



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 10:39 AM UTC

PDB ID : 6A2W / pdb_00006a2w
Title : Crystal structure of fucoxanthin chlorophyll a/c complex from *Phaeodactylum tricorutum*
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

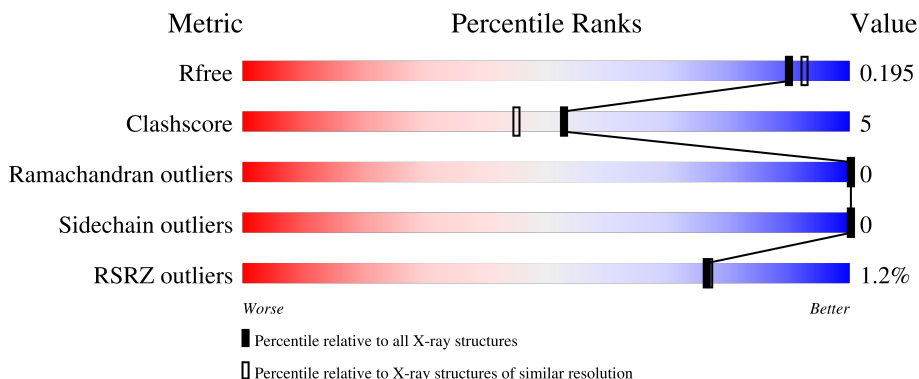
1 Overall quality at a glance

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 % 93% 6%

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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	A	402	X	-	-	-
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	-	-	-

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.

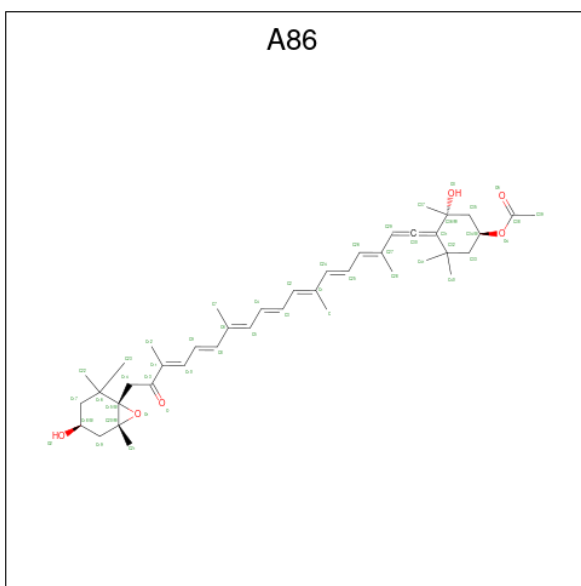
- Molecule 1 is a protein called Protein fucoxanthin chlorophyll a/c protein.

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

- Molecule 2 is CALCIUM ION (CCD ID: 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-h exahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



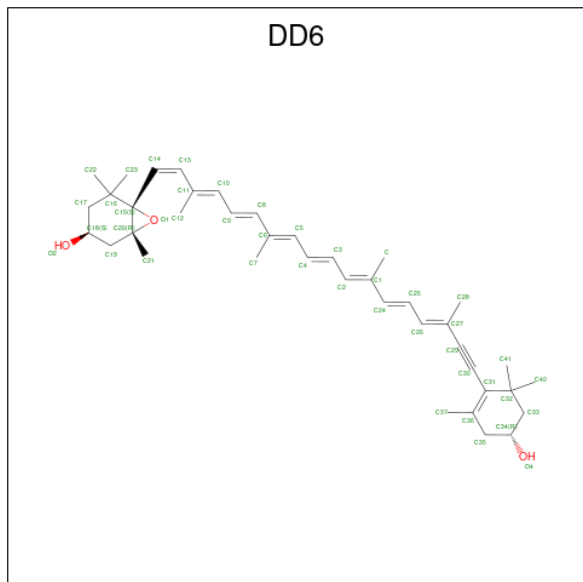
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		

Continued on next page...

Continued from previous page...

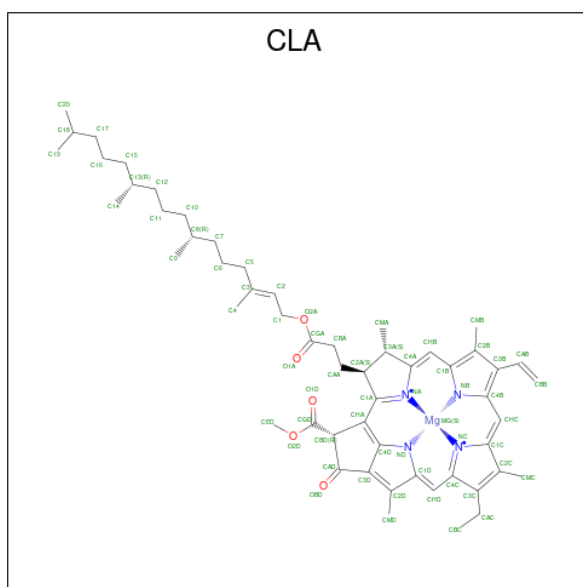
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		
3	A	1	Total	C	O	0	0
			48	42	6		

- Molecule 4 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃).



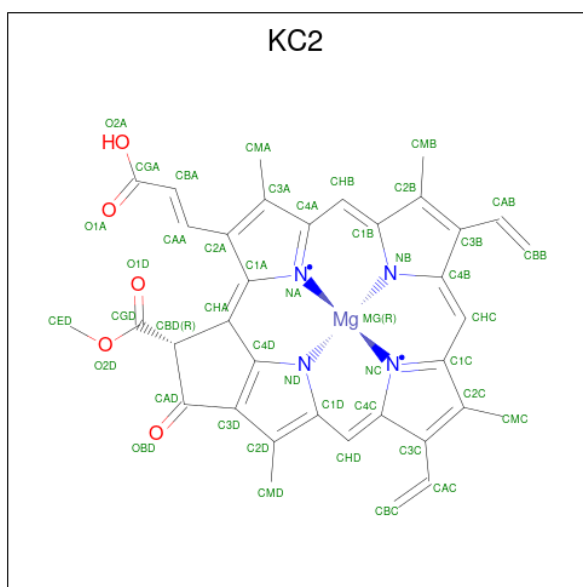
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			43	40	3		

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



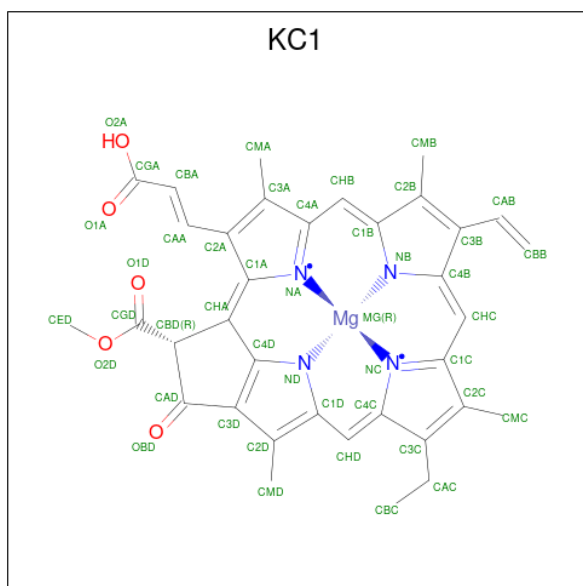
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A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

- Molecule 6 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



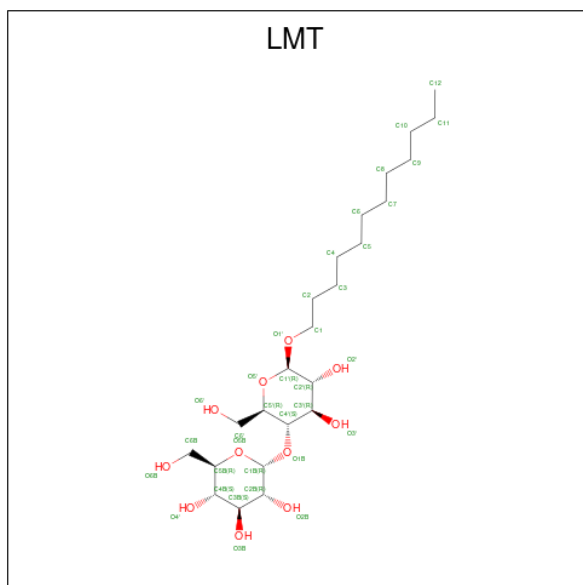
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	A	1	45	35	1	4	5	0	0

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



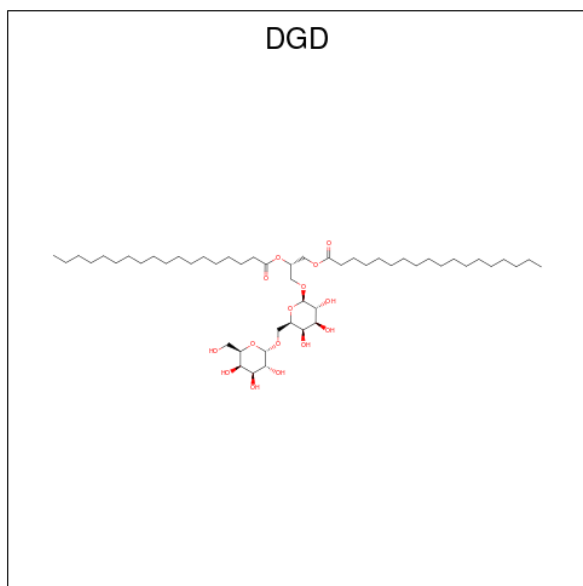
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
7	A	1	45	35	1	4	5	0	0

- Molecule 8 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



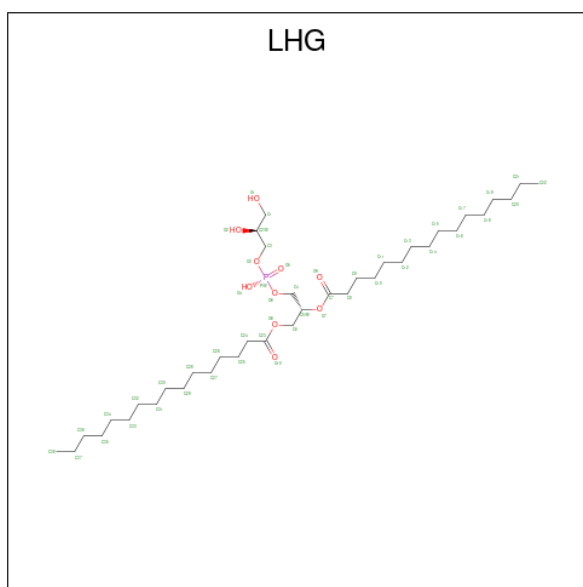
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
8	A	1	Total	C	O	0	0
			31	20	11		

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



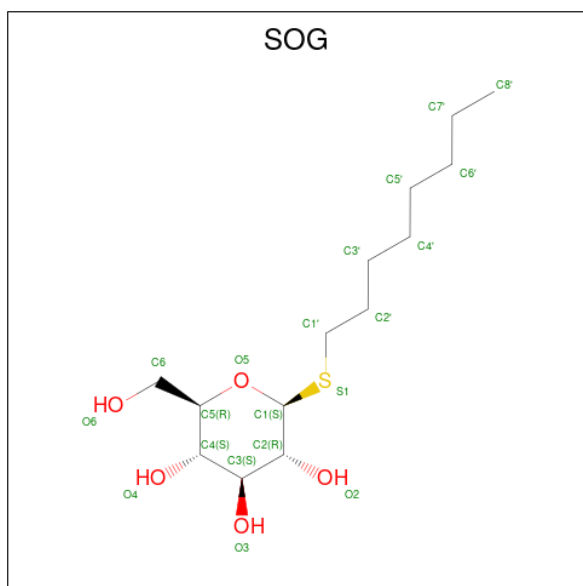
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
9	A	1	Total	C	O	0	0
			39	34	5		

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



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

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



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

Continued on next page...

Continued from previous page...

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

- Molecule 12 is UNKNOWN LIGAND (CCD ID: 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 [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 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:  % 93% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.175 , 0.197 0.173 , 0.195	Depositor DCC
R_{free} test set	2000 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 83.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2518	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: A86, LHG, SOG, CA, KC1, KC2, UNL, CLA, DGD, DD6, 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	A	0.36	0/1342	0.50	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	0	0
4	A	43	0	0	0	0
5	A	408	0	411	13	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	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 22 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:HBW2	9:A:411:DGD:HA92	1.76	0.68
1:A:91:LEU:HD23	5:A:405:CLA:HBC3	1.91	0.52
11:A:416:SOG:S1	11:A:416:SOG:O6	2.57	0.52
1:A:157:HIS:CE1	5:A:409:CLA:NA	2.78	0.52

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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.

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

Mol	Chain	Res	Type
1	A	26	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 2 are monoatomic and 7 are unknown - 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	$\# Z > 2$
5	CLA	A	406	1	69,73,73	1.13	4 (5%)	82,113,113	1.42	8 (9%)
3	A86	A	306	-	47,50,50	1.77	10 (21%)	51,76,76	2.19	15 (29%)
3	A86	A	307	-	47,50,50	1.28	4 (8%)	51,76,76	1.89	10 (19%)
8	LMT	A	410	-	32,32,36	1.01	2 (6%)	43,43,47	1.49	4 (9%)
3	A86	A	301	-	47,50,50	1.42	4 (8%)	51,76,76	2.38	17 (33%)
5	CLA	A	409	-	45,49,73	1.39	6 (13%)	54,84,113	1.47	6 (11%)
6	KC2	A	403	-	49,53,53	2.78	20 (40%)	60,89,89	3.68	33 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	LHG	A	412	-	32,32,48	0.87	2 (6%)	35,37,54	1.67	4 (11%)
3	A86	A	304	-	47,50,50	1.29	5 (10%)	51,76,76	2.00	10 (19%)
5	CLA	A	404	1	69,73,73	1.08	4 (5%)	82,113,113	1.33	9 (10%)
11	SOG	A	416	-	15,15,20	1.02	1 (6%)	19,20,25	1.33	1 (5%)
5	CLA	A	401	13	65,69,73	1.13	6 (9%)	77,108,113	1.24	6 (7%)
3	A86	A	305	-	47,50,50	1.45	4 (8%)	51,76,76	2.29	10 (19%)
5	CLA	A	402	1	69,73,73	1.16	6 (8%)	82,113,113	1.42	10 (12%)
9	DGD	A	411	-	38,38,67	0.70	1 (2%)	40,40,81	1.36	3 (7%)
3	A86	A	302	-	47,50,50	1.41	5 (10%)	51,76,76	1.88	10 (19%)
4	DD6	A	308	-	40,45,45	1.84	4 (10%)	51,67,67	2.57	17 (33%)
3	A86	A	303	-	47,50,50	1.40	5 (10%)	51,76,76	2.10	10 (19%)
5	CLA	A	407	1	69,73,73	1.07	4 (5%)	82,113,113	1.42	14 (17%)
11	SOG	A	413	-	20,20,20	0.87	1 (5%)	24,25,25	0.98	1 (4%)
11	SOG	A	414	-	20,20,20	1.04	1 (5%)	24,25,25	1.26	2 (8%)
5	CLA	A	405	1	50,54,73	1.34	7 (14%)	59,90,113	1.62	13 (22%)
11	SOG	A	415	-	20,20,20	0.84	1 (5%)	24,25,25	0.90	1 (4%)
7	KC1	A	408	1	49,53,53	2.56	19 (38%)	61,89,89	3.87	33 (54%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	A	406	1	1/1/15/20	5/39/115/115	-
3	A86	A	306	-	-	2/34/90/90	0/3/3/3
3	A86	A	307	-	-	3/34/90/90	0/3/3/3
8	LMT	A	410	-	-	8/17/57/61	0/2/2/2
3	A86	A	301	-	-	3/34/90/90	0/3/3/3
5	CLA	A	409	-	1/1/10/20	2/10/86/115	-
6	KC2	A	403	-	-	4/15/71/71	-
10	LHG	A	412	-	-	16/34/34/53	-
3	A86	A	304	-	-	0/34/90/90	0/3/3/3
5	CLA	A	404	1	1/1/15/20	4/39/115/115	-
11	SOG	A	416	-	-	3/6/26/31	0/1/1/1
5	CLA	A	401	13	1/1/14/20	6/35/111/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A86	A	305	-	-	3/34/90/90	0/3/3/3
5	CLA	A	402	1	1/1/15/20	12/39/115/115	-
9	DGD	A	411	-	-	24/40/40/95	-
3	A86	A	302	-	-	4/34/90/90	0/3/3/3
4	DD6	A	308	-	-	9/26/80/80	0/3/3/3
5	CLA	A	407	1	1/1/15/20	13/39/115/115	-
3	A86	A	303	-	-	2/34/90/90	0/3/3/3
11	SOG	A	413	-	-	2/11/31/31	0/1/1/1
11	SOG	A	414	-	-	5/11/31/31	0/1/1/1
5	CLA	A	405	1	1/1/11/20	8/17/93/115	-
11	SOG	A	415	-	-	3/11/31/31	0/1/1/1
7	KC1	A	408	1	-	1/15/71/71	-

