



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:00 AM BST

PDB ID : 6A2W  
Title : Crystal structure of fucoxanthin chlorophyll a/c complex from *Phaeodactylum tricornutum*  
Authors : Wang, W.; Yu, L.J.; Kuang, T.Y.; Shen, J.R.  
Deposited on : 2018-06-13  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

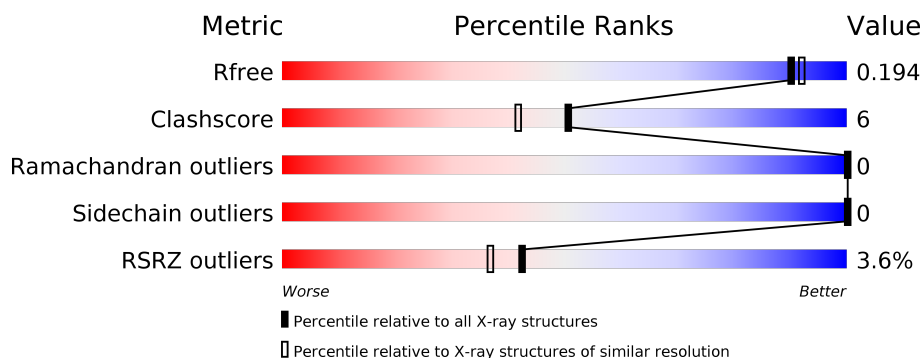
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	167	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>

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
5	CLA	A	401	X	-	-	-
5	CLA	A	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	A	404	X	-	-	-
5	CLA	A	405	X	-	-	-
5	CLA	A	406	X	-	-	-
5	CLA	A	407	X	-	-	-
5	CLA	A	409	X	-	-	-
8	LMT	A	410	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 2518 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

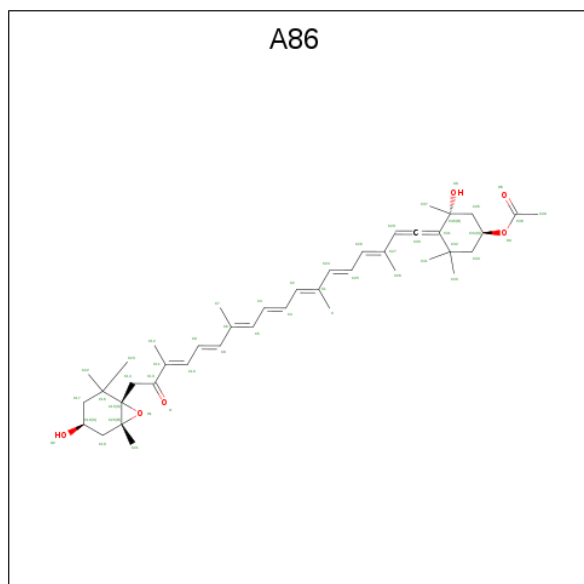
- Molecule 1 is a protein called Protein fucoxanthin chlorophyll a/c protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	3	0
			1308	847	216	241	4			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 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>).



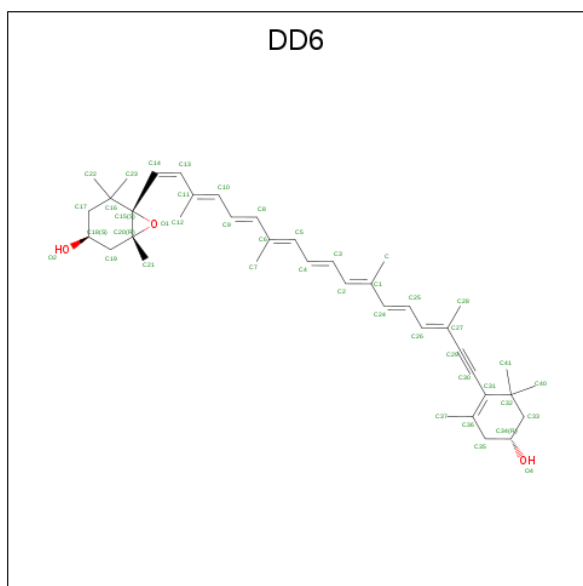
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			48	42	6		

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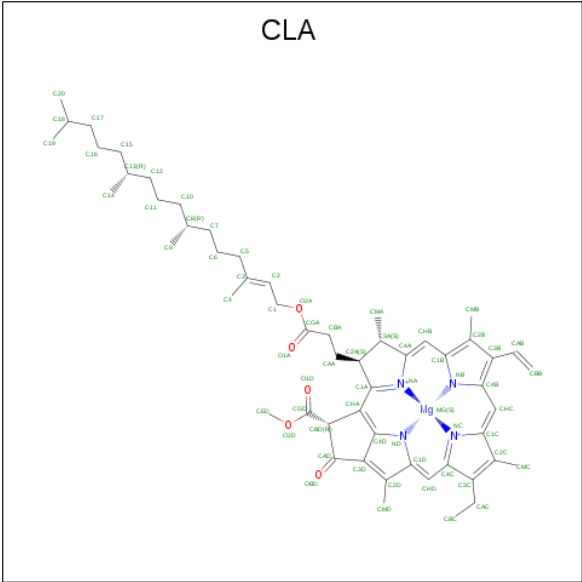
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		

- Molecule 4 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (three-letter code: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>).



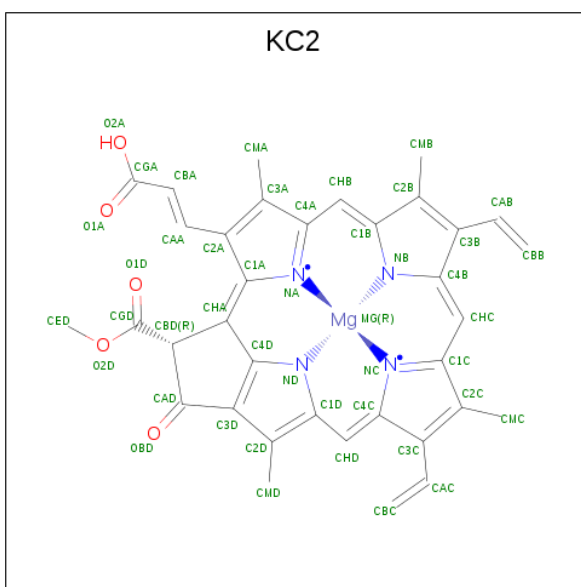
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			43	40	3		

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



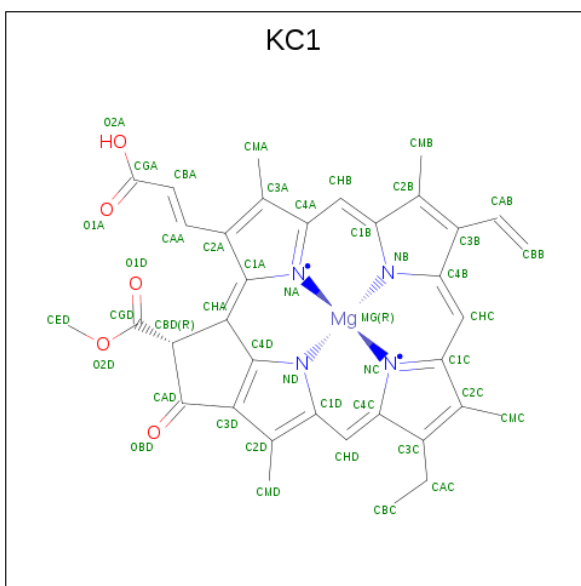
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		

- Molecule 6 is Chlorophyll c2 (three-letter code: KC2) (formula: C<sub>35</sub>H<sub>28</sub>MgN<sub>4</sub>O<sub>5</sub>).



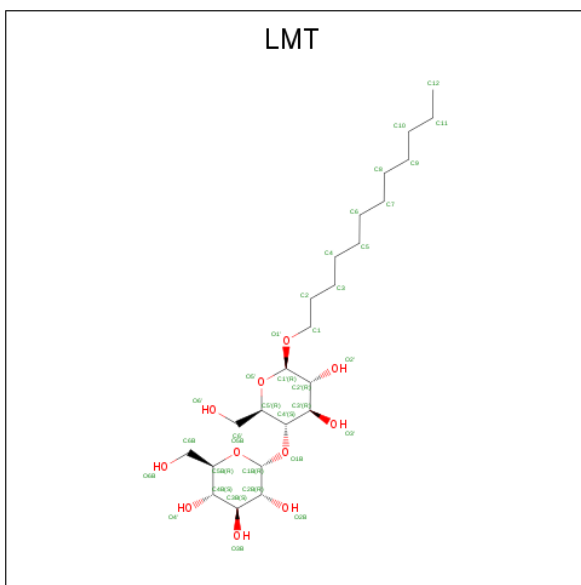
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 7 is Chlorophyll c1 (three-letter code: KC1) (formula:  $C_{35}H_{30}MgN_4O_5$ ).



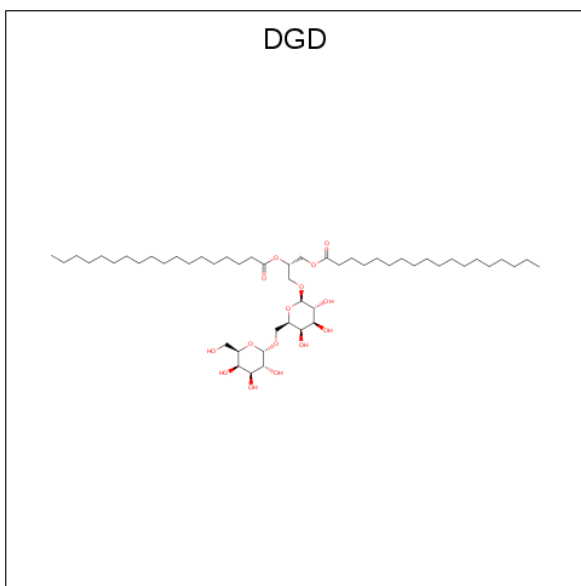
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 8 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			31	20	11		

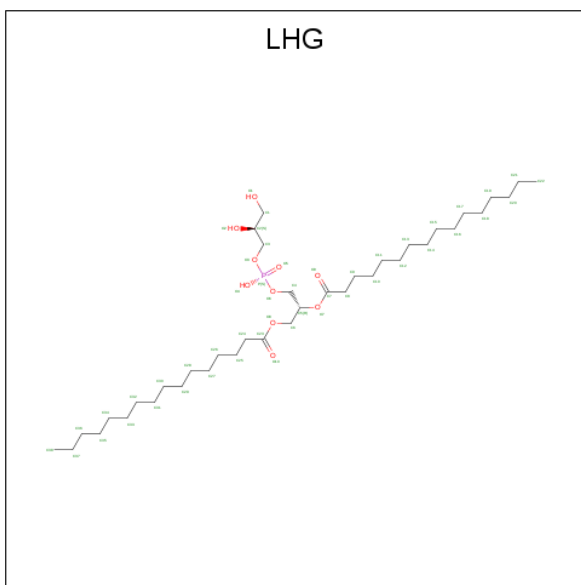
- Molecule 9 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			39	34	5		

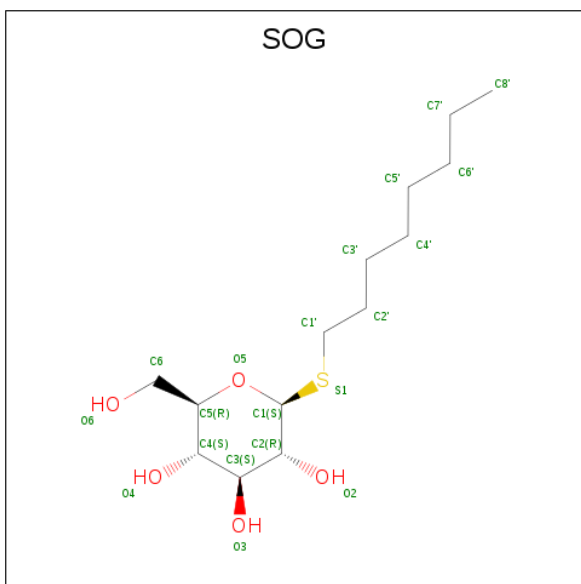
- Molecule 10 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	P	0	0
			33	24	8	1		

- Molecule 11 is octyl 1-thio-beta-D-glucopyranoside (three-letter code: SOG) (formula:  $C_{14}H_{28}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total 20	C 14	O 5	S 1	0	0
11	A	1	Total 20	C 14	O 5	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	S	0	0
			20	14	5	1		
11	A	1	Total	C	O	S	0	0
			15	9	5	1		

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	7	Total	C	0	0
			73	73		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	80	Total	O	0	0
			80	80		

### 3 Residue-property plots

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

- Molecule 1: Protein fucoxanthin chlorophyll a/c protein

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.75Å 115.72Å 141.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 1.80 19.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	67.0 (19.98-1.80) 67.0 (19.98-1.80)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.175 , 0.197 0.173 , 0.194	Depositor DCC
$R_{free}$ test set	1860 reflections (7.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 89.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, A86, DGD, SOG, CA, LMT, CLA, DD6, KC1, KC2, UNL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.43	0/1342	0.57	0/1811

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	A	1308	0	1297	9	0
2	A	2	0	0	0	0
3	A	336	0	0	1	0
4	A	43	0	0	0	0
5	A	408	0	411	17	0
6	A	45	0	0	0	0
7	A	45	0	0	0	0
8	A	31	0	35	0	0
9	A	39	0	62	4	0
10	A	33	0	42	1	0
11	A	75	0	99	4	0
12	A	73	0	0	0	0
13	A	80	0	0	1	0
All	All	2518	0	1946	25	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 (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:OD1	13:A:501:HOH:O	2.09	0.70
9:A:411:DGD:HA92	9:A:411:DGD:HBW2	1.76	0.68
5:A:401:CLA:HMB1	5:A:401:CLA:HBB1	1.85	0.57
1:A:91:LEU:HD23	5:A:405:CLA:HBC3	1.91	0.52
11:A:416:SOG:O6	11:A:416:SOG:S1	2.57	0.52
1:A:157:HIS:CE1	5:A:409:CLA:NA	2.78	0.52
9:A:411:DGD:HA51	9:A:411:DGD:HB61	1.92	0.51
5:A:406:CLA:H151	10:A:412:LHG:H132	1.92	0.50
5:A:409:CLA:HBD	11:A:413:SOG:H1	1.96	0.48
1:A:163:SER:O	11:A:414:SOG:H61	2.13	0.48
5:A:402:CLA:HMB1	5:A:402:CLA:HBB1	1.96	0.46
1:A:39:HIS:CE1	5:A:406:CLA:HMD1	2.52	0.45
1:A:91:LEU:HD23	5:A:405:CLA:CBC	2.47	0.45
5:A:406:CLA:H202	5:A:406:CLA:H161	1.79	0.44
5:A:402:CLA:H192	5:A:402:CLA:H161	1.81	0.44
9:A:411:DGD:HBT2	9:A:411:DGD:HA71	1.98	0.44
3:A:303:A86:C25	5:A:402:CLA:HMC2	2.47	0.44
1:A:162:VAL:HG21	5:A:409:CLA:HED3	2.01	0.42
9:A:411:DGD:HBE1	9:A:411:DGD:HBF1	1.40	0.42
5:A:404:CLA:H111	5:A:404:CLA:H91	1.67	0.42
5:A:409:CLA:CAA	11:A:413:SOG:H1'1	2.49	0.42
1:A:128:PHE:HB2	1:A:133:GLN:HG3	2.02	0.42
5:A:407:CLA:HMB1	5:A:407:CLA:HBB1	2.02	0.42
1:A:11:PRO:HD3	5:A:401:CLA:C4B	2.50	0.41
5:A:407:CLA:H111	5:A:407:CLA:H91	1.60	0.41

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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	167/167 (100%)	165 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/132 (102%)	134 (100%)	0	100	100

