



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 02:48 AM JST

PDB ID : 7DXH
EMDB ID : EMD-30909
Title : Cryo-EM structure of PSII intermediate Psb28-PSII complex
Authors : Sui, S.F.; Shen, J.R.; Han, G.Y.; Xiao, Y.N.; Huang, G.Q.
Deposited on : 2021-01-18
Resolution : 3.14 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:

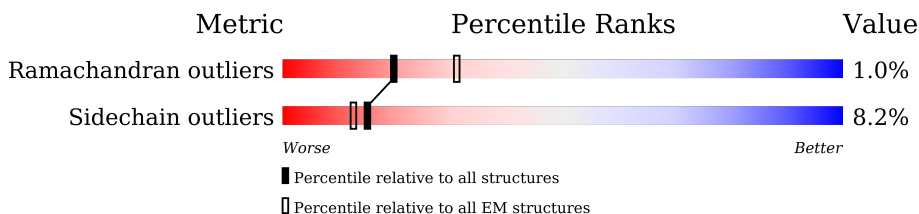
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.14 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.



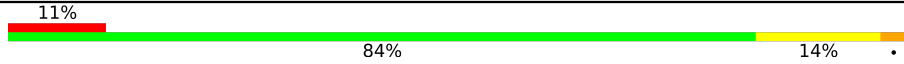




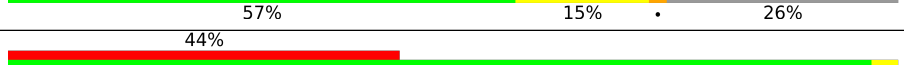

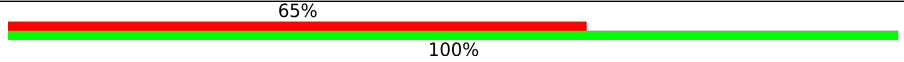

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	116	
2	B	56	
3	a	360	
4	b	505	
5	d	342	
6	e	84	
7	f	45	
8	h	65	
9	i	38	

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Mol	Chain	Length	Quality of chain
10	l	37	
11	m	36	
12	t	32	
13	x	40	
14	c	451	
15	k	46	
16	z	62	
17	y	30	
18	C	23	

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
21	CLA	a	402	X	-	-	-
21	CLA	b	601	X	-	-	-
21	CLA	b	602	X	-	-	-
21	CLA	b	603	X	-	-	-
21	CLA	b	604	X	-	-	-
21	CLA	b	605	X	-	-	-
21	CLA	b	606	X	-	-	-
21	CLA	b	609	X	-	-	-
21	CLA	b	611	X	-	-	-
21	CLA	b	612	X	-	-	-
21	CLA	b	613	X	-	-	-
21	CLA	b	614	X	-	-	-
21	CLA	b	615	X	-	-	-
21	CLA	c	503	X	-	-	-
21	CLA	c	504	X	-	-	-
21	CLA	c	508	X	-	-	-
21	CLA	c	509	X	-	-	-
21	CLA	c	510	X	-	-	-
21	CLA	c	511	X	-	-	-
21	CLA	d	402	X	-	-	-
21	CLA	d	406	X	-	-	-

2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 20054 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 reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	109	875	549	153	168	5	0	0

- Molecule 2 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	48	349	227	63	59	0	0

- Molecule 3 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	a	297	2304	1515	381	393	15	0	0

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	b	494	3886	2554	646	673	13	0	0

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	d	339	2694	1787	439	456	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	e	63	509	334	81	94	0	0

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	f	28	219	149	36	33	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	62	493	330	79	82	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	29	231	162	30	38	1	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	l	37	304	202	48	53	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	m	31	244	165	36	43	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	t	27	230	164	30	34	2	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	x	36	261	177	39	45	0	0

- Molecule 14 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	c	403	3130	2071	520	527	12	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	k	34	264	186	36	42	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	z	62	455	316	67	70	2	0	0

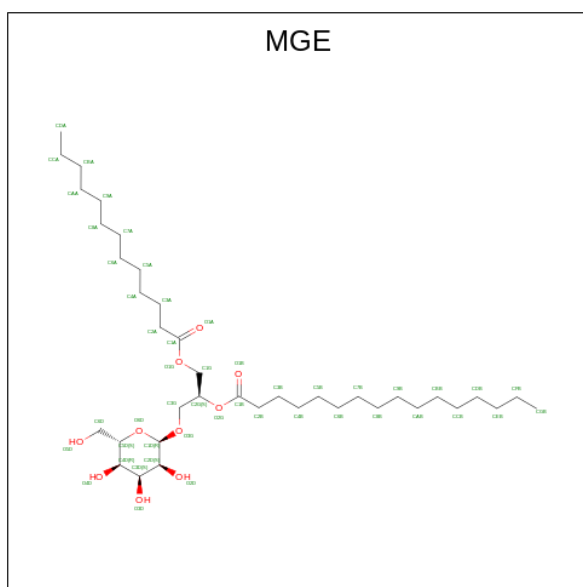
- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	y	28	137	81	28	28	0	0

- Molecule 18 is a protein called unidentified transmembrane protein.

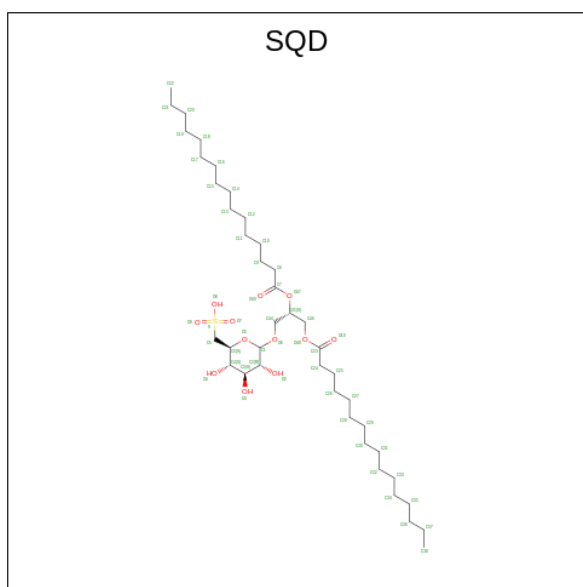
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	C	23	115	69	23	23	0	0

- Molecule 19 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: C₃₈H₇₂O₁₀).



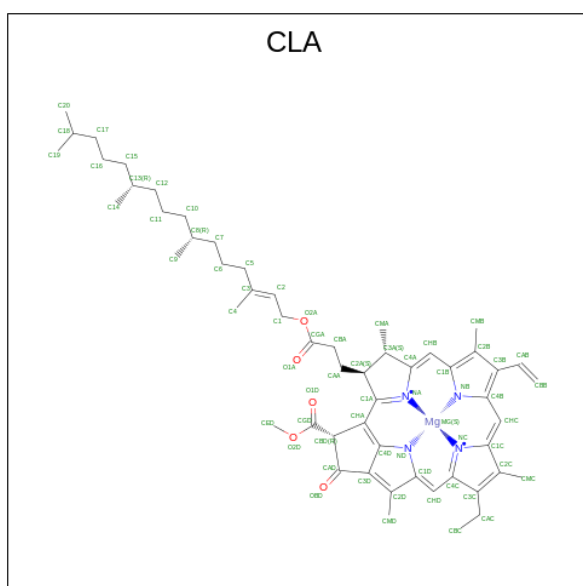
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
19	B	1	48	38	10	0
19	b	1	89	69	20	0
19	b	1	89	69	20	0
19	d	1	48	38	10	0
19	f	1	47	37	10	0
19	m	1	48	38	10	0
19	c	1	48	38	10	0

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
20	a	1	26	13	12	1	0
20	1	1	47	34	12	1	0

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	a	1	181	151	3	12	15	0
21	a	1	181	151	3	12	15	0

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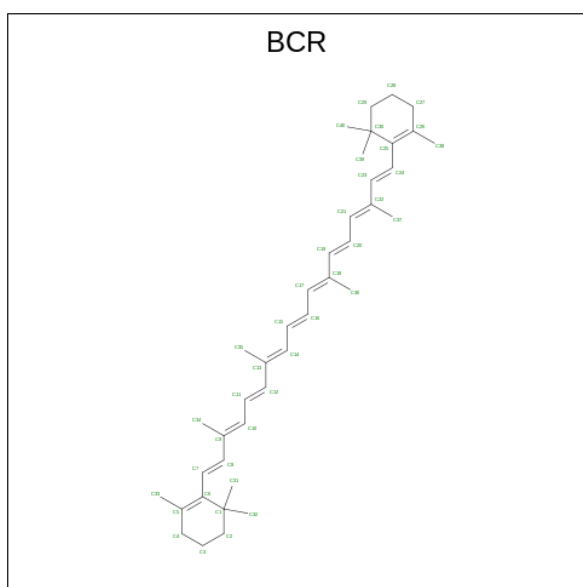
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	a	1	Total 181	C 151	Mg 3	N 12	O 15	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	b	1	Total 932	C 782	Mg 15	N 60	O 75	0
21	d	1	Total 176	C 146	Mg 3	N 12	O 15	0
21	d	1	Total 176	C 146	Mg 3	N 12	O 15	0
21	d	1	Total 176	C 146	Mg 3	N 12	O 15	0
21	h	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	c	1	Total 613	C 503	Mg 11	N 44	O 55	0
21	k	1	Total 46	C 36	Mg 1	N 4	O 5	0

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

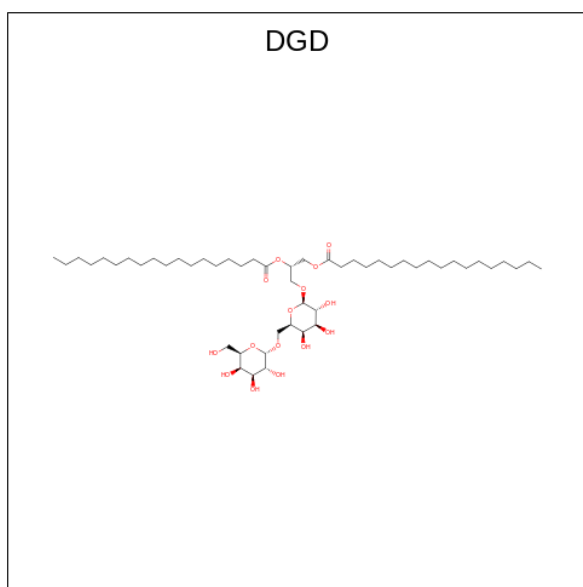


Mol	Chain	Residues	Atoms	AltConf
22	a	1	Total C 40 40	0
22	b	1	Total C 120 120	0
22	b	1	Total C 120 120	0
22	b	1	Total C 120 120	0
22	d	1	Total C 40 40	0
22	h	1	Total C 40 40	0
22	c	1	Total C 80 80	0
22	c	1	Total C 80 80	0
22	z	1	Total C 40 40	0

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

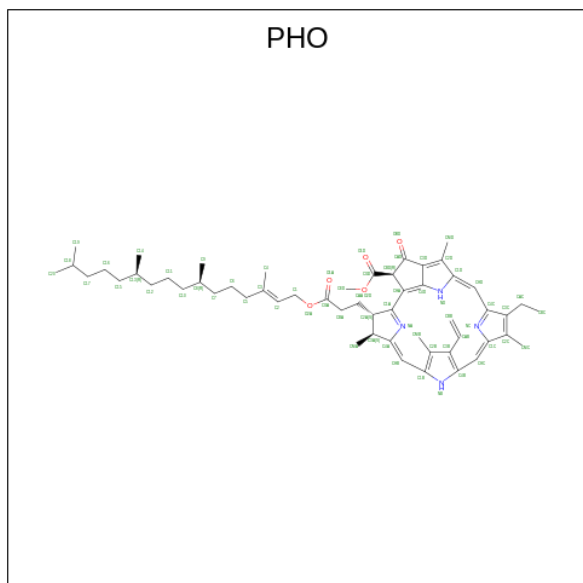
Mol	Chain	Residues	Atoms	AltConf
23	a	1	Total Cl 1 1	0
23	c	1	Total Cl 1 1	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



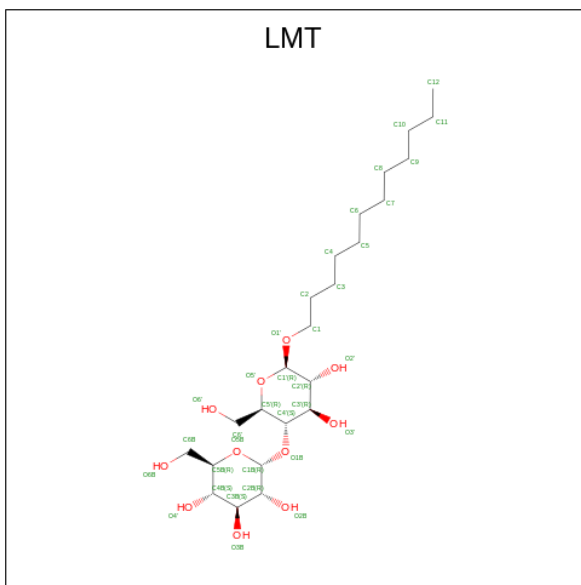
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	a	1	57	42	15	0
24	h	1	54	39	15	0
24	c	1	100	70	30	0
24	c	1	100	70	30	0

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
25	d	1	Total	C	N	O	0
			128	110	8	10	
25	d	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 26 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

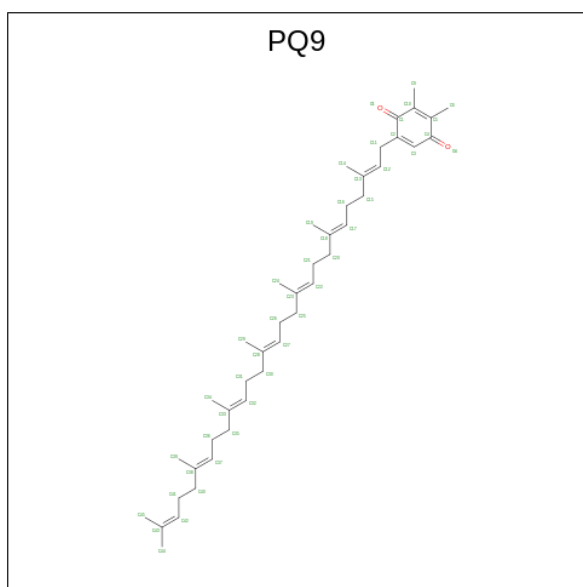


Mol	Chain	Residues	Atoms			AltConf
26	d	1	Total	C	O	0
			35	24	11	
26	m	1	Total	C	O	0
			35	24	11	
26	t	1	Total	C	O	0
			35	24	11	

- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
27	d	1	Total	Fe	0
			1	1	

- Molecule 28 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: $C_{43}H_{64}O_2$).

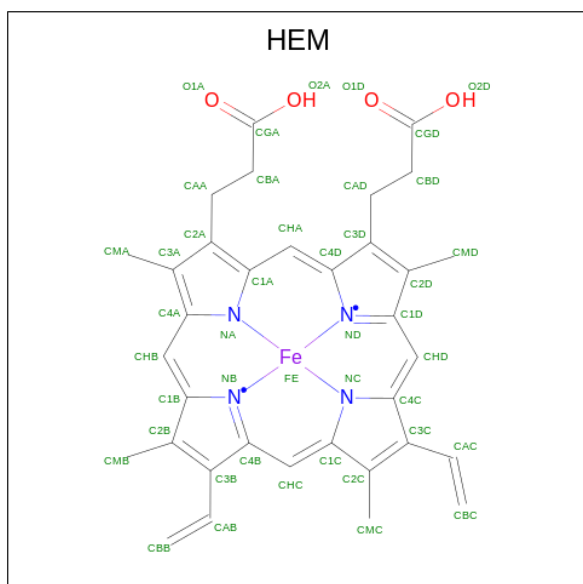


Mol	Chain	Residues	Atoms			AltConf
28	d	1	Total	C	O	0
			45	43	2	

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

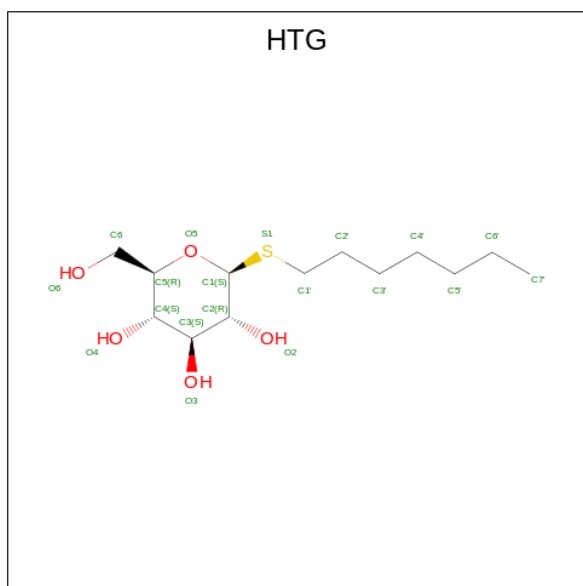
Mol	Chain	Residues	Atoms			AltConf
29	d	2	Total	C	O	0
			53	47	6	

- Molecule 30 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
30	e	1	43	34	1	4	4	0

- Molecule 31 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).

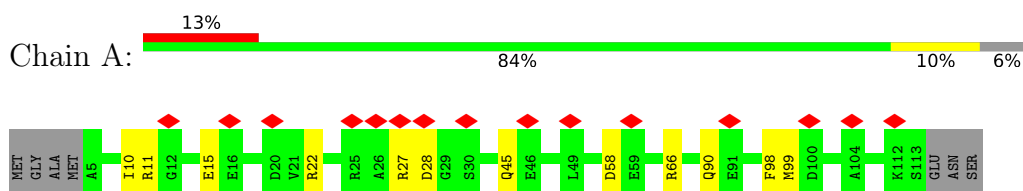


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
31	h	1	16	10	5	1	0

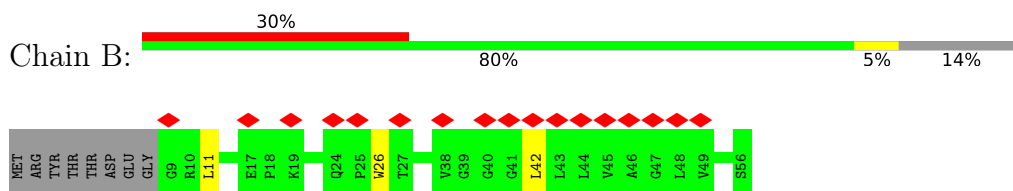
3 Residue-property plots [i](#)

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

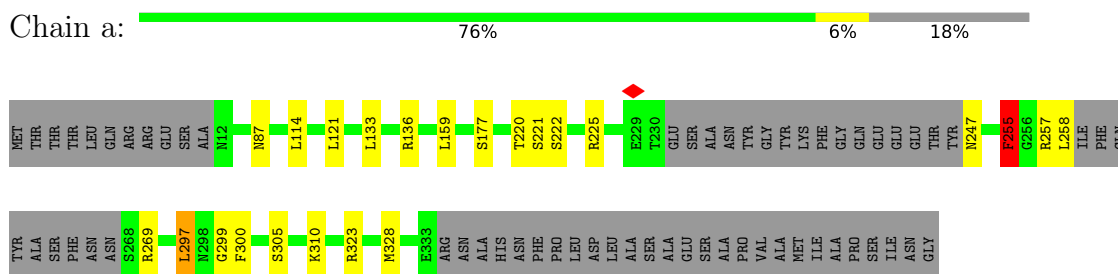
- Molecule 1: Photosystem II reaction center Psb28 protein



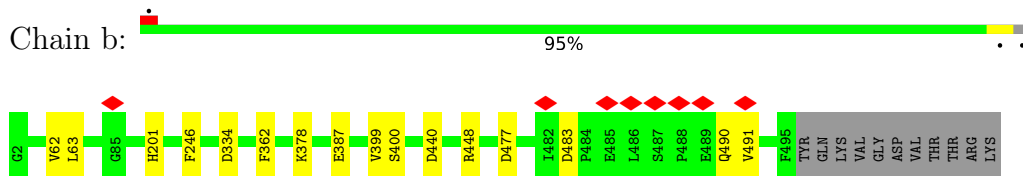
- Molecule 2: Tsl0063 protein



- Molecule 3: Photosystem II protein D1

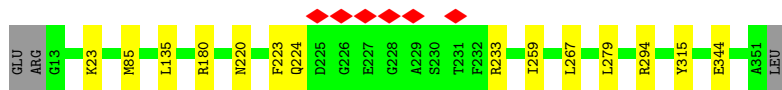


- Molecule 4: Photosystem II CP47 reaction center protein

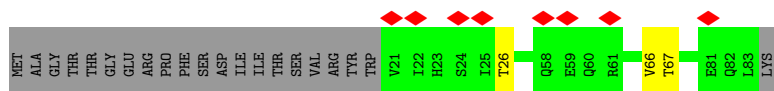


- Molecule 5: Photosystem II D2 protein

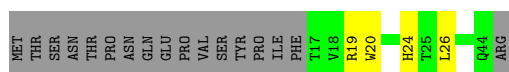




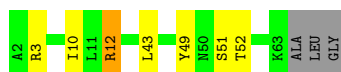
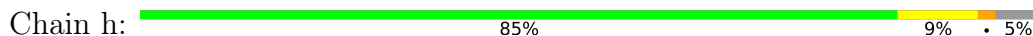
- Molecule 6: Cytochrome b559 subunit alpha



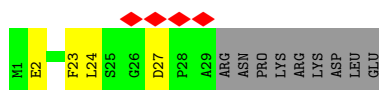
- Molecule 7: Cytochrome b559 subunit beta



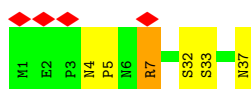
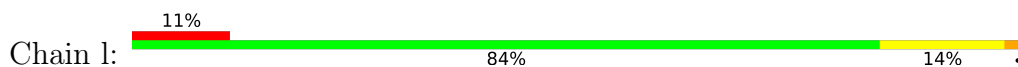
- Molecule 8: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein I



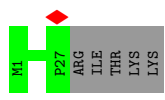
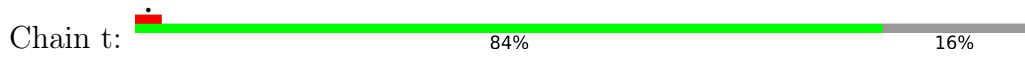
- Molecule 10: Photosystem II reaction center protein L



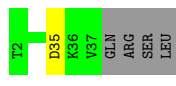
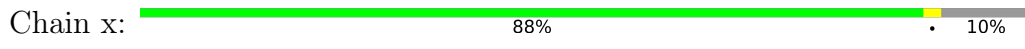
- Molecule 11: Photosystem II reaction center protein M



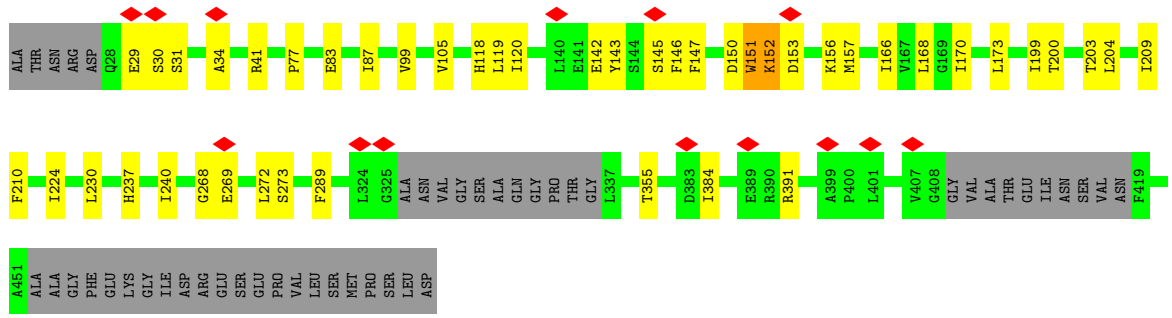
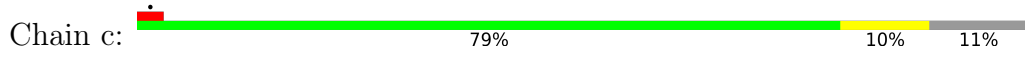
- Molecule 12: Photosystem II reaction center protein T



