA 3 316



Bond lengths



Bond angles

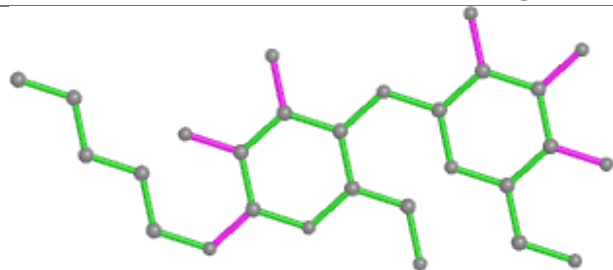


Torsions

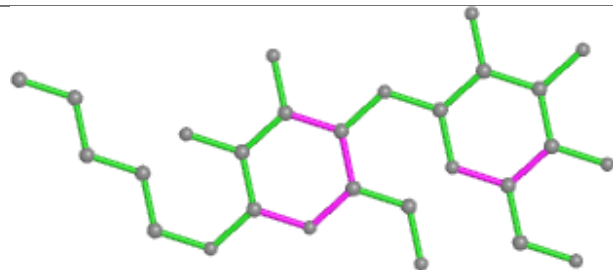


Rings

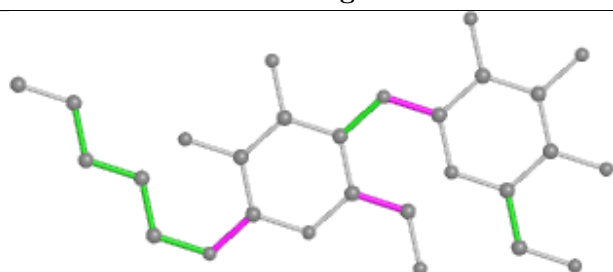
## Ligand LMT 3 317



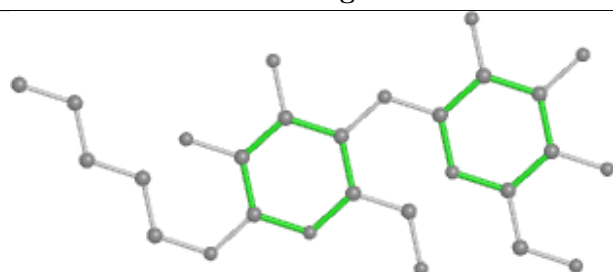
Bond lengths



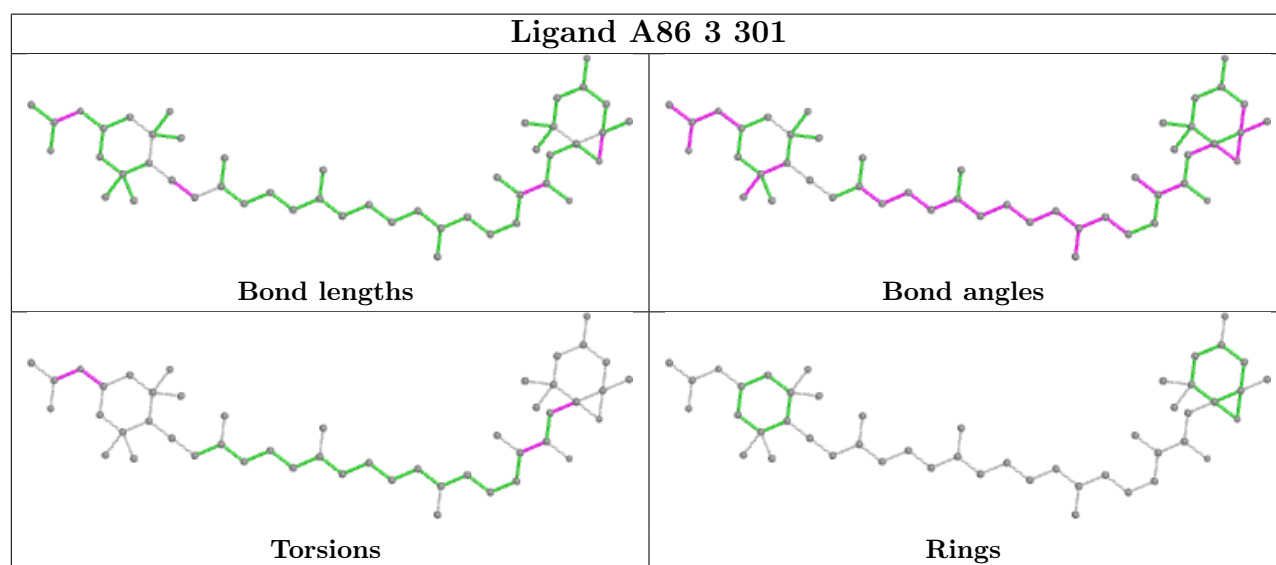
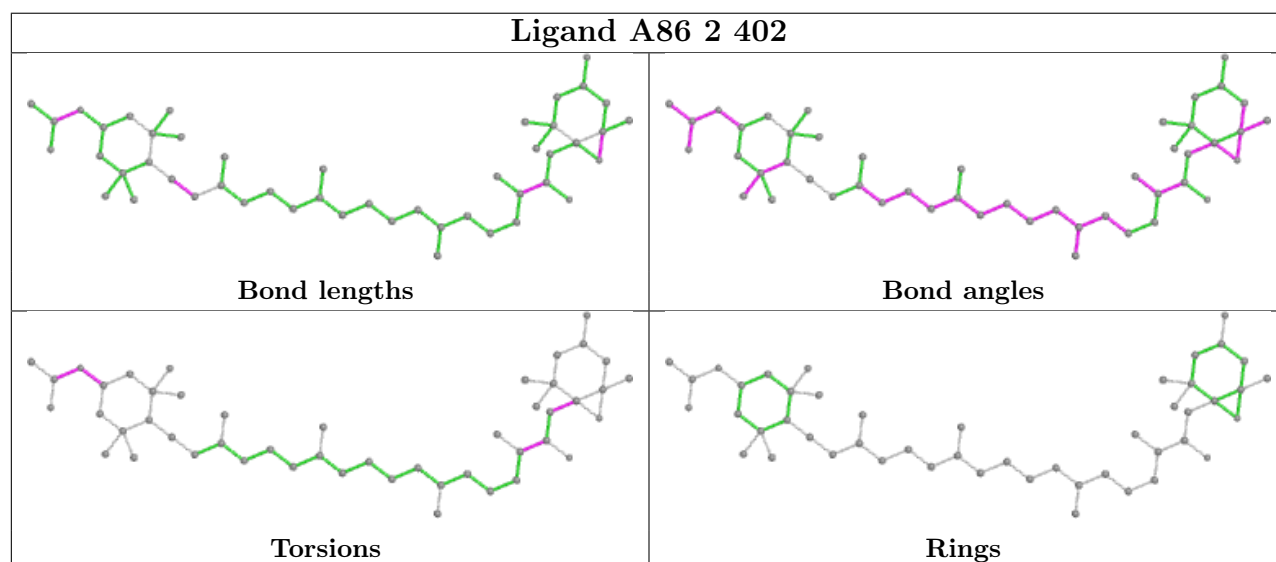
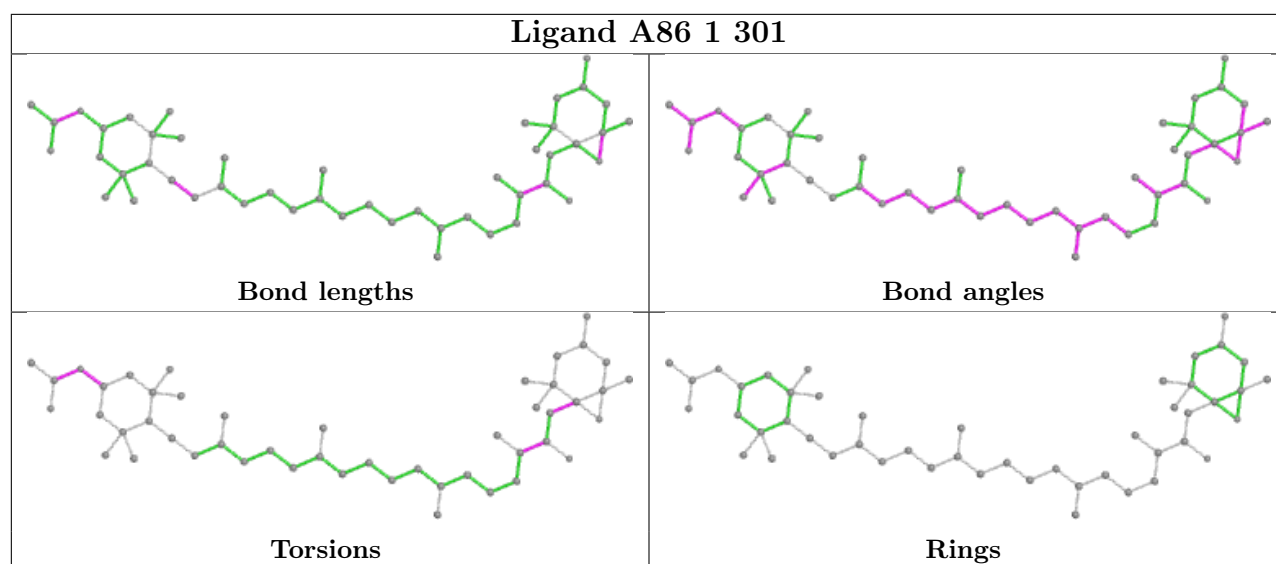
Bond angles

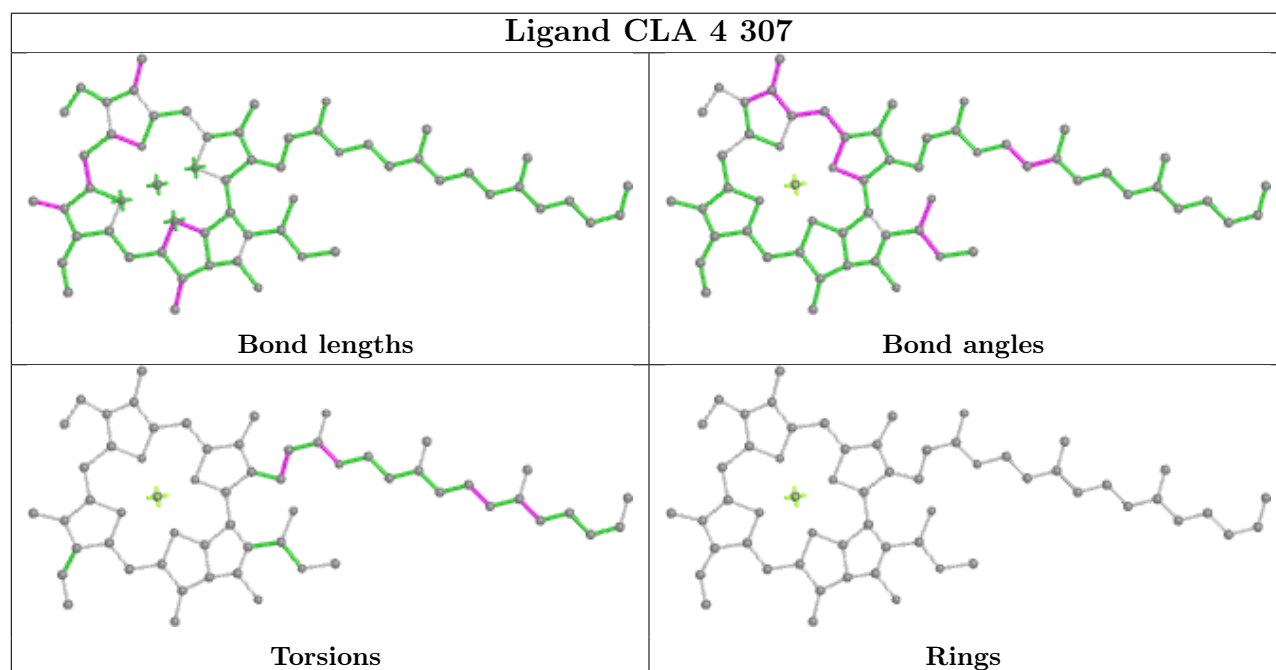
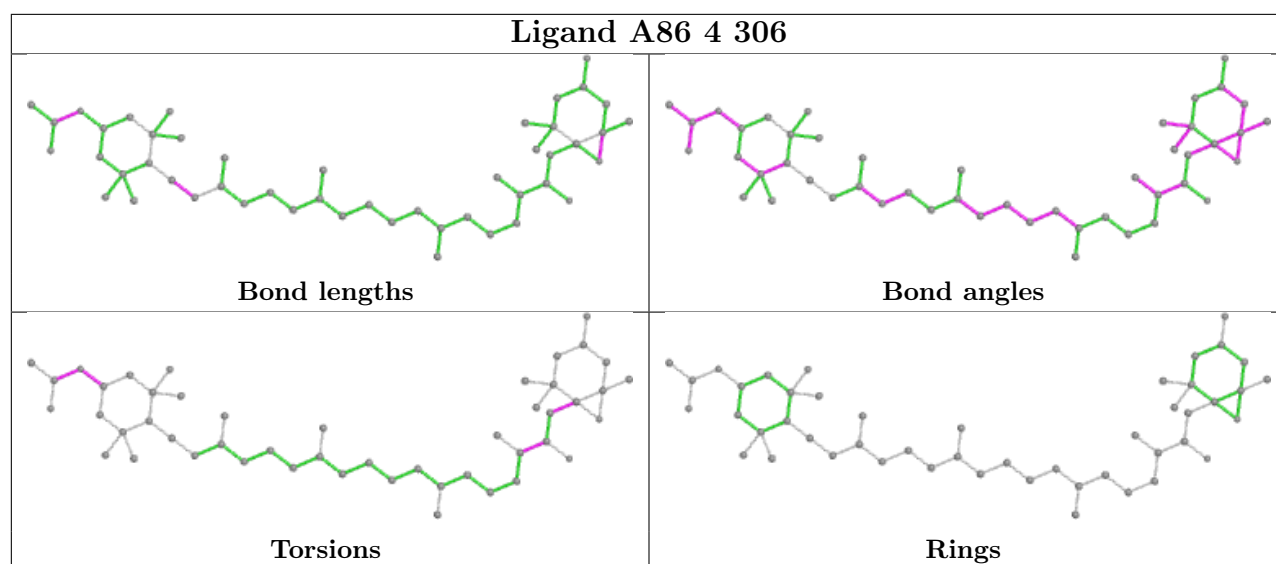