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

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 7 are unknown and 2 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	A86	A	303	-	44,50,50	1.15	3 (6%)	51,76,76	1.72	7 (13%)
9	DGD	A	411	-	38,38,67	0.68	1 (2%)	40,40,81	1.35	3 (7%)
4	DD6	A	308	-	39,45,45	2.24	4 (10%)	52,67,67	2.49	14 (26%)
3	A86	A	301	-	44,50,50	1.18	2 (4%)	51,76,76	2.34	18 (35%)
11	SOG	A	413	-	20,20,20	0.95	1 (5%)	24,25,25	1.03	1 (4%)
3	A86	A	302	-	44,50,50	1.13	2 (4%)	51,76,76	1.63	8 (15%)
11	SOG	A	414	-	20,20,20	1.13	1 (5%)	24,25,25	1.27	2 (8%)
5	CLA	A	401	13	55,69,73	1.33	3 (5%)	62,108,113	1.51	9 (14%)
5	CLA	A	409	-	35,49,73	1.76	6 (17%)	38,84,113	1.86	10 (26%)
11	SOG	A	415	-	20,20,20	0.91	1 (5%)	24,25,25	0.93	1 (4%)
3	A86	A	304	-	44,50,50	1.11	3 (6%)	51,76,76	1.69	10 (19%)
8	LMT	A	410	-	32,32,36	1.05	4 (12%)	43,43,47	1.48	4 (9%)
5	CLA	A	402	1	59,73,73	1.34	4 (6%)	67,113,113	1.65	11 (16%)
10	LHG	A	412	-	32,32,48	0.86	2 (6%)	36,37,54	1.63	4 (11%)
6	KC2	A	403	-	32,53,53	3.04	15 (46%)	23,89,89	4.00	12 (52%)
3	A86	A	306	-	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
7	KC1	A	408	1	33,53,53	2.65	14 (42%)	23,89,89	3.16	12 (52%)
5	CLA	A	406	1	59,73,73	1.38	4 (6%)	67,113,113	1.66	12 (17%)
5	CLA	A	404	1	59,73,73	1.34	3 (5%)	67,113,113	1.46	11 (16%)
11	SOG	A	416	-	15,15,20	1.11	1 (6%)	18,20,25	1.34	2 (11%)
3	A86	A	305	-	44,50,50	1.21	2 (4%)	51,76,76	2.23	8 (15%)
5	CLA	A	407	1	59,73,73	1.22	4 (6%)	67,113,113	1.50	13 (19%)
5	CLA	A	405	1	40,54,73	1.61	6 (15%)	44,90,113	1.98	15 (34%)
3	A86	A	307	-	44,50,50	1.10	2 (4%)	51,76,76	1.70	10 (19%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A86	A	303	-	-	2/34/90/90	0/3/3/3
9	DGD	A	411	-	-	25/40/40/95	-
4	DD6	A	308	-	-	9/26/80/80	0/3/3/3
3	A86	A	301	-	-	3/34/90/90	0/3/3/3
11	SOG	A	413	-	-	2/11/31/31	0/1/1/1
3	A86	A	302	-	-	4/34/90/90	0/3/3/3
11	SOG	A	414	-	-	5/11/31/31	0/1/1/1
3	A86	A	305	-	-	3/34/90/90	0/3/3/3
5	CLA	A	409	-	3/3/15/25	3/8/106/135	-
11	SOG	A	415	-	-	3/11/31/31	0/1/1/1
3	A86	A	304	-	-	0/34/90/90	0/3/3/3
8	LMT	A	410	-	-	9/17/57/61	0/2/2/2
5	CLA	A	402	1	3/3/20/25	12/37/135/135	-
10	LHG	A	412	-	-	16/34/34/53	-
6	KC2	A	403	-	-	0/9/71/71	-
3	A86	A	306	-	-	2/34/90/90	0/3/3/3
7	KC1	A	408	1	-	3/11/71/71	-
5	CLA	A	404	1	3/3/20/25	5/37/135/135	-
11	SOG	A	416	-	-	3/6/26/31	0/1/1/1
5	CLA	A	401	13	3/3/19/25	10/33/131/135	-
3	A86	A	307	-	-	3/34/90/90	0/3/3/3
5	CLA	A	407	1	3/3/20/25	12/37/135/135	-
5	CLA	A	406	1	3/3/20/25	5/37/135/135	-
5	CLA	A	405	1	3/3/16/25	5/15/113/135	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	308	DD6	C29-C27	-9.27	1.24	1.42
4	A	308	DD6	C30-C31	-7.95	1.25	1.42
5	A	406	CLA	C4B-NB	7.60	1.42	1.35
6	A	403	KC2	C4D-ND	7.55	1.41	1.35
5	A	409	CLA	C4B-NB	7.19	1.41	1.35
5	A	402	CLA	C4B-NB	7.15	1.41	1.35
5	A	401	CLA	C4B-NB	6.92	1.41	1.35
5	A	404	CLA	C4B-NB	6.69	1.41	1.35
5	A	405	CLA	C4B-NB	6.49	1.41	1.35
6	A	403	KC2	C2A-C3A	5.93	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	403	KC2	OBD-CAD	5.41	1.29	1.22
6	A	403	KC2	C3C-C2C	5.39	1.47	1.40
7	A	408	KC1	C4D-ND	5.34	1.40	1.35
7	A	408	KC1	C2A-C3A	5.33	1.47	1.40
7	A	408	KC1	C3B-C2B	5.31	1.47	1.40
5	A	407	CLA	C4B-NB	5.15	1.39	1.35
6	A	403	KC2	C3D-C2D	5.15	1.48	1.39
3	A	305	A86	O4-C38	5.09	1.46	1.35
3	A	301	A86	O4-C38	4.96	1.46	1.35
3	A	302	A86	O4-C38	4.84	1.46	1.35
7	A	408	KC1	C3D-C2D	4.79	1.48	1.39
6	A	403	KC2	C3B-C2B	4.73	1.46	1.40
6	A	403	KC2	O2D-CGD	4.61	1.44	1.33
3	A	306	A86	O4-C38	4.59	1.45	1.35
3	A	303	A86	O4-C38	4.43	1.45	1.35
7	A	408	KC1	C1A-CHA	4.40	1.46	1.38
3	A	306	A86	O1-C20	-4.31	1.40	1.46
11	A	414	SOG	C1'-S1	-4.30	1.75	1.81
7	A	408	KC1	OBD-CAD	4.30	1.28	1.22
3	A	307	A86	O4-C38	4.27	1.44	1.35
3	A	304	A86	O4-C38	4.21	1.44	1.35
6	A	403	KC2	C1A-CHA	4.20	1.46	1.38
7	A	408	KC1	O2D-CGD	4.13	1.43	1.33
11	A	413	SOG	C1'-S1	-3.74	1.76	1.81
3	A	306	A86	C30-C29	-3.66	1.25	1.32
11	A	416	SOG	C1'-S1	-3.50	1.77	1.81
5	A	404	CLA	C1B-NB	3.49	1.38	1.35
3	A	301	A86	C30-C29	-3.43	1.26	1.32
7	A	408	KC1	C4C-C3C	3.36	1.50	1.42
11	A	415	SOG	C1'-S1	-3.32	1.77	1.81
7	A	408	KC1	C1C-NC	-3.26	1.32	1.35
3	A	305	A86	C30-C29	-3.24	1.26	1.32
6	A	403	KC2	CBC-CAC	3.23	1.50	1.29
5	A	409	CLA	CHC-C1C	3.14	1.43	1.35
5	A	407	CLA	CHC-C1C	3.08	1.42	1.35
4	A	308	DD6	O1-C20	-3.06	1.41	1.46
5	A	402	CLA	CHC-C1C	3.00	1.42	1.35
7	A	408	KC1	C3C-C2C	2.94	1.46	1.37
3	A	306	A86	O1-C15	-2.94	1.40	1.45
7	A	408	KC1	C1B-C2B	2.93	1.49	1.42
5	A	405	CLA	CHC-C1C	2.89	1.42	1.35
3	A	303	A86	C30-C29	-2.78	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	403	KC2	C1B-C2B	2.76	1.48	1.42
5	A	402	CLA	C1D-C2D	2.76	1.48	1.42
6	A	403	KC2	C1D-CHD	2.73	1.48	1.41
7	A	408	KC1	C4D-CHA	2.71	1.48	1.45
5	A	401	CLA	CHC-C1C	2.69	1.41	1.35
3	A	307	A86	C30-C29	-2.69	1.27	1.32
5	A	407	CLA	C1D-C2D	2.63	1.48	1.42
5	A	404	CLA	CHC-C1C	2.62	1.41	1.35
3	A	306	A86	C13-C11	-2.60	1.44	1.49
5	A	405	CLA	C1D-C2D	2.58	1.48	1.42
5	A	409	CLA	C1D-C2D	2.56	1.48	1.42
3	A	302	A86	C30-C29	-2.56	1.27	1.32
6	A	403	KC2	C4D-CHA	2.54	1.48	1.45
5	A	405	CLA	CMB-C2B	-2.51	1.46	1.51
5	A	406	CLA	CHC-C1C	2.45	1.41	1.35
5	A	406	CLA	C1D-C2D	2.40	1.48	1.42
5	A	405	CLA	CMD-C2D	-2.34	1.46	1.51
7	A	408	KC1	C1D-CHD	2.33	1.47	1.41
3	A	303	A86	C13-C11	-2.30	1.45	1.49
4	A	308	DD6	C26-C27	-2.26	1.32	1.37
6	A	403	KC2	C1C-NC	-2.23	1.33	1.35
3	A	306	A86	C17-C18	-2.23	1.49	1.52
3	A	304	A86	C30-C29	-2.20	1.28	1.32
5	A	409	CLA	CMB-C2B	-2.19	1.47	1.51
8	A	410	LMT	O3'-C3'	-2.19	1.37	1.43
3	A	306	A86	C2-C1	-2.18	1.32	1.35
3	A	306	A86	C17-C16	-2.17	1.51	1.54
8	A	410	LMT	O2'-C2'	-2.14	1.37	1.43
7	A	408	KC1	C4A-CHB	2.13	1.46	1.41
5	A	405	CLA	C3B-C2B	-2.12	1.37	1.40
8	A	410	LMT	O3B-C3B	-2.10	1.38	1.43
5	A	406	CLA	CMB-C2B	-2.09	1.47	1.51
9	A	411	DGD	O2G-C2G	-2.09	1.41	1.46
5	A	402	CLA	CMB-C2B	-2.07	1.47	1.51
5	A	409	CLA	CMD-C2D	-2.07	1.46	1.51
5	A	401	CLA	C1D-C2D	2.06	1.47	1.42
10	A	412	LHG	P-O3	2.06	1.62	1.54
3	A	304	A86	C13-C11	-2.06	1.45	1.49
8	A	410	LMT	O4'-C4B	-2.04	1.38	1.43
10	A	412	LHG	P-O6	2.03	1.66	1.60
5	A	409	CLA	C3B-CAB	-2.03	1.43	1.47
6	A	403	KC2	C4A-CHB	2.01	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	403	KC2	C1C-CHC	2.01	1.46	1.41
5	A	407	CLA	O2A-CGA	2.00	1.39	1.33

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	306	A86	C17-C16-C15	10.05	119.41	109.16
3	A	305	A86	O1-C20-C19	-9.71	106.09	113.38
6	A	403	KC2	OBD-CAD-CBD	9.21	139.06	125.89
6	A	403	KC2	OBD-CAD-C3D	-7.68	115.23	127.98
6	A	403	KC2	C4C-C3C-C2C	-7.05	101.98	106.90
7	A	408	KC1	OBD-CAD-C3D	-6.92	116.49	127.98
4	A	308	DD6	O1-C20-C19	6.87	118.54	113.38
6	A	403	KC2	CMD-C2D-C1D	-6.70	118.16	128.46
5	A	402	CLA	C4A-NA-C1A	6.63	109.69	106.71
3	A	305	A86	O4-C38-C39	6.40	122.87	111.09
4	A	308	DD6	C21-C20-C19	6.39	121.47	114.28
5	A	406	CLA	C4A-NA-C1A	6.37	109.57	106.71
6	A	403	KC2	CMD-C2D-C3D	6.21	136.30	124.68
3	A	303	A86	O1-C20-C19	-6.11	108.79	113.38
7	A	408	KC1	CMD-C2D-C3D	5.85	135.63	124.68
5	A	409	CLA	C4A-NA-C1A	5.79	109.31	106.71
10	A	412	LHG	O4-P-O5	5.78	133.30	110.68
5	A	404	CLA	C4A-NA-C1A	5.77	109.30	106.71
4	A	308	DD6	C21-C20-C15	-5.72	112.68	122.26
3	A	301	A86	O1-C20-C19	-5.65	109.14	113.38
3	A	303	A86	O4-C38-C39	5.50	121.21	111.09
8	A	410	LMT	O5B-C5B-C4B	5.48	119.65	109.69
3	A	301	A86	C36-C31-C32	5.45	125.10	119.70
3	A	306	A86	O4-C38-C39	5.40	121.02	111.09
7	A	408	KC1	CMD-C2D-C1D	-5.26	120.38	128.46
4	A	308	DD6	C4-C5-C6	-5.24	119.83	127.31
3	A	307	A86	C17-C16-C15	5.24	114.51	109.16
7	A	408	KC1	OBD-CAD-CBD	5.21	133.33	125.89
5	A	401	CLA	C4A-NA-C1A	5.20	109.05	106.71
3	A	301	A86	O4-C38-C39	5.01	120.31	111.09
3	A	301	A86	C17-C16-C15	4.96	114.22	109.16
6	A	403	KC2	C4B-C3B-C2B	-4.88	103.49	106.90
5	A	405	CLA	C4A-NA-C1A	4.87	108.89	106.71
3	A	302	A86	C17-C16-C15	4.81	114.07	109.16
4	A	308	DD6	C8-C6-C5	4.76	126.24	118.94
3	A	301	A86	O1-C15-C14	-4.54	104.10	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	A86	O4-C38-C39	4.50	119.38	111.09
10	A	412	LHG	O3-P-O6	-4.49	94.77	106.73
3	A	305	A86	C17-C16-C15	4.47	113.72	109.16
4	A	308	DD6	C29-C30-C31	-4.46	164.12	175.43
3	A	304	A86	C17-C16-C15	4.36	113.61	109.16
3	A	307	A86	O4-C38-C39	4.35	119.09	111.09
3	A	302	A86	O1-C20-C19	-4.33	110.13	113.38
3	A	302	A86	O4-C38-C39	4.32	119.04	111.09
5	A	401	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
5	A	402	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
3	A	305	A86	C25-C26-C27	-4.10	121.46	127.31
7	A	408	KC1	C4B-C3B-C2B	-4.08	104.05	106.90
3	A	306	A86	C34-O4-C38	-4.08	110.30	117.90
4	A	308	DD6	C3-C2-C1	-4.07	121.50	127.31
7	A	408	KC1	C1A-C2A-CAA	4.01	135.00	126.97
5	A	405	CLA	CAC-C3C-C4C	4.00	130.00	124.81
11	A	416	SOG	C1-O5-C5	3.99	119.95	112.58
9	A	411	DGD	O3G-C3G-C2G	-3.99	101.21	111.78
5	A	405	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
3	A	304	A86	O1-C20-C19	-3.94	110.42	113.38
5	A	402	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
5	A	409	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
3	A	301	A86	C33-C32-C31	3.85	112.96	109.21
5	A	402	CLA	CMB-C2B-C3B	3.79	131.76	124.68
3	A	301	A86	C3-C2-C1	-3.77	121.93	127.31
5	A	406	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
6	A	403	KC2	CGA-CBA-CAA	-3.70	115.79	123.69
5	A	407	CLA	CMB-C2B-C3B	3.69	131.58	124.68
11	A	414	SOG	C1-O5-C5	3.68	119.36	112.58
3	A	307	A86	O1-C15-C14	-3.64	105.90	113.21
5	A	401	CLA	CMB-C2B-C3B	3.64	131.48	124.68
3	A	306	A86	O1-C15-C14	-3.60	105.98	113.21
5	A	407	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
5	A	409	CLA	CMB-C2B-C3B	3.53	131.28	124.68
5	A	406	CLA	CAC-C3C-C4C	3.47	129.31	124.81
6	A	403	KC2	O2D-CGD-CBD	3.44	117.39	111.27
5	A	406	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
3	A	301	A86	O1-C20-C21	-3.41	110.97	115.06
4	A	308	DD6	C10-C9-C8	-3.39	112.65	123.22
3	A	305	A86	O4-C38-O5	-3.37	116.27	122.96
5	A	405	CLA	CMB-C2B-C3B	3.34	130.93	124.68
7	A	408	KC1	O2D-CGD-O1D	-3.32	117.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	408	KC1	O2D-CGD-CBD	3.28	117.09	111.27
7	A	408	KC1	CGA-CBA-CAA	-3.26	116.72	123.69
8	A	410	LMT	C1B-O5B-C5B	3.24	120.05	113.69
3	A	302	A86	O1-C20-C21	-3.23	111.18	115.06
4	A	308	DD6	C25-C26-C27	-3.22	117.23	126.58
5	A	409	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
4	A	308	DD6	C14-C13-C11	-3.21	120.56	125.53
5	A	406	CLA	C4D-C3D-CAD	-3.16	106.71	108.47
5	A	407	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
8	A	410	LMT	O5'-C5'-C4'	3.13	116.35	109.75
4	A	308	DD6	C33-C32-C31	-3.09	103.35	109.62
3	A	304	A86	C25-C26-C27	-3.06	122.94	127.31
4	A	308	DD6	C7-C6-C5	-3.06	118.64	122.92
3	A	303	A86	O4-C38-O5	-3.05	116.90	122.96
5	A	405	CLA	CAA-C2A-C1A	3.04	121.95	111.97
5	A	405	CLA	C2A-C1A-CHA	3.03	129.16	123.86
5	A	402	CLA	O2D-CGD-CBD	3.00	116.60	111.27
3	A	307	A86	C14-C15-C16	2.98	130.18	118.75
5	A	407	CLA	O2A-CGA-O1A	-2.98	116.07	123.59
5	A	401	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
5	A	402	CLA	C1-C2-C3	2.95	131.14	126.04
5	A	407	CLA	C4A-NA-C1A	2.92	108.02	106.71
5	A	401	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
3	A	304	A86	C3-C4-C5	-2.92	117.50	123.47
5	A	404	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
5	A	406	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
3	A	301	A86	C4-C5-C6	-2.89	123.18	127.31
5	A	405	CLA	CHB-C4A-NA	2.89	128.51	124.51
11	A	414	SOG	O5-C5-C6	2.88	113.59	106.44
5	A	407	CLA	C5-C3-C2	2.88	126.94	121.12
5	A	407	CLA	C4-C3-C2	-2.87	116.32	123.68
5	A	401	CLA	O2A-CGA-O1A	-2.86	116.36	123.59
5	A	402	CLA	O2A-CGA-O1A	-2.85	116.39	123.59
3	A	301	A86	C41-C32-C31	-2.84	107.93	110.47
3	A	303	A86	C17-C16-C15	2.83	112.05	109.16
5	A	406	CLA	CMB-C2B-C3B	2.83	129.97	124.68
5	A	407	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
3	A	304	A86	O1-C20-C21	-2.82	111.68	115.06
3	A	307	A86	O4-C38-O5	-2.81	117.38	122.96
3	A	307	A86	C25-C26-C27	-2.80	123.32	127.31
5	A	404	CLA	CHB-C4A-NA	2.79	128.37	124.51
3	A	306	A86	C-C1-C2	-2.77	119.04	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	A86	C25-C26-C27	-2.76	123.38	127.31
5	A	407	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
4	A	308	DD6	C12-C11-C10	-2.75	119.08	122.92
3	A	304	A86	O1-C15-C14	-2.74	107.71	113.21
5	A	402	CLA	C1D-CHD-C4C	2.74	126.18	122.56
5	A	406	CLA	CMD-C2D-C3D	2.73	129.78	124.68
10	A	412	LHG	O8-C23-C24	2.71	120.41	111.91
5	A	406	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
5	A	405	CLA	CBA-CAA-C2A	-2.68	105.95	113.86
5	A	402	CLA	C1-O2A-CGA	2.68	123.47	116.44
5	A	405	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
11	A	413	SOG	O5-C1-C2	-2.63	107.00	110.31
3	A	301	A86	O4-C38-O5	-2.63	117.74	122.96
3	A	306	A86	C28-C27-C26	-2.62	119.25	122.92
6	A	403	KC2	CMA-C3A-C2A	2.62	129.57	124.68
5	A	405	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
7	A	408	KC1	CMA-C3A-C4A	-2.60	124.46	128.46
5	A	407	CLA	C1-O2A-CGA	-2.58	109.67	116.44
5	A	401	CLA	OBD-CAD-CBD	-2.55	122.25	125.89
3	A	303	A86	C10-C9-C8	-2.52	115.34	123.22
3	A	306	A86	O4-C34-C33	2.52	113.87	107.59
3	A	307	A86	O1-C20-C21	-2.52	112.04	115.06
5	A	409	CLA	CHB-C4A-NA	2.52	127.99	124.51
3	A	306	A86	C23-C16-C17	-2.51	104.62	108.98
3	A	301	A86	C14-C15-C16	2.49	128.28	118.75
3	A	306	A86	O4-C38-O5	-2.49	118.02	122.96
3	A	306	A86	C14-C15-C16	2.48	128.25	118.75
3	A	306	A86	C3-C2-C1	-2.48	123.77	127.31
5	A	402	CLA	CHB-C4A-NA	2.45	127.91	124.51
5	A	404	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
3	A	303	A86	C3-C2-C1	-2.44	123.83	127.31
3	A	301	A86	C34-O4-C38	-2.42	113.39	117.90
5	A	405	CLA	CAC-C3C-C2C	-2.41	123.41	127.53
11	A	415	SOG	O5-C1-C2	-2.40	107.29	110.31
3	A	302	A86	C4-C5-C6	-2.38	123.91	127.31
5	A	405	CLA	CMD-C2D-C3D	2.38	129.13	124.68
3	A	301	A86	C40-C32-C31	-2.37	108.35	110.47
6	A	403	KC2	CMC-C2C-C3C	2.37	129.11	124.68
3	A	306	A86	C41-C32-C31	-2.37	108.35	110.47
6	A	403	KC2	CMA-C3A-C4A	-2.36	124.83	128.46
3	A	304	A86	C4-C5-C6	-2.34	123.97	127.31
3	A	306	A86	C20-C19-C18	2.33	117.37	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	307	A86	C19-C18-C17	-2.33	106.27	110.77
5	A	405	CLA	C1D-CHD-C4C	2.33	125.63	122.56
3	A	301	A86	C26-C25-C24	-2.32	115.98	123.22
5	A	406	CLA	O1D-CGD-CBD	2.31	129.22	124.48
5	A	401	CLA	O1D-CGD-CBD	2.31	129.21	124.48
3	A	305	A86	C10-C9-C8	-2.29	116.08	123.22
5	A	409	CLA	CMD-C2D-C3D	2.28	128.95	124.68
5	A	404	CLA	OBD-CAD-CBD	-2.28	122.63	125.89
6	A	403	KC2	O2D-CGD-O1D	-2.28	119.38	123.84
4	A	308	DD6	C40-C32-C31	2.27	114.08	110.47
5	A	404	CLA	O1D-CGD-CBD	2.26	129.11	124.48
5	A	407	CLA	CHB-C4A-NA	2.23	127.59	124.51
3	A	307	A86	C4-C5-C6	-2.23	124.13	127.31
3	A	303	A86	C25-C26-C27	-2.22	124.14	127.31
3	A	301	A86	C21-C20-C19	-2.22	111.79	114.28
5	A	407	CLA	CHA-C1A-NA	-2.21	121.33	126.40
3	A	302	A86	O4-C38-O5	-2.20	118.60	122.96
5	A	404	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
7	A	408	KC1	C1C-C2C-C3C	-2.19	105.47	107.00
3	A	304	A86	O4-C38-O5	-2.18	118.64	122.96
3	A	307	A86	C10-C9-C8	-2.17	116.44	123.22
3	A	304	A86	C10-C9-C8	-2.16	116.47	123.22
3	A	306	A86	C25-C26-C27	-2.15	124.24	127.31
3	A	306	A86	O1-C20-C21	-2.15	112.48	115.06
5	A	404	CLA	C1-C2-C3	-2.15	122.33	126.04
8	A	410	LMT	C1-O1'-C1'	2.14	117.39	113.84
5	A	406	CLA	CHB-C4A-NA	2.14	127.47	124.51
3	A	305	A86	O1-C15-C14	-2.13	108.93	113.21
3	A	306	A86	O1-C15-C20	-2.13	57.32	59.40
11	A	416	SOG	O5-C1-C2	2.13	112.99	110.31
5	A	409	CLA	CAA-C2A-C3A	-2.12	111.14	116.10
5	A	405	CLA	OBD-CAD-CBD	-2.12	122.86	125.89
10	A	412	LHG	C11-C10-C9	-2.11	103.71	114.42
5	A	401	CLA	CMD-C2D-C3D	2.10	128.61	124.68
3	A	302	A86	C10-C9-C8	-2.10	116.66	123.22
3	A	305	A86	C3-C4-C5	-2.09	119.19	123.47
5	A	404	CLA	CMD-C2D-C3D	2.09	128.59	124.68
3	A	306	A86	O1-C20-C19	2.09	114.95	113.38
5	A	405	CLA	CHA-C1A-NA	-2.07	121.66	126.40
7	A	408	KC1	CMA-C3A-C2A	2.07	128.54	124.68
5	A	404	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
5	A	409	CLA	C4D-C3D-CAD	-2.06	107.32	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	A86	C3-C4-C5	-2.05	119.27	123.47
5	A	404	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
9	A	411	DGD	C1G-C2G-C3G	-2.05	107.00	111.80
5	A	409	CLA	C1D-CHD-C4C	2.04	125.25	122.56
5	A	402	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
5	A	407	CLA	C1D-CHD-C4C	2.02	125.23	122.56
5	A	409	CLA	OBD-CAD-CBD	-2.02	123.00	125.89
3	A	302	A86	C25-C26-C27	-2.02	124.43	127.31
9	A	411	DGD	CDB-CCB-CBB	-2.02	104.18	114.42
5	A	406	CLA	OBD-CAD-CBD	-2.02	123.01	125.89