The worst 5 of 126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	308	DD6	C30-C31	-8.62	1.25	1.42
6	A	403	KC2	C4C-NC	7.25	1.49	1.37
7	A	408	KC1	C4C-NC	6.61	1.48	1.37
6	A	403	KC2	C2A-C3A	5.63	1.48	1.37
6	A	403	KC2	CHD-C4C	5.38	1.49	1.38

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	403	KC2	C1A-NA-C4A	-10.42	101.92	106.68
7	A	408	KC1	CHD-C4C-C3C	-10.18	106.46	125.23
7	A	408	KC1	CHD-C4C-NC	9.84	139.13	124.31
3	A	306	A86	C20-O1-C15	9.27	65.01	61.03
6	A	403	KC2	CHD-C4C-NC	8.53	137.16	124.31

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	401	CLA	ND
5	A	402	CLA	ND
5	A	404	CLA	ND
5	A	405	CLA	ND
5	A	406	CLA	ND

5 of 142 torsion outliers are listed below:

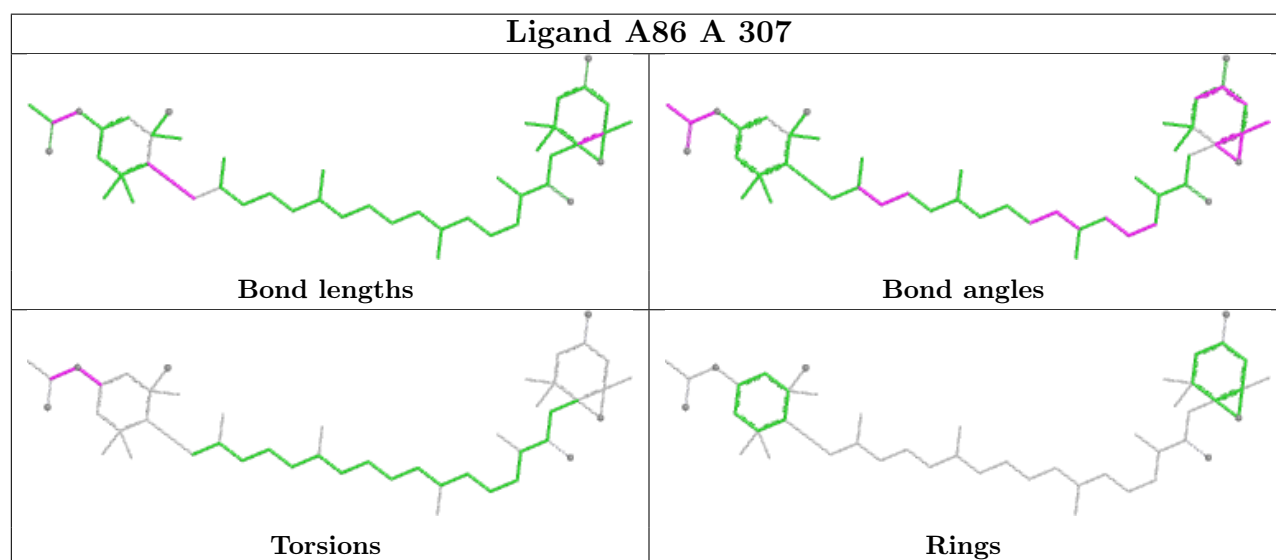
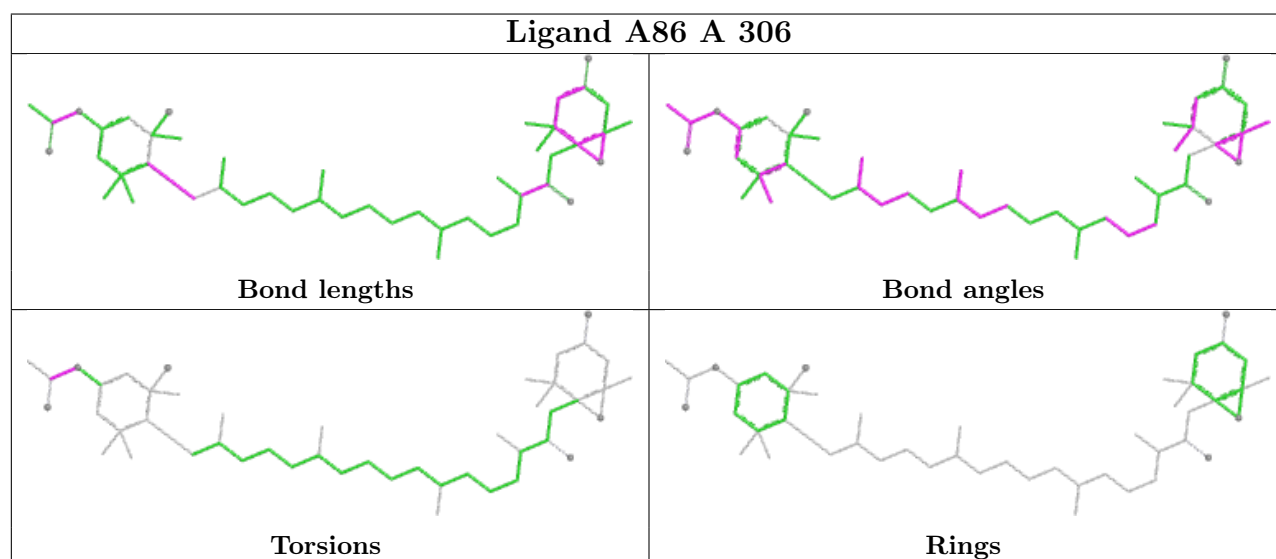
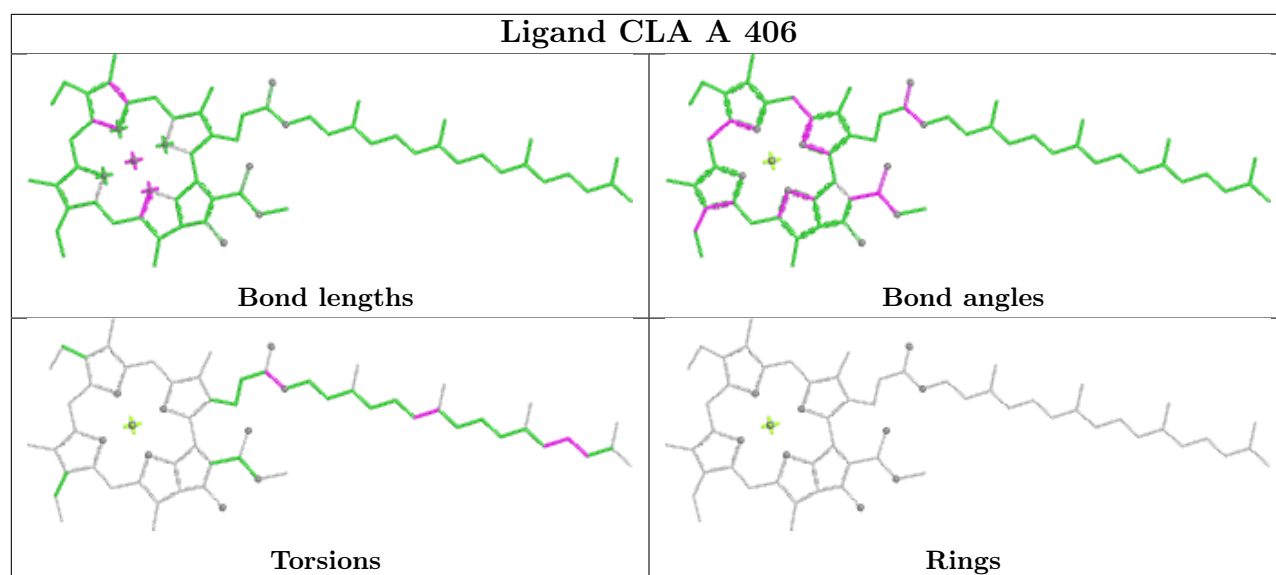
Mol	Chain	Res	Type	Atoms
3	A	301	A86	O5-C38-O4-C34
3	A	302	A86	C39-C38-O4-C34
3	A	306	A86	C39-C38-O4-C34
3	A	307	A86	C39-C38-O4-C34
4	A	308	DD6	C2-C1-C24-C25

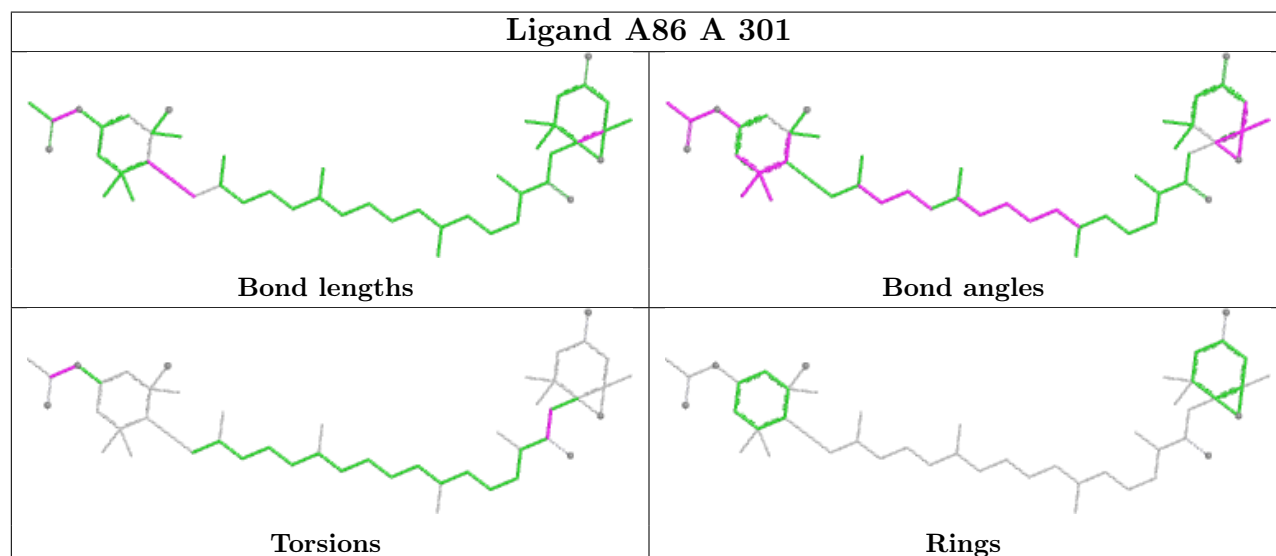
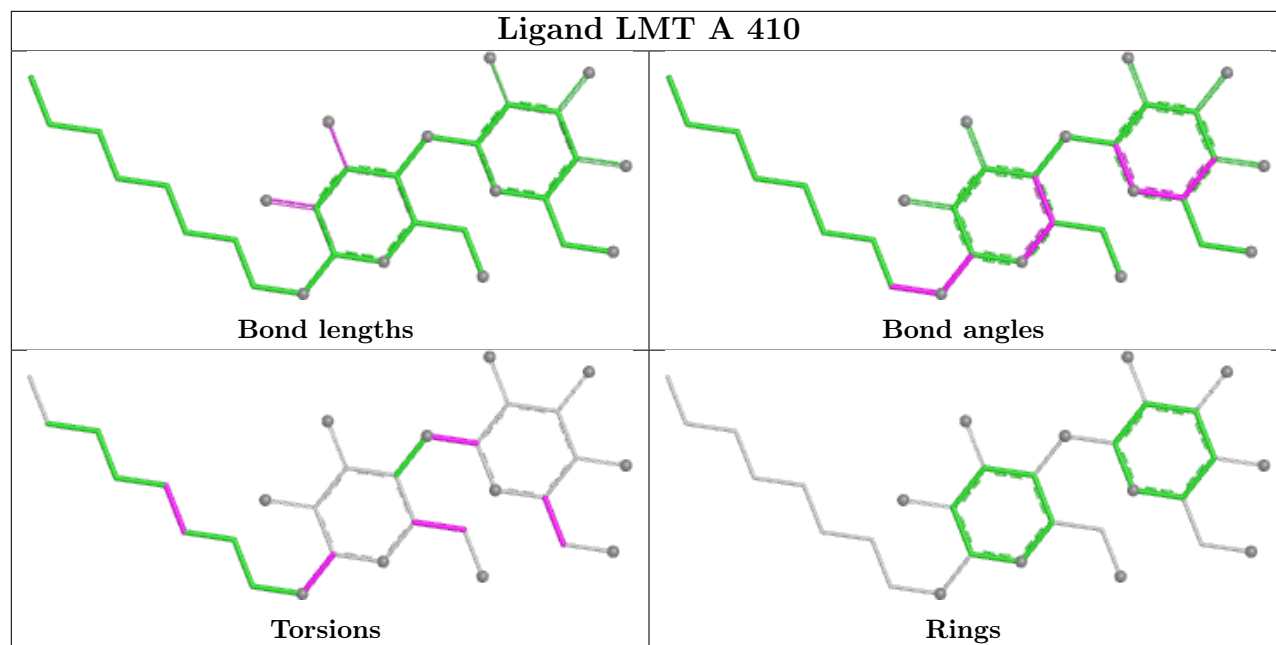
There are no ring outliers.