Torsions

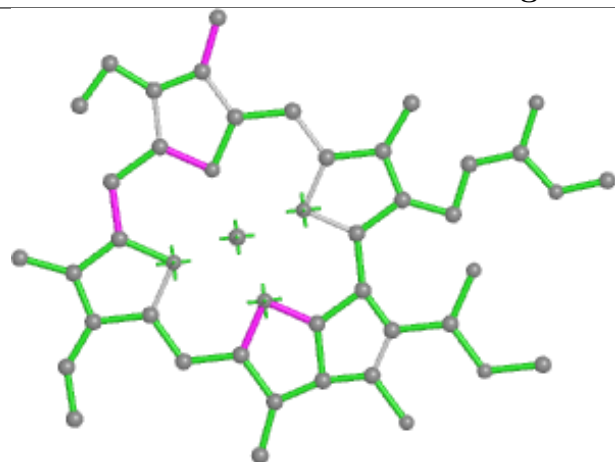


Rings

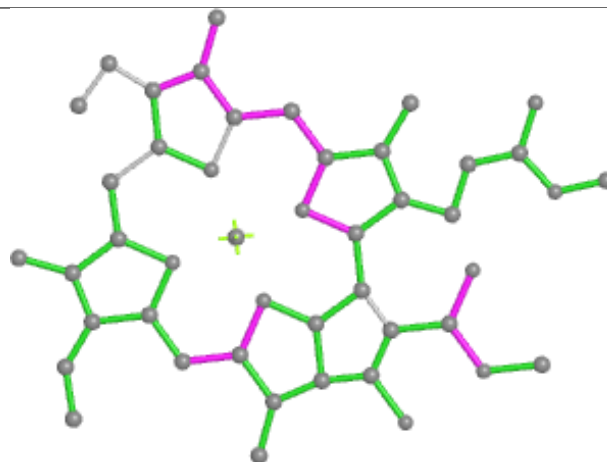




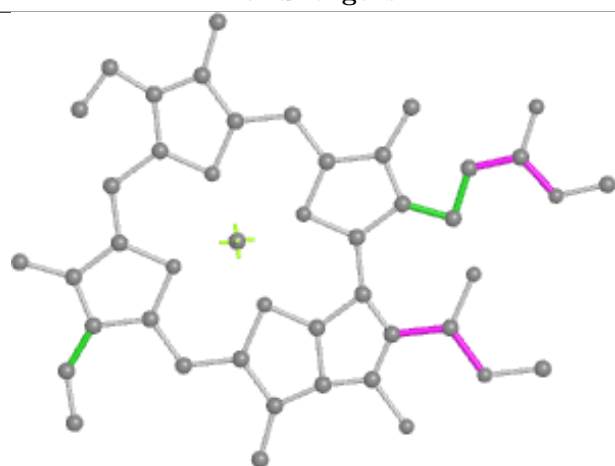
## Ligand CLA 1 315



Bond lengths



Bond angles



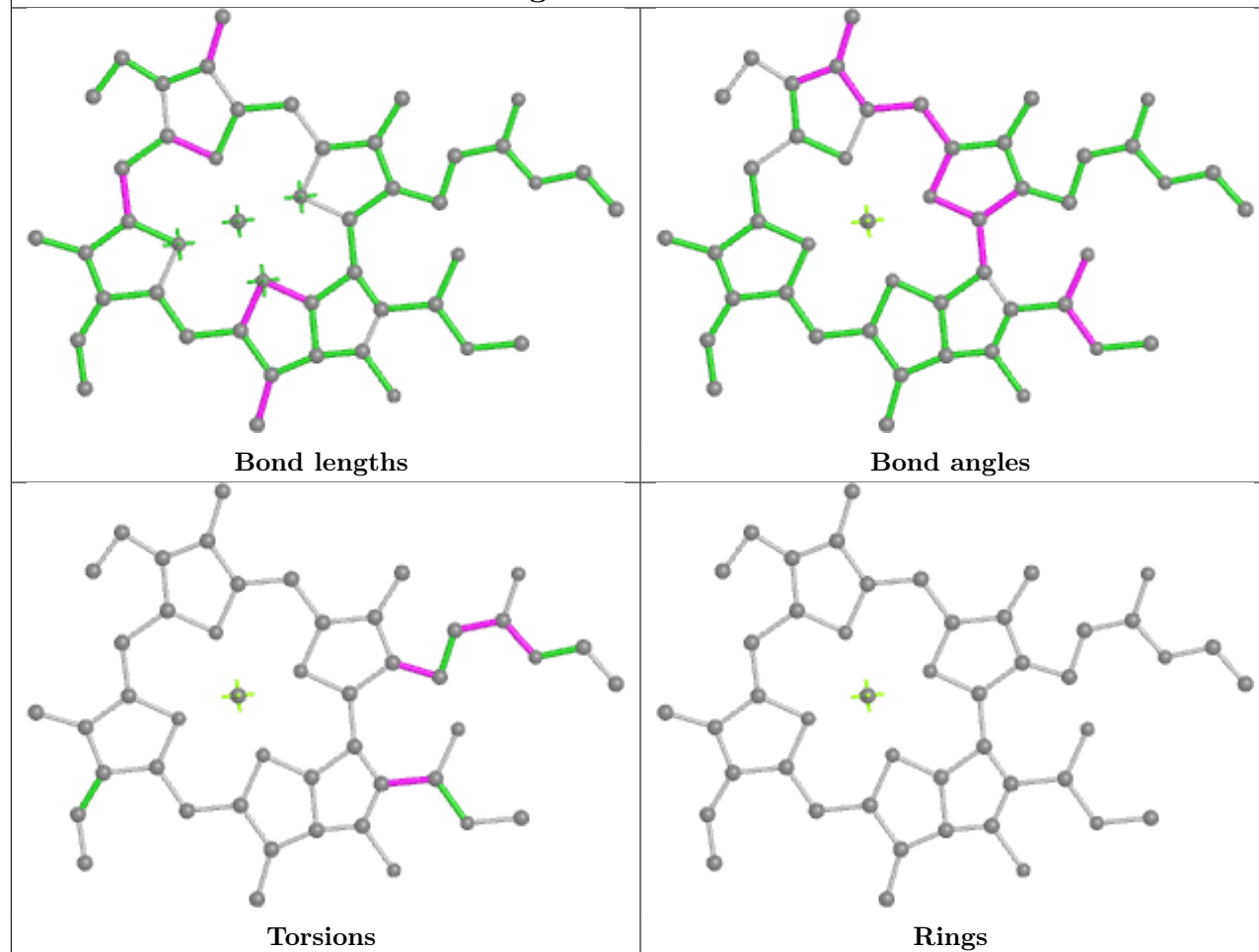
Torsions



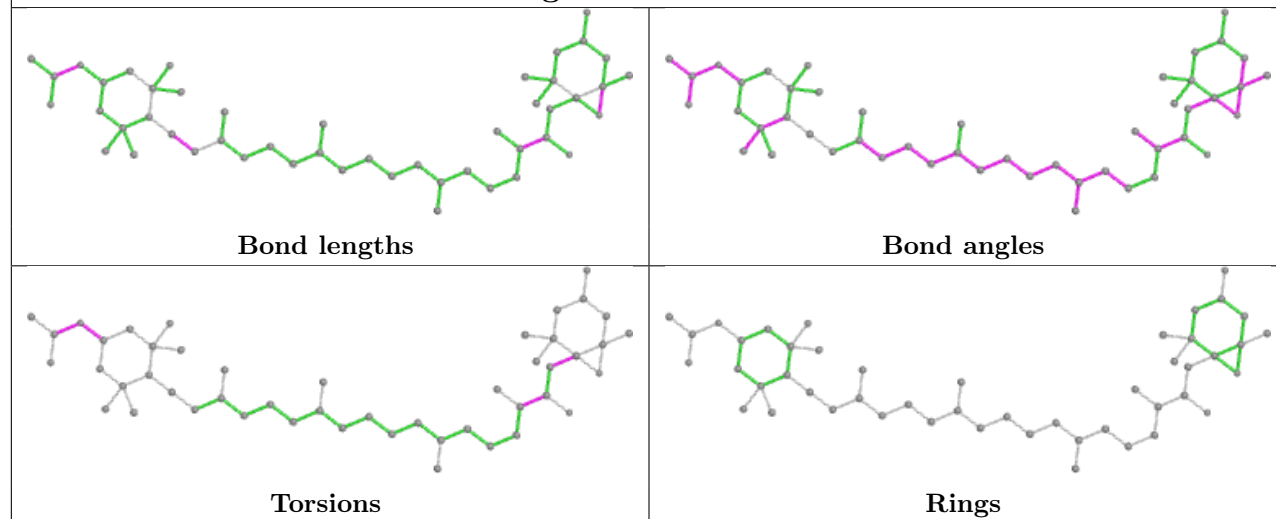
Rings

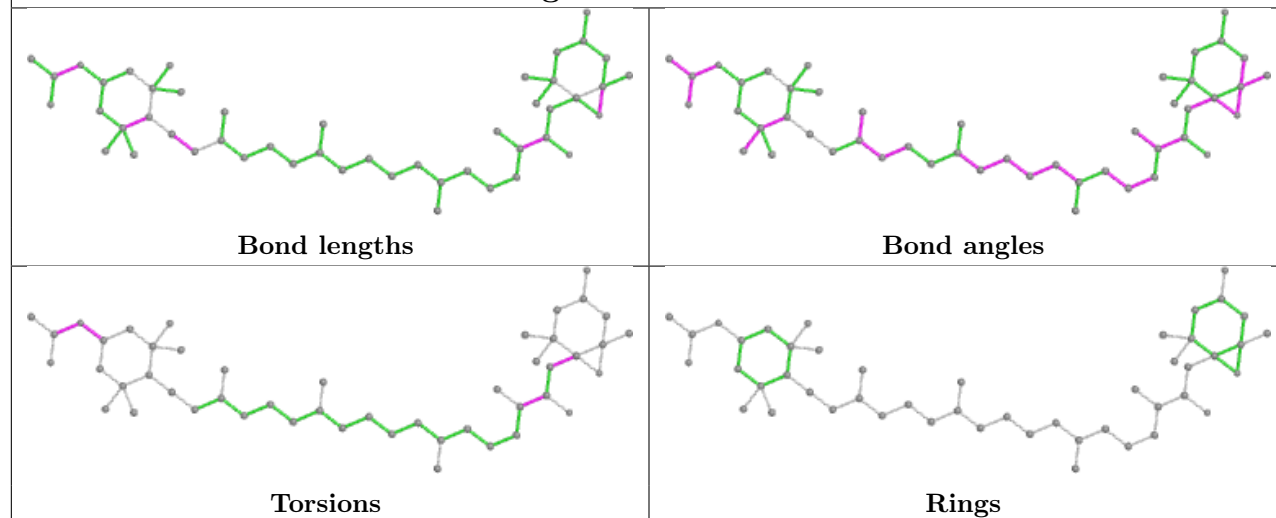
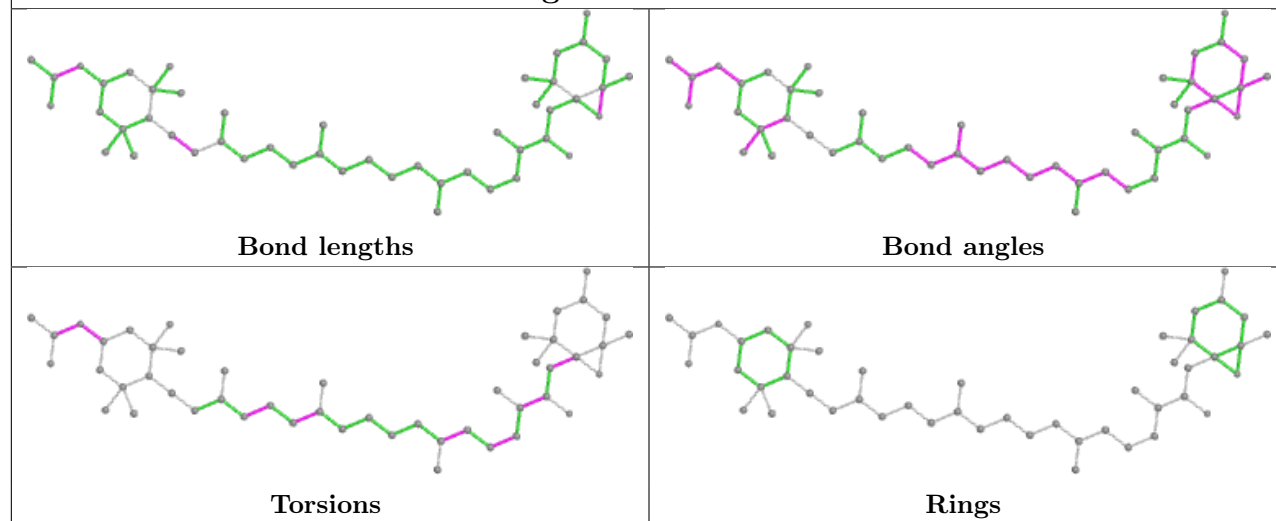