All (21) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	401	CLA	NC
5	A	401	CLA	ND
5	A	401	CLA	NA
5	A	409	CLA	NC
5	A	409	CLA	ND
5	A	409	CLA	NA
5	A	402	CLA	NC
5	A	402	CLA	ND
5	A	402	CLA	NA
5	A	404	CLA	NC
5	A	404	CLA	ND
5	A	404	CLA	NA
5	A	407	CLA	NC
5	A	407	CLA	ND
5	A	407	CLA	NA
5	A	406	CLA	NC
5	A	406	CLA	ND
5	A	406	CLA	NA
5	A	405	CLA	NC
5	A	405	CLA	ND
5	A	405	CLA	NA

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	308	DD6	C-C1-C24-C25
4	A	308	DD6	C2-C1-C24-C25
4	A	308	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
4	A	308	DD6	C12-C11-C13-C14
4	A	308	DD6	C5-C6-C8-C9
4	A	308	DD6	C7-C6-C8-C9
3	A	301	A86	O5-C38-O4-C34
3	A	302	A86	C-C1-C24-C25
11	A	414	SOG	O5-C1-S1-C1'
5	A	401	CLA	C2-C3-C5-C6
5	A	401	CLA	C4-C3-C5-C6
11	A	415	SOG	C2-C1-S1-C1'
11	A	415	SOG	O5-C1-S1-C1'
8	A	410	LMT	C2'-C1'-O1'-C1
8	A	410	LMT	O5'-C1'-O1'-C1
5	A	402	CLA	O2A-C1-C2-C3
10	A	412	LHG	C4-O6-P-O3
10	A	412	LHG	C4-O6-P-O5
7	A	408	KC1	C1A-C2A-CAA-CBA
7	A	408	KC1	C3A-C2A-CAA-CBA
11	A	416	SOG	O5-C1-S1-C1'
5	A	407	CLA	C1A-C2A-CAA-CBA
5	A	405	CLA	C1A-C2A-CAA-CBA
3	A	301	A86	C39-C38-O4-C34
3	A	302	A86	C39-C38-O4-C34
3	A	306	A86	C39-C38-O4-C34
3	A	305	A86	C39-C38-O4-C34
3	A	307	A86	C39-C38-O4-C34
3	A	306	A86	O5-C38-O4-C34
3	A	303	A86	C39-C38-O4-C34
3	A	305	A86	O5-C38-O4-C34
3	A	307	A86	O5-C38-O4-C34
3	A	303	A86	O5-C38-O4-C34
5	A	402	CLA	O1A-CGA-O2A-C1
10	A	412	LHG	O10-C23-O8-C6
5	A	406	CLA	O1A-CGA-O2A-C1
3	A	302	A86	O5-C38-O4-C34
5	A	405	CLA	CBA-CGA-O2A-C1
5	A	405	CLA	O1A-CGA-O2A-C1
10	A	412	LHG	C24-C23-O8-C6
5	A	402	CLA	C3-C5-C6-C7
5	A	402	CLA	CBA-CGA-O2A-C1
5	A	406	CLA	CBA-CGA-O2A-C1
5	A	404	CLA	C8-C10-C11-C12
5	A	407	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	A	402	CLA	C6-C7-C8-C9
5	A	407	CLA	C11-C10-C8-C9
5	A	409	CLA	CBD-CGD-O2D-CED
8	A	410	LMT	C4B-C5B-C6B-O6B
8	A	410	LMT	O5'-C5'-C6'-O6'
5	A	402	CLA	C5-C6-C7-C8
5	A	407	CLA	C8-C10-C11-C12
5	A	405	CLA	C2C-C3C-CAC-CBC
5	A	404	CLA	C11-C12-C13-C15
9	A	411	DGD	C1B-C2B-C3B-C4B
5	A	407	CLA	C5-C6-C7-C8
11	A	416	SOG	C4-C5-C6-O6
5	A	407	CLA	O1A-CGA-O2A-C1
11	A	414	SOG	C1'-C2'-C3'-C4'
5	A	406	CLA	C15-C16-C17-C18
10	A	412	LHG	C15-C16-C17-C18
9	A	411	DGD	C7B-C8B-C9B-CAB
9	A	411	DGD	CDB-CEB-CFB-CGB
5	A	402	CLA	C15-C16-C17-C18
10	A	412	LHG	C17-C18-C19-C20
9	A	411	DGD	C8B-C9B-CAB-CBB
5	A	404	CLA	C11-C12-C13-C14
9	A	411	DGD	C9B-CAB-CBB-CCB
9	A	411	DGD	C9A-CAA-CBA-CCA
8	A	410	LMT	C2-C3-C4-C5
9	A	411	DGD	C6A-C7A-C8A-C9A
9	A	411	DGD	C3B-C4B-C5B-C6B
9	A	411	DGD	C4B-C5B-C6B-C7B
9	A	411	DGD	C5A-C6A-C7A-C8A
10	A	412	LHG	C11-C10-C9-C8
9	A	411	DGD	C2B-C1B-O2G-C2G
10	A	412	LHG	C8-C7-O7-C5
9	A	411	DGD	C4A-C5A-C6A-C7A
5	A	401	CLA	C11-C12-C13-C14
5	A	405	CLA	C4C-C3C-CAC-CBC
5	A	402	CLA	C1A-C2A-CAA-CBA
11	A	416	SOG	O5-C5-C6-O6
5	A	402	CLA	C13-C15-C16-C17
5	A	407	CLA	C10-C11-C12-C13
10	A	412	LHG	C11-C12-C13-C14
8	A	410	LMT	C2B-C1B-O1B-C4'
9	A	411	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
5	A	409	CLA	O1D-CGD-O2D-CED
5	A	401	CLA	C11-C12-C13-C15
10	A	412	LHG	C24-C25-C26-C27
8	A	410	LMT	O5B-C5B-C6B-O6B
11	A	414	SOG	C4'-C5'-C6'-C7'
9	A	411	DGD	CBB-CCB-CDB-CEB
3	A	301	A86	O-C13-C14-C15
3	A	305	A86	O-C13-C14-C15
11	A	413	SOG	C5'-C6'-C7'-C8'
5	A	404	CLA	C11-C10-C8-C9
5	A	407	CLA	C11-C12-C13-C14
9	A	411	DGD	C6B-C7B-C8B-C9B
3	A	302	A86	C2-C1-C24-C25
11	A	414	SOG	C3'-C4'-C5'-C6'
5	A	402	CLA	C6-C7-C8-C10
5	A	407	CLA	C11-C12-C13-C15
11	A	415	SOG	S1-C1'-C2'-C3'
9	A	411	DGD	O2G-C2G-C3G-O3G
5	A	406	CLA	C13-C15-C16-C17
7	A	408	KC1	CAD-CBD-CGD-O2D
5	A	404	CLA	CAD-CBD-CGD-O2D
9	A	411	DGD	O1G-C1G-C2G-C3G
9	A	411	DGD	O1G-C1G-C2G-O2G
4	A	308	DD6	C24-C25-C26-C27
10	A	412	LHG	C23-C24-C25-C26
9	A	411	DGD	CEB-CFB-CGB-CHB
9	A	411	DGD	CCB-CDB-CEB-CFB
9	A	411	DGD	C3A-C4A-C5A-C6A
10	A	412	LHG	C13-C14-C15-C16
5	A	402	CLA	C16-C17-C18-C19
5	A	401	CLA	O1D-CGD-O2D-CED
3	A	307	A86	C33-C34-O4-C38
11	A	413	SOG	C4'-C5'-C6'-C7'
5	A	406	CLA	C6-C7-C8-C9
5	A	407	CLA	C15-C16-C17-C18
5	A	401	CLA	C11-C10-C8-C7
4	A	308	DD6	C11-C10-C9-C8
4	A	308	DD6	C3-C4-C5-C6
9	A	411	DGD	C1G-C2G-C3G-O3G
11	A	414	SOG	C5'-C6'-C7'-C8'
10	A	412	LHG	C12-C13-C14-C15
5	A	407	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	409	CLA	CAD-CBD-CGD-O2D
9	A	411	DGD	C5B-C6B-C7B-C8B
5	A	401	CLA	CHA-CBD-CGD-O1D
5	A	401	CLA	CHA-CBD-CGD-O2D
8	A	410	LMT	O5B-C1B-O1B-C4'
10	A	412	LHG	O7-C7-C8-C9
10	A	412	LHG	C16-C17-C18-C19
5	A	407	CLA	C11-C10-C8-C7
10	A	412	LHG	O9-C7-C8-C9
9	A	411	DGD	C8A-C9A-CAA-CBA
5	A	401	CLA	CAD-CBD-CGD-O1D
5	A	402	CLA	CAA-CBA-CGA-O2A
5	A	401	CLA	CBD-CGD-O2D-CED
8	A	410	LMT	C2-C1-O1'-C1'
9	A	411	DGD	O1A-C1A-C2A-C3A

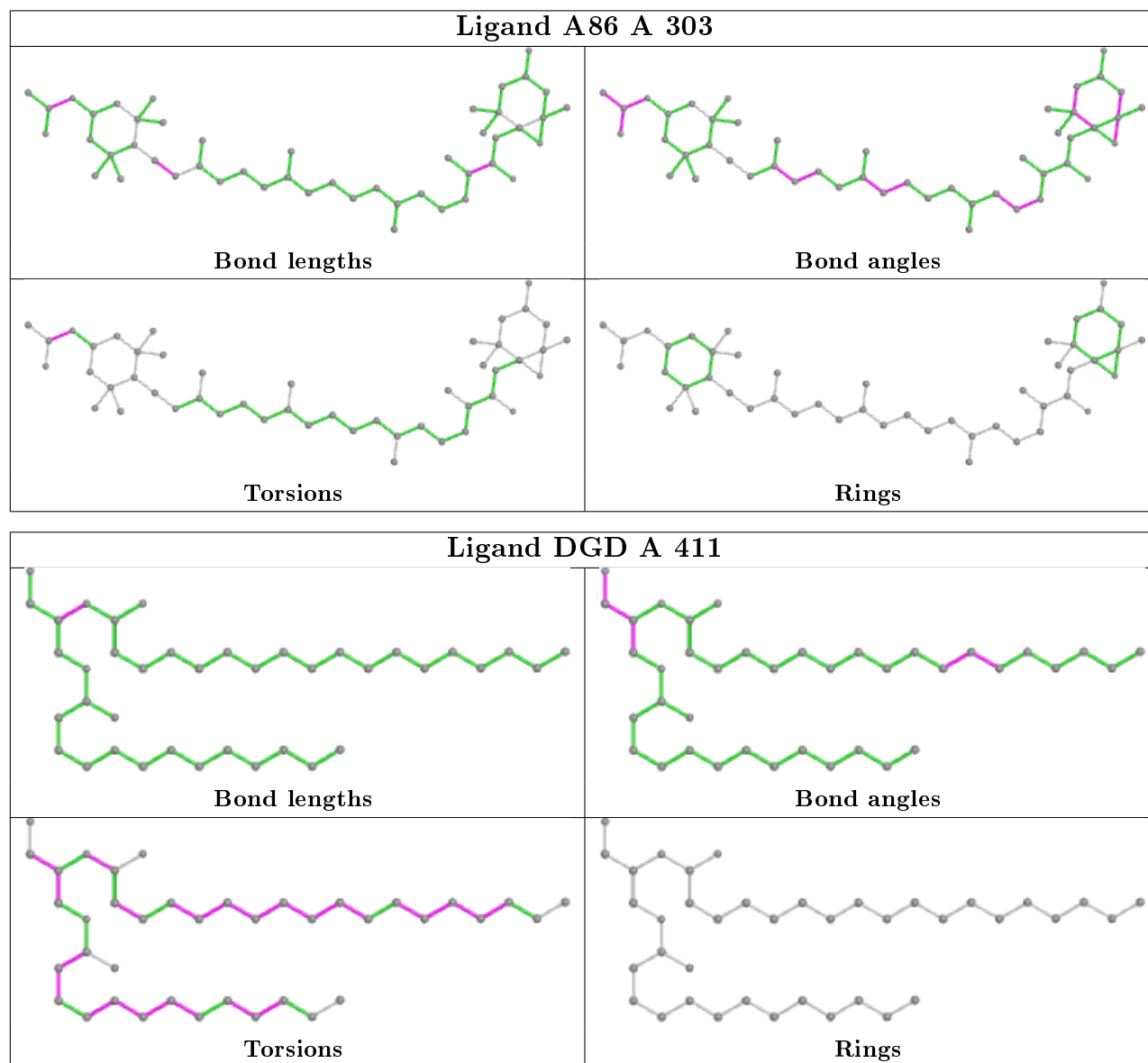
There are no ring outliers.

13 monomers are involved in 23 short contacts:

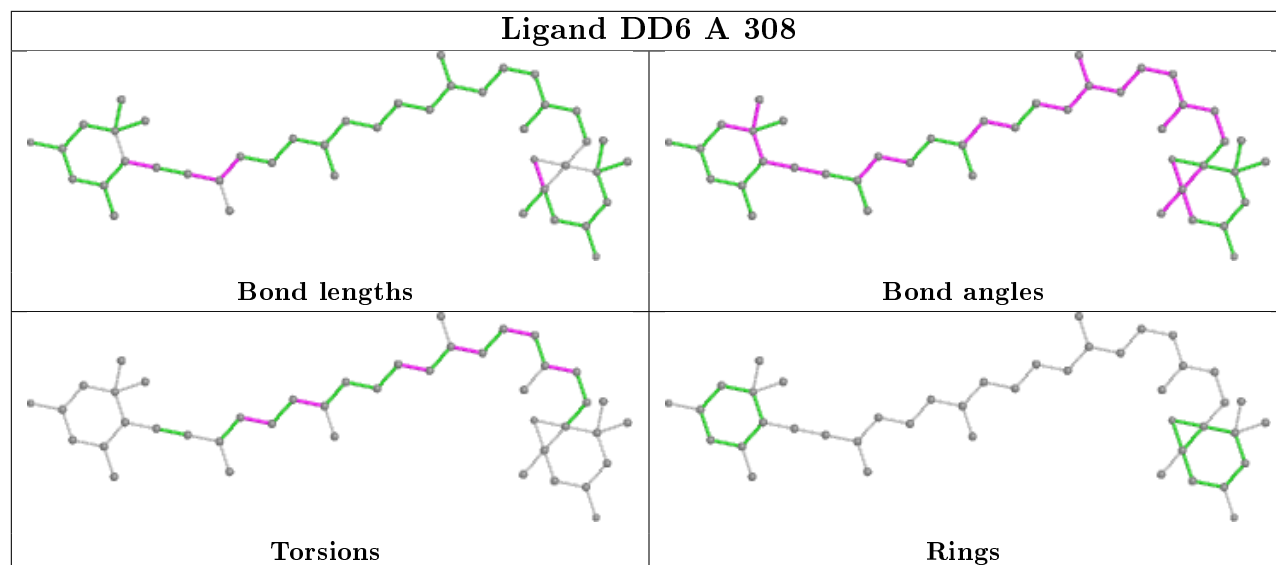
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	A86	1	0
9	A	411	DGD	4	0
11	A	413	SOG	2	0
11	A	414	SOG	1	0
5	A	401	CLA	2	0
5	A	409	CLA	4	0
5	A	402	CLA	3	0
10	A	412	LHG	1	0
5	A	406	CLA	3	0
5	A	404	CLA	1	0
11	A	416	SOG	1	0
5	A	407	CLA	2	0
5	A	405	CLA	2	0

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

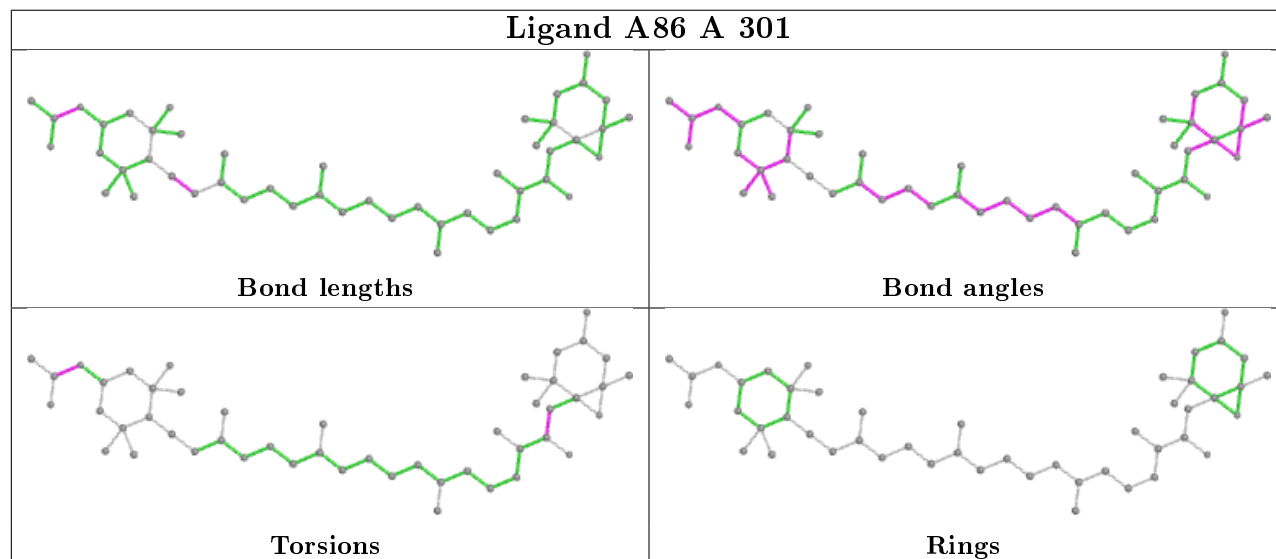
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



