



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:06 PM UTC

PDB ID : 8R2I / pdb_00008r2i
EMDB ID : EMD-18848
Title : Cryo-EM Structure of native Photosystem II assembly intermediate from Chlamydomonas reinhardtii
Authors : Fadeeva, M.; Klaiman, D.; Kandiah, E.; Nelson, N.
Deposited on : 2023-11-06
Resolution : 2.90 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

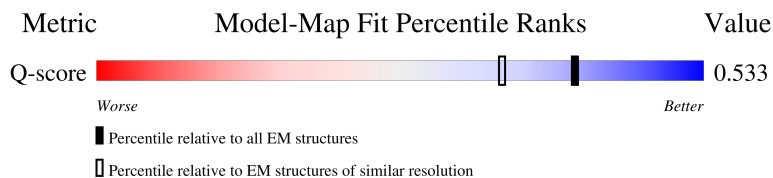
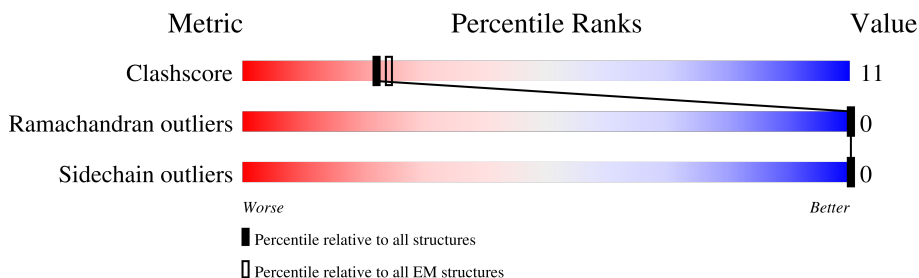
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	 73% 21% 6%
2	B	487	 82% 18%
3	C	423	 79% 21%
4	D	350	 73% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	76	
6	F	33	
7	H	65	
8	I	28	
9	K	37	
10	2	101	
11	1	32	

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
13	CLA	A	402	X	-	-	-
13	CLA	A	403	X	-	-	-
13	CLA	A	405	X	-	-	-
13	CLA	B	501	X	-	-	-
13	CLA	B	502	X	-	-	-
13	CLA	B	503	X	-	-	-
13	CLA	B	504	X	-	-	-
13	CLA	B	505	X	-	-	-
13	CLA	B	506	X	-	-	-
13	CLA	B	507	X	-	-	-
13	CLA	B	508	X	-	-	-
13	CLA	B	509	X	-	-	-
13	CLA	B	510	X	-	-	-
13	CLA	B	511	X	-	-	-
13	CLA	B	512	X	-	-	-
13	CLA	B	513	X	-	-	-
13	CLA	B	514	X	-	-	-
13	CLA	B	515	X	-	-	-
13	CLA	B	516	X	-	-	-
13	CLA	C	501	X	-	-	-
13	CLA	C	502	X	-	-	-
13	CLA	C	503	X	-	-	-
13	CLA	C	504	X	-	-	-
13	CLA	C	505	X	-	-	-
13	CLA	C	506	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	C	507	X	-	-	-
13	CLA	C	508	X	-	-	-
13	CLA	C	509	X	-	-	-
13	CLA	C	510	X	-	-	-
13	CLA	C	511	X	-	-	-
13	CLA	C	512	X	-	-	-
13	CLA	C	513	X	-	-	-
13	CLA	D	401	X	-	-	-
13	CLA	D	404	X	-	-	-
13	CLA	D	405	X	-	-	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 18054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2390	1570	396	409	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3811	2494	638	667	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	423	Total	C	N	O	S	0	0
			3292	2164	547	565	16		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	335	Total	C	N	O	S	0	0
			2674	1770	437	455	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	76	Total	C	N	O	0	0
			619	404	102	113		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	33	Total	C	N	O	S	0	0
			269	185	44	39	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			497	332	73	90	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	28	Total	C	N	O	S	0	0
			231	163	30	36	2		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			296	209	43	44		

- Molecule 10 is a protein called Chain U, Predicted protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	2	101	Total	C	N	O	0	0
			790	501	137	152		

- Molecule 11 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	32	Total	C	N	O	S	0	0
			224	146	37	40	1		

- Molecule 12 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Fe	0
			1	1	

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).

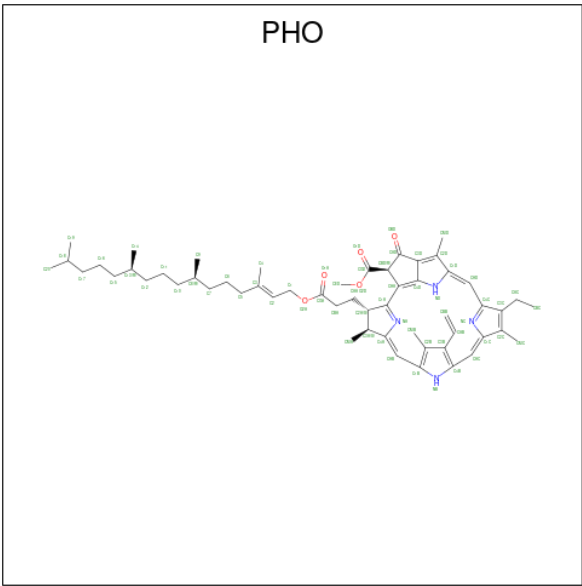


Continued on next page...

Continued from previous page...

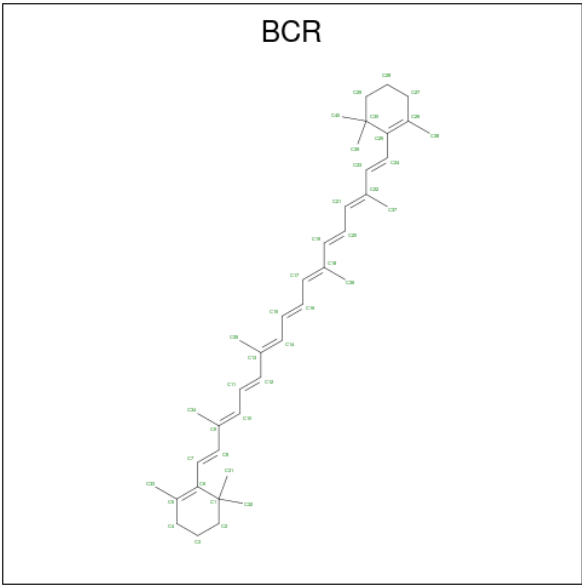
Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 14 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	N	O	0
			64	55	4	5	
14	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



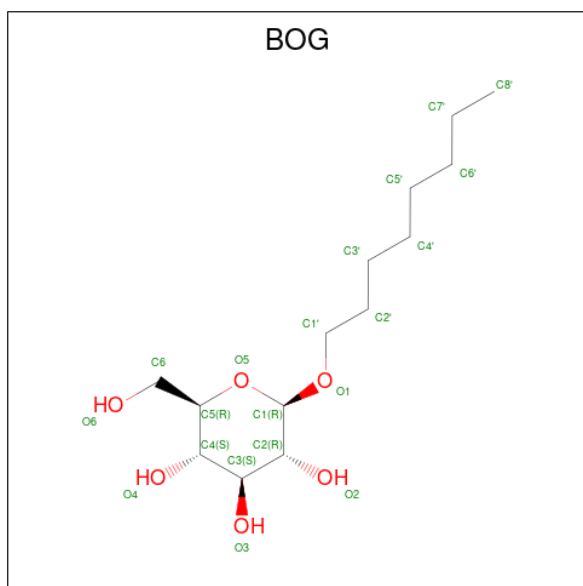
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

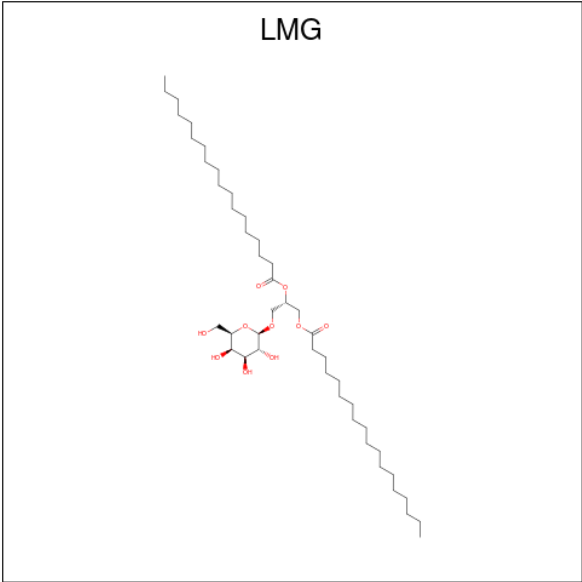
Mol	Chain	Residues	Atoms	AltConf
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	C	1	Total C 40 40	0
15	C	1	Total C 40 40	0
15	C	1	Total C 40 40	0
15	D	1	Total C 40 40	0
15	H	1	Total C 40 40	0

- Molecule 16 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



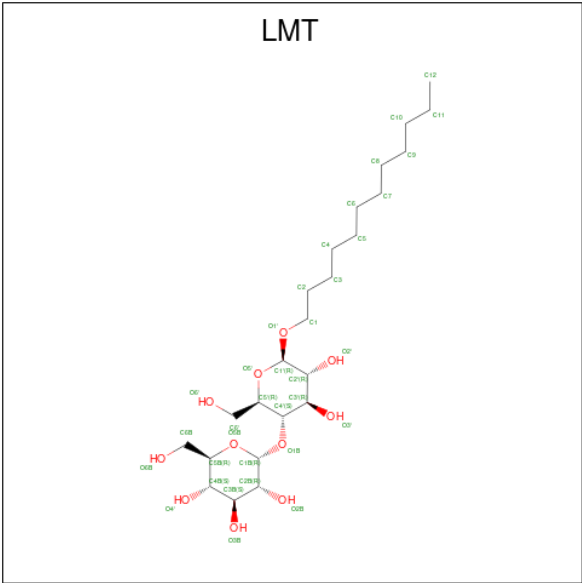
Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C O 20 14 6	0
16	C	1	Total C O 20 14 6	0
16	D	1	Total C O 20 14 6	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



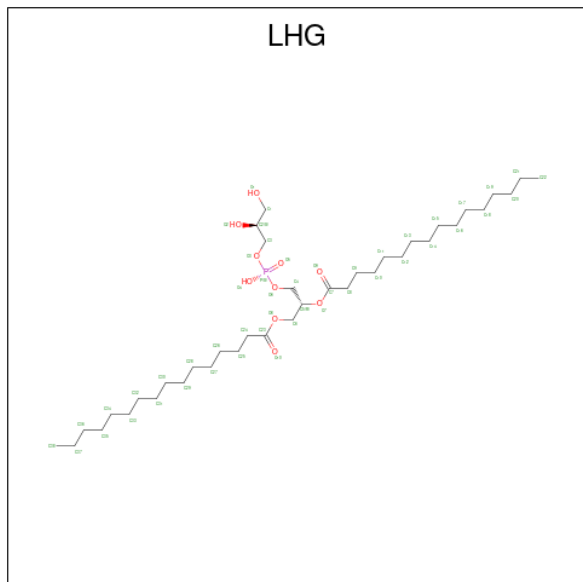
Mol	Chain	Residues	Atoms			AltConf
17	B	1	Total	C	O	0
			41	31	10	
17	H	1	Total	C	O	0
			48	38	10	

- Molecule 18 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



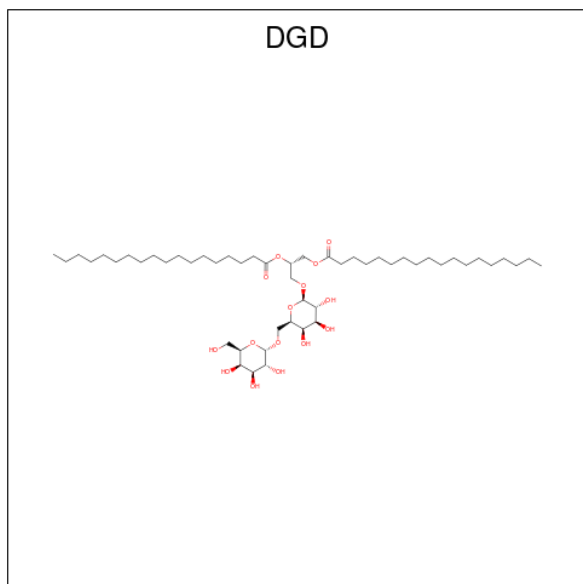
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			35	24	11	
18	B	1	Total	C	O	0
			35	24	11	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



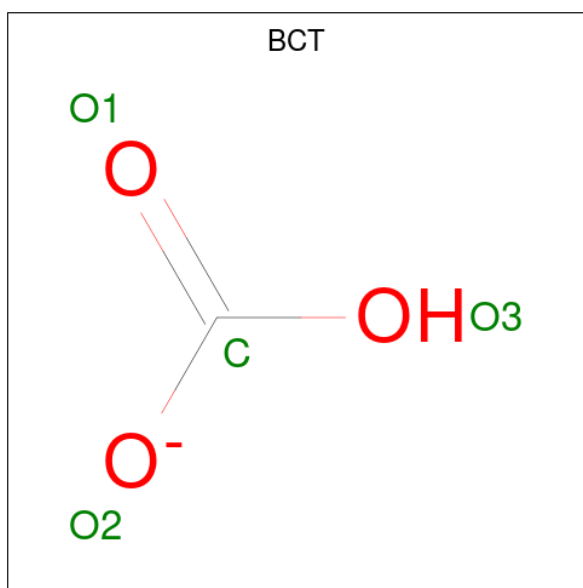
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	B	1	44	33	10	1	0

- Molecule 20 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



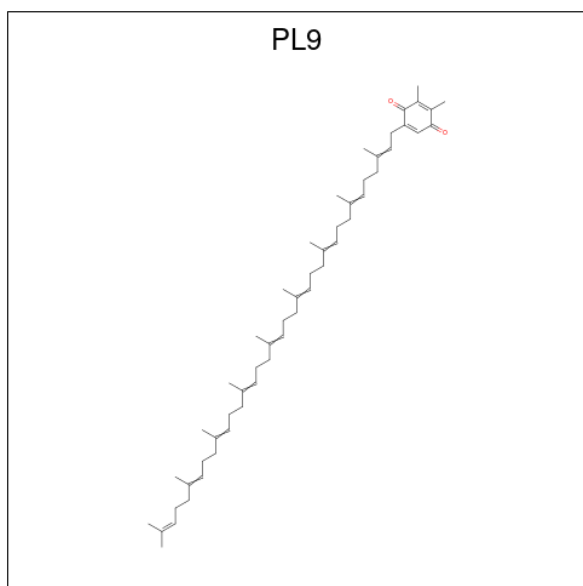
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
20	C	1	55	40	15		0

- Molecule 21 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
21	D	1	Total	C	O	0
			4	1	3	

- Molecule 22 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



Mol	Chain	Residues	Atoms			AltConf
22	D	1	Total	C	O	0
			55	53	2	

-
- Chemical structure of HEM (heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme label.

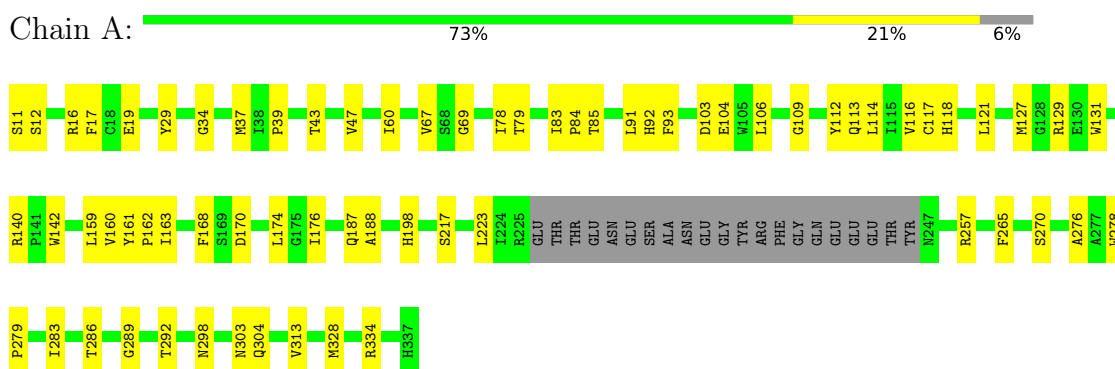
- Molecule 24 is water.



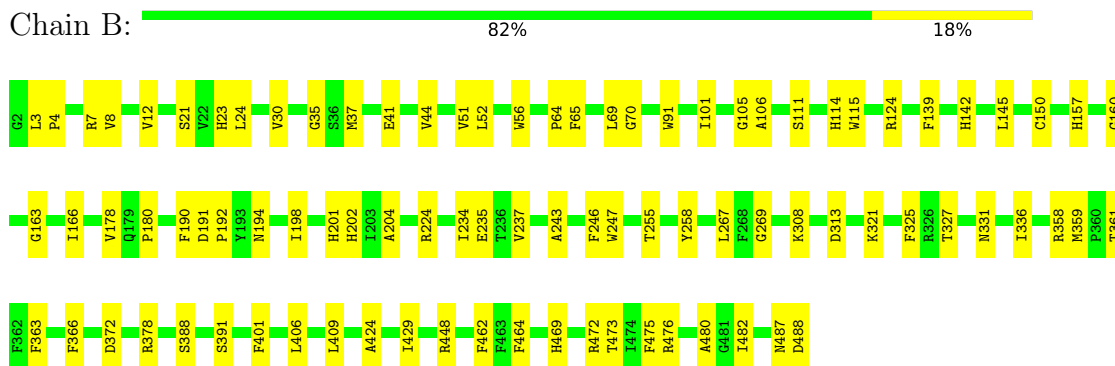
3 Residue-property plots

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 atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

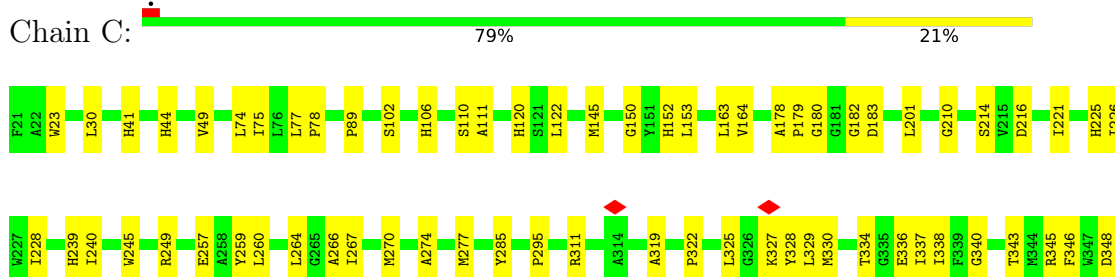
• Molecule 1: Photosystem II protein D1

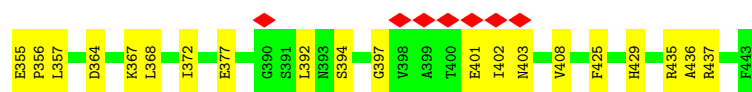


• Molecule 2: Photosystem II CP47 reaction center protein



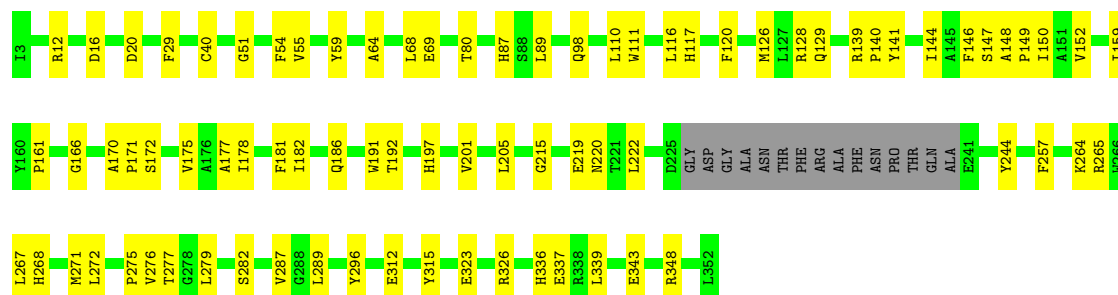
• Molecule 3: Photosystem II CP43 reaction center protein





• Molecule 4: Photosystem II D2 protein

Chain D: 73% 23%



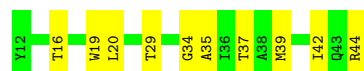
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 79% 21%



• Molecule 6: Cytochrome b559 subunit beta

Chain F: 70% 30%



• Molecule 7: Photosystem II reaction center protein H

Chain H: 85% 15%



• Molecule 8: Photosystem II reaction center protein I

Chain I: 86% 14%

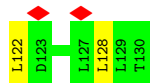
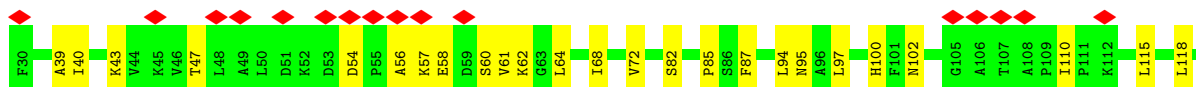
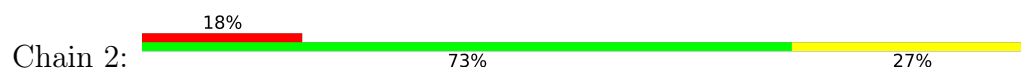


• Molecule 9: Photosystem II reaction center protein K

Chain K: 65% 35%



- Molecule 10: Chain U, Predicted protein



- Molecule 11: Photosystem II reaction center protein Ycf12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	327737	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.07	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	285.6, 285.6, 285.6	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84000003, 0.84000003, 0.84000003	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, LHG, CLA, BCT, LMT, DGD, LMG, FE2, BOG, HEM, PL9, BCR

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	0.14	0/2466	0.29	0/3362
2	B	0.12	0/3939	0.27	0/5363
3	C	0.11	0/3410	0.26	0/4650
4	D	0.12	0/2765	0.27	0/3770
5	E	0.13	0/637	0.31	0/869
6	F	0.14	0/278	0.34	0/379
7	H	0.16	0/508	0.29	0/696
8	I	0.10	0/238	0.26	0/323
9	K	0.16	0/308	0.43	0/425
10	2	0.13	0/804	0.35	0/1086
11	1	0.15	0/224	0.49	0/306
All	All	0.13	0/15577	0.29	0/21229

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	2390	0	2328	56	0
2	B	3811	0	3686	75	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3292	0	3176	68	0
4	D	2674	0	2573	72	0
5	E	619	0	605	23	0
6	F	269	0	279	10	0
7	H	497	0	520	10	0
8	I	231	0	240	4	0
9	K	296	0	308	8	0
10	2	790	0	805	20	0
11	1	224	0	257	19	0
12	A	1	0	0	0	0
13	A	169	0	158	19	0
13	B	960	0	969	78	0
13	C	782	0	786	45	0
13	D	176	0	175	19	0
14	A	64	0	74	3	0
14	D	64	0	74	2	0
15	A	40	0	56	3	0
15	B	80	0	112	7	0
15	C	120	0	168	10	0
15	D	40	0	56	1	0
15	H	40	0	56	3	0
16	A	20	0	28	1	0
16	C	20	0	28	2	0
16	D	20	0	28	1	0
17	B	41	0	52	1	0
17	H	48	0	66	2	0
18	B	70	0	92	5	0
19	B	44	0	61	5	0
20	C	55	0	68	1	0
21	D	4	0	1	0	0
22	D	55	0	80	1	0
23	E	43	0	30	2	0
24	A	1	0	0	0	0
24	B	2	0	0	0	0
24	C	1	0	0	0	0
24	D	1	0	0	0	0
All	All	18054	0	17995	413	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 11.