## Ligand CLA 3 313

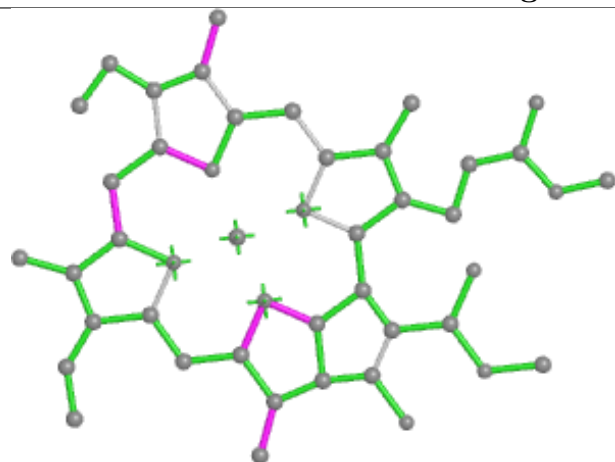


## Ligand A86 4 301

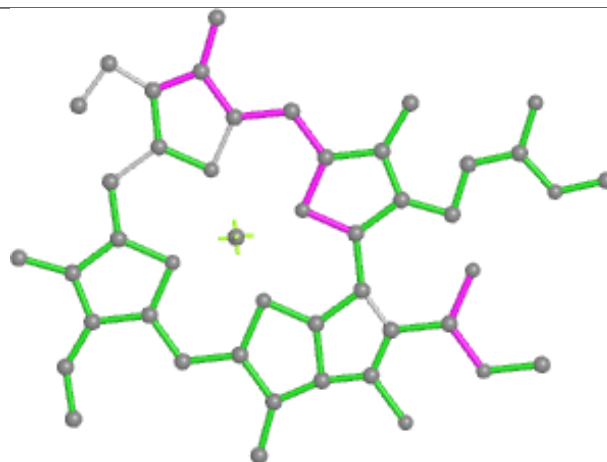


**Ligand A86 3 302****Ligand A86 4 305**

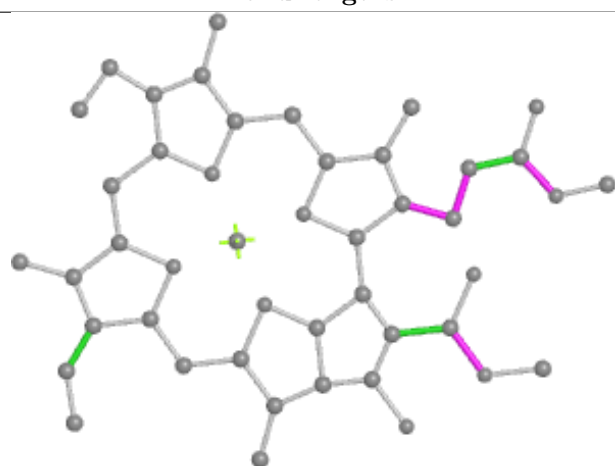
## Ligand CLA 3 315



Bond lengths



Bond angles

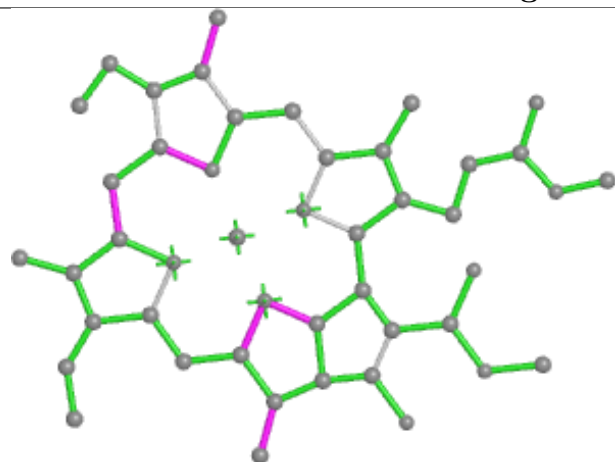


Torsions

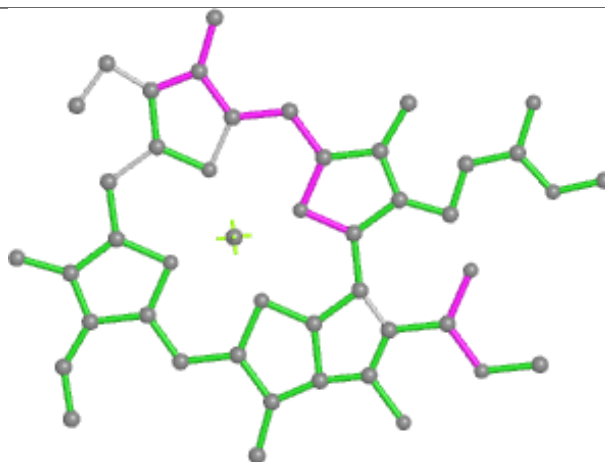


Rings

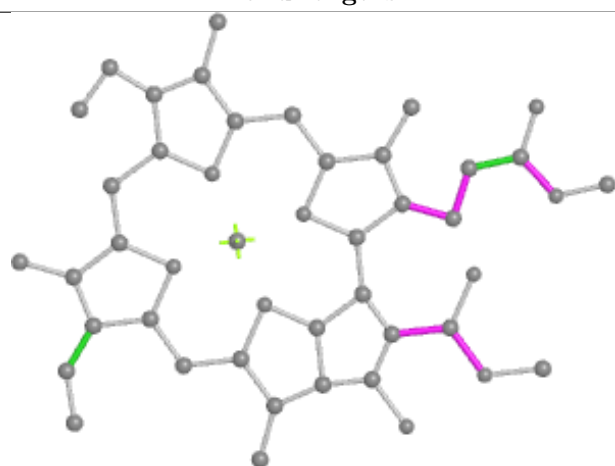
## Ligand CLA 1 314



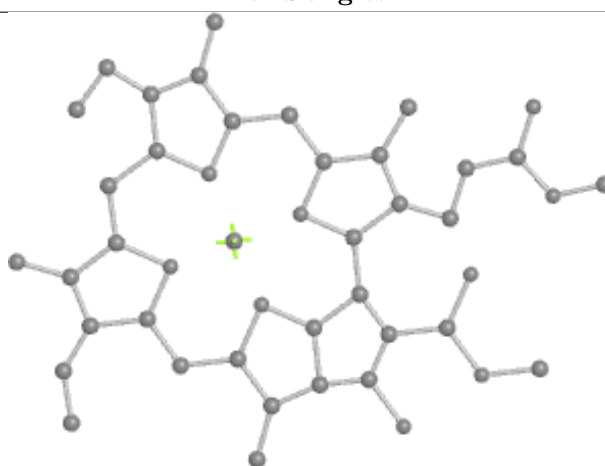
Bond lengths



Bond angles

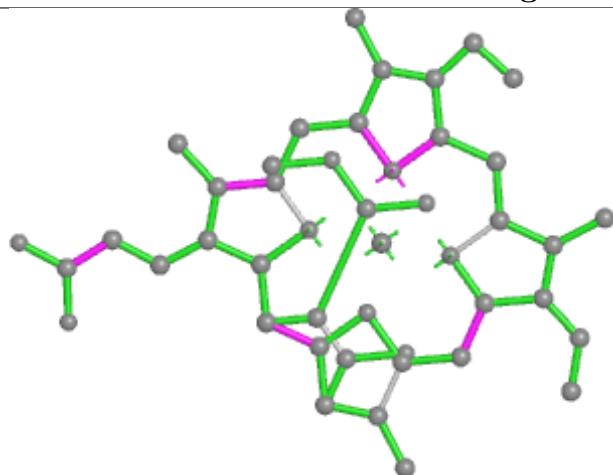


Torsions

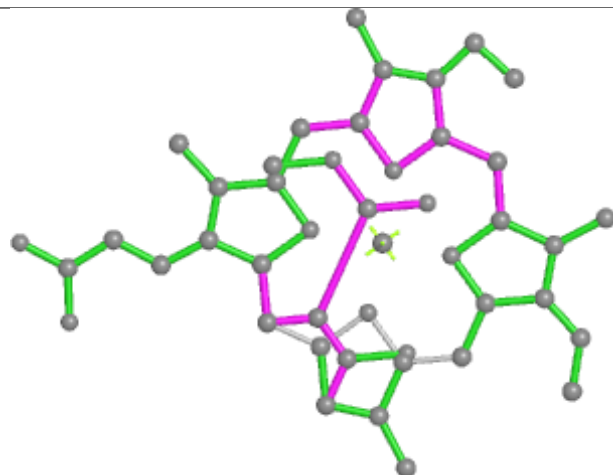


Rings

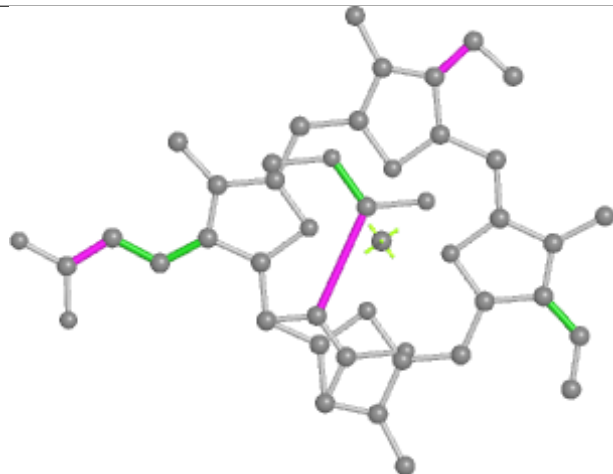
## Ligand KC1 2 415



Bond lengths



Bond angles

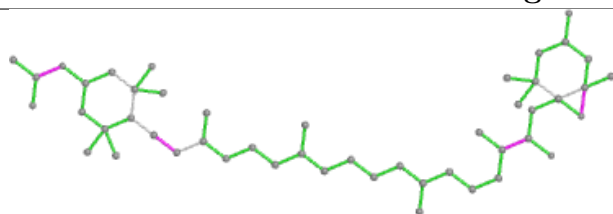


Torsions

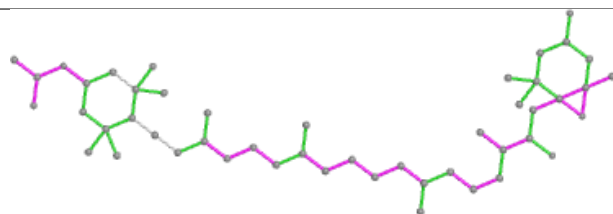


Rings

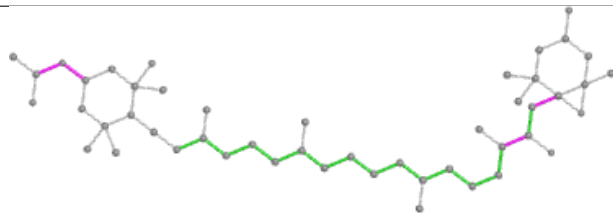
## Ligand A86 2 404



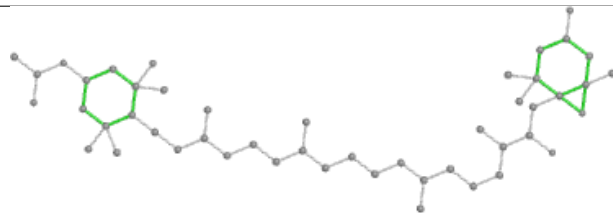
Bond lengths



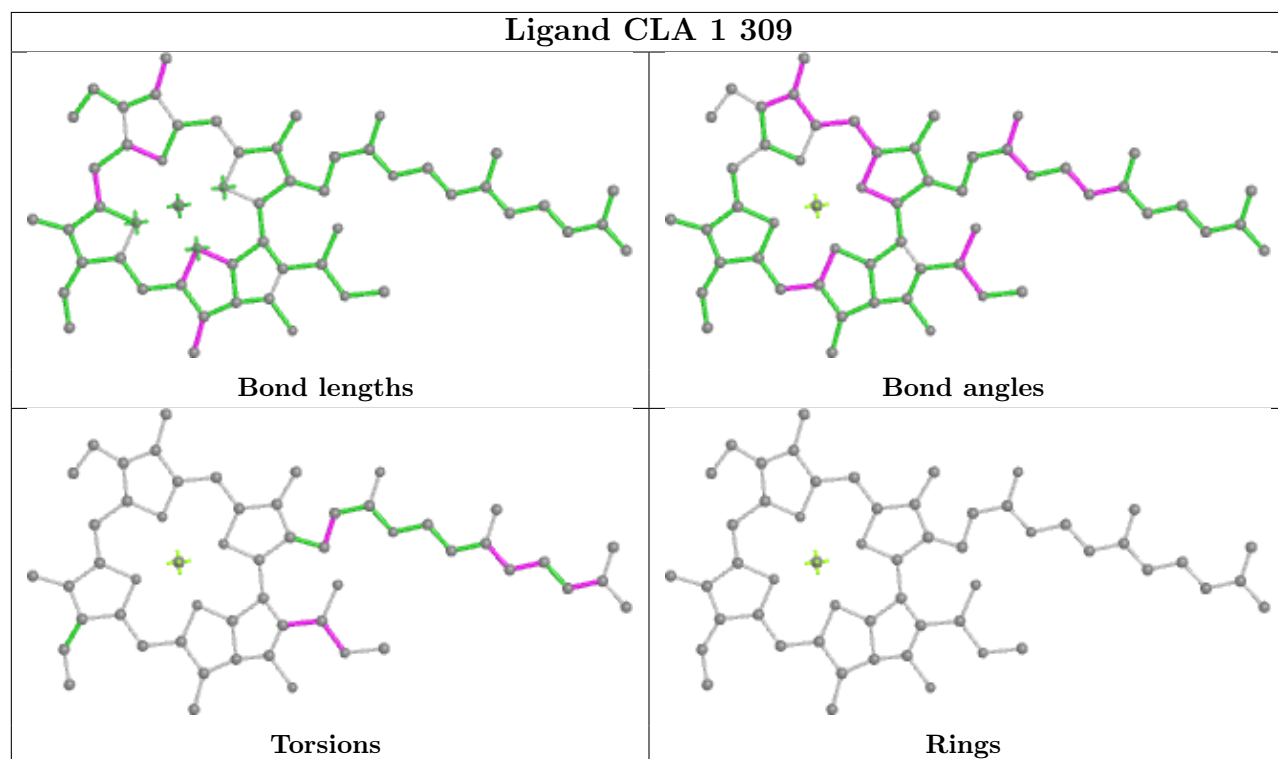
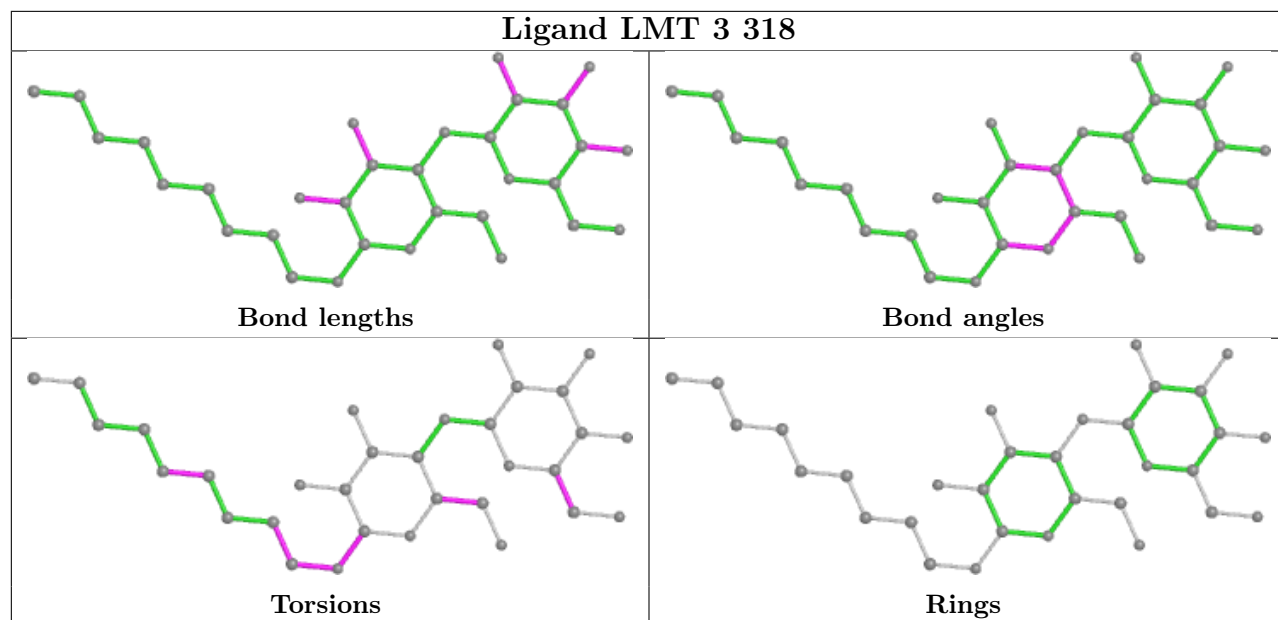
Bond angles

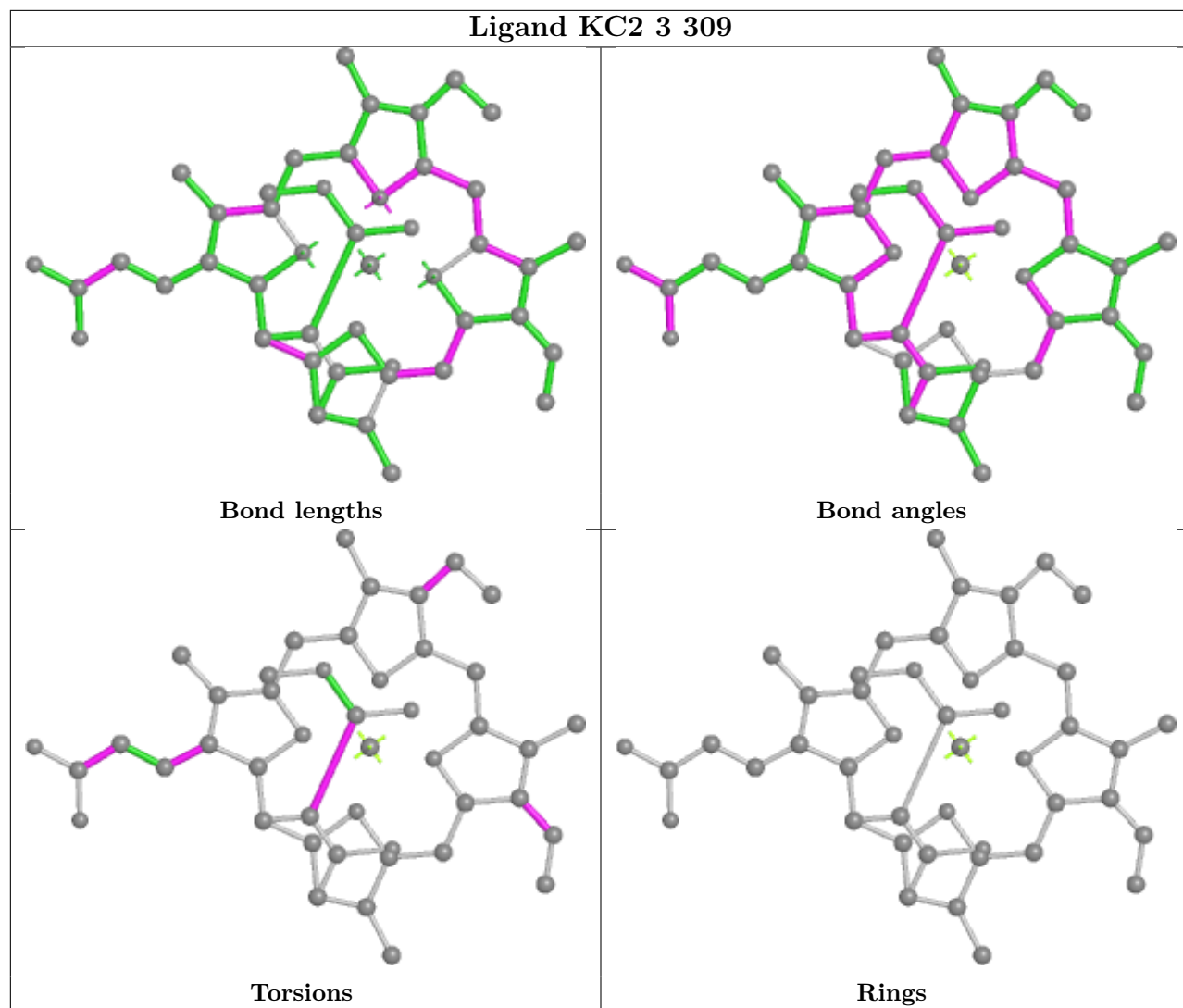


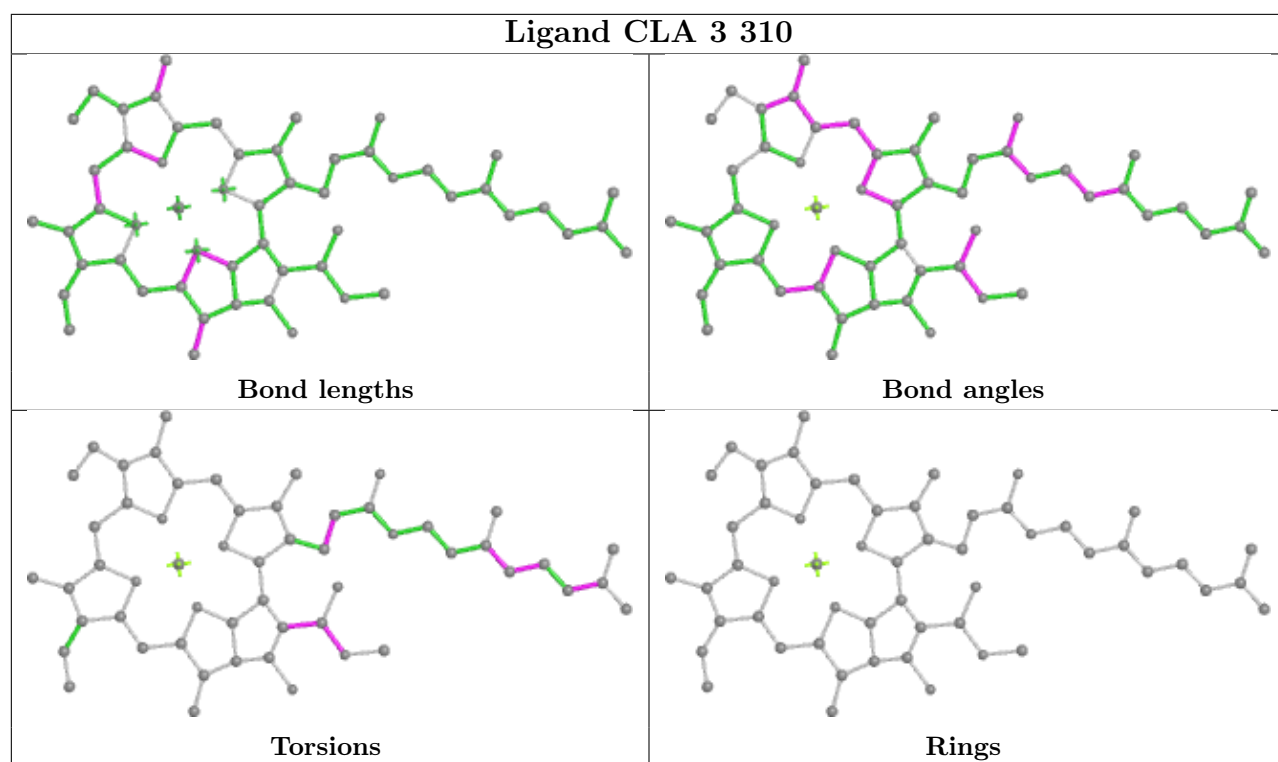
Torsions



Rings

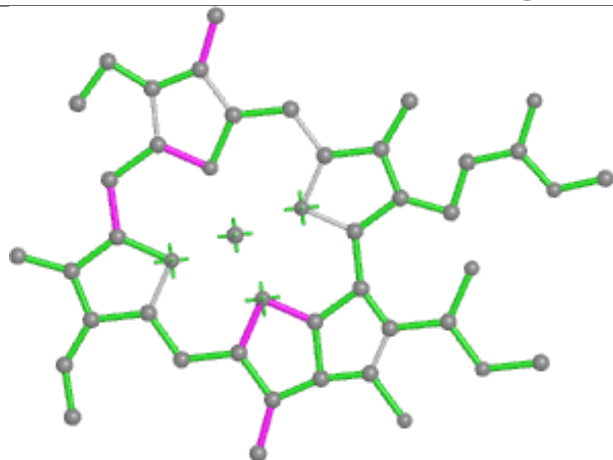




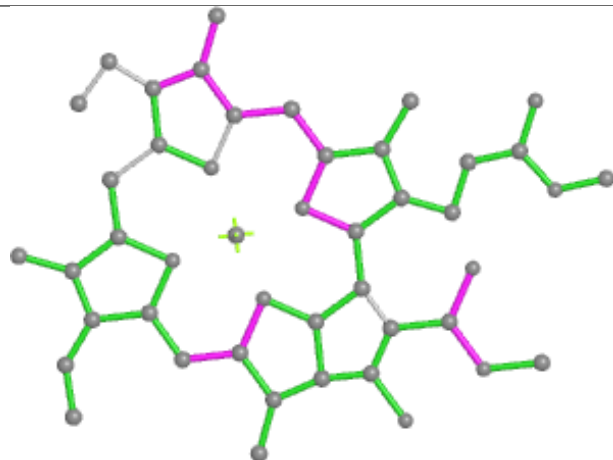




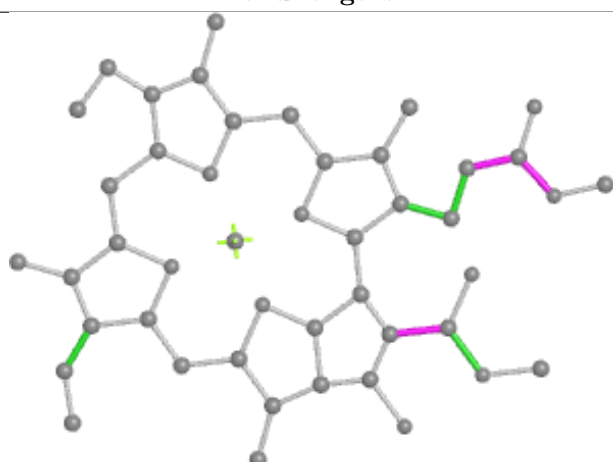
## Ligand CLA 2 417



Bond lengths



Bond angles

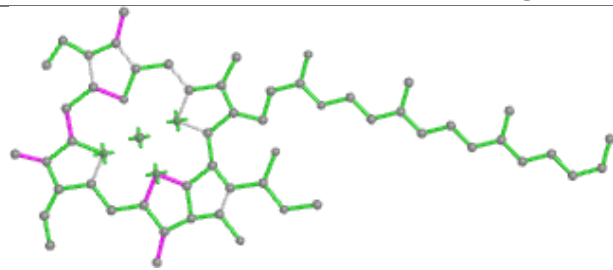


Torsions

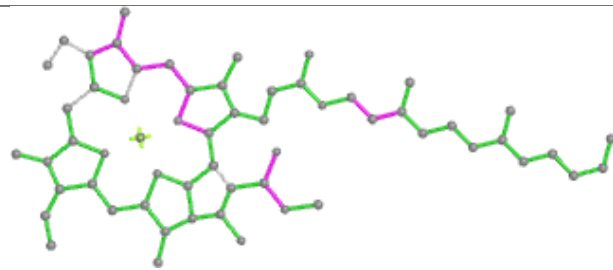


Rings

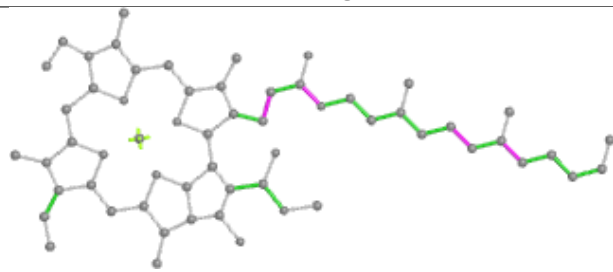
## Ligand CLA 2 409



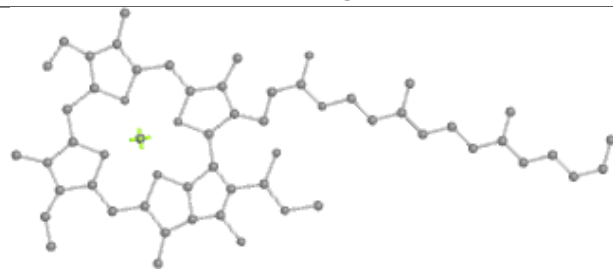
Bond lengths



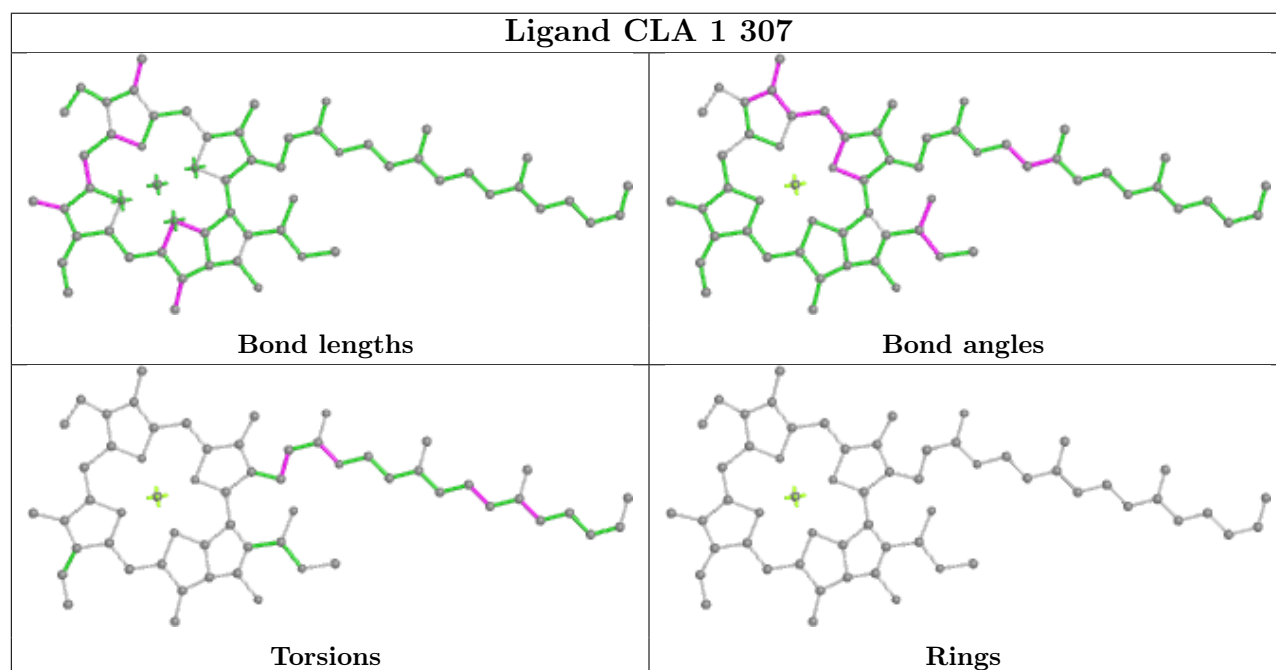
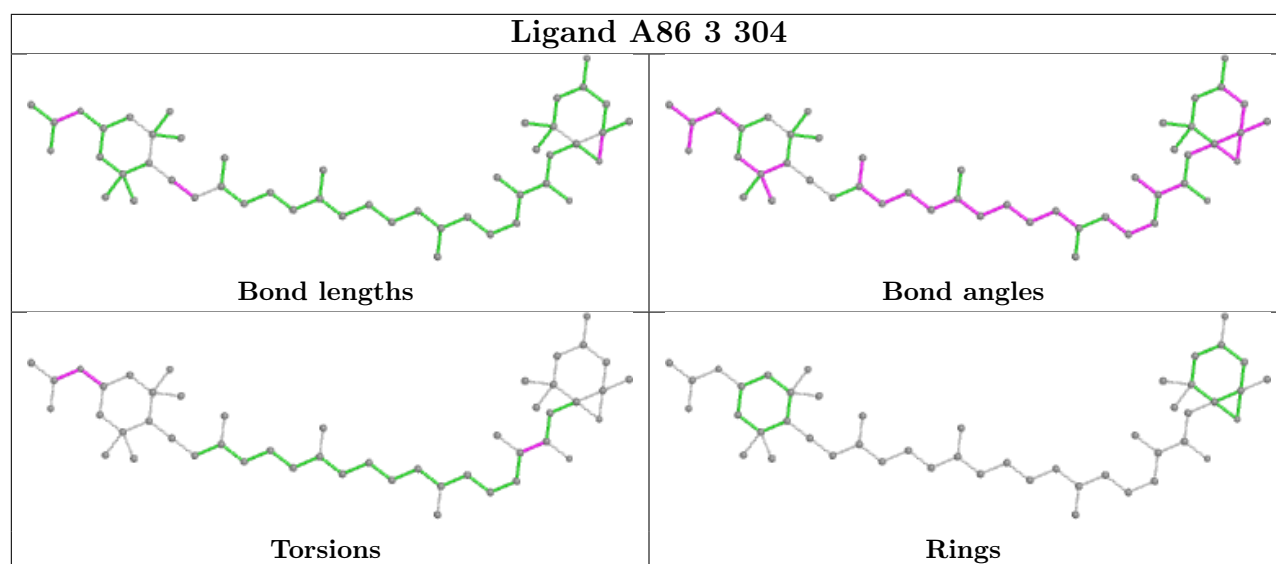
Bond angles