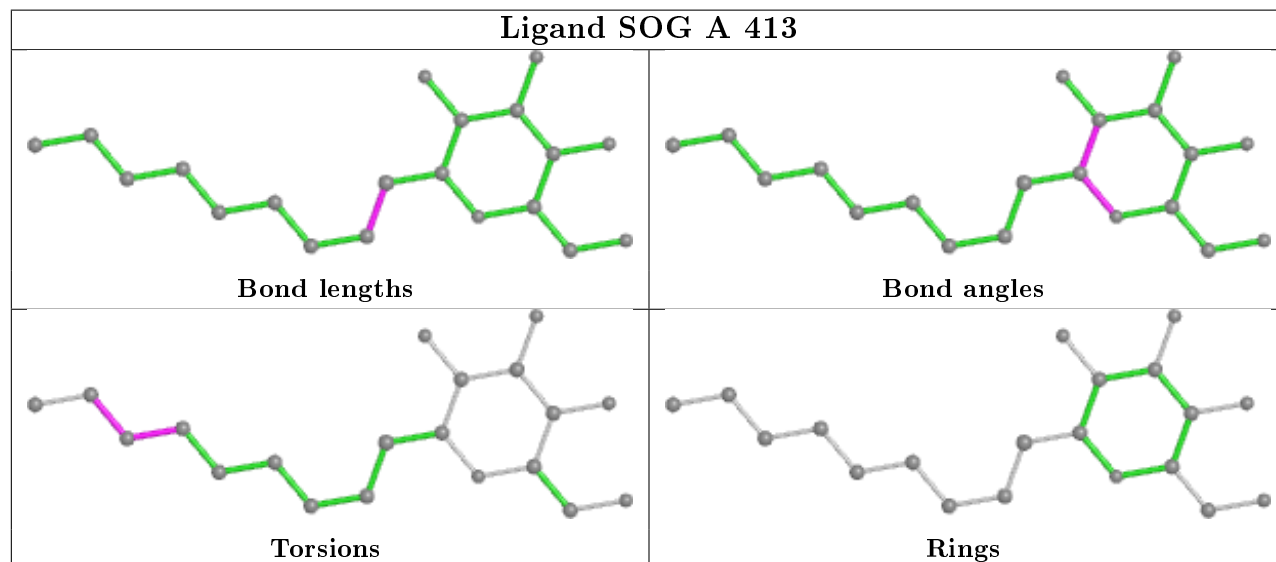
## Ligand DD6 A 308



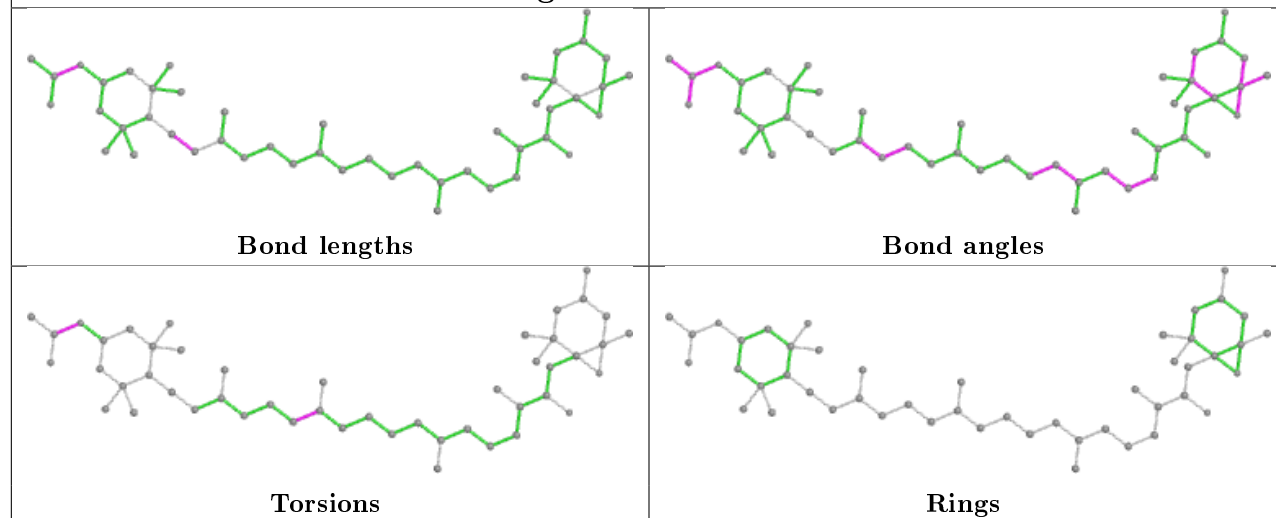
## Ligand A86 A 301



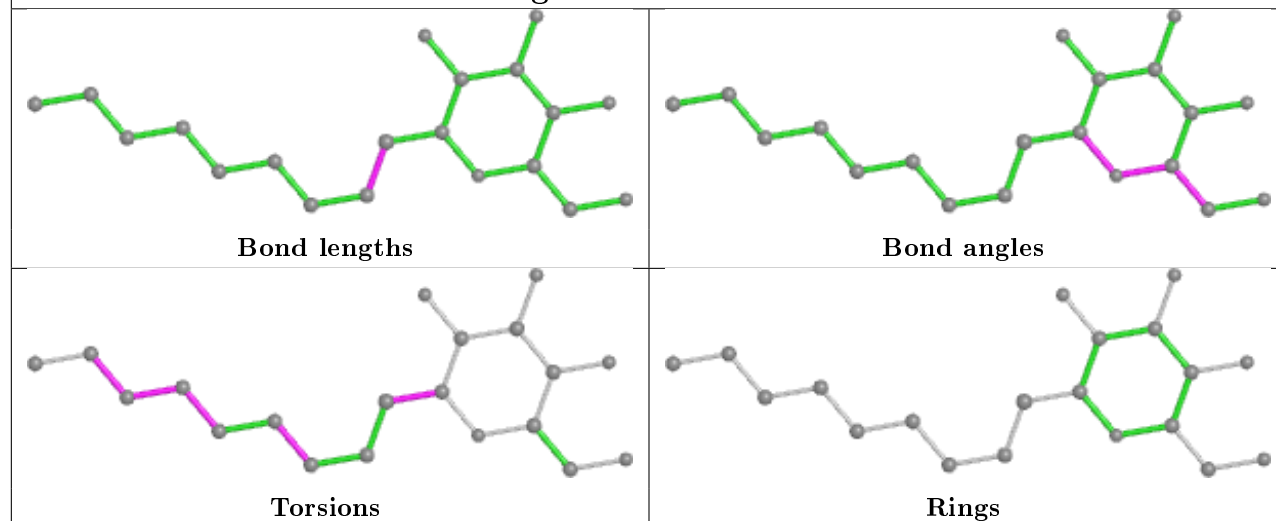
## Ligand SOG A 413



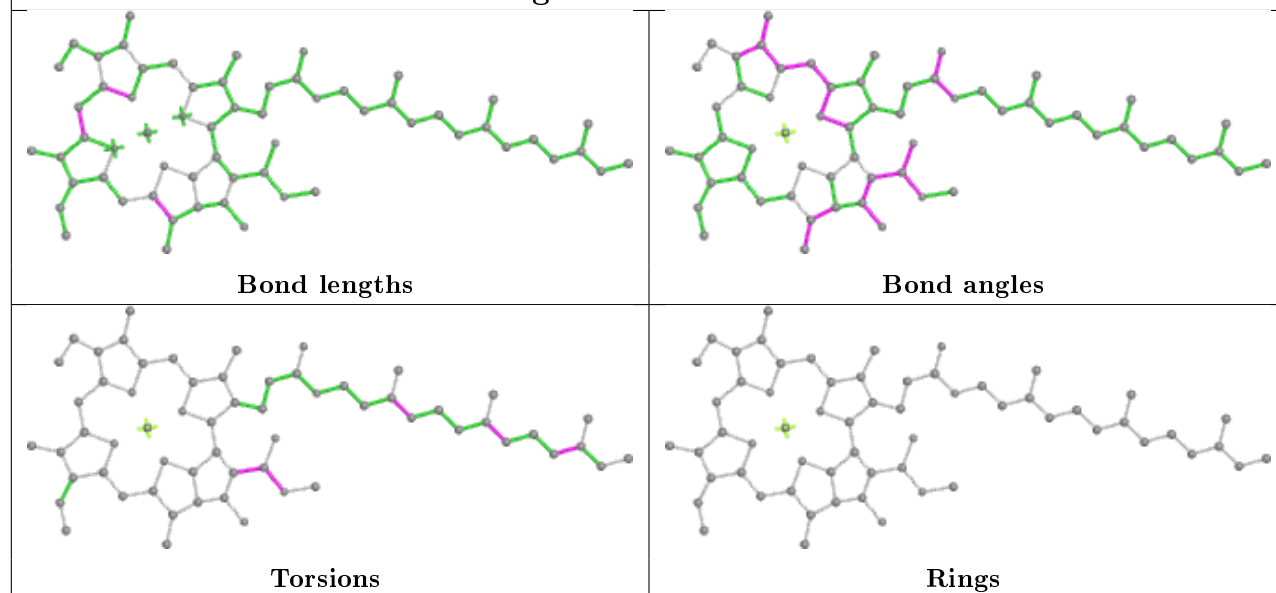
## Ligand A86 A 302



## Ligand SOG A 414

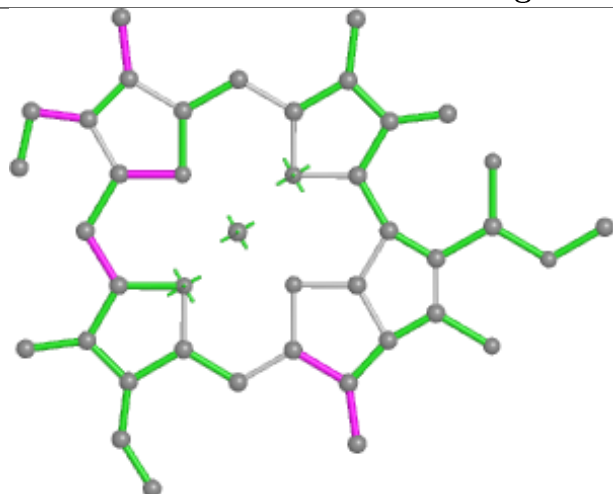


## Ligand CLA A 401

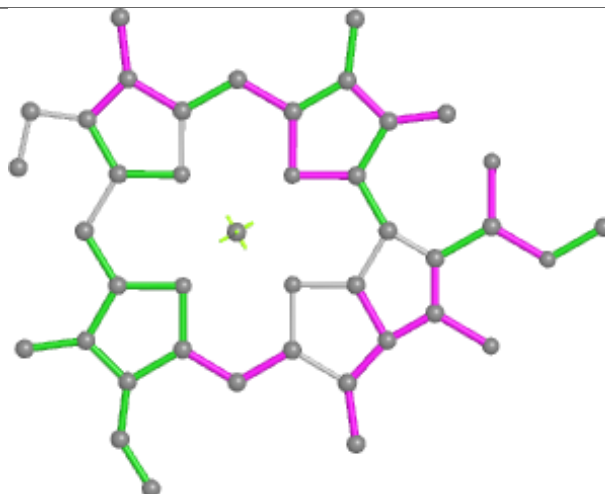




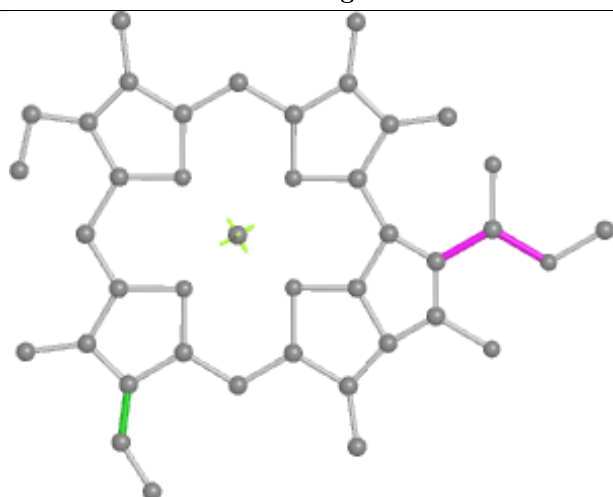
## Ligand CLA A 409



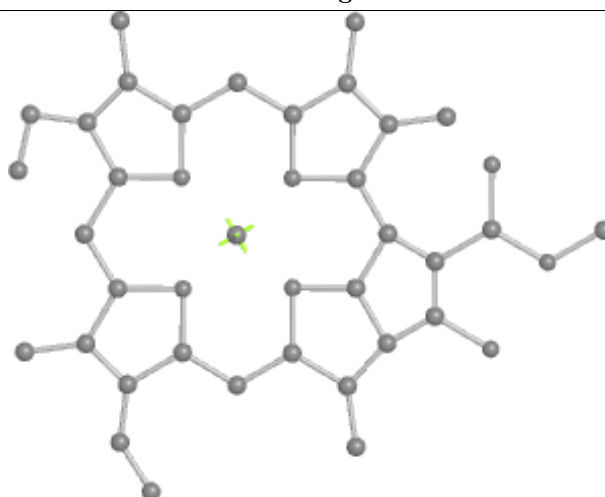
Bond lengths



Bond angles

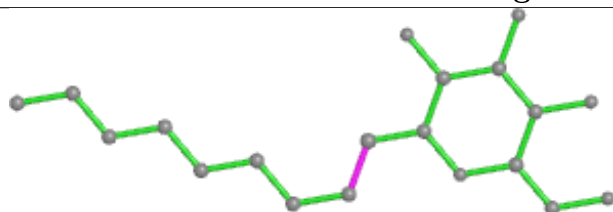


Torsions

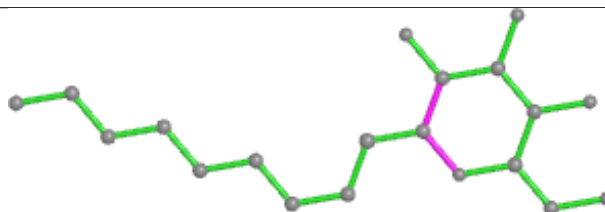


Rings

## Ligand SOG A 415



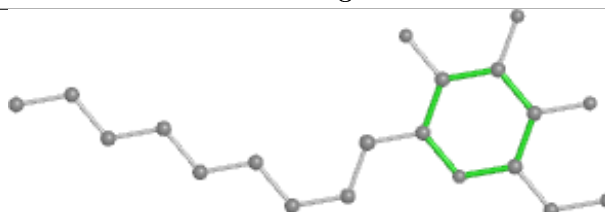
Bond lengths



Bond angles

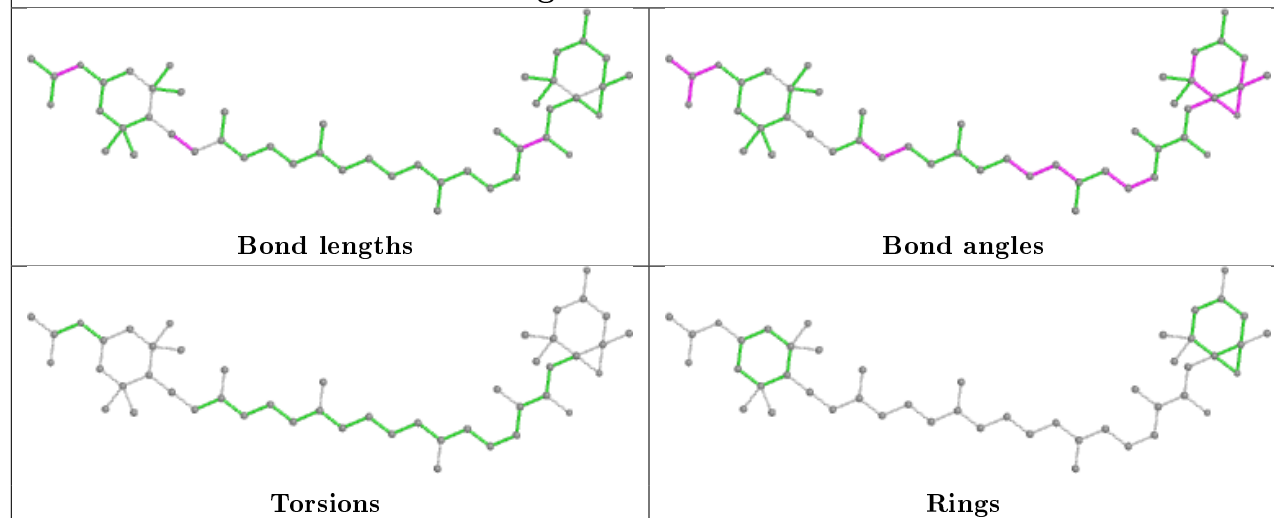


Torsions

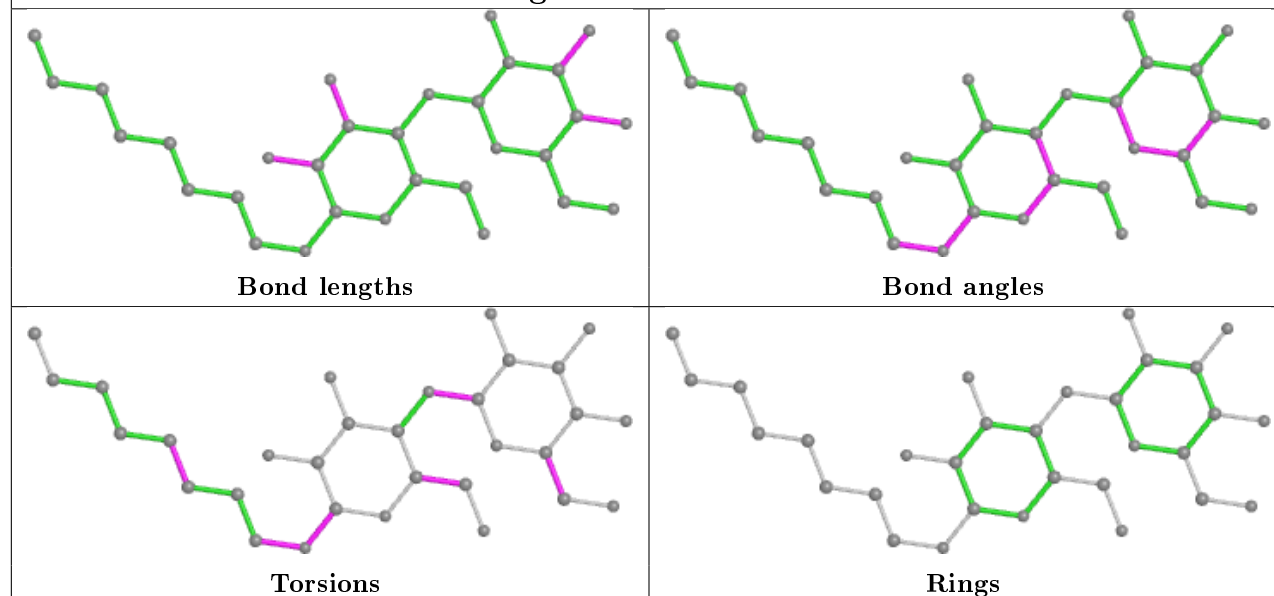


Rings

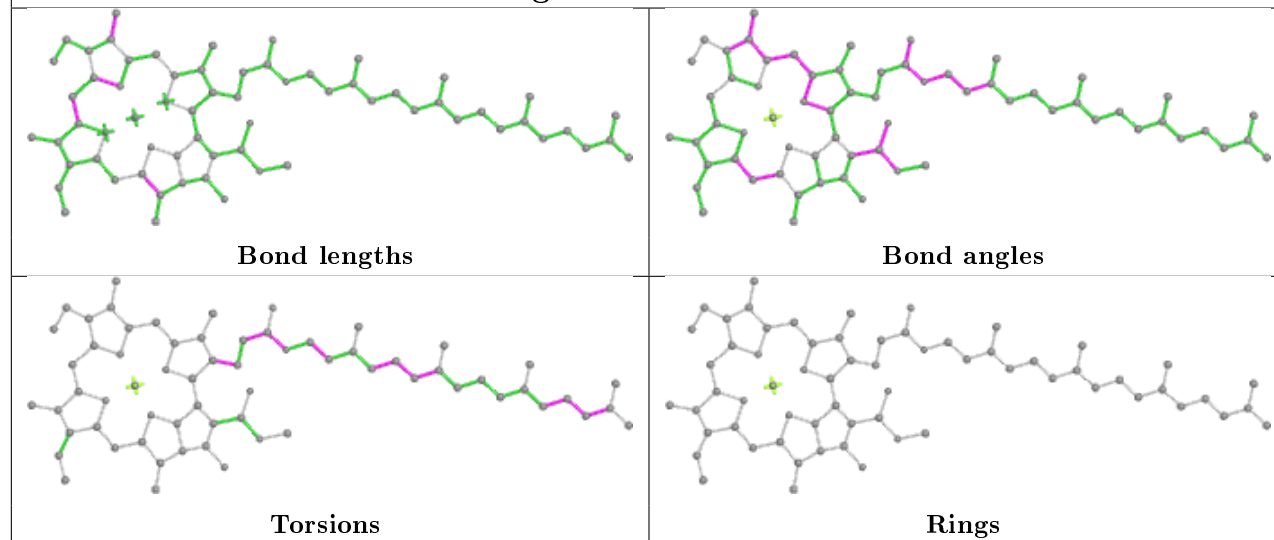
## Ligand A86 A 304

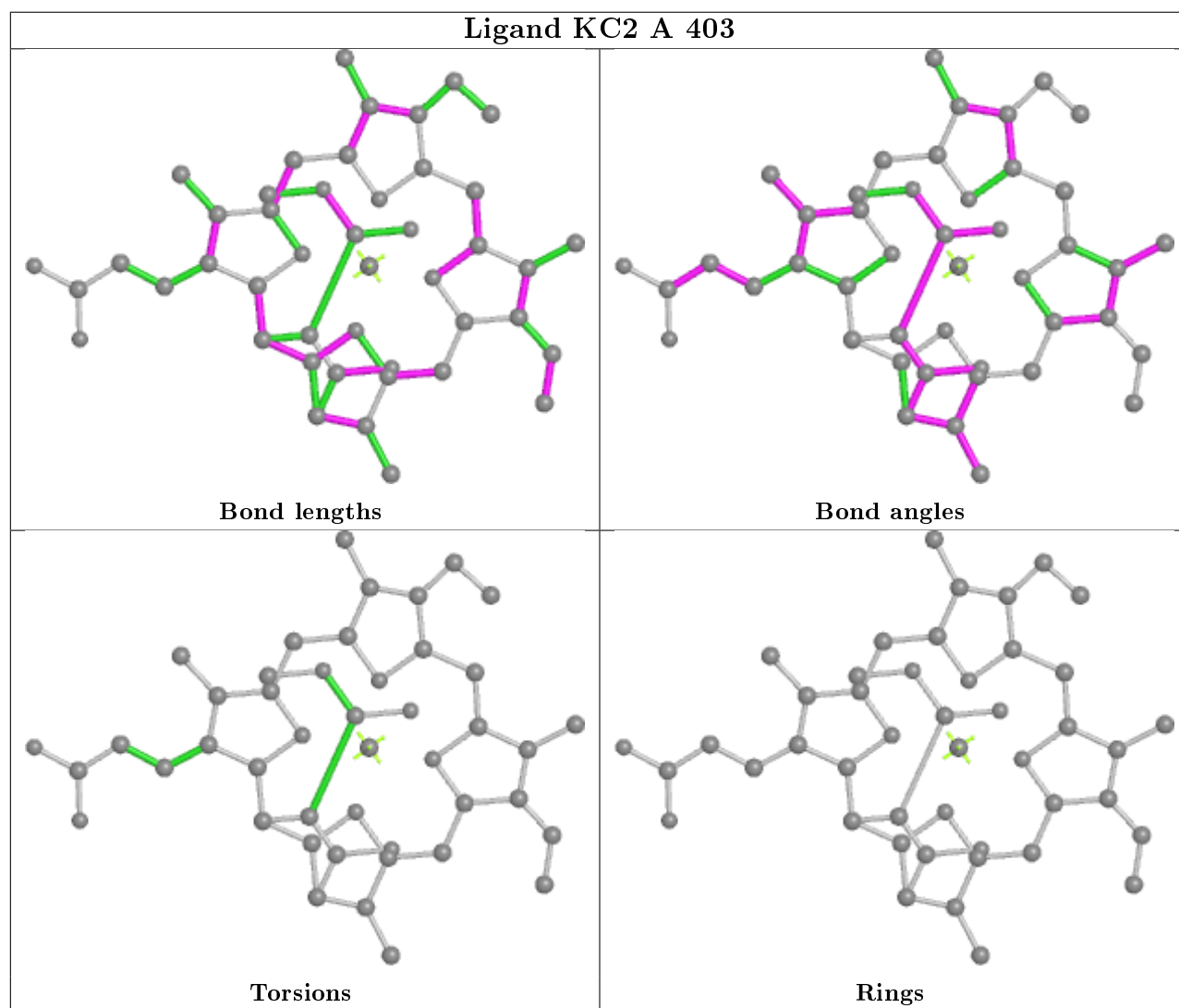
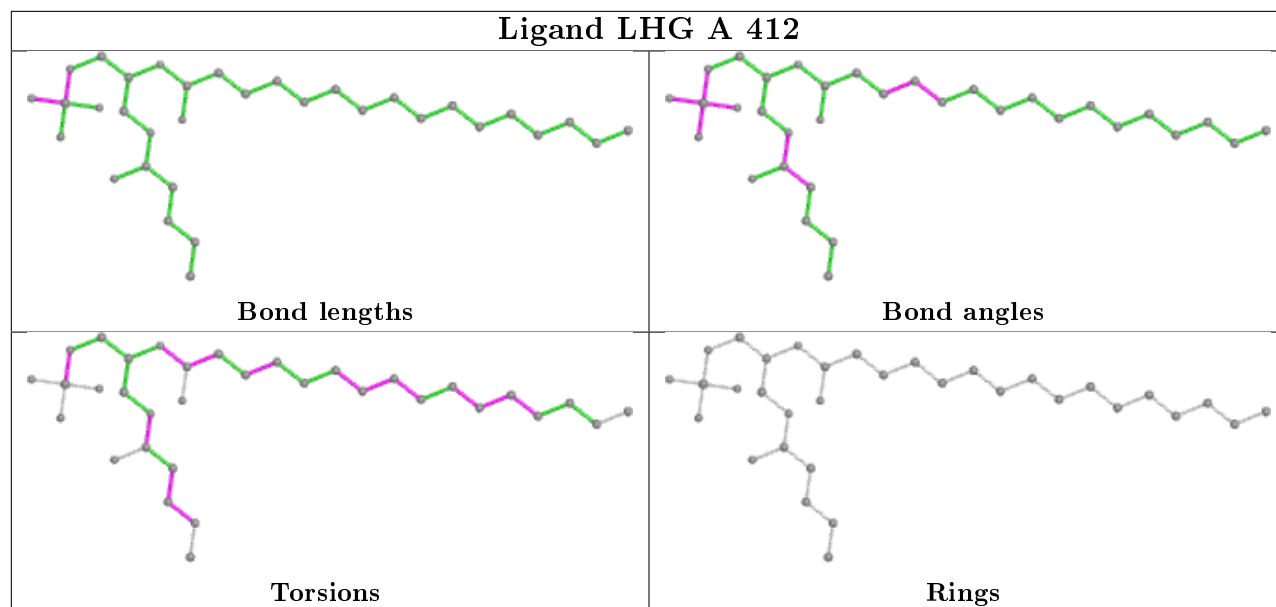