• Molecule 13: Photosystem II reaction center protein X



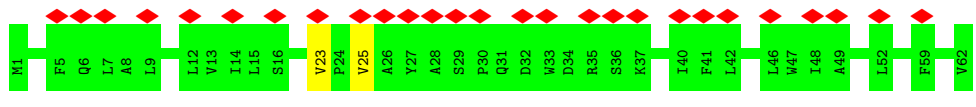
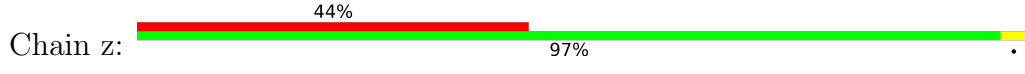
• Molecule 14: Photosystem II CP43 reaction center protein



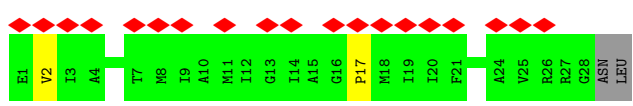
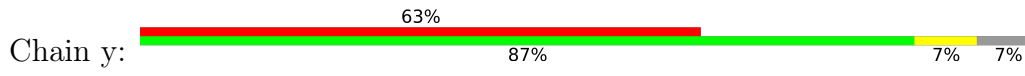
• Molecule 15: Photosystem II reaction center protein K



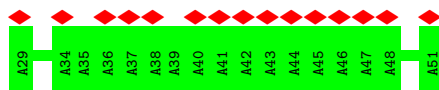
• Molecule 16: Photosystem II reaction center protein Z



• Molecule 17: Photosystem II reaction center protein Ycf12



• Molecule 18: unidentified transmembrane protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194738	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (\AA)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.30654, 1.30654, 1.30654	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: PQ9, BCR, CLA, FE2, DGD, SQD, CL, HTG, MGE, UNL, LMT, PHO, HEM

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	0.39	0/892	0.59	0/1202
2	B	0.28	0/355	0.65	1/484 (0.2%)
3	a	0.37	0/2376	0.62	2/3239 (0.1%)
4	b	0.39	0/4025	0.57	0/5486
5	d	0.42	0/2789	0.61	2/3803 (0.1%)
6	e	0.34	0/523	0.53	0/714
7	f	0.33	0/225	0.66	0/308
8	h	0.34	0/506	0.60	0/690
9	i	0.42	0/237	0.63	0/322
10	l	0.34	0/311	0.53	0/422
11	m	0.37	0/248	0.55	0/339
12	t	0.39	0/239	0.48	0/324
13	x	0.29	0/264	0.51	0/358
14	c	0.35	0/3237	0.56	0/4408
15	k	0.39	0/274	0.75	1/379 (0.3%)
16	z	0.33	0/466	0.65	0/641
17	y	0.34	0/136	0.77	1/187 (0.5%)
18	C	0.15	0/114	0.34	0/158
All	All	0.37	0/17217	0.59	7/23464 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	k	31	LEU	CA-CB-CG	7.04	131.48	115.30
3	a	297	LEU	N-CA-C	-6.51	93.44	111.00
17	y	17	PRO	N-CA-CB	6.11	110.64	103.30
5	d	267	LEU	CA-CB-CG	6.09	129.30	115.30
2	B	42	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/116 (92%)	95 (89%)	11 (10%)	1 (1%)	17	50
2	B	46/56 (82%)	44 (96%)	2 (4%)	0	100	100
3	a	291/360 (81%)	279 (96%)	10 (3%)	2 (1%)	22	56
4	b	492/505 (97%)	470 (96%)	21 (4%)	1 (0%)	47	78
5	d	337/342 (98%)	323 (96%)	14 (4%)	0	100	100
6	e	61/84 (73%)	56 (92%)	5 (8%)	0	100	100
7	f	26/45 (58%)	22 (85%)	4 (15%)	0	100	100
8	h	60/65 (92%)	54 (90%)	5 (8%)	1 (2%)	9	34
9	i	27/38 (71%)	25 (93%)	2 (7%)	0	100	100
10	l	35/37 (95%)	31 (89%)	2 (6%)	2 (6%)	1	9
11	m	29/36 (81%)	28 (97%)	1 (3%)	0	100	100
12	t	25/32 (78%)	24 (96%)	1 (4%)	0	100	100
13	x	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
14	c	397/451 (88%)	355 (89%)	32 (8%)	10 (2%)	5	25
15	k	32/46 (70%)	26 (81%)	4 (12%)	2 (6%)	1	7
16	z	60/62 (97%)	48 (80%)	10 (17%)	2 (3%)	4	19
17	y	26/30 (87%)	20 (77%)	5 (19%)	1 (4%)	3	17
18	C	21/23 (91%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2106/2368 (89%)	1950 (93%)	134 (6%)	22 (1%)	20 47

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	l	7	ARG
14	c	151	TRP
14	c	153	ASP
14	c	210	PHE
16	z	23	VAL

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 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	92/97 (95%)	81 (88%)	11 (12%)	5 19
2	B	34/42 (81%)	32 (94%)	2 (6%)	19 48
3	a	236/290 (81%)	214 (91%)	22 (9%)	9 31
4	b	392/403 (97%)	377 (96%)	15 (4%)	33 64
5	d	272/277 (98%)	259 (95%)	13 (5%)	25 56
6	e	55/73 (75%)	52 (94%)	3 (6%)	21 51
7	f	22/39 (56%)	18 (82%)	4 (18%)	1 7
8	h	53/54 (98%)	46 (87%)	7 (13%)	4 16
9	i	26/35 (74%)	22 (85%)	4 (15%)	2 11
10	l	35/35 (100%)	30 (86%)	5 (14%)	3 13
11	m	28/33 (85%)	21 (75%)	7 (25%)	0 2
12	t	24/29 (83%)	24 (100%)	0	100 100
13	x	29/33 (88%)	28 (97%)	1 (3%)	37 67
14	c	312/352 (89%)	274 (88%)	38 (12%)	5 19
15	k	27/37 (73%)	21 (78%)	6 (22%)	1 4
16	z	45/52 (86%)	45 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1682/1881 (89%)	1544 (92%)	138 (8%)	15 36

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	c	170	ILE
14	c	203	THR
14	c	384	ILE
4	b	483	ASP
4	b	477	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
4	b	455	HIS
7	f	41	GLN
5	d	332	GLN
11	m	28	GLN
3	a	215	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 3 are monoatomic and 2 are unknown - leaving 64 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
21	CLA	k	501	-	46,54,73	2.32	13 (28%)	53,90,113	4.72	29 (54%)
19	MGE	f	101	-	47,47,48	0.99	2 (4%)	55,55,56	1.33	7 (12%)
24	DGD	c	517	-	48,48,67	1.02	2 (4%)	62,62,81	1.11	5 (8%)
21	CLA	b	606	-	65,73,73	2.22	15 (23%)	76,113,113	2.08	24 (31%)
19	MGE	b	620	-	41,41,48	1.03	2 (4%)	49,49,56	1.20	6 (12%)
22	BCR	b	617	-	41,41,41	0.69	0	56,56,56	1.86	15 (26%)
19	MGE	d	410	-	48,48,48	0.95	2 (4%)	56,56,56	1.28	5 (8%)
21	CLA	c	505	-	65,73,73	2.51	18 (27%)	76,113,113	2.28	25 (32%)
21	CLA	c	506	-	46,54,73	2.35	14 (30%)	53,90,113	4.82	26 (49%)
19	MGE	b	619	-	48,48,48	0.99	2 (4%)	56,56,56	1.18	5 (8%)
21	CLA	b	613	-	52,60,73	2.10	16 (30%)	60,97,113	3.19	31 (51%)
21	CLA	c	513	-	50,58,73	2.30	13 (26%)	58,95,113	3.81	34 (58%)
21	CLA	b	602	-	65,73,73	2.03	16 (24%)	76,113,113	2.53	24 (31%)
21	CLA	c	507	-	51,59,73	2.25	14 (27%)	59,96,113	3.60	27 (45%)
21	CLA	c	512	-	51,59,73	2.26	13 (25%)	59,96,113	4.15	26 (44%)
22	BCR	b	618	-	41,41,41	0.71	0	56,56,56	2.04	17 (30%)
22	BCR	b	616	-	41,41,41	0.71	0	56,56,56	1.89	20 (35%)
25	PHO	d	403	-	51,69,69	1.54	8 (15%)	47,99,99	1.99	11 (23%)
21	CLA	b	615	-	46,54,73	2.57	18 (39%)	53,90,113	2.76	24 (45%)
22	BCR	a	404	-	41,41,41	0.70	0	56,56,56	2.29	17 (30%)
21	CLA	b	604	-	65,73,73	1.90	14 (21%)	76,113,113	2.54	25 (32%)
26	LMT	d	404	-	36,36,36	0.44	0	47,47,47	0.83	1 (2%)
20	SQD	l	101	-	46,47,54	1.30	4 (8%)	55,58,65	3.86	9 (16%)
21	CLA	b	607	-	65,73,73	2.06	17 (26%)	76,113,113	2.15	23 (30%)
21	CLA	b	601	-	65,73,73	2.12	13 (20%)	76,113,113	2.30	27 (35%)
22	BCR	c	515	-	41,41,41	0.82	1 (2%)	56,56,56	2.60	20 (35%)
21	CLA	b	610	-	65,73,73	2.08	15 (23%)	76,113,113	2.30	26 (34%)
24	DGD	c	516	-	54,54,67	0.99	2 (3%)	68,68,81	1.48	14 (20%)
19	MGE	m	102	-	48,48,48	0.99	2 (4%)	56,56,56	1.13	3 (5%)
21	CLA	b	605	-	65,73,73	2.42	19 (29%)	76,113,113	2.48	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMT	m	101	-	36,36,36	0.47	0	47,47,47	0.95	3 (6%)
28	PQ9	d	408	-	45,45,45	0.69	1 (2%)	56,57,57	1.49	13 (23%)
21	CLA	a	407	-	65,73,73	1.81	16 (24%)	76,113,113	2.37	29 (38%)
31	HTG	h	102	-	16,16,19	1.18	2 (12%)	20,21,24	1.68	1 (5%)
21	CLA	c	511	-	65,73,73	2.12	16 (24%)	76,113,113	2.12	23 (30%)
21	CLA	c	503	-	65,73,73	2.12	16 (24%)	76,113,113	2.70	24 (31%)
30	HEM	e	101	-	41,50,50	1.32	5 (12%)	45,82,82	1.76	9 (20%)
21	CLA	d	407	-	50,58,73	2.22	12 (24%)	58,95,113	4.21	30 (51%)
22	BCR	z	101	-	41,41,41	0.70	0	56,56,56	2.06	16 (28%)
22	BCR	d	409	-	41,41,41	0.69	0	56,56,56	1.73	9 (16%)
21	CLA	b	612	-	54,62,73	2.14	16 (29%)	62,99,113	2.54	21 (33%)
21	CLA	a	402	-	65,73,73	1.89	14 (21%)	76,113,113	2.31	24 (31%)
21	CLA	c	509	-	63,71,73	2.38	21 (33%)	73,110,113	2.51	26 (35%)
24	DGD	a	406	-	58,58,67	0.91	2 (3%)	72,72,81	1.00	4 (5%)
21	CLA	d	402	-	65,73,73	1.97	17 (26%)	76,113,113	2.17	22 (28%)
22	BCR	h	103	-	41,41,41	0.75	0	56,56,56	1.93	15 (26%)
21	CLA	b	603	-	65,73,73	2.09	16 (24%)	76,113,113	2.52	24 (31%)
21	CLA	h	101	-	41,49,73	2.47	12 (29%)	47,84,113	5.07	27 (57%)
21	CLA	c	510	-	46,54,73	2.86	20 (43%)	53,90,113	2.70	25 (47%)
21	CLA	b	608	-	65,73,73	2.25	18 (27%)	76,113,113	1.98	19 (25%)
25	PHO	d	401	-	51,69,69	1.65	8 (15%)	47,99,99	1.88	9 (19%)
24	DGD	h	104	-	55,55,67	0.92	2 (3%)	69,69,81	1.06	4 (5%)
20	SQD	a	401	-	25,26,54	1.68	4 (16%)	34,37,65	4.81	7 (20%)
26	LMT	t	301	-	36,36,36	0.49	0	47,47,47	0.89	1 (2%)
21	CLA	a	403	-	51,59,73	2.17	16 (31%)	59,96,113	2.86	29 (49%)
21	CLA	b	614	-	65,73,73	2.12	16 (24%)	76,113,113	2.38	25 (32%)
21	CLA	b	609	-	65,73,73	2.13	16 (24%)	76,113,113	2.47	20 (26%)
22	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.99	13 (23%)
19	MGE	B	101	-	48,48,48	0.94	2 (4%)	56,56,56	1.29	6 (10%)
21	CLA	c	504	-	65,73,73	2.26	17 (26%)	76,113,113	2.59	26 (34%)
21	CLA	d	406	-	61,69,73	1.95	8 (13%)	71,108,113	3.91	31 (43%)
21	CLA	b	611	-	65,73,73	2.12	15 (23%)	76,113,113	2.55	21 (27%)
19	MGE	c	502	-	48,48,48	0.97	2 (4%)	56,56,56	1.09	4 (7%)
21	CLA	c	508	-	46,54,73	2.54	16 (34%)	53,90,113	2.95	24 (45%)

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
21	CLA	k	501	-	-	7/15/93/115	-
19	MGE	f	101	-	-	3/42/62/63	0/1/1/1
24	DGD	c	517	-	-	8/36/76/95	0/2/2/2
21	CLA	b	606	-	1/1/15/20	2/37/115/115	-
19	MGE	c	502	-	-	13/43/63/63	0/1/1/1
19	MGE	b	620	-	-	6/36/56/63	0/1/1/1
22	BCR	b	617	-	-	0/29/63/63	0/2/2/2
19	MGE	d	410	-	-	14/43/63/63	0/1/1/1
21	CLA	c	505	-	-	2/37/115/115	-
21	CLA	c	506	-	-	4/15/93/115	-
19	MGE	b	619	-	-	9/43/63/63	0/1/1/1
21	CLA	b	613	-	1/1/12/20	9/22/100/115	-
21	CLA	c	513	-	-	9/19/97/115	-
21	CLA	b	602	-	1/1/15/20	4/37/115/115	-
21	CLA	c	507	-	-	10/21/99/115	-
21	CLA	c	512	-	-	8/21/99/115	-
22	BCR	b	618	-	-	3/29/63/63	0/2/2/2
22	BCR	b	616	-	-	0/29/63/63	0/2/2/2
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6
21	CLA	b	615	-	1/1/11/20	2/15/93/115	-
22	BCR	a	404	-	-	10/29/63/63	0/2/2/2
21	CLA	b	604	-	1/1/15/20	4/37/115/115	-
26	LMT	d	404	-	-	4/21/61/61	0/2/2/2
20	SQD	l	101	-	-	7/42/62/69	0/1/1/1
21	CLA	b	607	-	-	1/37/115/115	-
21	CLA	b	601	-	1/1/15/20	4/37/115/115	-
22	BCR	c	515	-	-	4/29/63/63	0/2/2/2
21	CLA	b	610	-	-	6/37/115/115	-
24	DGD	c	516	-	-	12/42/82/95	0/2/2/2
19	MGE	m	102	-	-	10/43/63/63	0/1/1/1
21	CLA	b	605	-	1/1/15/20	12/37/115/115	-
26	LMT	m	101	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PQ9	d	408	-	-	7/41/61/61	0/1/1/1
21	CLA	a	407	-	-	6/37/115/115	-
31	HTG	h	102	-	-	0/7/27/30	0/1/1/1
21	CLA	c	511	-	1/1/15/20	9/37/115/115	-
21	CLA	c	503	-	1/1/15/20	4/37/115/115	-
30	HEM	e	101	-	-	5/12/54/54	-
21	CLA	d	407	-	-	4/19/97/115	-
22	BCR	z	101	-	-	6/29/63/63	0/2/2/2
22	BCR	d	409	-	-	8/29/63/63	0/2/2/2
21	CLA	b	612	-	1/1/12/20	0/24/102/115	-
21	CLA	c	509	-	1/1/14/20	7/35/113/115	-
21	CLA	a	402	-	1/1/15/20	5/37/115/115	-
24	DGD	a	406	-	-	19/46/86/95	0/2/2/2
21	CLA	d	402	-	1/1/15/20	5/37/115/115	-
22	BCR	h	103	-	-	7/29/63/63	0/2/2/2
21	CLA	b	603	-	1/1/15/20	7/37/115/115	-
21	CLA	h	101	-	-	2/8/86/115	-
21	CLA	c	510	-	1/1/11/20	3/15/93/115	-
21	CLA	b	608	-	-	0/37/115/115	-
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6
24	DGD	h	104	-	-	13/43/83/95	0/2/2/2
20	SQD	a	401	-	-	4/19/39/69	0/1/1/1
26	LMT	t	301	-	-	7/21/61/61	0/2/2/2
21	CLA	a	403	-	-	1/21/99/115	-
21	CLA	b	614	-	1/1/15/20	9/37/115/115	-
22	BCR	c	514	-	-	8/29/63/63	0/2/2/2
21	CLA	c	504	-	1/1/15/20	7/37/115/115	-
19	MGE	B	101	-	-	17/43/63/63	0/1/1/1
21	CLA	d	406	-	1/1/14/20	9/33/111/115	-
21	CLA	b	611	-	1/1/15/20	7/37/115/115	-
21	CLA	b	609	-	1/1/15/20	4/37/115/115	-
21	CLA	c	508	-	1/1/11/20	3/15/93/115	-

The worst 5 of 581 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	611	CLA	MG-NA	10.39	2.31	2.06
21	b	605	CLA	MG-NA	10.30	2.30	2.06
21	c	505	CLA	MG-NA	9.83	2.29	2.06
21	c	506	CLA	C1D-ND	8.70	1.48	1.37
21	c	505	CLA	MG-NC	8.62	2.26	2.06

The worst 5 of 1134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	l	101	SQD	O9-S-C6	-19.47	83.80	106.94
20	a	401	SQD	O9-S-C6	-18.75	84.65	106.94
21	k	501	CLA	C1D-ND-C4D	-18.13	93.46	106.33
21	c	506	CLA	C1D-ND-C4D	-17.32	94.03	106.33
21	d	407	CLA	C1D-ND-C4D	-16.66	94.50	106.33

5 of 21 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	a	402	CLA	ND
21	b	601	CLA	ND
21	b	602	CLA	ND
21	b	603	CLA	ND
21	b	604	CLA	ND

5 of 387 torsion outliers are listed below:

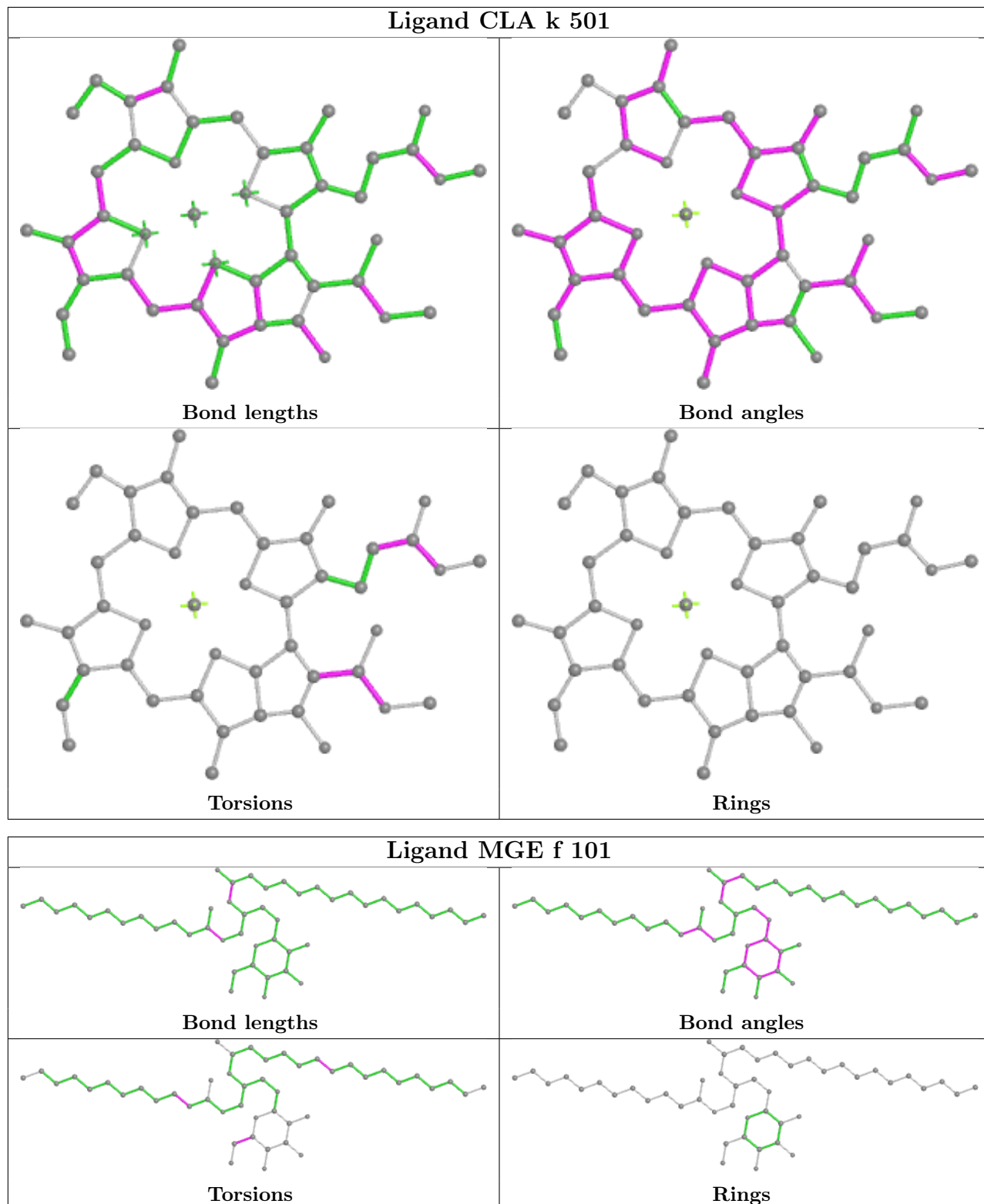
Mol	Chain	Res	Type	Atoms
19	B	101	MGE	O2G-C2G-C3G-O3G
19	d	410	MGE	O6D-C1D-O3G-C3G
19	m	102	MGE	C2B-C1B-O2G-C2G
20	a	401	SQD	C5-C6-S-O8
20	l	101	SQD	O47-C45-C46-O48

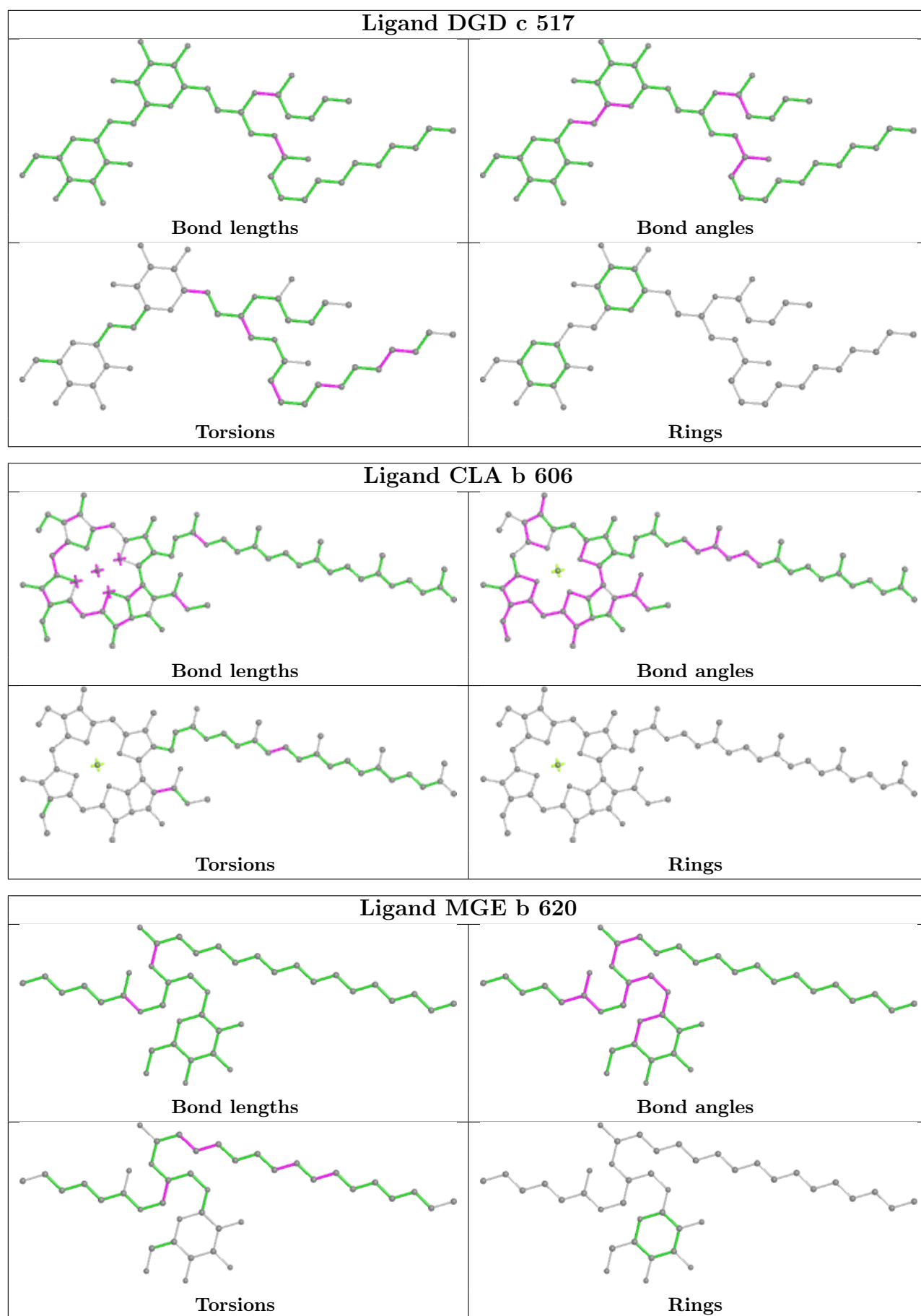
There are no ring outliers.

