



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 05:29 AM JST

PDB ID : 7DXH / pdb_00007dxh
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:

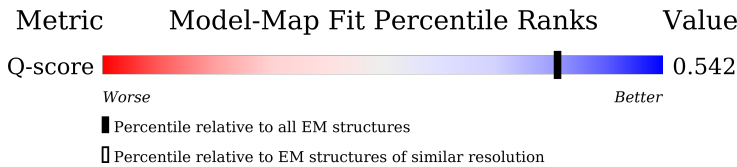
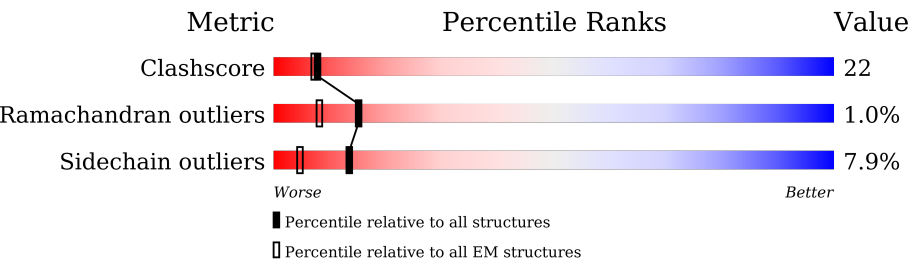
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14483 (2.64 - 3.64)

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	13% 57% 31% 6% 6%
2	B	56	30% 64% 18% • 14%
3	a	360	61% 19% •• 18%
4	b	505	69% 27% ••

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Mol	Chain	Length	Quality of chain
5	d	342	
6	e	84	
7	f	45	
8	h	65	
9	i	38	
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	b	605	-	-	X	-
21	CLA	c	503	-	-	X	-
21	CLA	c	507	-	-	X	-
21	CLA	c	510	-	-	X	-
21	CLA	d	406	X	-	-	-
22	BCR	c	515	-	-	X	-
23	CL	a	405	-	-	X	-
31	HTG	h	102	-	-	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
1	A	109	Total	C	N	O	S	0	0
			875	549	153	168	5		

- Molecule 2 is a protein called Tsl0063 protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

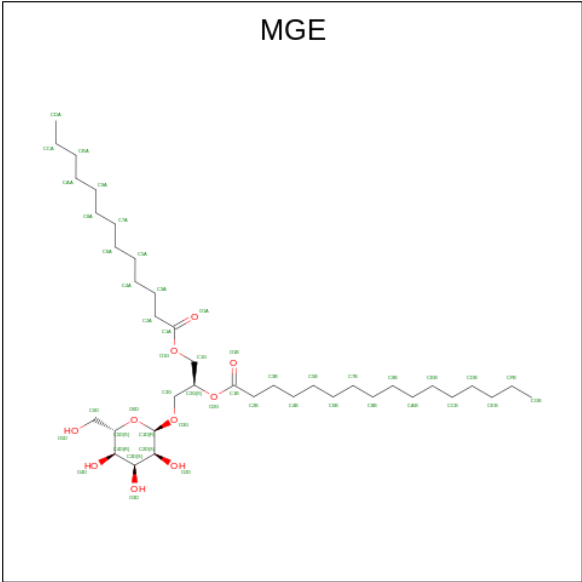
- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

- Molecule 18 is a protein called unidentified transmembrane protein.

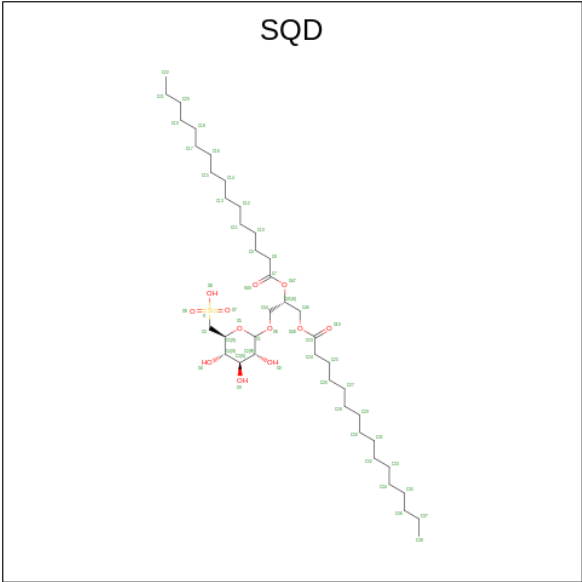
Mol	Chain	Residues	Atoms				AltConf	Trace
18	C	23	Total	C	N	O	0	0
			115	69	23	23		

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



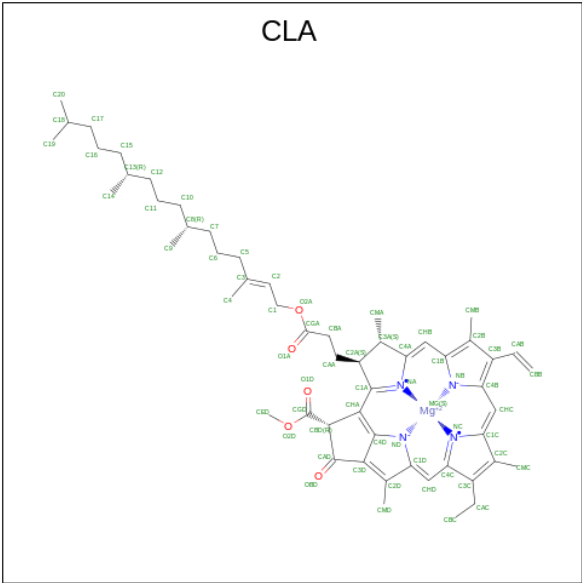
Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			48	38	10	
19	b	1	Total	C	O	0
			48	38	10	
19	b	1	Total	C	O	0
			41	31	10	
19	d	1	Total	C	O	0
			48	38	10	
19	f	1	Total	C	O	0
			47	37	10	
19	m	1	Total	C	O	0
			48	38	10	
19	c	1	Total	C	O	0
			48	38	10	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



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

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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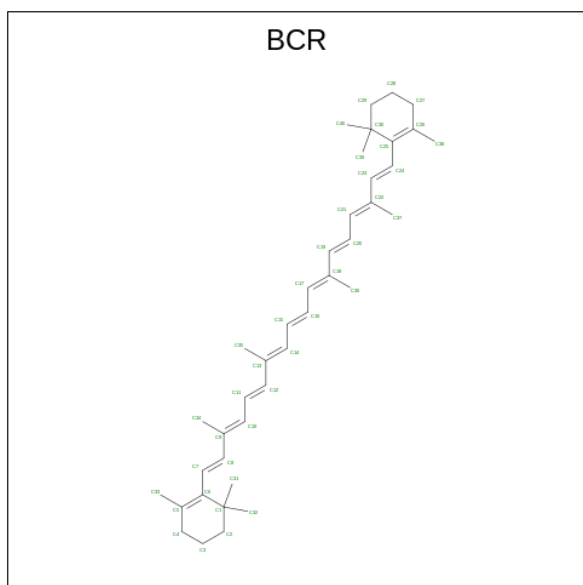
Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	d	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	h	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