## Ligand LMT A 410

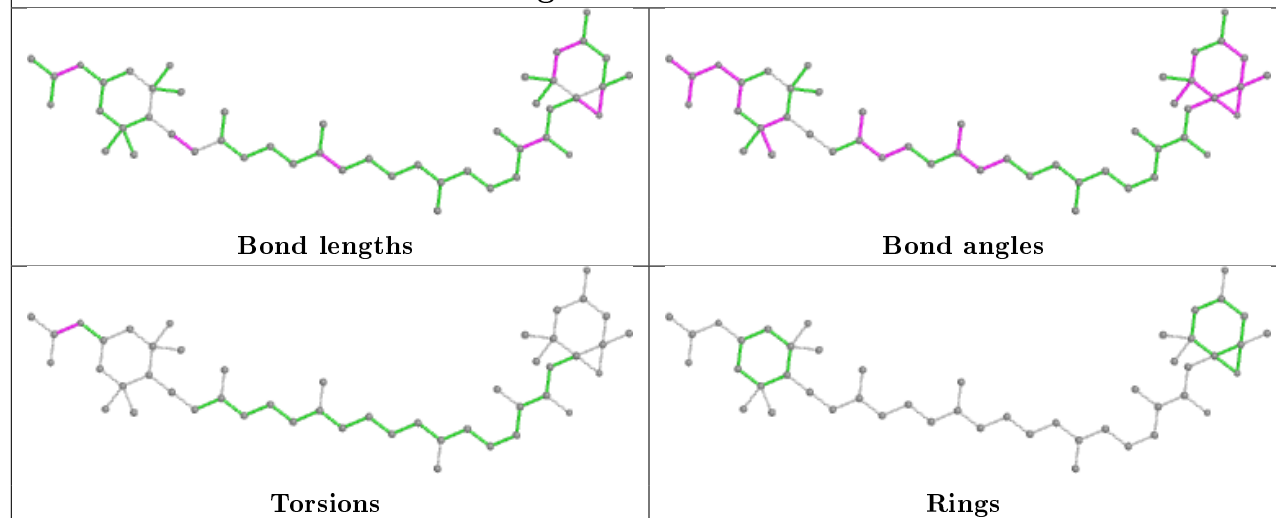


## Ligand CLA A 402

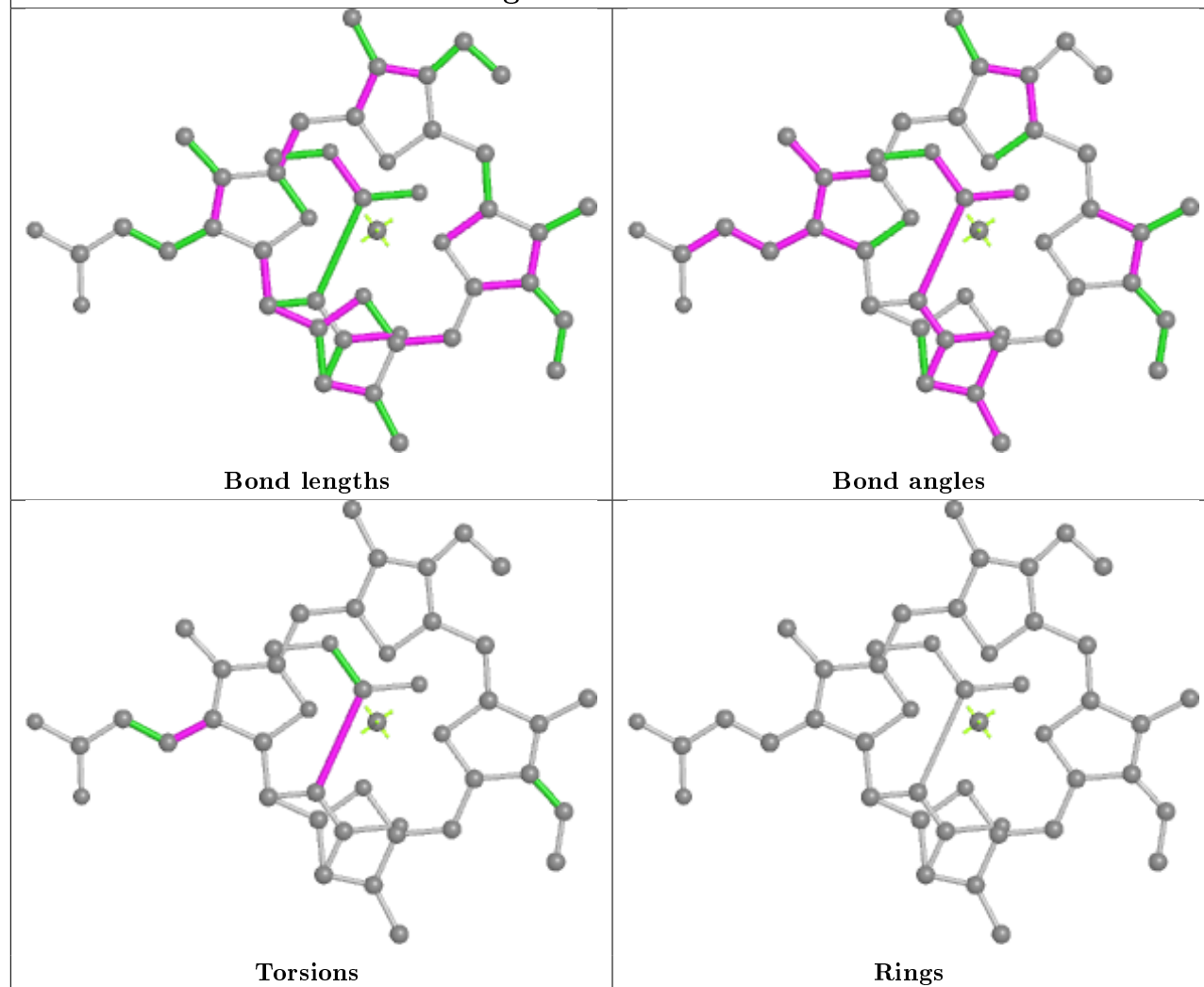




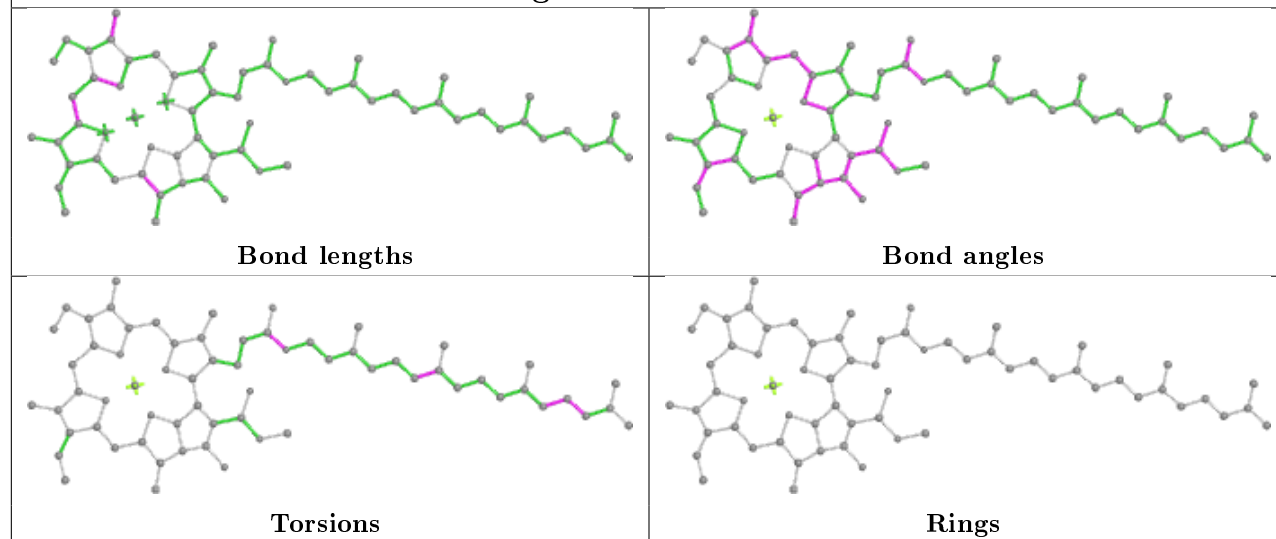
## Ligand A86 A 306



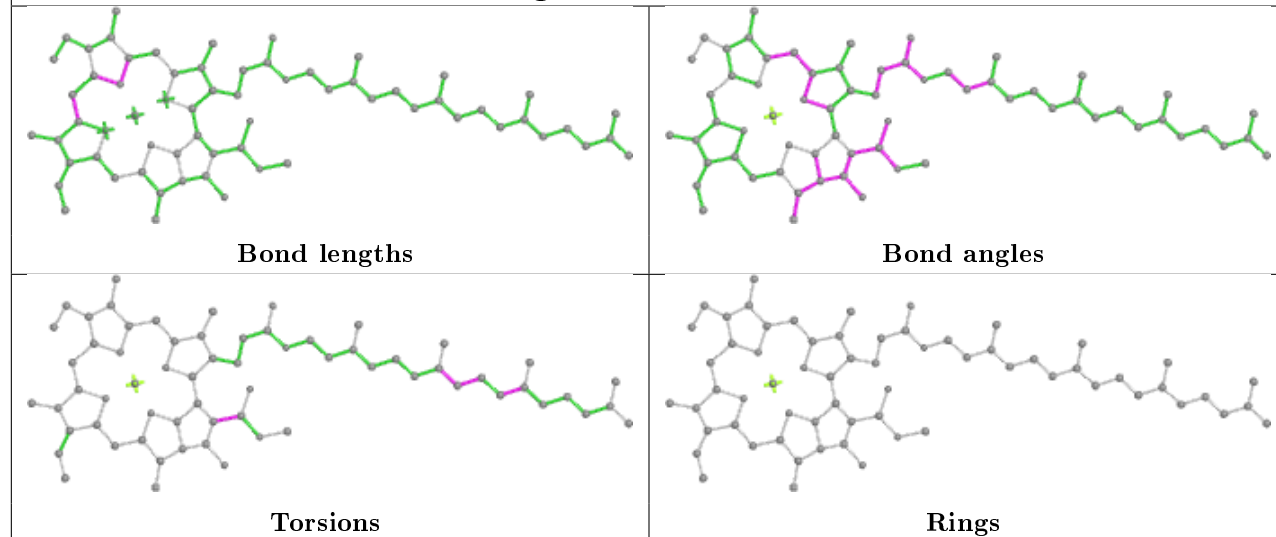
## Ligand KC1 A 408

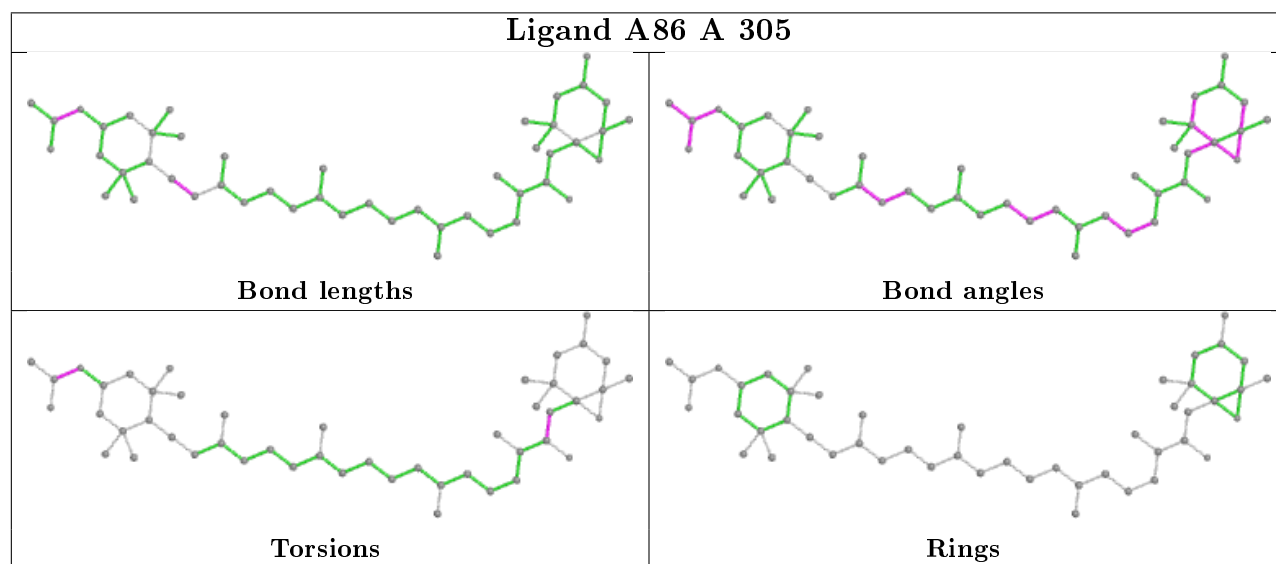
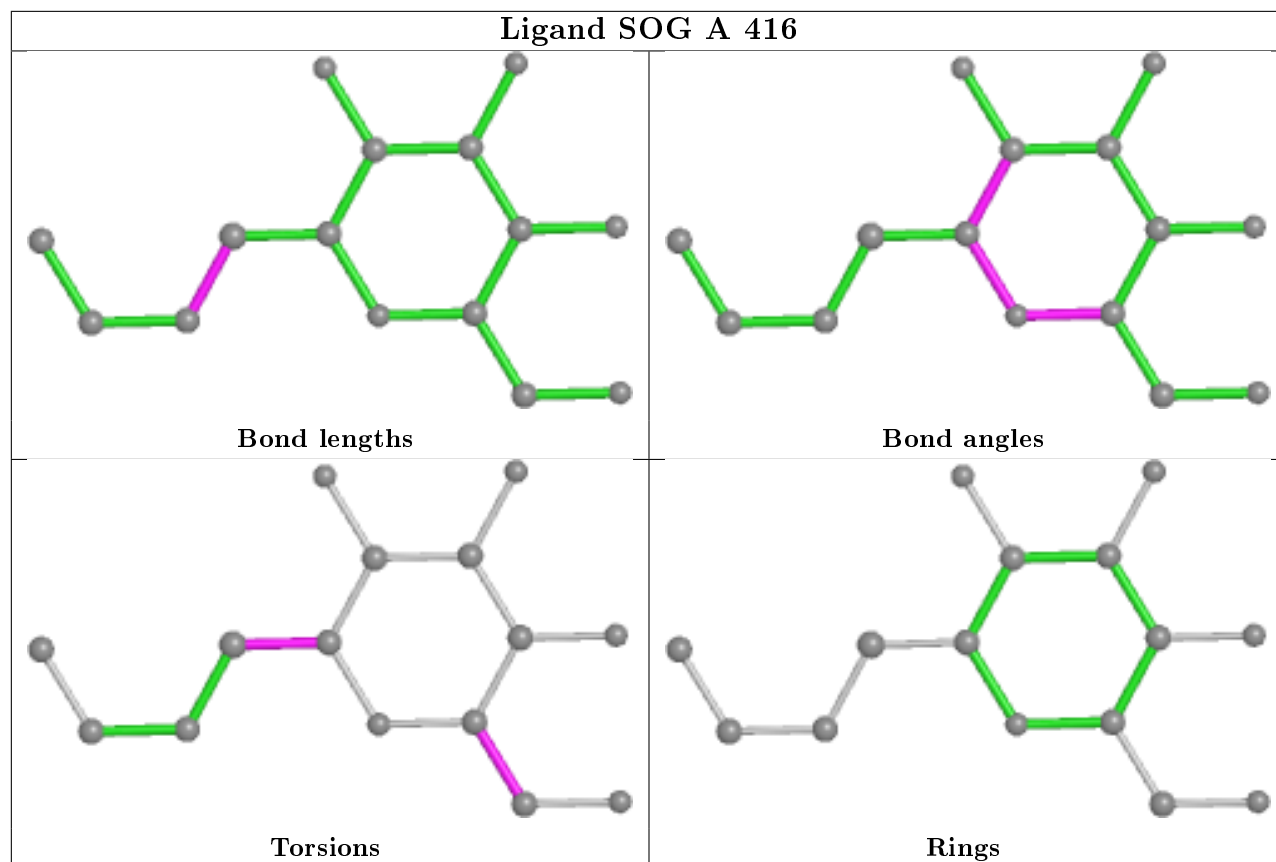


## Ligand CLA A 406

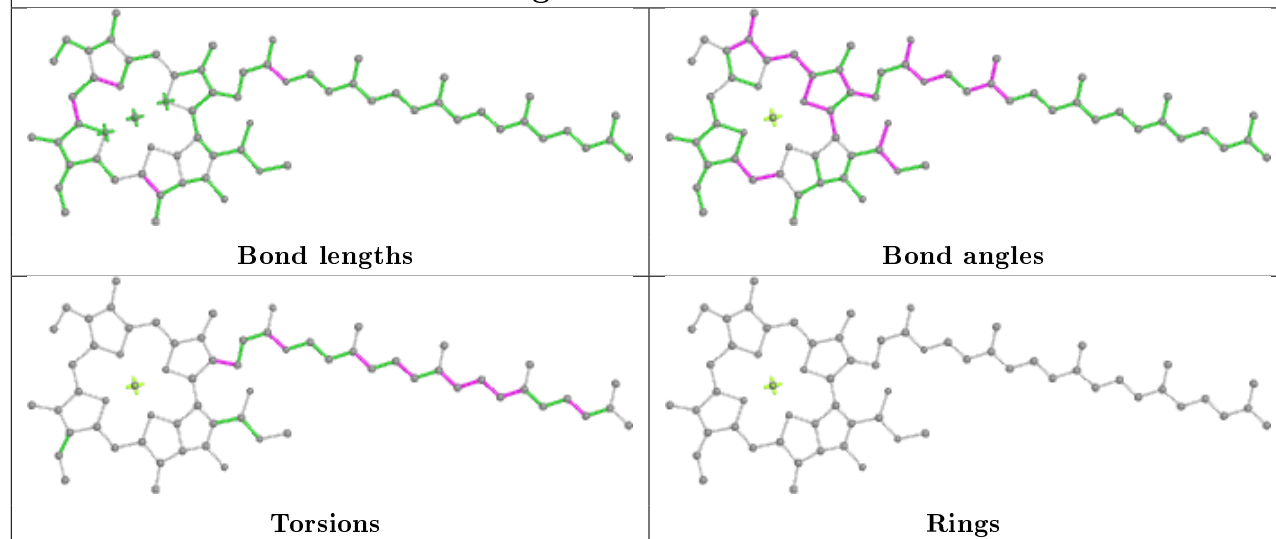


## Ligand CLA A 404

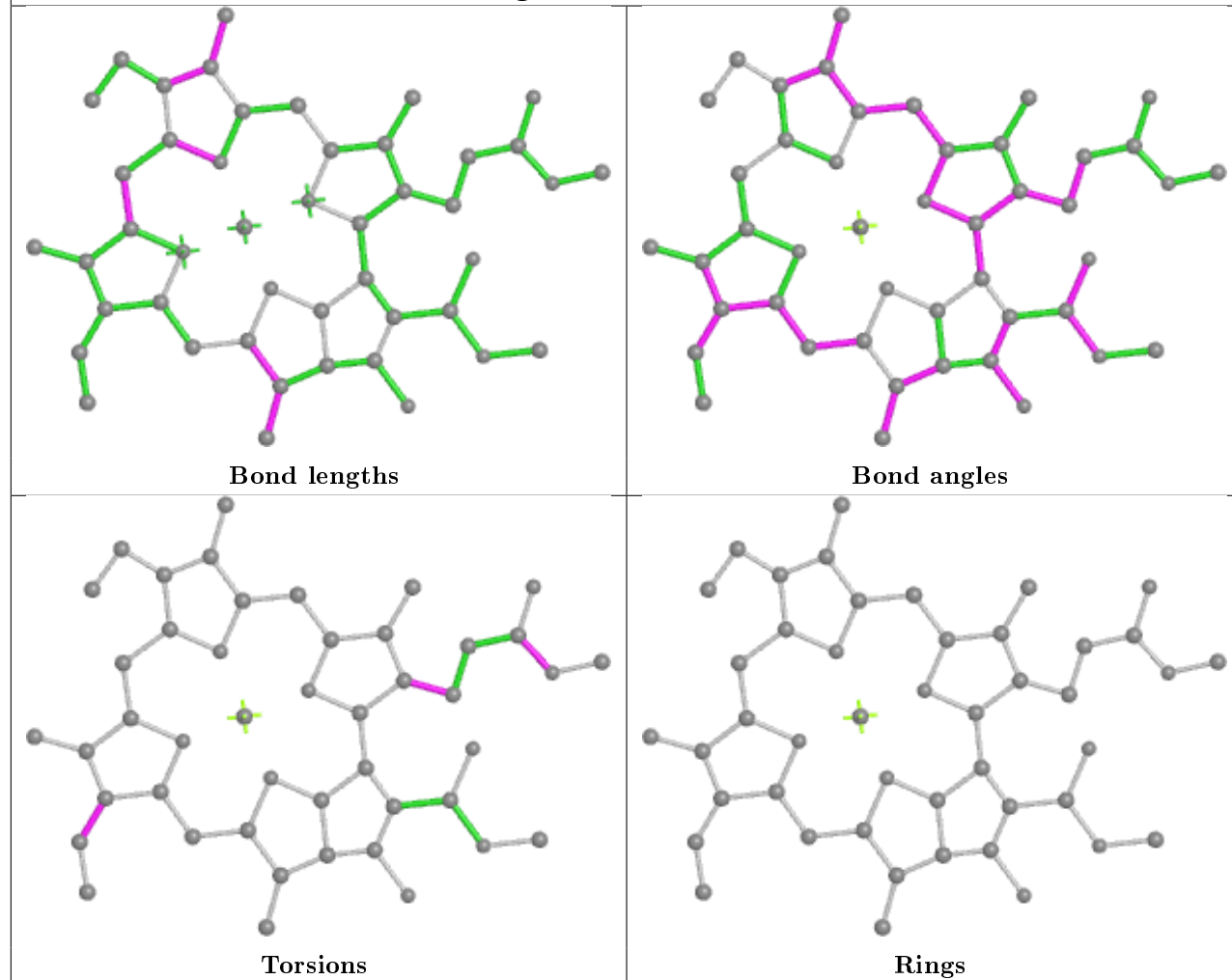


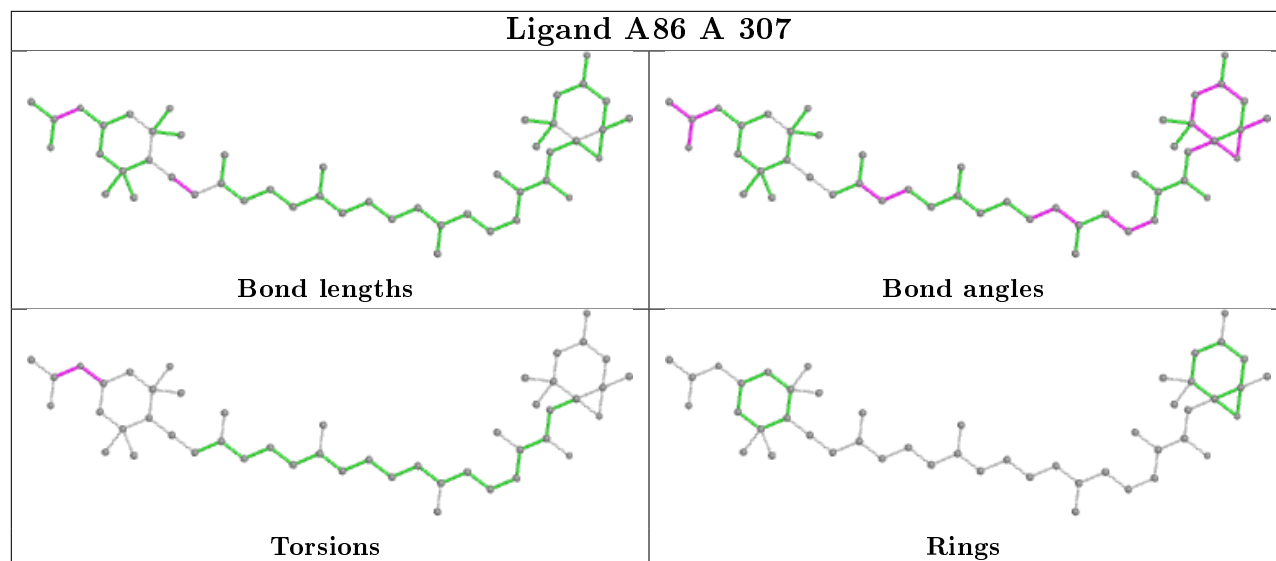


## Ligand CLA A 407



## Ligand CLA A 405





## 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	166/167 (99%)	-0.10	6 (3%) 42 37	18, 36, 63, 79	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	GLU	3.3
1	A	25	ASP	2.5
1	A	23	ASP	2.4
1	A	66	SER	2.3
1	A	26	GLN	2.3
1	A	108	GLY	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	LMT	A	410	31/35	0.51	0.40	49,110,124,127	0

*Continued on next page...*

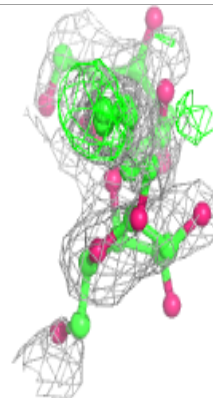
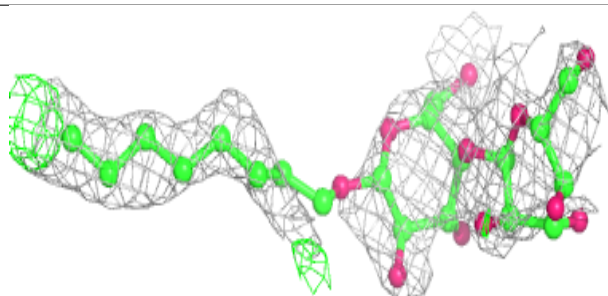
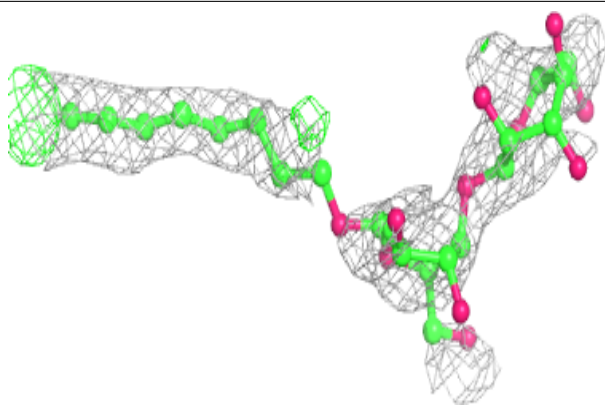
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DD6	A	308	43/43	0.52	0.30	70,84,104,109	0
9	DGD	A	411	39/66	0.59	0.33	68,86,99,105	0
10	LHG	A	412	33/49	0.62	0.20	45,66,123,127	0
11	SOG	A	414	20/20	0.65	0.24	43,93,104,109	0
11	SOG	A	415	20/20	0.66	0.20	55,100,105,110	0