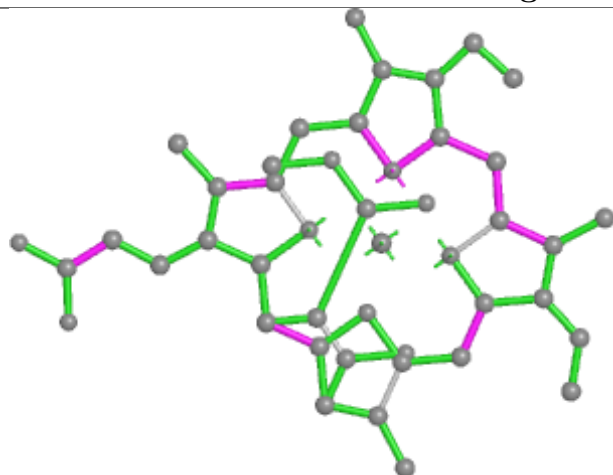
Torsions



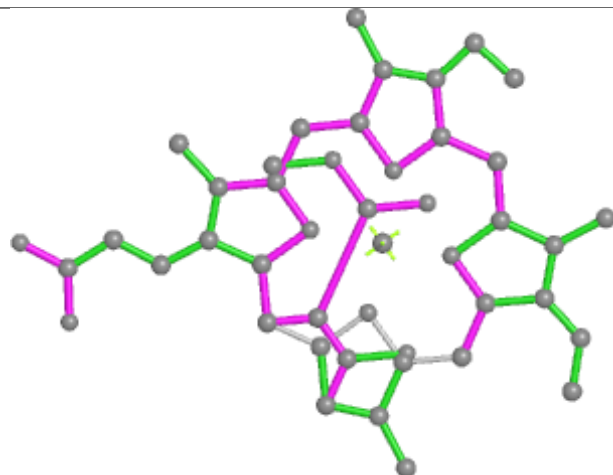
Rings



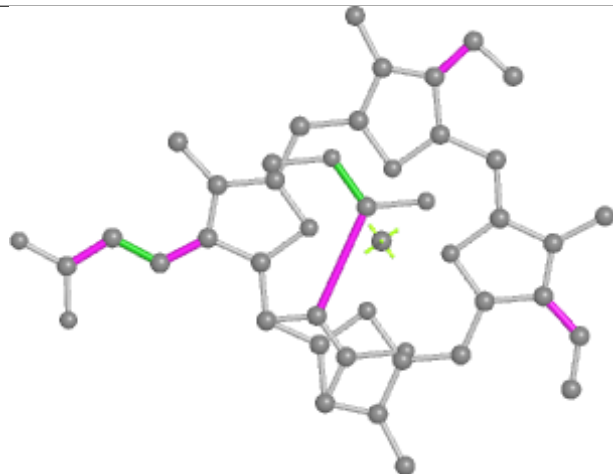
## Ligand KC2 4 308



Bond lengths



Bond angles

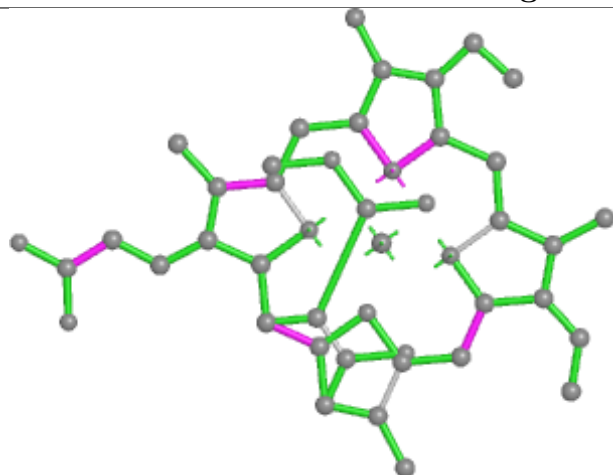


Torsions

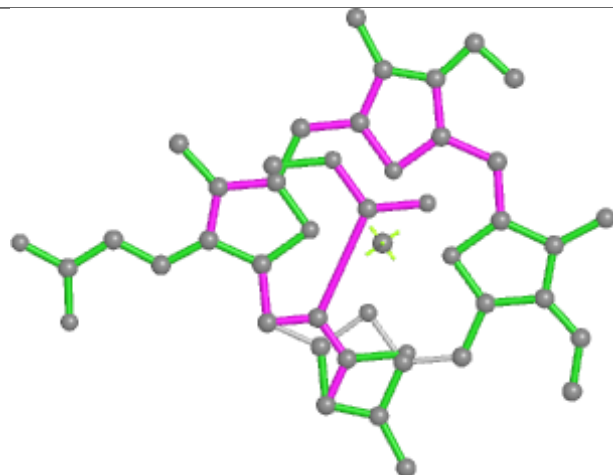


Rings

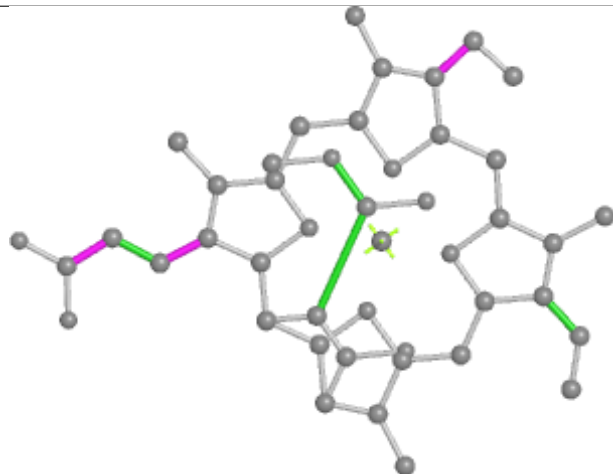
## Ligand KC1 1 311



Bond lengths



Bond angles

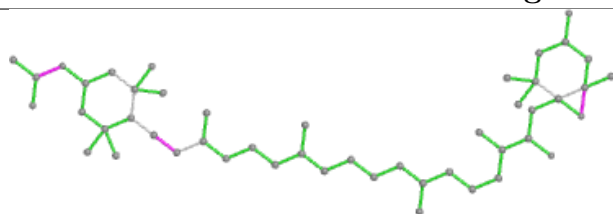


Torsions

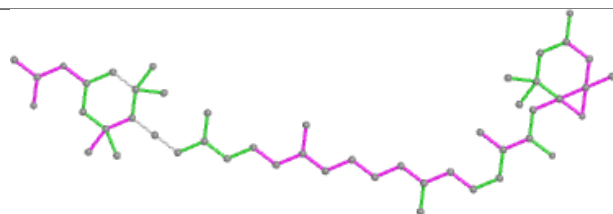


Rings

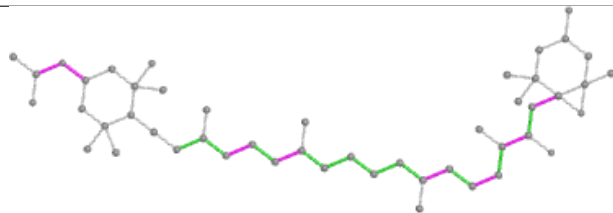
## Ligand A86 1 305



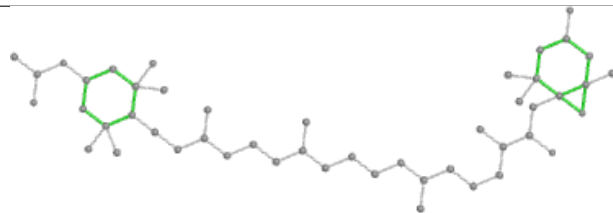
Bond lengths



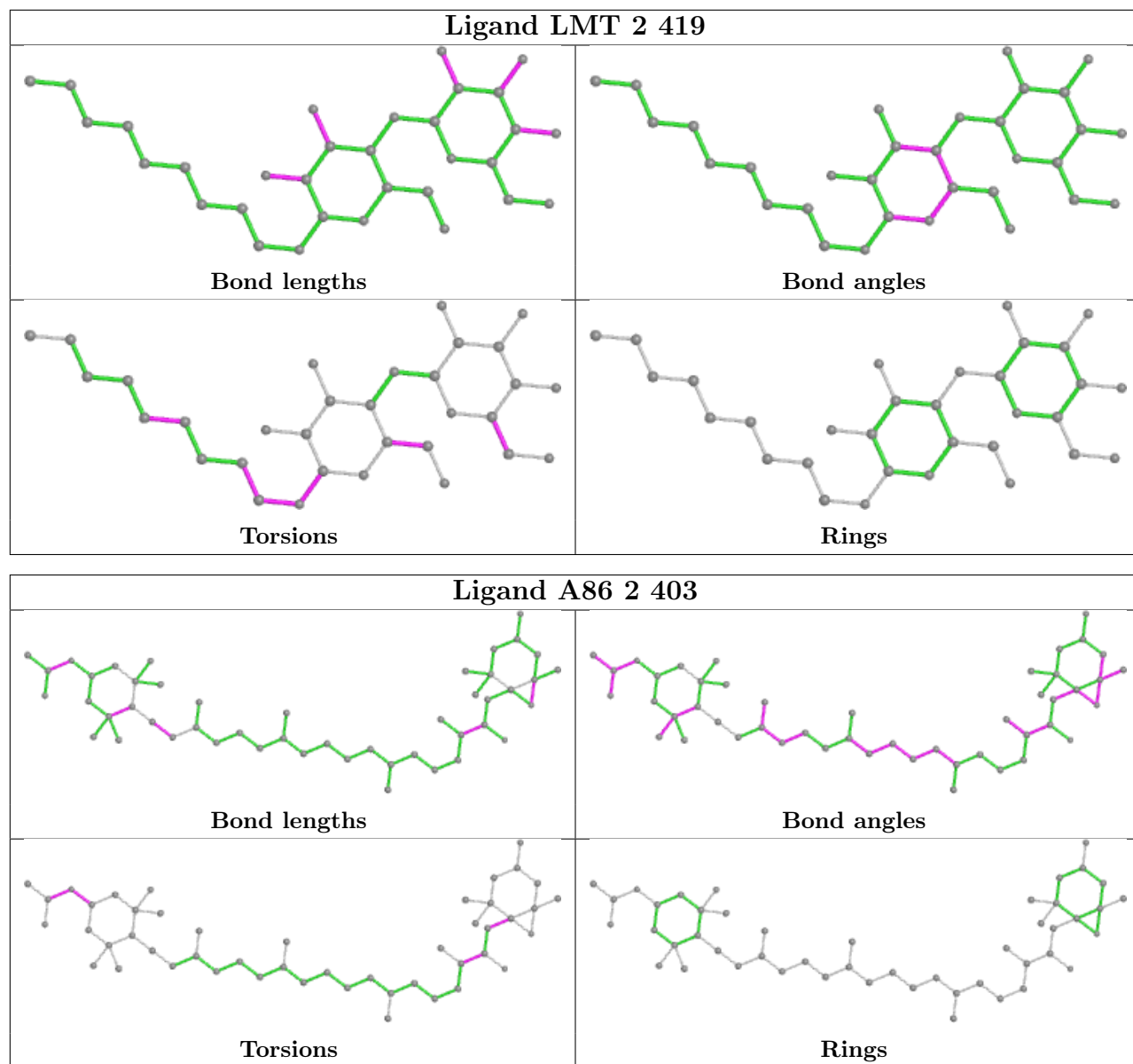
Bond angles



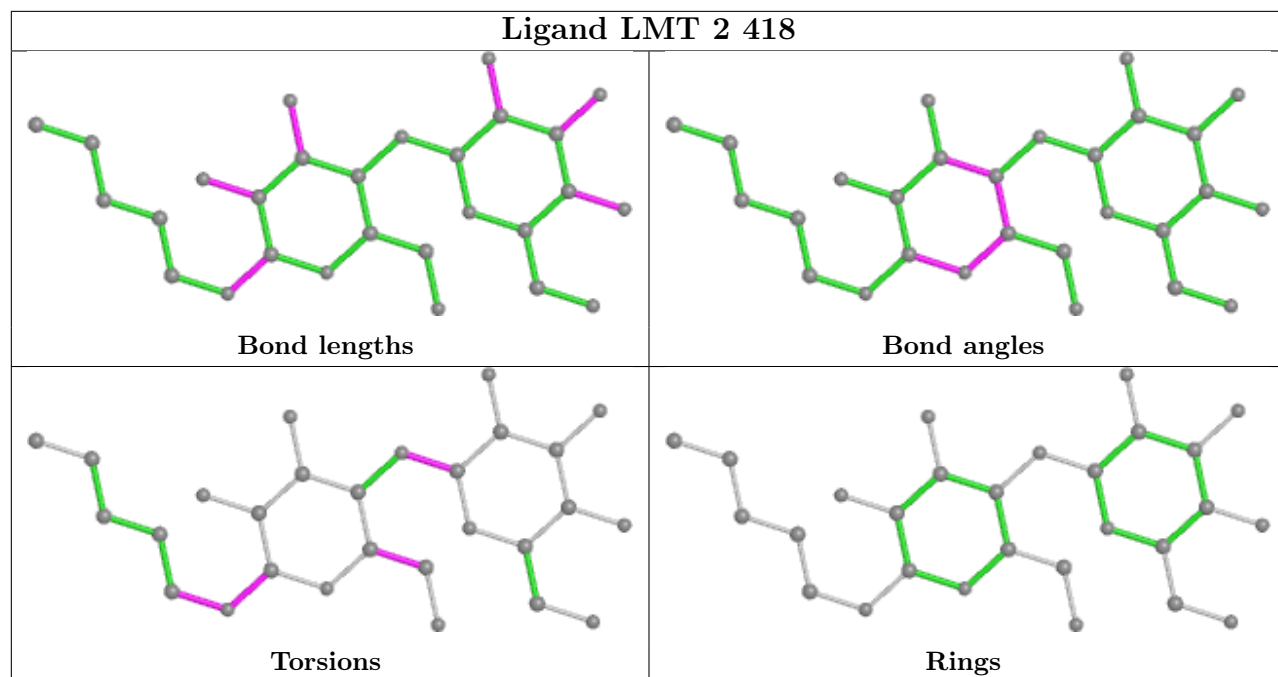
Torsions



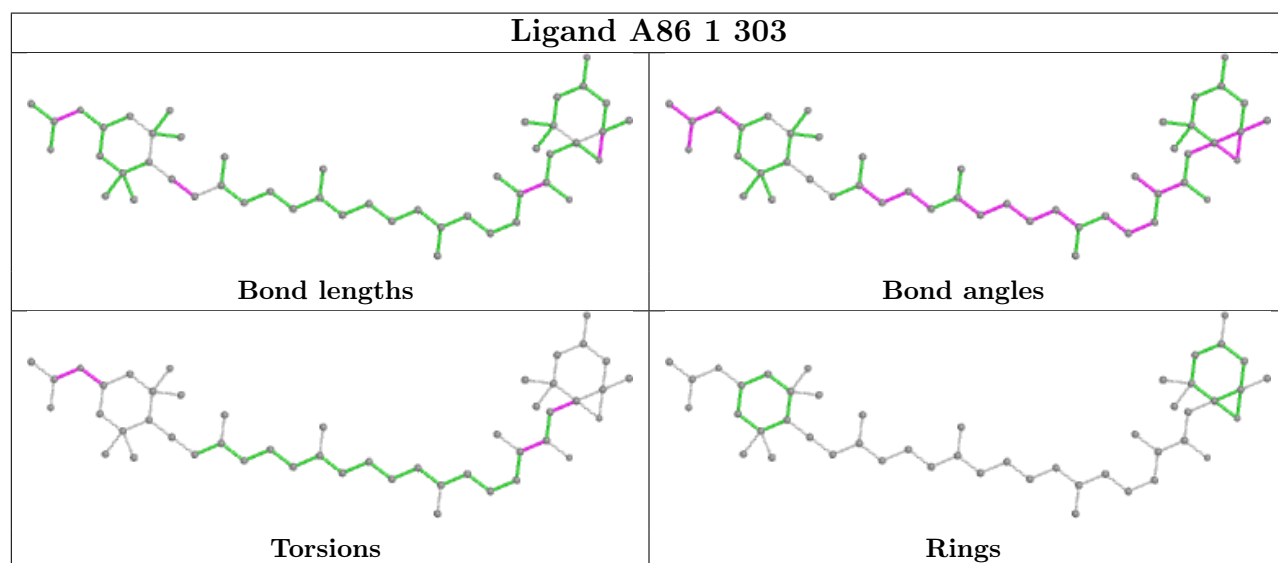
Rings



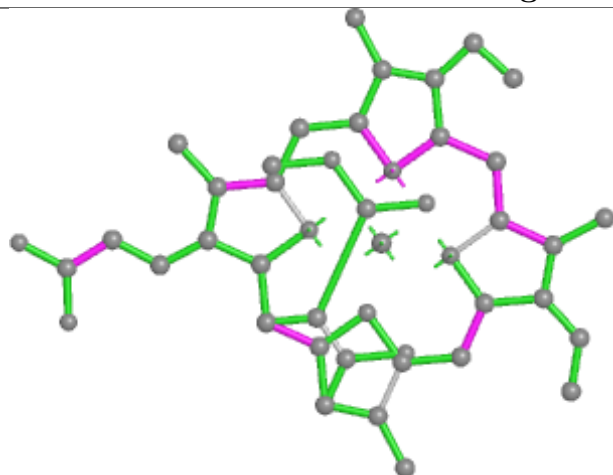