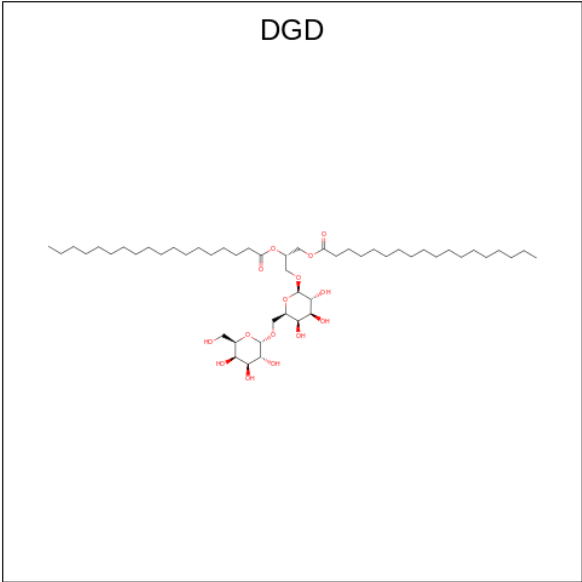


Mol	Chain	Residues	Atoms	AltConf
22	a	1	Total C 40 40	0
22	b	1	Total C 40 40	0
22	b	1	Total C 40 40	0
22	b	1	Total C 40 40	0
22	d	1	Total C 40 40	0
22	h	1	Total C 40 40	0
22	c	1	Total C 40 40	0
22	c	1	Total C 40 40	0
22	z	1	Total C 40 40	0

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

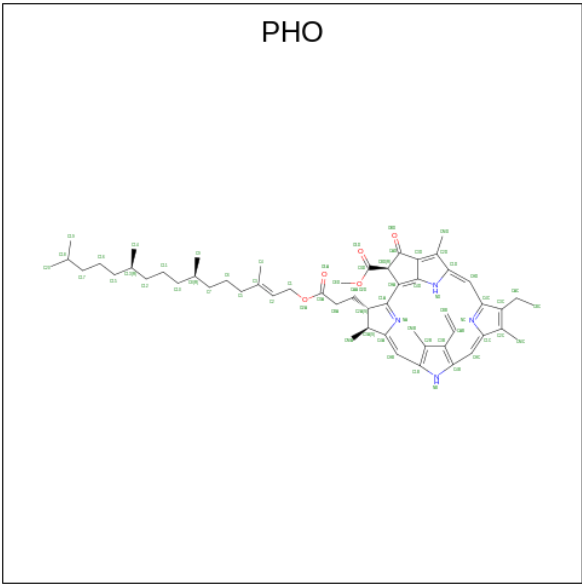
Mol	Chain	Residues	Atoms	AltConf
23	a	1	Total Cl 1 1	0
23	c	1	Total Cl 1 1	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



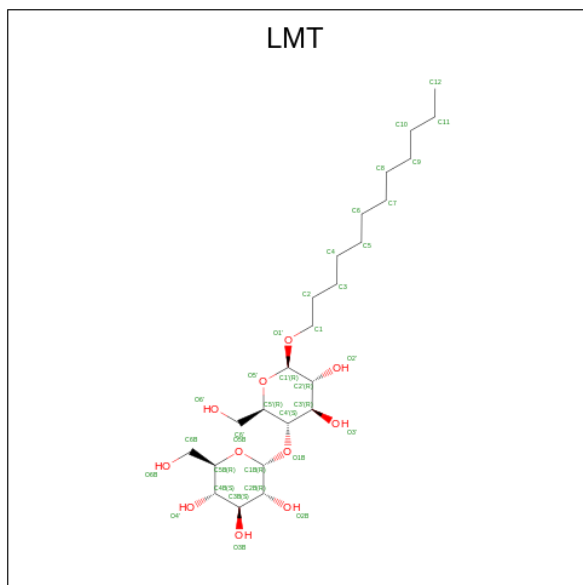
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			57	42	15	
24	h	1	Total	C	O	0
			54	39	15	
24	c	1	Total	C	O	0
			53	38	15	
24	c	1	Total	C	O	0
			47	32	15	

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
25	d	1	Total	C	N	O	0
			64	55	4	5	
25	d	1	Total	C	N	O	0
			64	55	4	5	

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

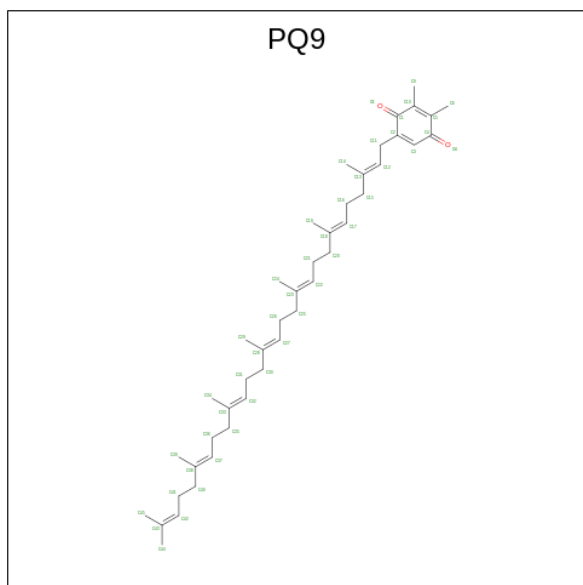


Mol	Chain	Residues	Atoms			AltConf
26	d	1	Total	C	O	0
			35	24	11	
26	m	1	Total	C	O	0
			35	24	11	
26	t	1	Total	C	O	0
			35	24	11	

- Molecule 27 is FE (II) ION (CCD ID: 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-HEPTAMETHYLOCTACO SA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: $C_{43}H_{64}O_2$).