12	UNL	A	423	10/-	0.68	0.16	62,64,65,65	0
12	UNL	A	420	12/-	0.69	0.21	56,60,64,64	0
11	SOG	A	416	15/20	0.70	0.30	90,96,104,105	0
12	UNL	A	422	7/-	0.71	0.15	43,54,60,61	0
11	SOG	A	413	20/20	0.73	0.30	48,105,119,120	0
12	UNL	A	418	12/-	0.79	0.12	58,61,68,69	0
12	UNL	A	421	12/-	0.79	0.30	52,55,67,69	0
3	A86	A	304	48/48	0.87	0.13	21,28,59,76	0
12	UNL	A	417	12/-	0.89	0.11	47,52,59,60	0
3	A86	A	306	48/48	0.89	0.12	35,49,72,85	0
12	UNL	A	419	8/-	0.89	0.11	49,54,56,59	0
2	CA	A	202	1/1	0.90	0.08	76,76,76,76	0
3	A86	A	301	48/48	0.90	0.14	26,43,93,105	0
5	CLA	A	407	65/65	0.93	0.14	15,25,75,83	0
5	CLA	A	405	46/65	0.93	0.10	31,43,60,75	0
3	A86	A	302	48/48	0.94	0.09	18,28,66,73	0
5	CLA	A	402	65/65	0.94	0.14	25,37,74,79	0
3	A86	A	303	48/48	0.95	0.09	20,27,51,58	0
3	A86	A	307	48/48	0.95	0.08	23,31,55,58	0
5	CLA	A	404	65/65	0.95	0.10	18,25,51,59	0
5	CLA	A	406	65/65	0.95	0.10	19,28,70,78	0
5	CLA	A	409	41/65	0.95	0.10	31,44,61,67	0
3	A86	A	305	48/48	0.96	0.09	17,28,50,63	0
5	CLA	A	401	61/65	0.96	0.09	21,35,66,71	0
7	KC1	A	408	45/45	0.97	0.09	19,24,31,56	0
6	KC2	A	403	45/45	0.97	0.07	24,30,43,57	0
2	CA	A	201	1/1	0.99	0.05	39,39,39,39	0

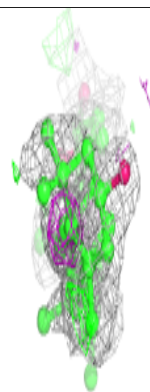
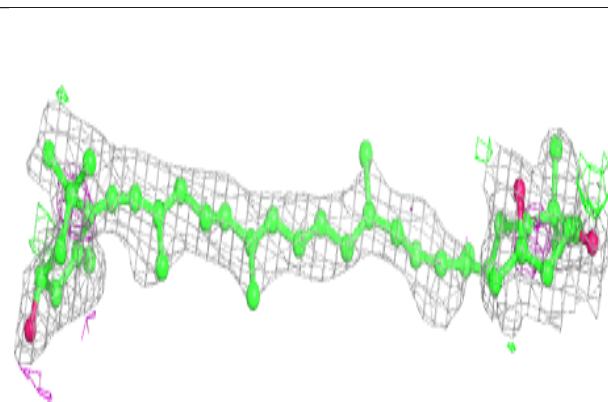
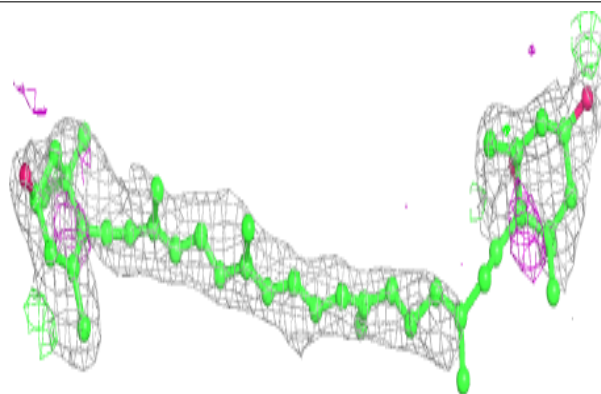
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around LMT A 410:**