The worst 5 of 413 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)
5:E:31:PHE:HB3	11:1:10:VAL:HG12	1.36	1.01
2:B:24:LEU:HD21	13:B:516:CLA:HAB	1.47	0.94
4:D:282:SER:HB2	13:D:404:CLA:HED3	1.51	0.88
7:H:60:PHE:HB2	15:H:101:BCR:H16C	1.62	0.81
3:C:397:GLY:HA3	3:C:401:GLU:HG3	1.63	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/327 (92%)	290 (96%)	12 (4%)	0	100	100
2	B	485/487 (100%)	473 (98%)	12 (2%)	0	100	100
3	C	421/423 (100%)	406 (96%)	15 (4%)	0	100	100
4	D	331/350 (95%)	320 (97%)	11 (3%)	0	100	100
5	E	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
6	F	31/33 (94%)	31 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
8	I	26/28 (93%)	25 (96%)	1 (4%)	0	100	100
9	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	2	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
11	1	30/32 (94%)	27 (90%)	3 (10%)	0	100	100
All	All	1897/1959 (97%)	1834 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/266 (93%)	248 (100%)	0	100	100
2	B	389/389 (100%)	389 (100%)	0	100	100
3	C	329/329 (100%)	329 (100%)	0	100	100
4	D	269/279 (96%)	269 (100%)	0	100	100
5	E	67/67 (100%)	67 (100%)	0	100	100
6	F	27/27 (100%)	27 (100%)	0	100	100
7	H	56/56 (100%)	56 (100%)	0	100	100
8	I	27/27 (100%)	27 (100%)	0	100	100
9	K	31/31 (100%)	31 (100%)	0	100	100
10	2	85/85 (100%)	85 (100%)	0	100	100
11	1	26/26 (100%)	26 (100%)	0	100	100
All	All	1554/1582 (98%)	1554 (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. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	186	GLN
4	D	220	ASN
10	2	102	ASN
6	F	40	GLN
4	D	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 58 ligands modelled in this entry, 1 is monoatomic - leaving 57 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	$\# Z > 2$
13	CLA	C	502	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	19 (23%)
13	CLA	B	501	24	49,53,73	1.60	7 (14%)	58,89,113	2.06	17 (29%)
13	CLA	B	515	-	69,73,73	1.35	6 (8%)	82,113,113	1.97	21 (25%)
13	CLA	B	504	-	69,73,73	1.37	6 (8%)	82,113,113	1.96	16 (19%)
13	CLA	C	506	-	52,56,73	1.56	7 (13%)	61,92,113	2.07	17 (27%)
13	CLA	C	513	-	69,73,73	1.36	7 (10%)	82,113,113	4.99	20 (24%)
15	BCR	B	517	-	41,41,41	4.96	28 (68%)	56,56,56	2.35	20 (35%)
13	CLA	B	502	-	69,73,73	1.35	7 (10%)	82,113,113	4.03	23 (28%)
15	BCR	A	406	-	41,41,41	4.97	27 (65%)	56,56,56	2.31	20 (35%)
13	CLA	B	506	-	60,64,73	1.44	6 (10%)	71,102,113	2.02	18 (25%)
13	CLA	B	505	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
13	CLA	B	509	-	65,69,73	1.38	7 (10%)	77,108,113	1.92	18 (23%)
19	LHG	B	522	-	43,43,48	0.40	0	46,49,54	1.11	3 (6%)
15	BCR	D	406	-	41,41,41	4.94	27 (65%)	56,56,56	2.40	19 (33%)
13	CLA	D	405	-	50,54,73	1.58	7 (14%)	59,90,113	2.18	15 (25%)
15	BCR	C	514	-	41,41,41	4.93	27 (65%)	56,56,56	2.39	18 (32%)
15	BCR	C	516	-	41,41,41	4.93	27 (65%)	56,56,56	2.47	19 (33%)
21	BCT	D	403	12	3,3,3	1.10	0	2,3,3	4.20	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	C	512	-	59,63,73	1.47	7 (11%)	70,101,113	2.02	18 (25%)
15	BCR	H	101	-	41,41,41	4.96	27 (65%)	56,56,56	2.47	22 (39%)
13	CLA	D	404	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	20 (24%)
15	BCR	B	518	-	41,41,41	4.93	27 (65%)	56,56,56	3.25	24 (42%)
18	LMT	B	521	-	36,36,36	1.11	2 (5%)	47,47,47	0.99	1 (2%)
13	CLA	C	510	-	69,73,73	1.35	7 (10%)	82,113,113	2.08	21 (25%)
13	CLA	C	507	24	69,73,73	1.36	7 (10%)	82,113,113	1.87	16 (19%)
17	LMG	H	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.09	2 (3%)
14	PHO	A	404	-	58,69,69	2.15	10 (17%)	55,99,99	1.42	5 (9%)
14	PHO	D	402	-	58,69,69	2.17	9 (15%)	55,99,99	1.43	6 (10%)
13	CLA	B	511	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	20 (24%)
13	CLA	B	503	-	69,73,73	1.36	6 (8%)	82,113,113	1.85	16 (19%)
20	DGD	C	517	-	56,56,67	1.06	4 (7%)	70,70,81	0.96	3 (4%)
16	BOG	C	518	-	20,20,20	1.29	2 (10%)	25,25,25	0.80	0
17	LMG	B	519	-	41,41,55	1.01	3 (7%)	49,49,63	1.18	4 (8%)
13	CLA	C	505	-	69,73,73	1.35	6 (8%)	82,113,113	1.83	15 (18%)
13	CLA	A	402	-	69,73,73	1.34	6 (8%)	82,113,113	1.90	19 (23%)
18	LMT	B	520	-	36,36,36	1.11	2 (5%)	47,47,47	1.10	2 (4%)
13	CLA	B	514	-	50,54,73	1.58	7 (14%)	59,90,113	2.00	15 (25%)
13	CLA	B	510	24	69,73,73	1.37	7 (10%)	82,113,113	1.84	18 (21%)
13	CLA	B	508	-	69,73,73	1.36	8 (11%)	82,113,113	1.93	17 (20%)
13	CLA	C	511	3	56,60,73	1.51	7 (12%)	65,97,113	2.09	16 (24%)
13	CLA	B	507	-	59,63,73	1.47	6 (10%)	70,101,113	2.01	17 (24%)
13	CLA	A	403	24	53,57,73	1.55	8 (15%)	61,93,113	2.19	18 (29%)
13	CLA	C	501	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	21 (25%)
13	CLA	A	405	-	59,63,73	1.47	7 (11%)	70,101,113	2.10	19 (27%)
13	CLA	C	504	-	59,63,73	1.46	6 (10%)	70,101,113	2.07	18 (25%)
23	HEM	E	101	6,5	50,50,50	1.50	7 (14%)	67,82,82	1.13	3 (4%)
13	CLA	C	508	-	56,60,73	1.51	6 (10%)	65,97,113	2.06	18 (27%)
16	BOG	A	407	-	20,20,20	1.30	2 (10%)	25,25,25	0.78	0
13	CLA	B	513	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	17 (22%)
13	CLA	D	401	24	69,73,73	1.35	6 (8%)	82,113,113	1.92	18 (21%)
13	CLA	B	512	-	69,73,73	1.37	8 (11%)	82,113,113	1.92	16 (19%)
15	BCR	C	515	-	41,41,41	4.95	27 (65%)	56,56,56	2.35	20 (35%)
13	CLA	C	503	-	69,73,73	1.37	8 (11%)	82,113,113	1.87	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	C	509	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	19 (23%)
16	BOG	D	408	-	20,20,20	1.31	2 (10%)	25,25,25	0.76	0
13	CLA	B	516	-	56,60,73	1.51	7 (12%)	65,97,113	2.09	18 (27%)
22	PL9	D	407	-	55,55,55	1.05	4 (7%)	68,69,69	1.48	12 (17%)

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
13	CLA	C	502	-	1/1/15/20	15/39/115/115	-
13	CLA	B	501	24	1/1/11/20	8/15/91/115	-
13	CLA	B	515	-	1/1/15/20	10/39/115/115	-
13	CLA	B	504	-	1/1/15/20	12/39/115/115	-
13	CLA	C	506	-	1/1/11/20	11/19/95/115	-
13	CLA	C	513	-	1/1/15/20	19/39/115/115	-
15	BCR	B	517	-	-	12/29/63/63	0/2/2/2
13	CLA	B	502	-	1/1/15/20	15/39/115/115	-
15	BCR	A	406	-	-	11/29/63/63	0/2/2/2
13	CLA	B	506	-	1/1/13/20	8/29/105/115	-
13	CLA	B	505	-	1/1/15/20	20/39/115/115	-
13	CLA	B	509	-	1/1/14/20	16/35/111/115	-
19	LHG	B	522	-	-	29/48/48/53	-
15	BCR	D	406	-	-	15/29/63/63	0/2/2/2
13	CLA	D	405	-	1/1/11/20	9/17/93/115	-
15	BCR	C	514	-	-	13/29/63/63	0/2/2/2
15	BCR	C	516	-	-	12/29/63/63	0/2/2/2
22	PL9	D	407	-	-	15/53/73/73	0/1/1/1
13	CLA	C	512	-	1/1/13/20	10/27/103/115	-
15	BCR	H	101	-	-	15/29/63/63	0/2/2/2
13	CLA	D	404	-	1/1/15/20	20/39/115/115	-
15	BCR	B	518	-	-	9/29/63/63	0/2/2/2
18	LMT	B	521	-	-	13/21/61/61	0/2/2/2
13	CLA	C	510	-	1/1/15/20	10/39/115/115	-
13	CLA	C	507	24	1/1/15/20	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LMG	H	102	-	-	8/43/63/70	0/1/1/1
14	PHO	A	404	-	-	11/37/103/103	0/5/6/6
14	PHO	D	402	-	-	7/37/103/103	0/5/6/6
13	CLA	B	511	-	1/1/15/20	14/39/115/115	-
13	CLA	B	503	-	1/1/15/20	16/39/115/115	-
20	DGD	C	517	-	-	10/44/84/95	0/2/2/2
16	BOG	C	518	-	-	1/11/31/31	0/1/1/1
17	LMG	B	519	-	-	10/36/56/70	0/1/1/1
13	CLA	C	505	-	1/1/15/20	13/39/115/115	-
13	CLA	A	402	-	1/1/15/20	11/39/115/115	-
18	LMT	B	520	-	-	11/21/61/61	0/2/2/2
13	CLA	B	514	-	1/1/11/20	6/17/93/115	-
13	CLA	B	510	24	1/1/15/20	12/39/115/115	-
13	CLA	B	508	-	1/1/15/20	13/39/115/115	-
13	CLA	C	511	3	1/1/12/20	7/24/100/115	-
13	CLA	B	507	-	1/1/13/20	17/27/103/115	-
13	CLA	A	403	24	1/1/11/20	11/20/96/115	-
13	CLA	C	501	-	1/1/15/20	19/39/115/115	-
13	CLA	A	405	-	1/1/13/20	12/27/103/115	-
13	CLA	C	504	-	1/1/13/20	12/27/103/115	-
23	HEM	E	101	6,5	-	2/14/54/54	-
13	CLA	C	508	-	1/1/12/20	7/24/100/115	-
16	BOG	A	407	-	-	4/11/31/31	0/1/1/1
13	CLA	B	513	-	1/1/14/20	10/33/109/115	-
13	CLA	D	401	24	1/1/15/20	20/39/115/115	-
13	CLA	B	512	-	1/1/15/20	16/39/115/115	-
15	BCR	C	515	-	-	9/29/63/63	0/2/2/2
13	CLA	C	503	-	1/1/15/20	15/39/115/115	-
13	CLA	C	509	-	1/1/15/20	14/39/115/115	-
16	BOG	D	408	-	-	3/11/31/31	0/1/1/1
13	CLA	B	516	-	1/1/12/20	10/24/100/115	-

The worst 5 of 506 bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	517	BCR	C26-C25	16.12	1.61	1.34
15	H	101	BCR	C26-C25	15.94	1.61	1.34
15	C	515	BCR	C26-C25	15.89	1.61	1.34
15	C	516	BCR	C26-C25	15.85	1.61	1.34
15	A	406	BCR	C26-C25	15.84	1.61	1.34

The worst 5 of 836 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	513	CLA	O2D-CGD-CBD	27.53	159.37	111.23
13	C	513	CLA	O2D-CGD-O1D	-22.98	79.12	123.85
13	C	513	CLA	O1D-CGD-CBD	-22.38	80.37	124.52
13	B	502	CLA	C4-C3-C5	-21.96	77.11	115.23
13	B	502	CLA	C5-C3-C2	16.82	158.93	121.17

5 of 35 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	402	CLA	ND
13	A	403	CLA	ND
13	A	405	CLA	ND
13	B	501	CLA	ND
13	B	502	CLA	ND

5 of 673 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	402	CLA	CAD-CBD-CGD-O1D
13	A	402	CLA	CAD-CBD-CGD-O2D
13	A	403	CLA	C1A-C2A-CAA-CBA
13	A	403	CLA	CHA-CBD-CGD-O1D
13	A	403	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

55 monomers are involved in 197 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	502	CLA	7	0
13	B	501	CLA	2	0
13	B	515	CLA	4	0

Continued on next page...

Continued from previous page...

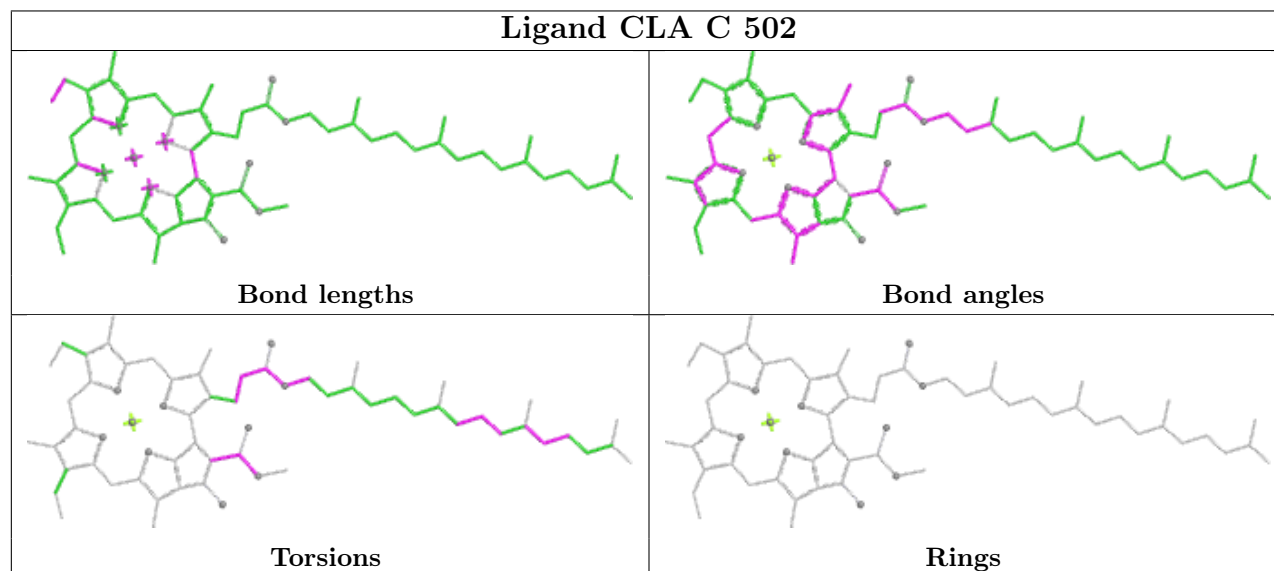
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	504	CLA	9	0
13	C	506	CLA	2	0
13	C	513	CLA	5	0
15	B	517	BCR	2	0
13	B	502	CLA	5	0
15	A	406	BCR	3	0
13	B	506	CLA	3	0
13	B	505	CLA	8	0
13	B	509	CLA	8	0
19	B	522	LHG	5	0
15	D	406	BCR	1	0
13	D	405	CLA	3	0
15	C	514	BCR	2	0
15	C	516	BCR	3	0
13	C	512	CLA	3	0
15	H	101	BCR	3	0
13	D	404	CLA	10	0
15	B	518	BCR	5	0
18	B	521	LMT	3	0
13	C	510	CLA	7	0
17	H	102	LMG	2	0
14	A	404	PHO	3	0
14	D	402	PHO	2	0
13	B	511	CLA	4	0
13	B	503	CLA	7	0
20	C	517	DGD	1	0
16	C	518	BOG	2	0
17	B	519	LMG	1	0
13	C	505	CLA	5	0
13	A	402	CLA	6	0
18	B	520	LMT	2	0
13	B	514	CLA	5	0
13	B	510	CLA	8	0
13	B	508	CLA	4	0
13	C	511	CLA	1	0
13	B	507	CLA	7	0
13	A	403	CLA	2	0
13	C	501	CLA	4	0
13	A	405	CLA	11	0
13	C	504	CLA	2	0
23	E	101	HEM	2	0
13	C	508	CLA	6	0

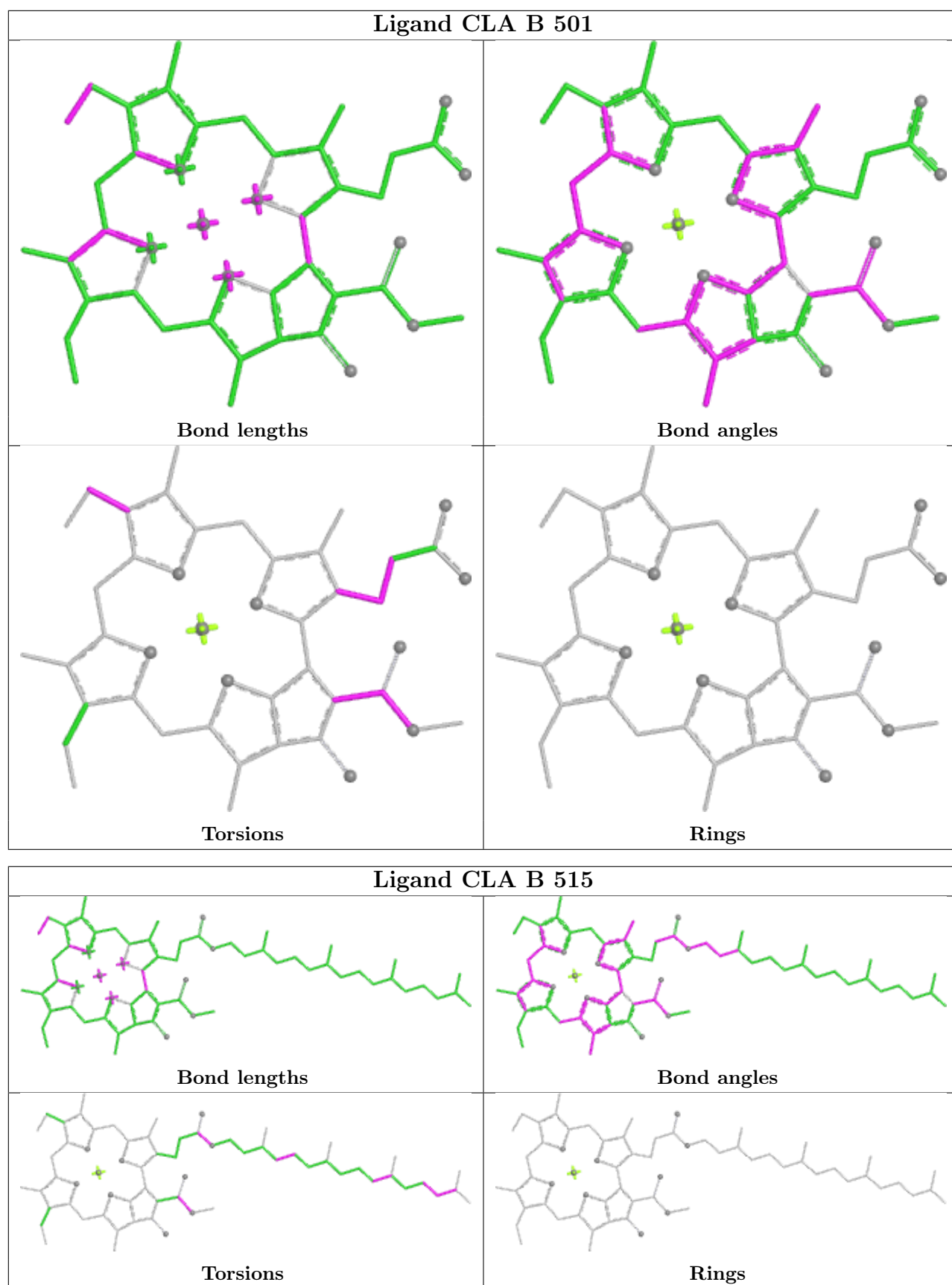
Continued on next page...

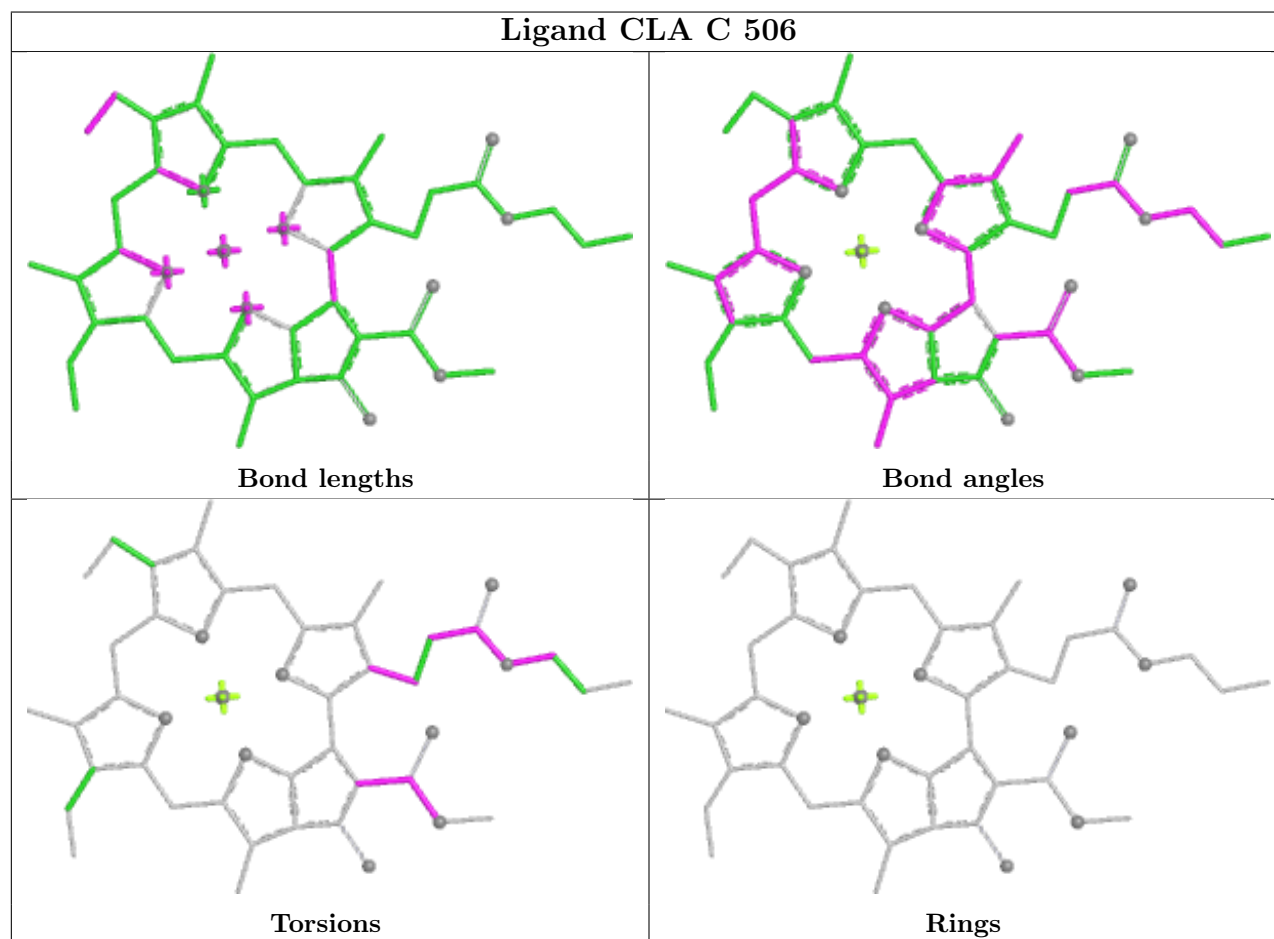
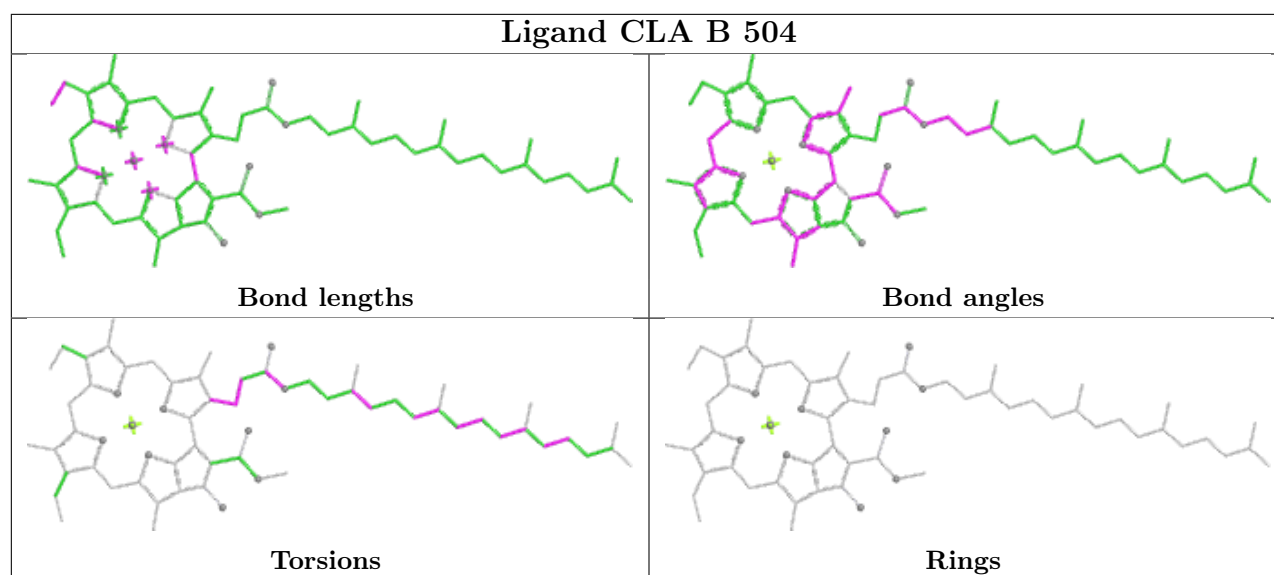
Continued from previous page...