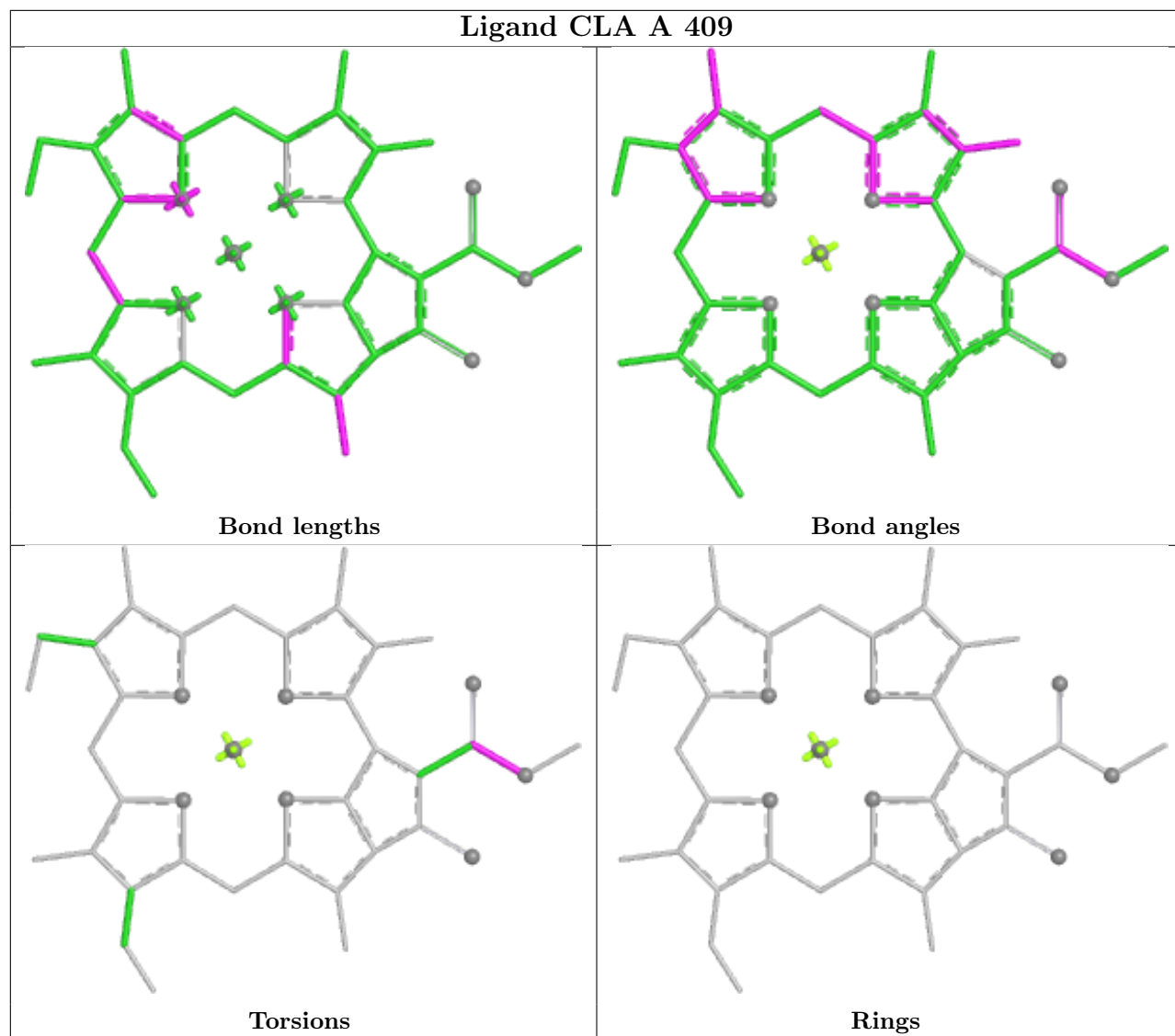
12 monomers are involved in 19 short contacts:

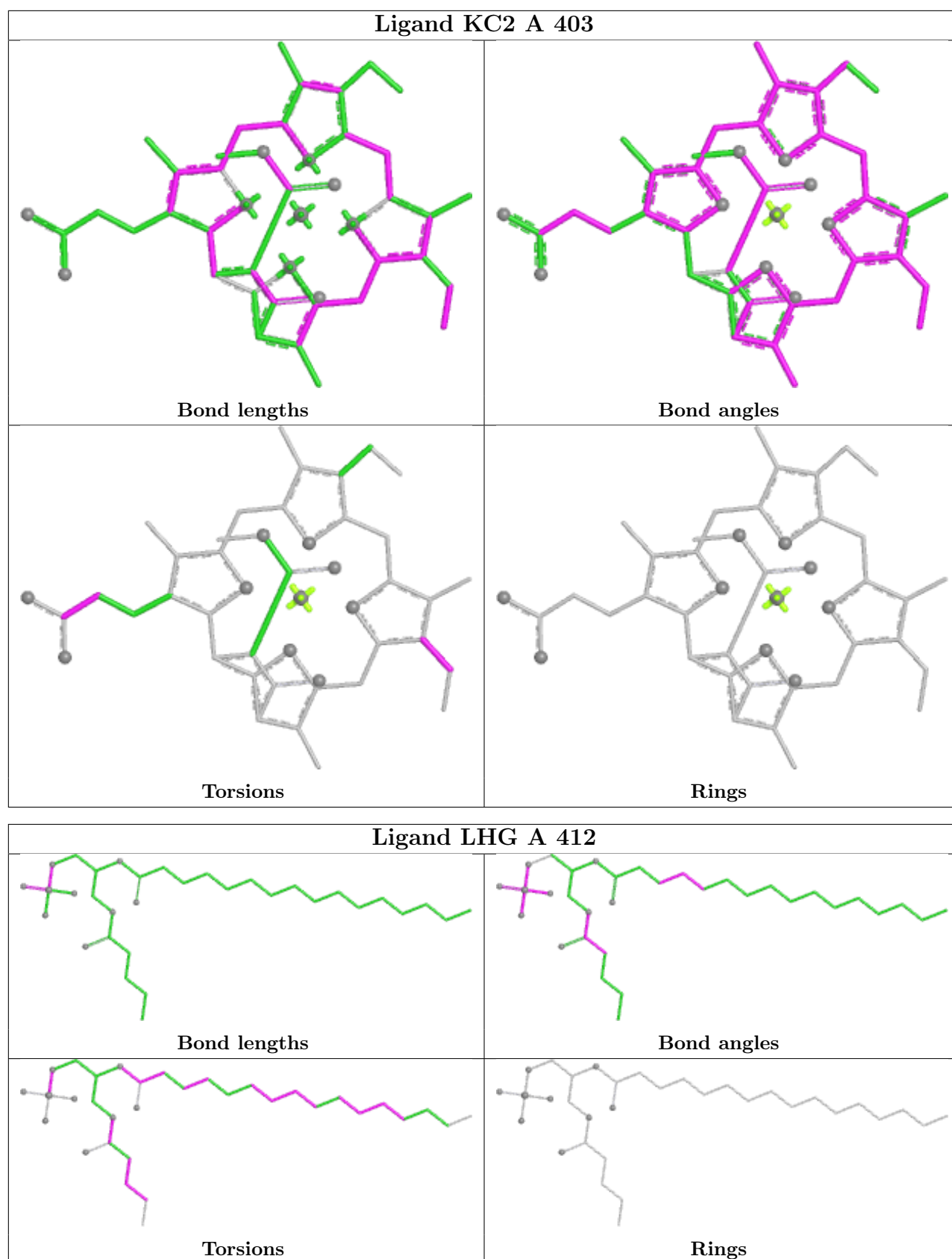
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	CLA	2	0
5	A	409	CLA	4	0
10	A	412	LHG	1	0
5	A	404	CLA	1	0
11	A	416	SOG	1	0
5	A	401	CLA	1	0
5	A	402	CLA	1	0
9	A	411	DGD	4	0
5	A	407	CLA	2	0
11	A	413	SOG	2	0
11	A	414	SOG	1	0
5	A	405	CLA	2	0

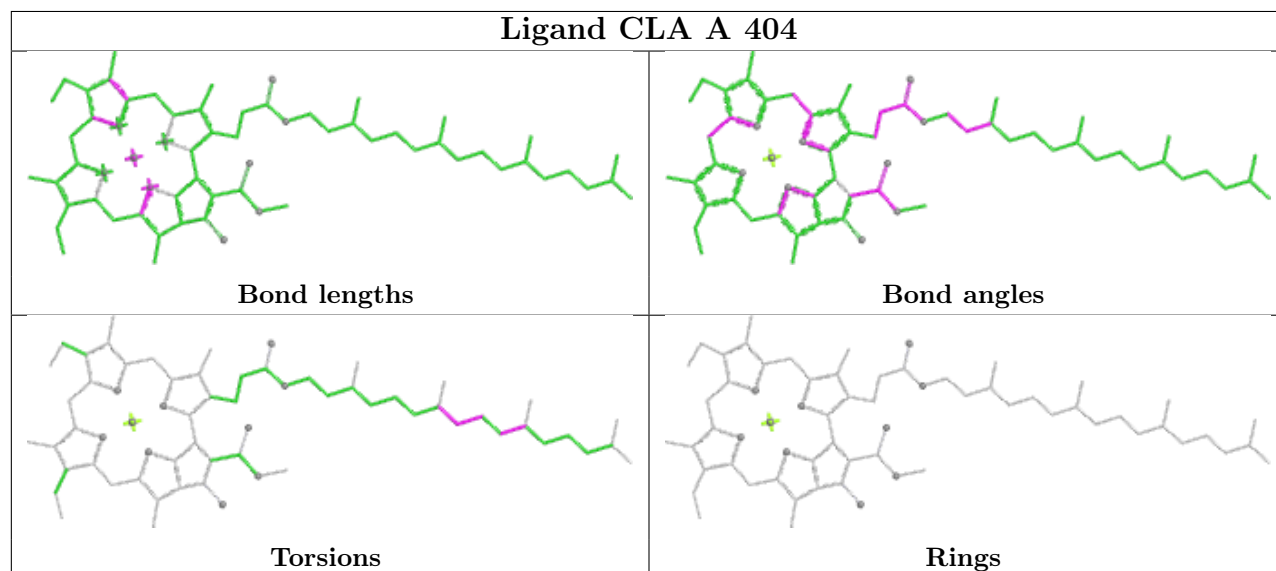
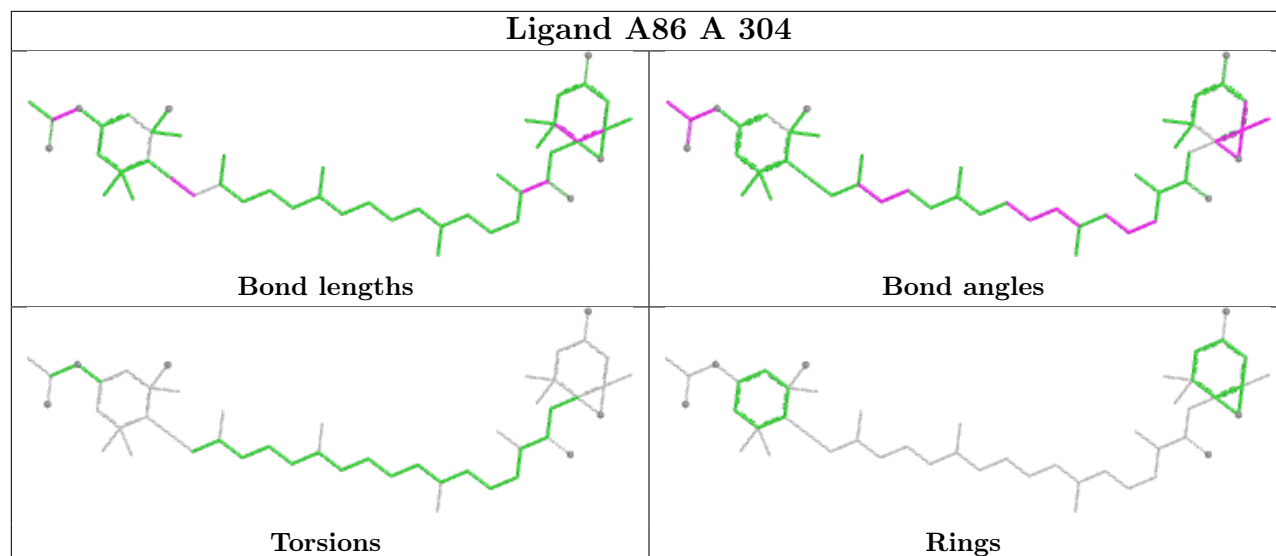
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