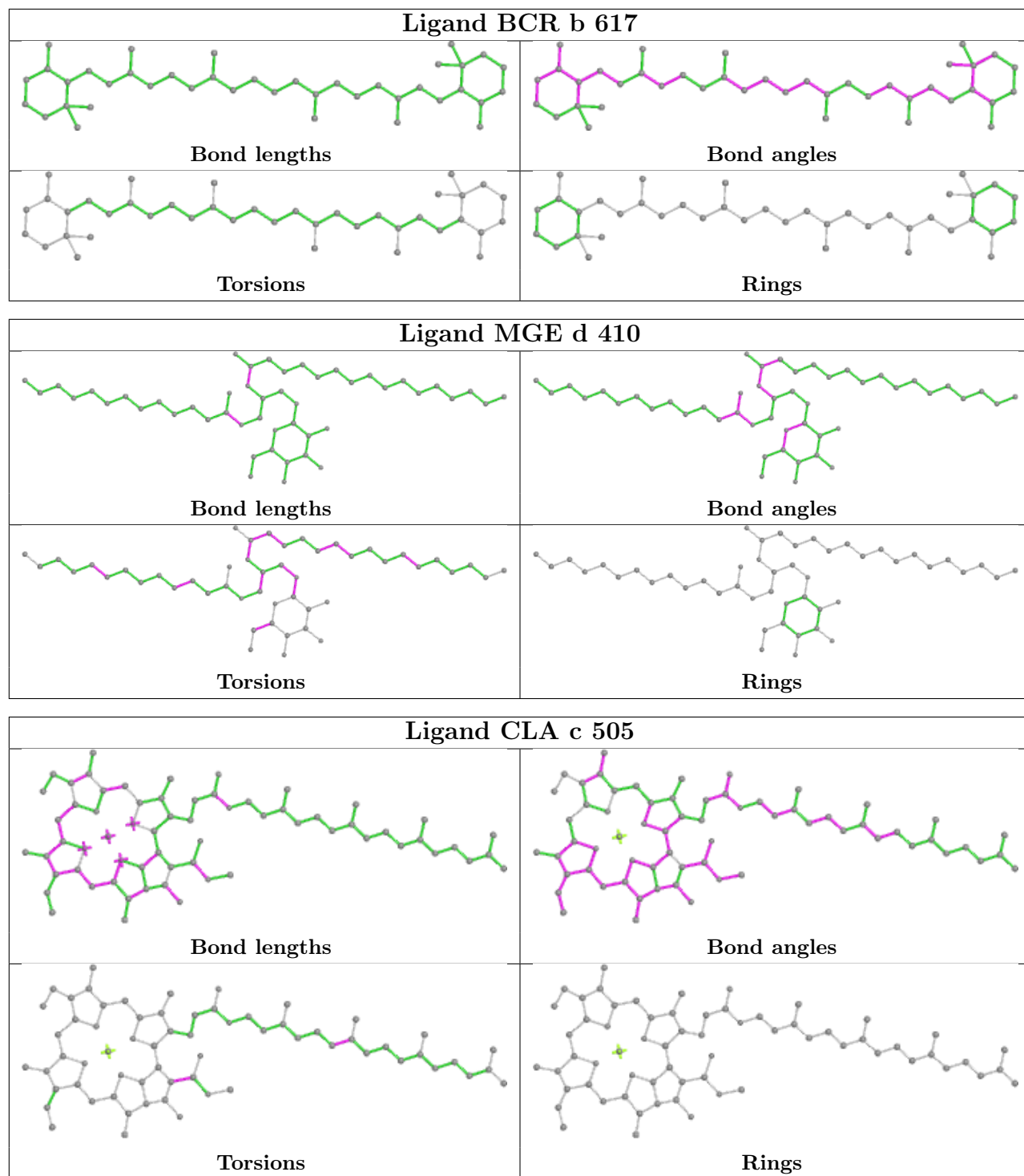
No monomer is involved in short contacts.

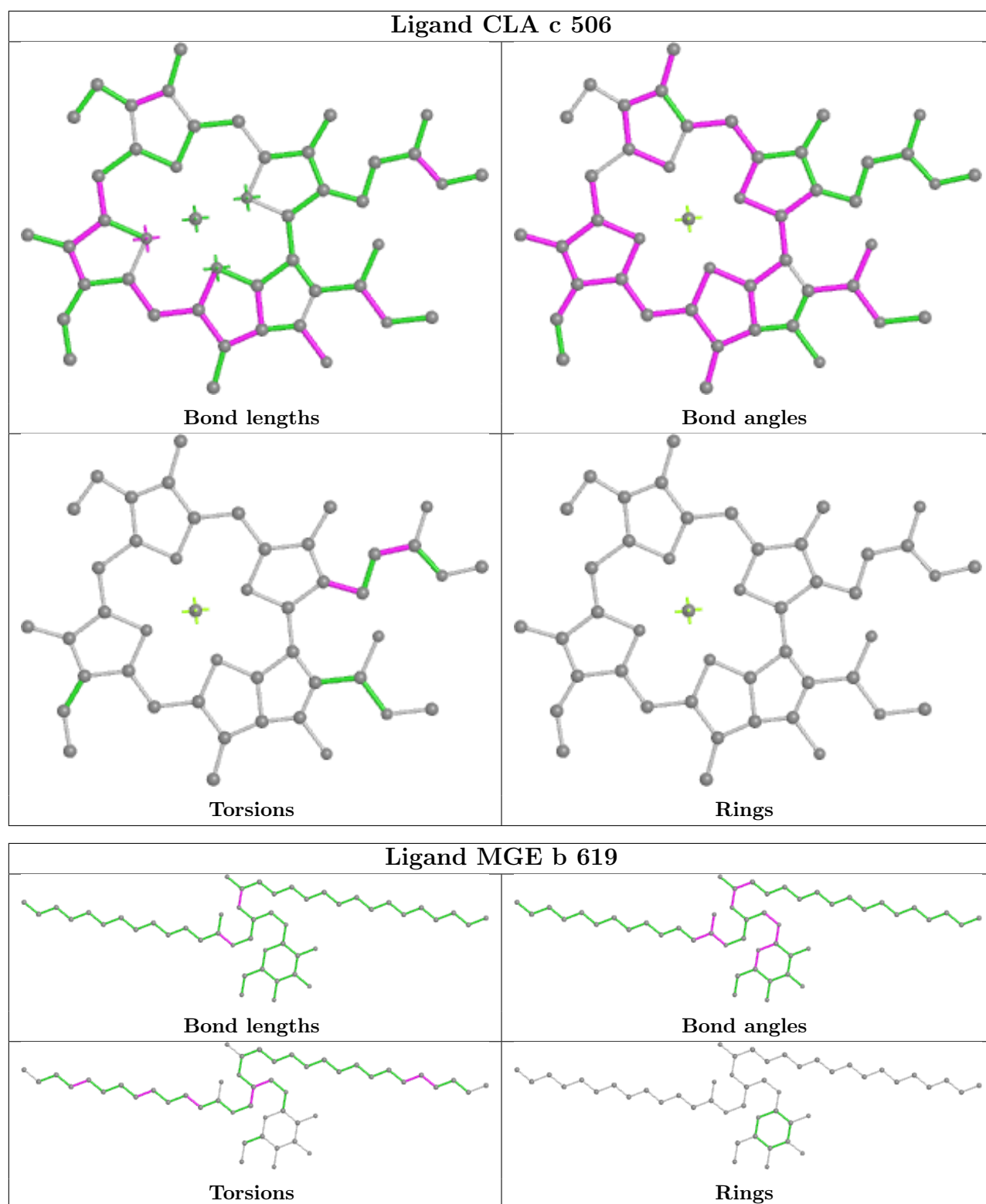
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

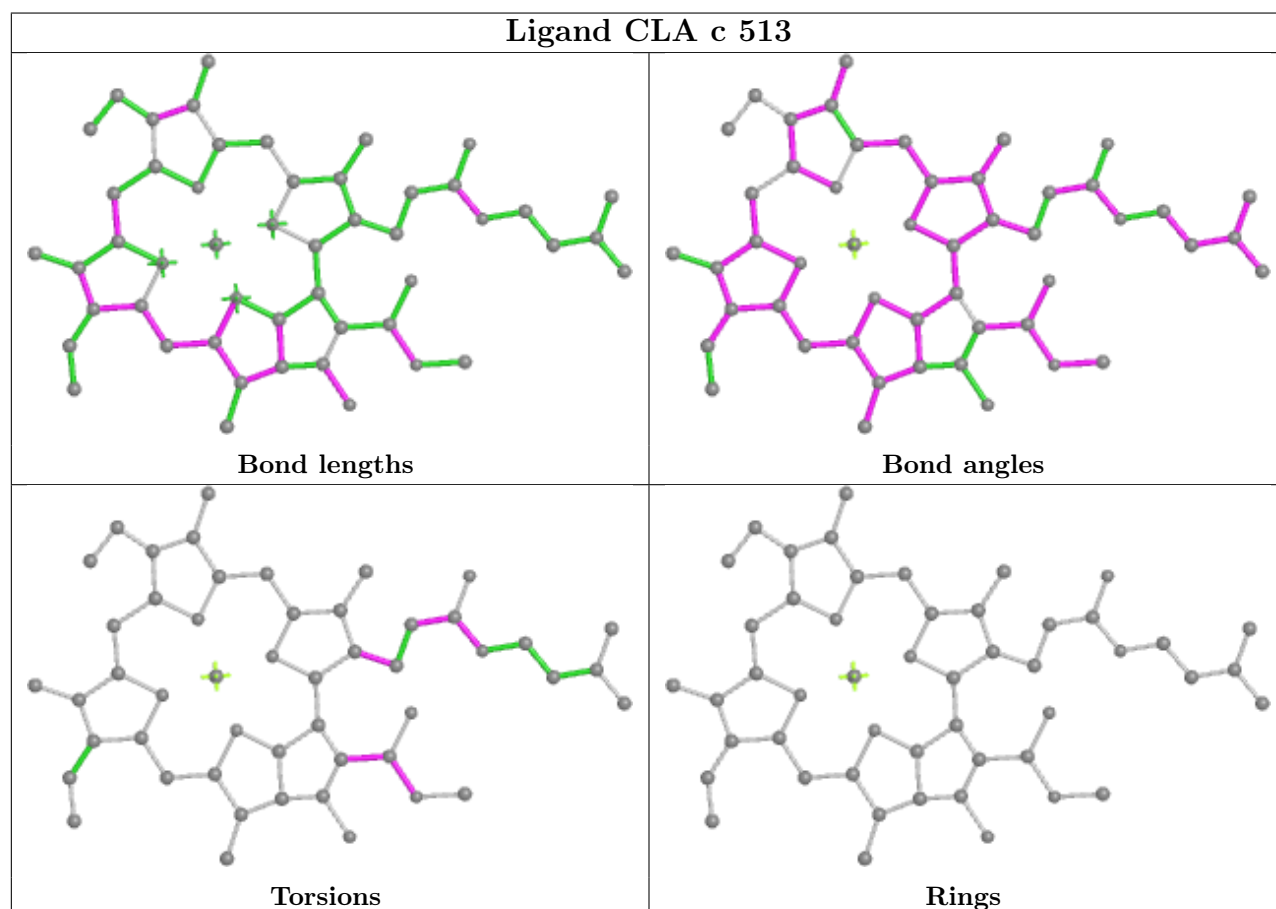
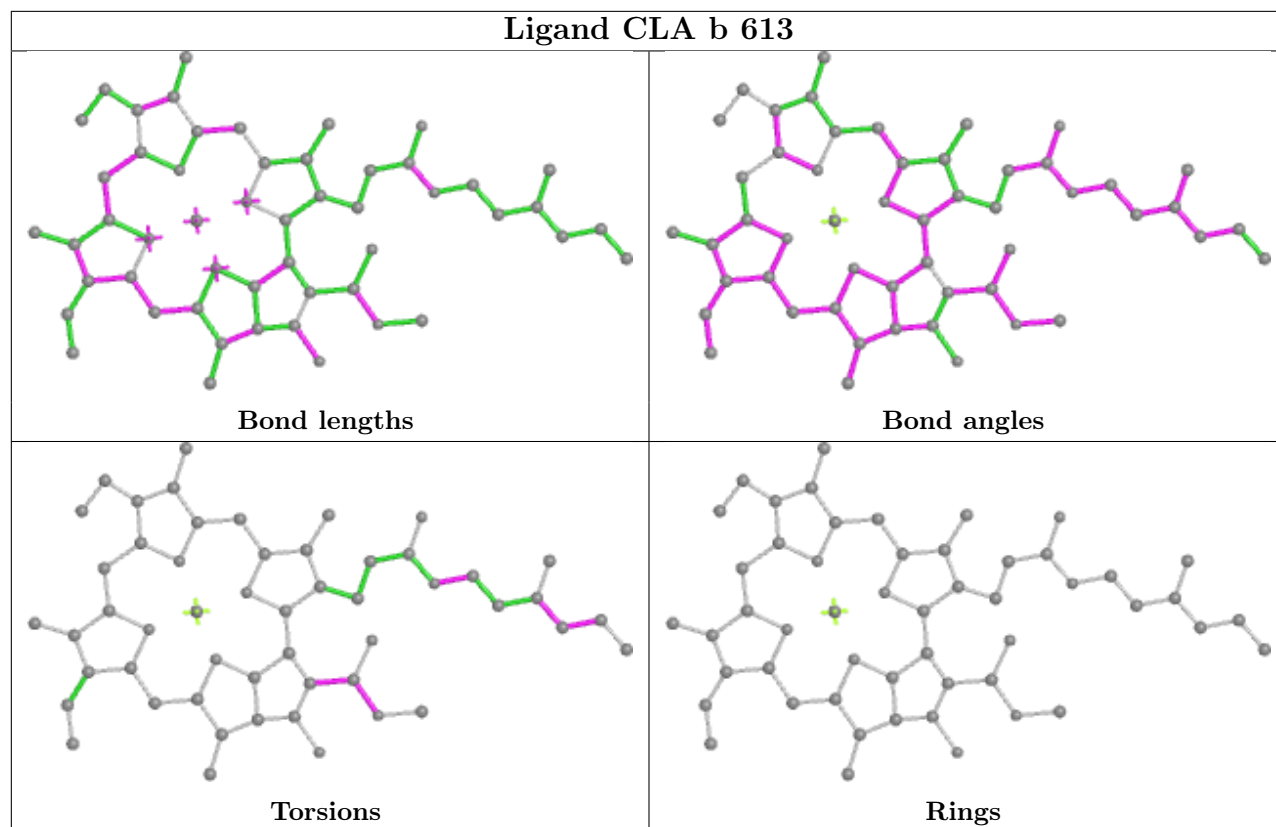
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

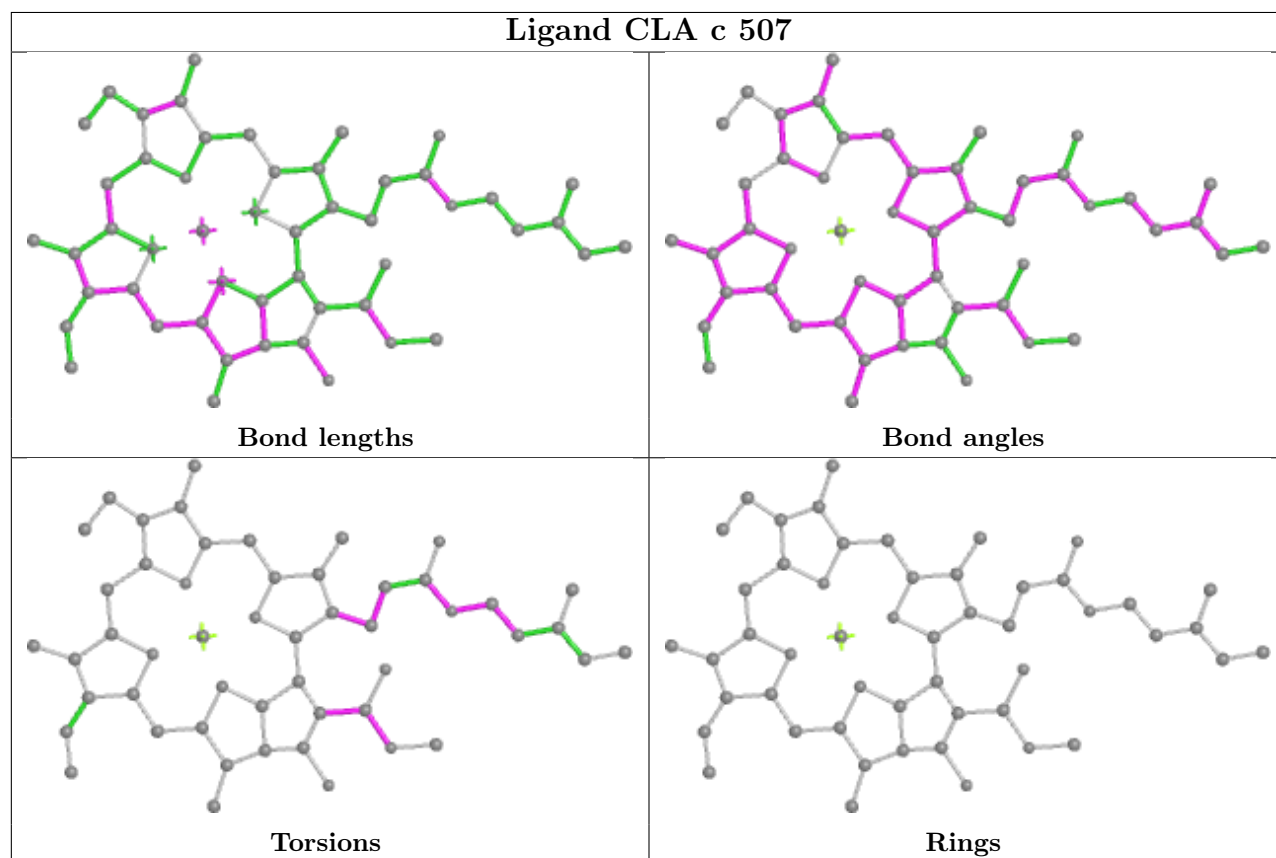
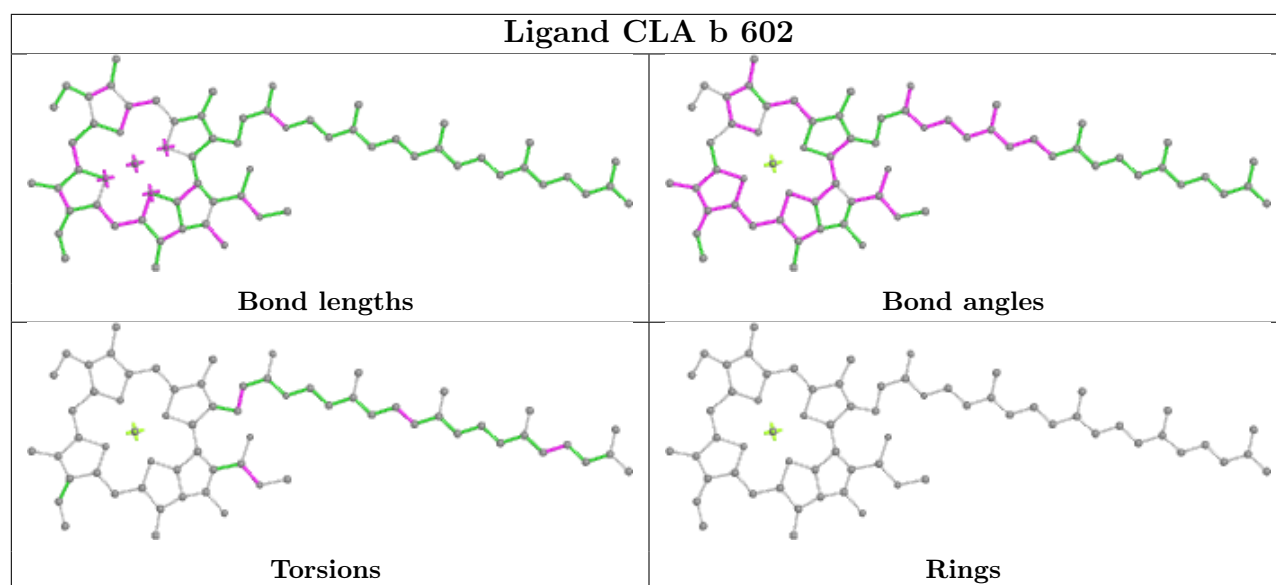