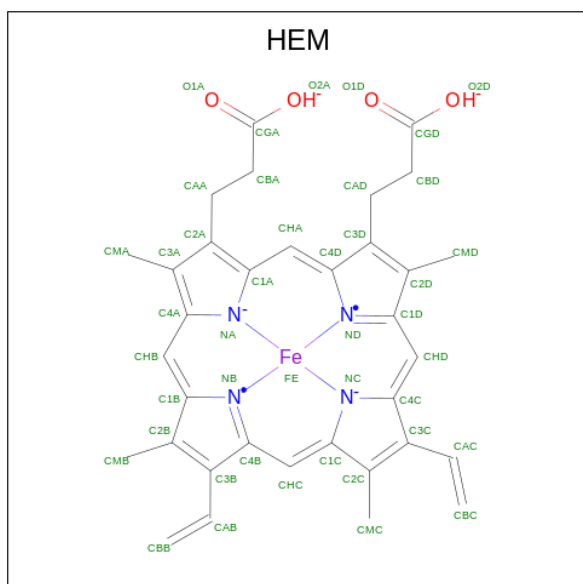


Mol	Chain	Residues	Atoms			AltConf
28	d	1	Total	C	O	0
			45	43	2	

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

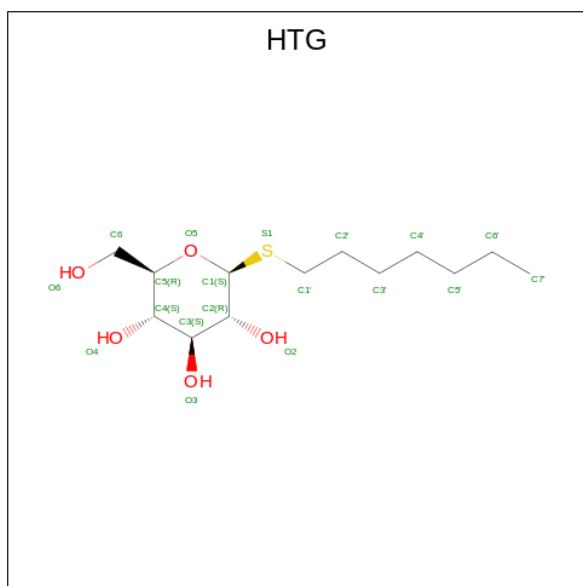
Mol	Chain	Residues	Atoms			AltConf
29	d	2	Total	C	O	0
			53	47	6	

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



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

- Molecule 31 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).

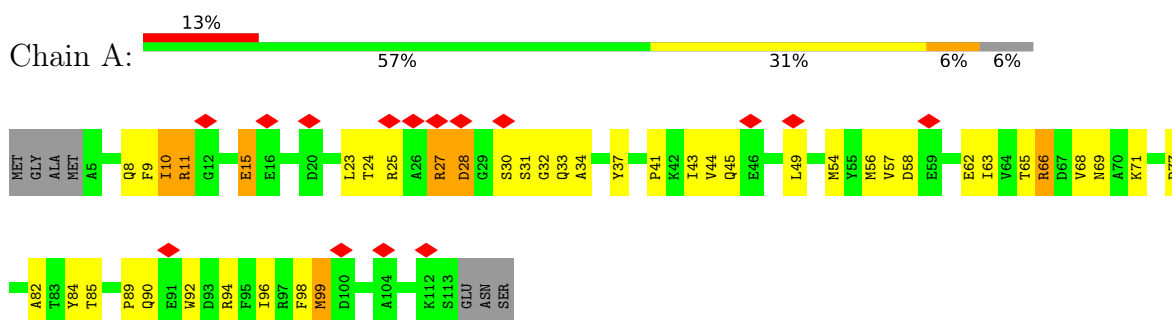


Mol	Chain	Residues	Atoms				AltConf
31	h	1	Total	C	O	S	0
			16	10	5	1	

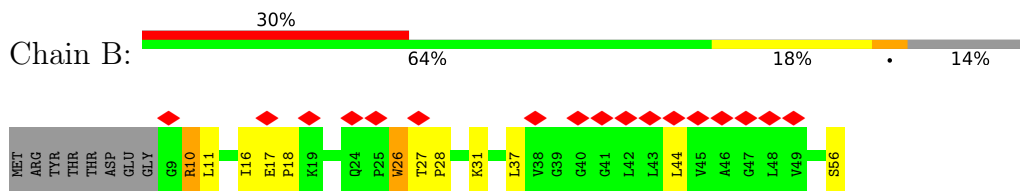
3 Residue-property plots

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.

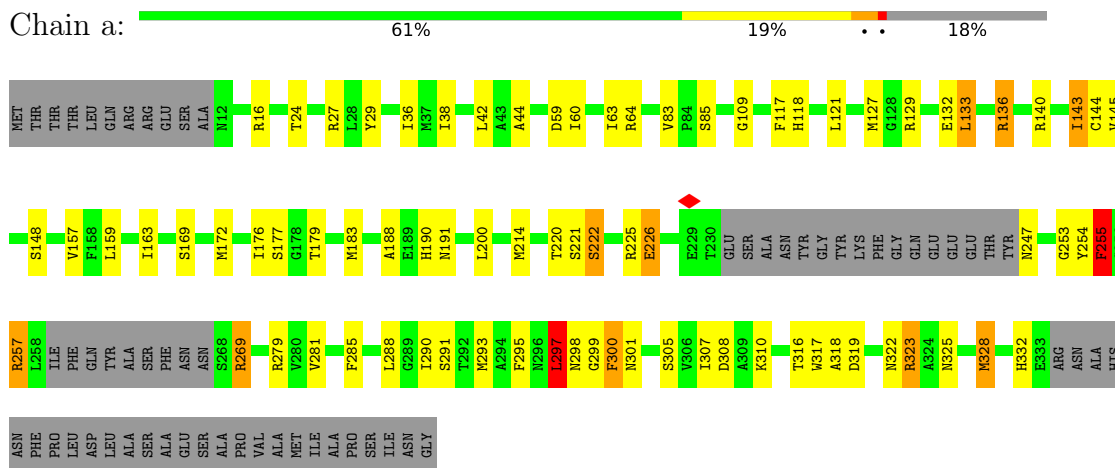
- Molecule 1: Photosystem II reaction center Psb28 protein