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

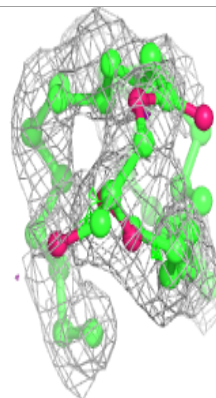
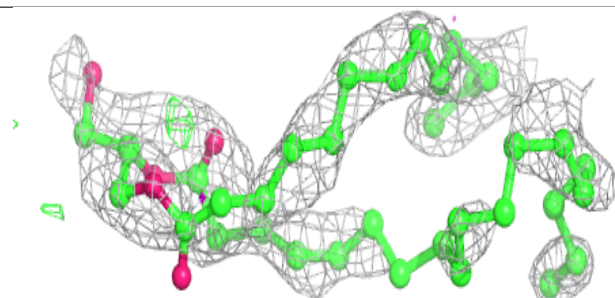
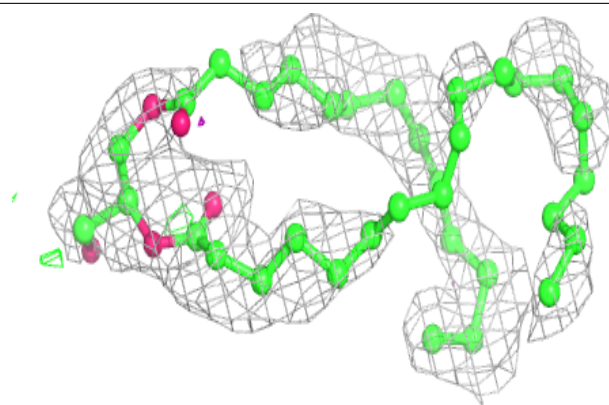
**Electron density around DD6 A 308:**

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

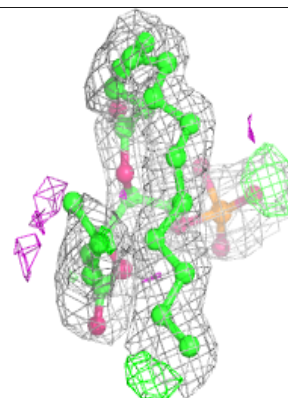
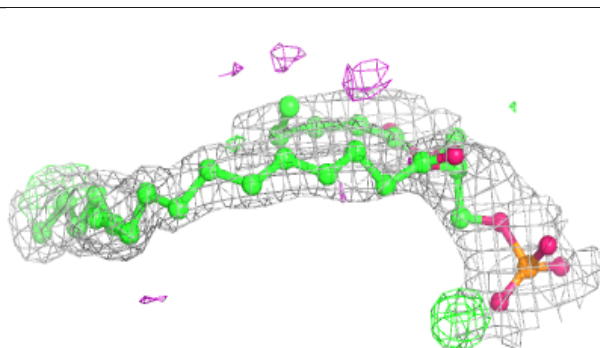
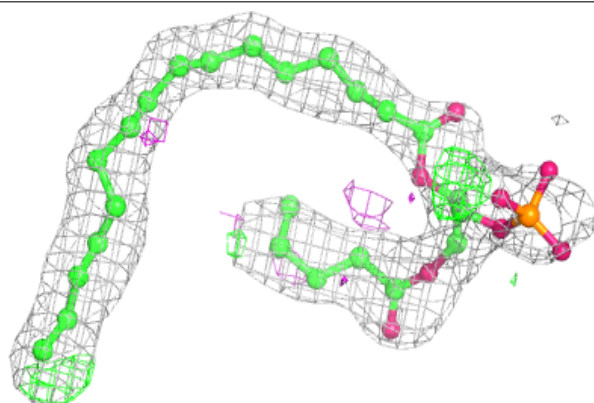


**Electron density around DGD A 411:**

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

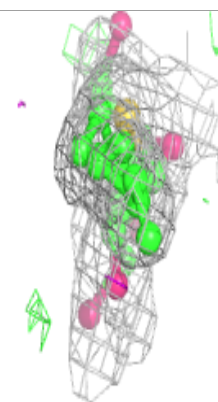
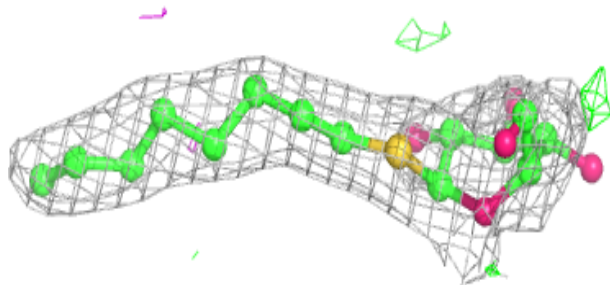
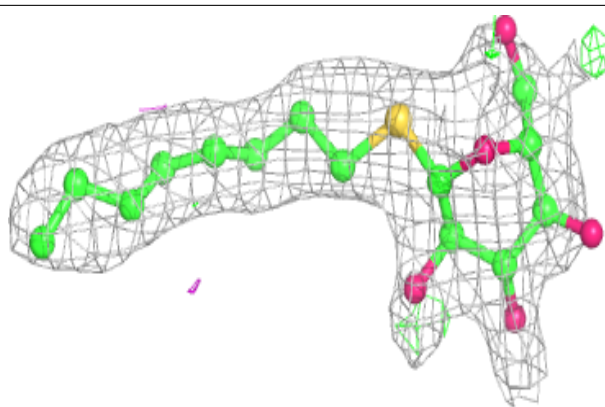
**Electron density around LHG A 412:**

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

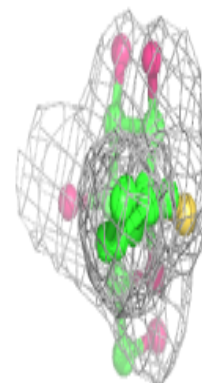
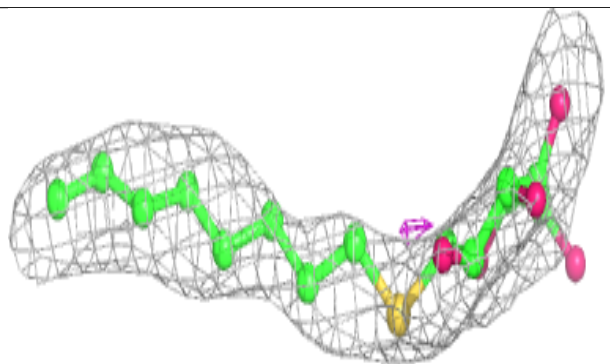
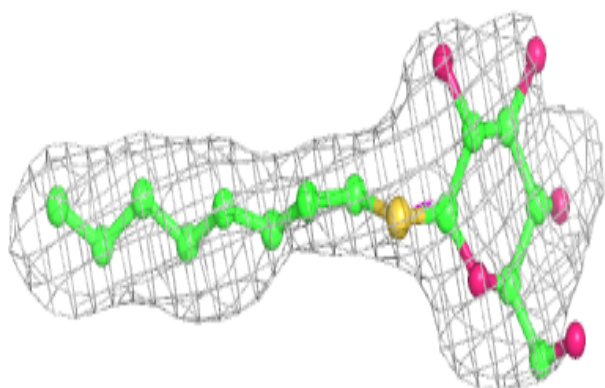


**Electron density around SOG A 414:**

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

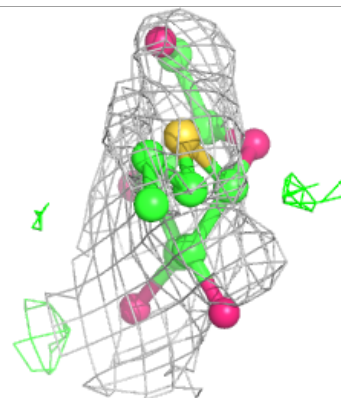
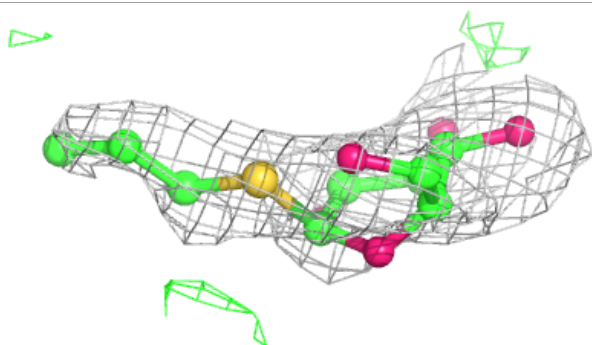
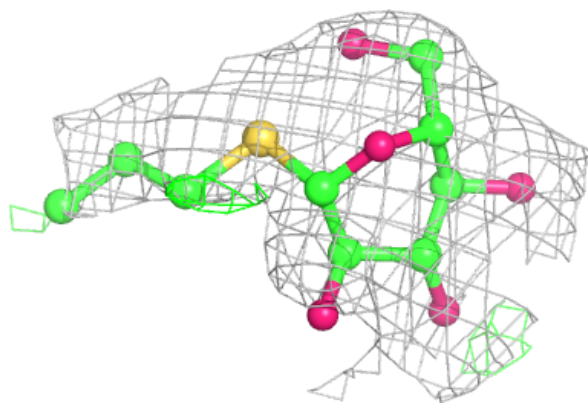
**Electron density around SOG A 415:**

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

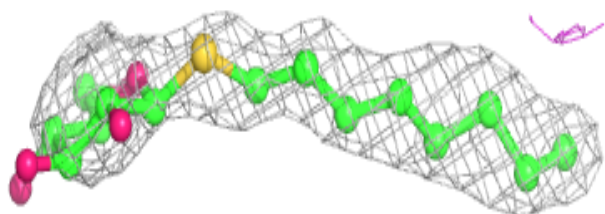
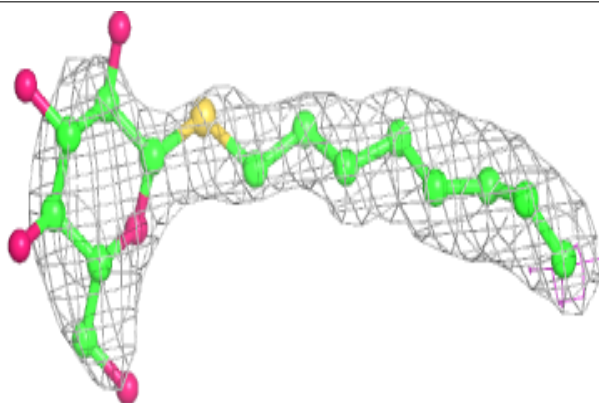


**Electron density around SOG A 416:**

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

**Electron density around SOG A 413:**

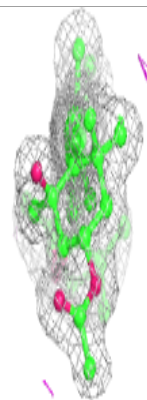
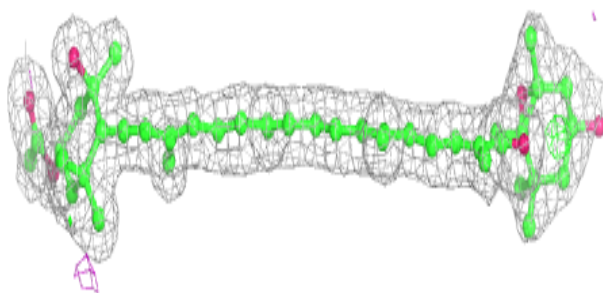
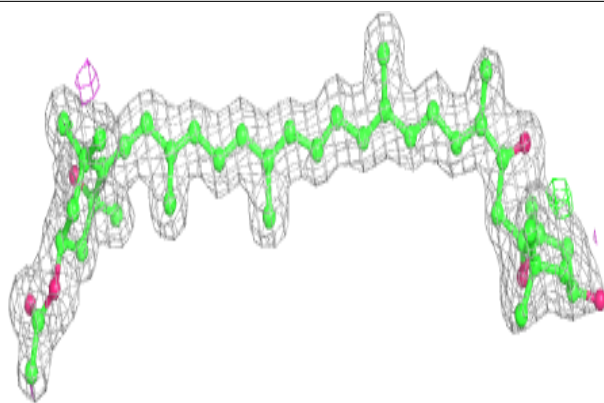
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



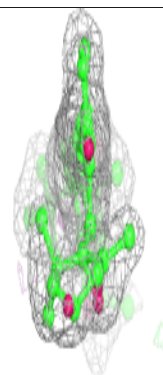
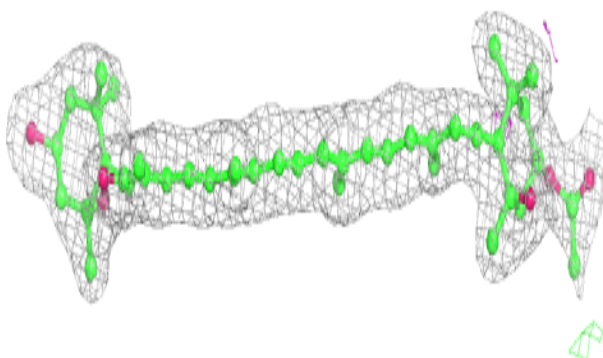
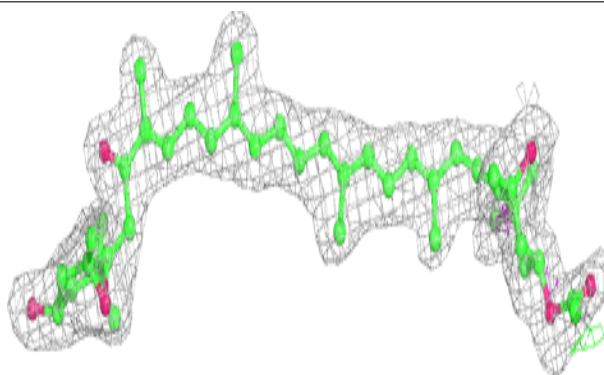


**Electron density around A86 A 304:**

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

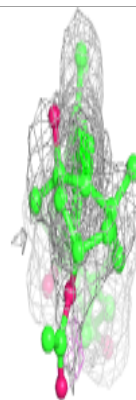
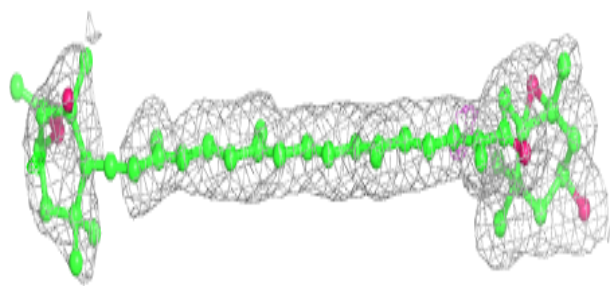
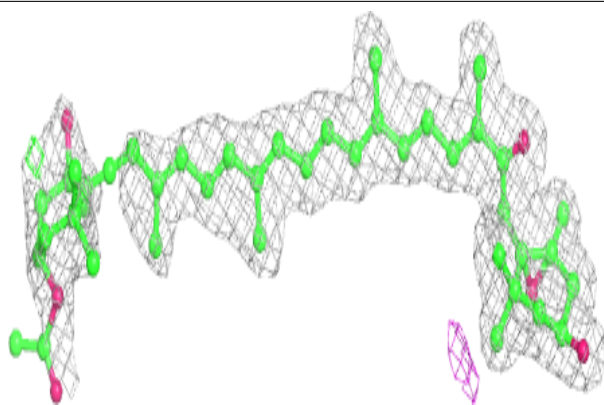
**Electron density around A86 A 306:**

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



**Electron density around A86 A 301:**

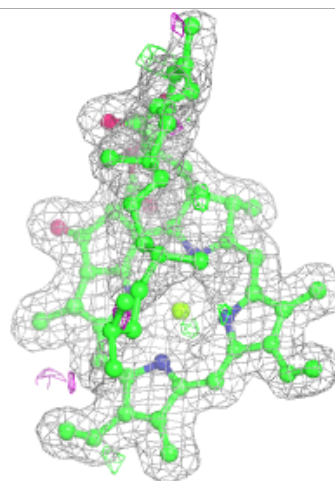
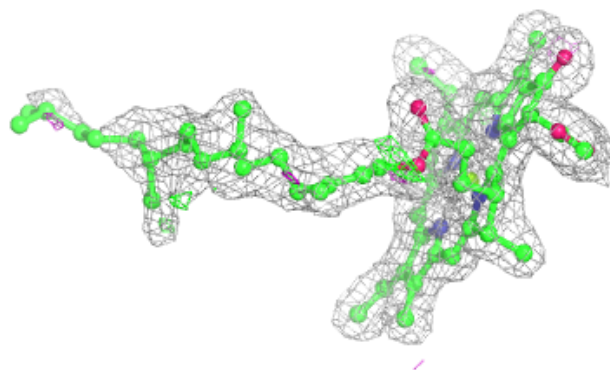
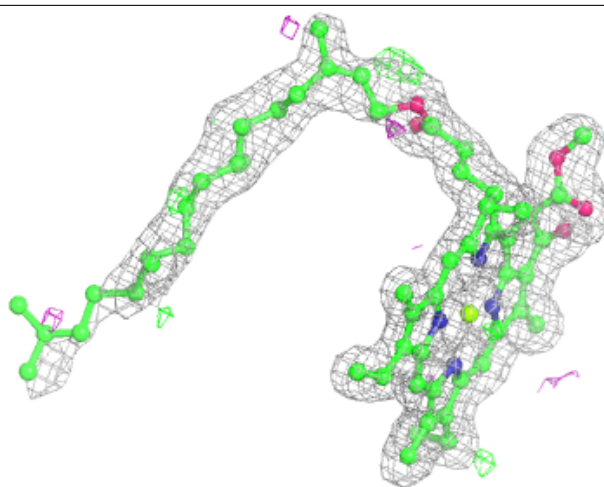
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





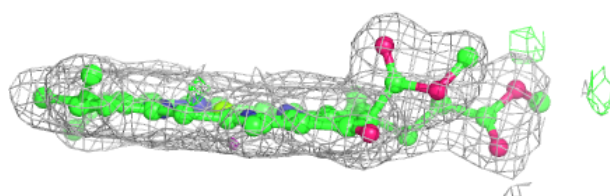
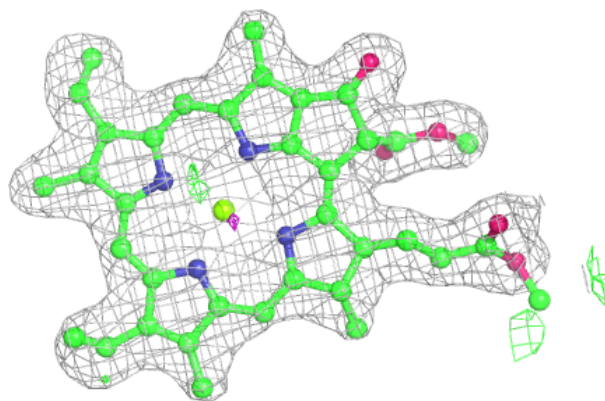
**Electron density around CLA A 407:**