## Ligand LMT 2 418



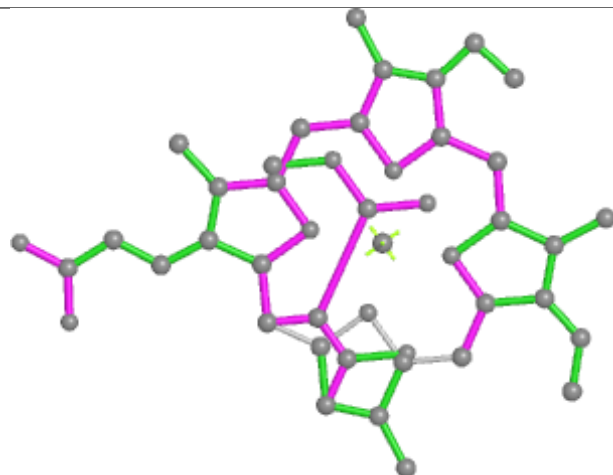
## Ligand A86 1 303



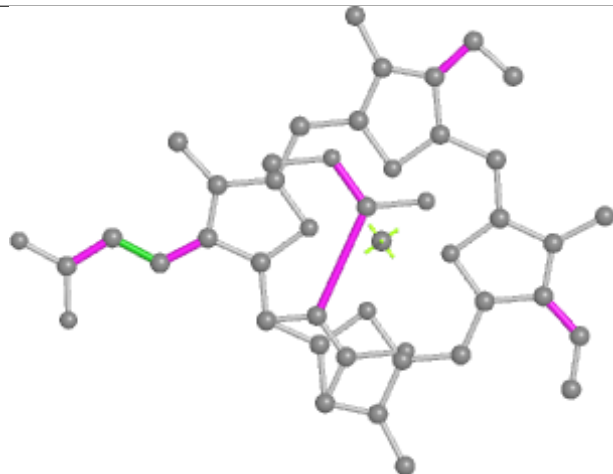
## Ligand KC2 1 308



Bond lengths



Bond angles

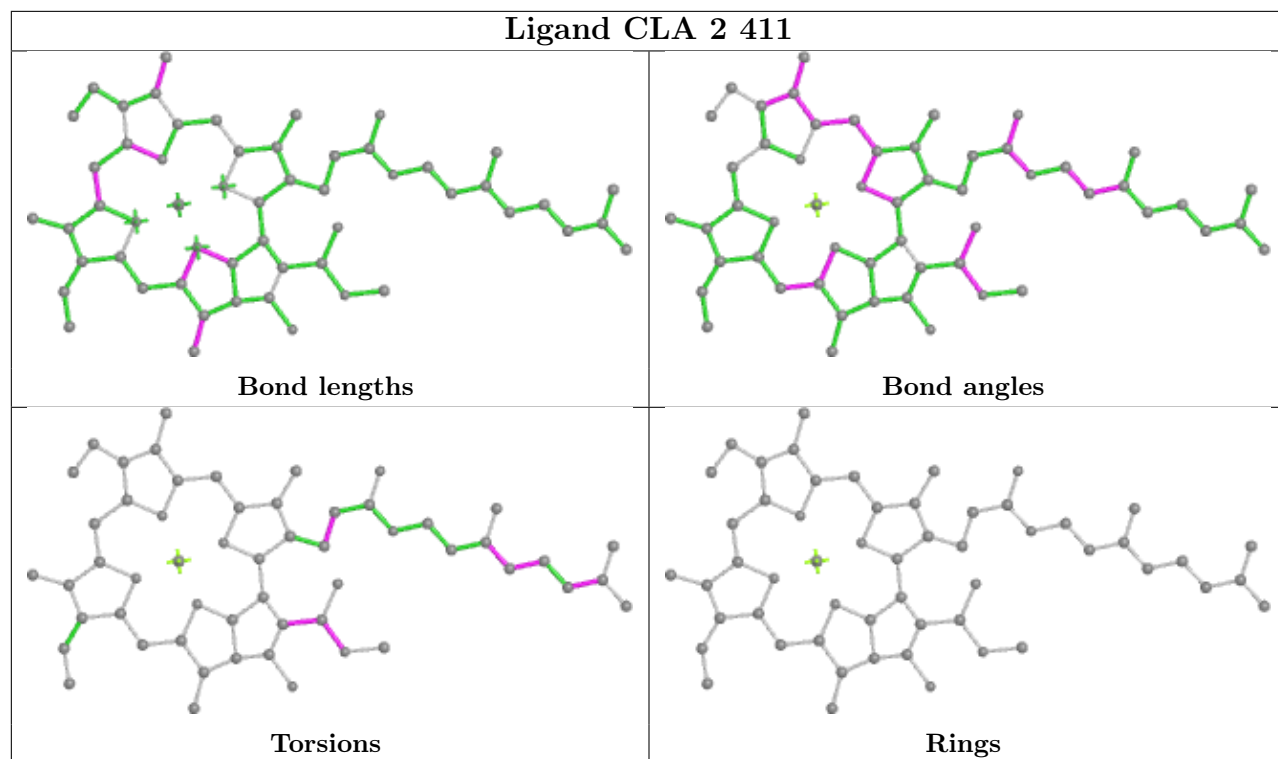


Torsions

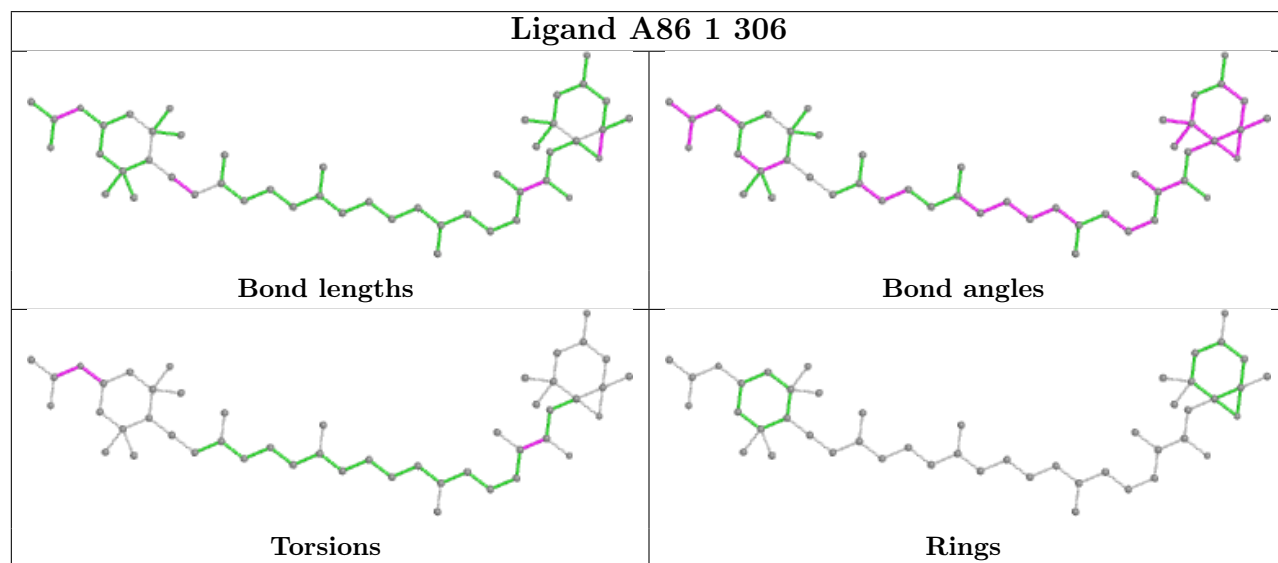


Rings

## Ligand CLA 2 411

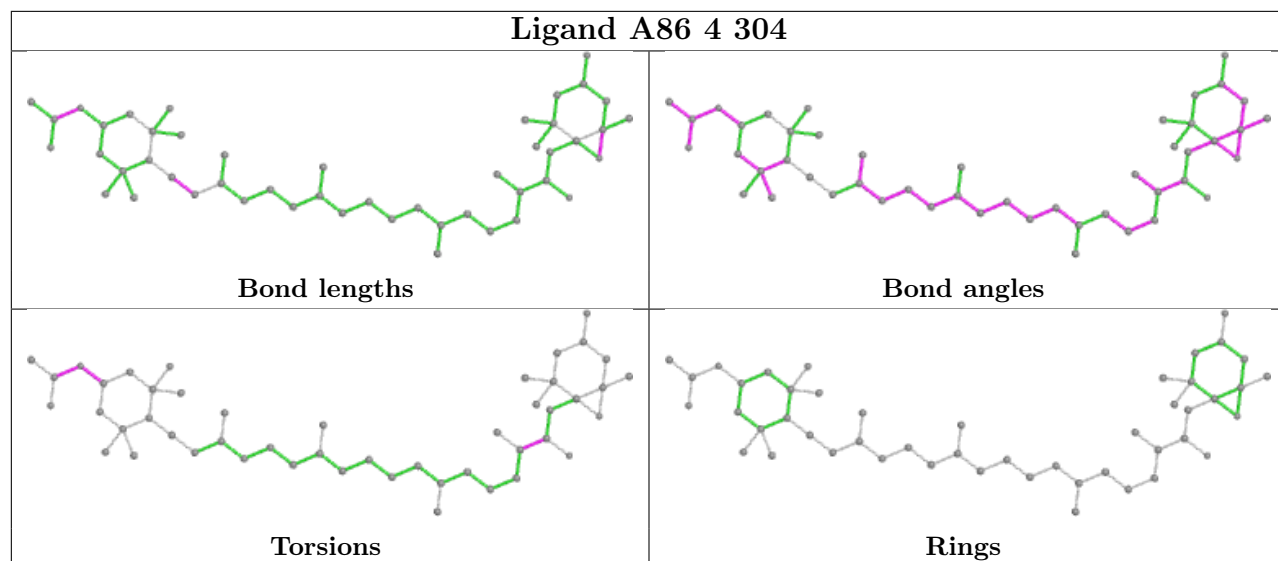


## Ligand A86 1 306

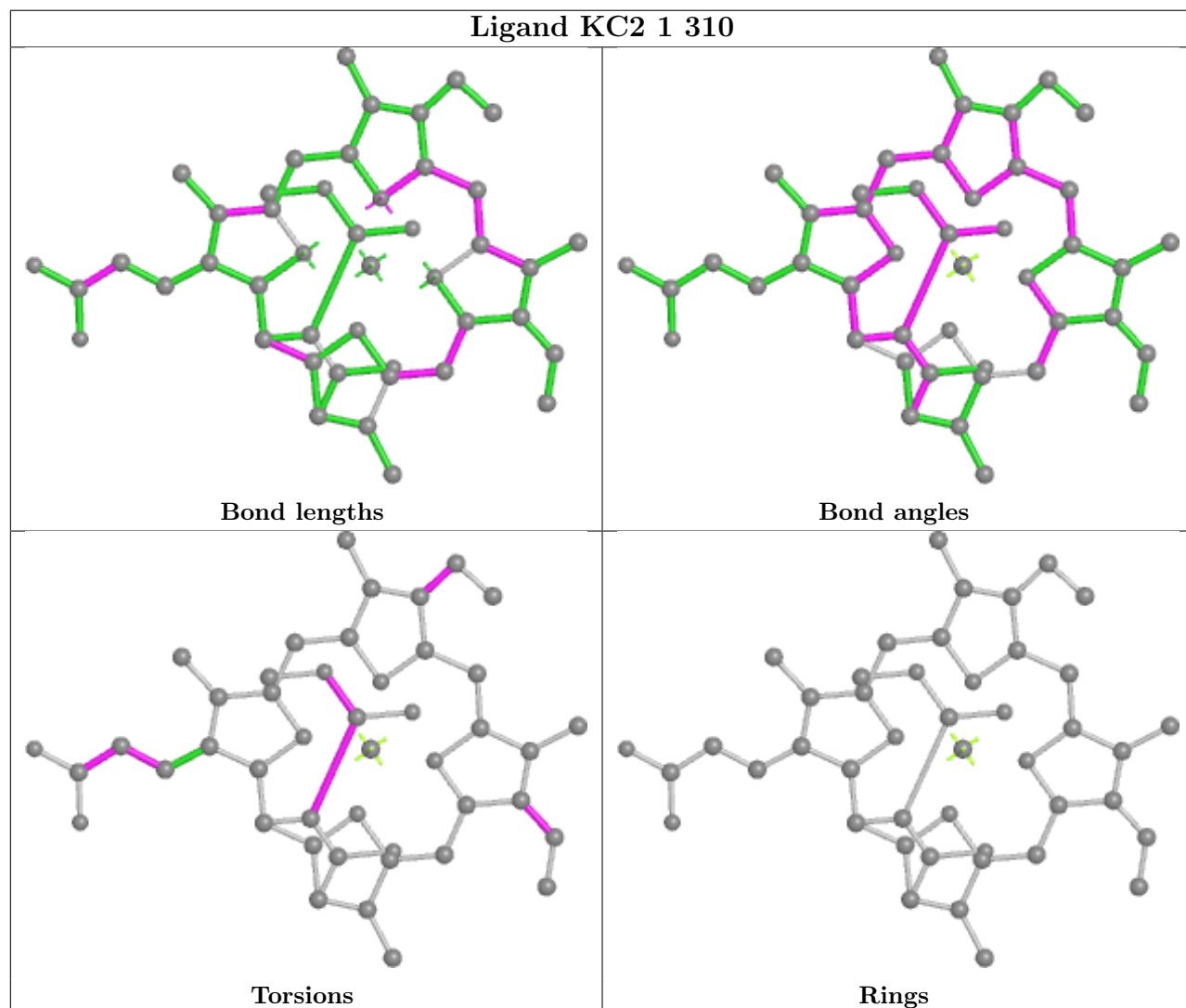




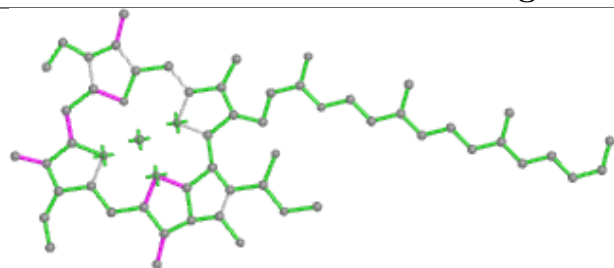
## Ligand A86 4 304



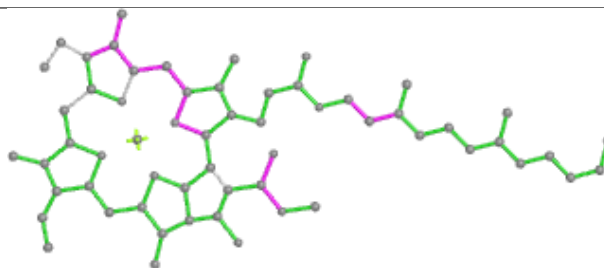
## Ligand KC2 1 310



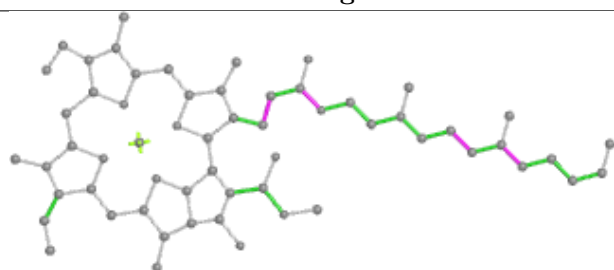
## Ligand CLA 3 308



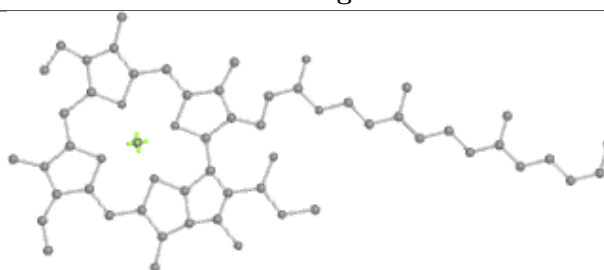
Bond lengths



Bond angles

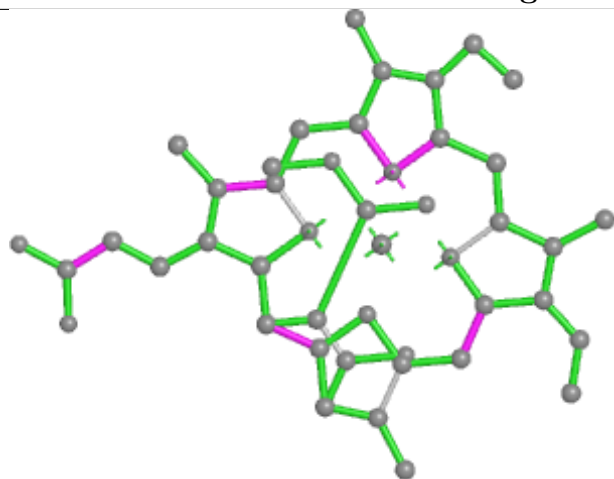


Torsions

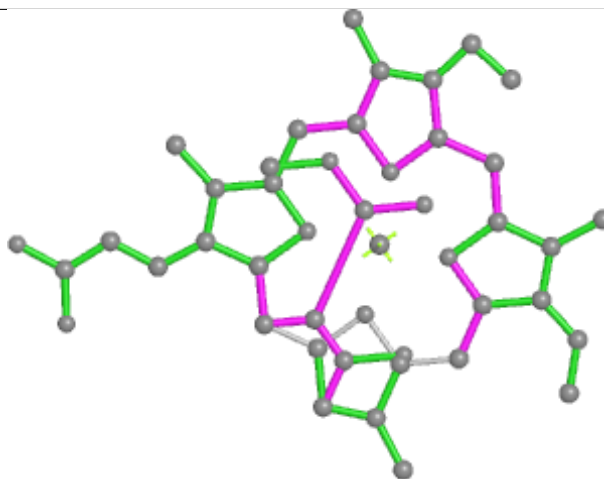


Rings

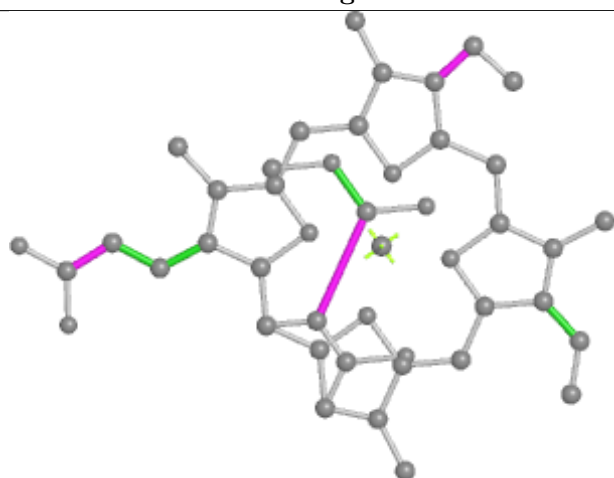