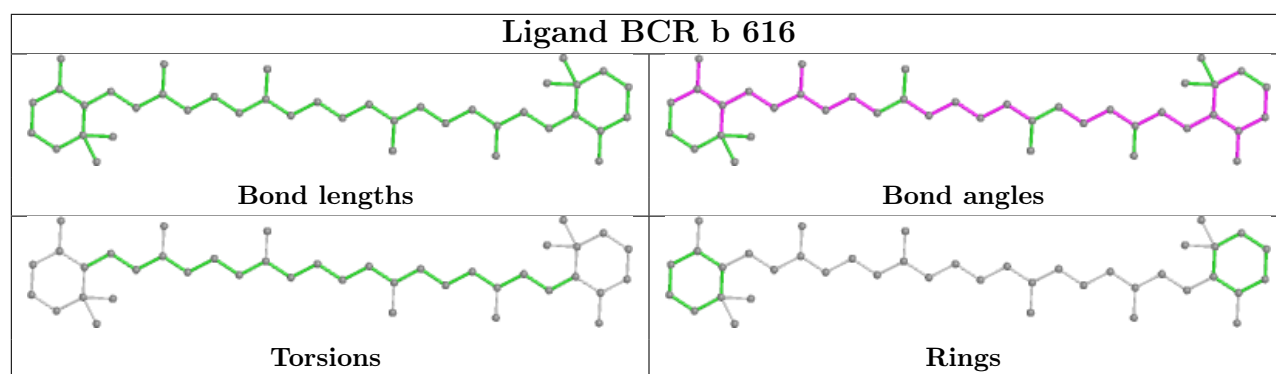
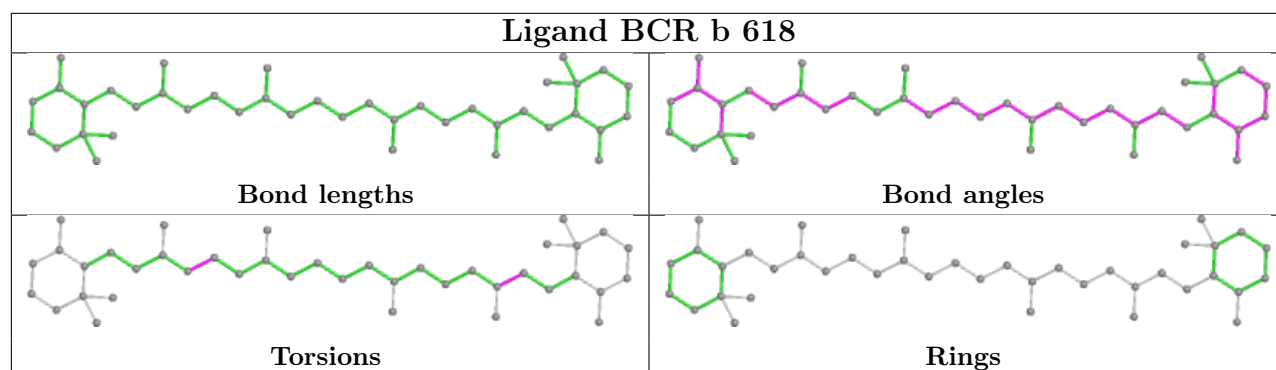
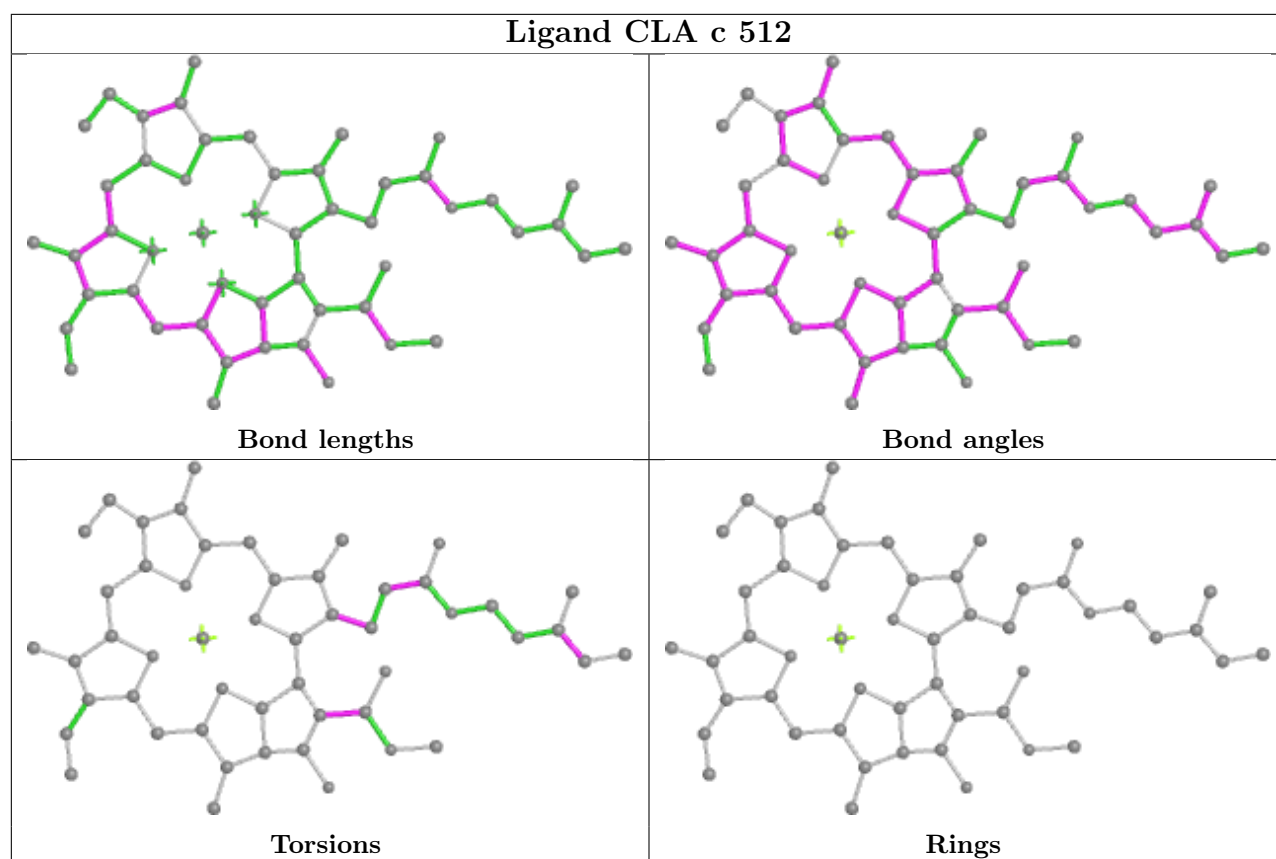


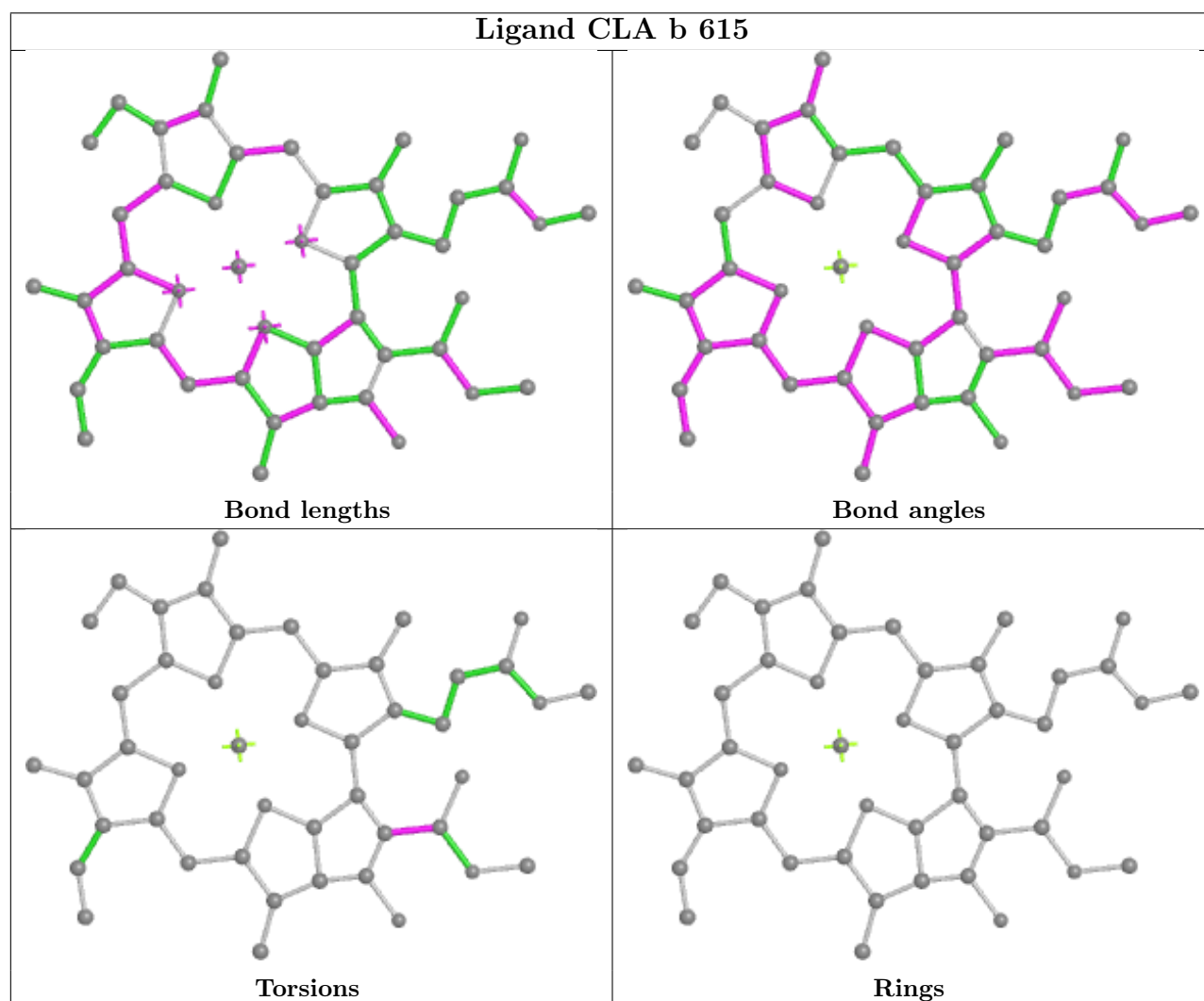
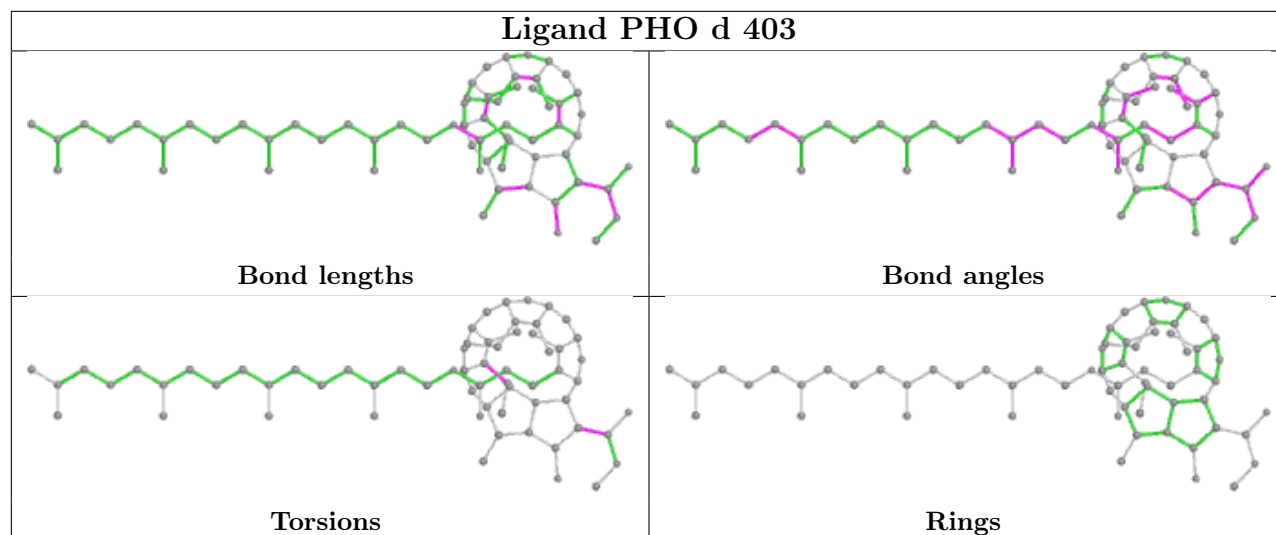


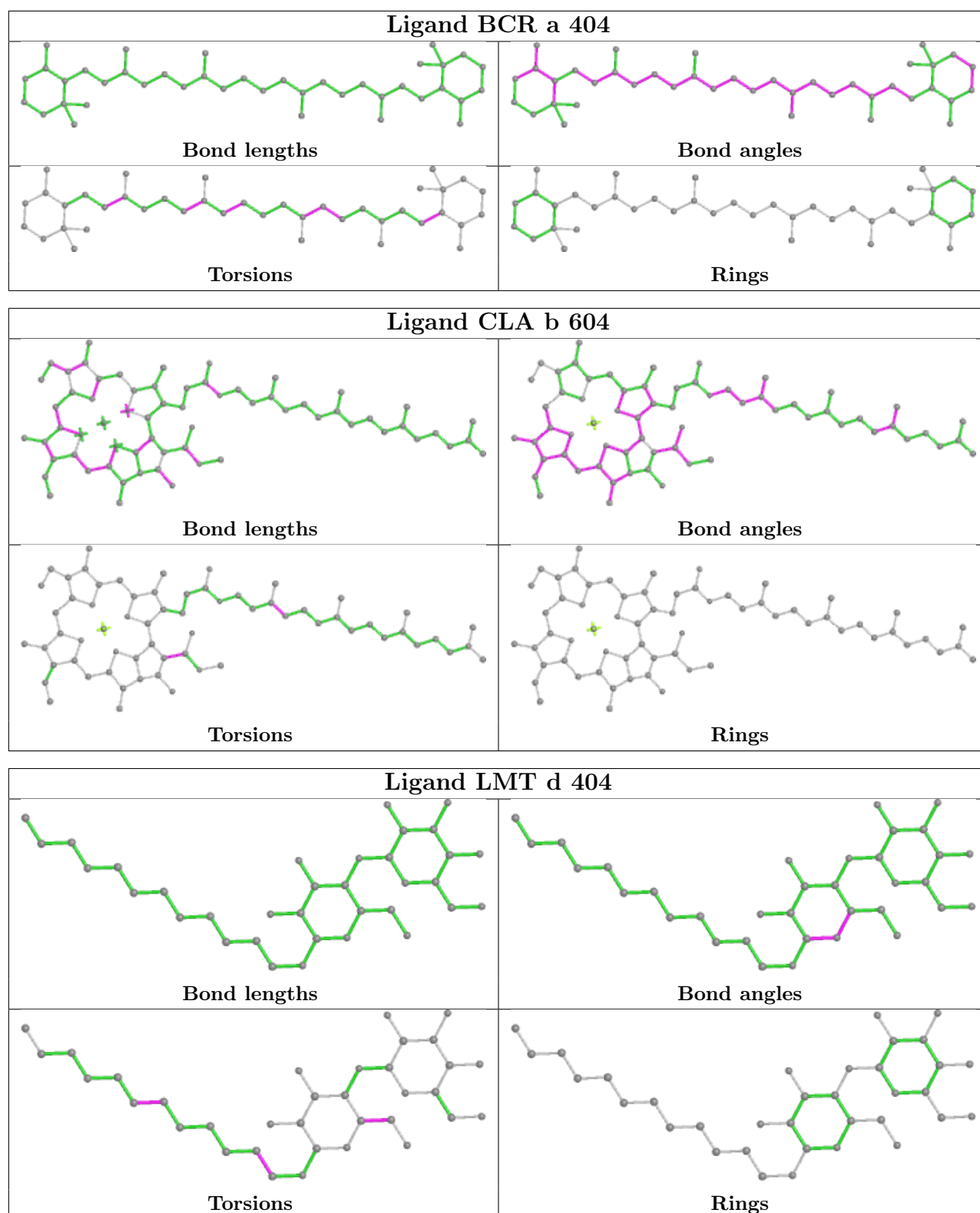


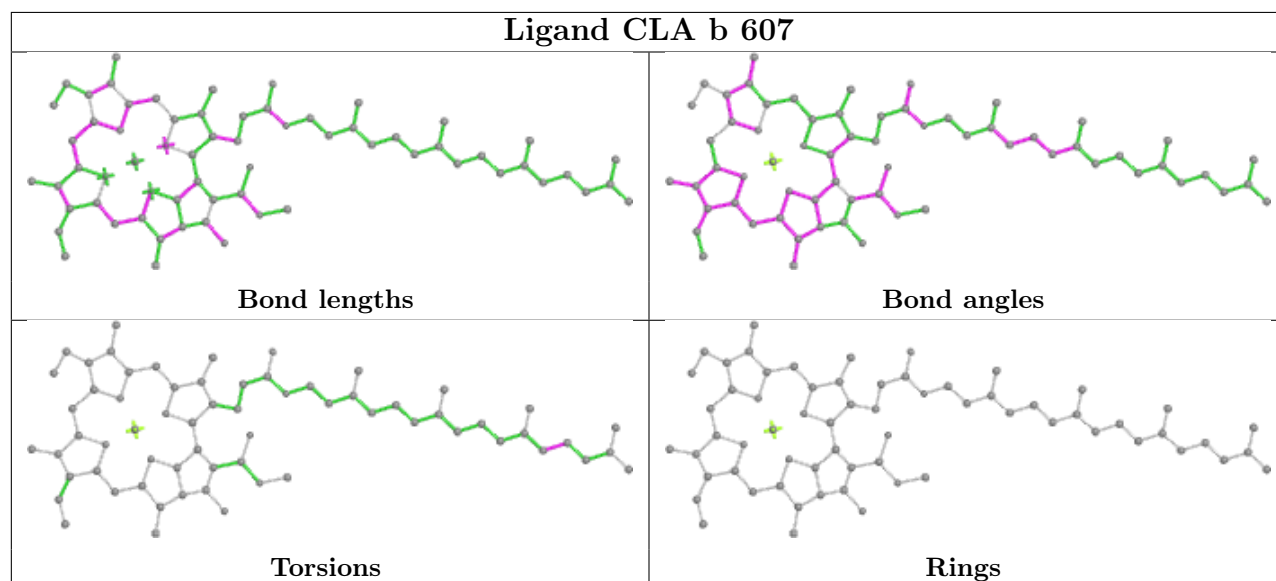
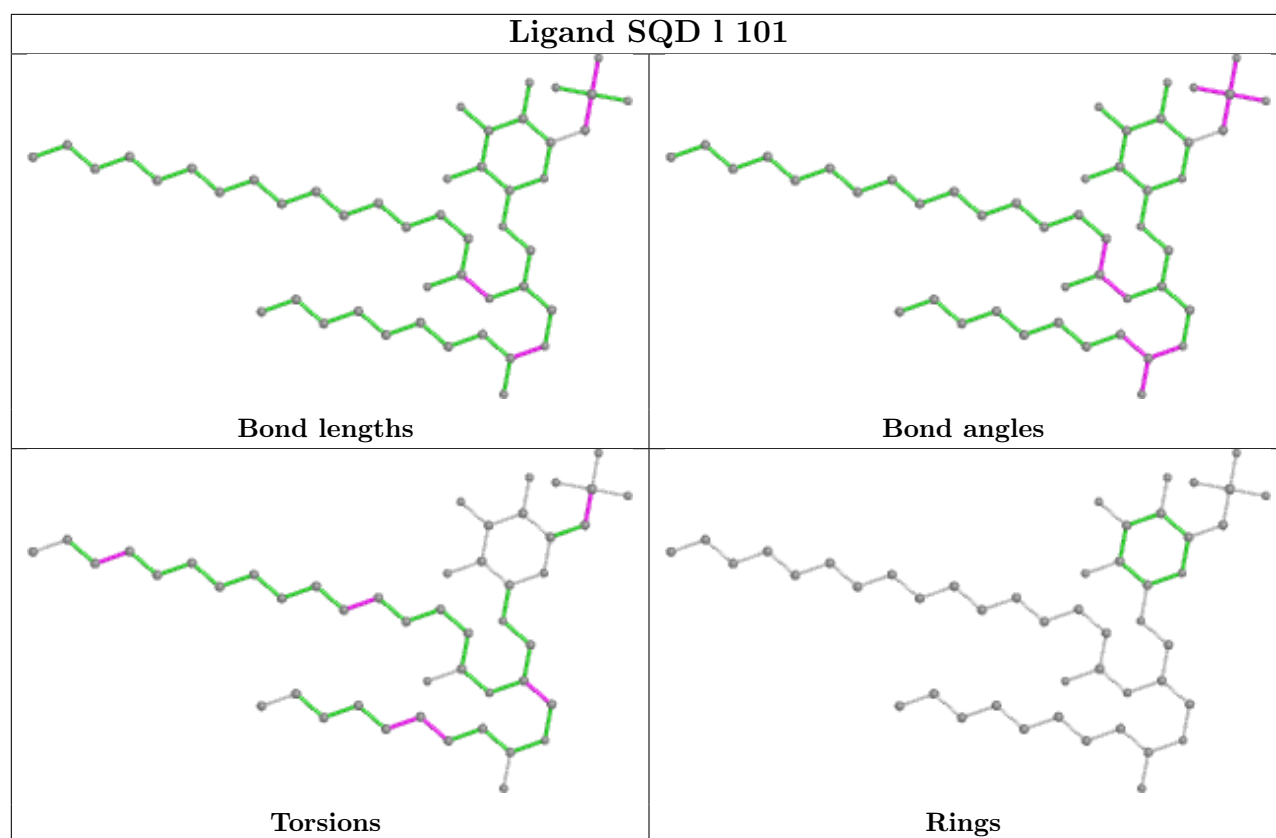