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and green (positive)

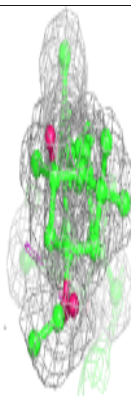
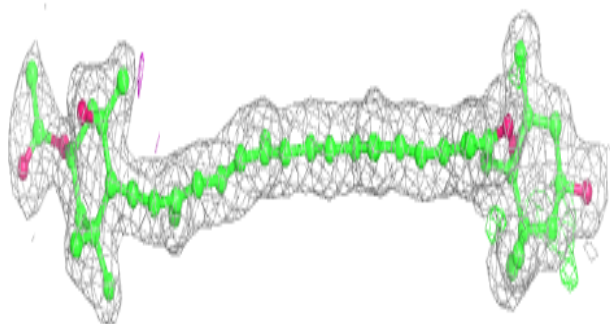
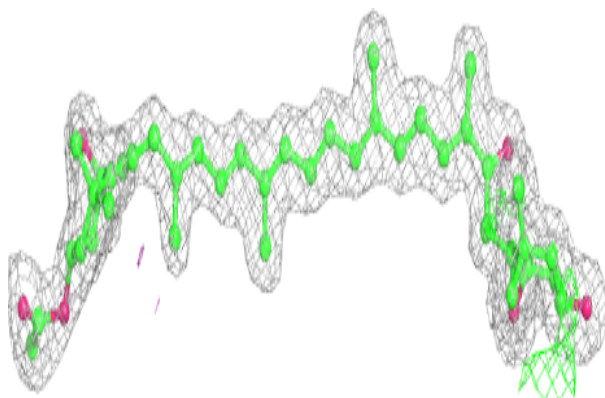


**Electron density around CLA A 405:**

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and green (positive)

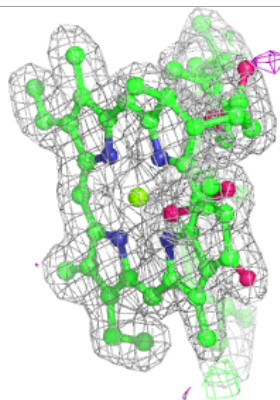
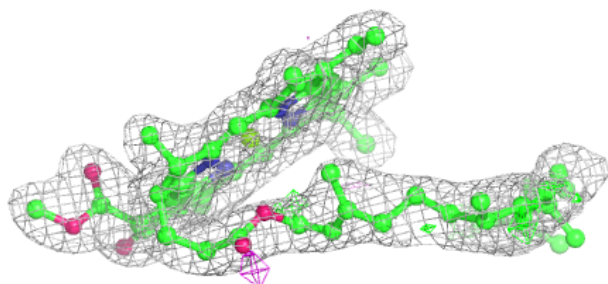
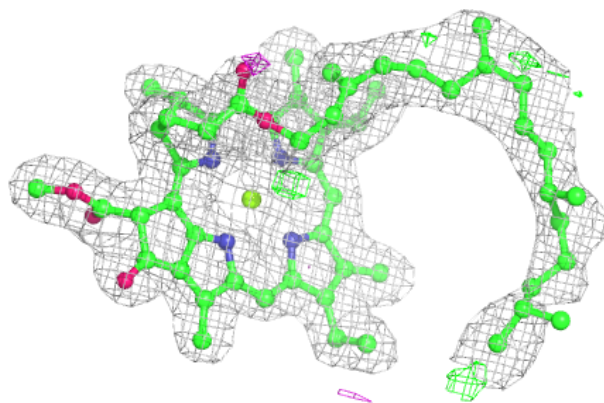
**Electron density around A86 A 302:**

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

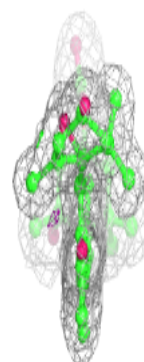
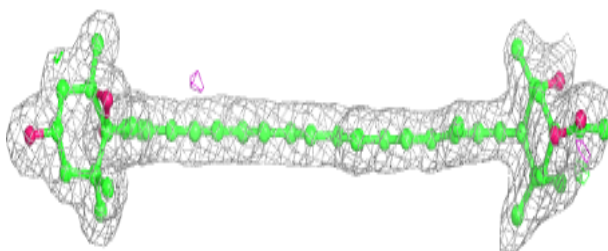
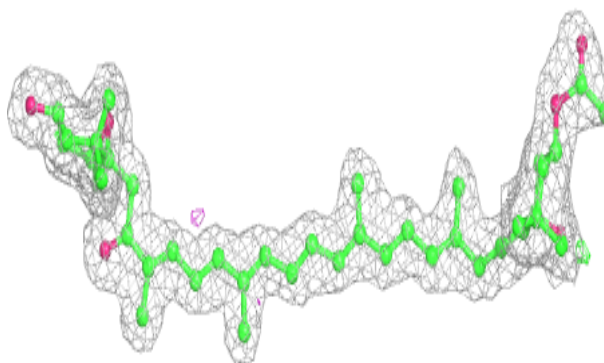


**Electron density around CLA A 402:**

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and green (positive)

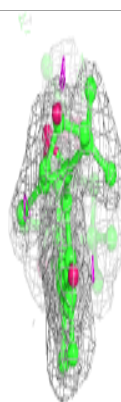
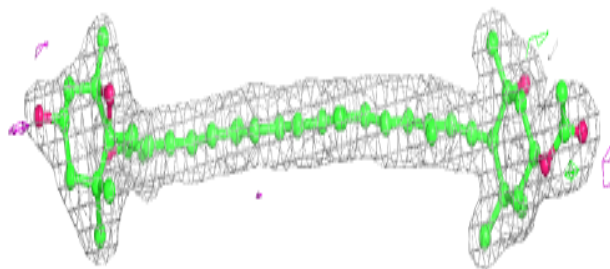
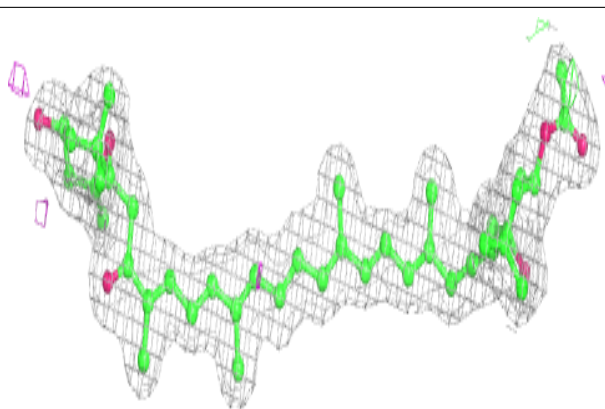
**Electron density around A86 A 303:**

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

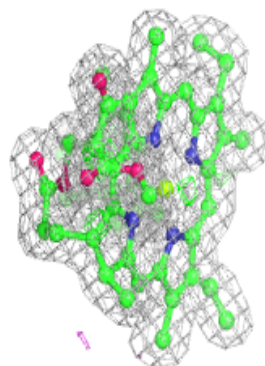
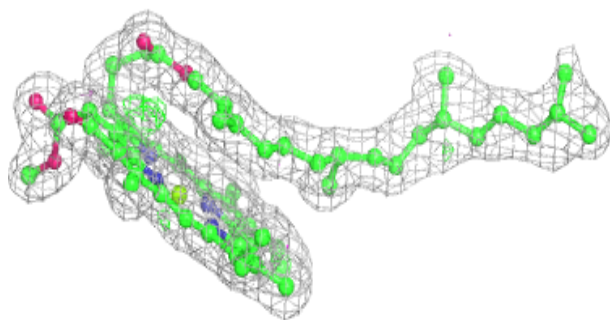
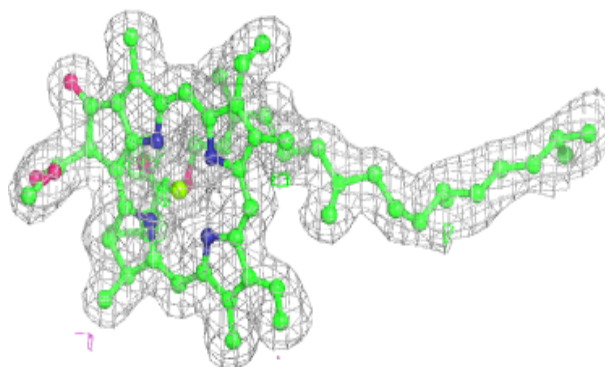


**Electron density around A86 A 307:**

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

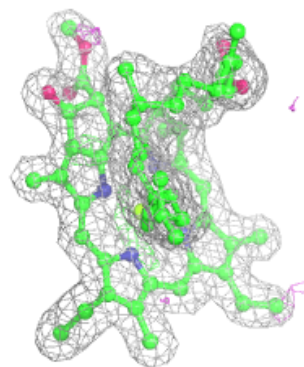
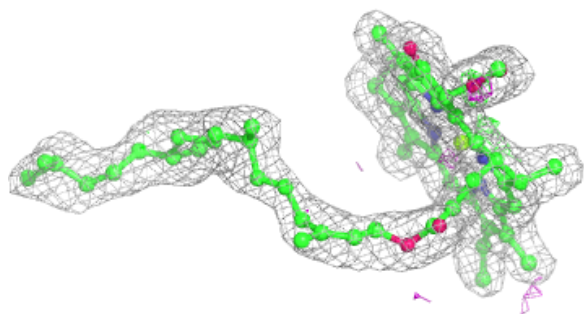
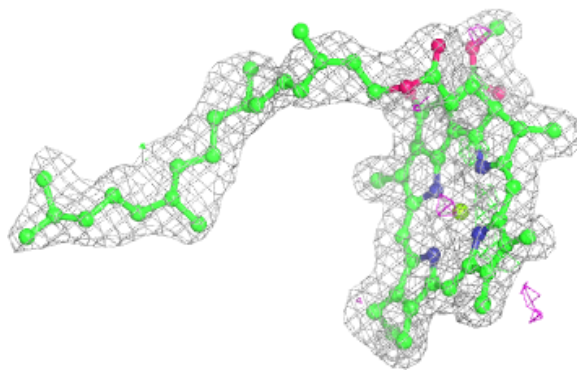
**Electron density around CLA A 404:**

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



**Electron density around CLA A 406:**

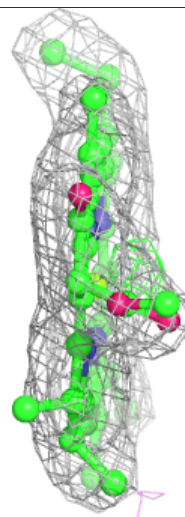
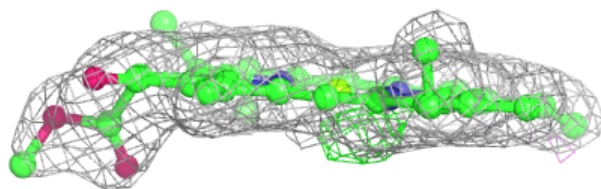
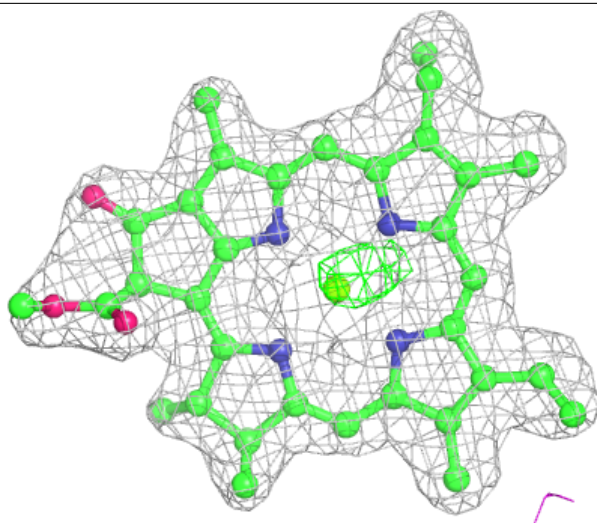
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





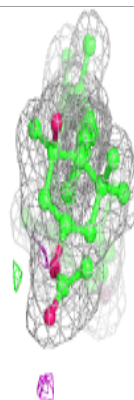
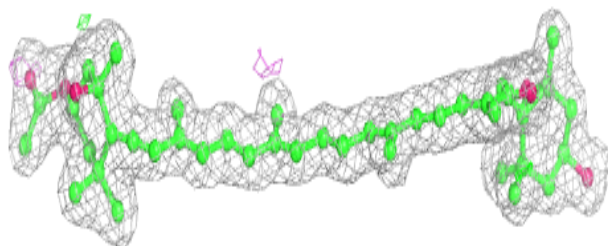
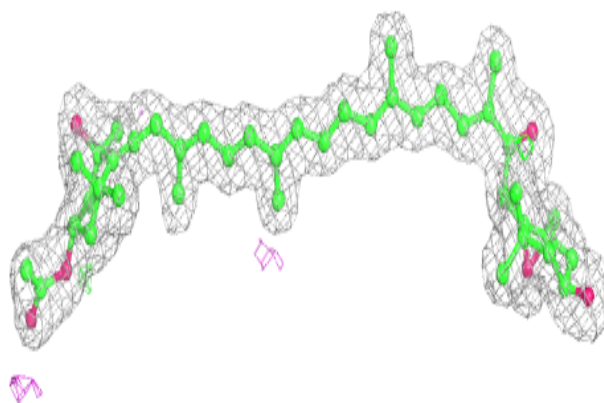
**Electron density around CLA A 409:**

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



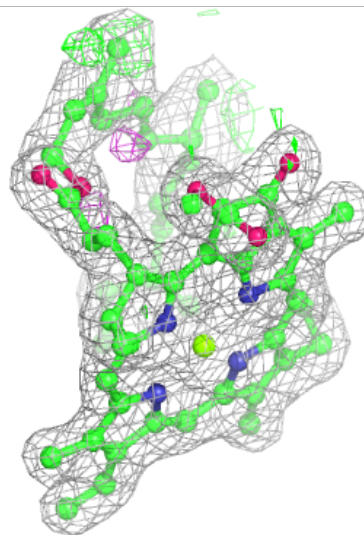
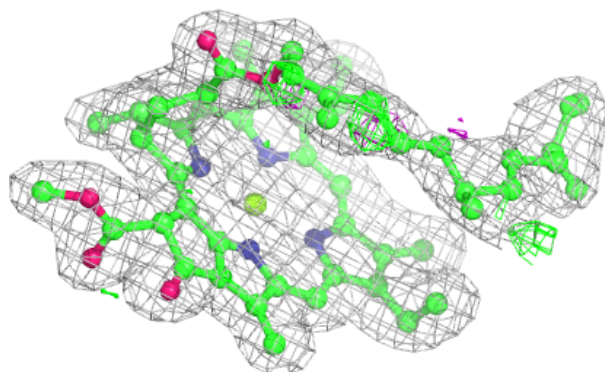
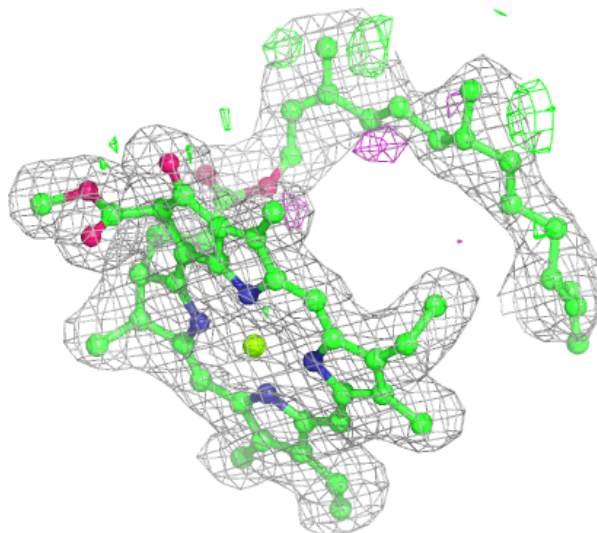
**Electron density around A86 A 305:**

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



**Electron density around CLA A 401:**

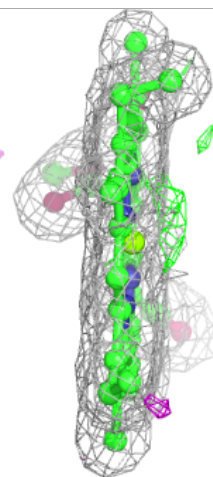
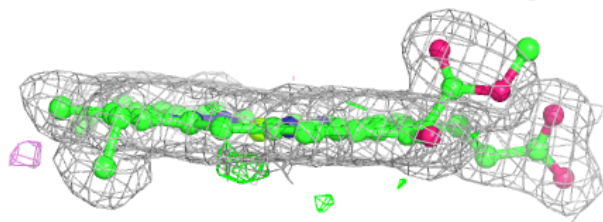
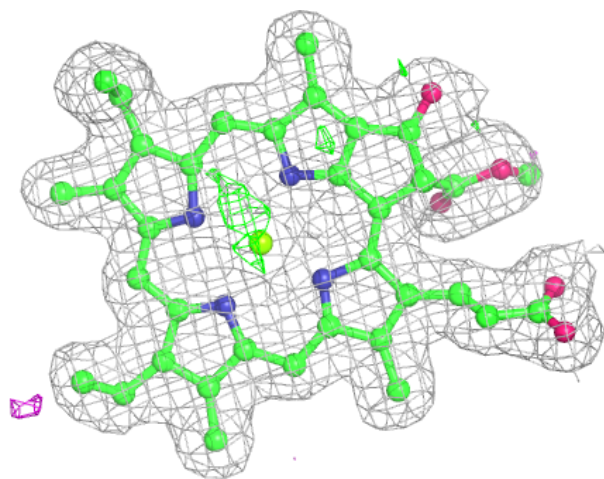
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





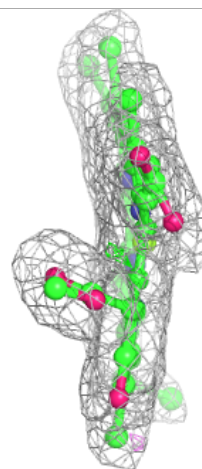
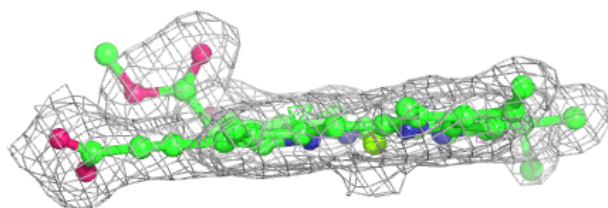
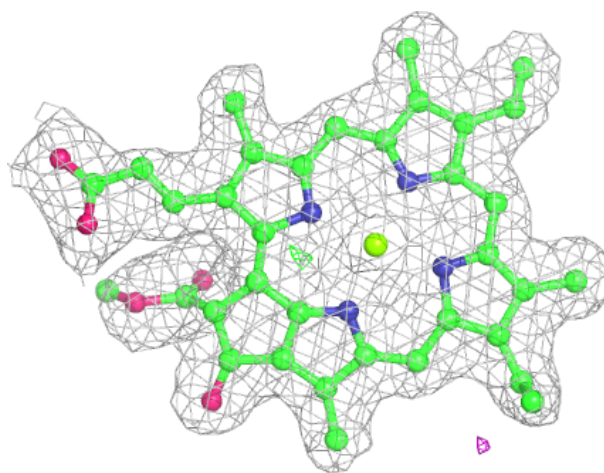
**Electron density around KC1 A 408:**

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



**Electron density around KC2 A 403:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.