## Ligand KC1 4 313



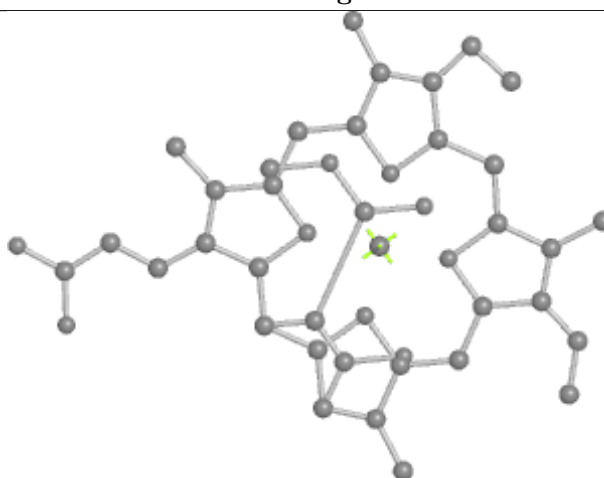
Bond lengths



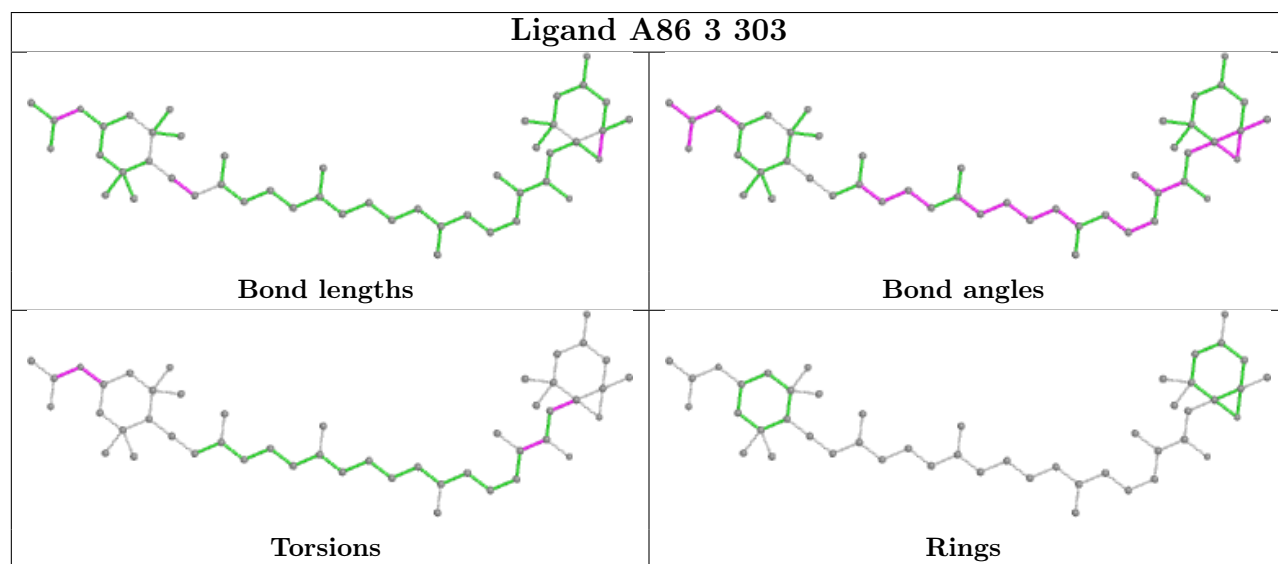
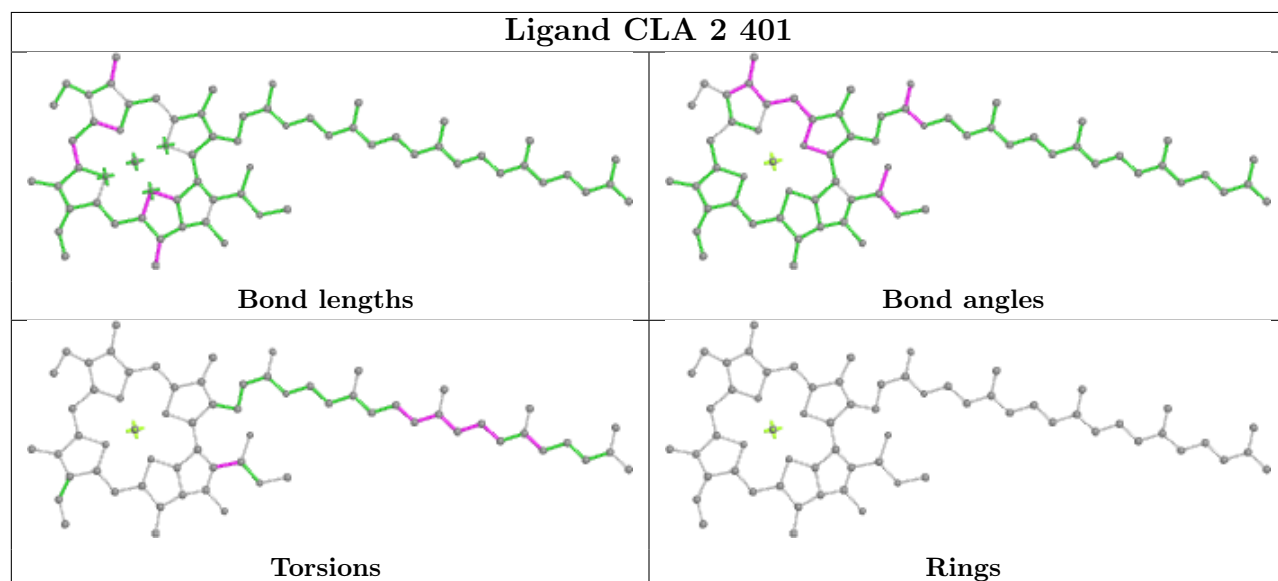
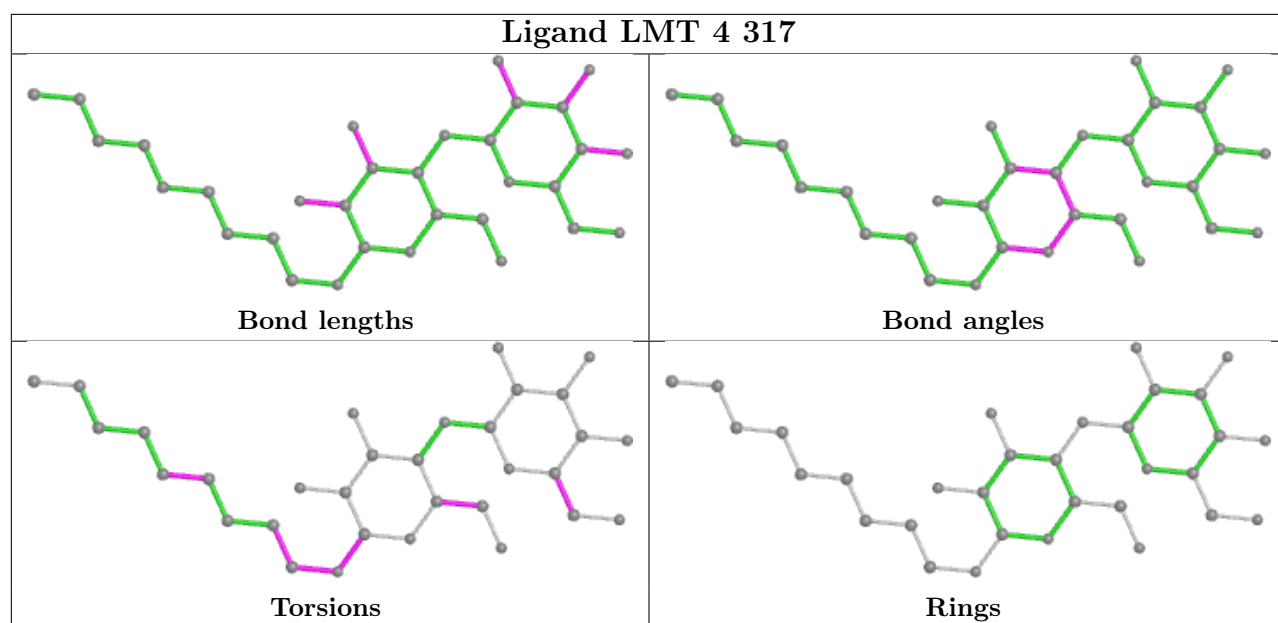
Bond angles



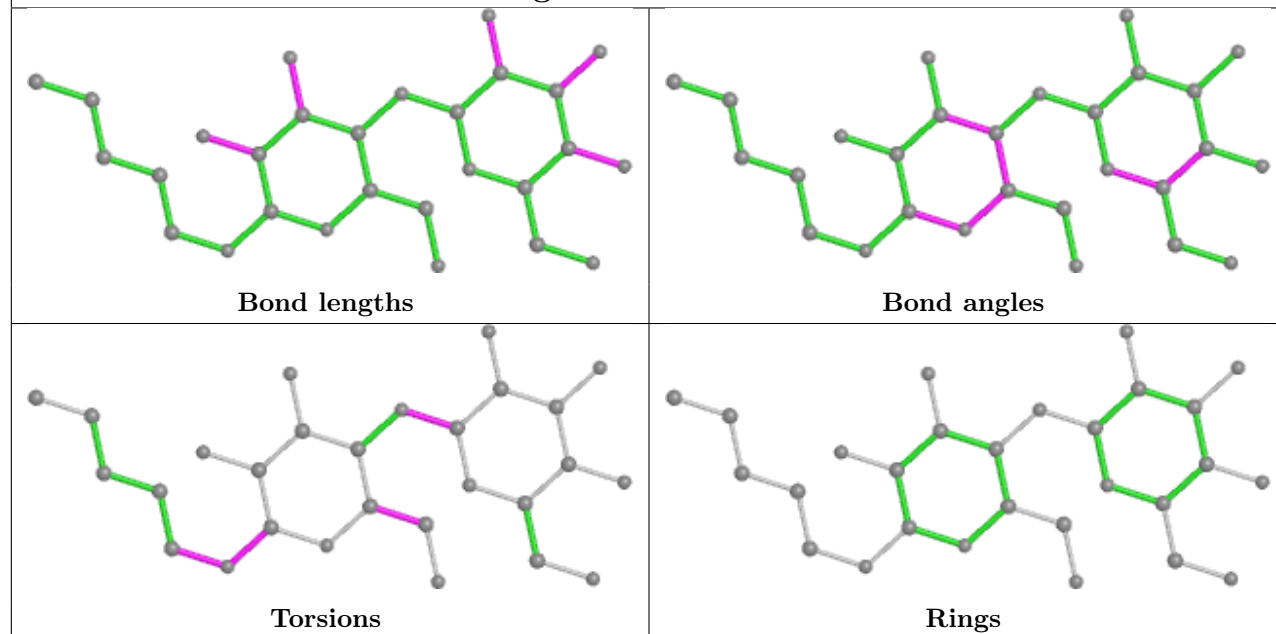
Torsions



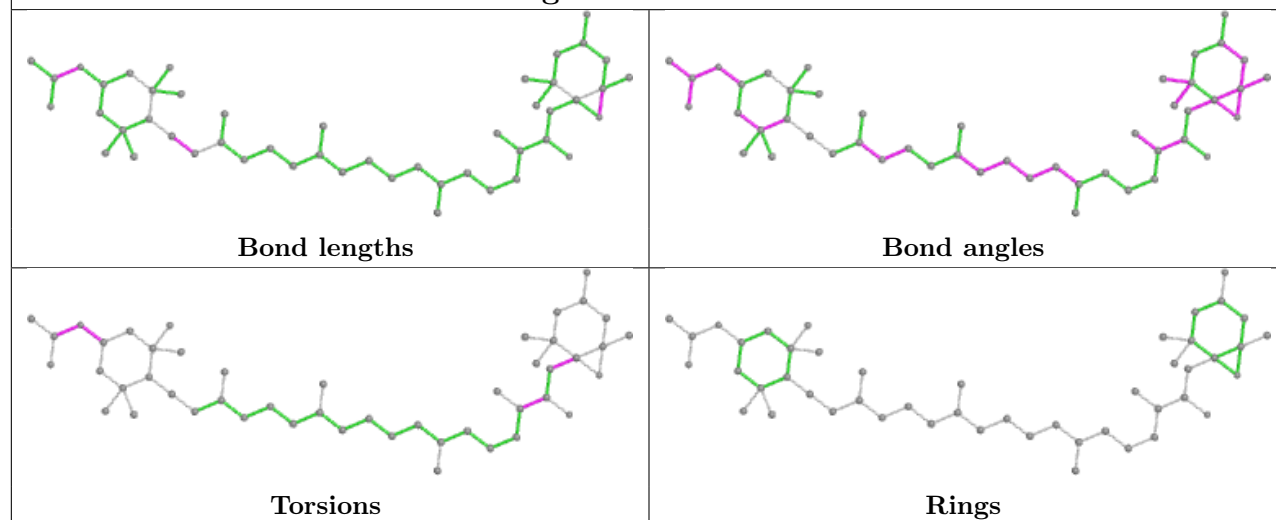
Rings



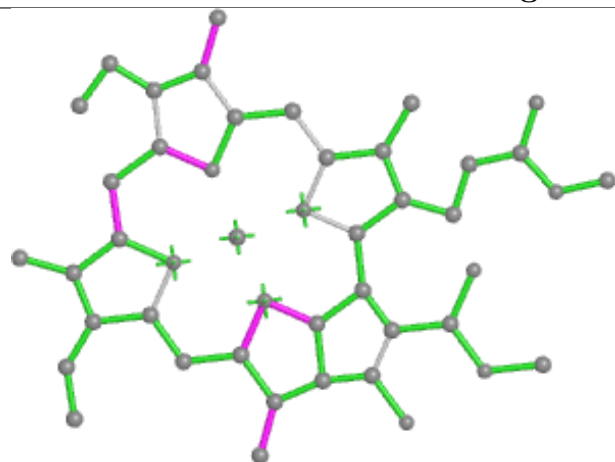
## Ligand LMT 4 316



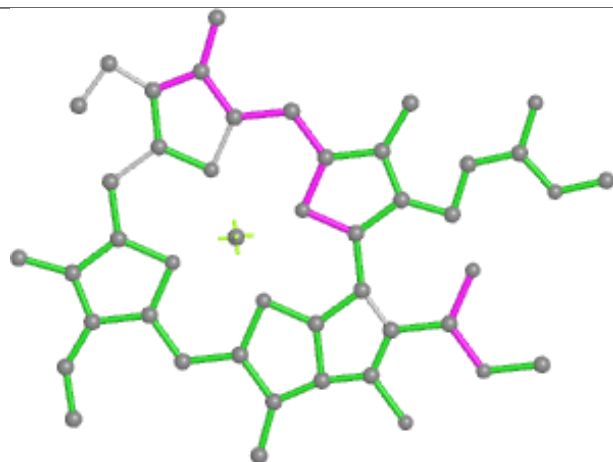
## Ligand A86 2 407



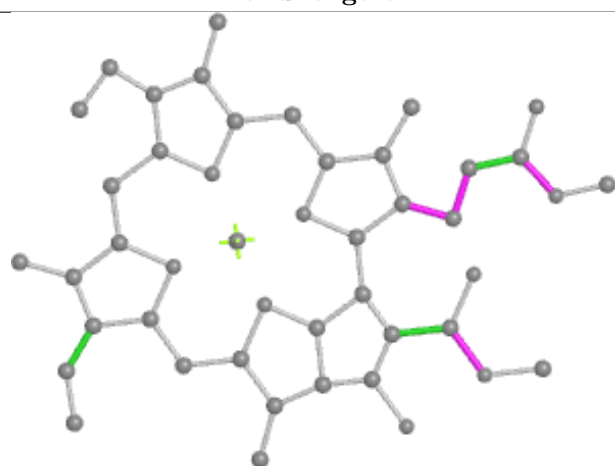
## Ligand CLA 2 416



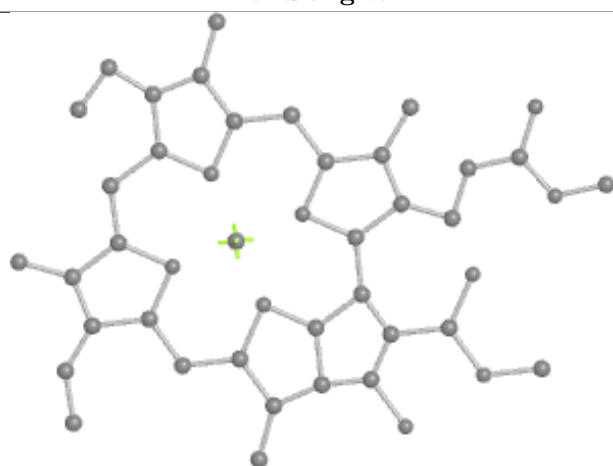
Bond lengths



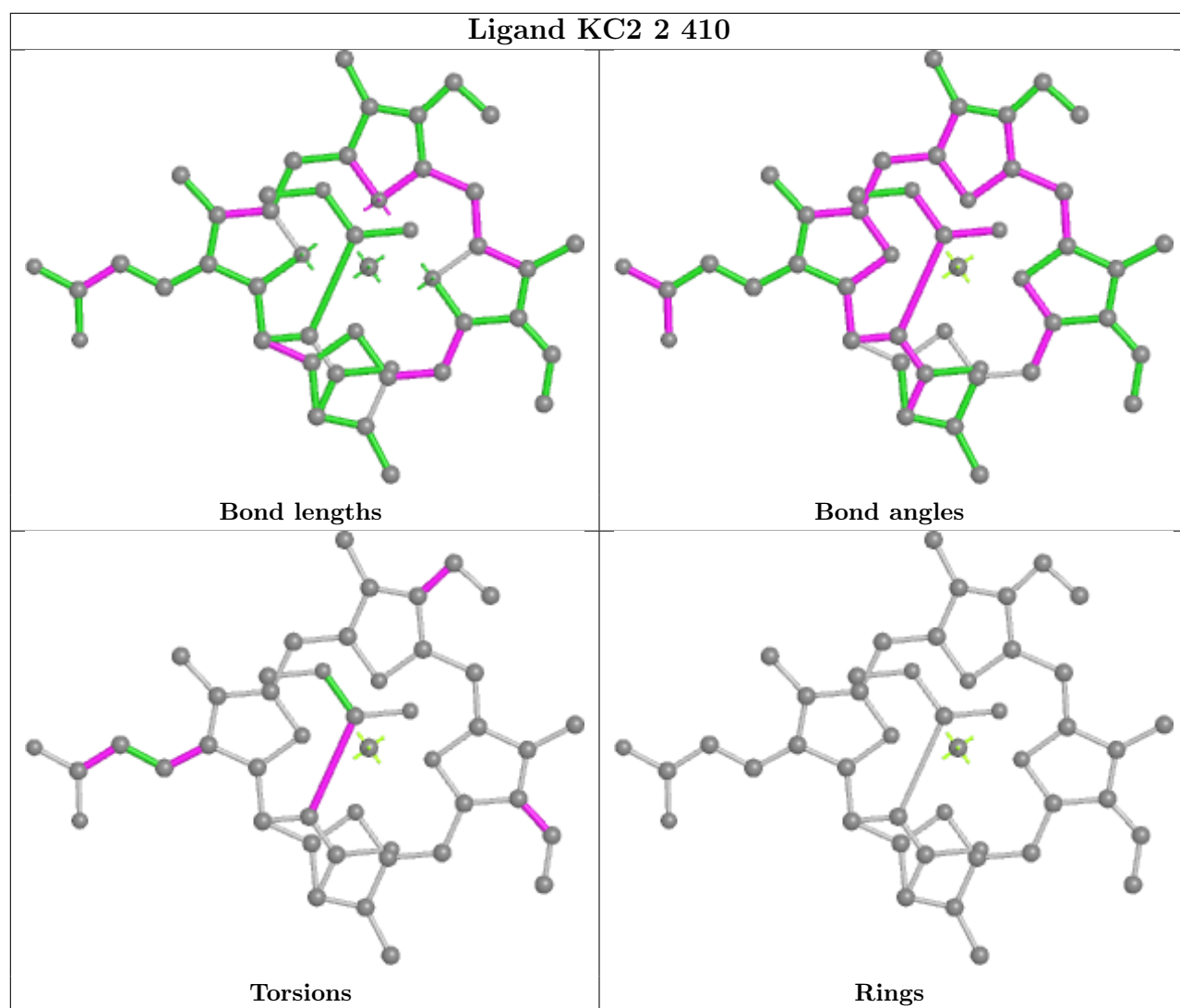
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

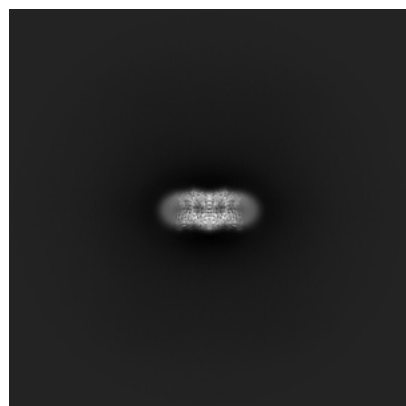
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37441. These allow visual inspection of the internal detail of the map and identification of artifacts.