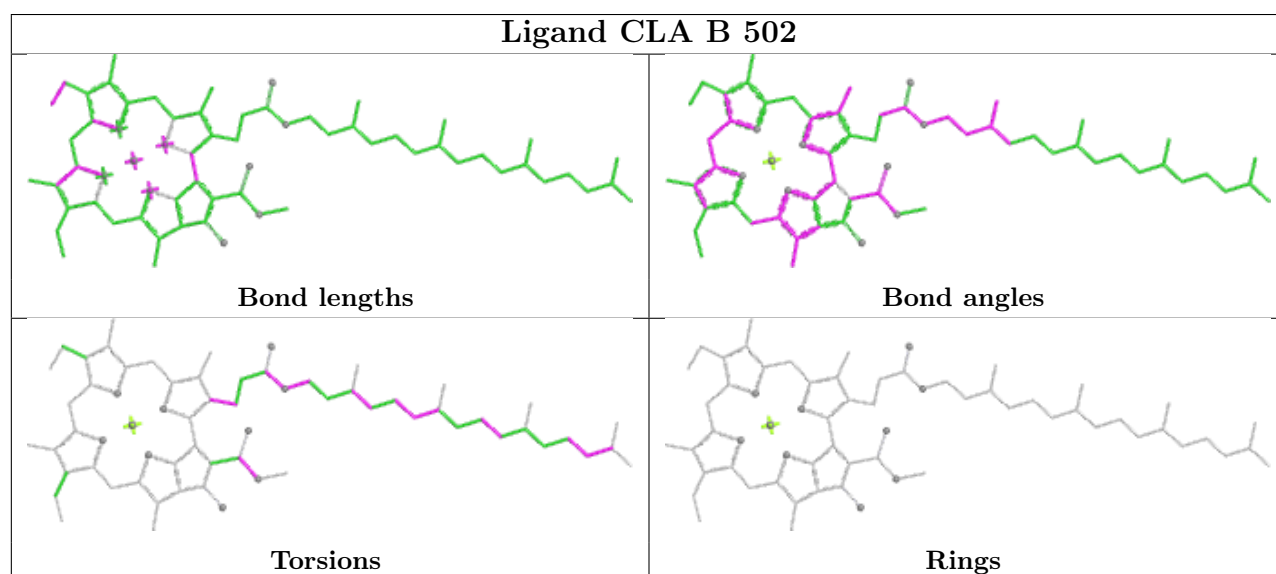
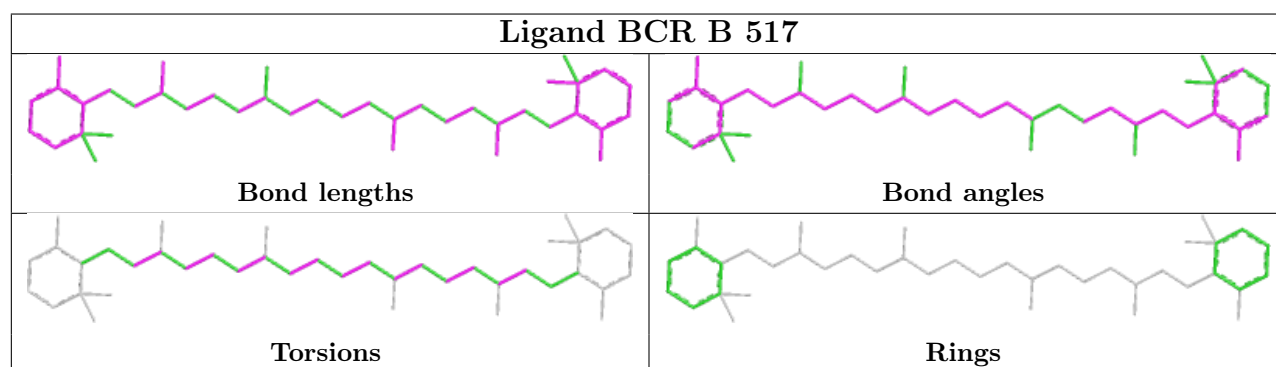
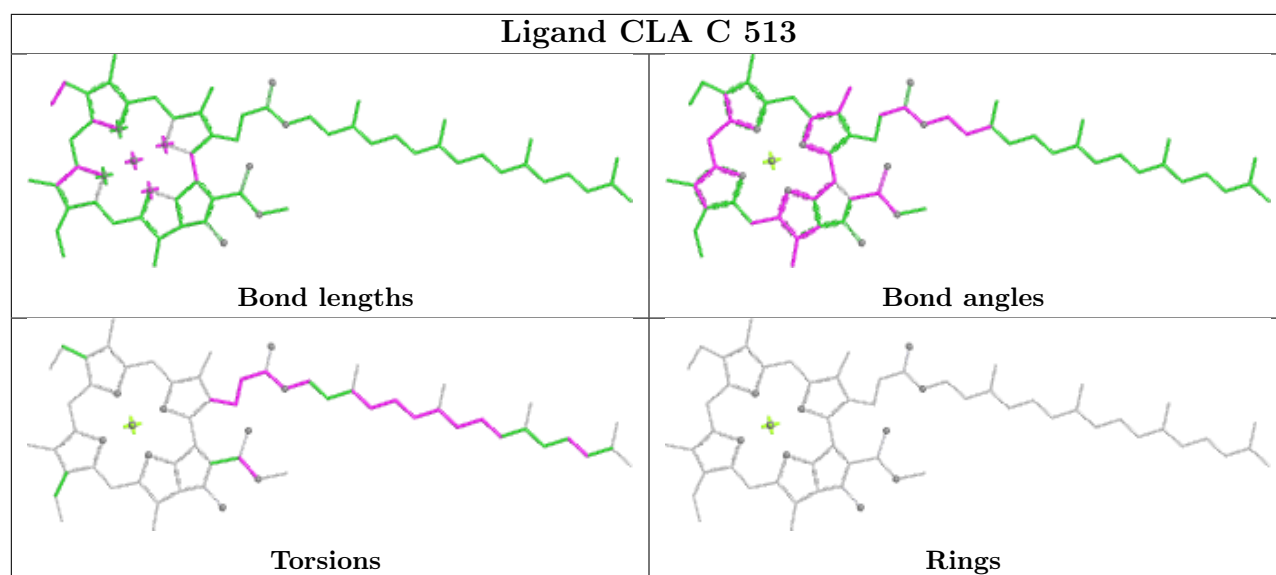
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	407	BOG	1	0
13	B	513	CLA	5	0
13	D	401	CLA	6	0
13	B	512	CLA	9	0
15	C	515	BCR	5	0
13	C	503	CLA	5	0
13	C	509	CLA	6	0
16	D	408	BOG	1	0
13	B	516	CLA	3	0
22	D	407	PL9	1	0

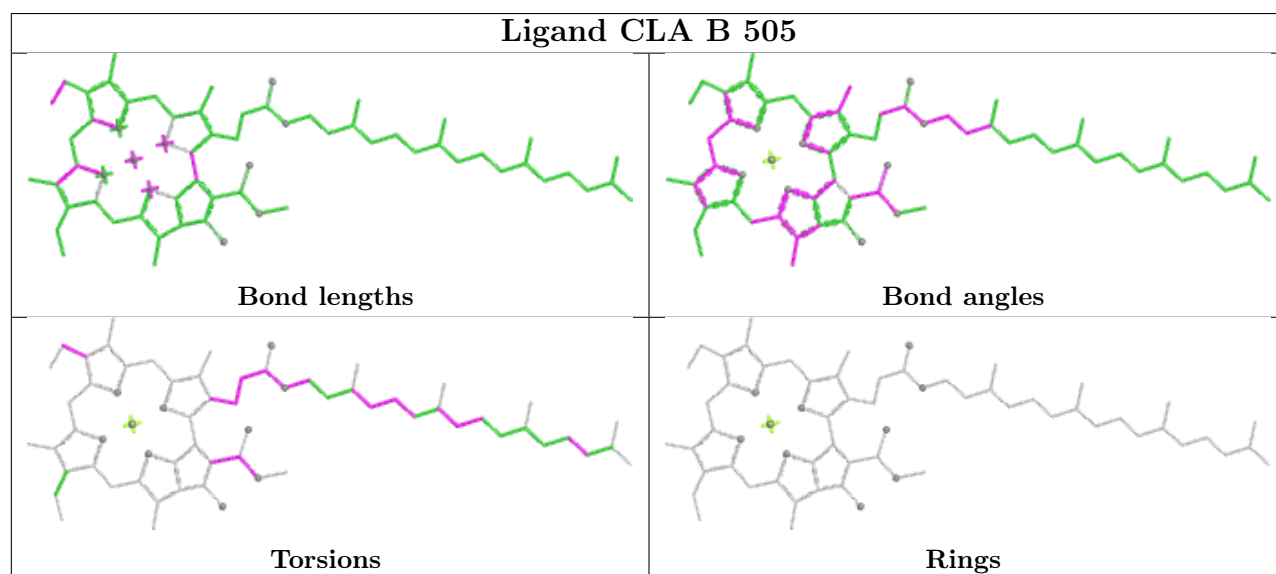
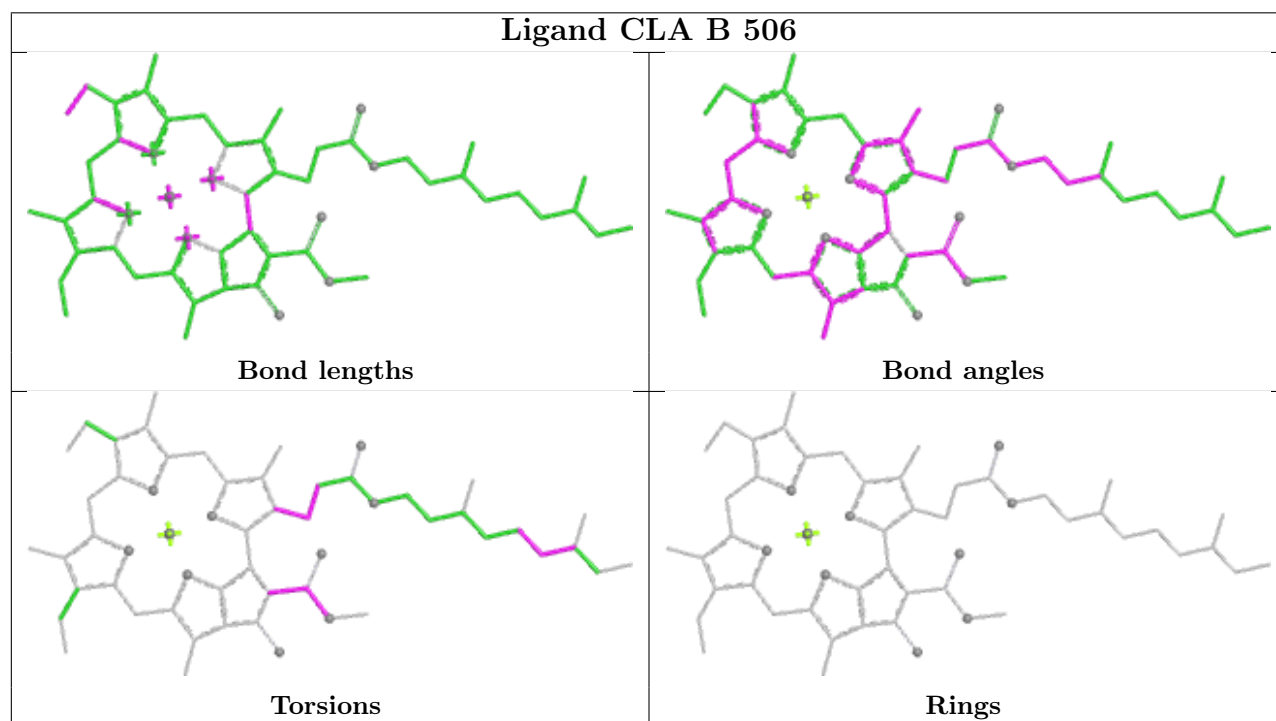
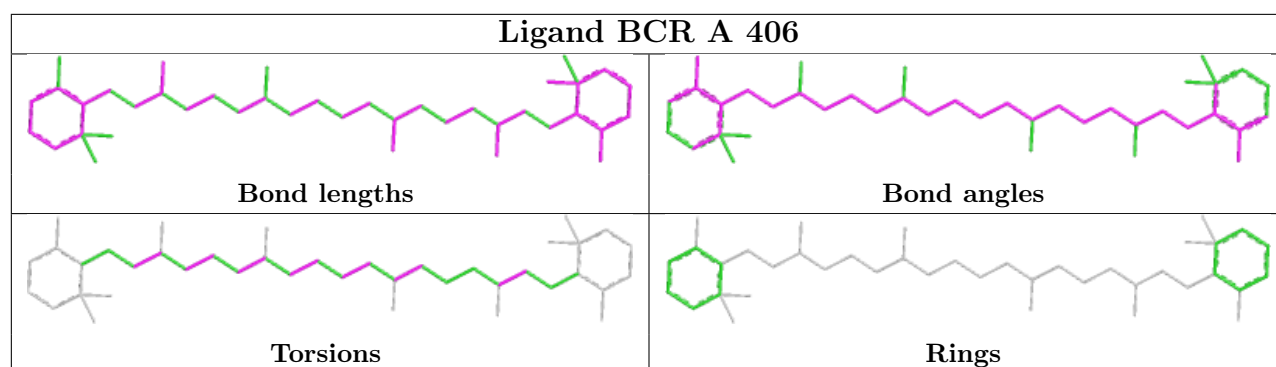
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

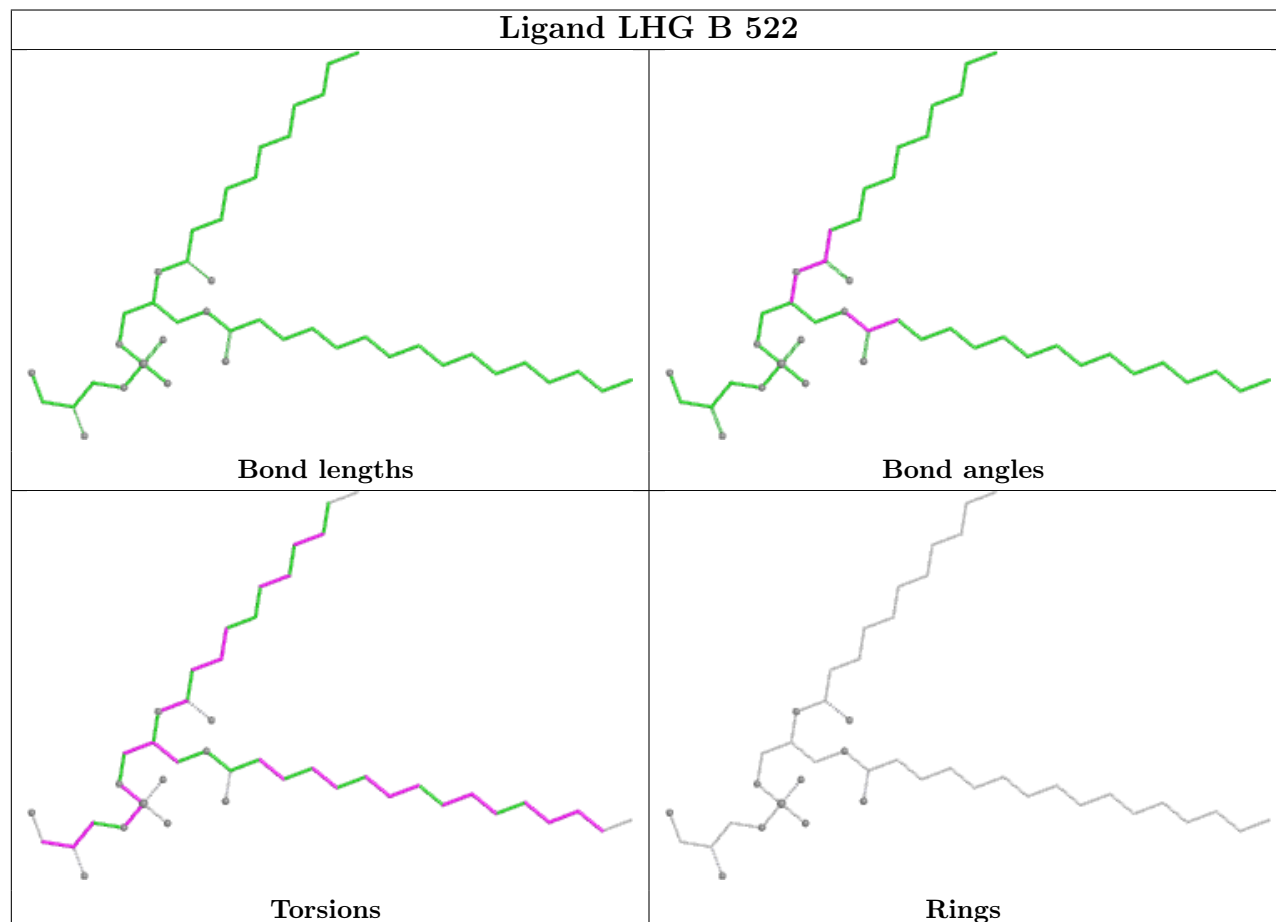
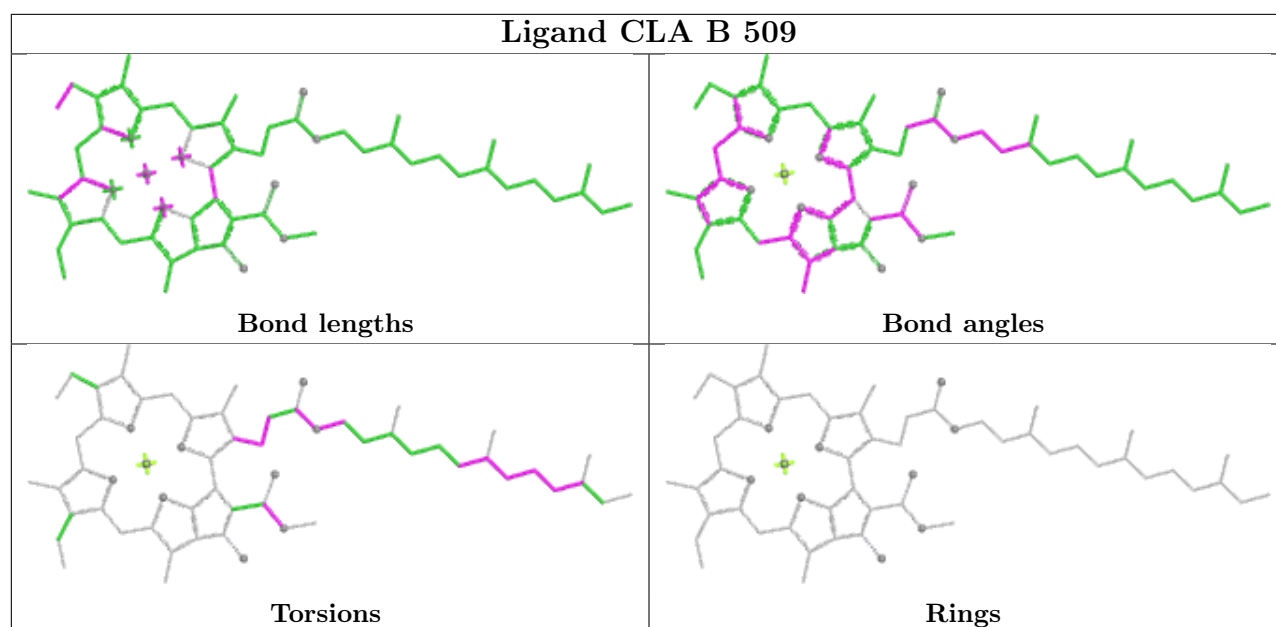


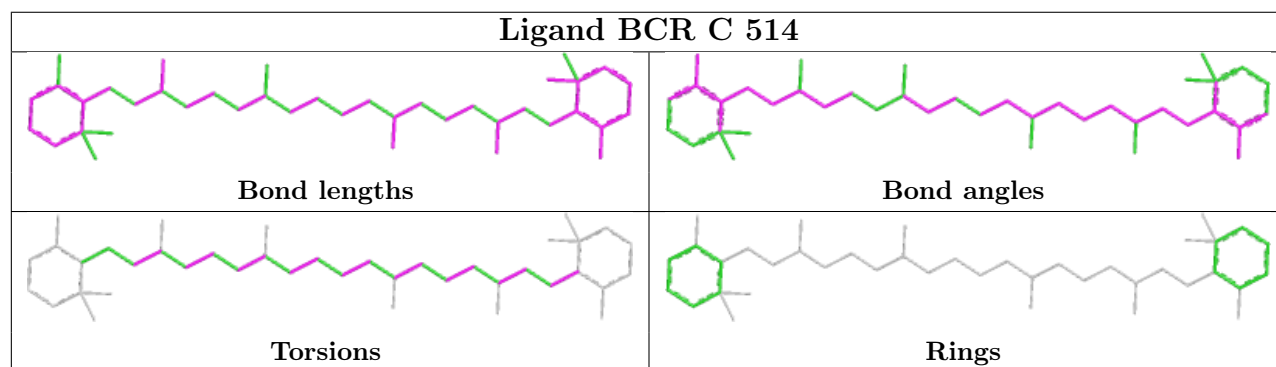
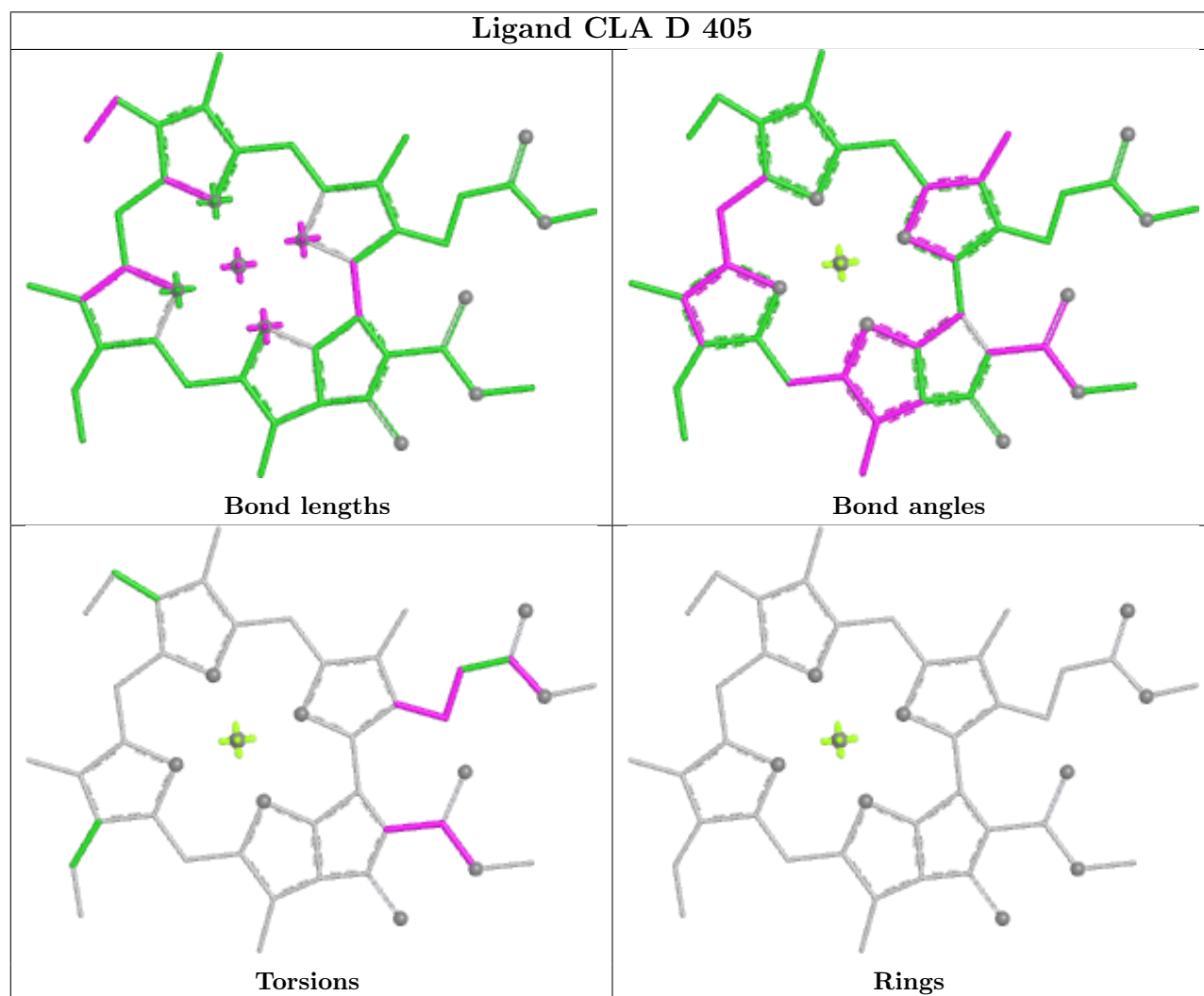
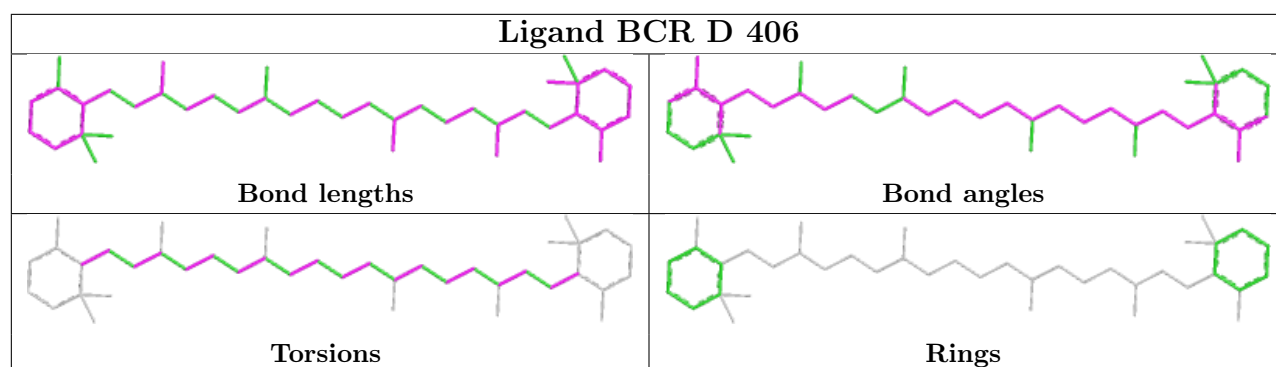