- Molecule 2: Tsl0063 protein

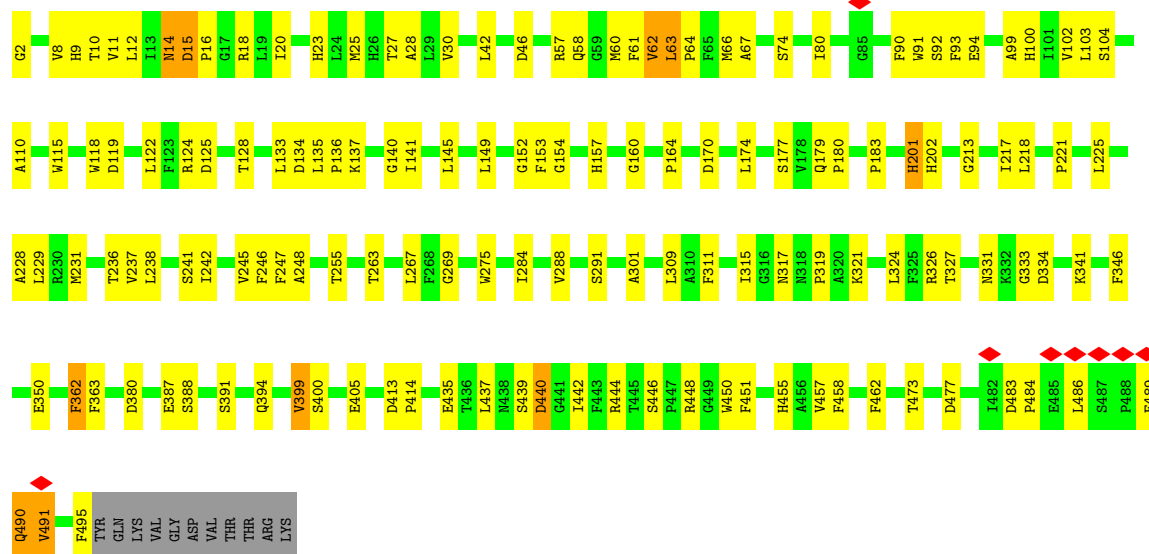


- Molecule 3: Photosystem II protein D1



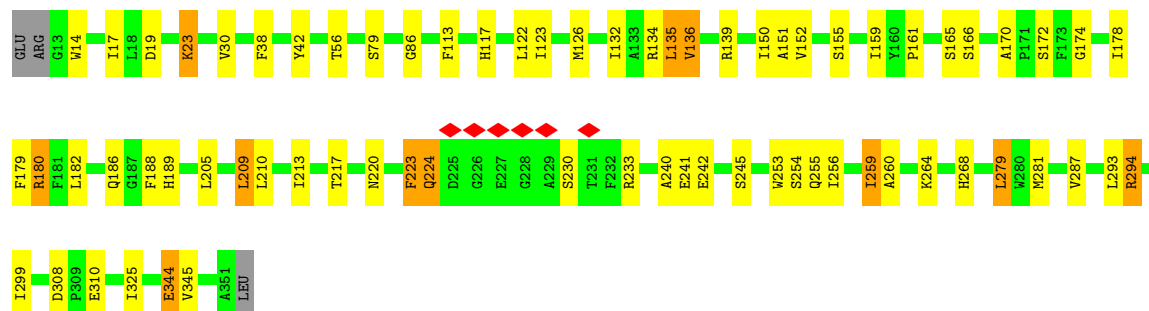
- Molecule 4: Photosystem II CP47 reaction center protein

Chain b:  69% 27% ..



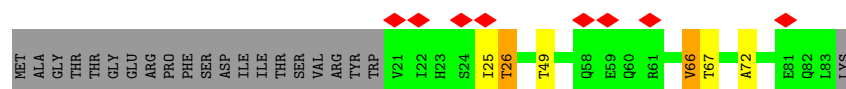
• Molecule 5: Photosystem II D2 protein

Chain d:  78% 18% ..

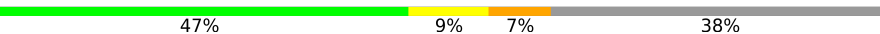


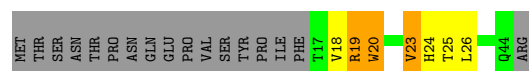
• Molecule 6: Cytochrome b559 subunit alpha

Chain e:  10% 68% 5% 25%



• Molecule 7: Cytochrome b559 subunit beta

Chain f:  47% 9% 7% 38%



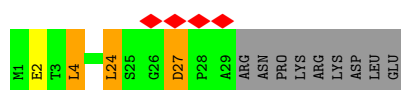
• Molecule 8: Photosystem II reaction center protein H

Chain h:  68% 23% • • 5%



• Molecule 9: Photosystem II reaction center protein I

Chain i:  11% 66% • 8% 24%



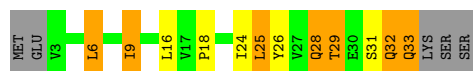
• Molecule 10: Photosystem II reaction center protein L

Chain l:  11% 59% 32% 8%



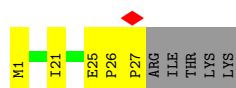
• Molecule 11: Photosystem II reaction center protein M

Chain m:  53% 14% 19% 14%



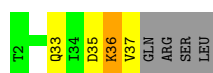
• Molecule 12: Photosystem II reaction center protein T

Chain t:  69% 16% 16%



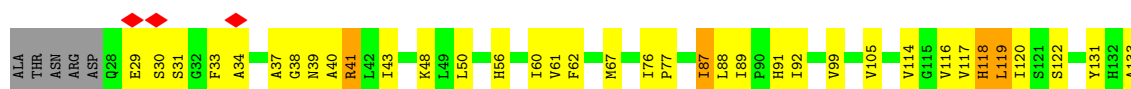
• Molecule 13: Photosystem II reaction center protein X

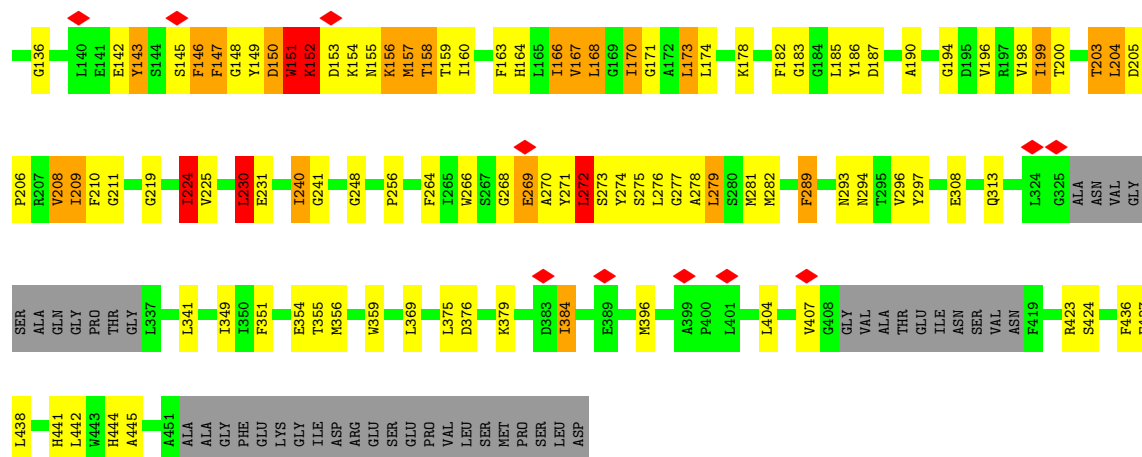
Chain x:  80% 8% • 10%



• Molecule 14: Photosystem II CP43 reaction center protein

Chain c:  58% 24% 6% • 11%

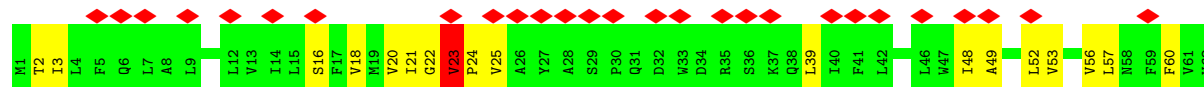
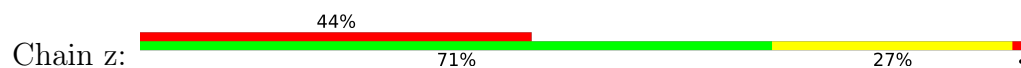




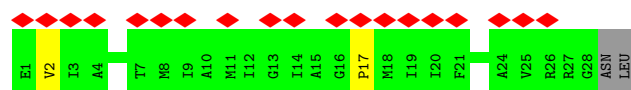
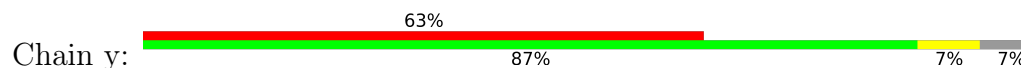
• Molecule 15: Photosystem II reaction center protein K