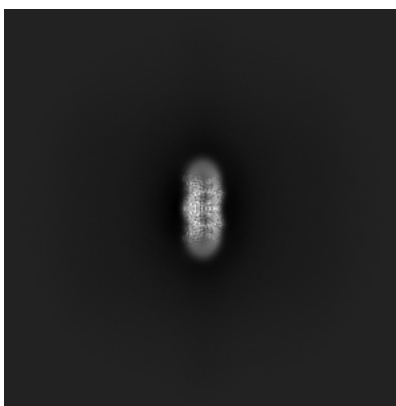
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

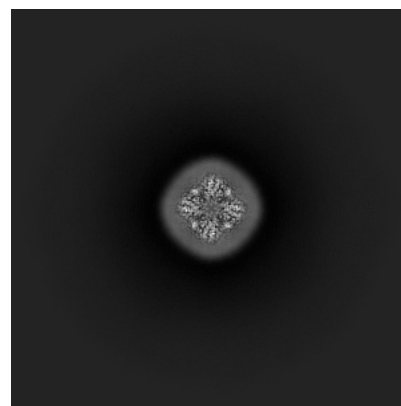
#### 6.1.1 Primary map



X

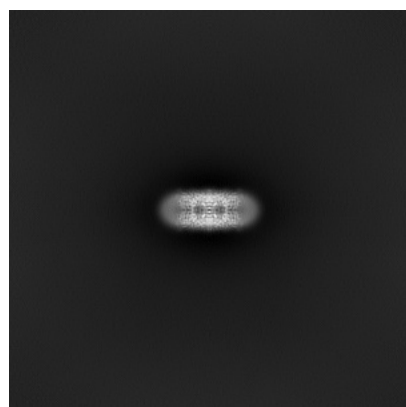


Y

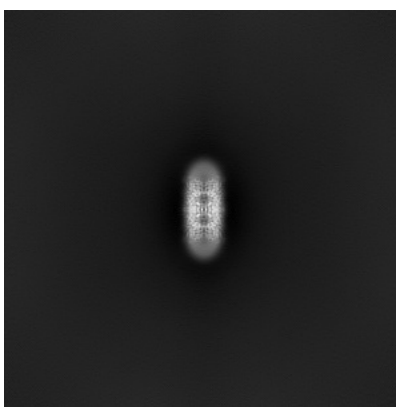


Z

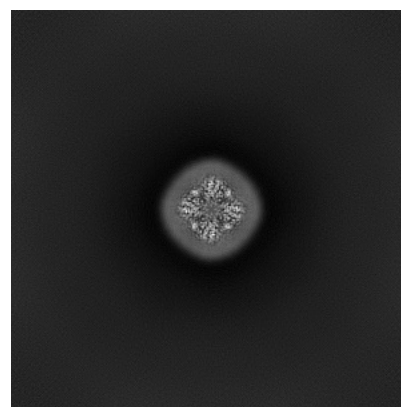
#### 6.1.2 Raw map



X



Y

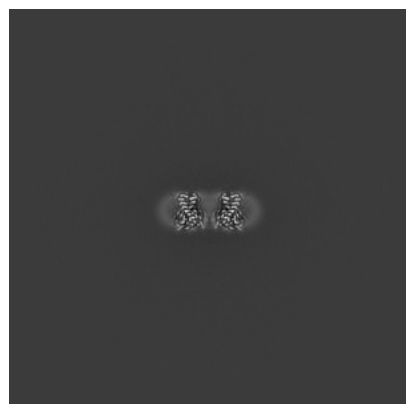


Z

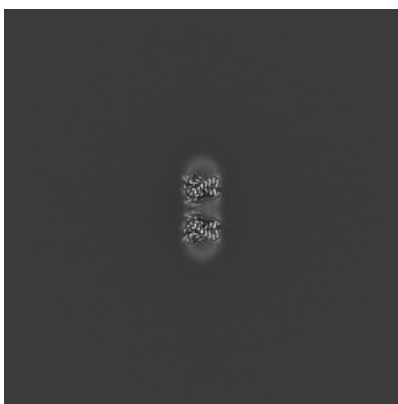
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

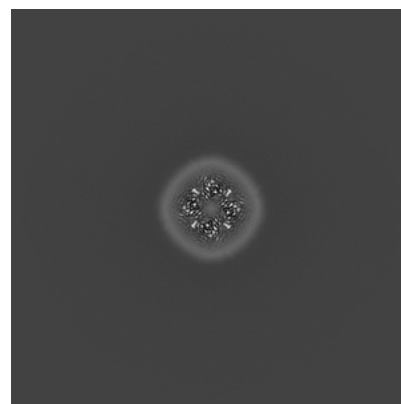
### 6.2.1 Primary map



X Index: 240

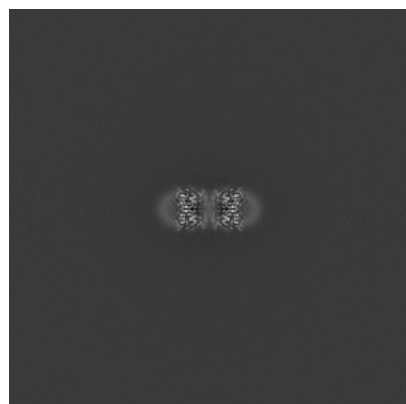


Y Index: 240

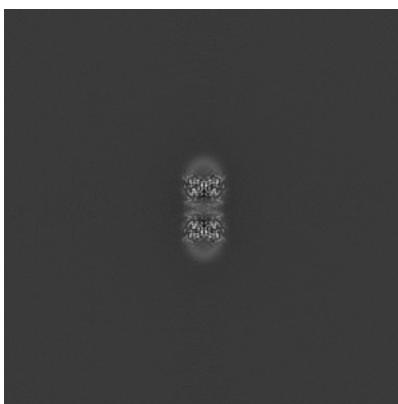


Z Index: 240

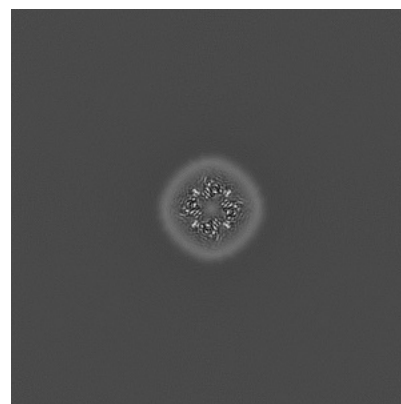
### 6.2.2 Raw map



X Index: 240



Y Index: 240



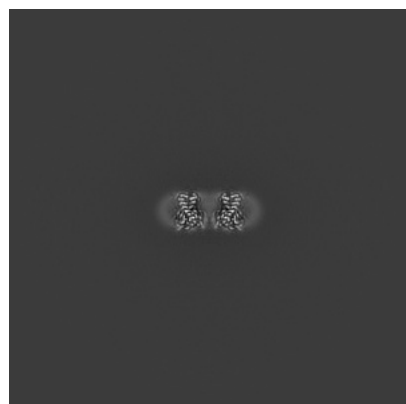
Z Index: 240

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

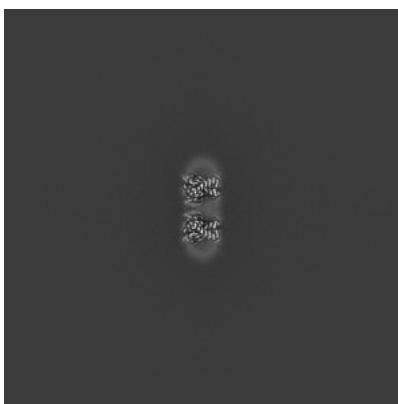


## 6.3 Largest variance slices [i](#)

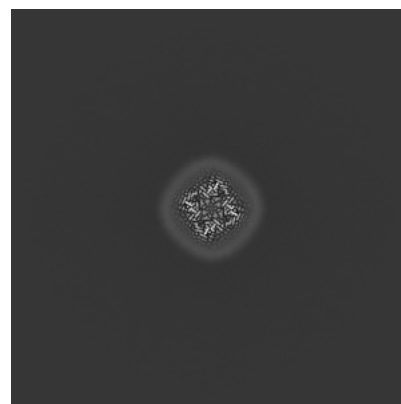
### 6.3.1 Primary map



X Index: 240

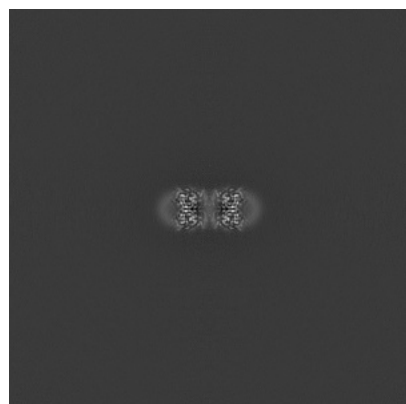


Y Index: 240

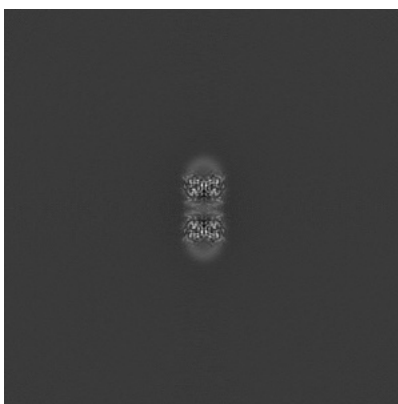


Z Index: 233

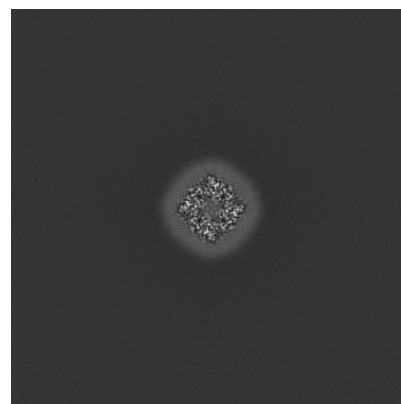
### 6.3.2 Raw map



X Index: 240



Y Index: 240

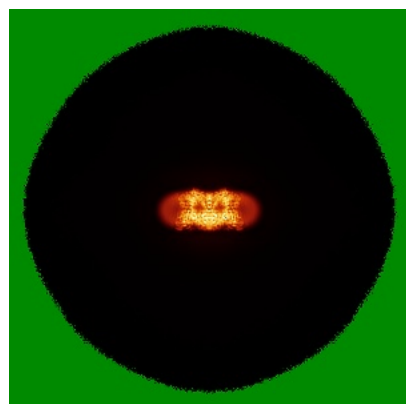


Z Index: 251

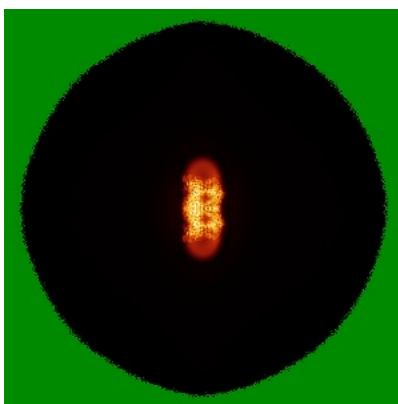
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

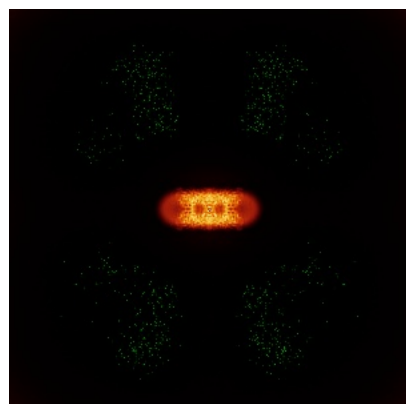


Y

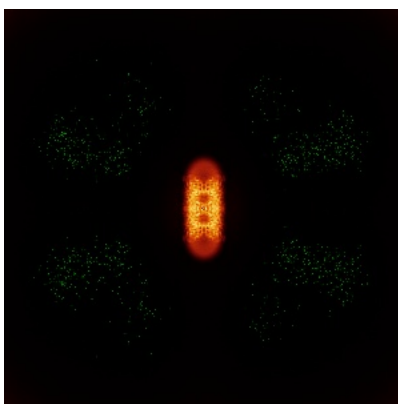


Z

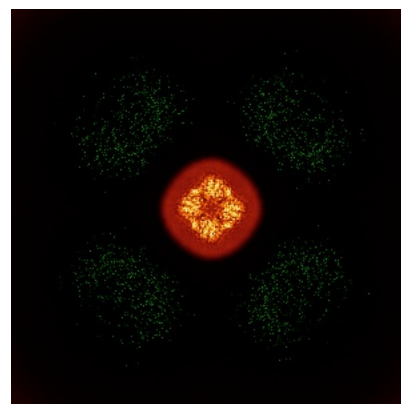
### 6.4.2 Raw map



X



Y

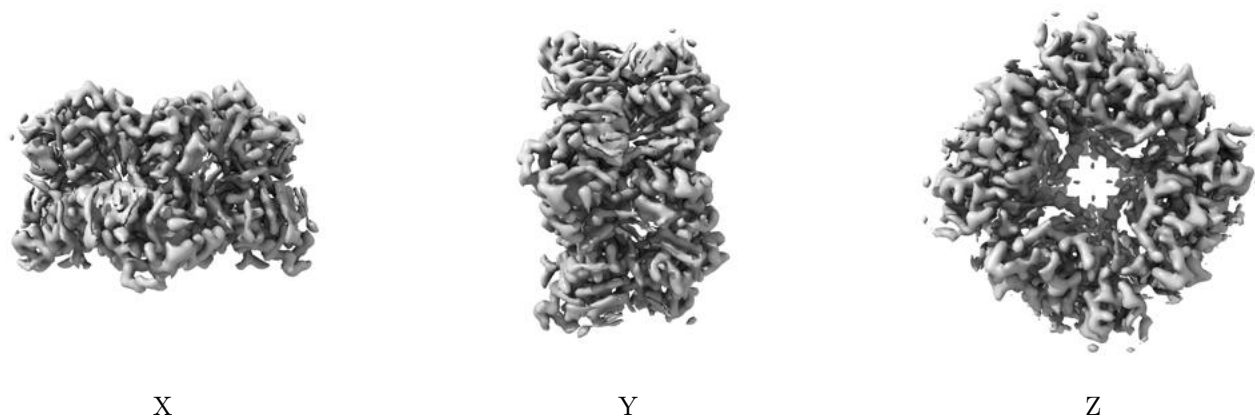


Z

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.

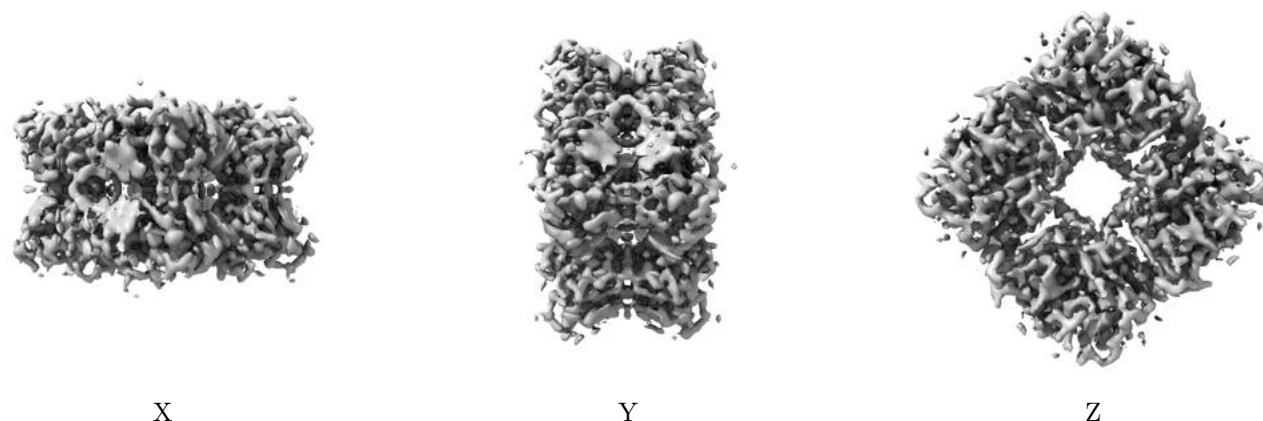
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. 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.

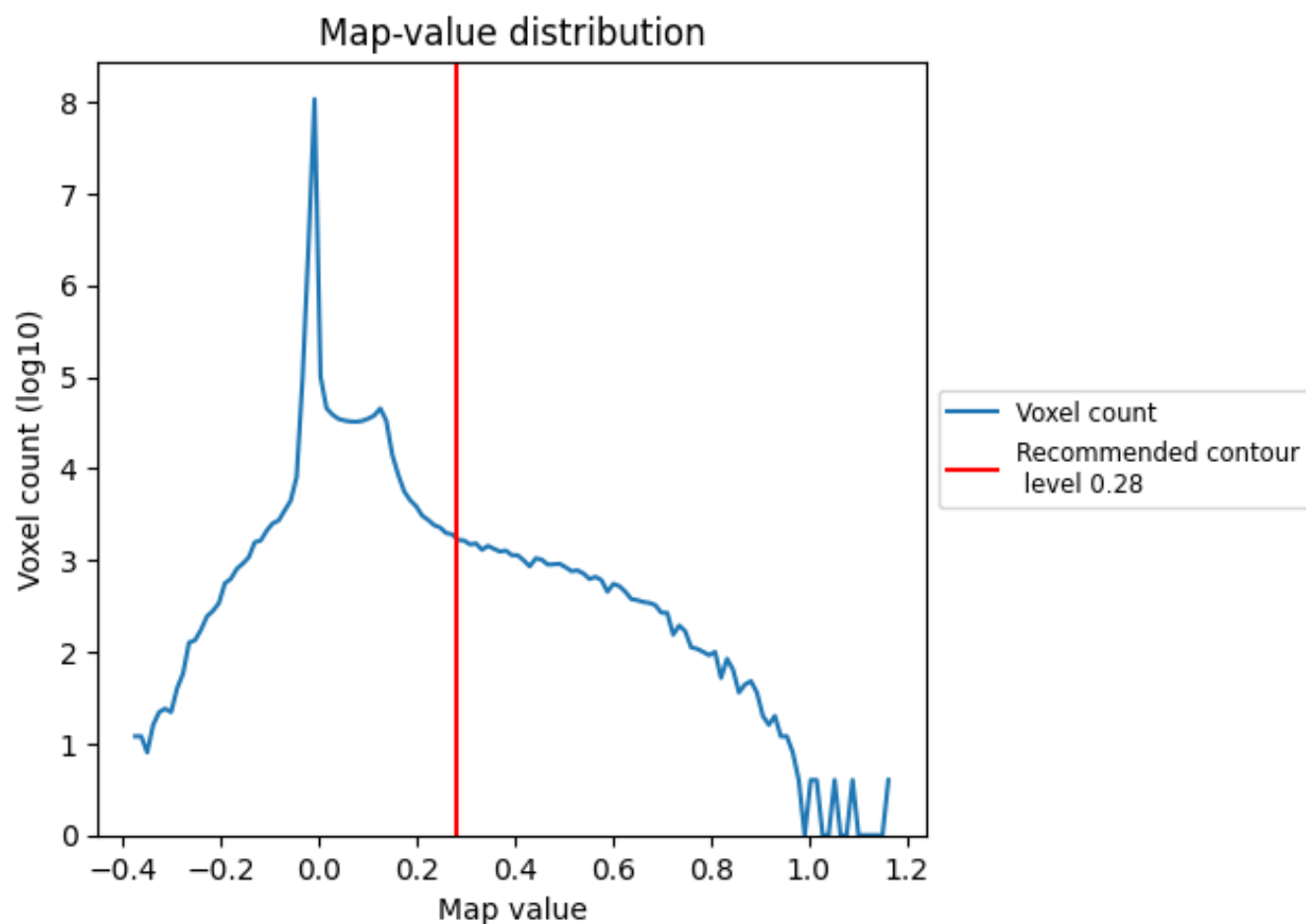
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

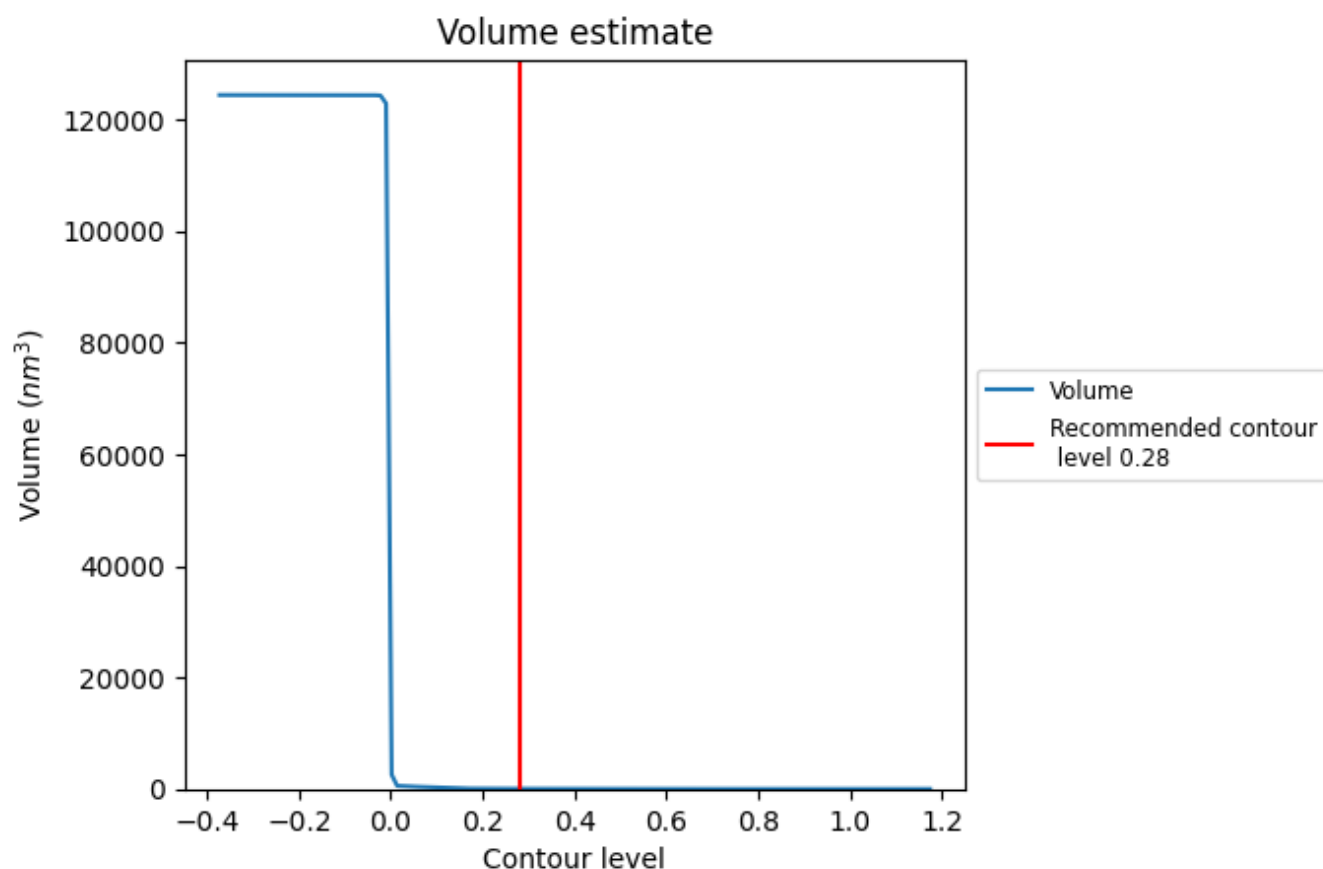
This section contains the results of statistical analysis of the map.