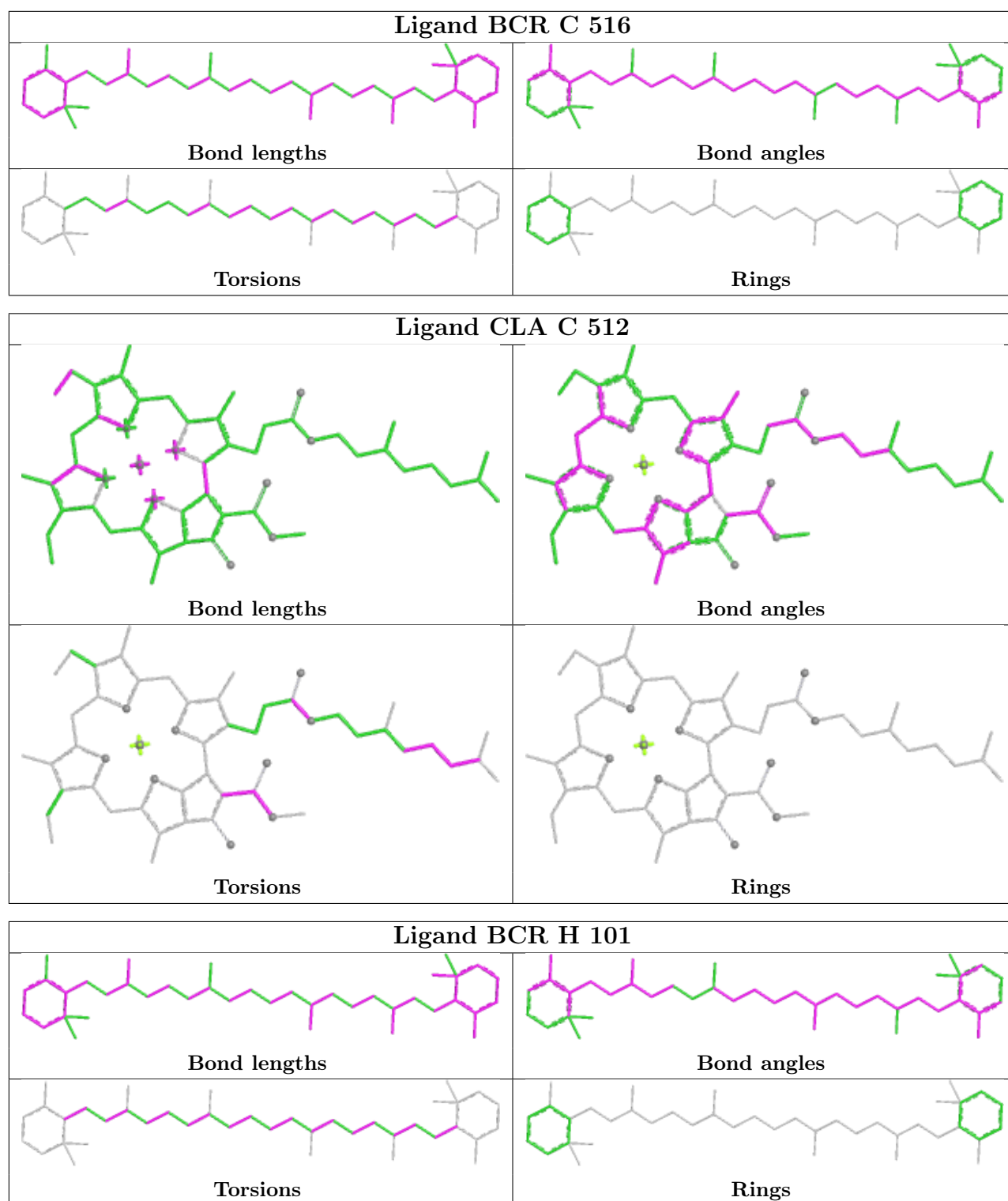


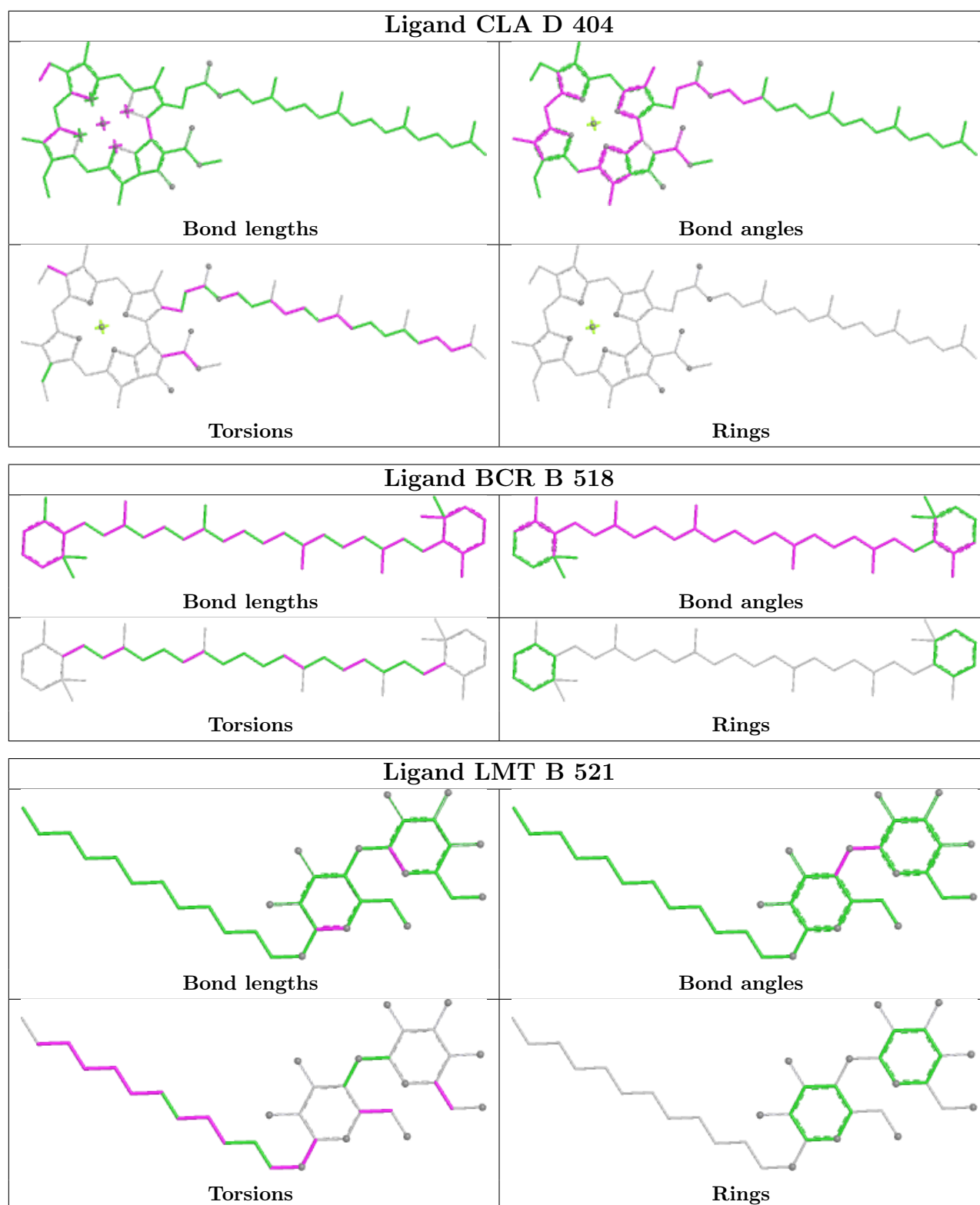


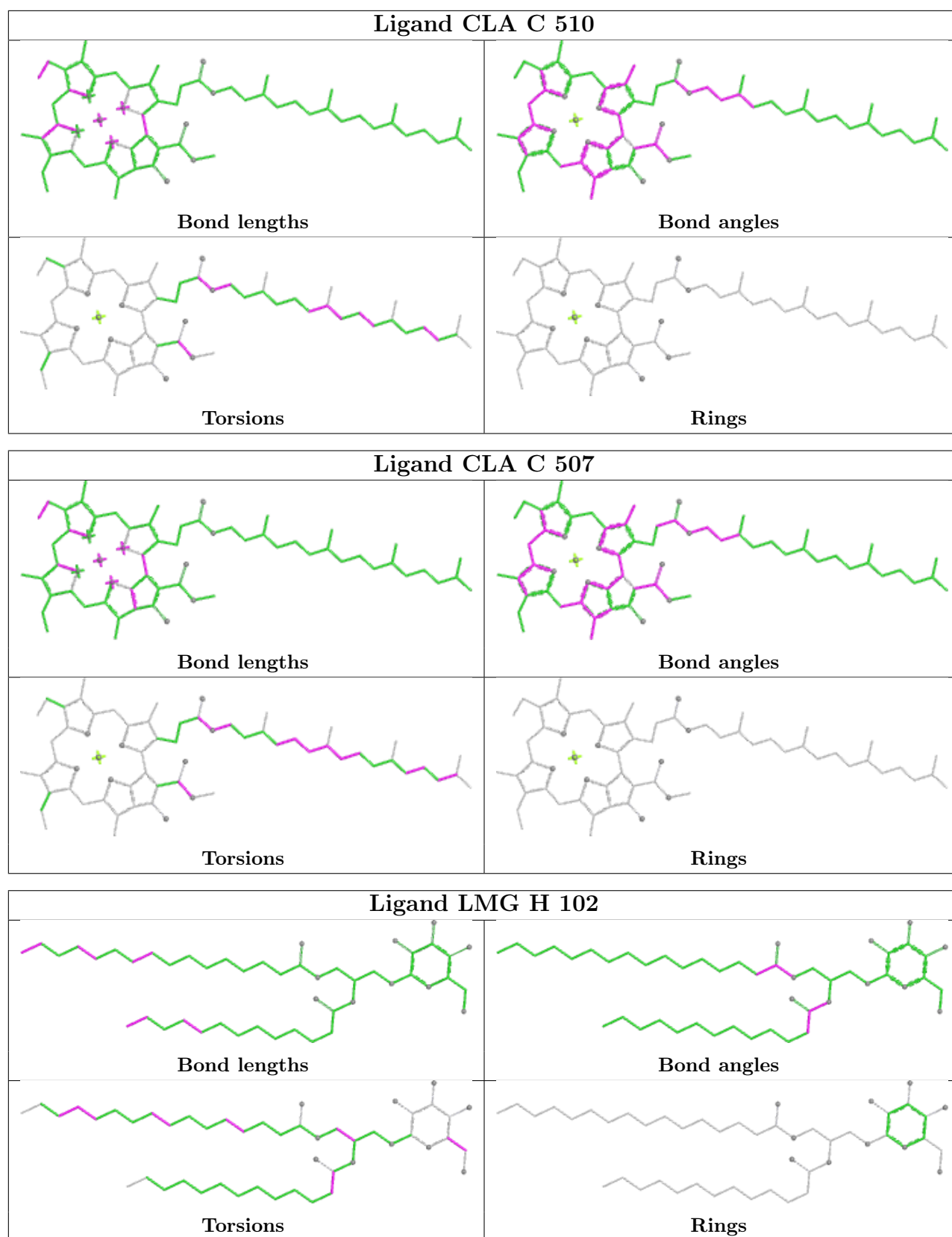


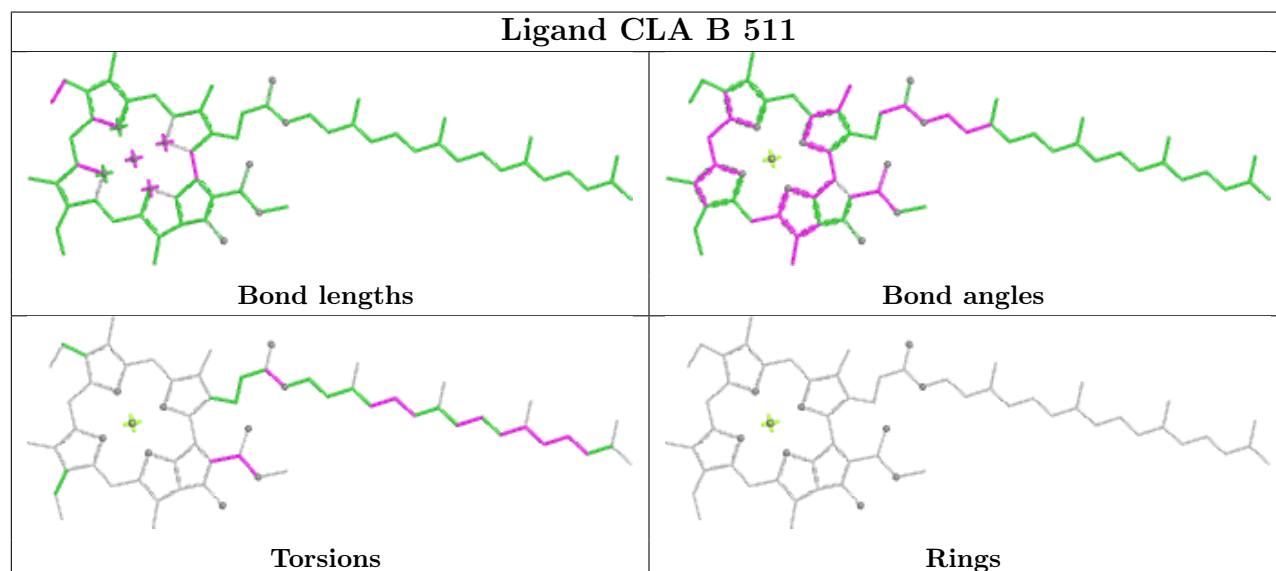
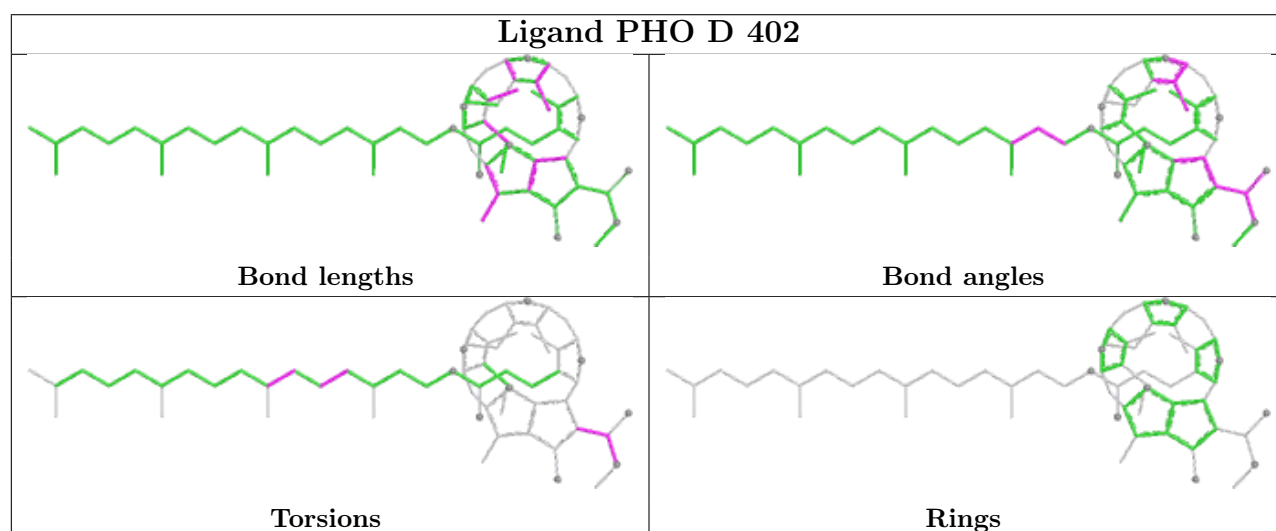
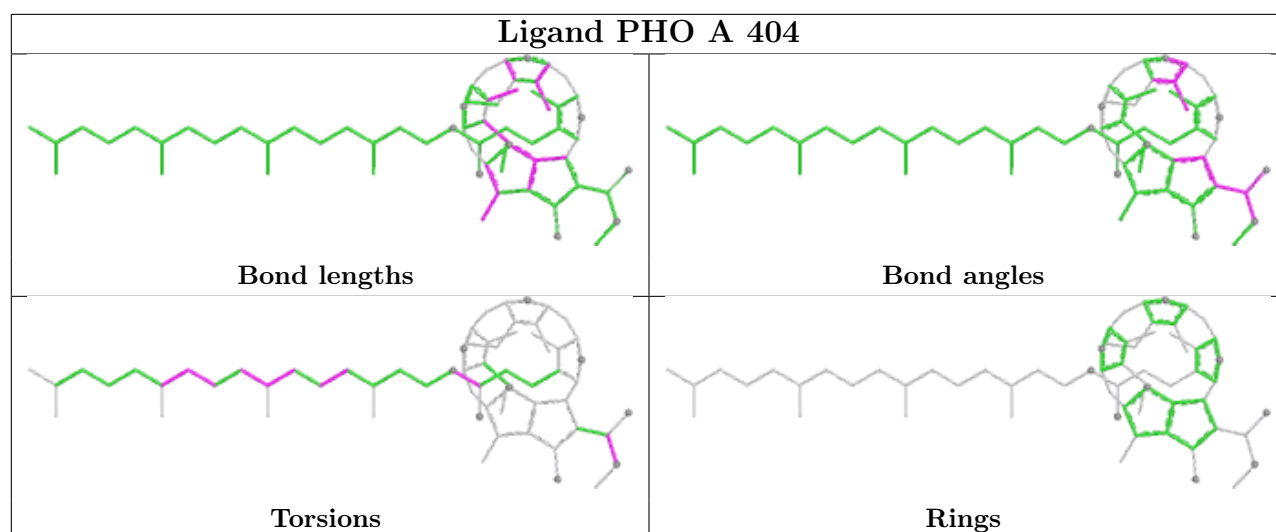


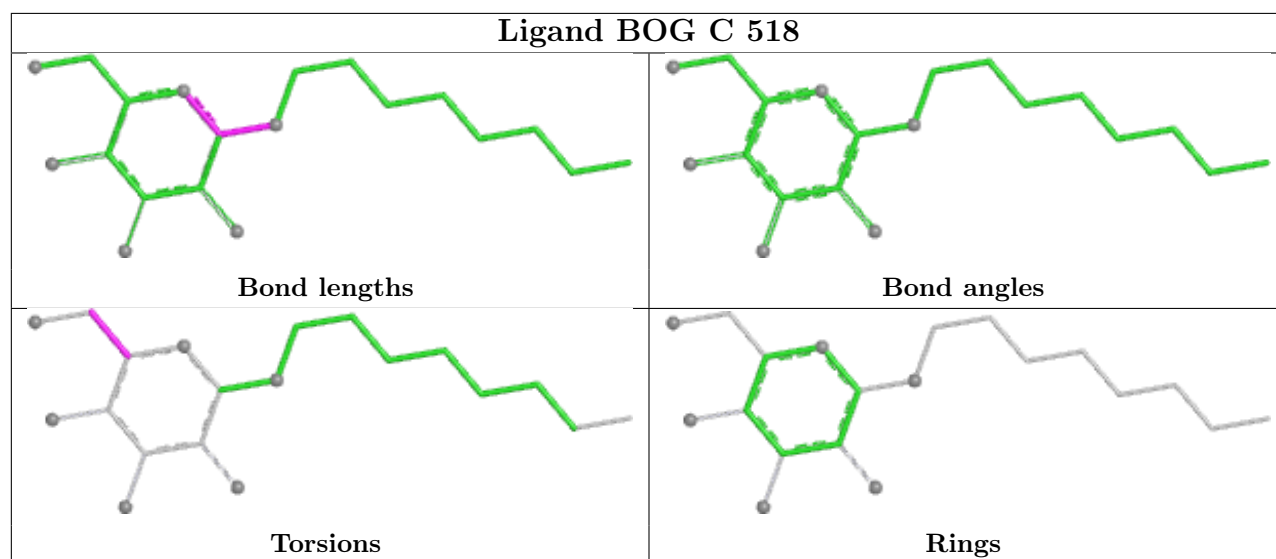
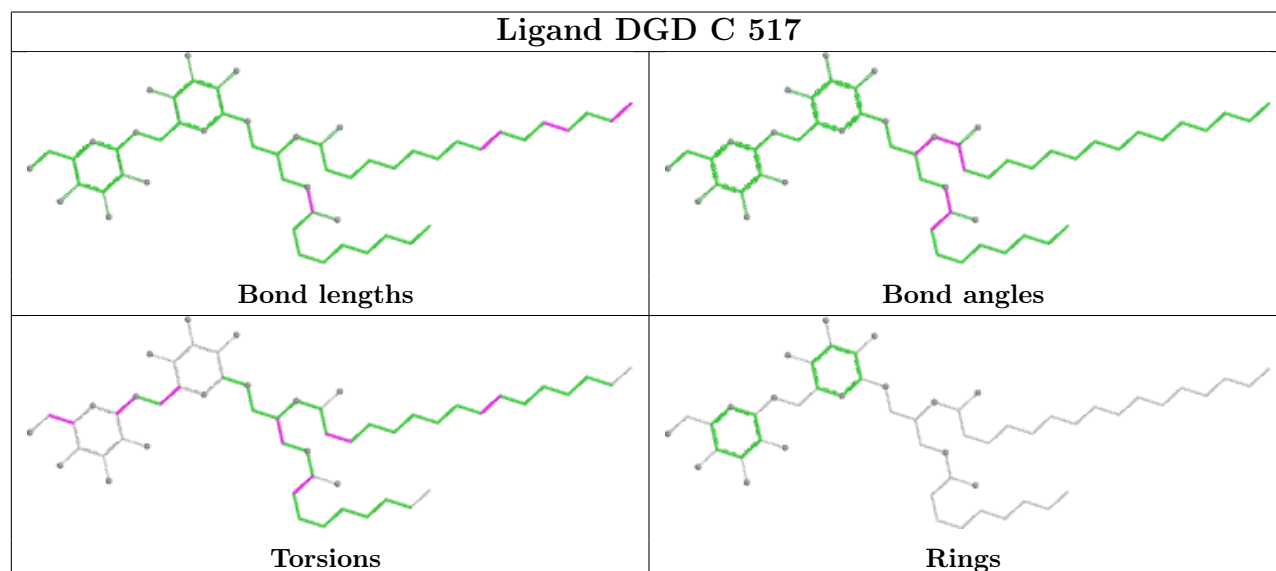
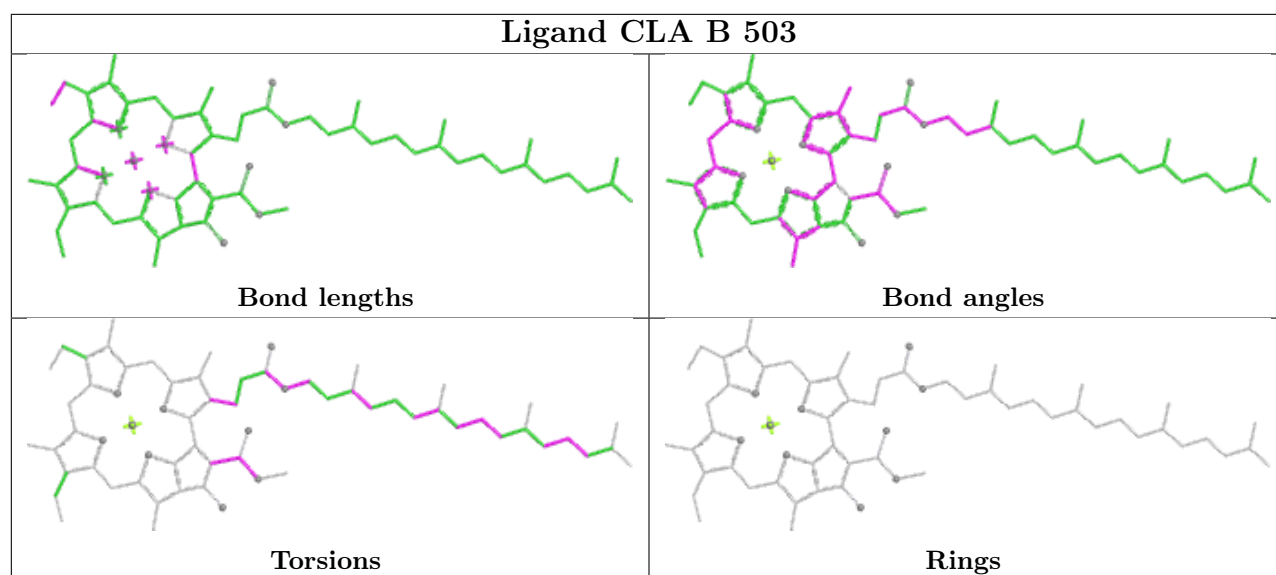