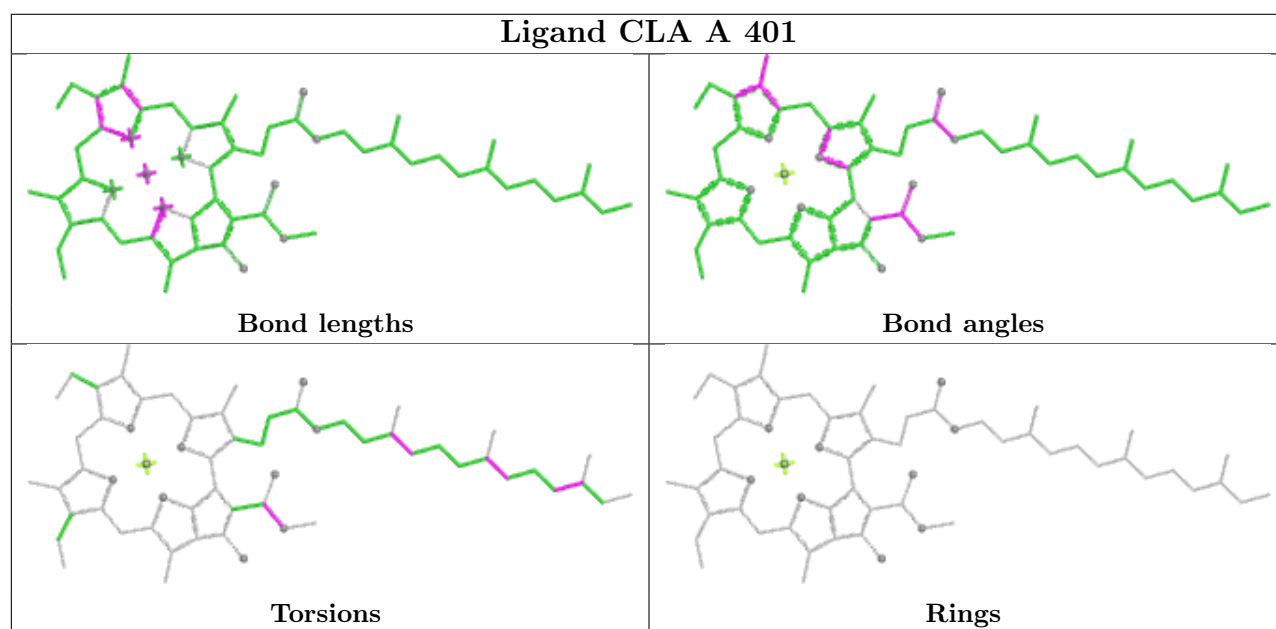
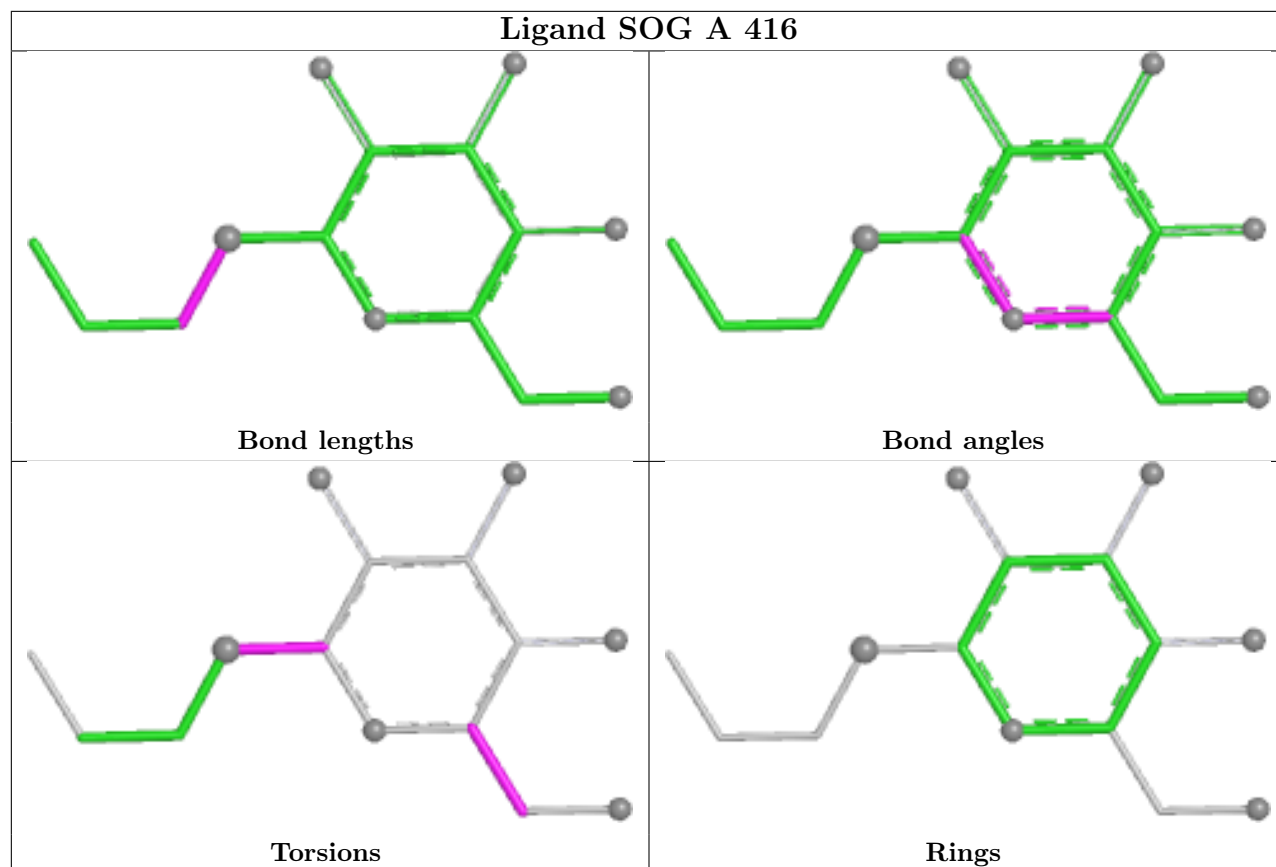


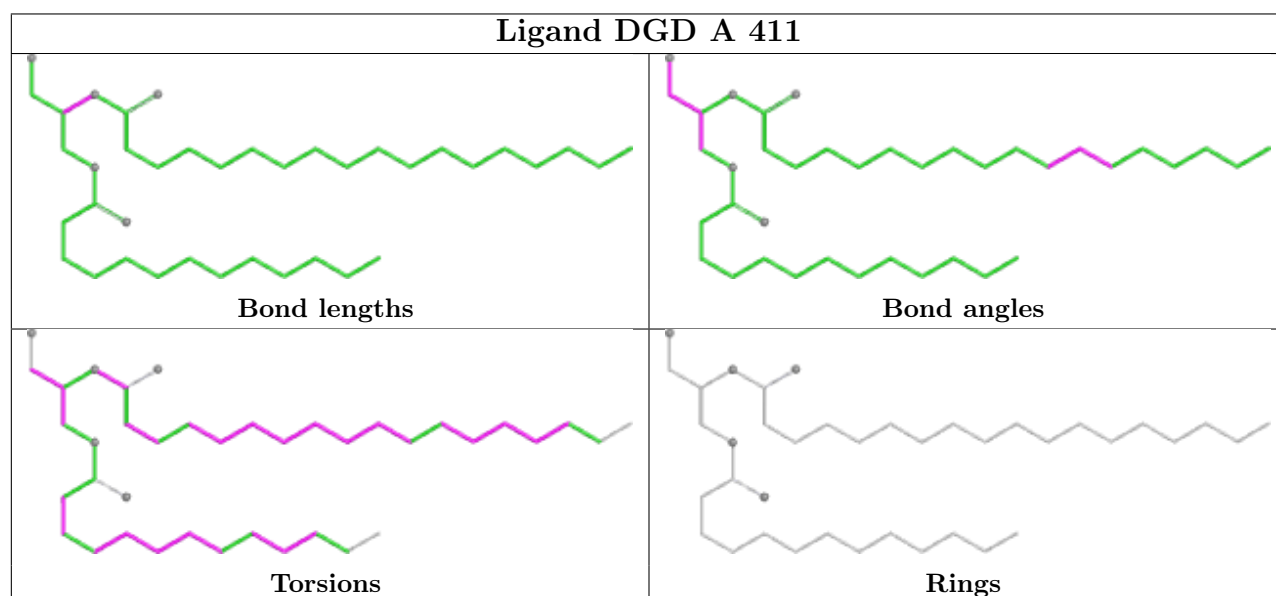
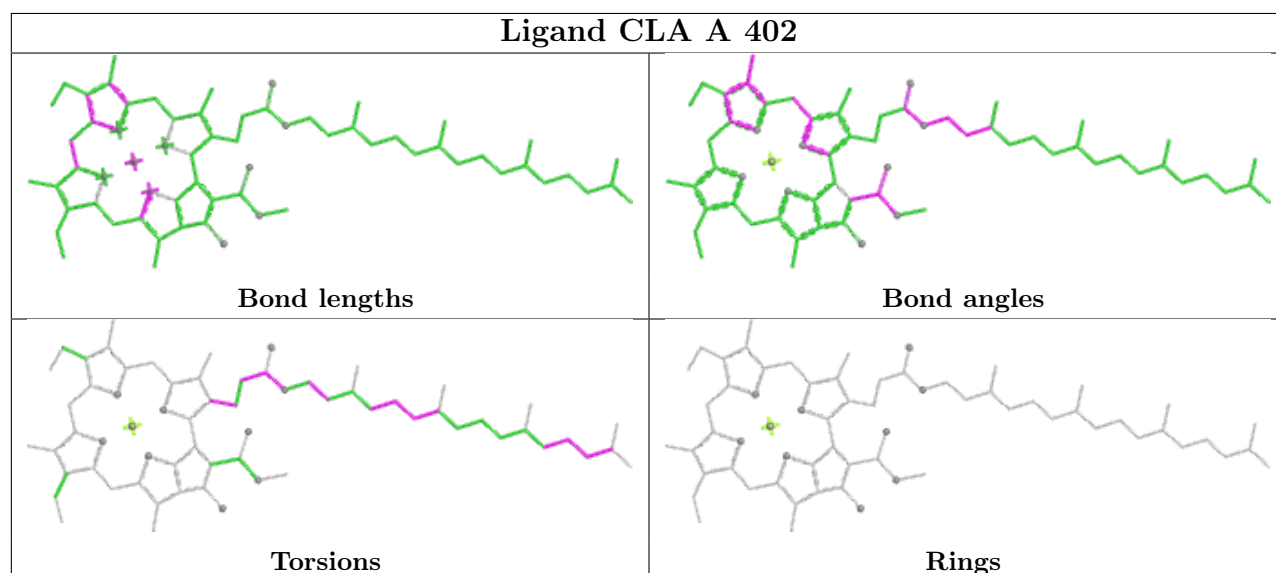
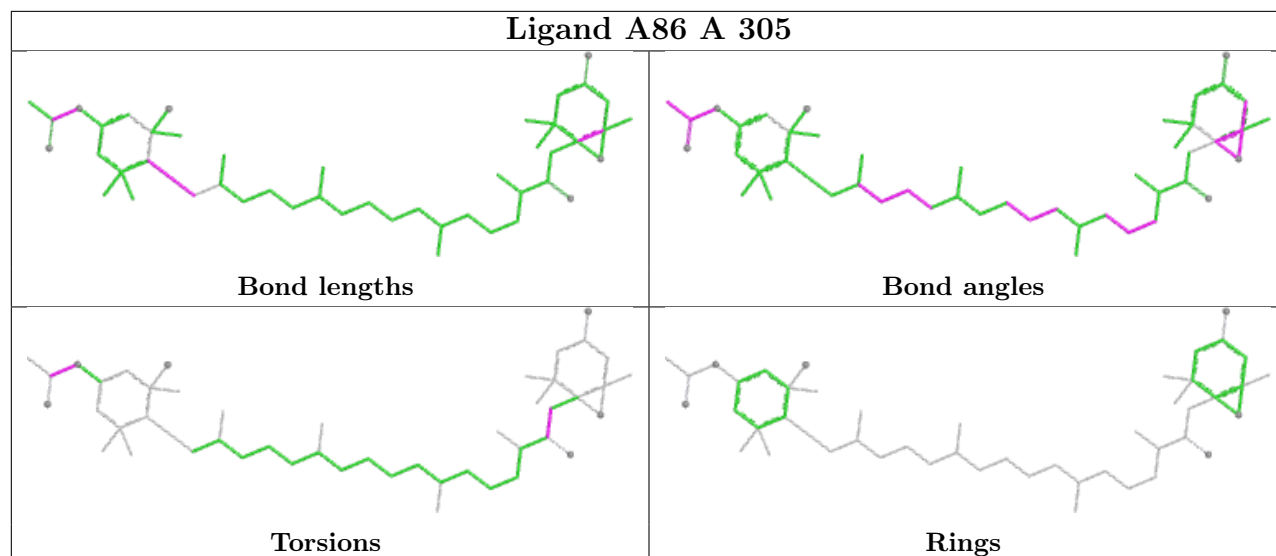


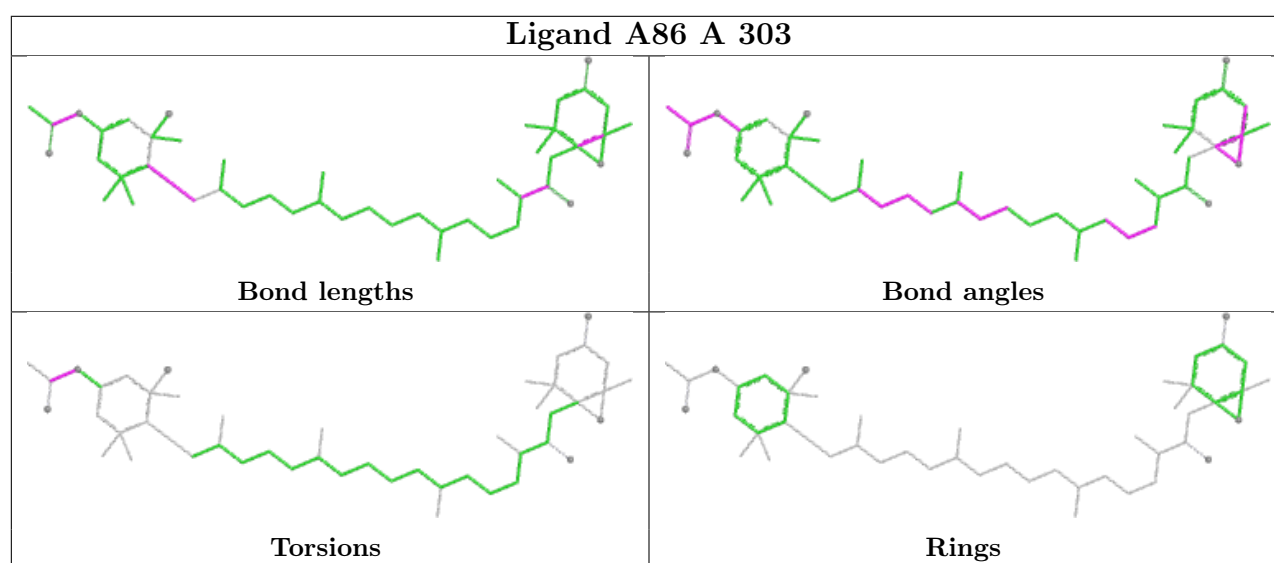
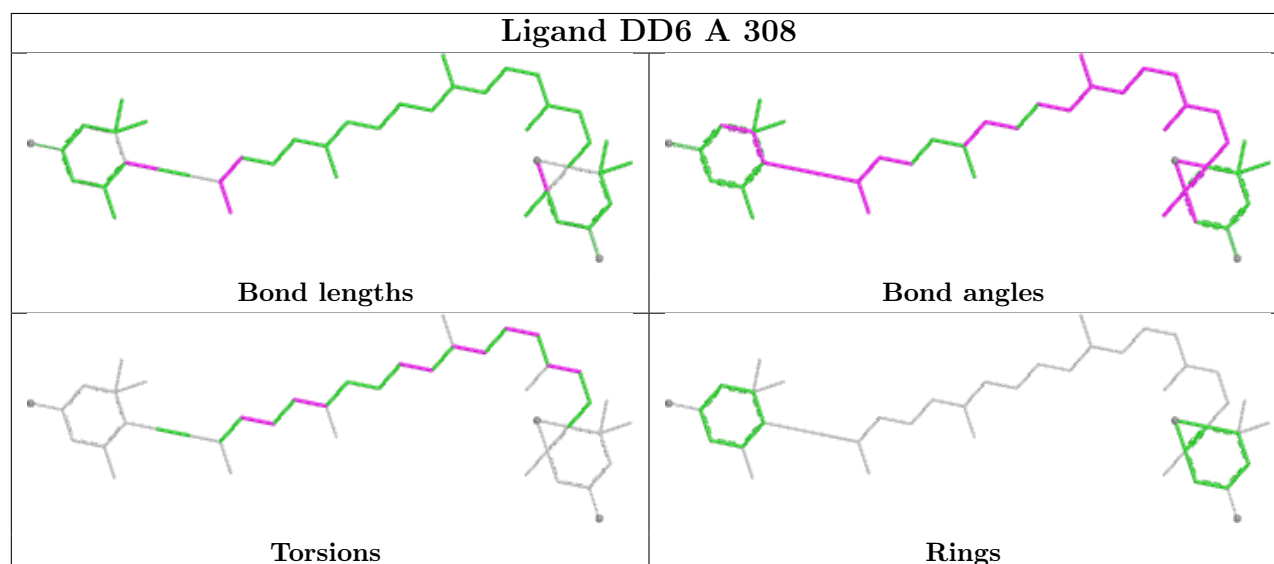
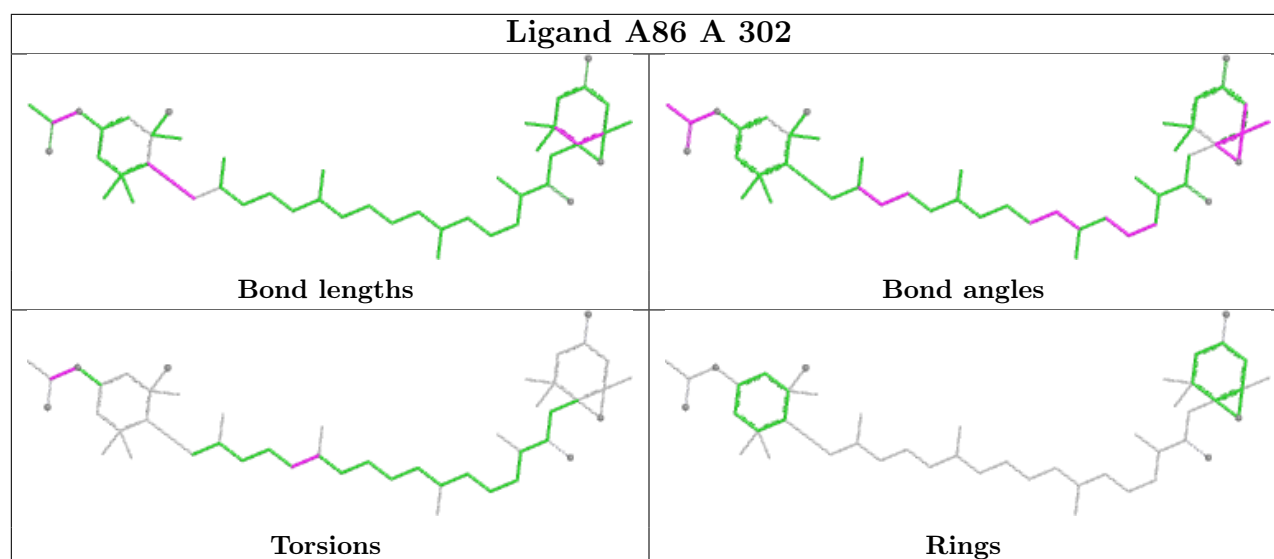