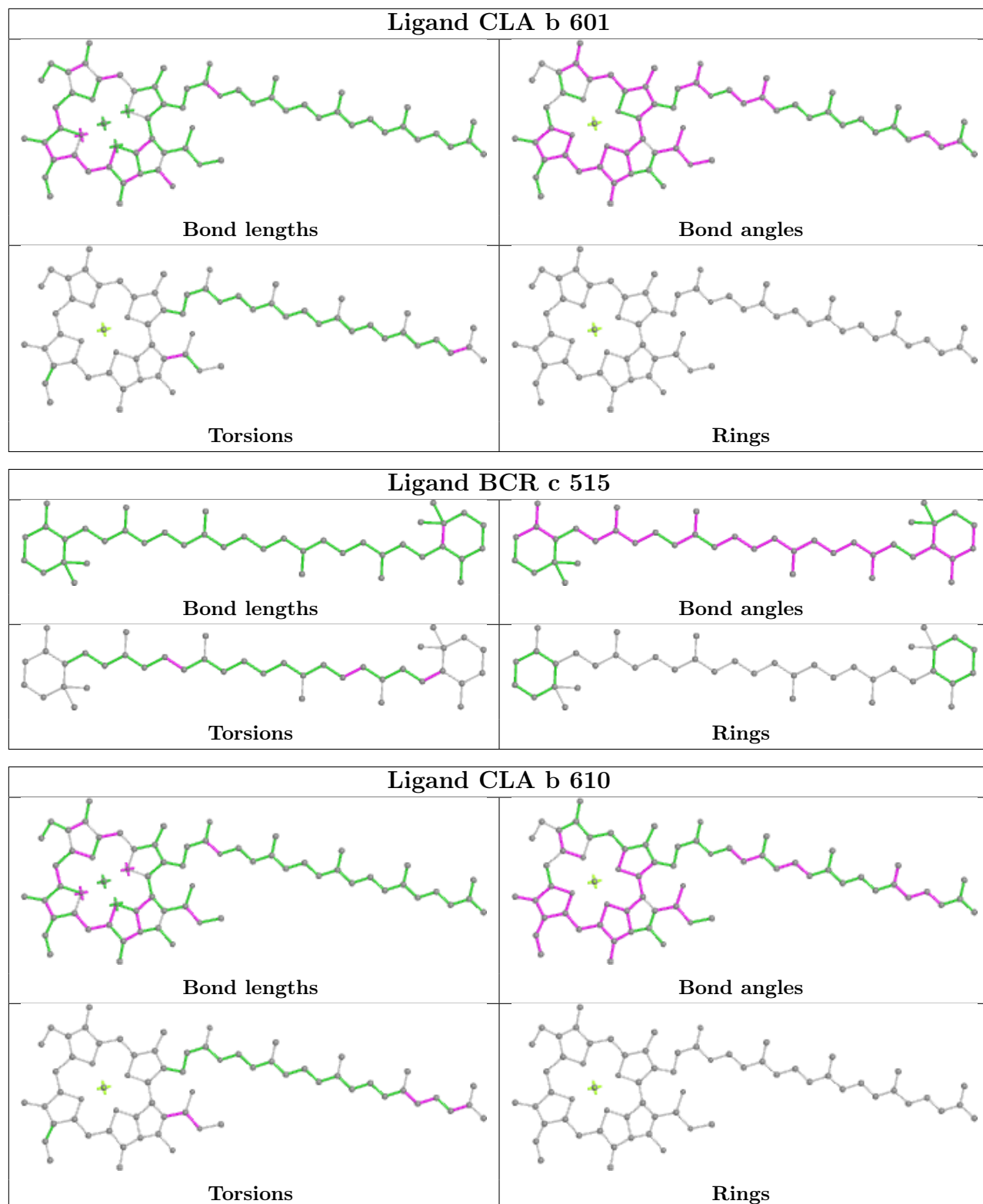


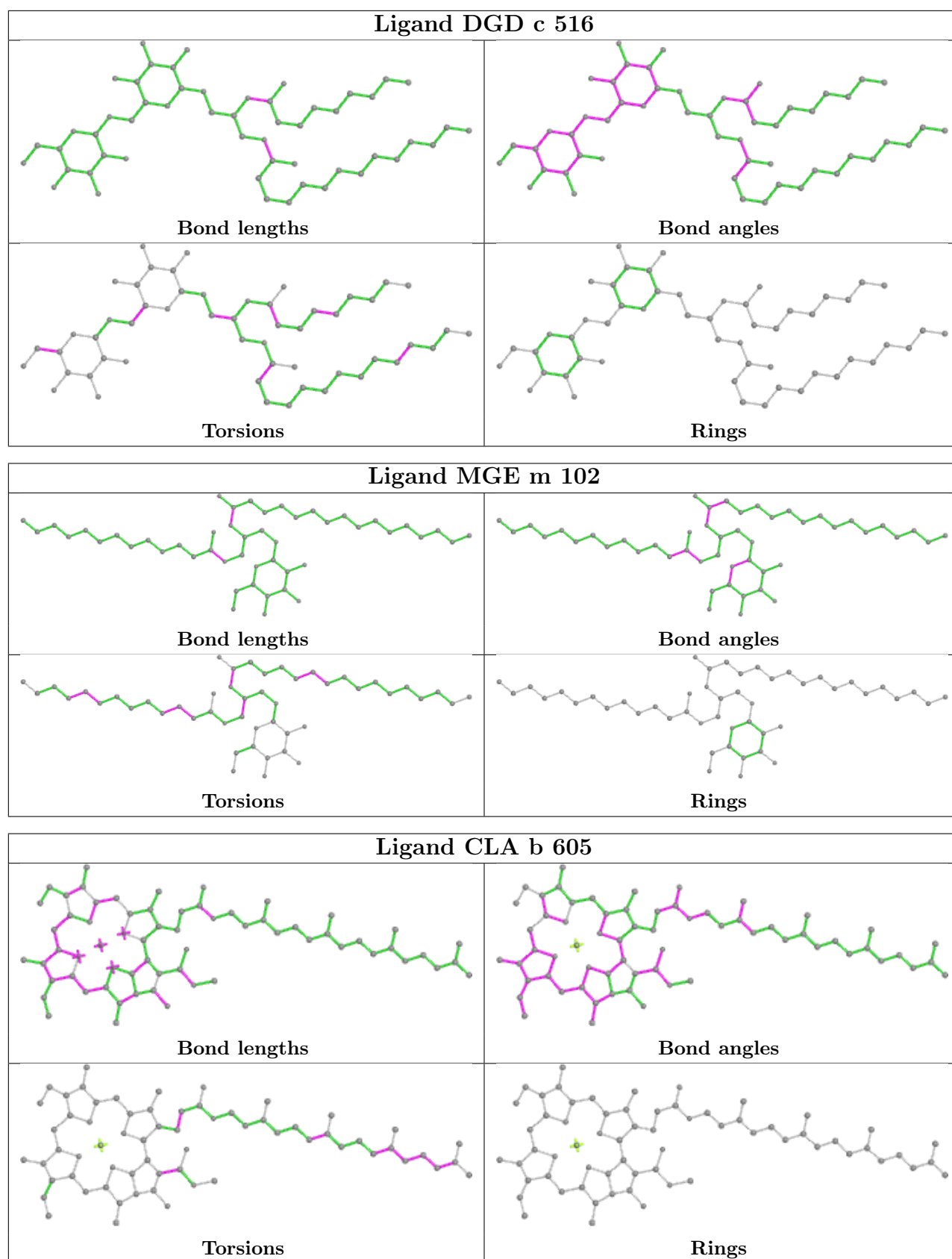


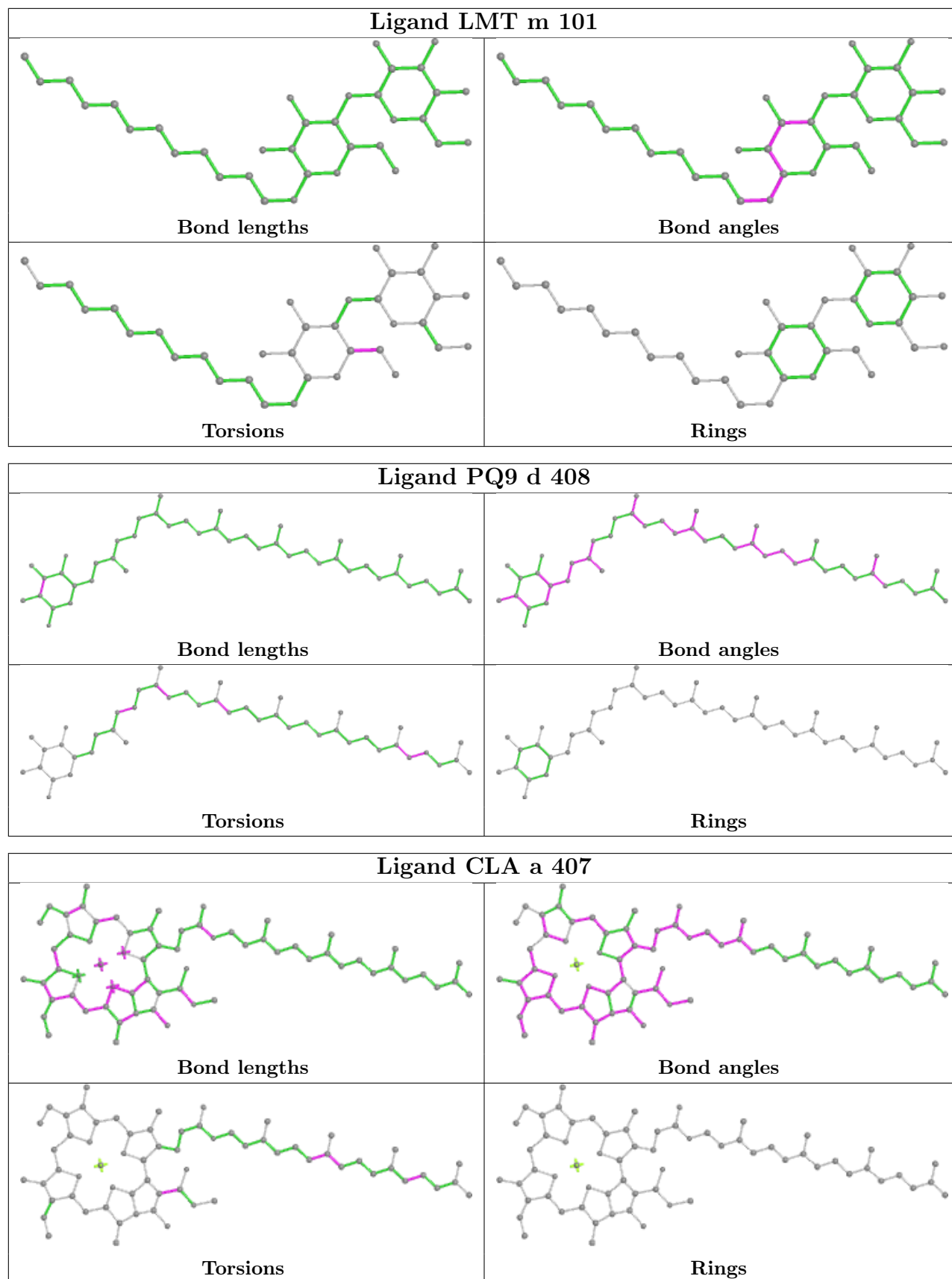


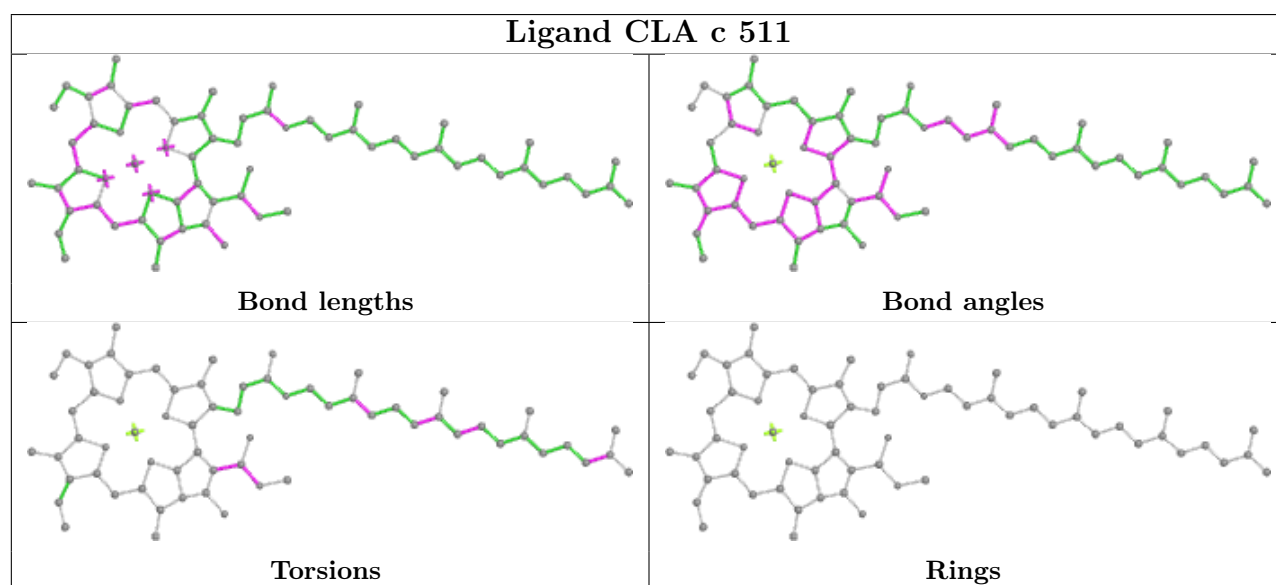
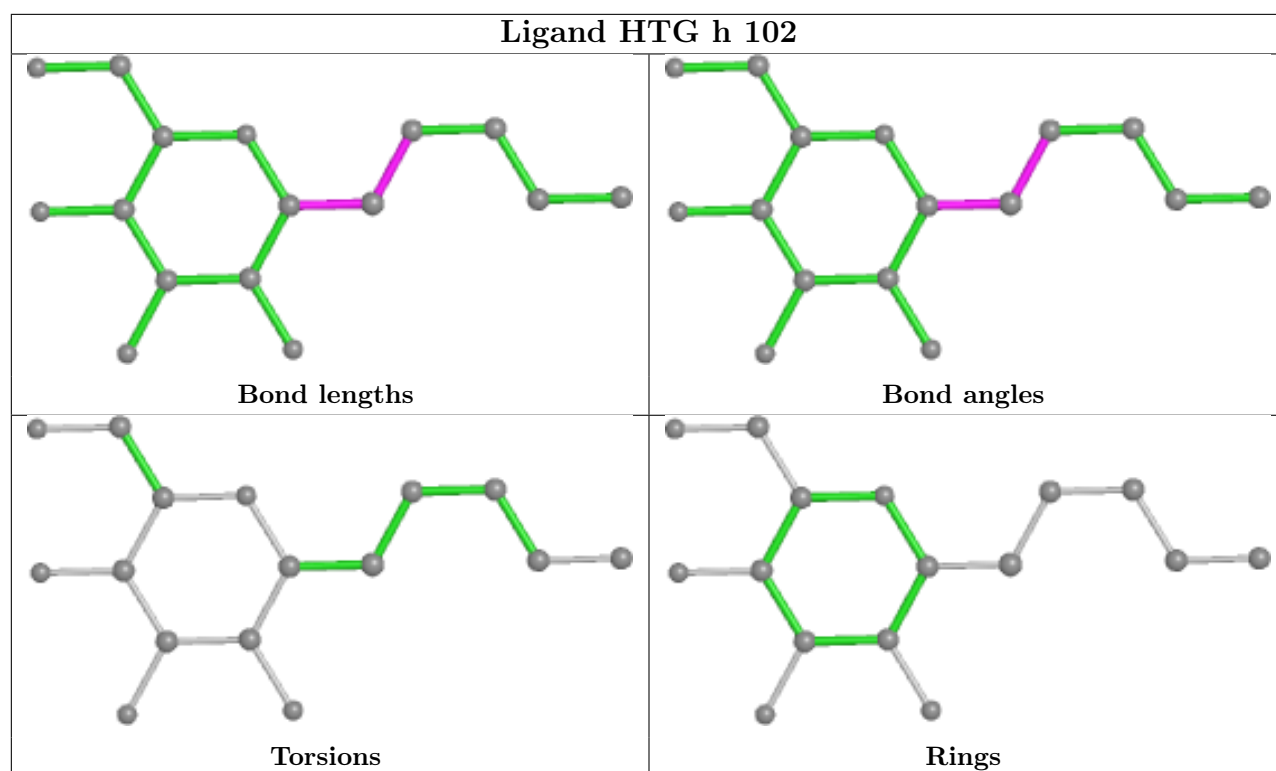


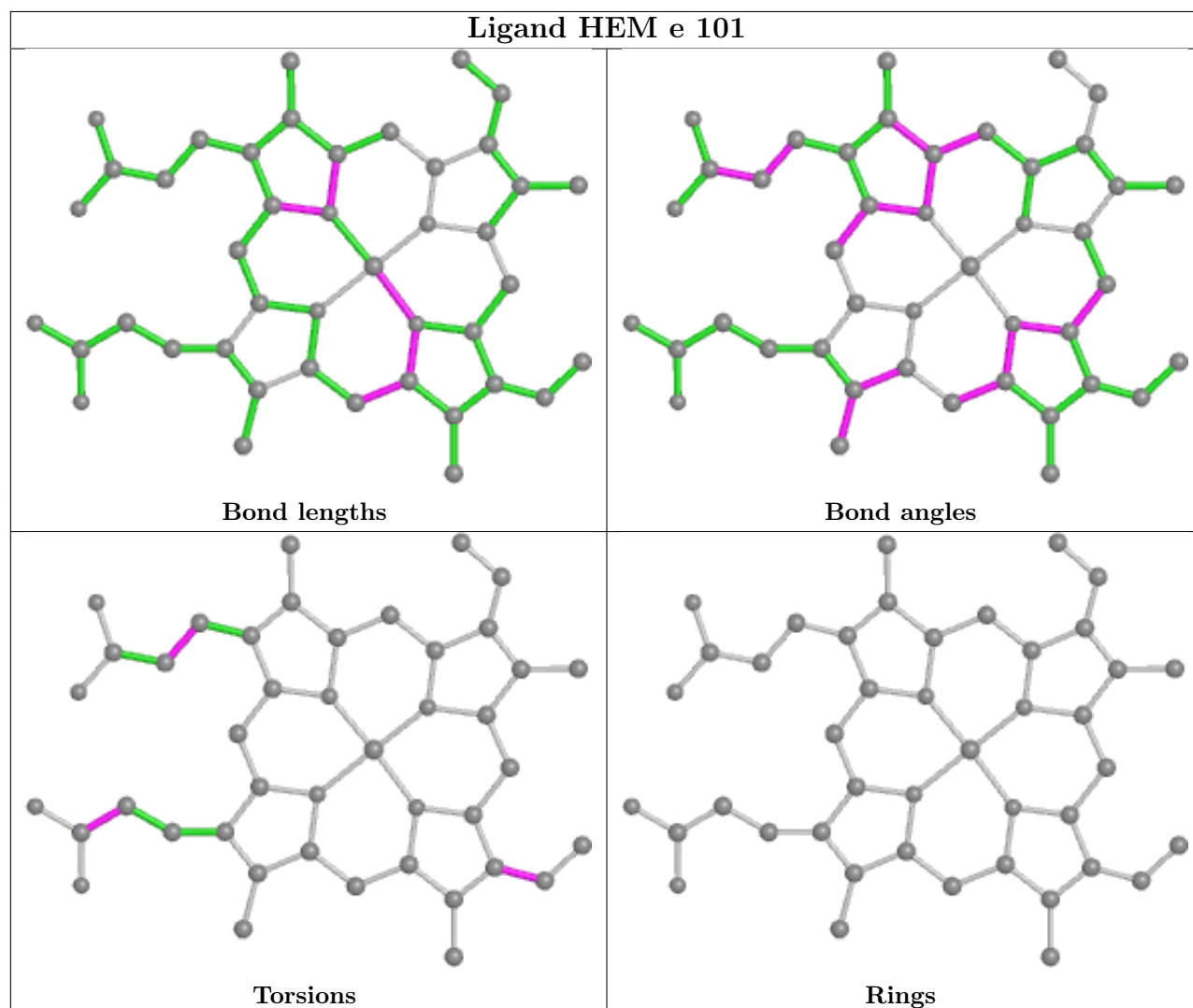
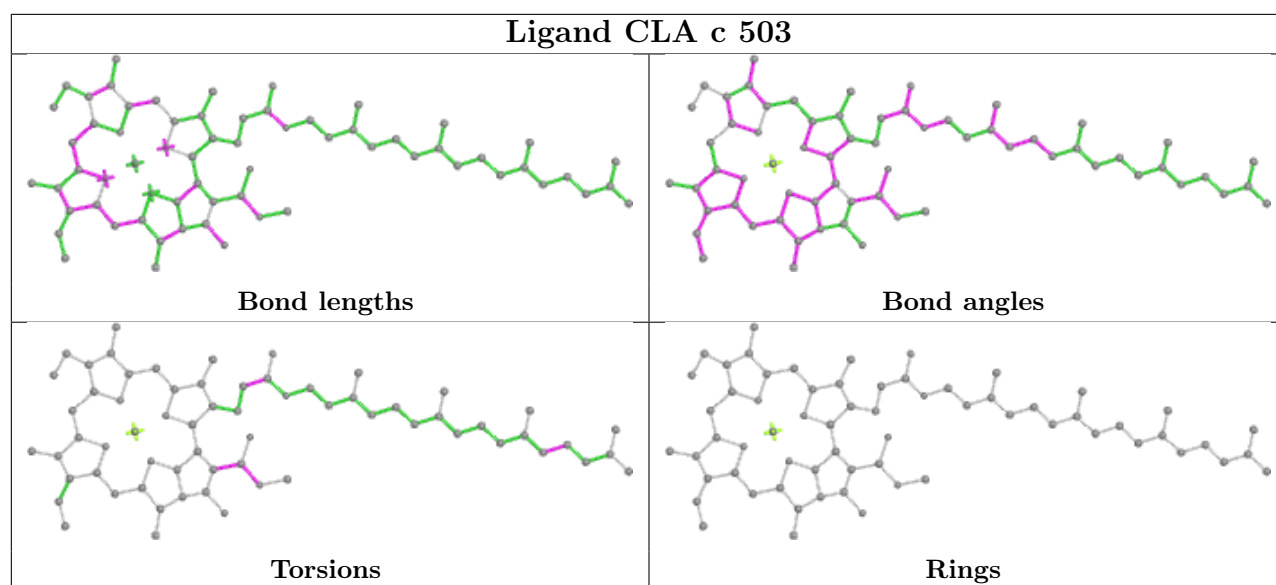