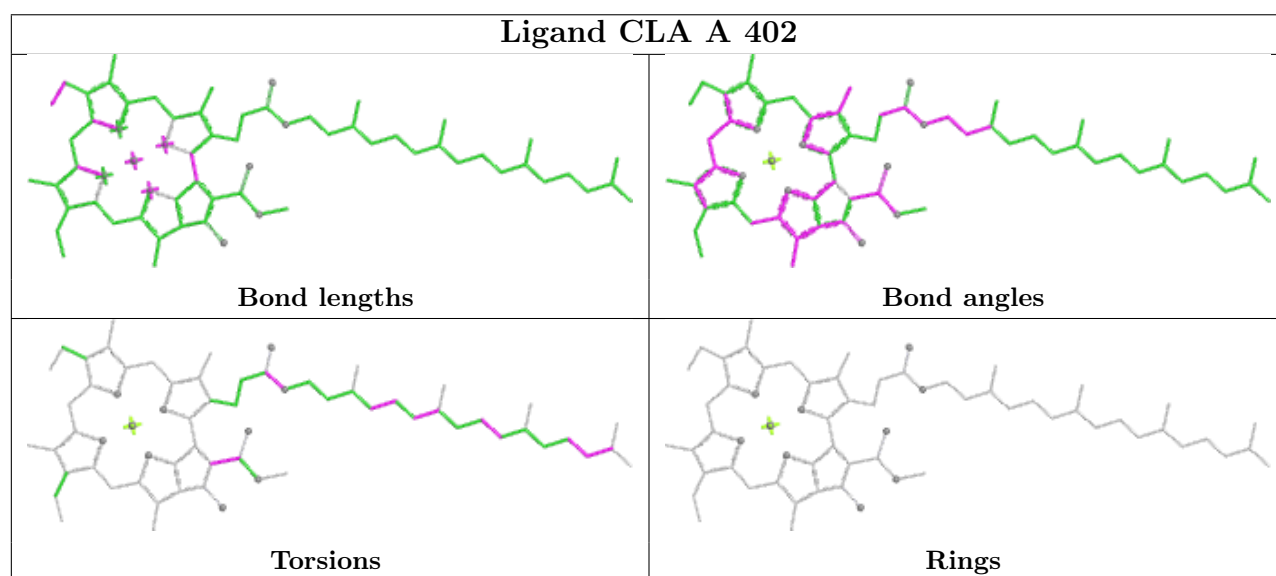
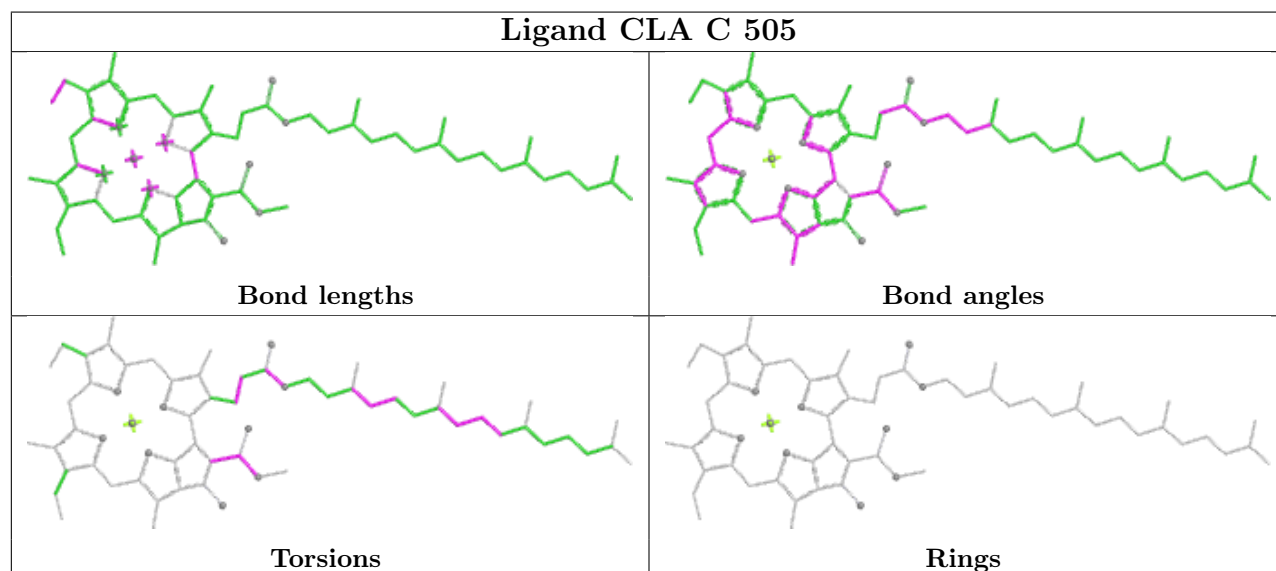
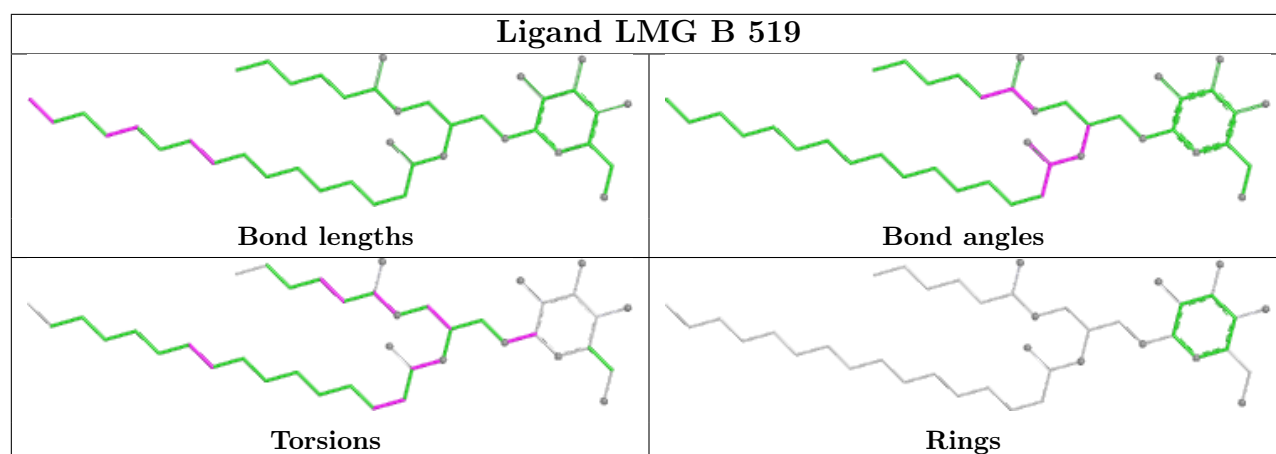


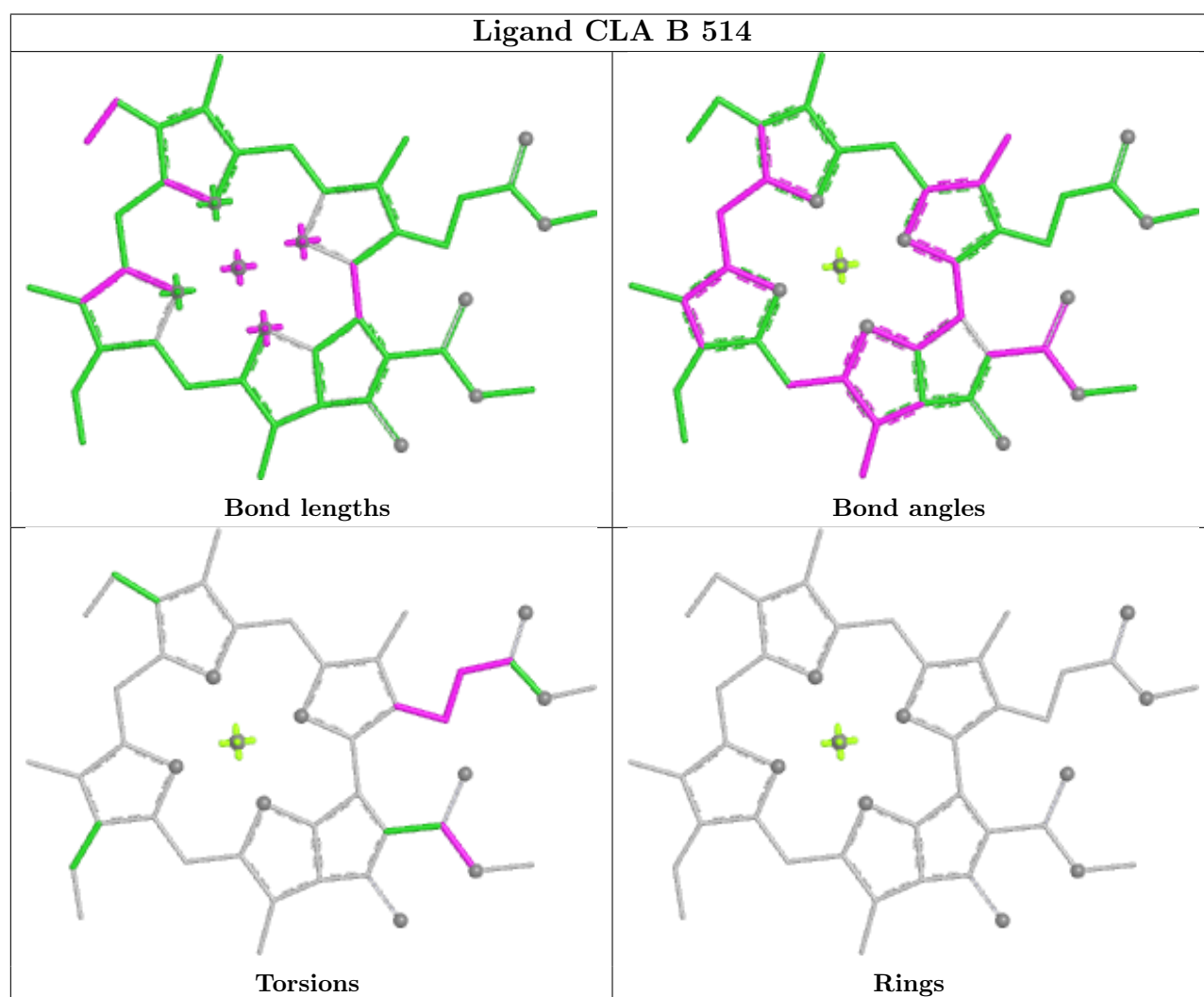
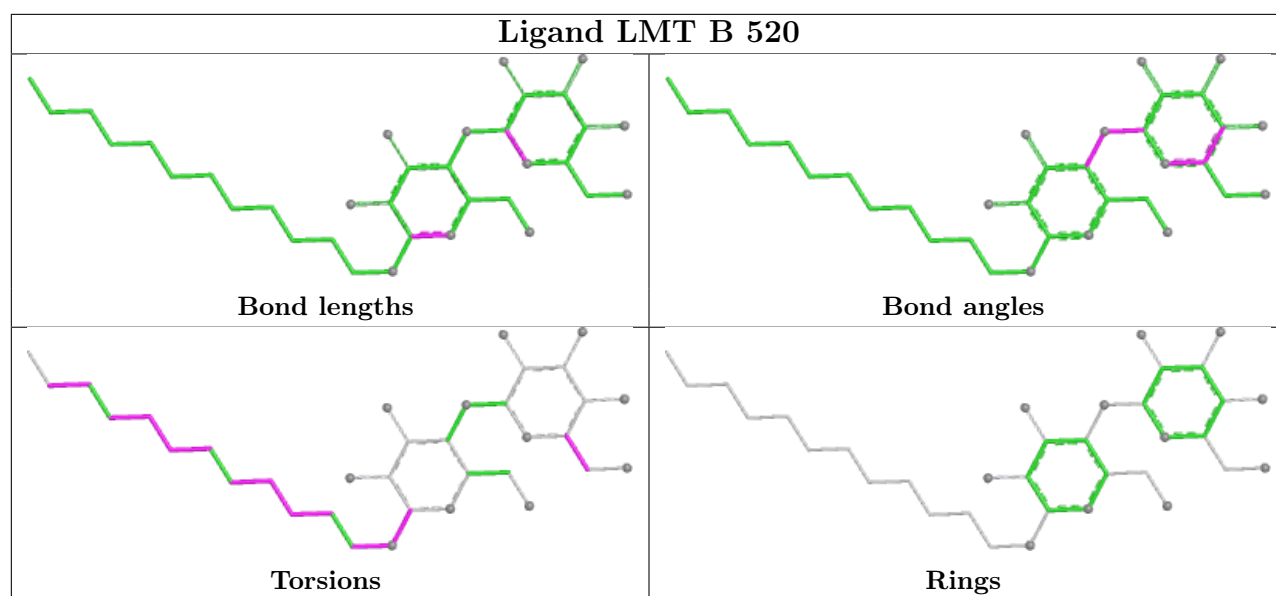


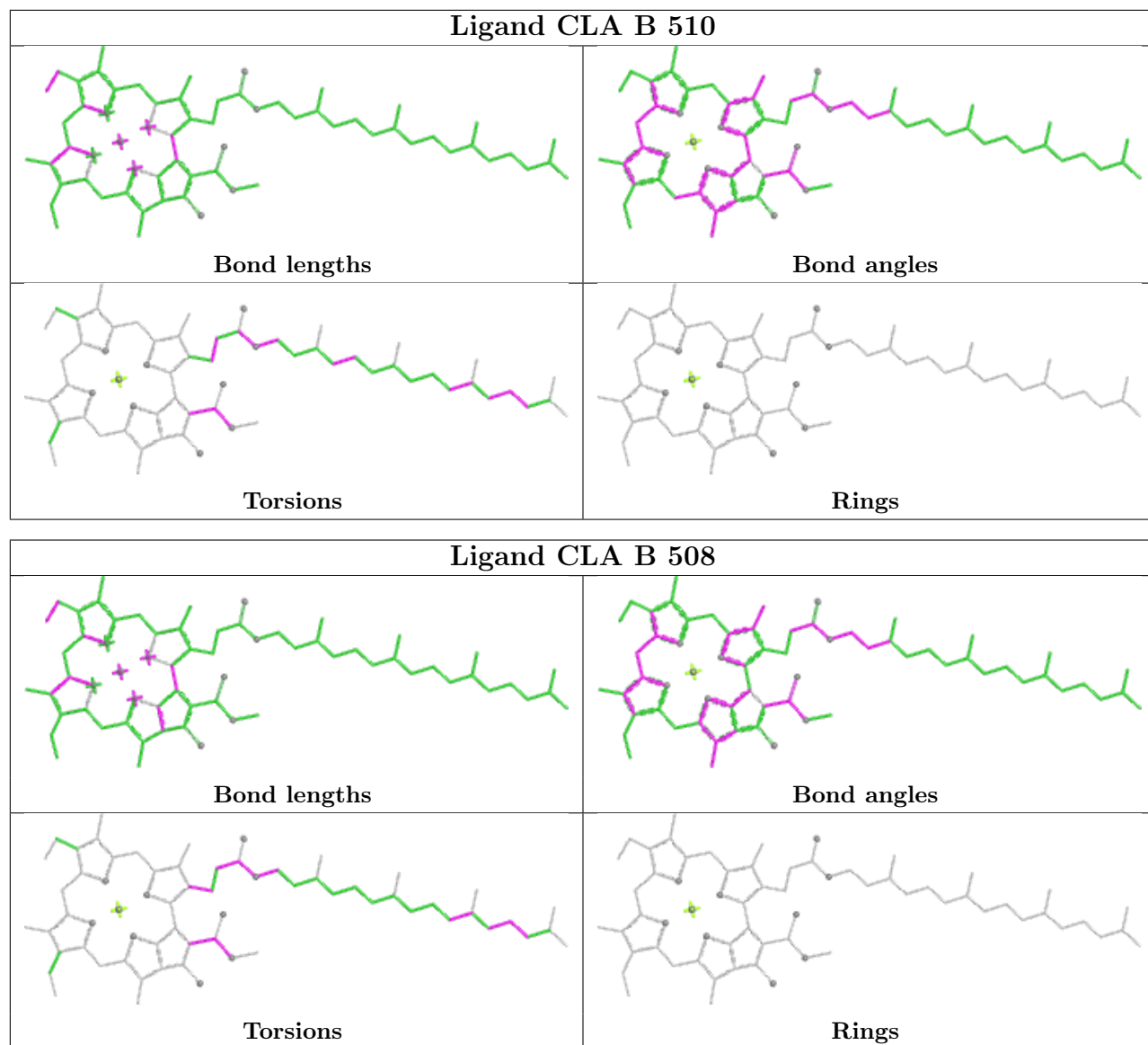


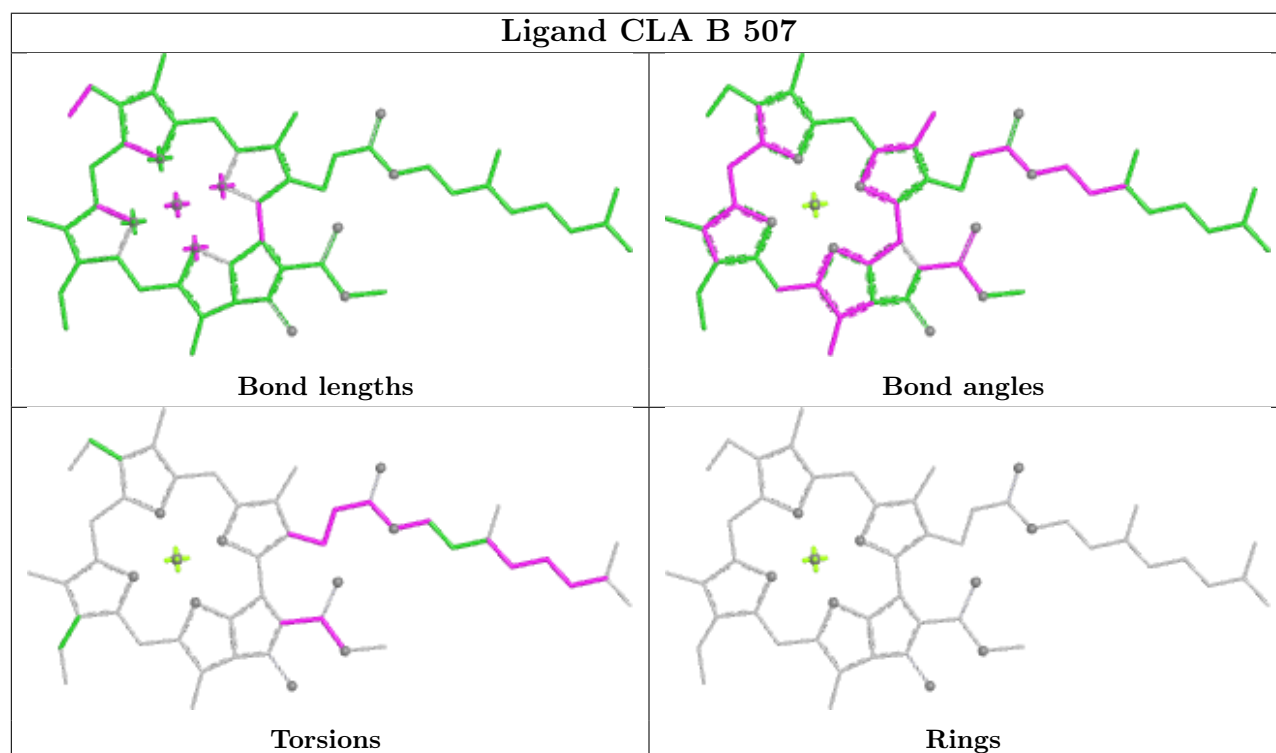
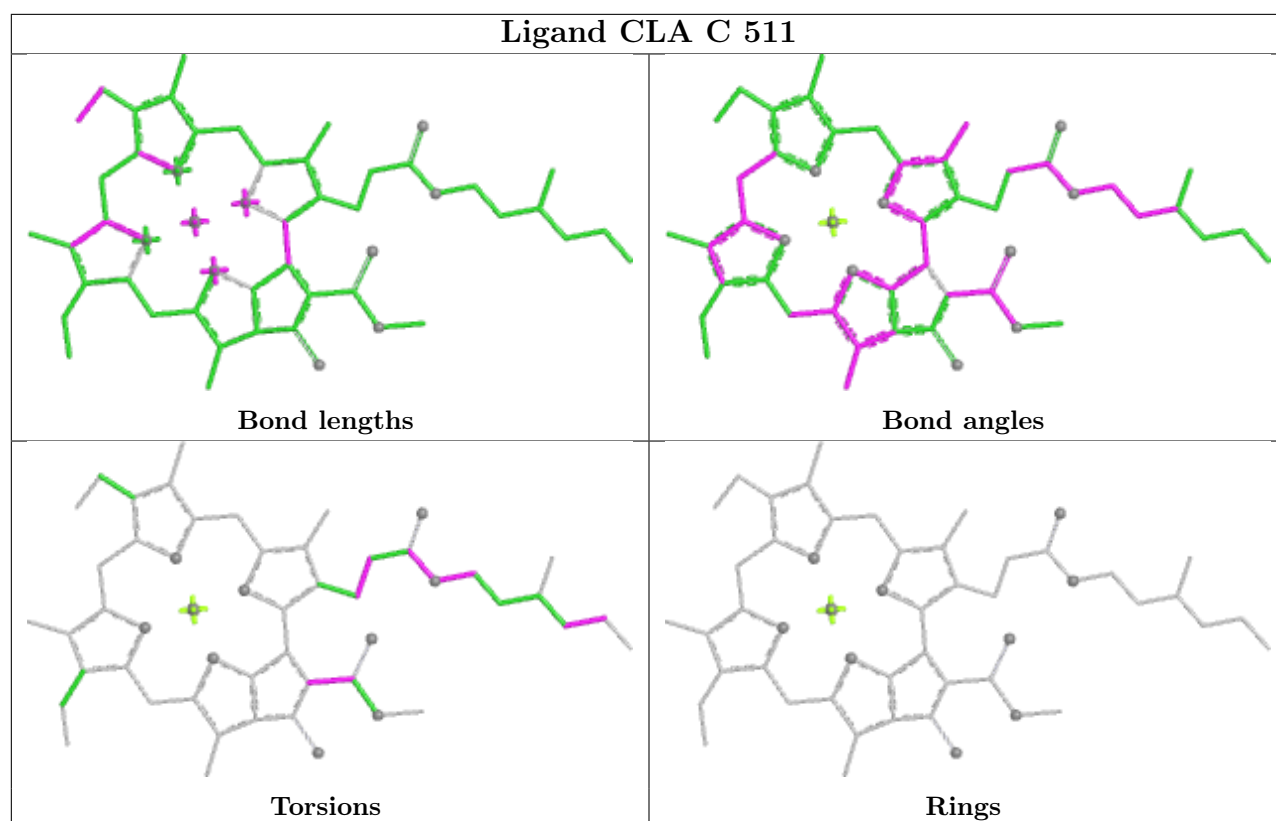