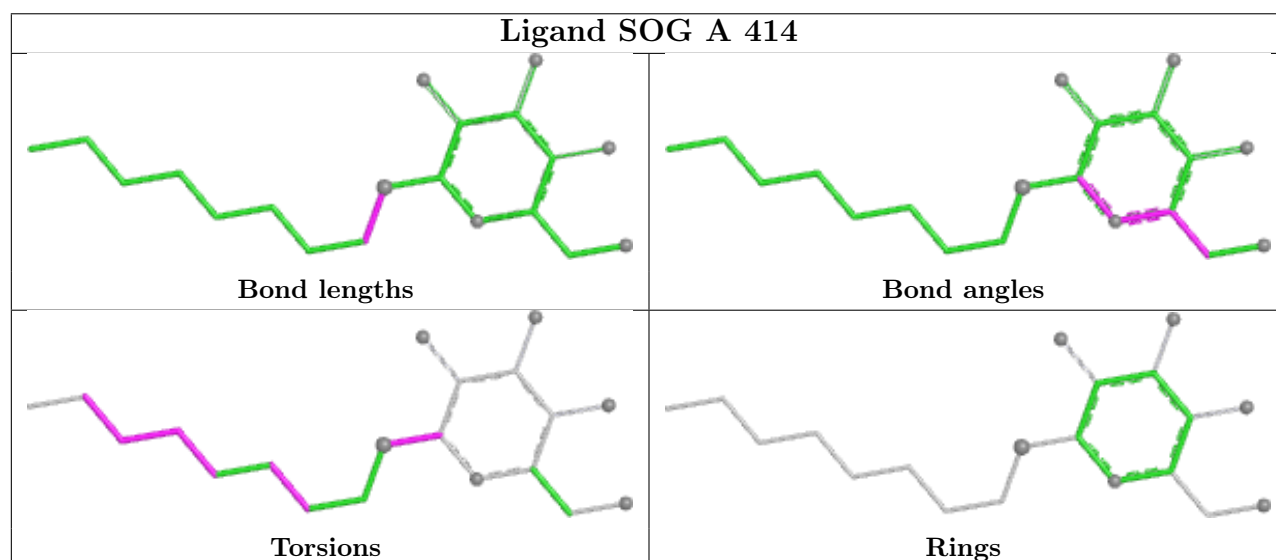
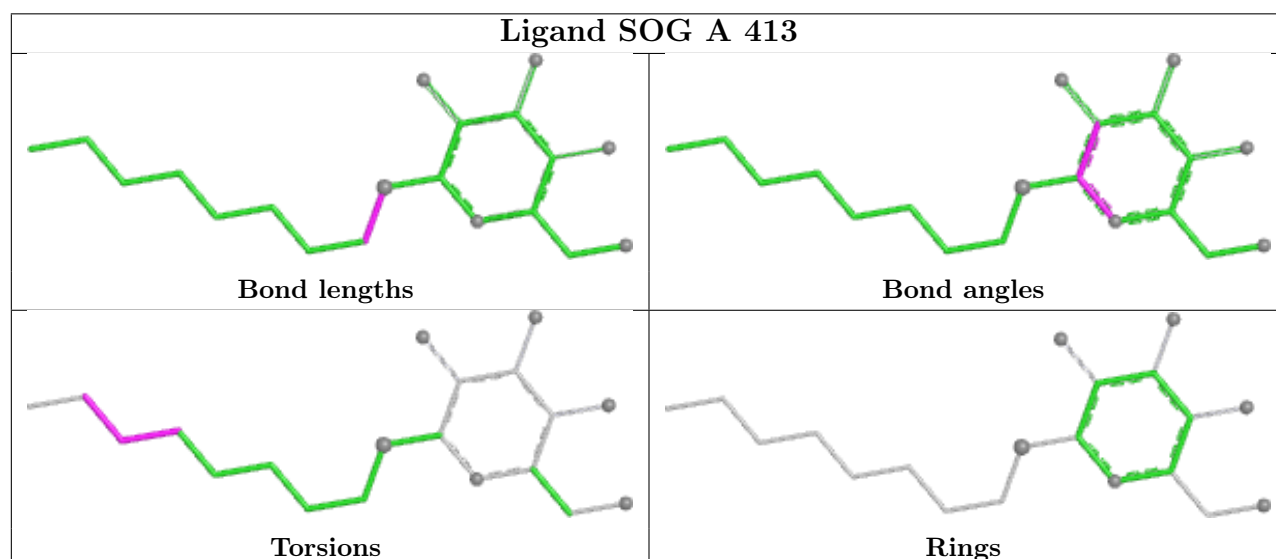
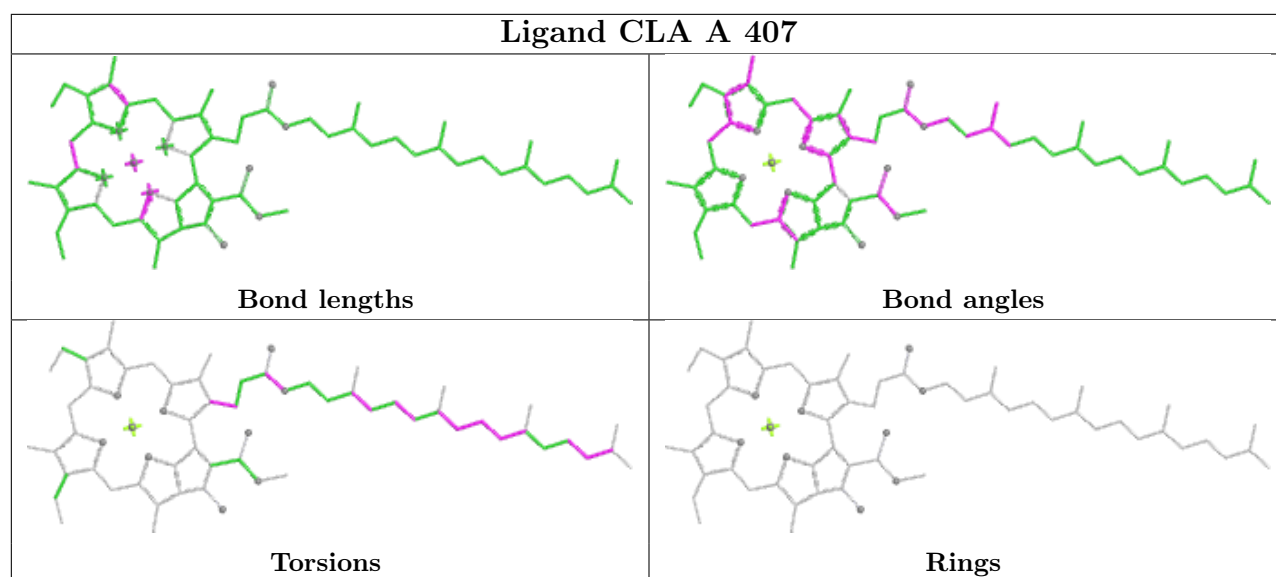


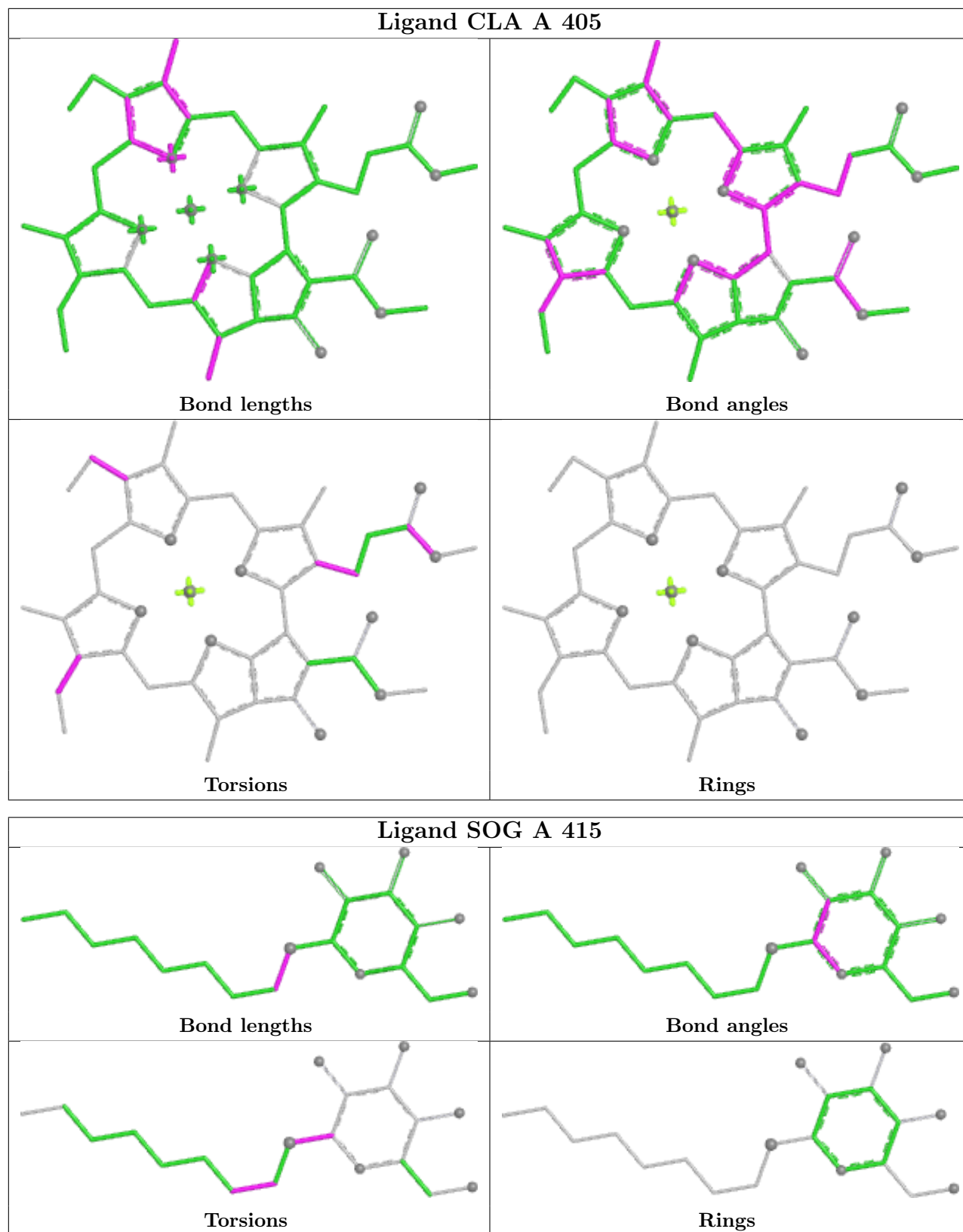


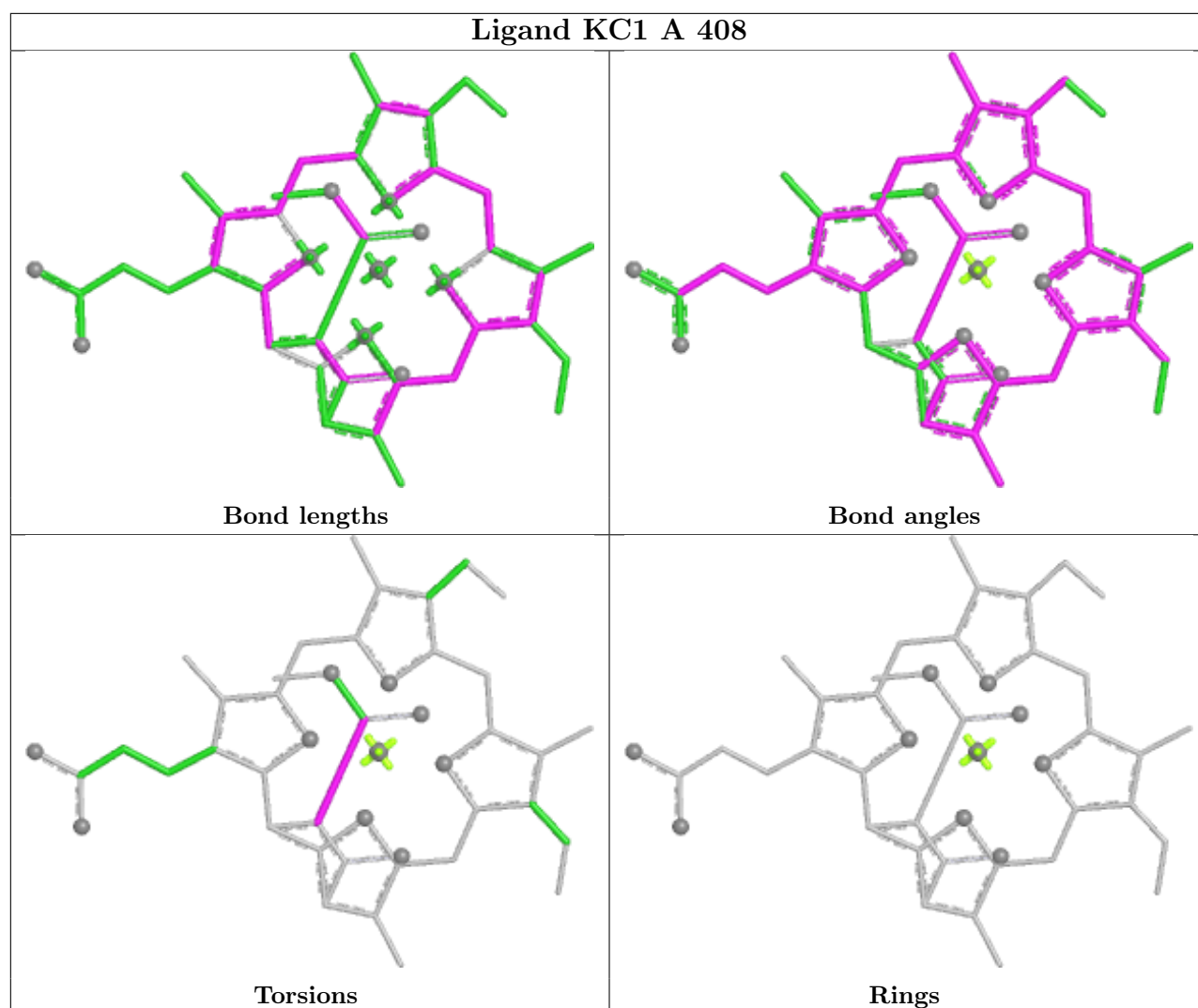












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	166/167 (99%)	-0.14	2 (1%) 76 77	13, 35, 63, 79	3 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	3.3
1	A	166	PRO	2.5

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
8	LMT	A	410	31/35	0.66	0.15	49,110,124,127	0
4	DD6	A	308	43/43	0.67	0.20	70,84,104,109	0
12	UNL	A	423	10/-	0.68	0.17	62,64,65,65	0
12	UNL	A	420	12/-	0.69	0.19	56,60,64,64	0
9	DGD	A	411	39/66	0.74	0.18	68,86,99,105	0

Continued on next page...