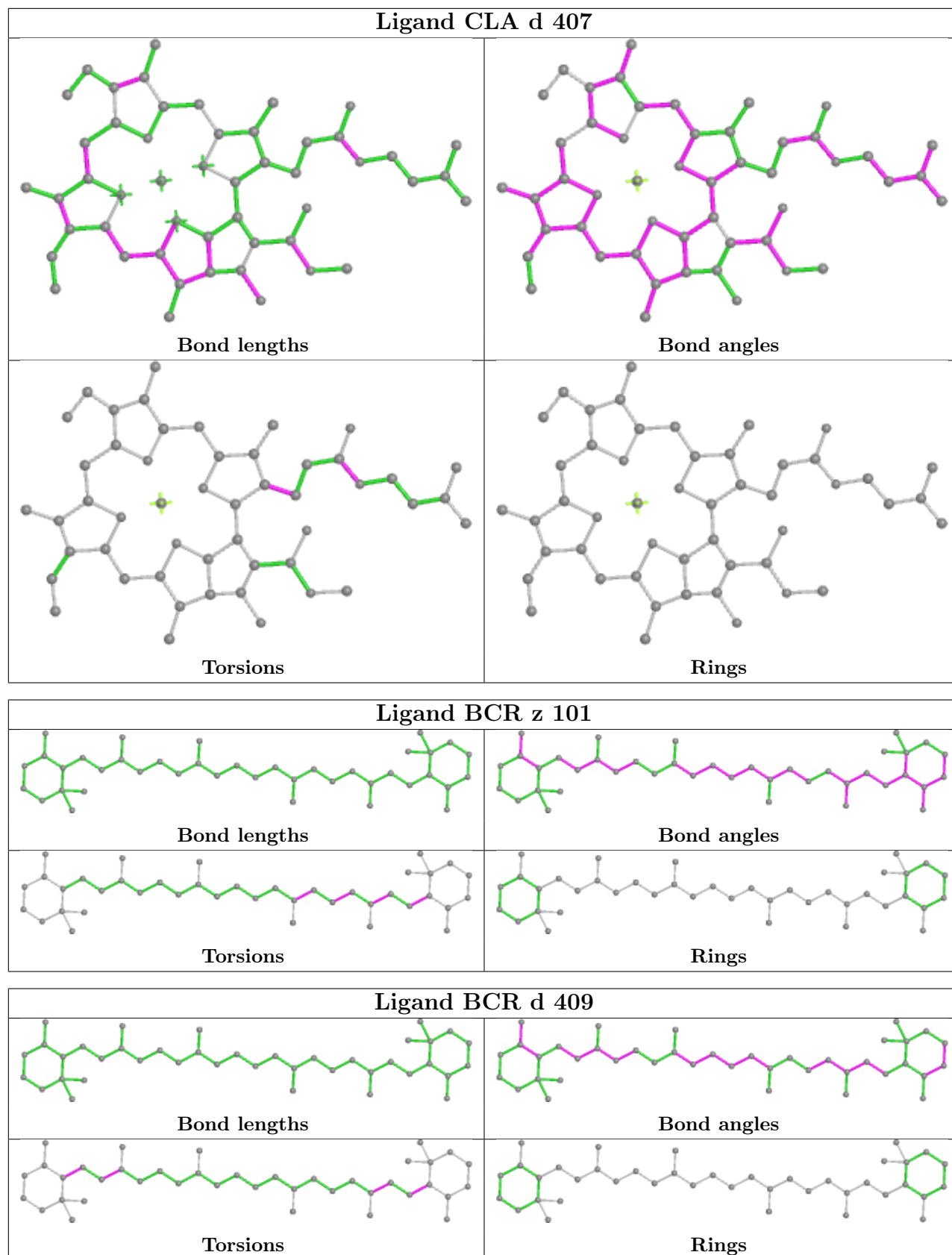


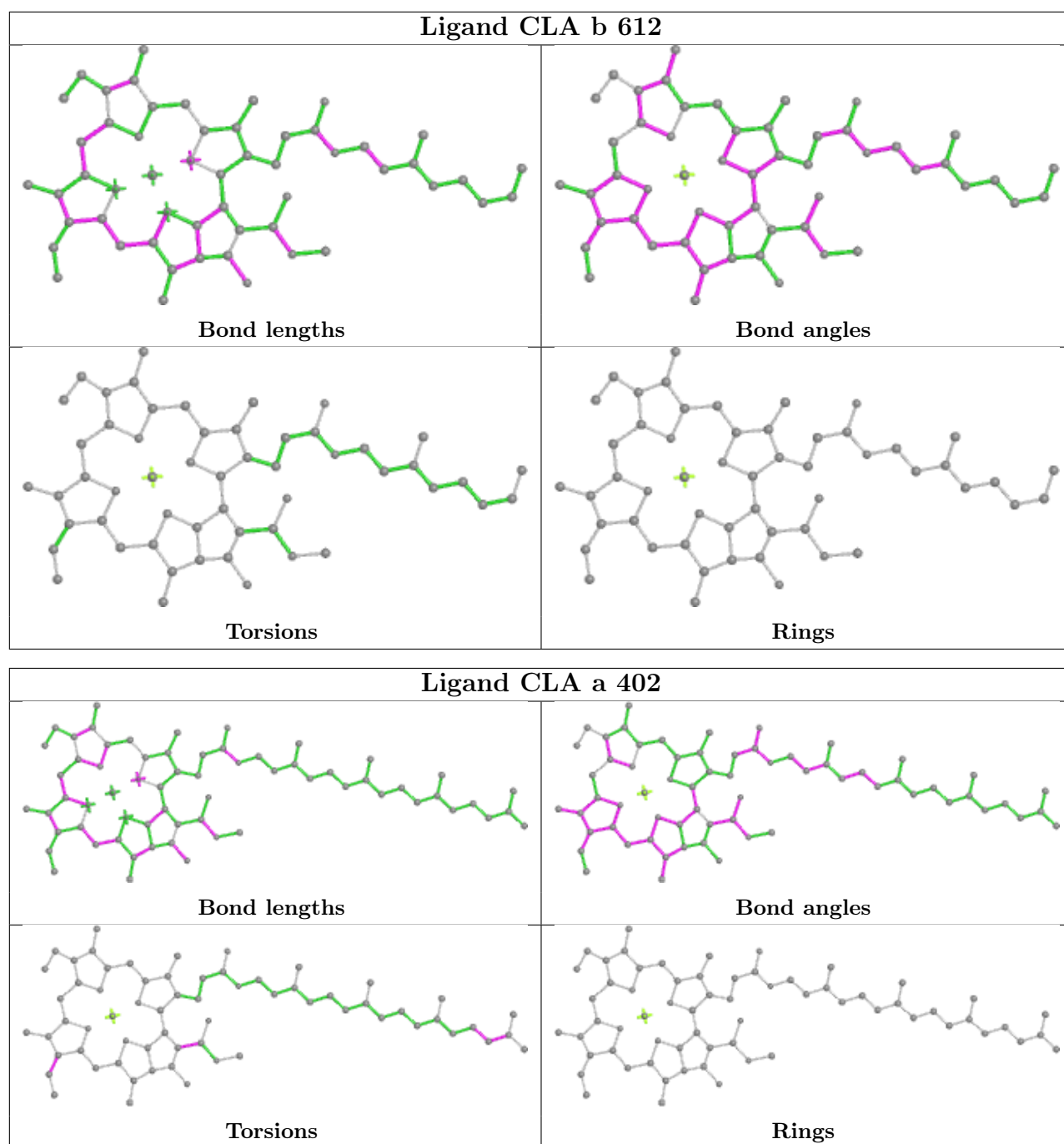


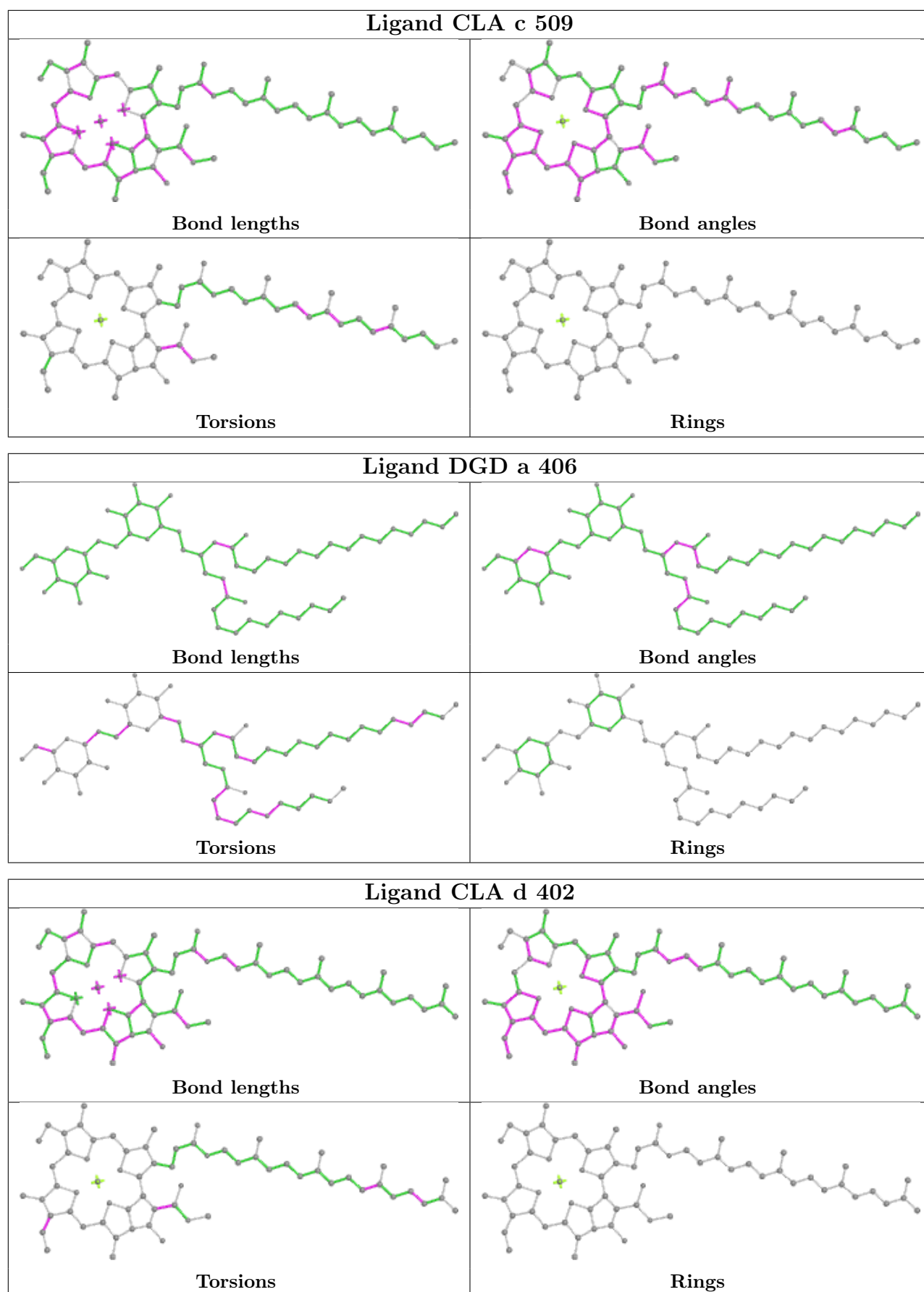


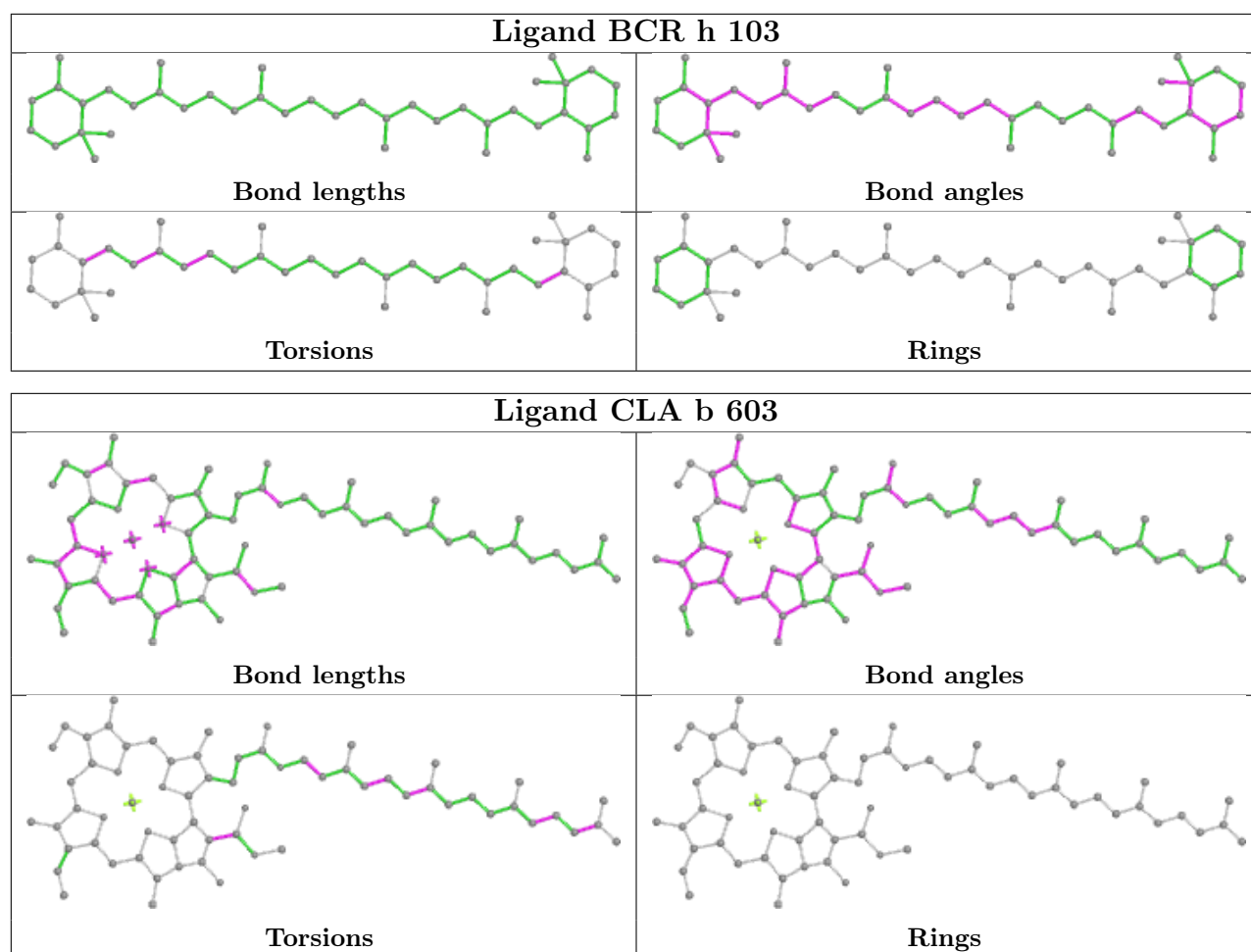


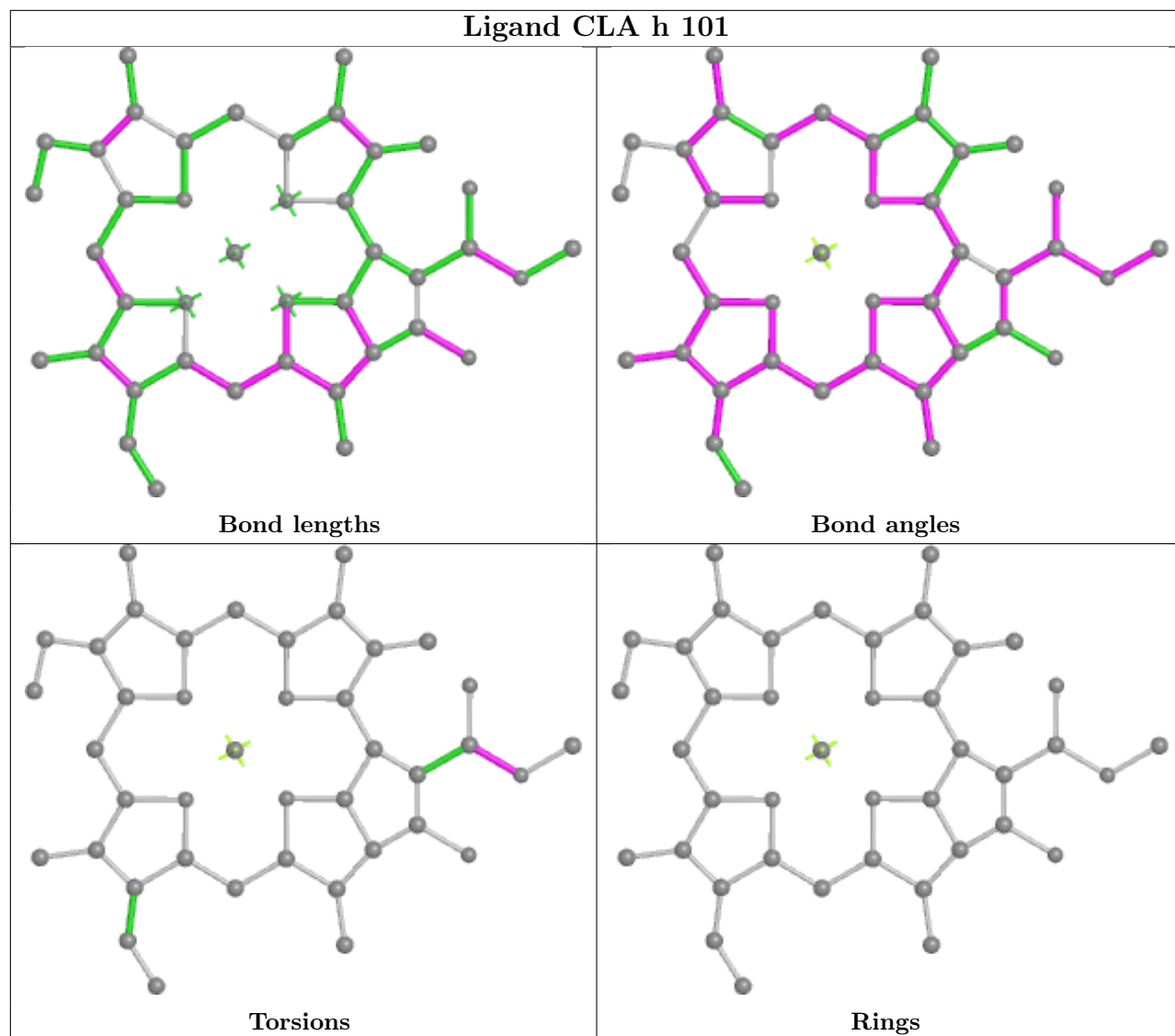


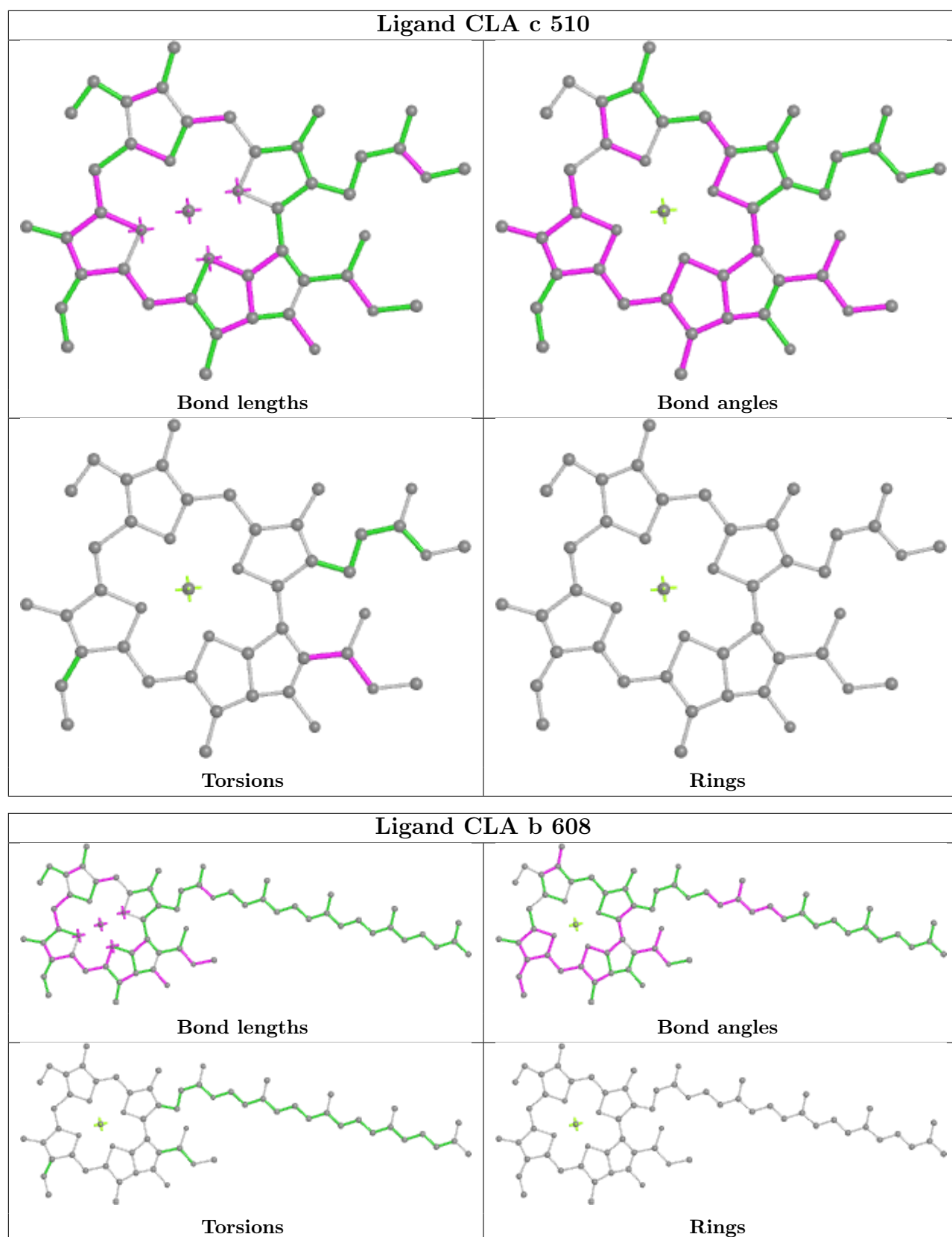


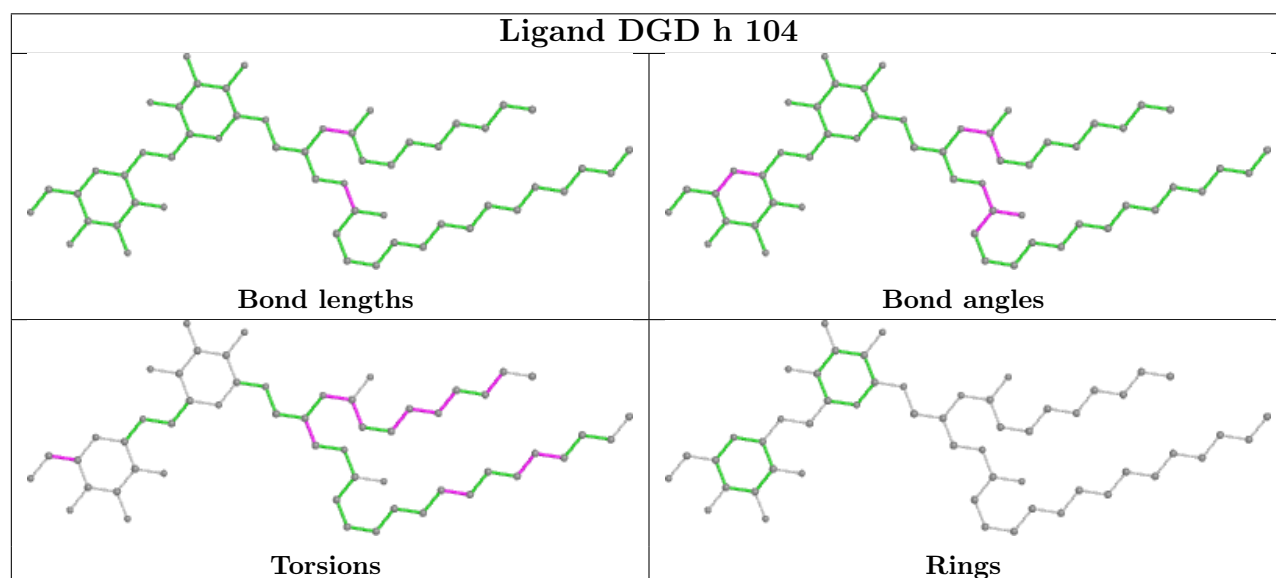
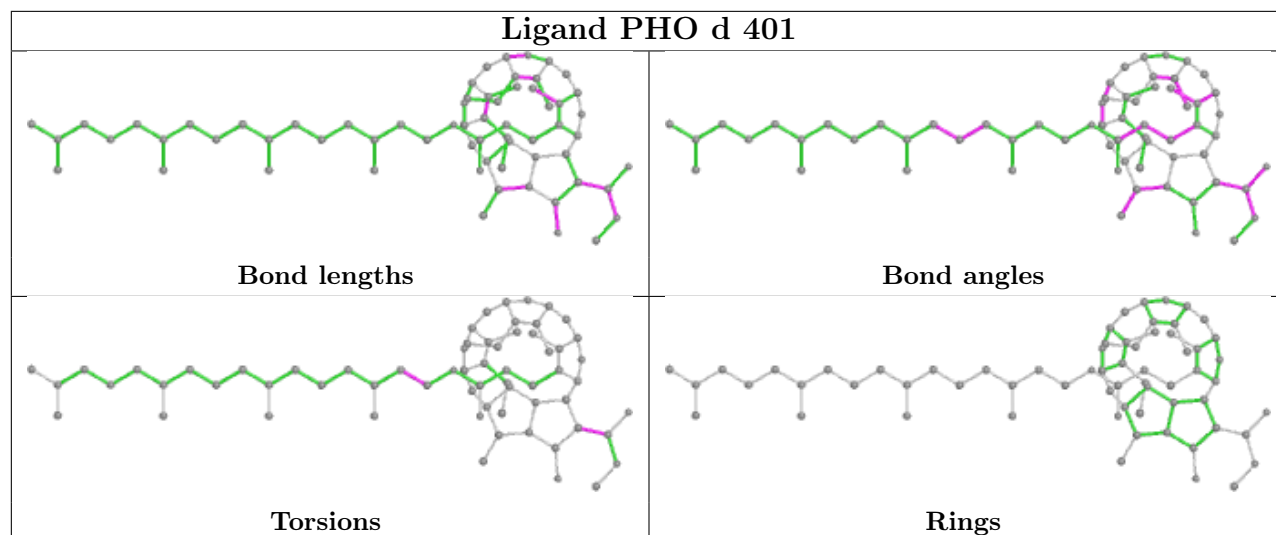


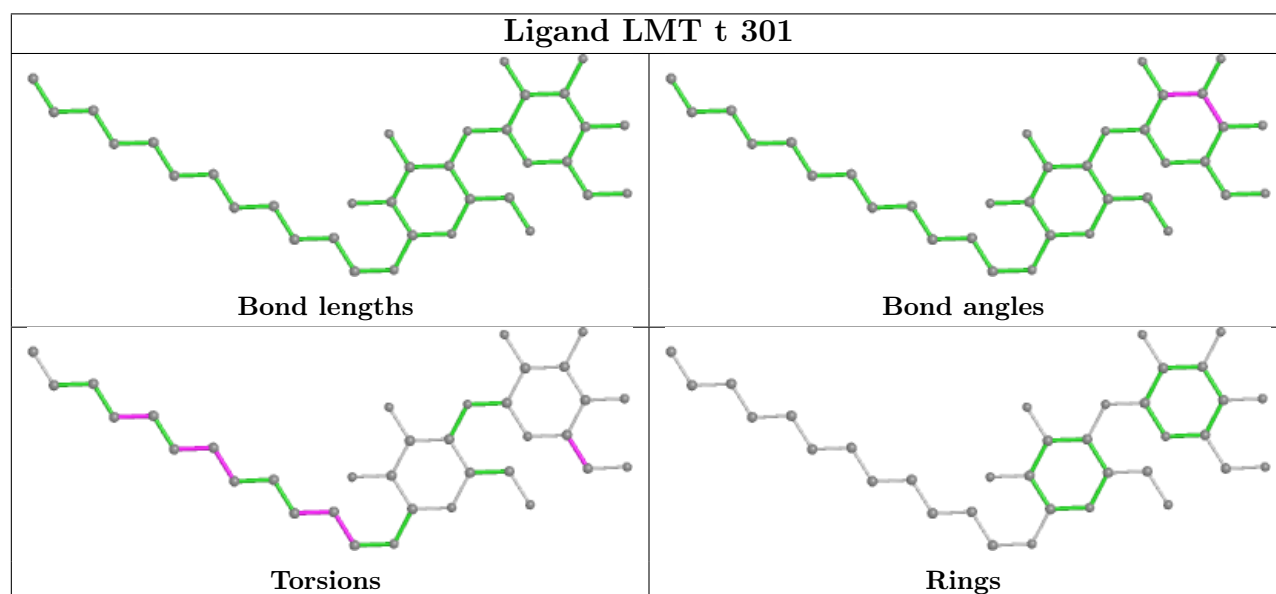
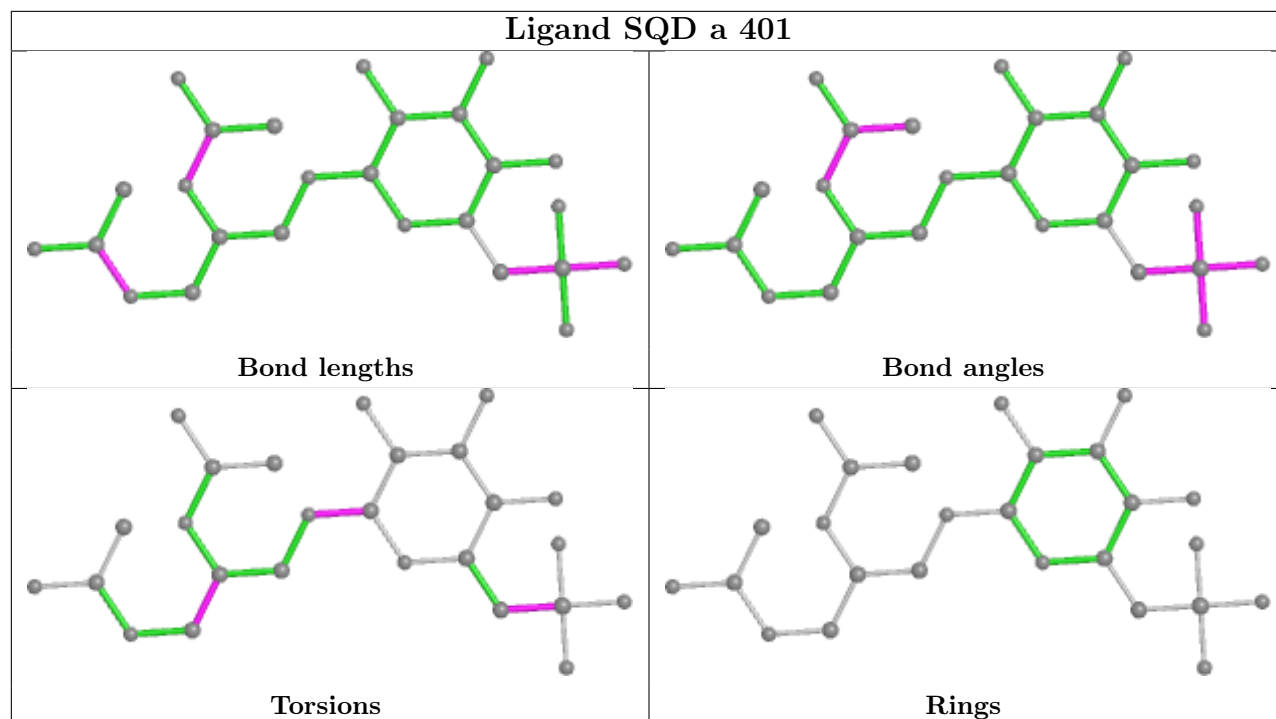