### 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.

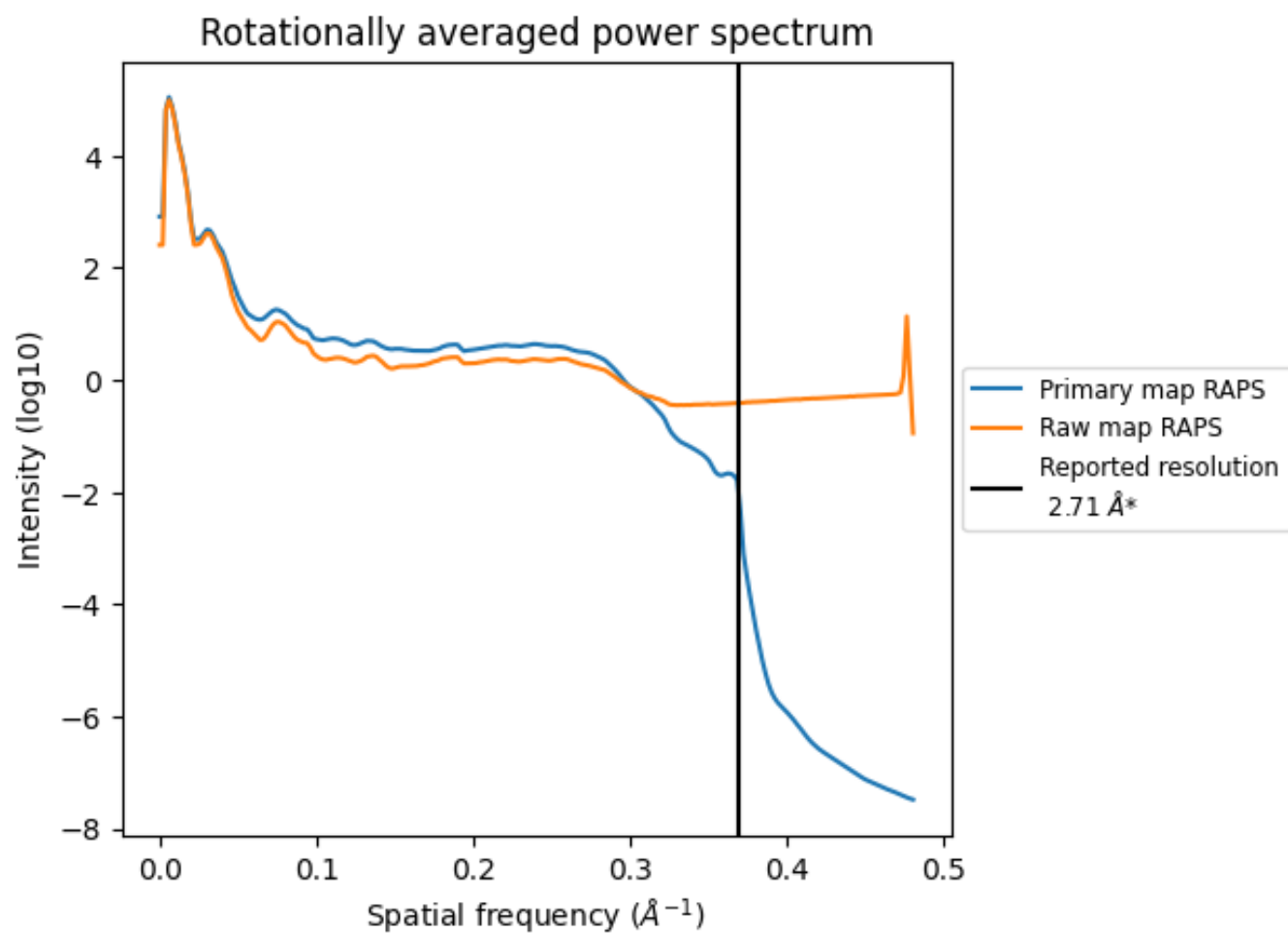
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38  $\text{nm}^3$ ; this corresponds to an approximate mass of 34 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 ⓘ

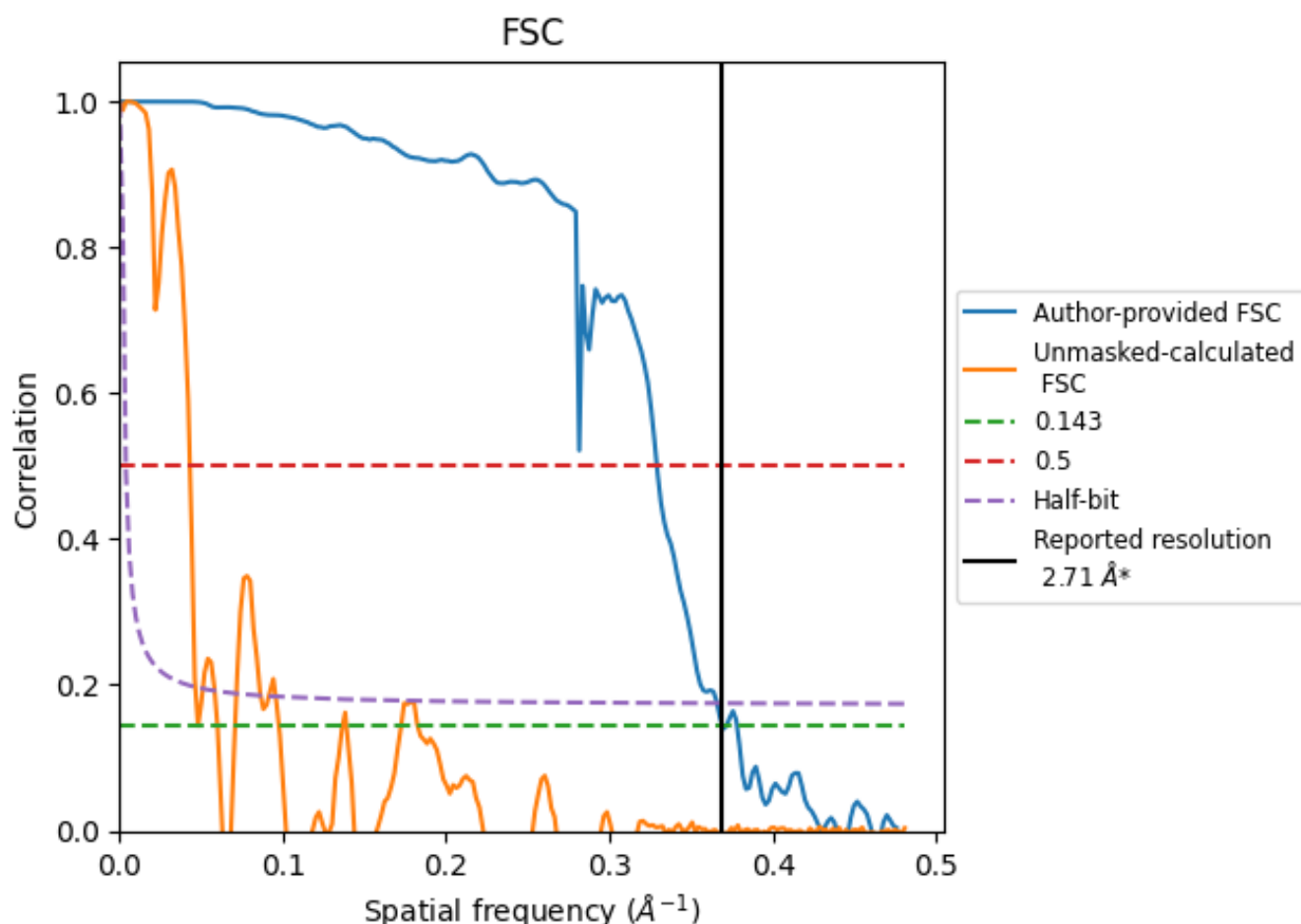


\*Reported resolution corresponds to spatial frequency of 0.369 Å<sup>-1</sup>

## 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 0.369  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.71	3.04	2.73
Unmasked-calculated*	16.67	23.20	21.55

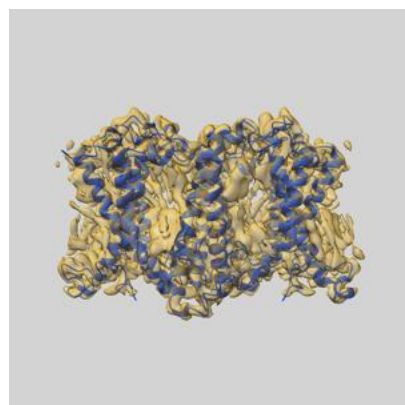
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 16.67 differs from the reported value 2.71 by more than 10 %



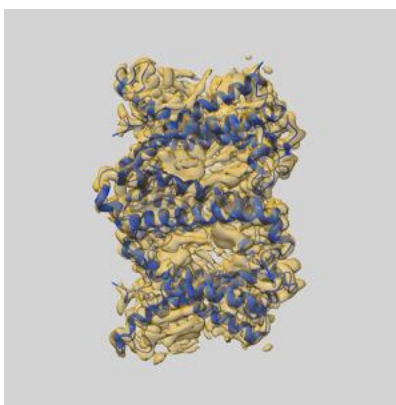
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37441 and PDB model 8WCK. Per-residue inclusion information can be found in section [3](#) on page [11](#).

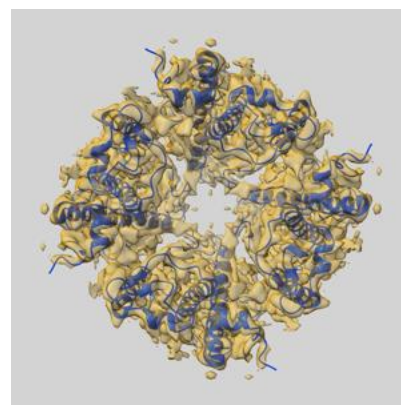
### 9.1 Map-model overlay [i](#)



X



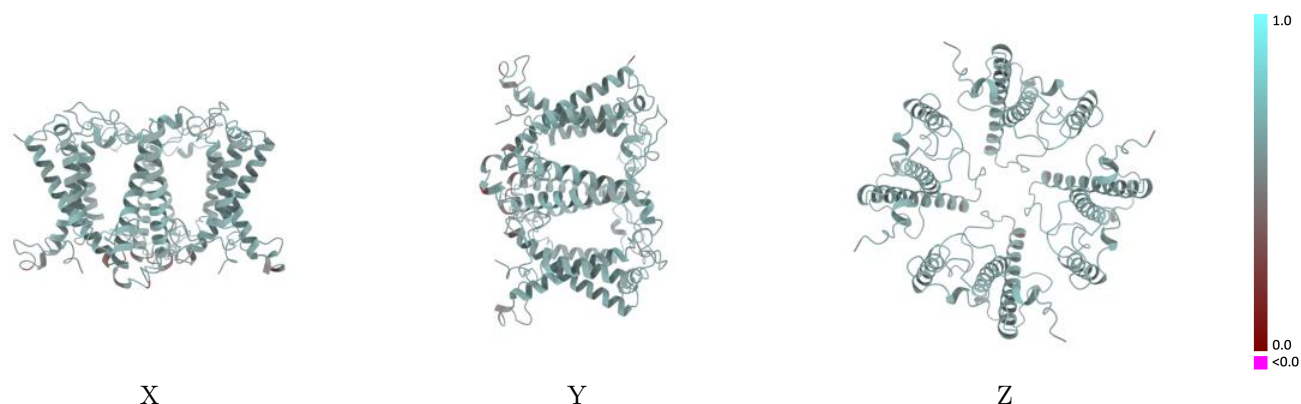
Y



Z

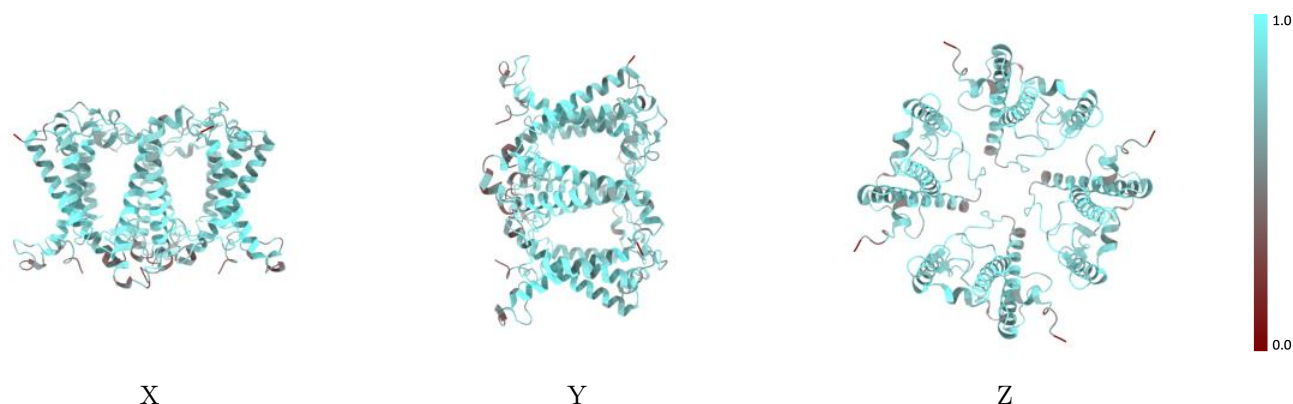
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



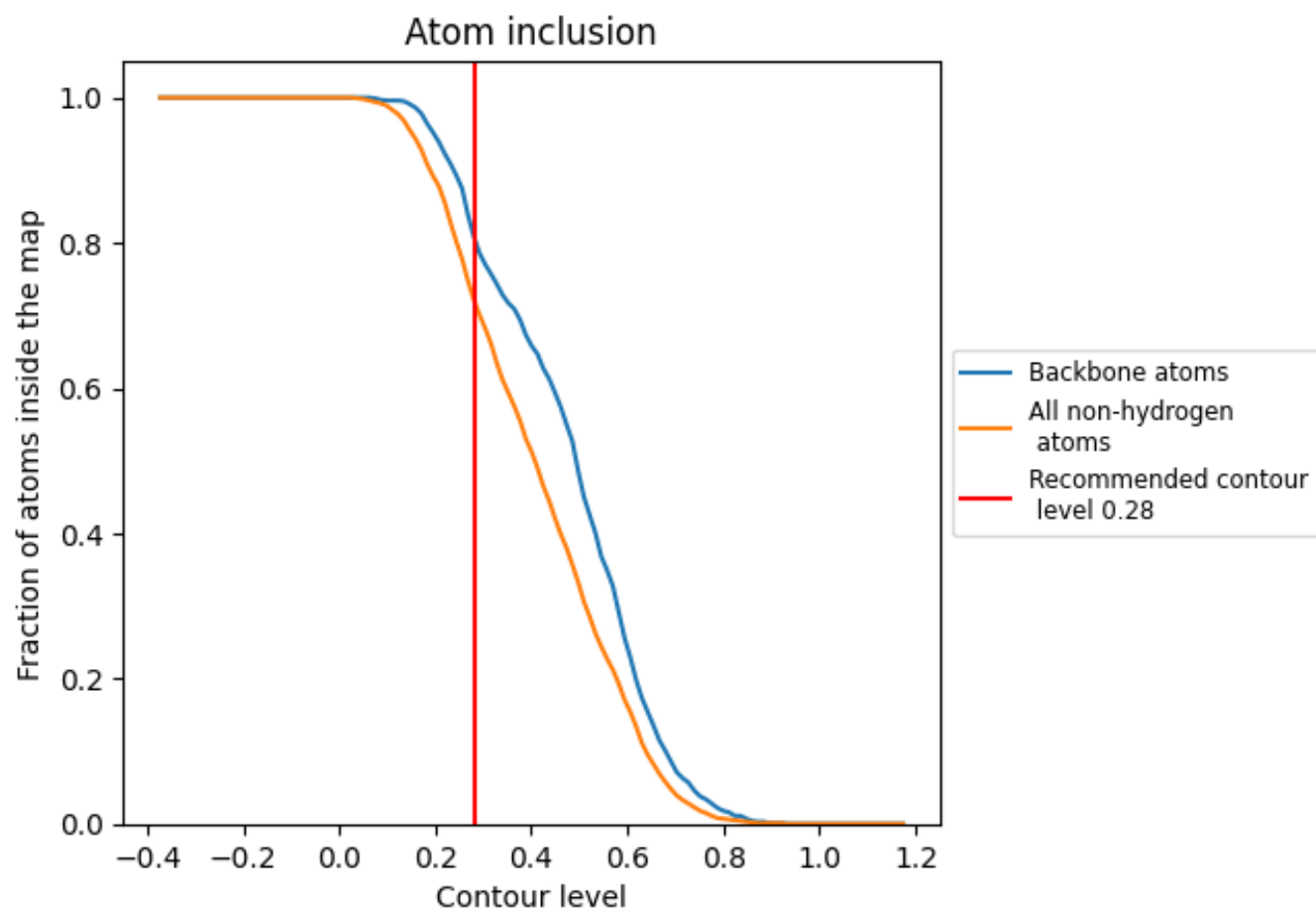
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 72% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7220	<div></div> 0.5860
1	<div></div> 0.7230	<div></div> 0.5840
2	<div></div> 0.7240	<div></div> 0.5860
3	<div></div> 0.7210	<div></div> 0.5860
4	<div></div> 0.7210	<div></div> 0.5860