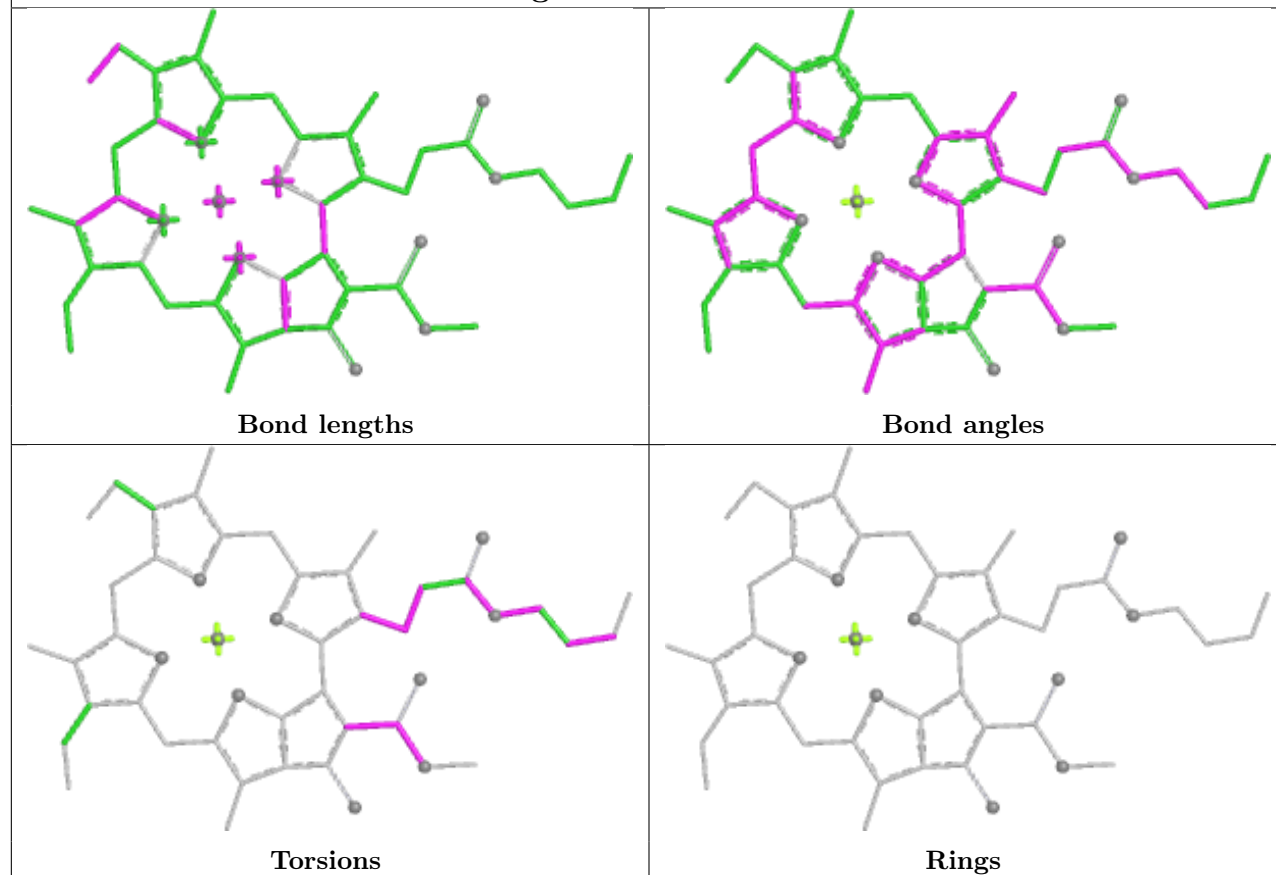




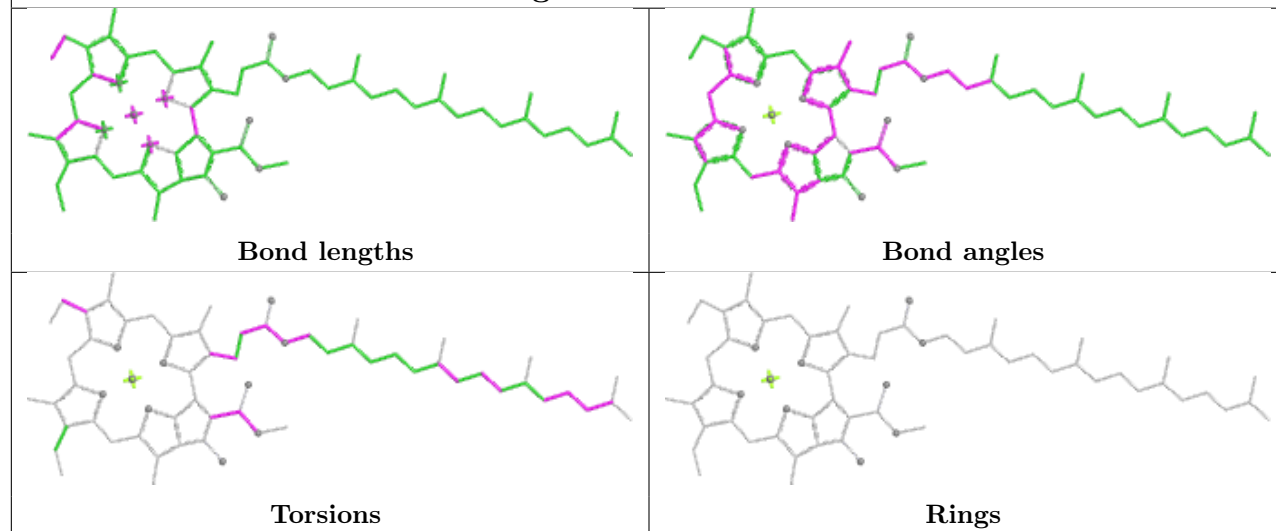


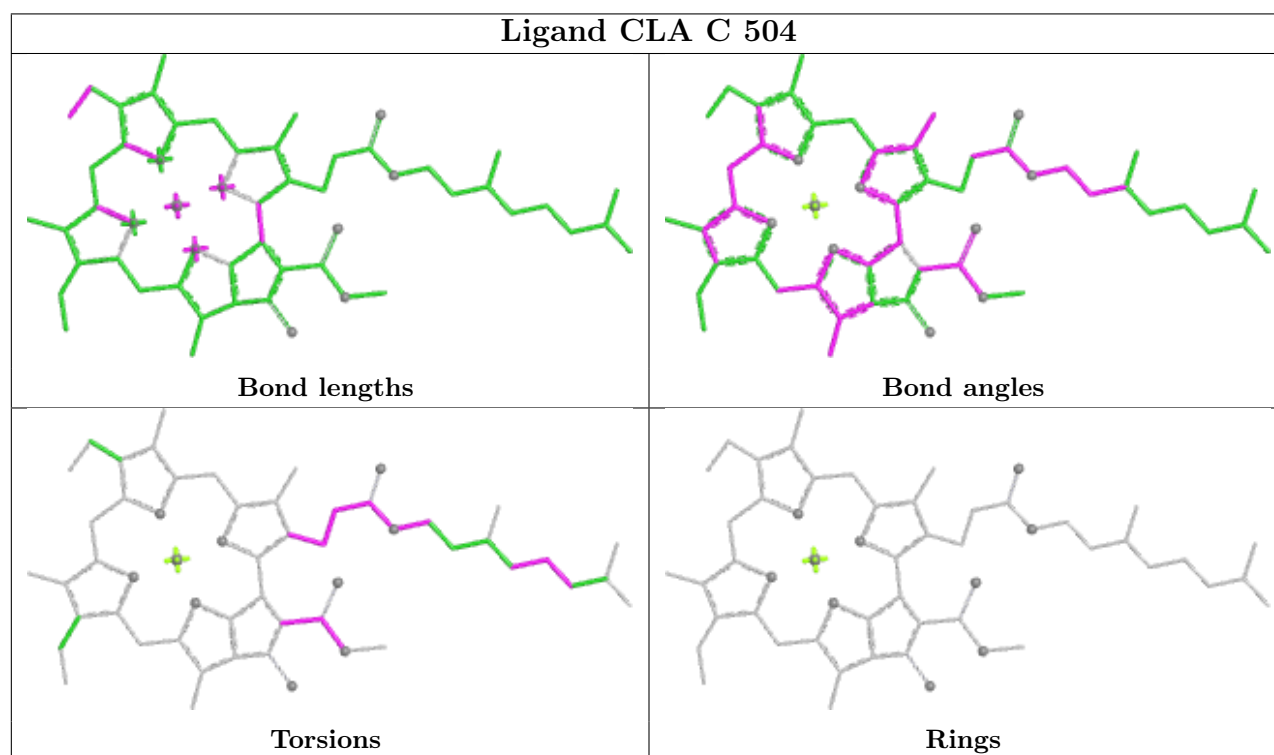
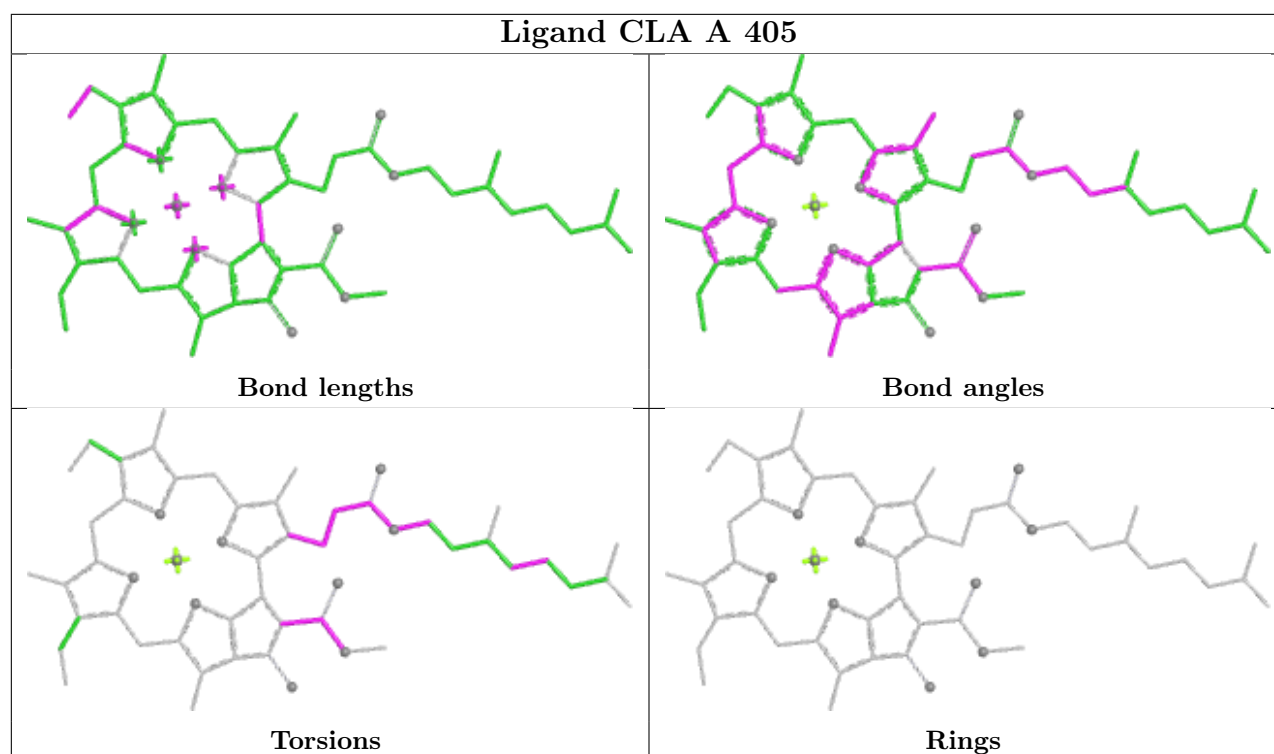


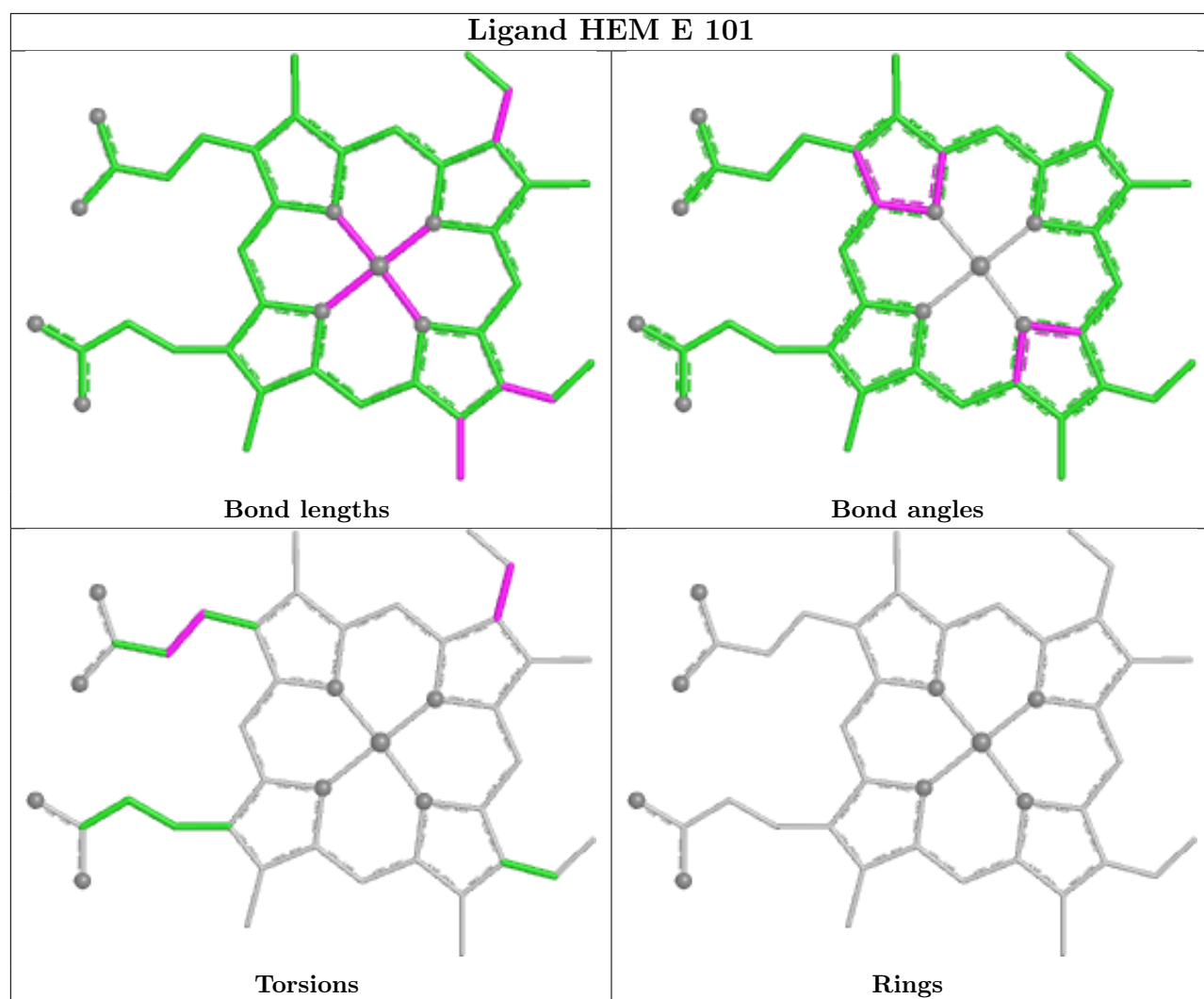
Ligand CLA A 403

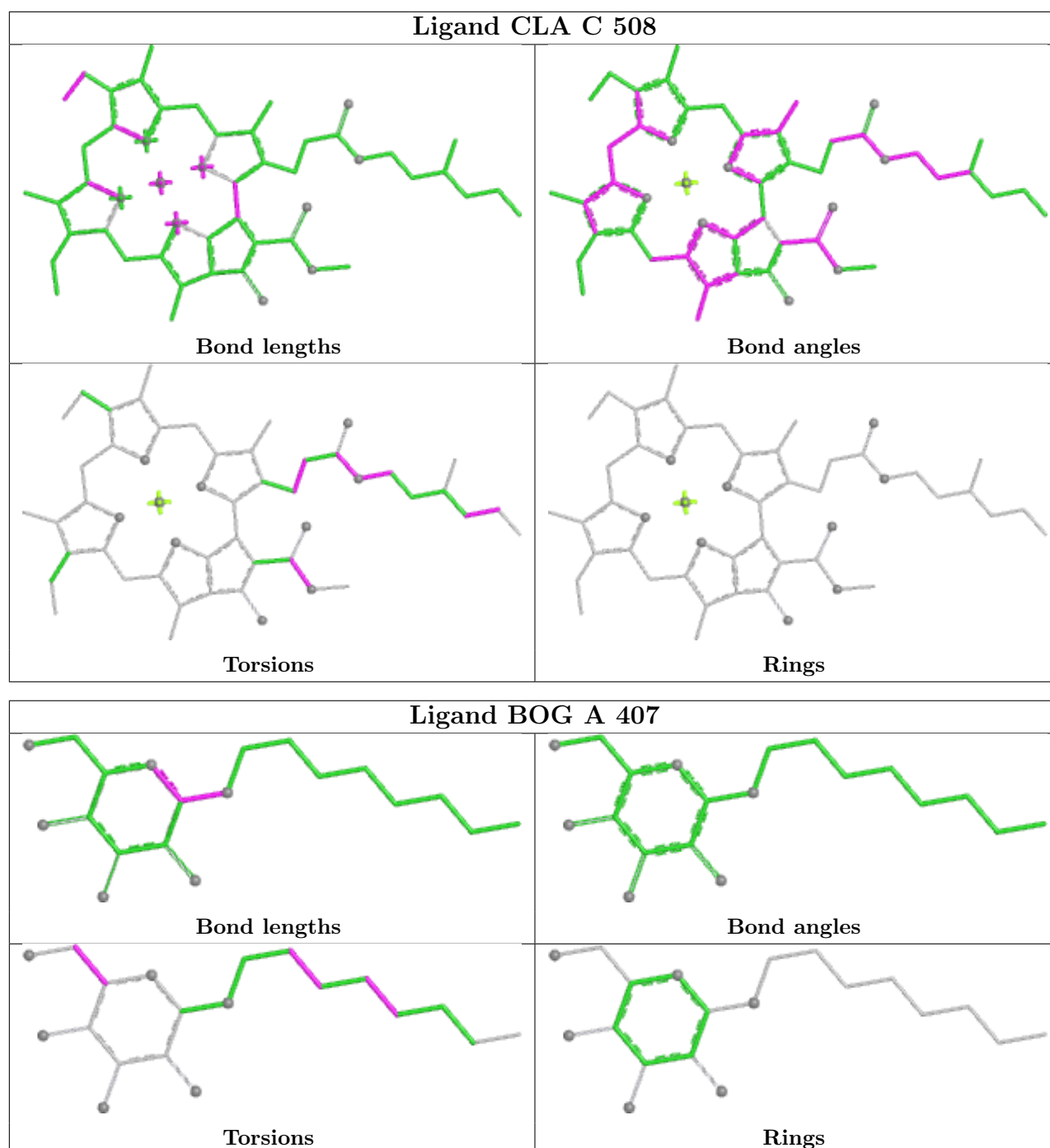


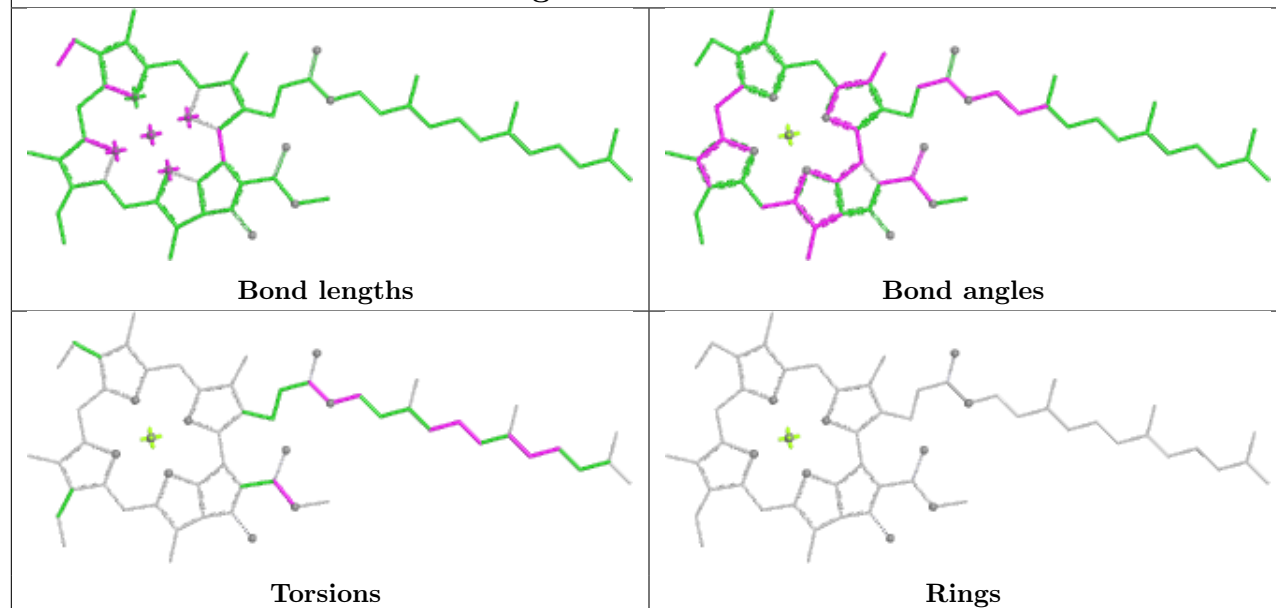
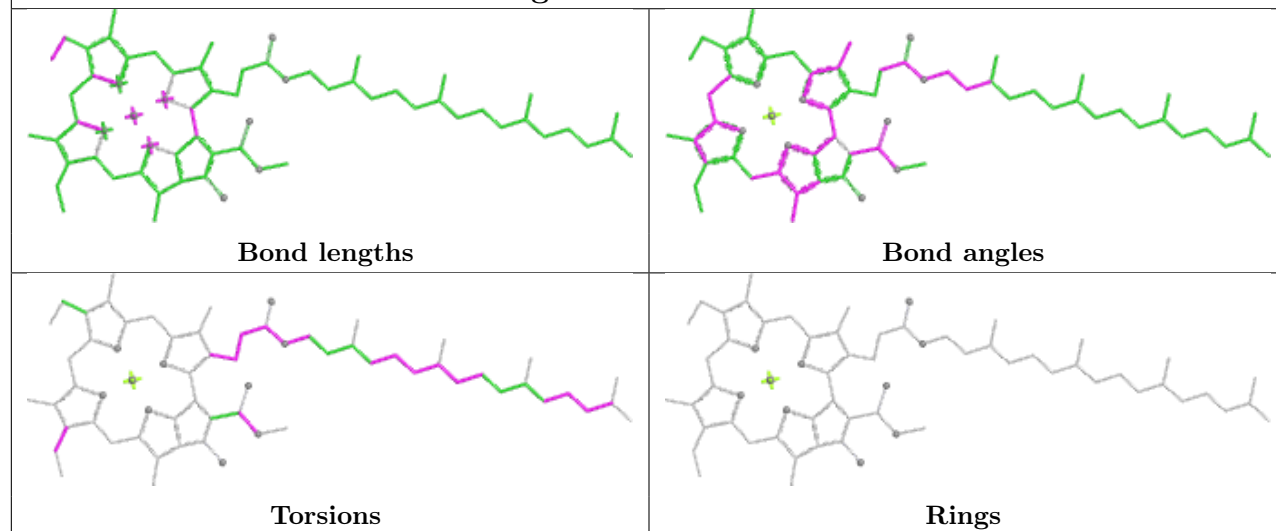
Ligand CLA C 501

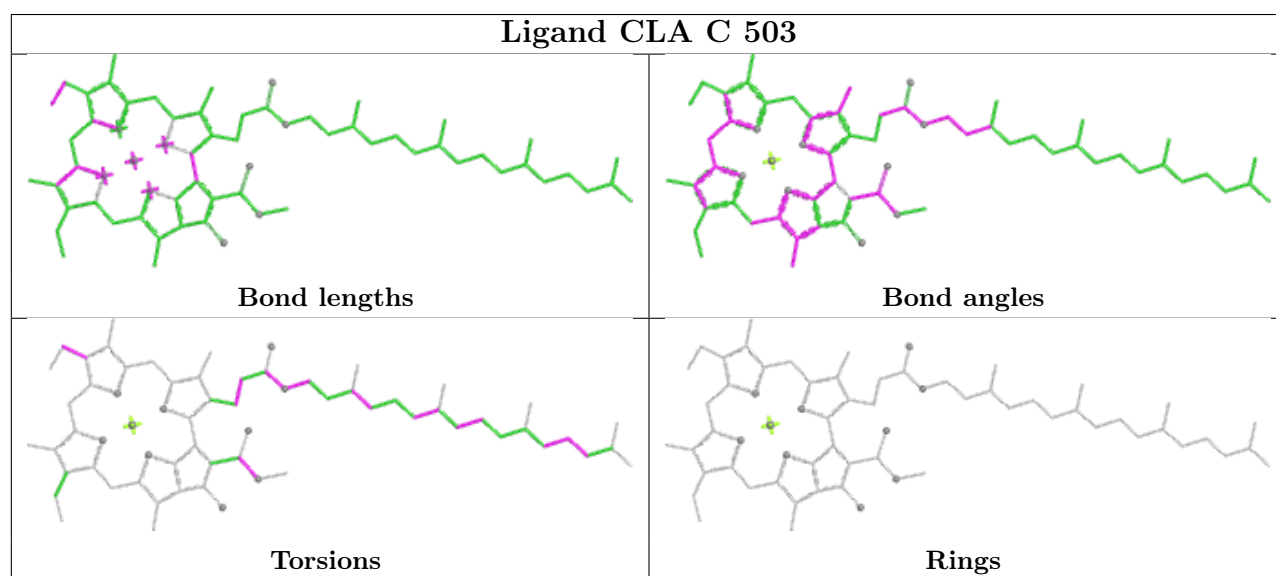
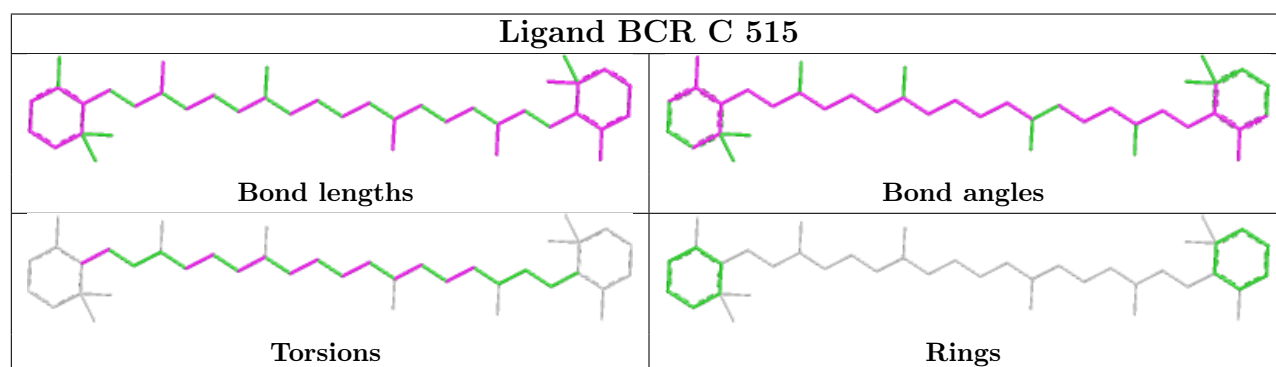
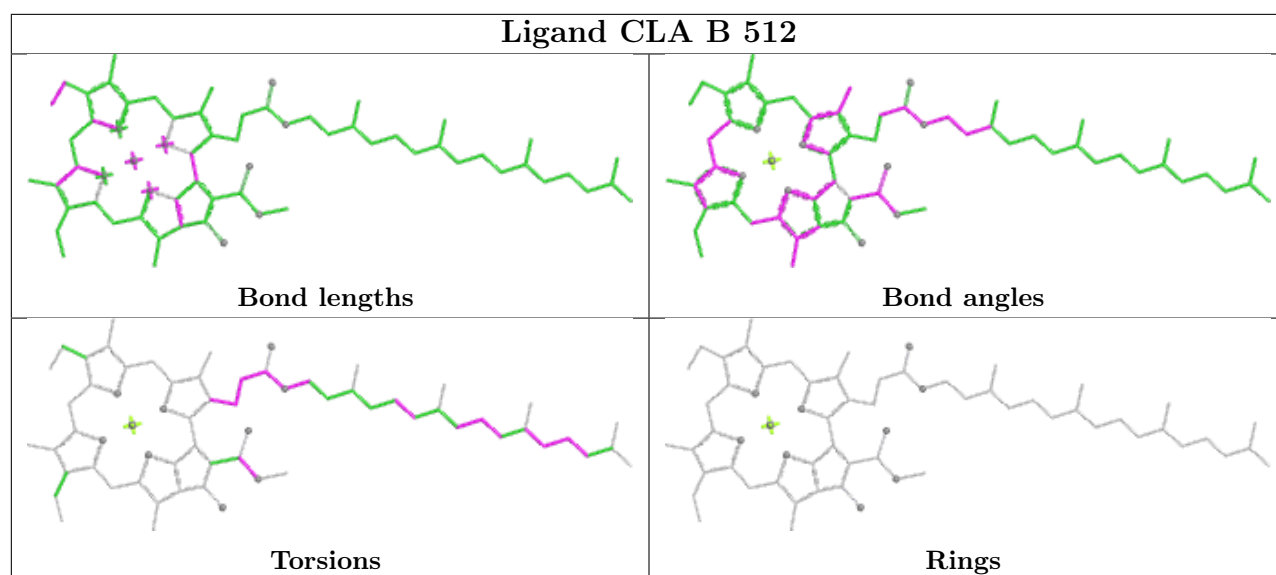