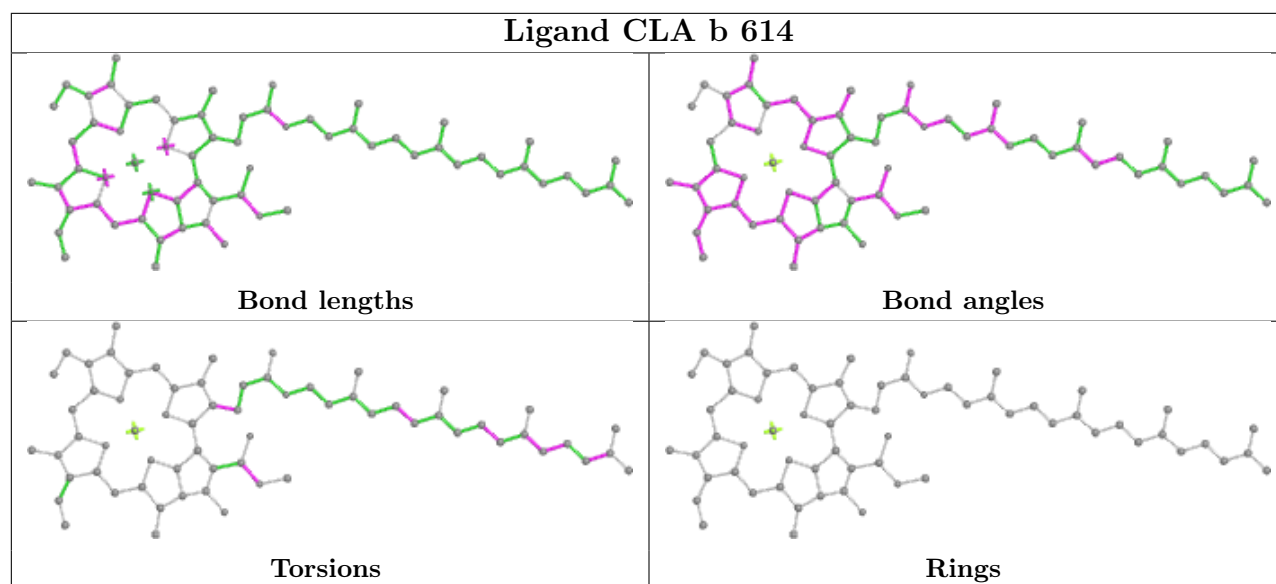
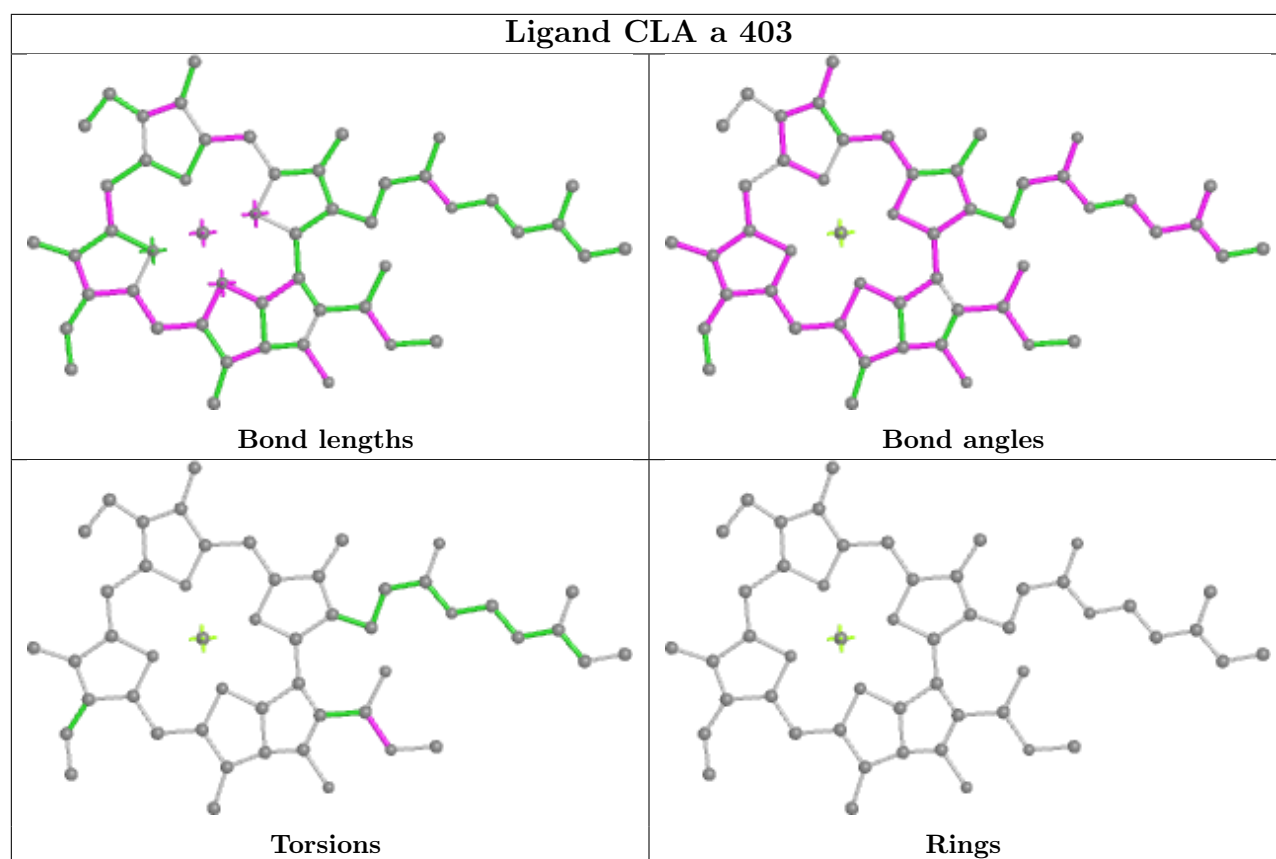


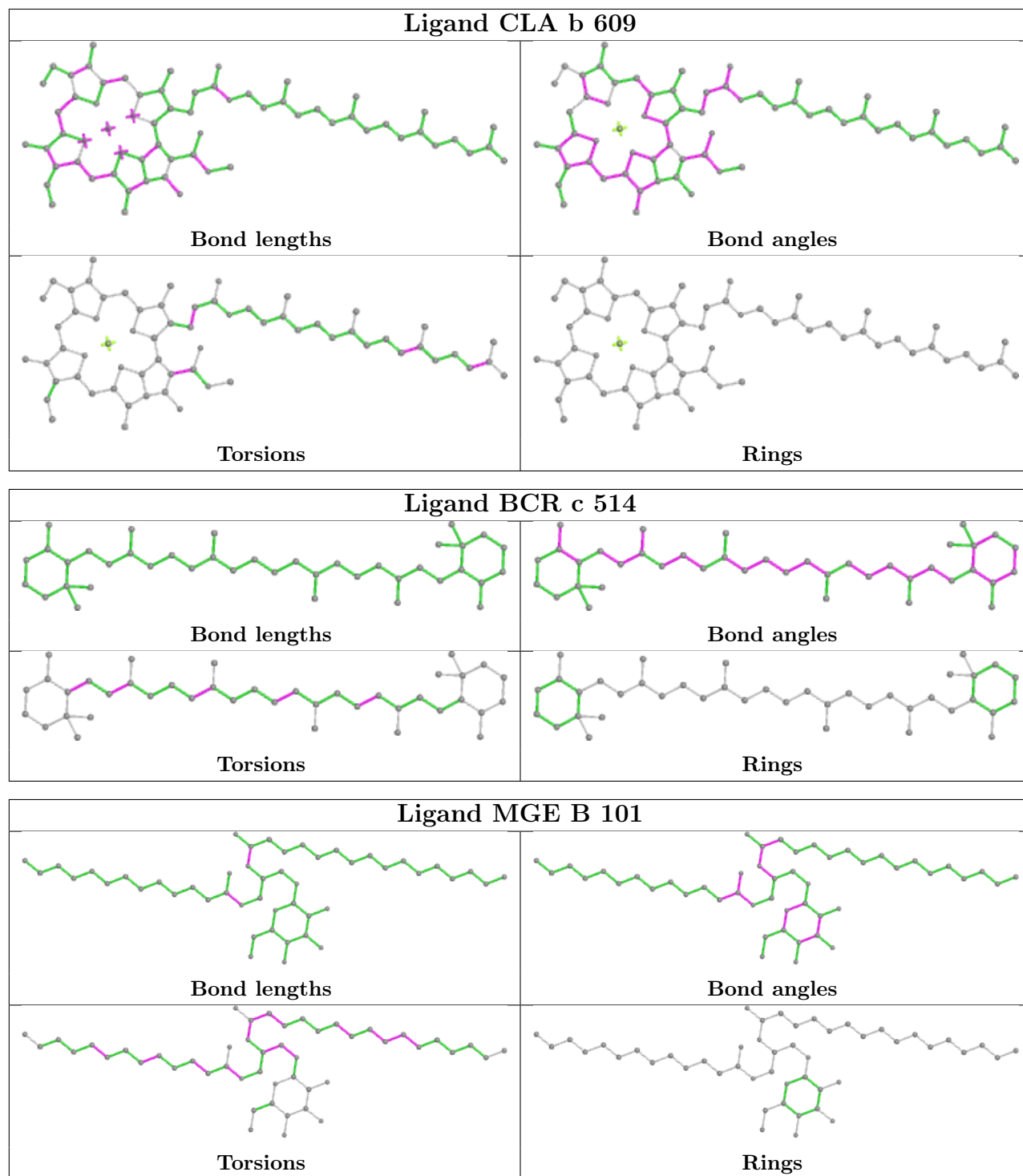


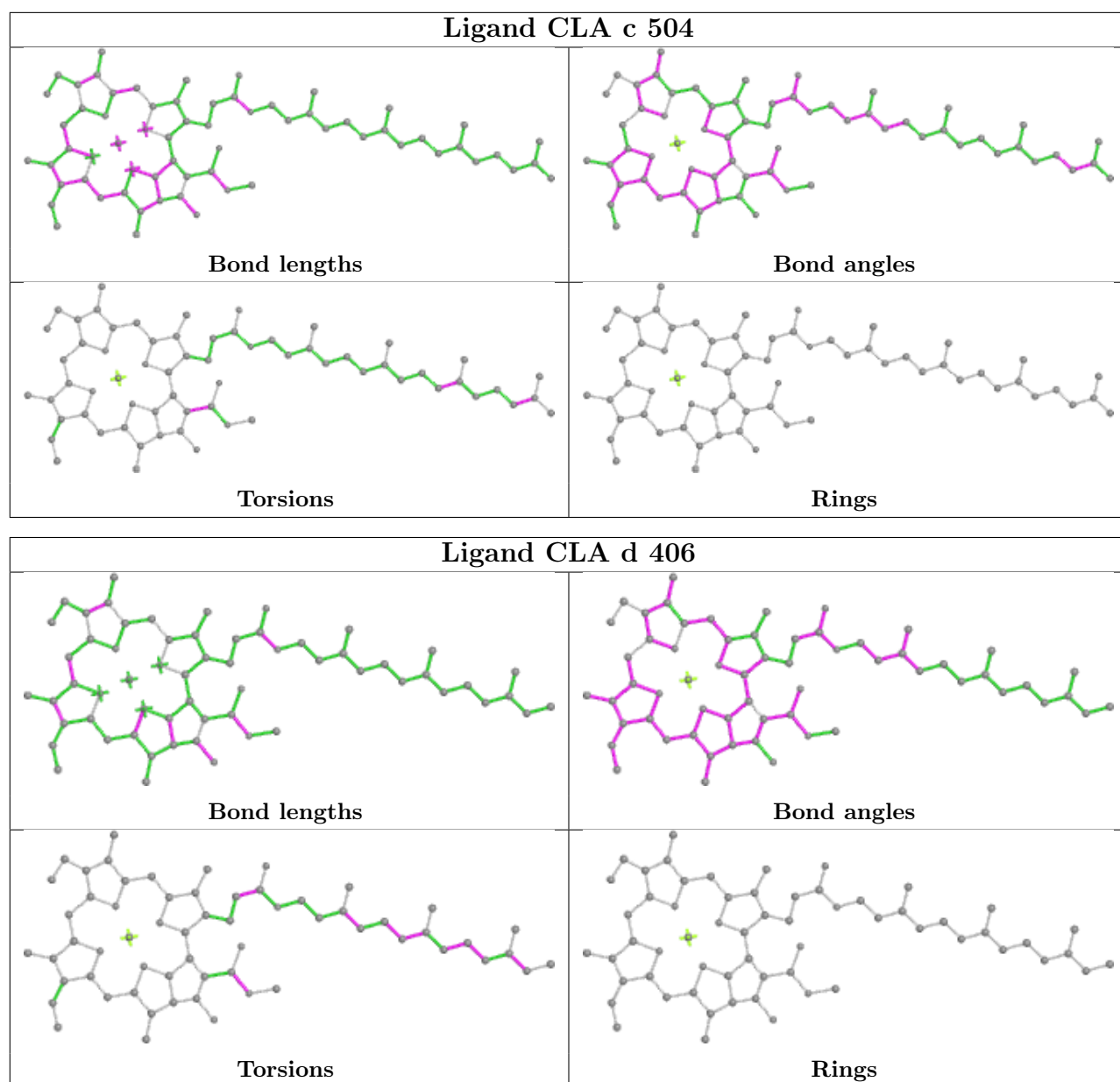


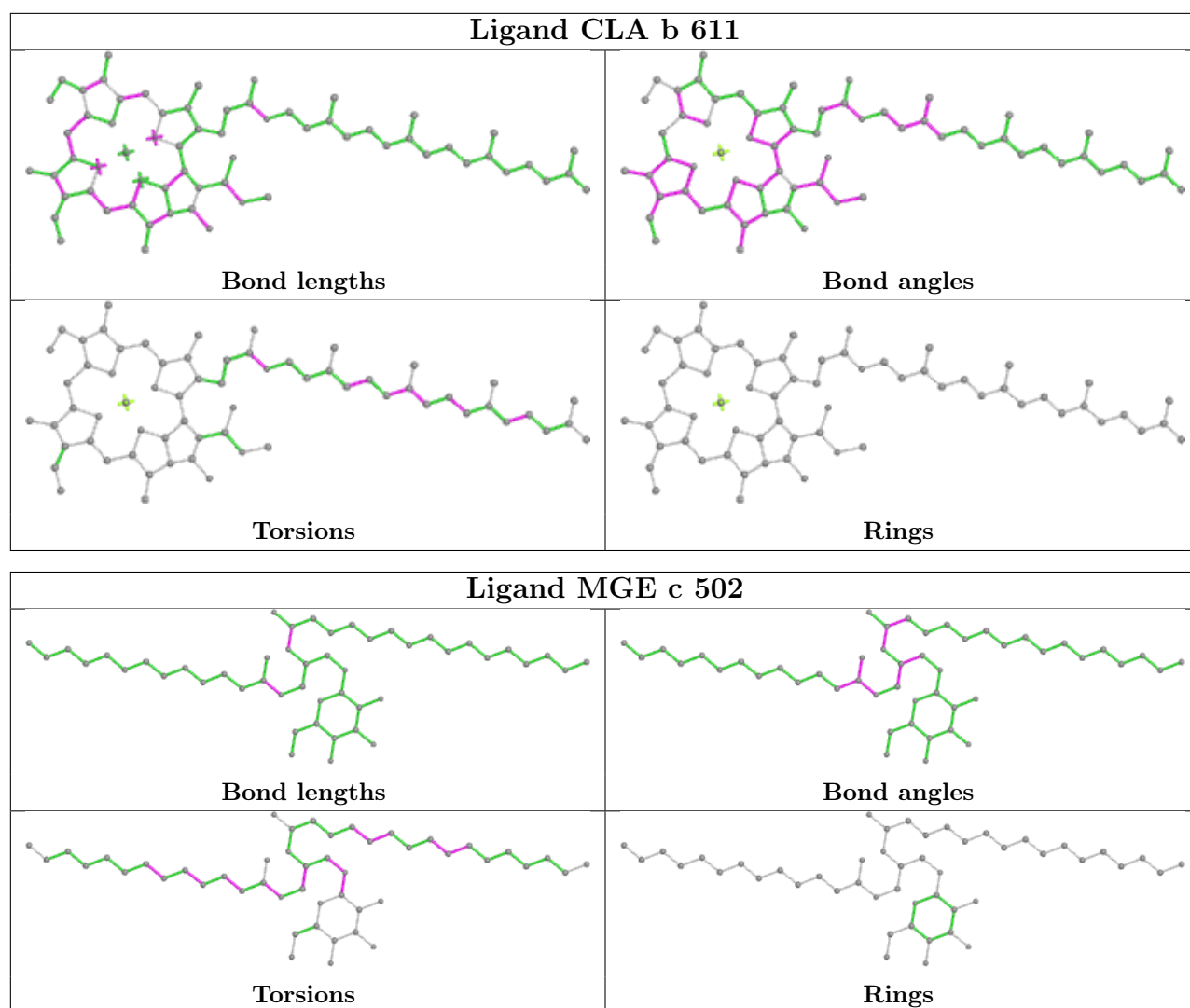


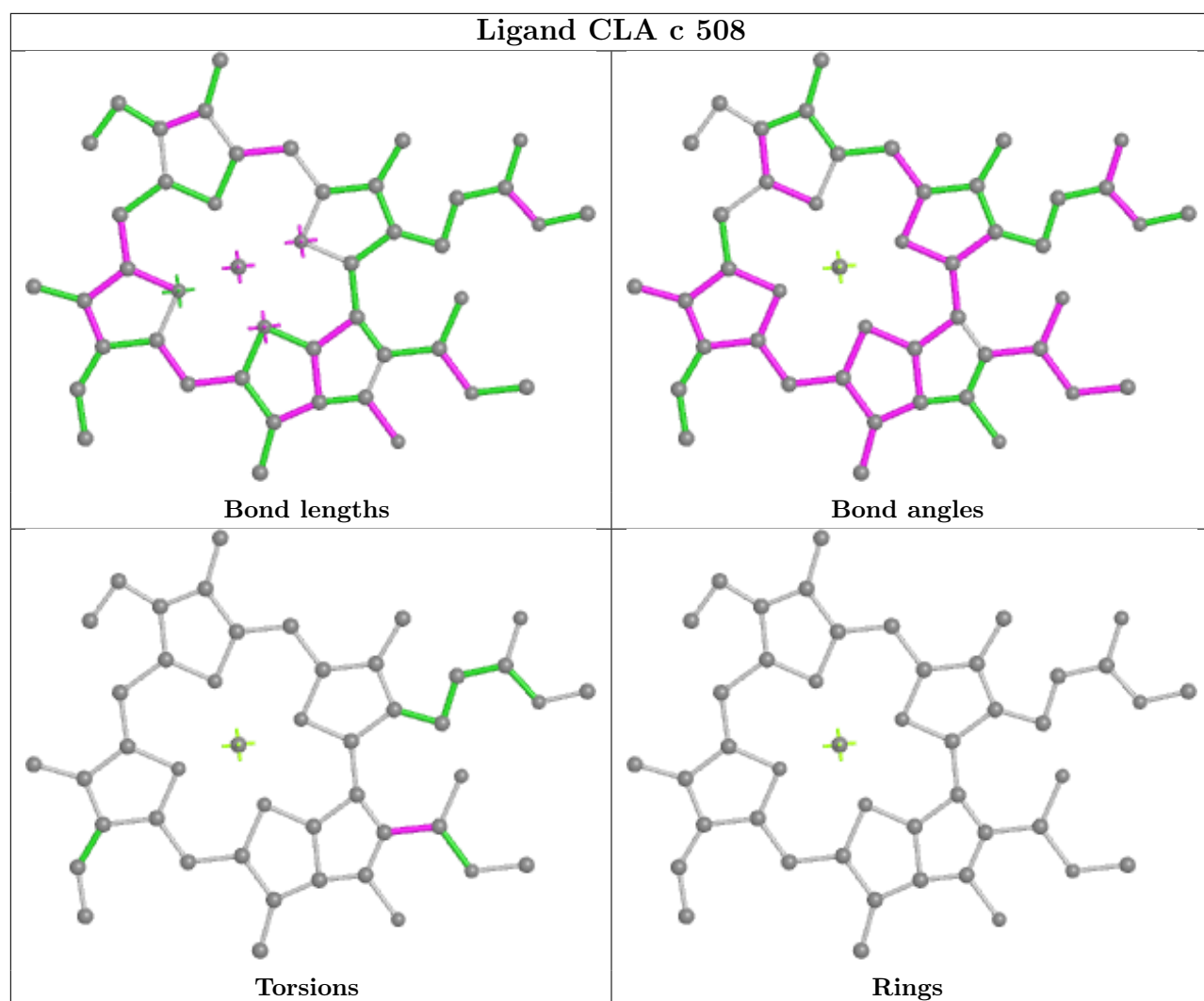












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

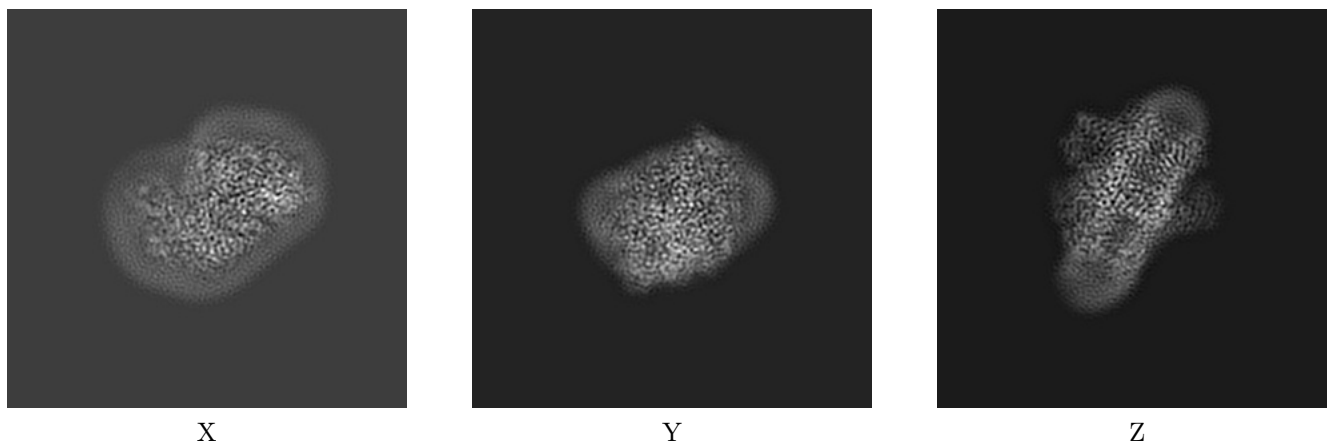
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30909. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