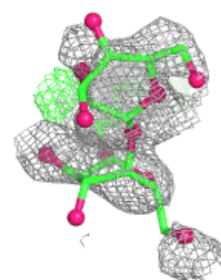
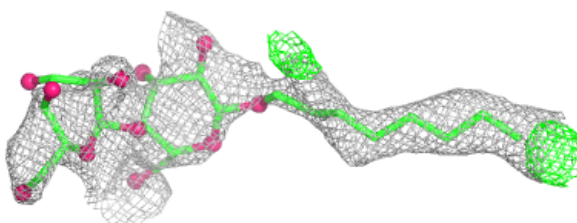
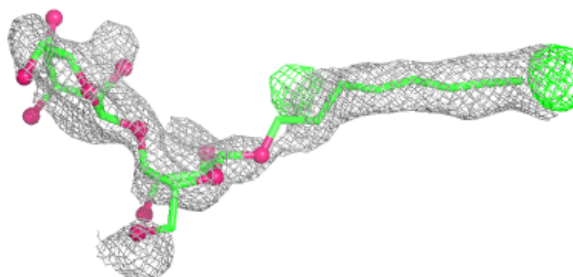
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	UNL	A	422	7/-	0.76	0.19	43,54,60,61	0
11	SOG	A	416	15/20	0.76	0.18	90,96,104,105	0
11	SOG	A	413	20/20	0.77	0.16	48,105,119,120	0
12	UNL	A	421	12/-	0.78	0.14	52,55,67,69	0
10	LHG	A	412	33/49	0.80	0.15	45,66,123,127	0
12	UNL	A	418	12/-	0.80	0.12	58,61,68,69	0
12	UNL	A	417	12/-	0.84	0.14	47,52,59,60	0
11	SOG	A	415	20/20	0.85	0.13	55,100,105,110	0
11	SOG	A	414	20/20	0.87	0.13	43,93,104,109	0
12	UNL	A	419	8/-	0.87	0.10	49,54,56,59	0
3	A86	A	306	48/48	0.91	0.09	35,49,72,85	0
2	CA	A	202	1/1	0.92	0.10	76,76,76,76	0
5	CLA	A	402	65/65	0.94	0.09	25,37,74,79	0
5	CLA	A	405	46/65	0.94	0.08	31,43,60,75	0
3	A86	A	301	48/48	0.95	0.09	26,43,93,105	0
5	CLA	A	406	65/65	0.95	0.09	19,28,70,78	0
5	CLA	A	401	61/65	0.95	0.07	21,35,66,71	0
3	A86	A	307	48/48	0.95	0.07	23,31,55,58	0
3	A86	A	305	48/48	0.96	0.06	17,28,50,63	0
3	A86	A	303	48/48	0.96	0.06	20,27,51,58	0
5	CLA	A	407	65/65	0.96	0.08	15,25,75,83	0
5	CLA	A	409	41/65	0.96	0.07	31,44,61,67	0
3	A86	A	304	48/48	0.96	0.07	21,28,59,76	0
5	CLA	A	404	65/65	0.96	0.06	18,25,51,59	0
7	KC1	A	408	45/45	0.97	0.05	19,24,31,56	0
3	A86	A	302	48/48	0.97	0.06	18,28,66,73	0
6	KC2	A	403	45/45	0.97	0.05	24,30,43,57	0
2	CA	A	201	1/1	0.99	0.04	39,39,39,39	0

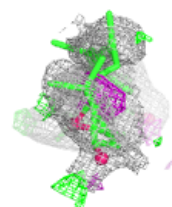
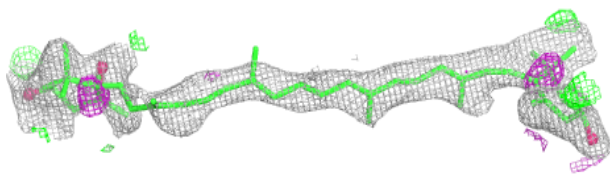
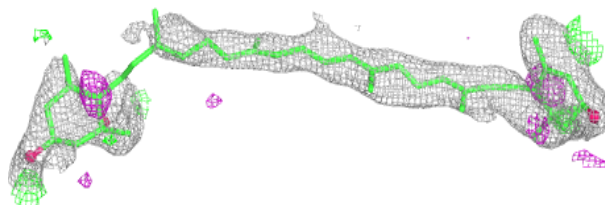
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

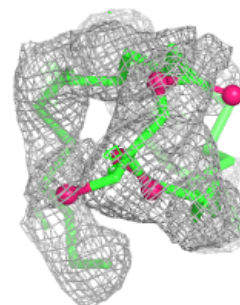
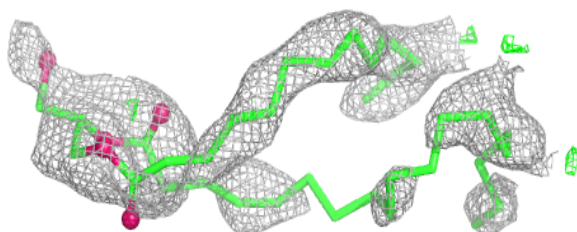
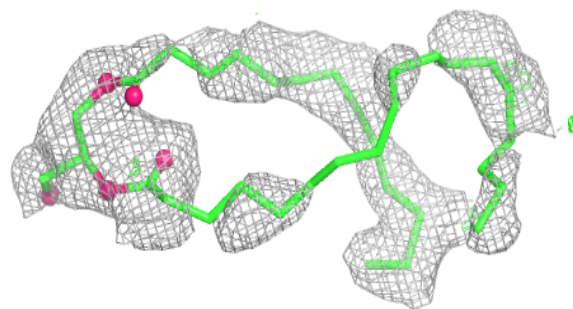
**Electron density around DD6 A 308:**

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

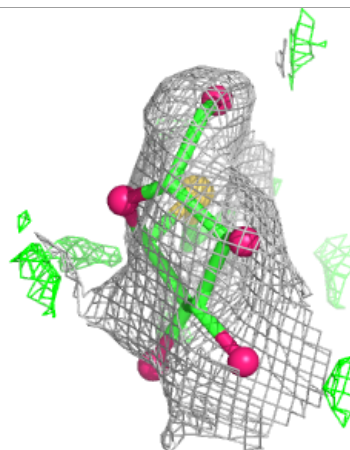
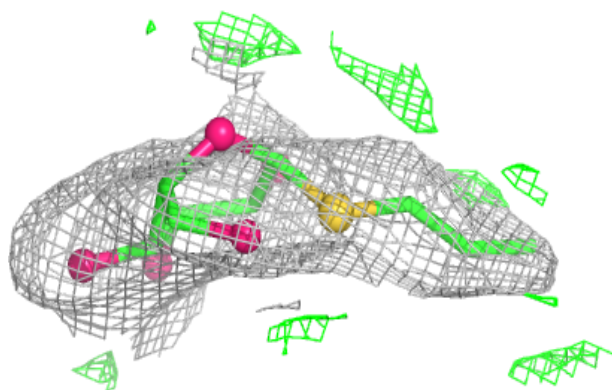
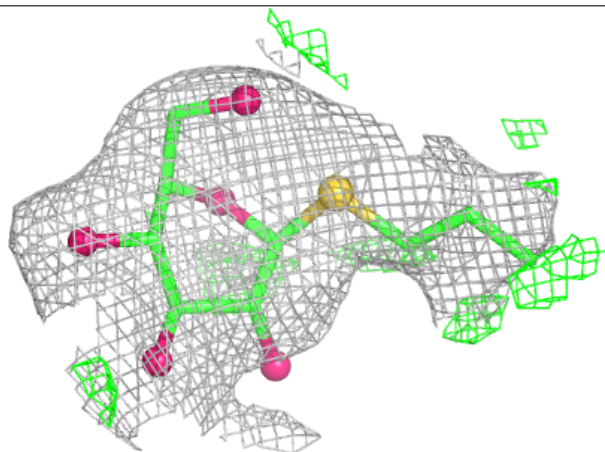


Electron density around DGD A 411:

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

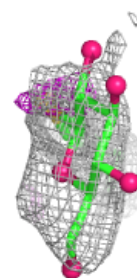
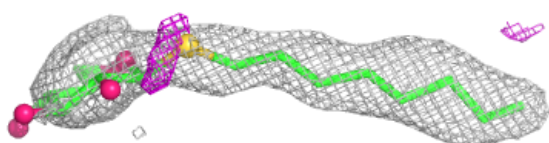
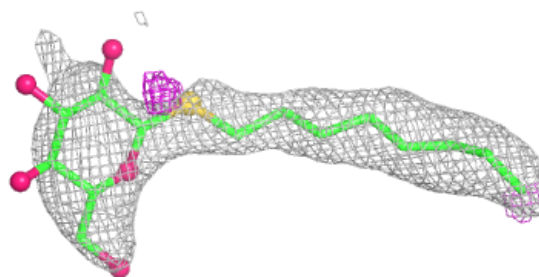
**Electron density around SOG A 416:**

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

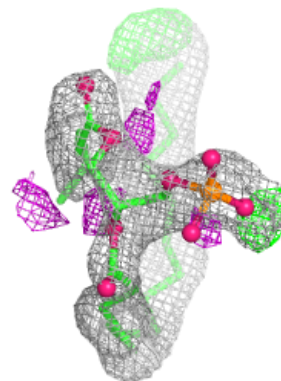
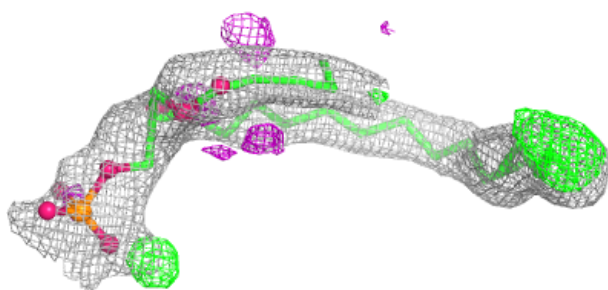
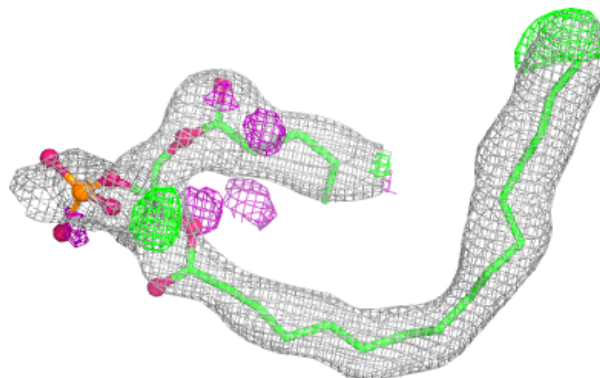


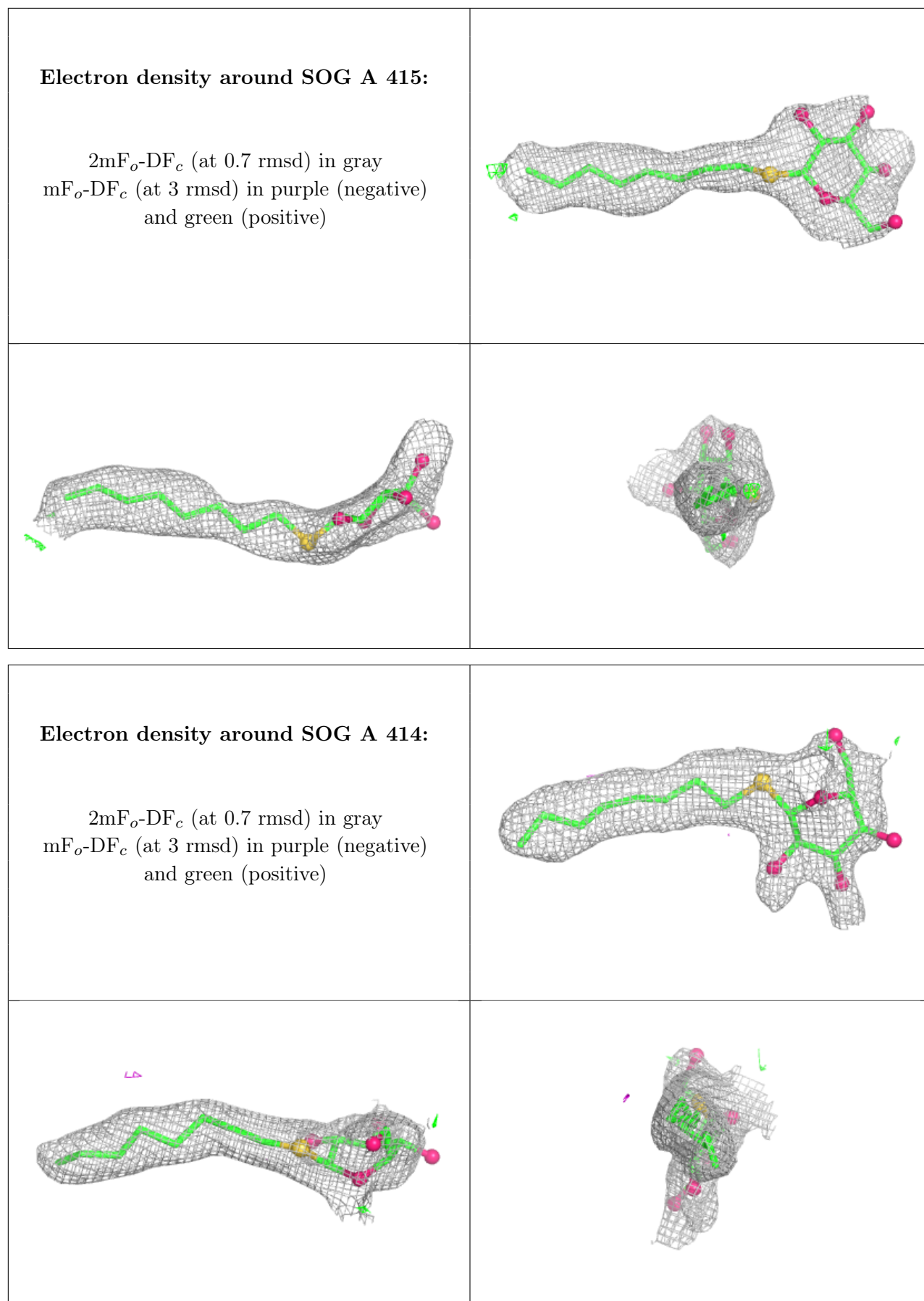
Electron density around SOG A 413:

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

**Electron density around LHG A 412:**

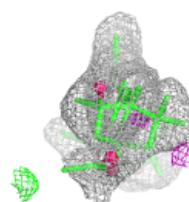
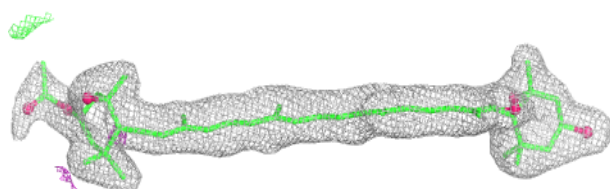
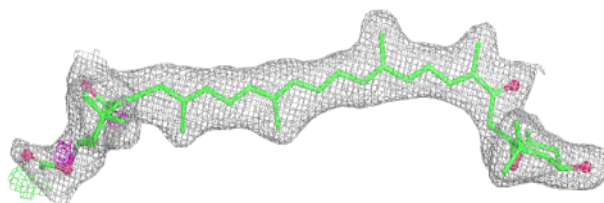
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



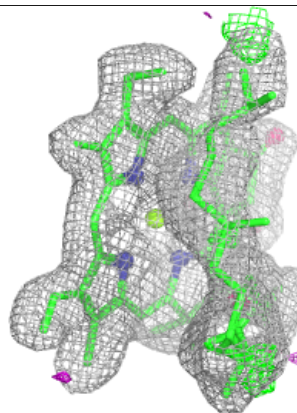
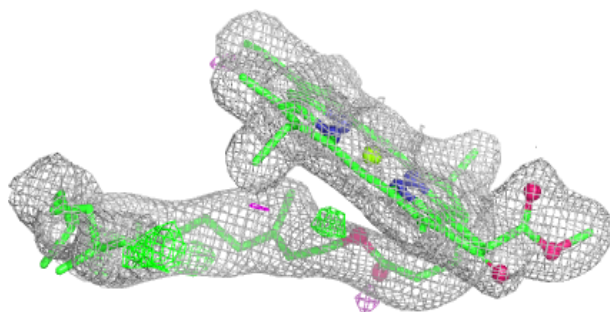
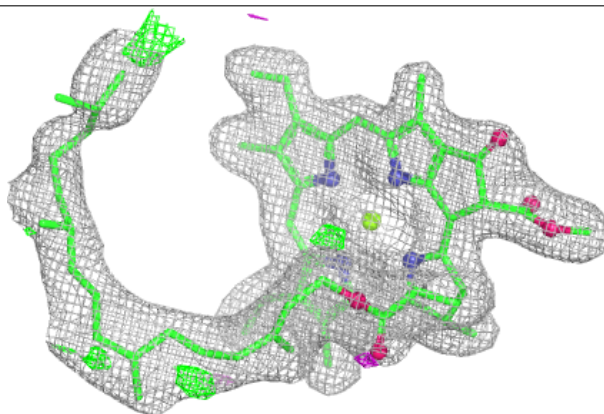


Electron density around A86 A 306:

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

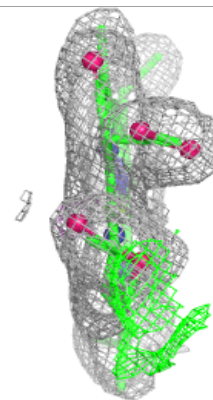
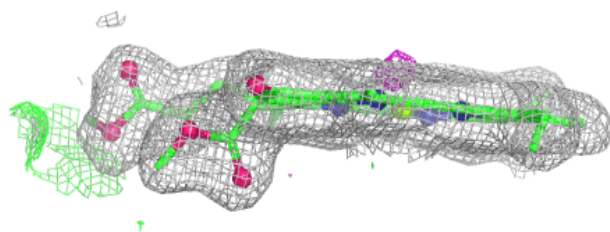
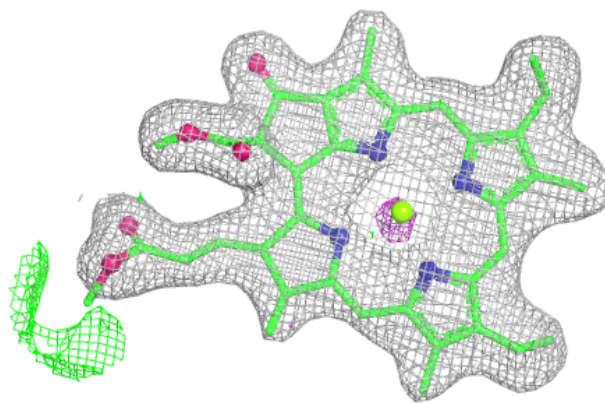
**Electron density around CLA A 402:**

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

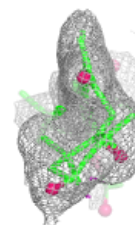
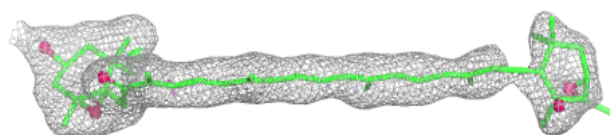
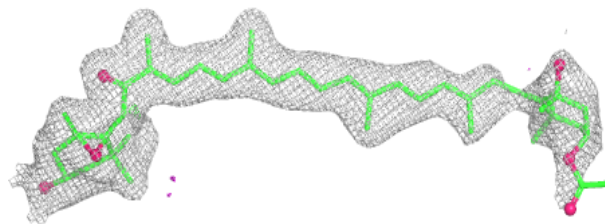


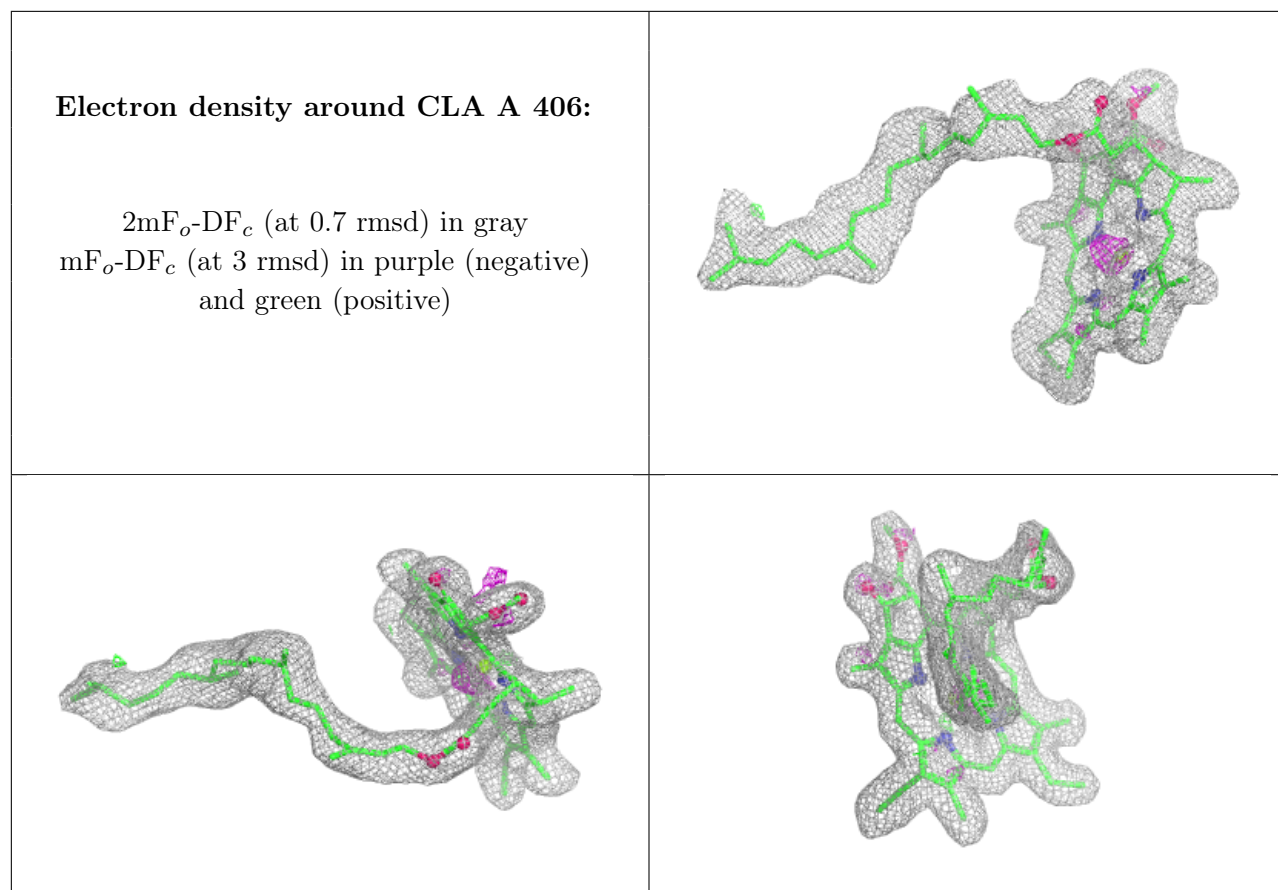
Electron density around CLA A 405:

$2mF_o-DF_c$ (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:**

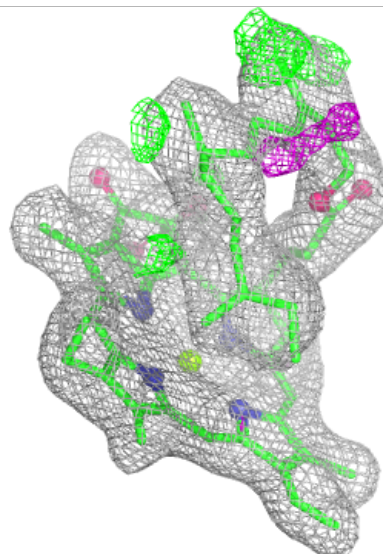
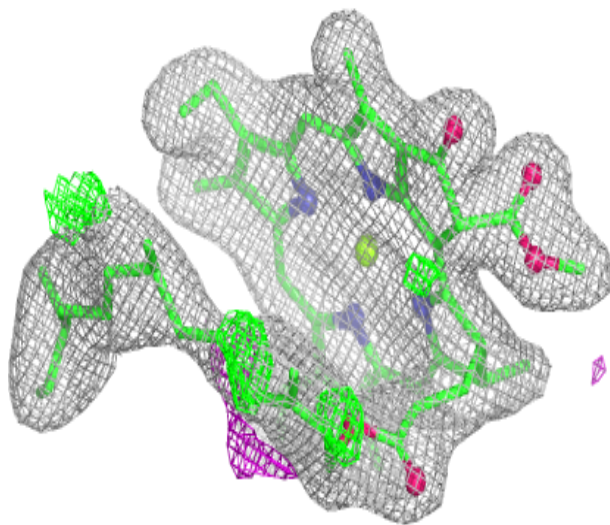
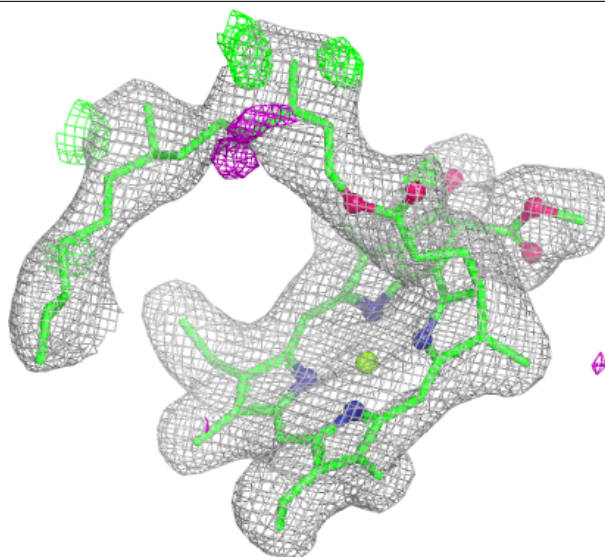
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





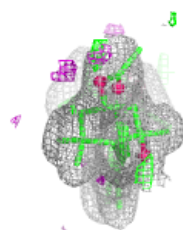
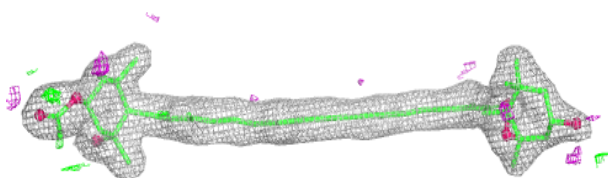
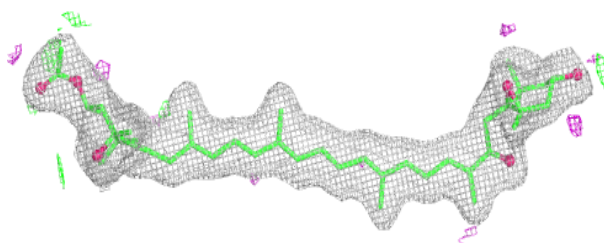
Electron density around CLA A 401:

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

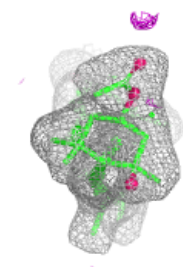
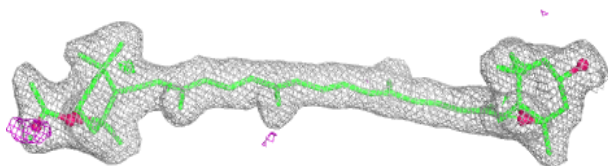
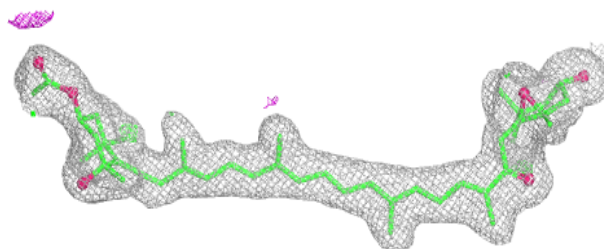


Electron density around A86 A 307:

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

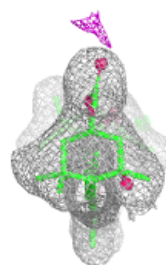
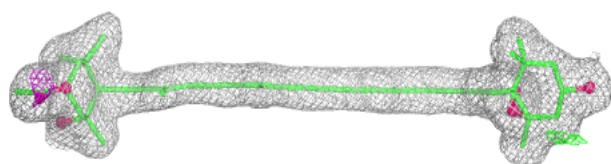
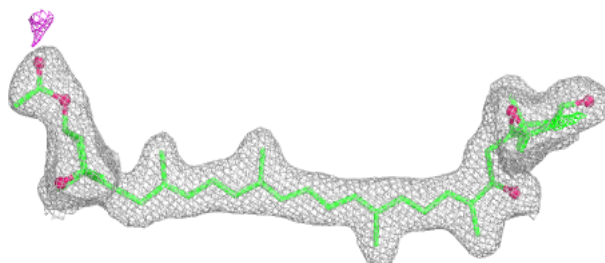
**Electron density around A86 A 305:**

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

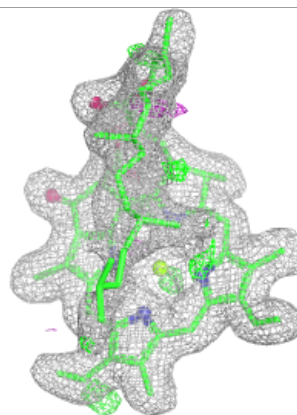
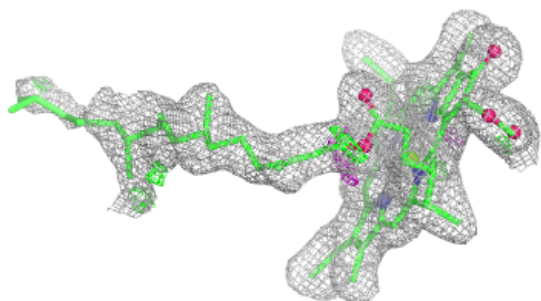
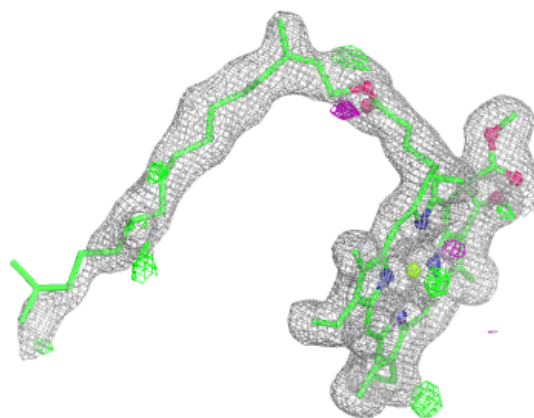


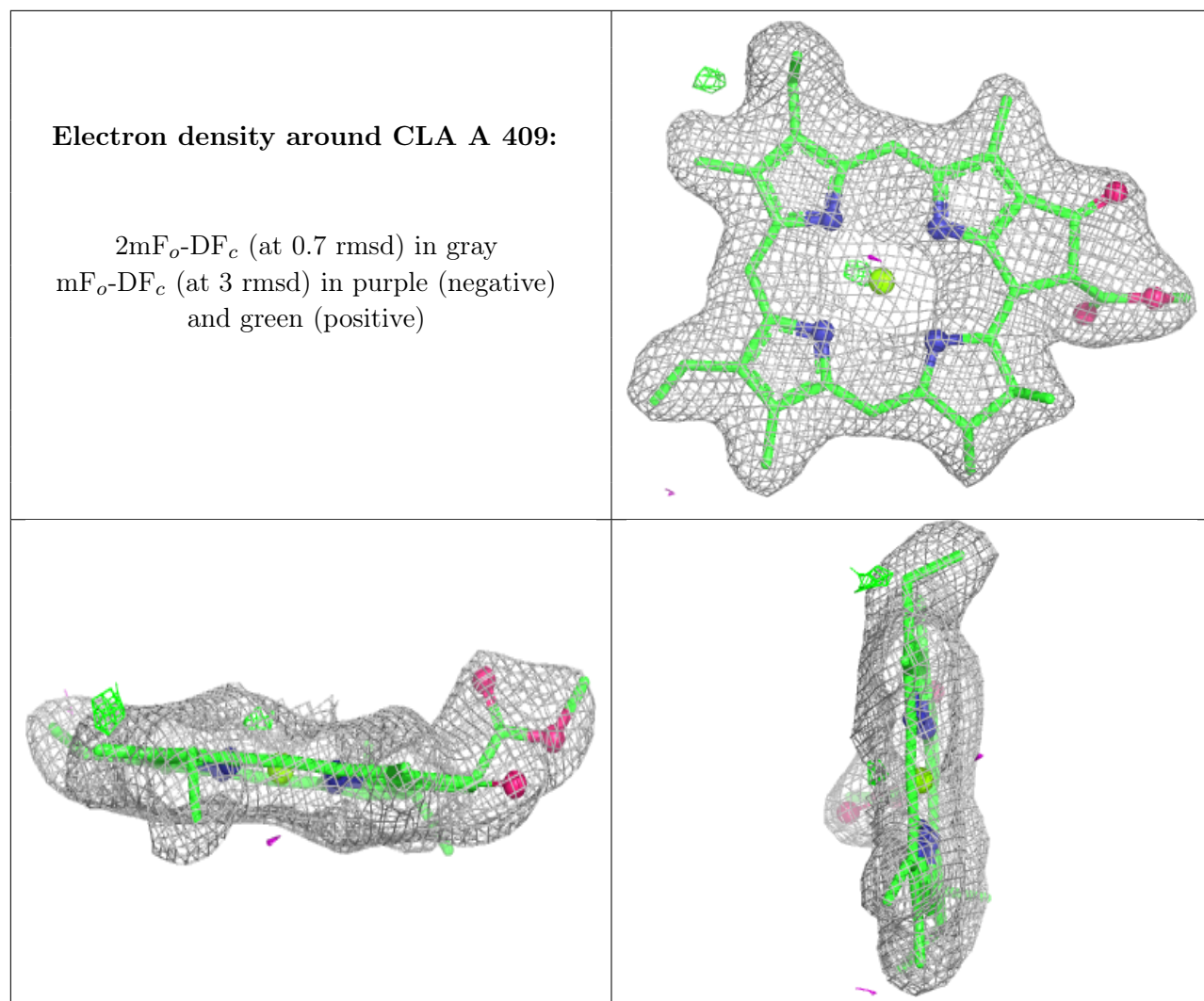
Electron density around A86 A 303:

$2mF_o-DF_c$ (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:**

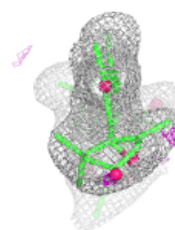
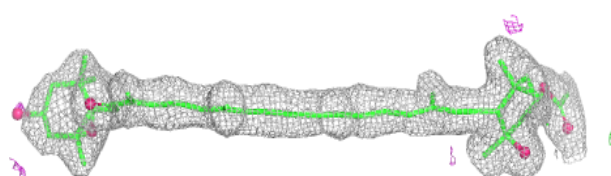
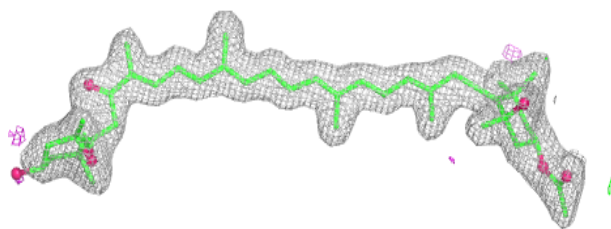
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



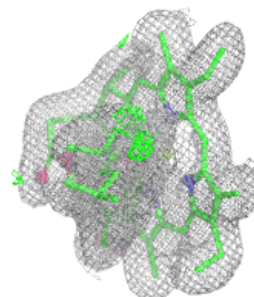
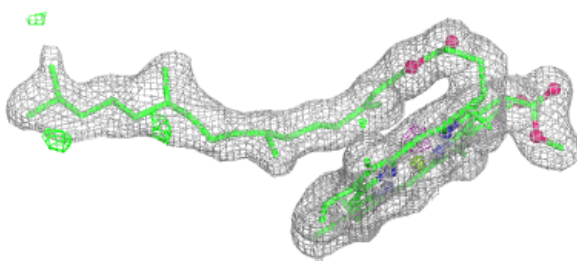
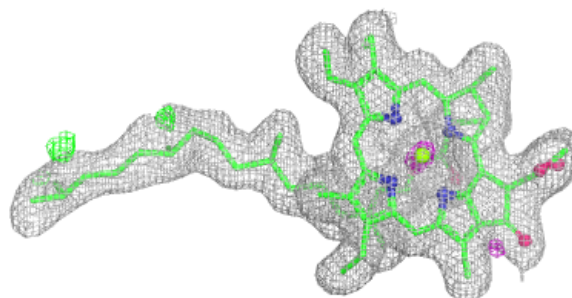


Electron density around A86 A 304:

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

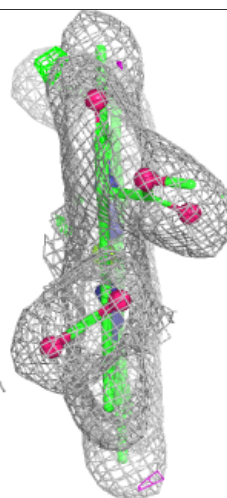
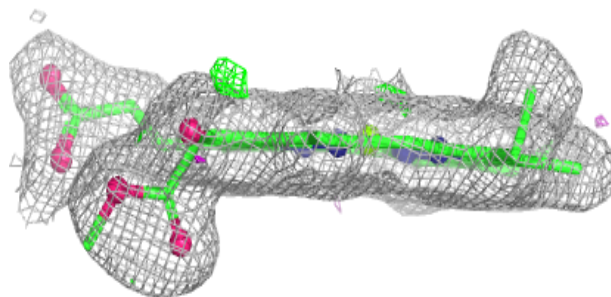
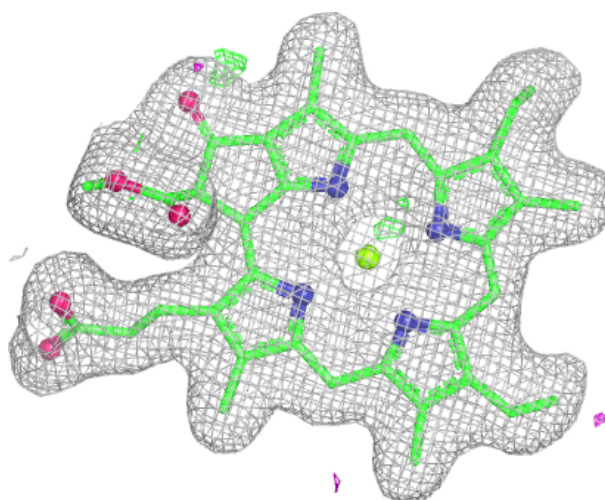
**Electron density around CLA A 404:**

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



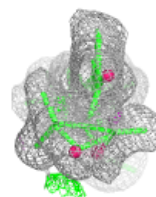
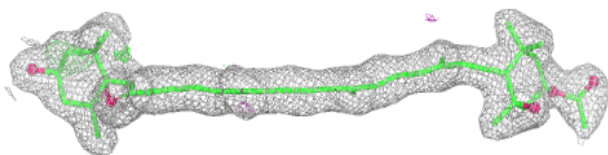
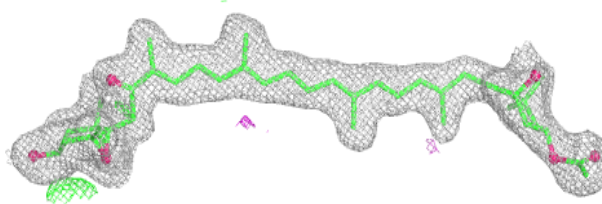
Electron density around KC1 A 408:

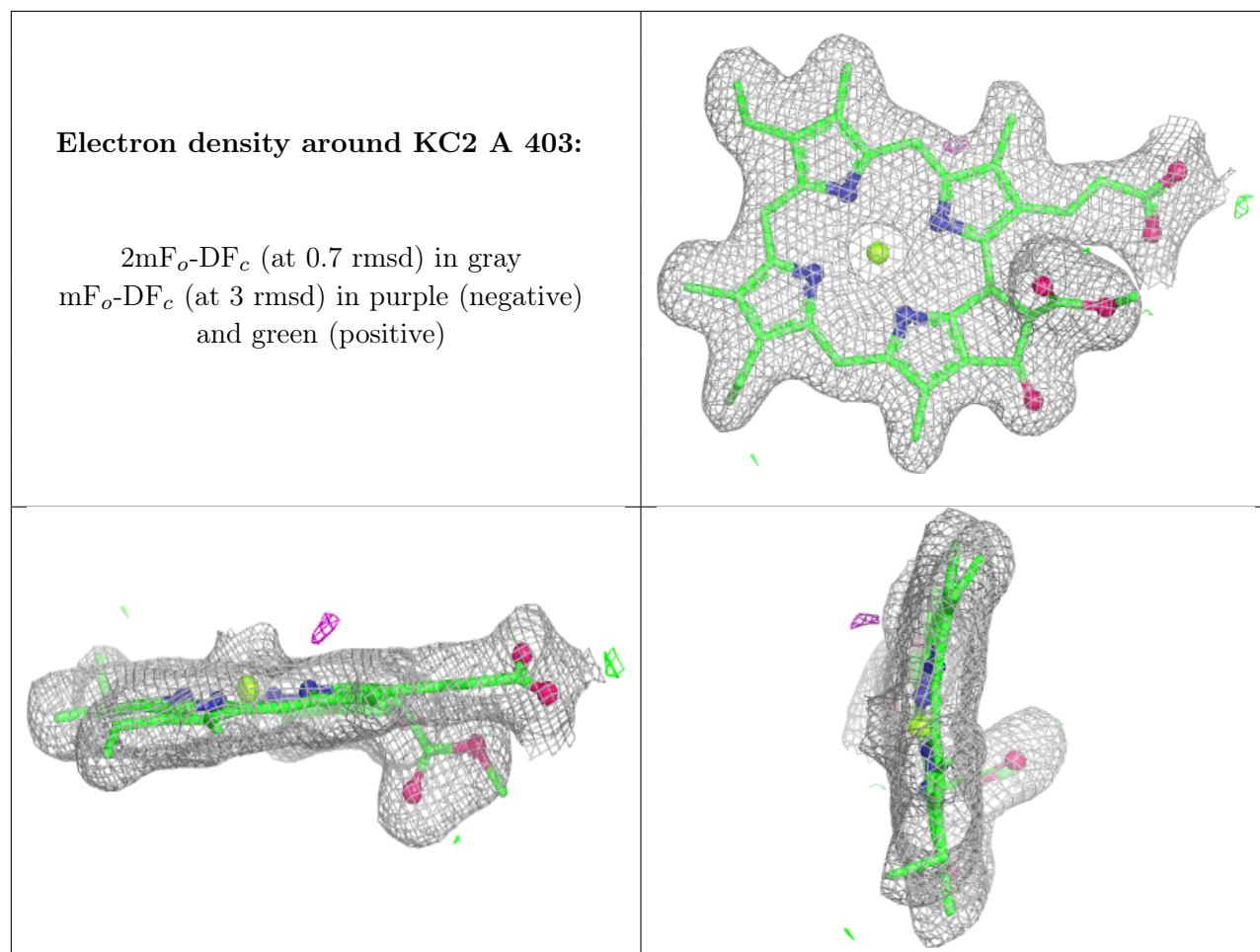
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.