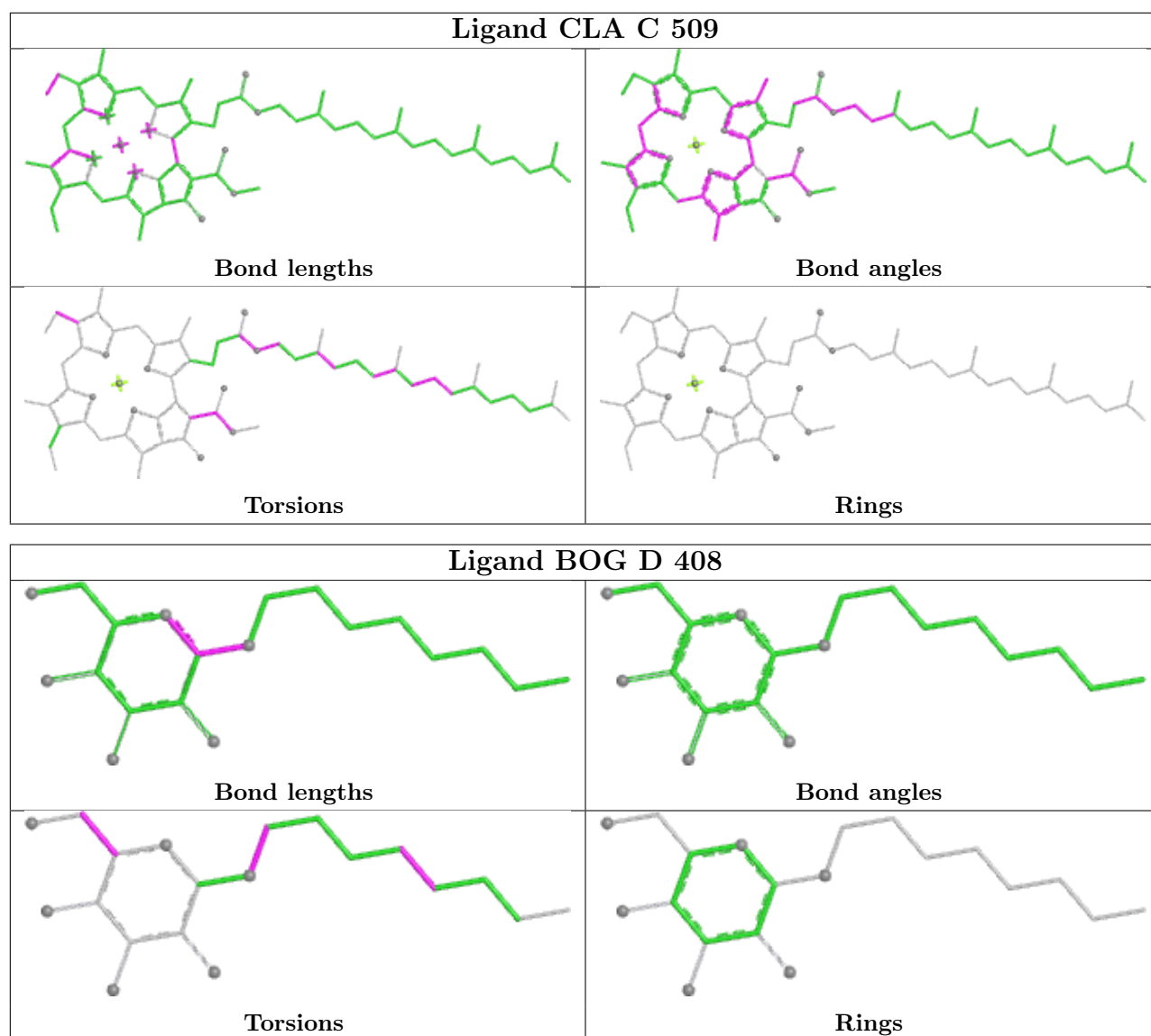


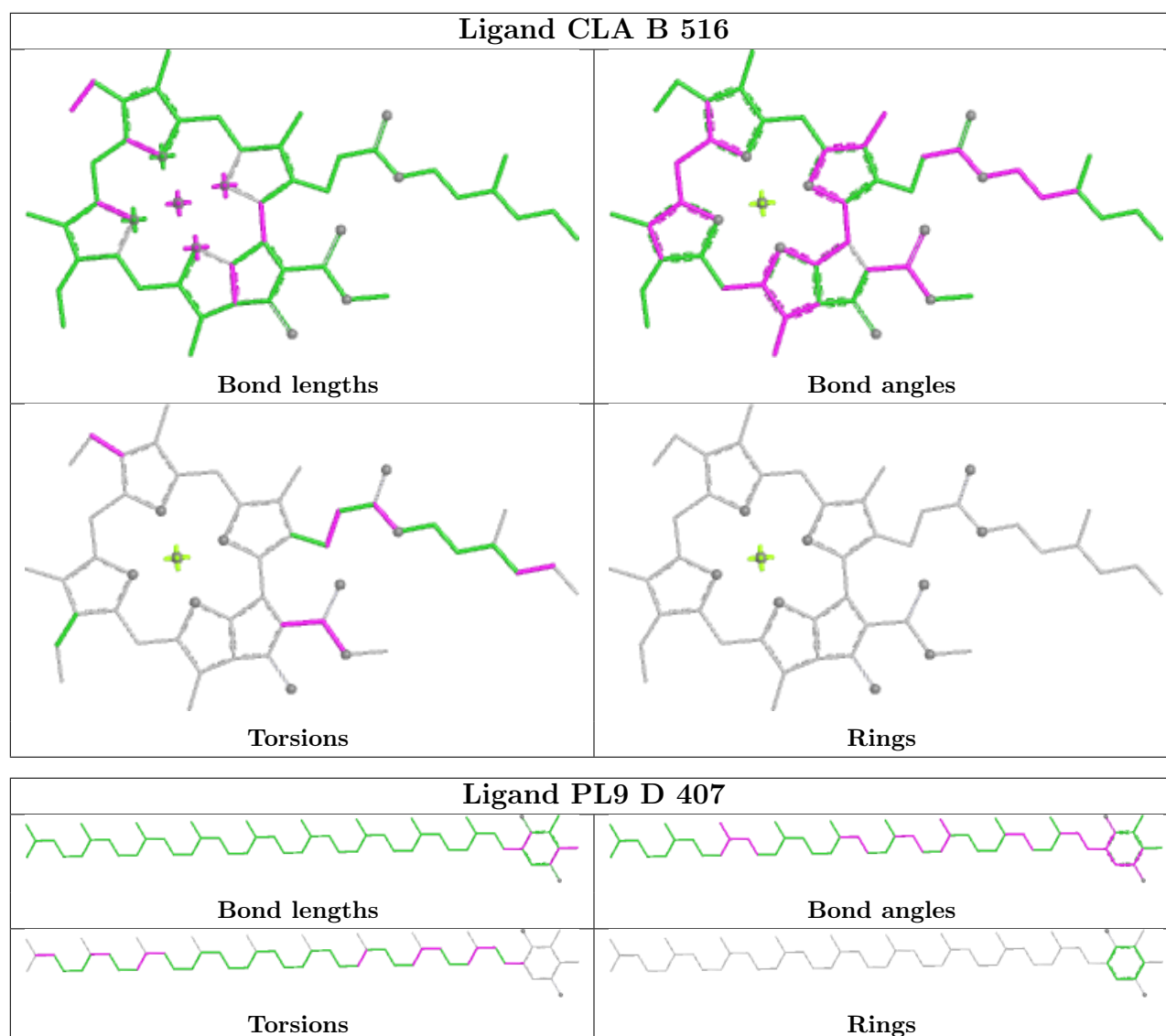




Ligand CLA B 513**Ligand CLA D 401**







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

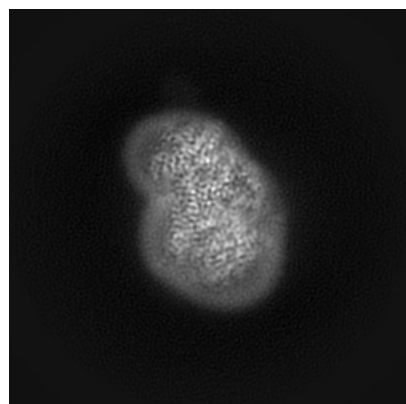
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18848. These allow visual inspection of the internal detail of the map and identification of artifacts.

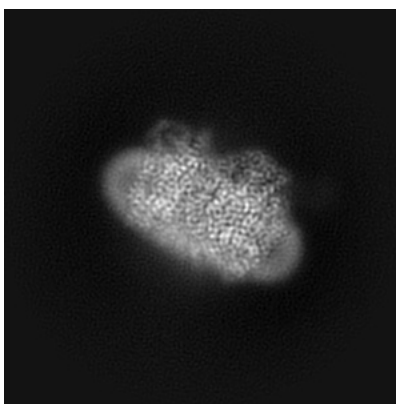
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

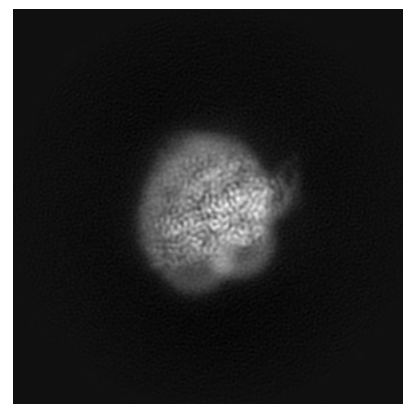
6.1.1 Primary map



X

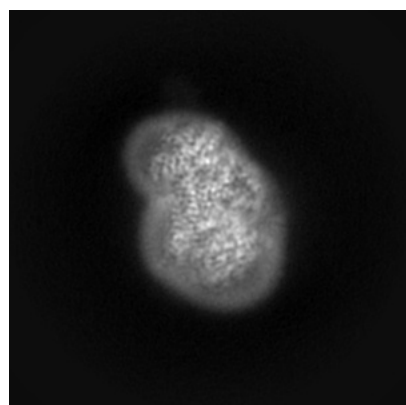


Y

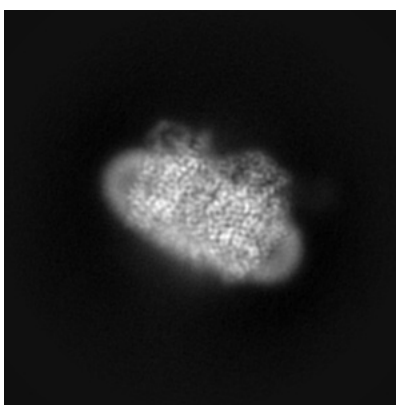


Z

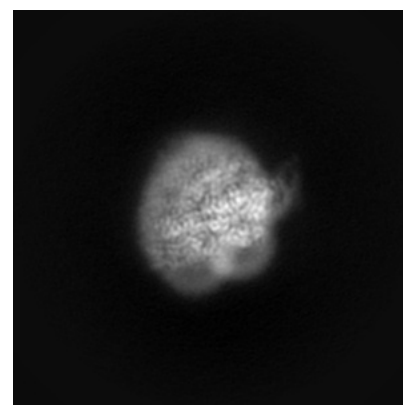
6.1.2 Raw map



X



Y

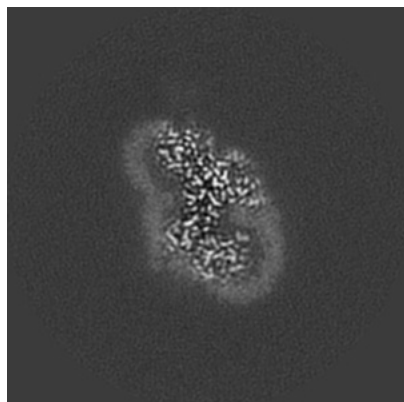


Z

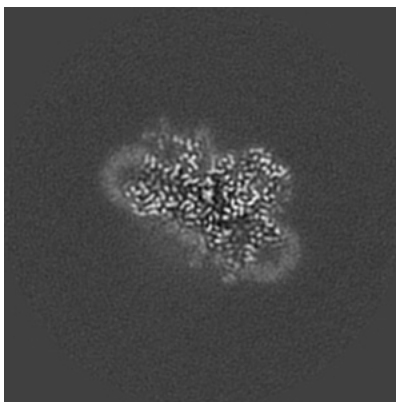
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

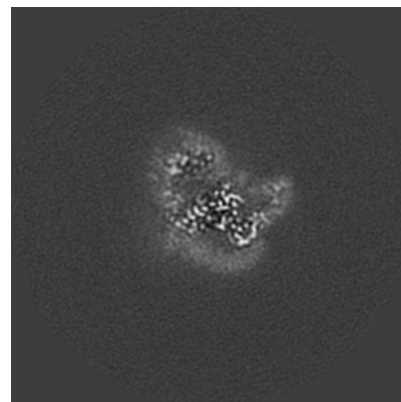
6.2.1 Primary map



X Index: 170

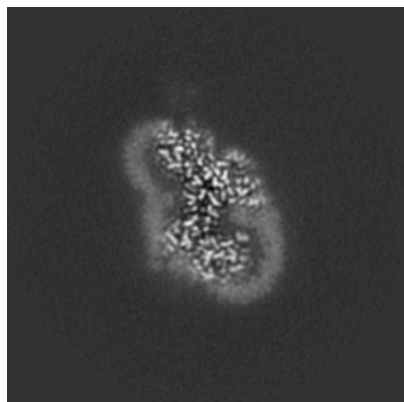


Y Index: 170

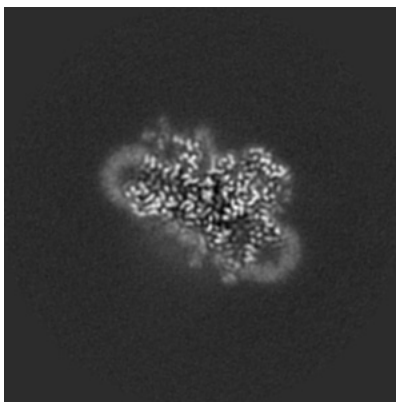


Z Index: 170

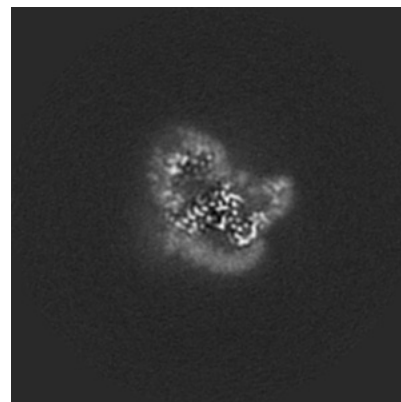
6.2.2 Raw map



X Index: 170



Y Index: 170

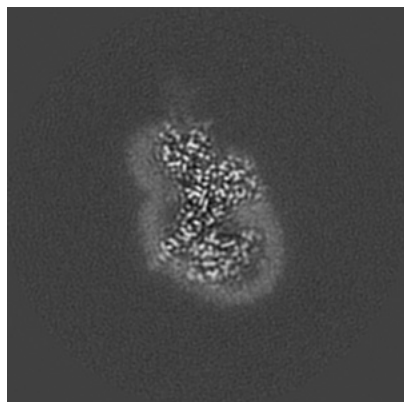


Z Index: 170

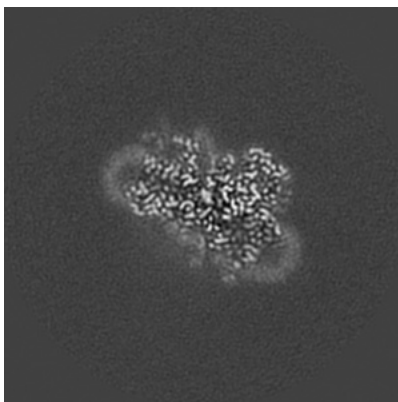
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

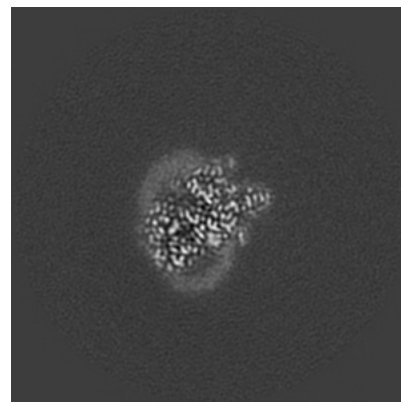
6.3.1 Primary map



X Index: 175

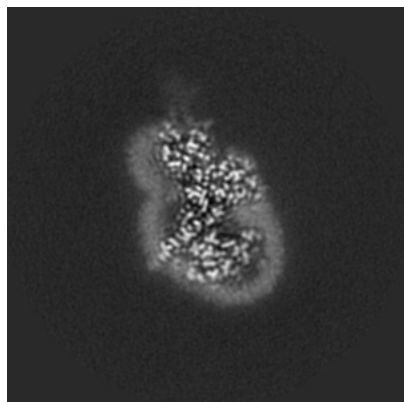


Y Index: 169

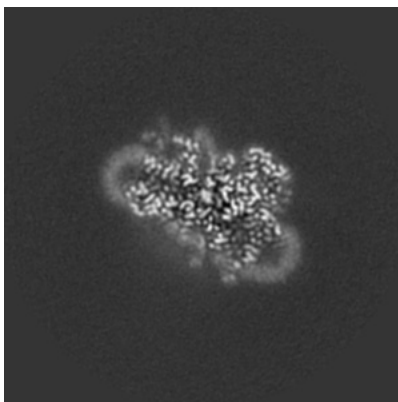


Z Index: 205

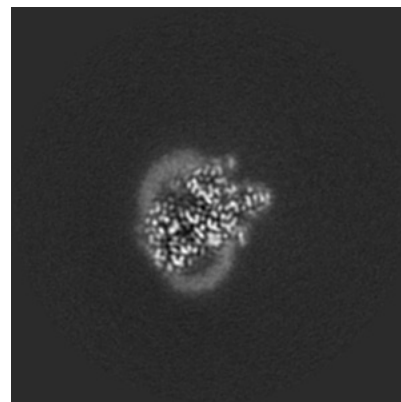
6.3.2 Raw map



X Index: 175



Y Index: 169

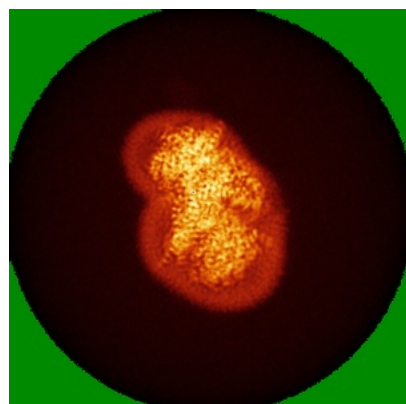


Z Index: 205

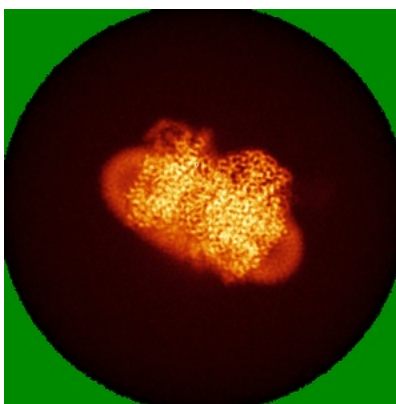
The images above show the largest variance slices of the map in three orthogonal directions.

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

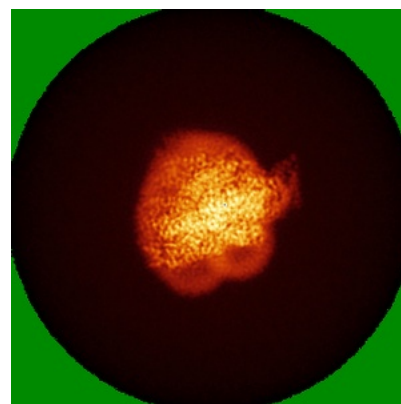
6.4.1 Primary map



X

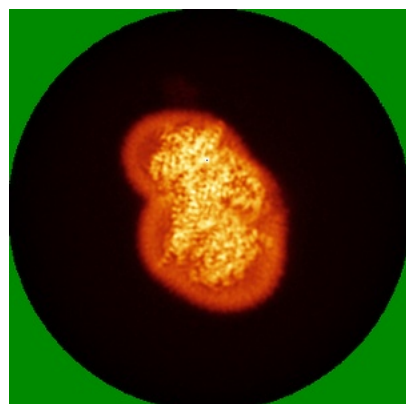


Y

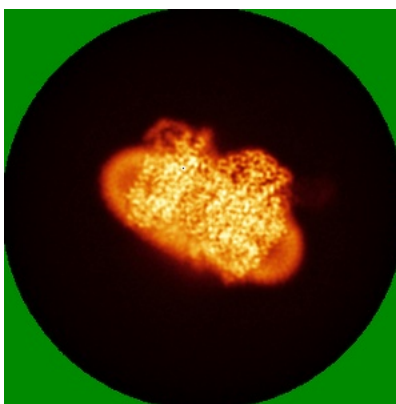


Z

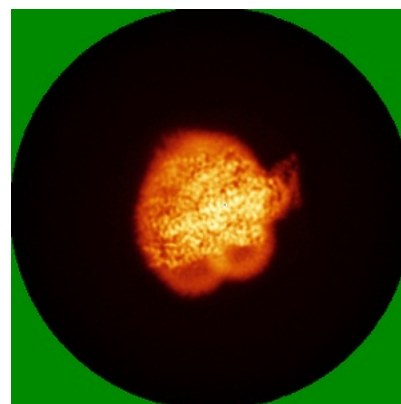
6.4.2 Raw map



X



Y

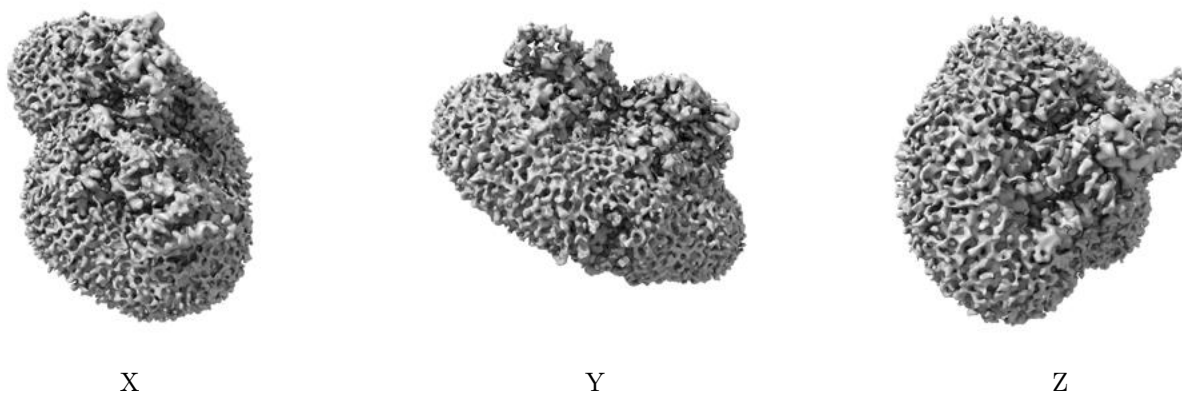


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

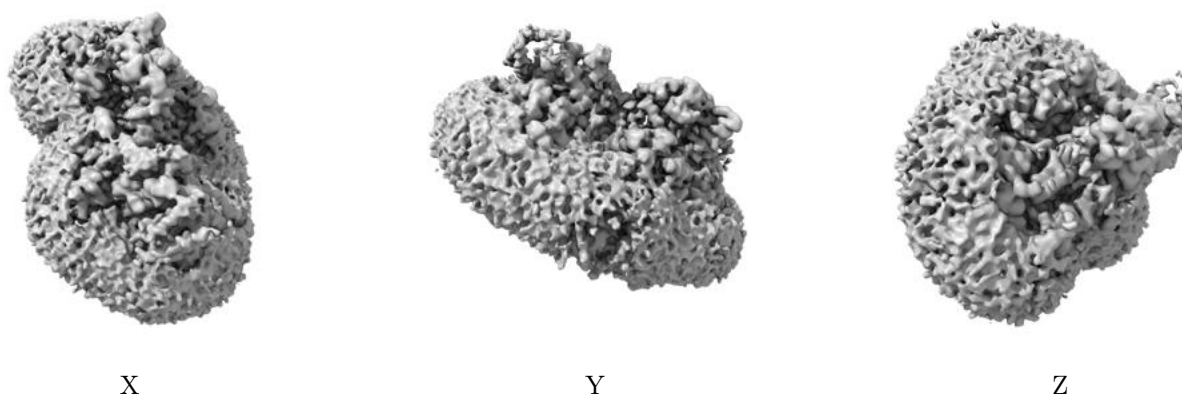
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