• Molecule 16: Photosystem II reaction center protein Z



• Molecule 17: Photosystem II reaction center protein Ycf12



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 ($\text{\AA}$)	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 ($\text{\AA}$)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, PQ9, CL, DGD, PHO, HTG, LMT, FE2, CLA, HEM, MGE, SQD, UNL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/892	0.76	0/1202
2	B	0.27	0/355	0.72	1/484 (0.2%)
3	a	0.36	0/2376	0.74	2/3239 (0.1%)
4	b	0.36	0/4025	0.67	6/5486 (0.1%)
5	d	0.40	0/2789	0.69	1/3803 (0.0%)
6	e	0.27	0/523	0.60	0/714
7	f	0.37	0/225	0.79	0/308
8	h	0.36	0/506	0.70	0/690
9	i	0.38	0/237	0.90	1/322 (0.3%)
10	l	0.32	0/311	0.73	1/422 (0.2%)
11	m	0.46	0/248	1.01	2/339 (0.6%)
12	t	0.28	0/239	0.50	0/324
13	x	0.26	0/264	0.60	0/358
14	c	0.36	0/3237	0.79	7/4408 (0.2%)
15	k	0.34	0/274	1.12	3/379 (0.8%)
16	z	0.28	0/466	0.70	1/641 (0.2%)
17	y	0.39	0/136	1.05	1/187 (0.5%)
18	C	0.41	0/114	0.76	0/158
All	All	0.37	0/17217	0.73	26/23464 (0.1%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	k	25	LEU	CA-C-N	8.36	130.29	119.84
15	k	25	LEU	C-N-CA	8.36	130.29	119.84
5	d	242	GLU	N-CA-C	-8.28	104.05	114.56
11	m	16	LEU	CA-C-N	7.76	125.13	120.24
11	m	16	LEU	C-N-CA	7.76	125.13	120.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	875	0	839	83	0
2	B	349	0	368	18	0
3	a	2304	0	2235	119	0
4	b	3886	0	3741	198	0
5	d	2694	0	2588	94	0
6	e	509	0	499	3	0
7	f	219	0	228	6	0
8	h	493	0	513	30	0
9	i	231	0	243	4	0
10	l	304	0	316	14	0
11	m	244	0	256	15	0
12	t	230	0	231	4	0
13	x	261	0	291	2	0
14	c	3130	0	3059	231	0
15	k	264	0	269	25	0
16	z	455	0	474	16	0
17	y	137	0	72	0	0
18	C	115	0	114	3	0
19	B	48	0	72	8	0
19	b	89	0	127	9	0
19	c	48	0	69	0	0
19	d	48	0	71	11	0
19	f	47	0	67	0	0
19	m	48	0	72	1	0
20	a	26	0	16	0	0
20	l	47	0	61	3	0
21	a	181	0	185	13	0
21	b	932	0	988	109	0
21	c	613	0	573	128	0
21	d	176	0	172	16	0
21	h	41	0	29	0	0
21	k	46	0	33	1	0
22	a	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	b	120	0	168	12	0
22	c	80	0	112	49	0
22	d	40	0	56	2	0
22	h	40	0	56	2	0
22	z	40	0	56	4	0
23	a	1	0	0	2	0
23	c	1	0	0	1	0
24	a	57	0	72	5	0
24	c	100	0	112	3	0
24	h	54	0	66	3	0
25	d	128	0	148	16	0
26	d	35	0	46	1	0
26	m	35	0	46	0	0
26	t	35	0	46	2	0
27	d	1	0	0	0	0
28	d	45	0	64	6	0
29	d	53	0	0	2	0
30	e	43	0	30	1	0
31	h	16	0	17	10	0
All	All	20054	0	20022	901	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 22.

The worst 5 of 901 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)
3:a:293:MET:HE1	3:a:298:ASN:CB	1.23	1.64
14:c:157:MET:HE1	14:c:271:TYR:CD2	1.46	1.49
3:a:269:ARG:CD	5:d:240:ALA:HB2	1.46	1.45
21:b:606:CLA:H201	19:b:620:MGE:C6A	1.51	1.40
14:c:157:MET:HE1	14:c:271:TYR:CE2	1.54	1.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/116 (92%)	95 (89%)	11 (10%)	1 (1%)	14	41
2	B	46/56 (82%)	44 (96%)	2 (4%)	0	100	100
3	a	291/360 (81%)	279 (96%)	10 (3%)	2 (1%)	18	47
4	b	492/505 (97%)	470 (96%)	21 (4%)	1 (0%)	43	70
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%)	7	27
9	i	27/38 (71%)	25 (93%)	2 (7%)	0	100	100
10	l	35/37 (95%)	31 (89%)	2 (6%)	2 (6%)	1	7
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%)	4	19
15	k	32/46 (70%)	26 (81%)	4 (12%)	2 (6%)	1	6
16	z	60/62 (97%)	48 (80%)	10 (17%)	2 (3%)	3	14
17	y	26/30 (87%)	20 (77%)	5 (19%)	1 (4%)	2	13
18	C	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
All	All	2106/2368 (89%)	1950 (93%)	134 (6%)	22 (1%)	15	38

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

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Mol	Chain	Res	Type
16	z	23	VAL

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	92/97 (95%)	84 (91%)	8 (9%)	9	30
2	B	34/42 (81%)	32 (94%)	2 (6%)	18	44
3	a	236/290 (81%)	215 (91%)	21 (9%)	9	29
4	b	392/403 (97%)	380 (97%)	12 (3%)	35	60
5	d	272/277 (98%)	258 (95%)	14 (5%)	21	48
6	e	55/73 (75%)	52 (94%)	3 (6%)	19	46
7	f	22/39 (56%)	17 (77%)	5 (23%)	1	4
8	h	53/54 (98%)	48 (91%)	5 (9%)	8	28
9	i	26/35 (74%)	23 (88%)	3 (12%)	5	20
10	l	35/35 (100%)	30 (86%)	5 (14%)	3	13
11	m	28/33 (85%)	20 (71%)	8 (29%)	0	1
12	t	24/29 (83%)	24 (100%)	0	100	100
13	x	29/33 (88%)	26 (90%)	3 (10%)	7	24
14	c	312/352 (89%)	275 (88%)	37 (12%)	5	19
15	k	27/37 (73%)	21 (78%)	6 (22%)	1	4
16	z	45/52 (86%)	44 (98%)	1 (2%)	45	67
All	All	1682/1881 (89%)	1549 (92%)	133 (8%)	13	34

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	c	204	LEU
14	c	240	ILE
15	k	27	VAL
5	d	209	LEU