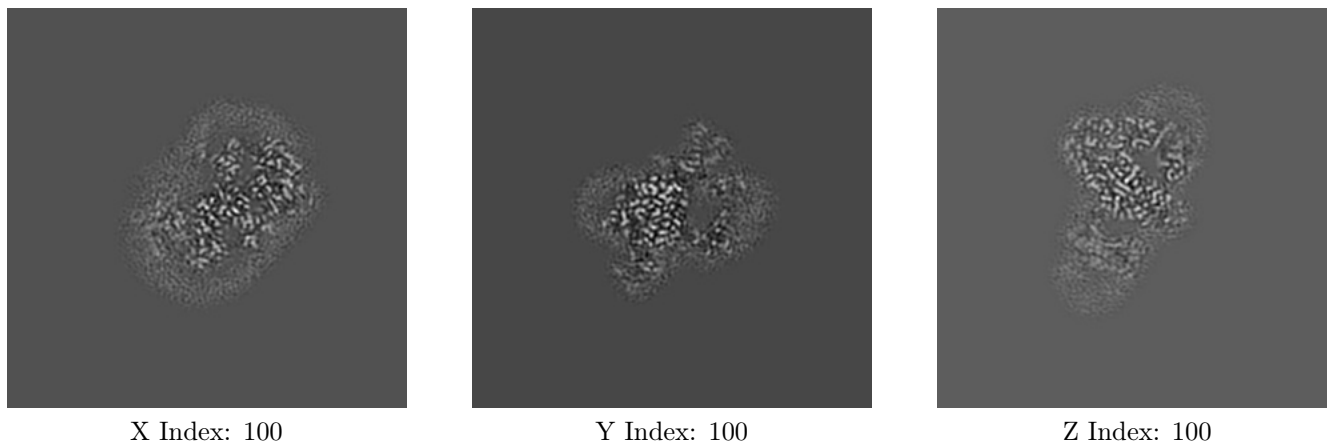
6.1.1 Primary map



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

6.2 Central slices [i](#)

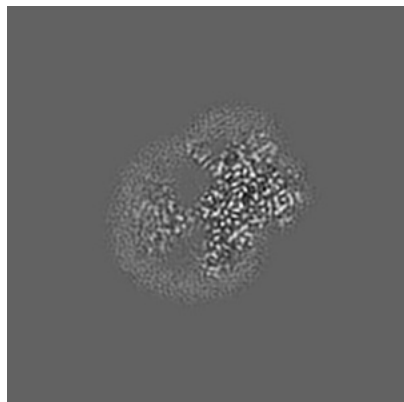
6.2.1 Primary map



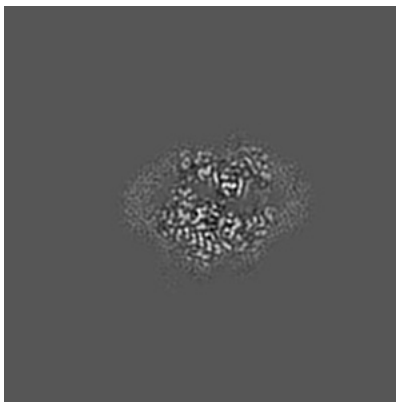
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

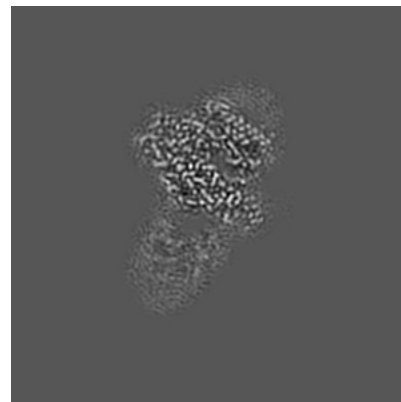
6.3.1 Primary map



X Index: 91



Y Index: 118

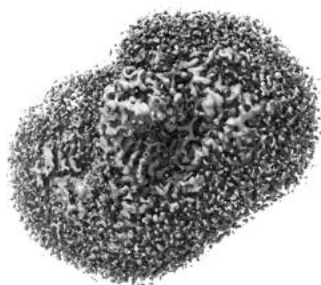


Z Index: 104

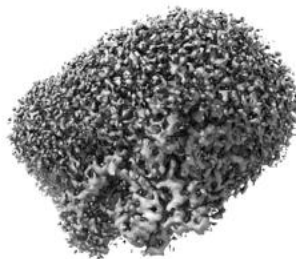
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

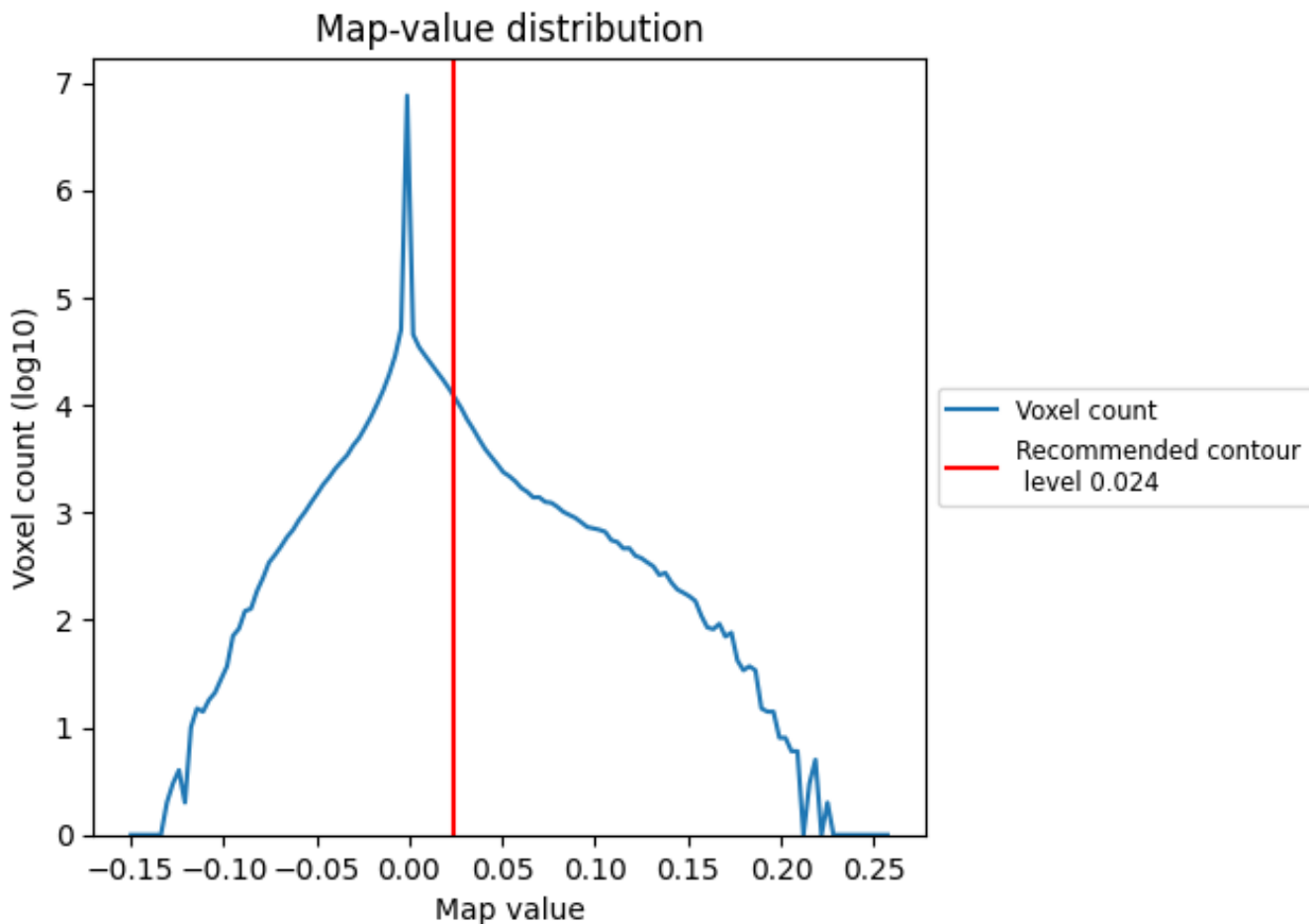
6.5 Mask visualisation

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

7 Map analysis [i](#)

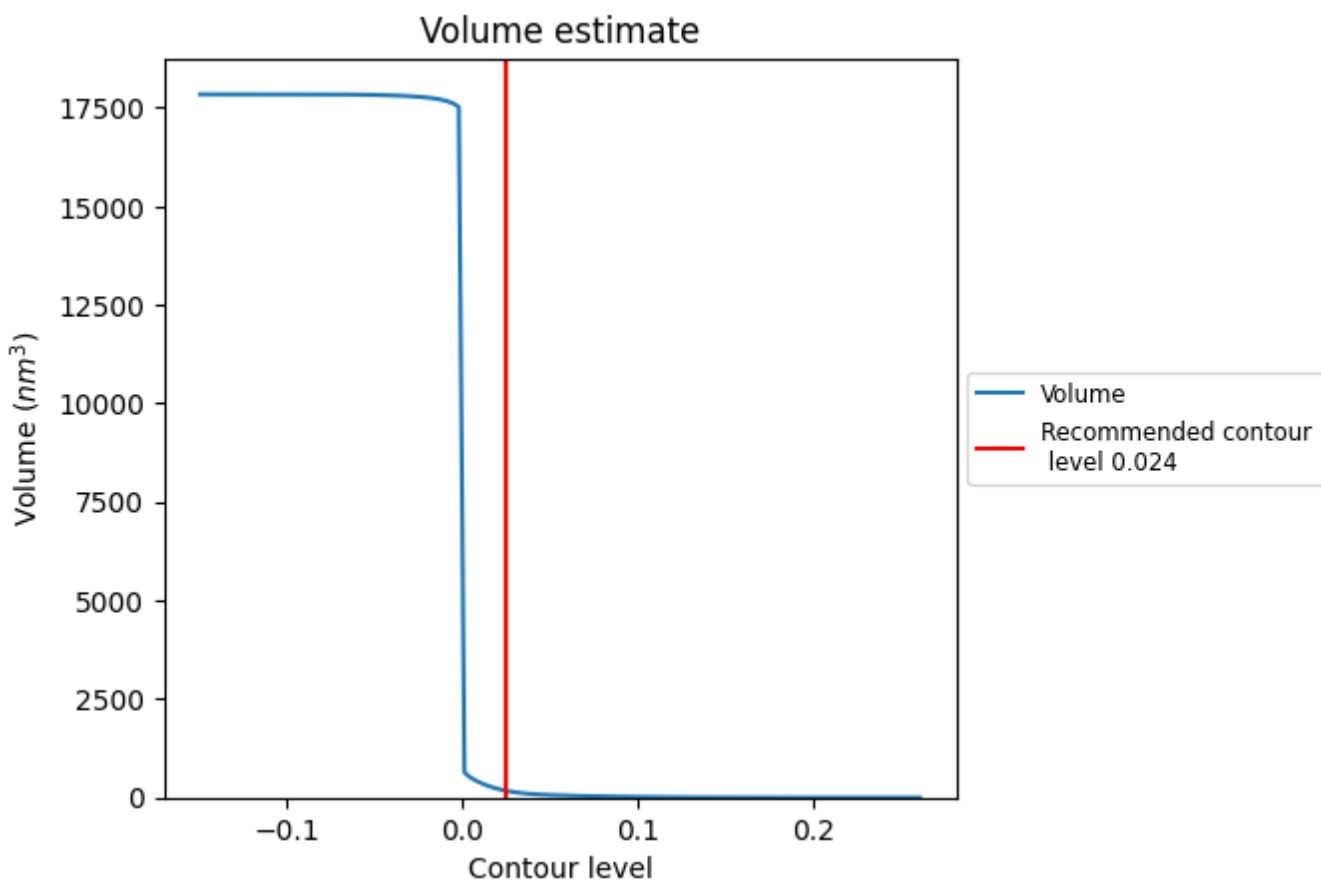
This section contains the results of statistical analysis of the map.

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.

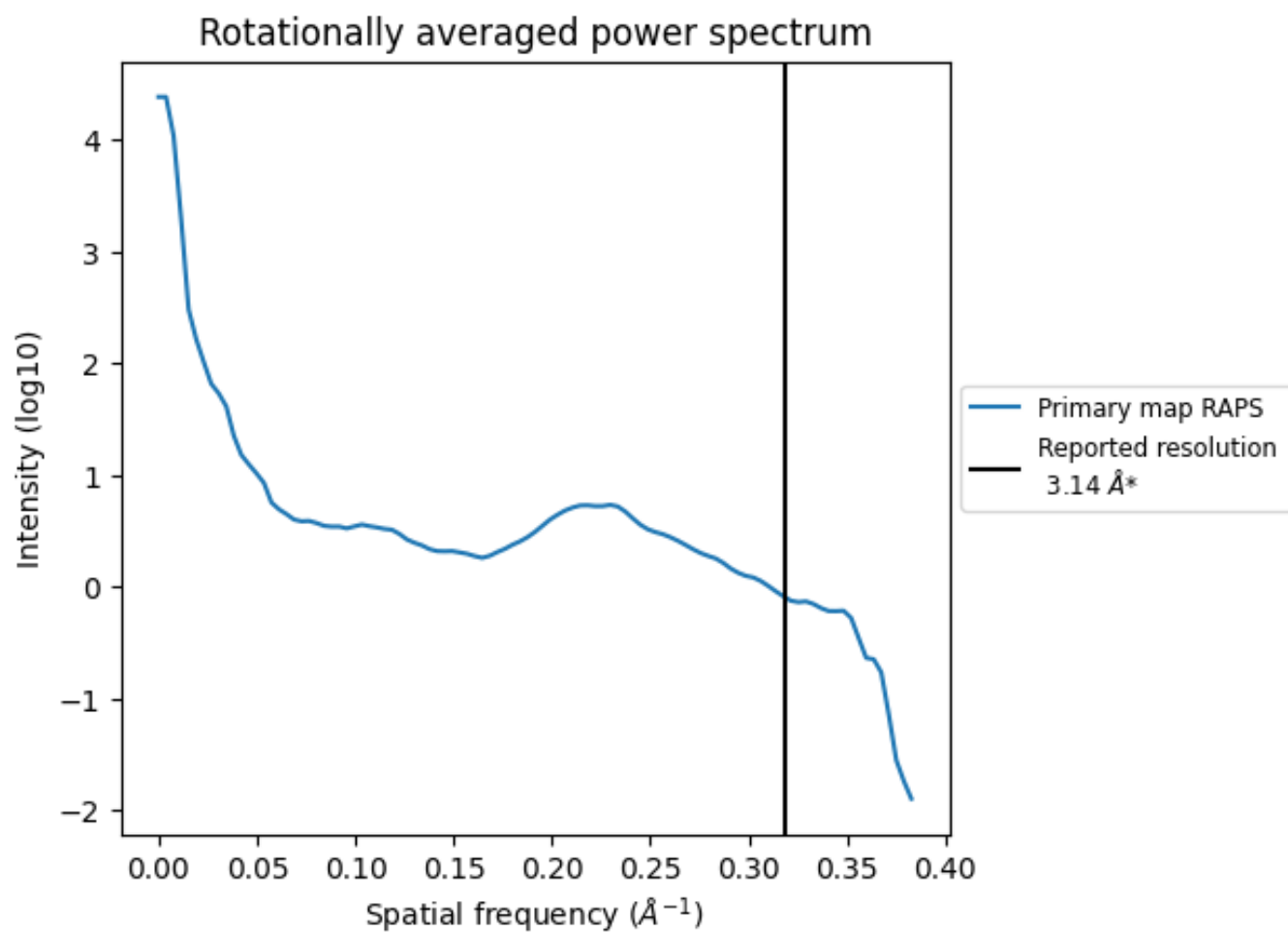
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 179 nm³; this corresponds to an approximate mass of 162 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

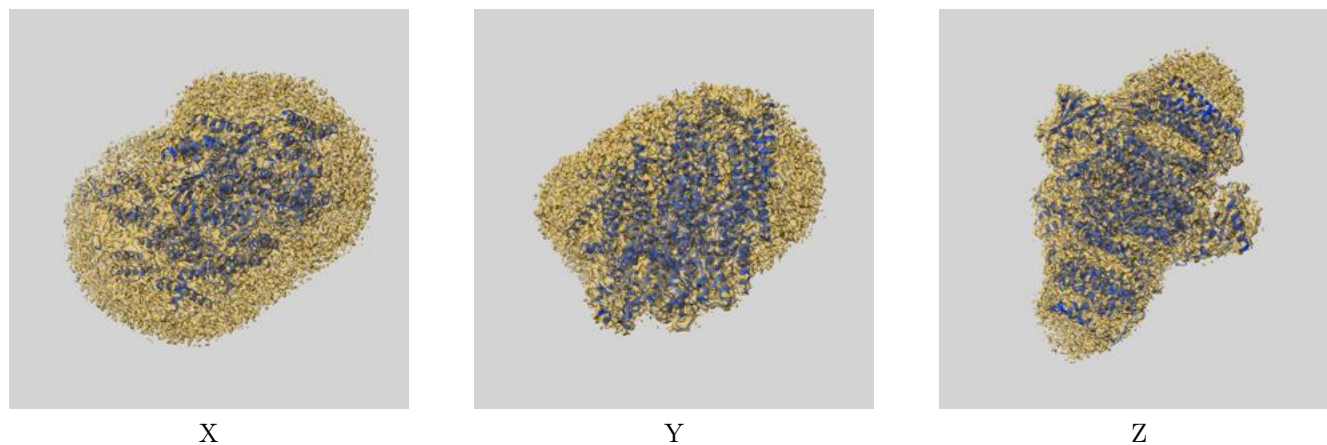
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

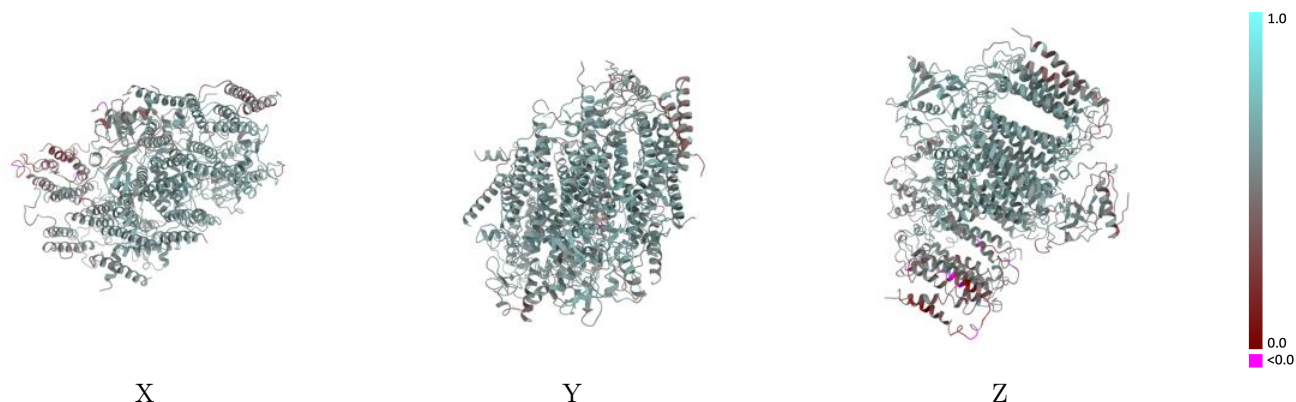
This section contains information regarding the fit between EMDB map EMD-30909 and PDB model 7DXH. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



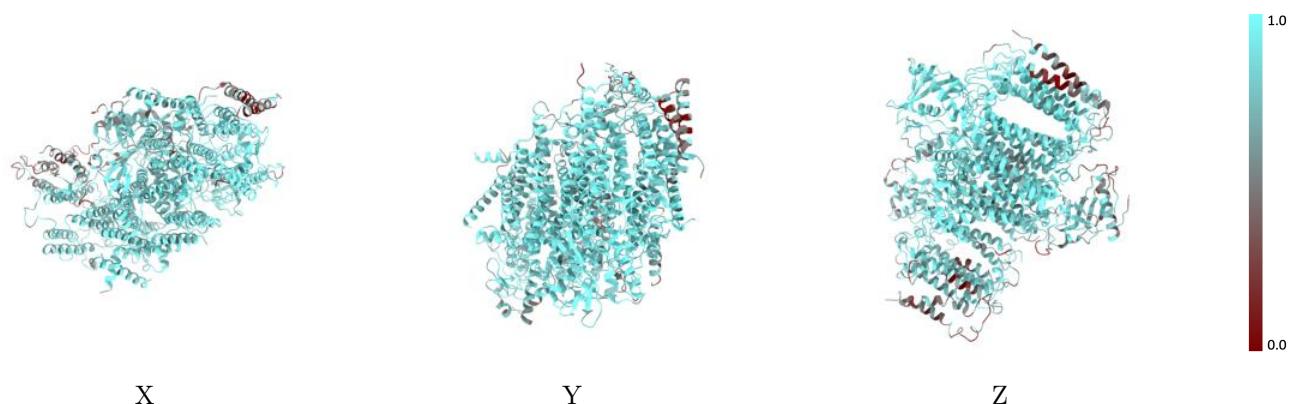
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



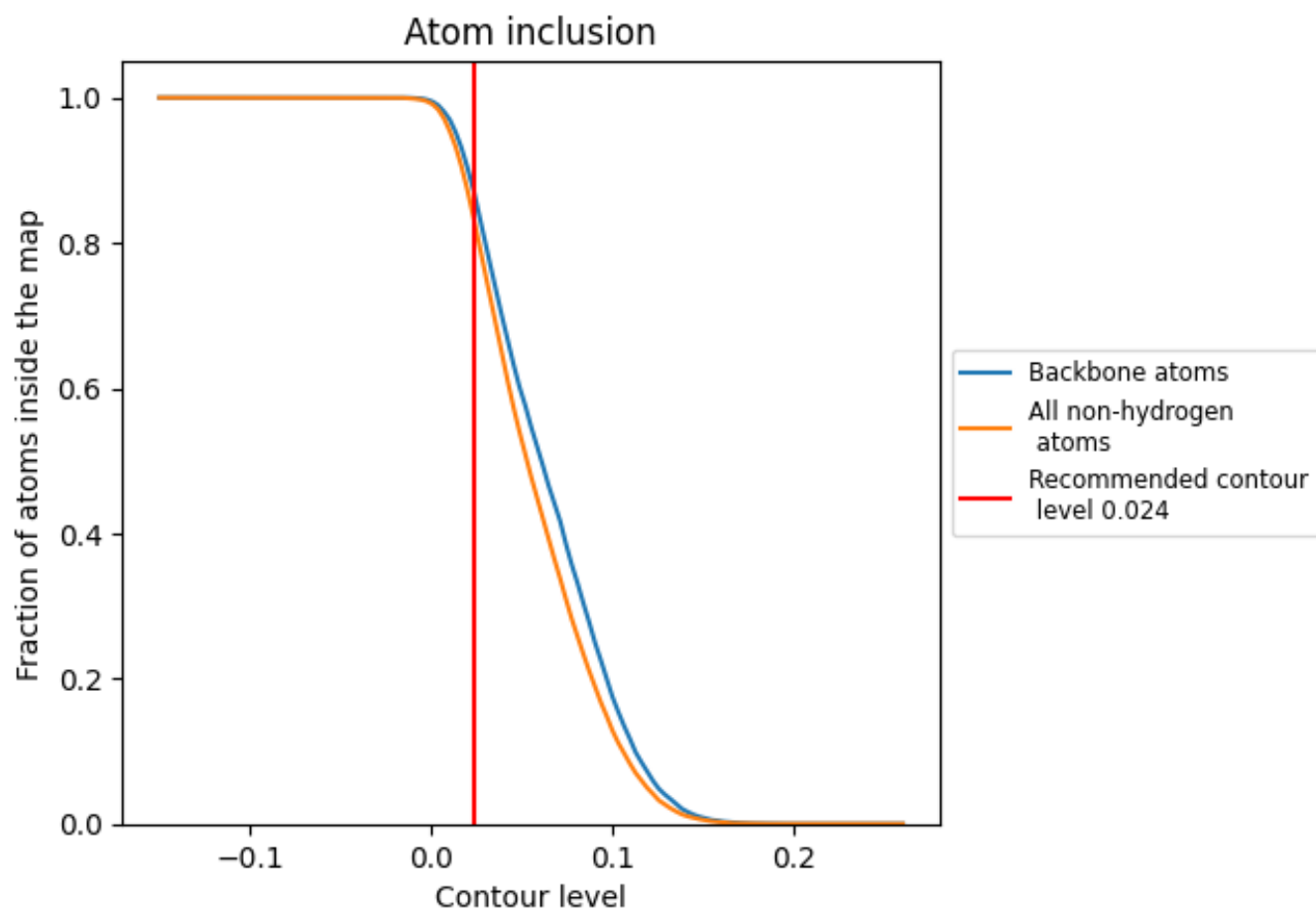
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8307	 0.5420
A	 0.6925	 0.4890
B	 0.5422	 0.4840
C	 0.4348	 0.4330
a	 0.8936	 0.5730
b	 0.8879	 0.5800
c	 0.8261	 0.5060
d	 0.9105	 0.5950
e	 0.7528	 0.4920
f	 0.8099	 0.5440
h	 0.8919	 0.5710
i	 0.8130	 0.5100
k	 0.6908	 0.4490
l	 0.7739	 0.5510
m	 0.6656	 0.5040
t	 0.7710	 0.5220
x	 0.8314	 0.5580
y	 0.3358	 0.2240
z	 0.4533	 0.3120