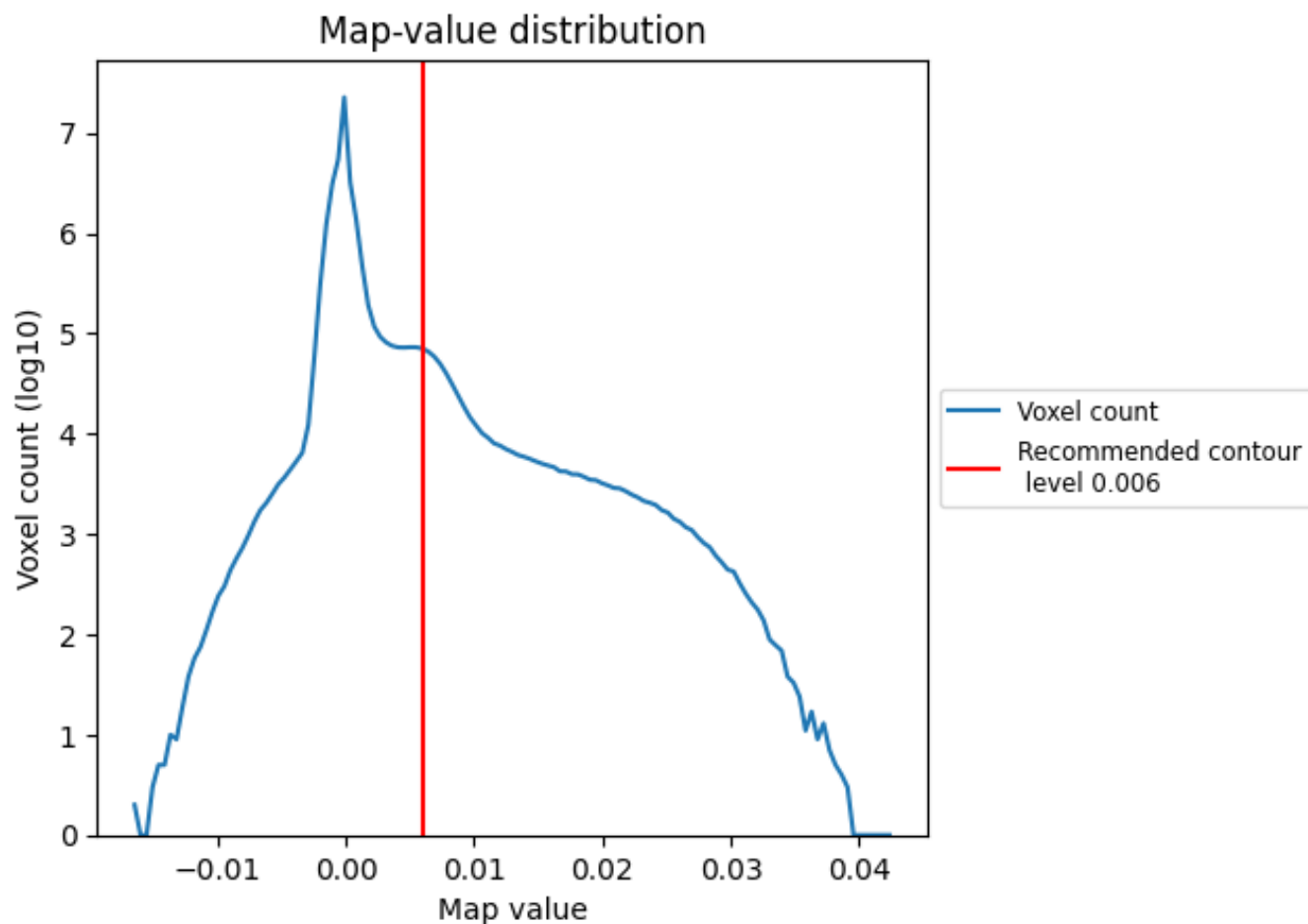
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

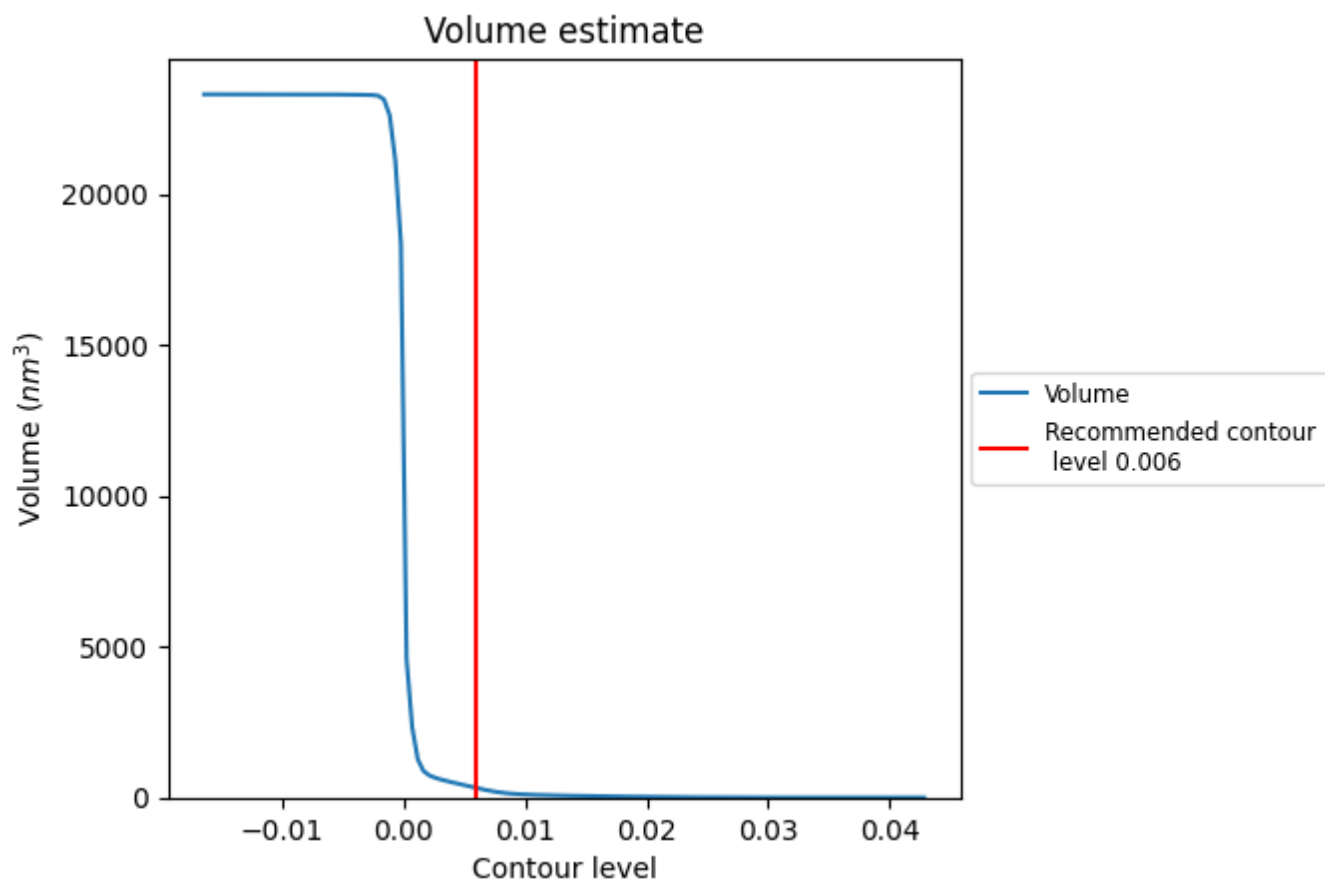
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

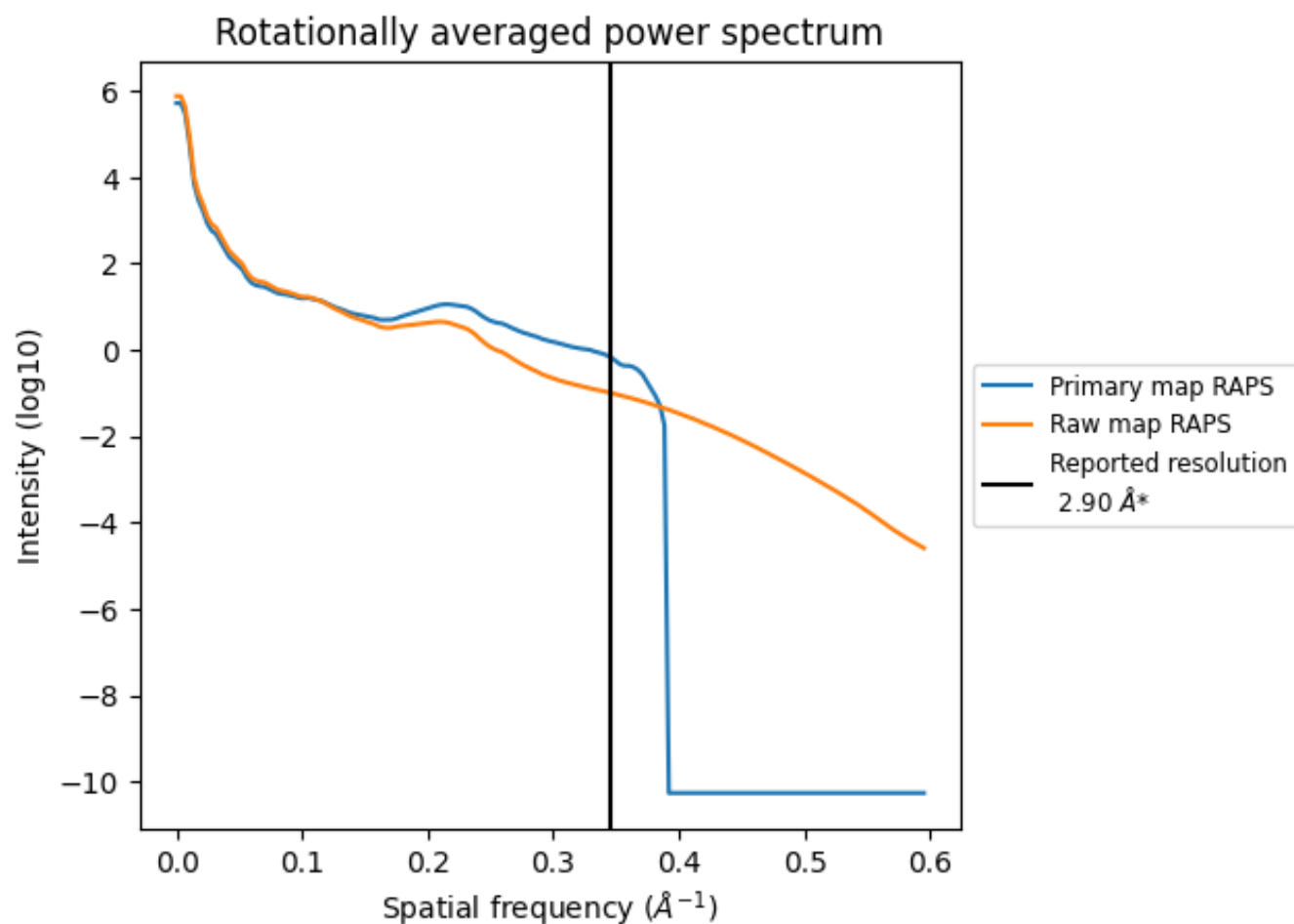
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 318 nm^3 ; this corresponds to an approximate mass of 287 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

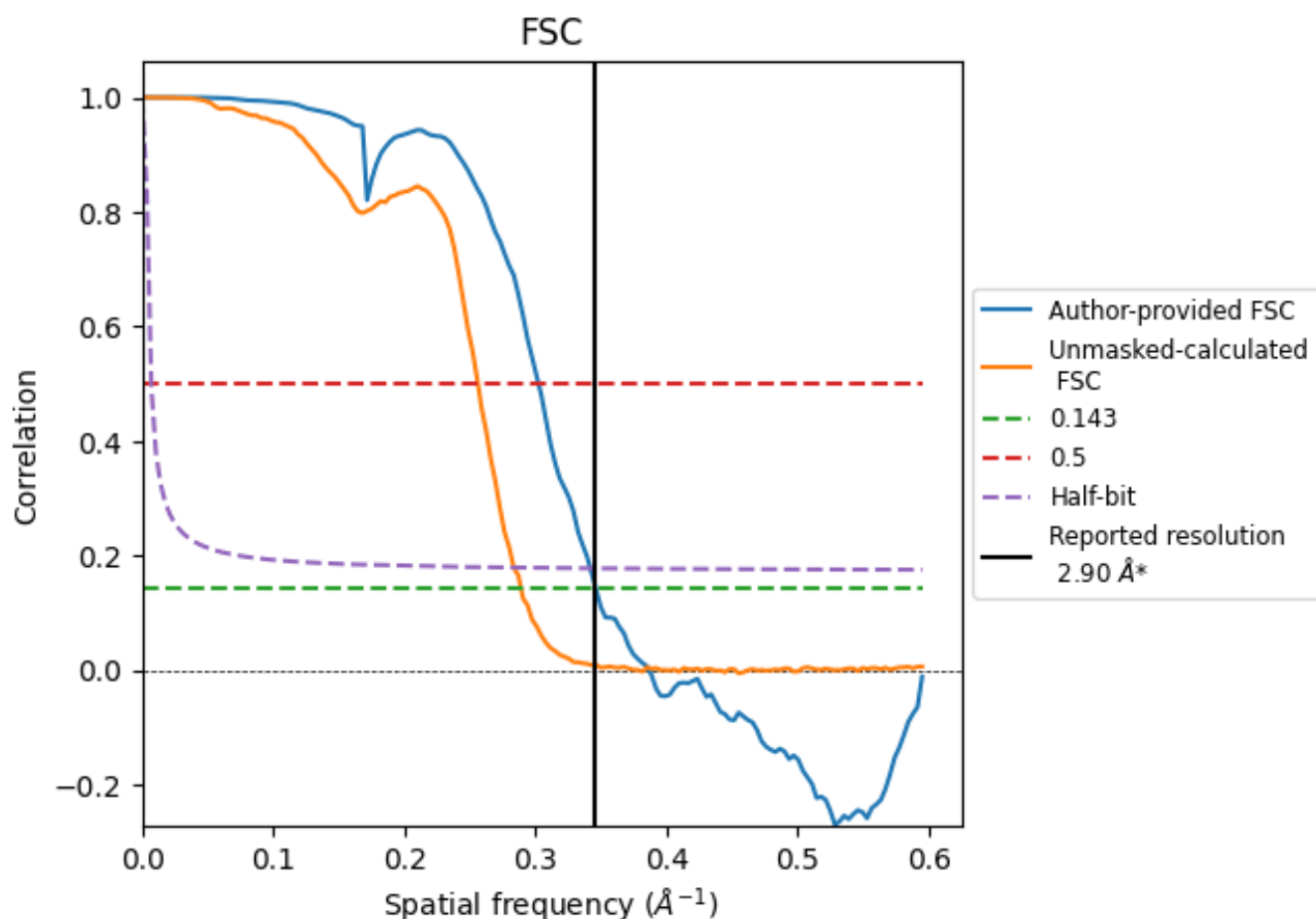


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

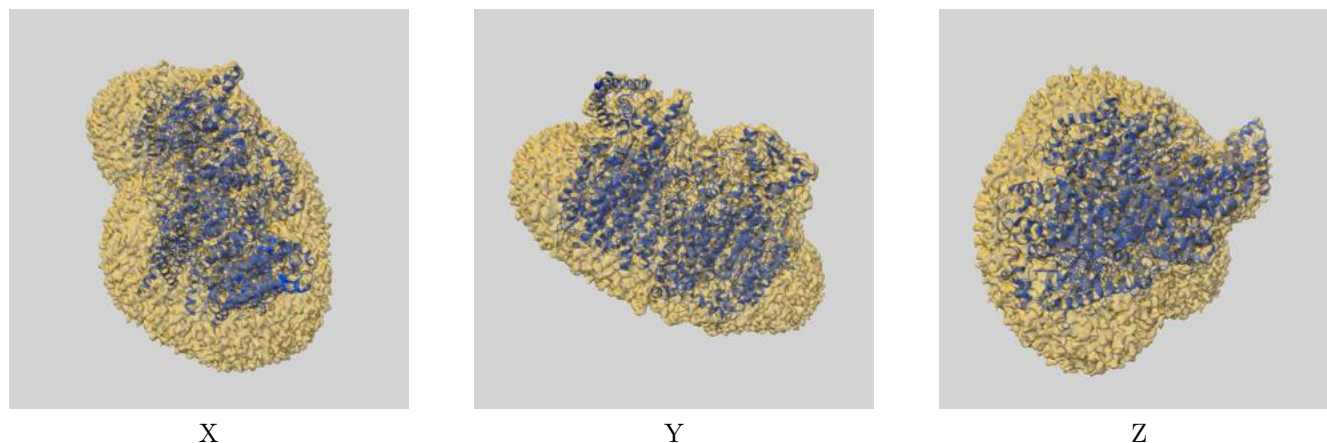
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.31	2.92
Unmasked-calculated*	3.46	3.90	3.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

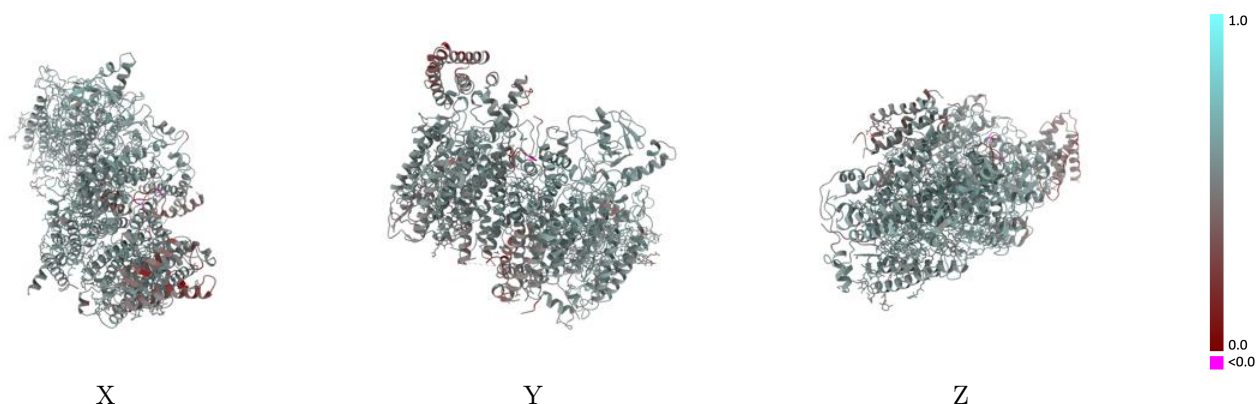
This section contains information regarding the fit between EMDB map EMD-18848 and PDB model 8R2I. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



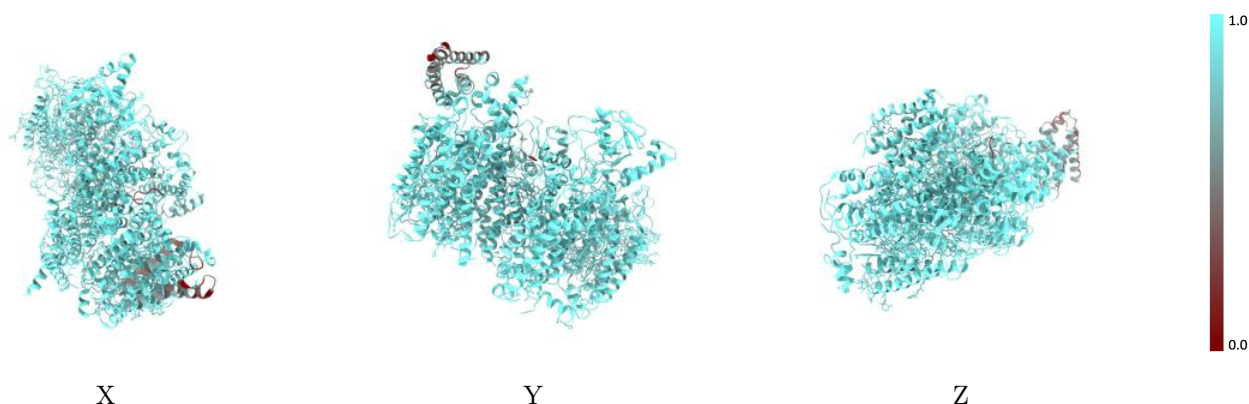
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



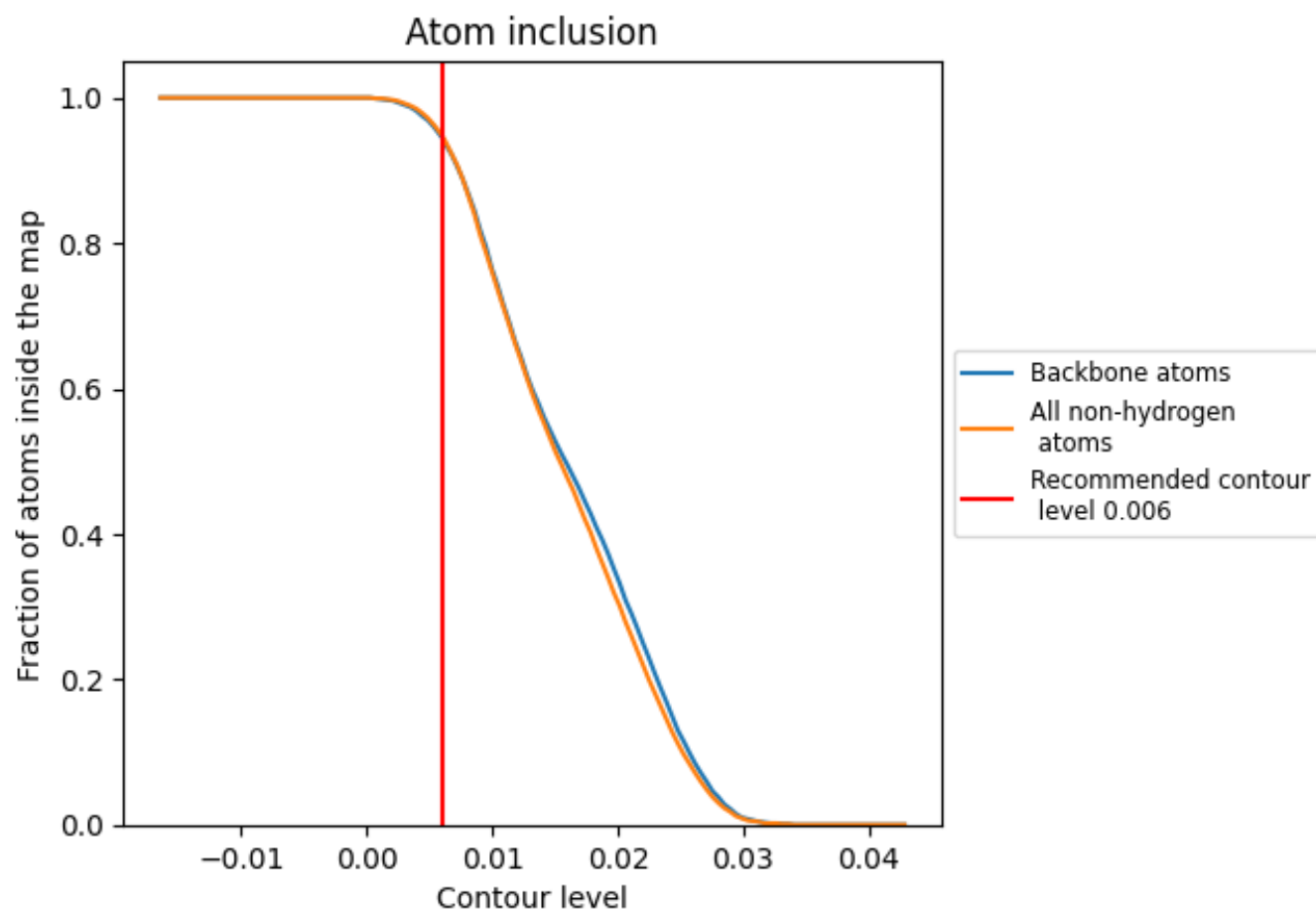
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.5330
1	0.9230	0.3870
2	0.6220	0.4050
A	0.9770	0.5490
B	0.9690	0.5590
C	0.9480	0.5200
D	0.9670	0.5610
E	0.9460	0.4980
F	0.9660	0.4780
H	0.9520	0.5360
I	0.9960	0.5050
K	0.9800	0.4670

1.0

0.0

<0.0