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Mol	Chain	Res	Type
5	d	180	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
6	e	82	GLN
14	c	441	HIS
7	f	41	GLN
14	c	293	ASN
3	a	247	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	c	506	-	50,54,73	2.34	18 (36%)	60,90,113	4.94	29 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	c	508	14	50,54,73	2.61	19 (38%)	60,90,113	3.20	30 (50%)
26	LMT	d	404	-	36,36,36	0.44	0	47,47,47	0.83	1 (2%)
21	CLA	b	610	-	69,73,73	2.06	15 (21%)	83,113,113	2.37	30 (36%)
20	SQD	l	101	-	46,47,54	1.30	4 (8%)	55,58,65	3.86	9 (16%)
21	CLA	b	607	-	69,73,73	2.12	18 (26%)	83,113,113	2.21	24 (28%)
21	CLA	d	407	-	54,58,73	2.21	16 (29%)	65,95,113	4.41	35 (53%)
19	MGE	b	619	-	48,48,48	0.99	2 (4%)	56,56,56	1.18	5 (8%)
21	CLA	c	505	14	69,73,73	2.48	20 (28%)	83,113,113	2.38	28 (33%)
21	CLA	c	509	-	67,71,73	2.41	22 (32%)	80,110,113	2.64	31 (38%)
22	BCR	b	617	-	41,41,41	0.69	0	56,56,56	1.86	15 (26%)
30	HEM	e	101	-	50,50,50	1.54	8 (16%)	66,82,82	1.68	14 (21%)
21	CLA	b	613	-	56,60,73	2.10	16 (28%)	67,97,113	3.24	38 (56%)
21	CLA	c	513	-	54,58,73	2.31	16 (29%)	65,95,113	4.29	38 (58%)
24	DGD	c	516	14	54,54,67	0.99	2 (3%)	68,68,81	1.48	14 (20%)
22	BCR	c	515	-	41,41,41	0.82	1 (2%)	56,56,56	2.60	20 (35%)
21	CLA	b	605	-	69,73,73	2.32	20 (28%)	83,113,113	2.55	28 (33%)
19	MGE	d	410	5	48,48,48	0.95	2 (4%)	56,56,56	1.28	5 (8%)
24	DGD	c	517	-	48,48,67	1.02	2 (4%)	62,62,81	1.11	5 (8%)
21	CLA	c	504	-	69,73,73	2.20	19 (27%)	83,113,113	2.77	30 (36%)
21	CLA	b	609	-	69,73,73	2.16	18 (26%)	83,113,113	2.65	25 (30%)
22	BCR	d	409	-	41,41,41	0.69	0	56,56,56	1.73	9 (16%)
21	CLA	d	402	-	69,73,73	2.00	21 (30%)	83,113,113	2.37	26 (31%)
22	BCR	b	616	-	41,41,41	0.71	0	56,56,56	1.89	20 (35%)
21	CLA	c	510	14	50,54,73	2.76	22 (44%)	60,90,113	3.01	31 (51%)
26	LMT	t	301	-	36,36,36	0.49	0	47,47,47	0.89	1 (2%)
25	PHO	d	403	-	58,69,69	2.58	15 (25%)	56,99,99	2.96	18 (32%)
21	CLA	c	511	14	69,73,73	2.14	20 (28%)	83,113,113	2.22	27 (32%)
21	CLA	b	614	4	69,73,73	2.07	18 (26%)	83,113,113	2.57	30 (36%)
26	LMT	m	101	-	36,36,36	0.47	0	47,47,47	0.95	3 (6%)
31	HTG	h	102	-	16,16,19	1.18	2 (12%)	20,21,24	1.68	1 (5%)
22	BCR	b	618	-	41,41,41	0.71	0	56,56,56	2.04	17 (30%)
21	CLA	b	602	-	69,73,73	2.08	19 (27%)	83,113,113	2.70	29 (34%)
21	CLA	b	615	4	50,54,73	2.54	19 (38%)	60,90,113	2.87	27 (45%)
21	CLA	b	603	-	69,73,73	2.13	20 (28%)	83,113,113	2.58	28 (33%)
24	DGD	a	406	-	58,58,67	0.91	2 (3%)	72,72,81	1.00	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	b	611	4	69,73,73	2.21	18 (26%)	83,113,113	2.58	27 (32%)
21	CLA	a	407	-	69,73,73	1.83	18 (26%)	83,113,113	2.47	35 (42%)
21	CLA	a	403	-	55,59,73	2.18	19 (34%)	66,96,113	2.96	32 (48%)
28	PQ9	d	408	-	45,45,45	0.69	1 (2%)	56,57,57	1.49	13 (23%)
22	BCR	z	101	-	41,41,41	0.70	0	56,56,56	2.06	16 (28%)
19	MGE	B	101	-	48,48,48	0.94	2 (4%)	56,56,56	1.29	6 (10%)
21	CLA	b	608	-	69,73,73	2.39	22 (31%)	83,113,113	2.09	23 (27%)
24	DGD	h	104	-	55,55,67	0.92	2 (3%)	69,69,81	1.06	4 (5%)
21	CLA	d	406	-	65,69,73	1.95	13 (20%)	78,108,113	4.10	36 (46%)
19	MGE	f	101	-	47,47,48	0.99	2 (4%)	55,55,56	1.33	7 (12%)
21	CLA	b	612	4	58,62,73	2.13	18 (31%)	69,99,113	2.61	24 (34%)
19	MGE	b	620	-	41,41,48	1.03	2 (4%)	49,49,56	1.20	6 (12%)
21	CLA	h	101	8	45,49,73	2.44	17 (37%)	54,84,113	4.93	30 (55%)
22	BCR	h	103	-	41,41,41	0.75	0	56,56,56	1.93	15 (26%)
21	CLA	a	402	-	69,73,73	1.92	17 (24%)	83,113,113	2.43	28 (33%)
19	MGE	m	102	-	48,48,48	0.99	2 (4%)	56,56,56	1.13	3 (5%)
21	CLA	b	604	-	69,73,73	1.99	18 (26%)	83,113,113	2.61	29 (34%)
21	CLA	k	501	15	50,54,73	2.28	17 (34%)	60,90,113	4.94	34 (56%)
21	CLA	c	507	-	55,59,73	2.24	18 (32%)	66,96,113	3.93	31 (46%)
19	MGE	c	502	14	48,48,48	0.97	2 (4%)	56,56,56	1.09	4 (7%)
22	BCR	a	404	-	41,41,41	0.70	0	56,56,56	2.29	17 (30%)
22	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.99	13 (23%)
21	CLA	c	512	-	55,59,73	2.24	17 (30%)	66,96,113	4.39	31 (46%)
20	SQD	a	401	-	25,26,54	1.68	4 (16%)	34,37,65	4.81	7 (20%)
21	CLA	b	606	-	69,73,73	2.33	18 (26%)	83,113,113	2.13	26 (31%)
21	CLA	c	503	-	69,73,73	2.08	19 (27%)	83,113,113	2.87	29 (34%)
21	CLA	b	601	-	69,73,73	2.14	17 (24%)	83,113,113	2.33	29 (34%)
25	PHO	d	401	-	58,69,69	2.30	13 (22%)	56,99,99	2.63	14 (25%)

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	c	506	-	-	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	c	508	14	-	3/17/93/115	-
26	LMT	d	404	-	-	4/21/61/61	0/2/2/2
21	CLA	b	610	-	-	6/39/115/115	-
20	SQD	l	101	-	-	7/42/62/69	0/1/1/1
21	CLA	b	607	-	-	1/39/115/115	-
21	CLA	d	407	-	-	6/21/97/115	-
19	MGE	b	619	-	-	9/43/63/63	0/1/1/1
21	CLA	c	505	14	-	2/39/115/115	-
21	CLA	c	509	-	-	7/37/113/115	-
22	BCR	b	617	-	-	0/29/63/63	0/2/2/2
30	HEM	e	101	-	-	7/14/54/54	-
21	CLA	b	613	-	-	9/24/100/115	-
21	CLA	c	513	-	-	11/21/97/115	-
24	DGD	c	516	14	-	12/42/82/95	0/2/2/2
22	BCR	c	515	-	-	4/29/63/63	0/2/2/2
21	CLA	b	605	-	-	12/39/115/115	-
19	MGE	d	410	5	-	14/43/63/63	0/1/1/1
24	DGD	c	517	-	-	8/36/76/95	0/2/2/2
21	CLA	c	504	-	-	7/39/115/115	-
21	CLA	b	609	-	-	4/39/115/115	-
22	BCR	d	409	-	-	8/29/63/63	0/2/2/2
21	CLA	d	402	-	-	5/39/115/115	-
22	BCR	b	616	-	-	0/29/63/63	0/2/2/2
21	CLA	c	510	14	-	3/17/93/115	-
26	LMT	t	301	-	-	7/21/61/61	0/2/2/2
25	PHO	d	403	-	-	2/37/103/103	0/5/6/6
21	CLA	c	511	14	-	9/39/115/115	-
21	CLA	b	614	4	-	9/39/115/115	-
26	LMT	m	101	-	-	2/21/61/61	0/2/2/2
31	HTG	h	102	-	-	0/7/27/30	0/1/1/1
22	BCR	b	618	-	-	3/29/63/63	0/2/2/2
21	CLA	b	602	-	-	4/39/115/115	-
21	CLA	b	615	4	-	2/17/93/115	-
21	CLA	b	603	-	-	7/39/115/115	-
24	DGD	a	406	-	-	19/46/86/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	611	4	-	7/39/115/115	-
21	CLA	a	407	-	-	8/39/115/115	-
21	CLA	a	403	-	-	1/23/99/115	-
28	PQ9	d	408	-	-	7/41/61/61	0/1/1/1
22	BCR	z	101	-	-	6/29/63/63	0/2/2/2
19	MGE	B	101	-	-	17/43/63/63	0/1/1/1
21	CLA	b	608	-	-	2/39/115/115	-
24	DGD	h	104	-	-	13/43/83/95	0/2/2/2
21	CLA	d	406	-	1/1/14/20	9/35/111/115	-
19	MGE	f	101	-	-	3/42/62/63	0/1/1/1
21	CLA	b	612	4	-	0/26/102/115	-
19	MGE	b	620	-	-	6/36/56/63	0/1/1/1
21	CLA	h	101	8	-	4/10/86/115	-
22	BCR	h	103	-	-	7/29/63/63	0/2/2/2
21	CLA	a	402	-	-	5/39/115/115	-
19	MGE	m	102	-	-	10/43/63/63	0/1/1/1
21	CLA	b	604	-	-	4/39/115/115	-
21	CLA	k	501	15	-	9/17/93/115	-
21	CLA	c	507	-	-	12/23/99/115	-
19	MGE	c	502	14	-	13/43/63/63	0/1/1/1
22	BCR	a	404	-	-	10/29/63/63	0/2/2/2
22	BCR	c	514	-	-	8/29/63/63	0/2/2/2
21	CLA	c	512	-	-	10/23/99/115	-
20	SQD	a	401	-	-	4/19/39/69	0/1/1/1
21	CLA	b	606	-	-	2/39/115/115	-
21	CLA	c	503	-	-	4/39/115/115	-
21	CLA	b	601	-	-	4/39/115/115	-
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6

The worst 5 of 692 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
25	d	403	PHO	C1B-C2B	8.99	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	506	CLA	C1D-ND	8.70	1.48	1.37

The worst 5 of 1294 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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	d	406	CLA	C8

5 of 406 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.

57 monomers are involved in 369 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	c	506	CLA	4	0
21	c	508	CLA	4	0
26	d	404	LMT	1	0
21	b	610	CLA	2	0
20	l	101	SQD	3	0
21	b	607	CLA	3	0
19	b	619	MGE	6	0
21	c	505	CLA	10	0
21	c	509	CLA	10	0
22	b	617	BCR	1	0
30	e	101	HEM	1	0
21	b	613	CLA	5	0

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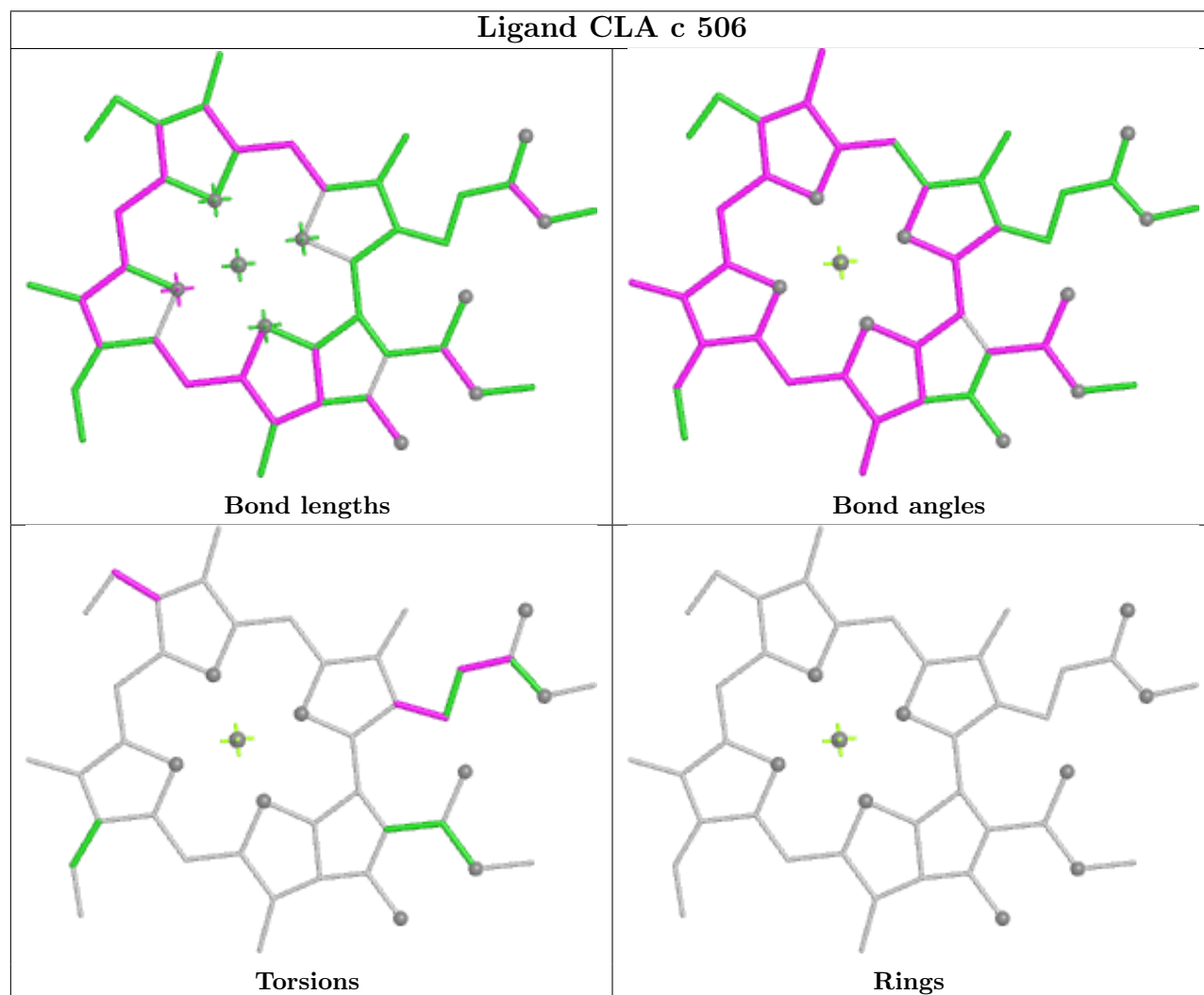
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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24	c	516	DGD	3	0
22	c	515	BCR	48	0
21	b	605	CLA	34	0
19	d	410	MGE	11	0
21	c	504	CLA	3	0
21	b	609	CLA	6	0
22	d	409	BCR	2	0
21	d	402	CLA	2	0
22	b	616	BCR	2	0
21	c	510	CLA	22	0
26	t	301	LMT	2	0
25	d	403	PHO	12	0
21	c	511	CLA	18	0
21	b	614	CLA	9	0
31	h	102	HTG	10	0
22	b	618	BCR	9	0
21	b	602	CLA	5	0
21	b	615	CLA	2	0
21	b	603	CLA	14	0
24	a	406	DGD	5	0
21	b	611	CLA	9	0
21	a	407	CLA	2	0
21	a	403	CLA	4	0
28	d	408	PQ9	6	0
22	z	101	BCR	4	0
19	B	101	MGE	8	0
21	b	608	CLA	1	0
24	h	104	DGD	3	0
21	d	406	CLA	14	0
21	b	612	CLA	5	0
19	b	620	MGE	3	0
22	h	103	BCR	2	0
21	a	402	CLA	7	0
19	m	102	MGE	1	0
21	b	604	CLA	7	0
21	k	501	CLA	1	0
21	c	507	CLA	26	0
22	a	404	BCR	2	0
22	c	514	BCR	1	0
21	c	512	CLA	4	0
21	b	606	CLA	10	0

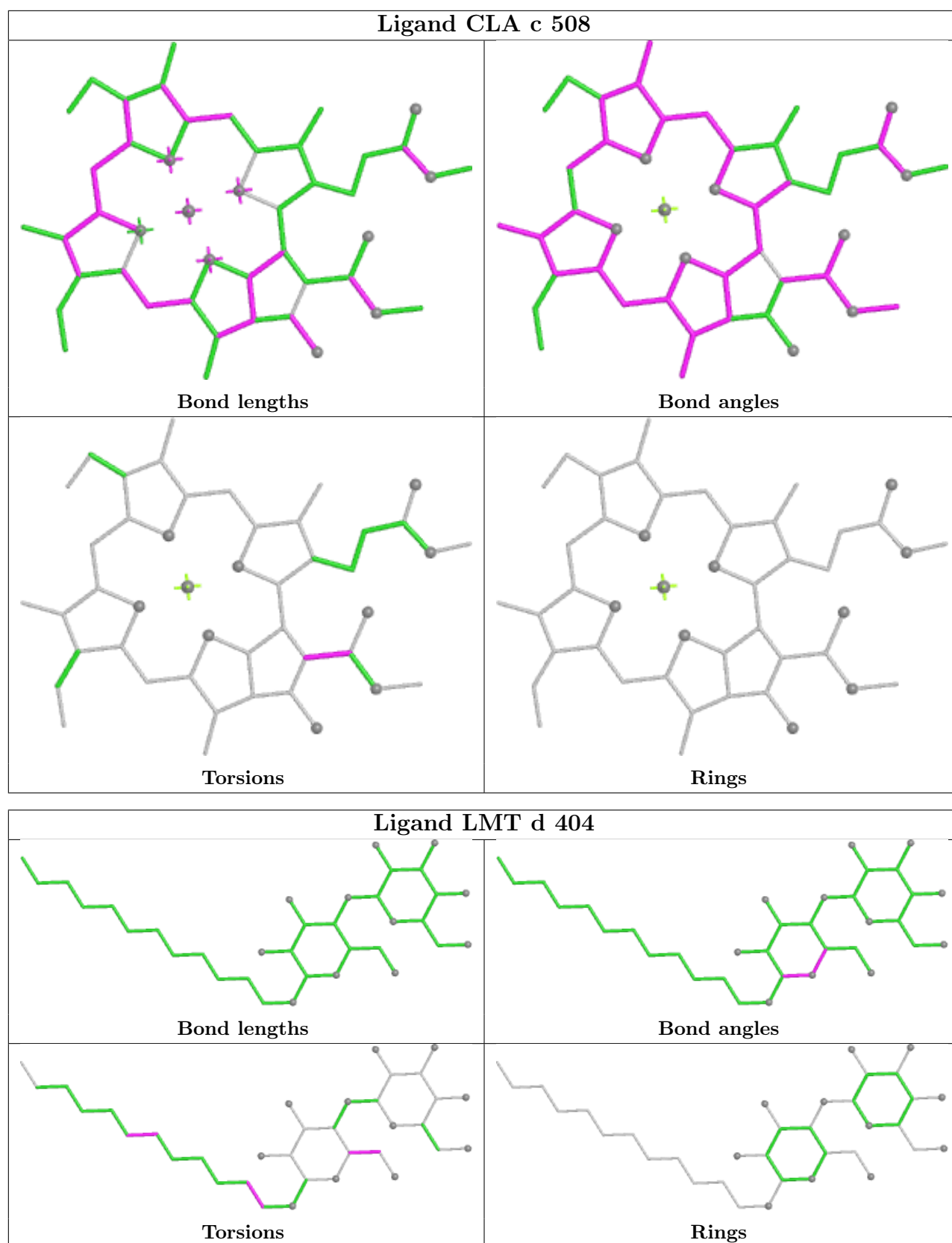
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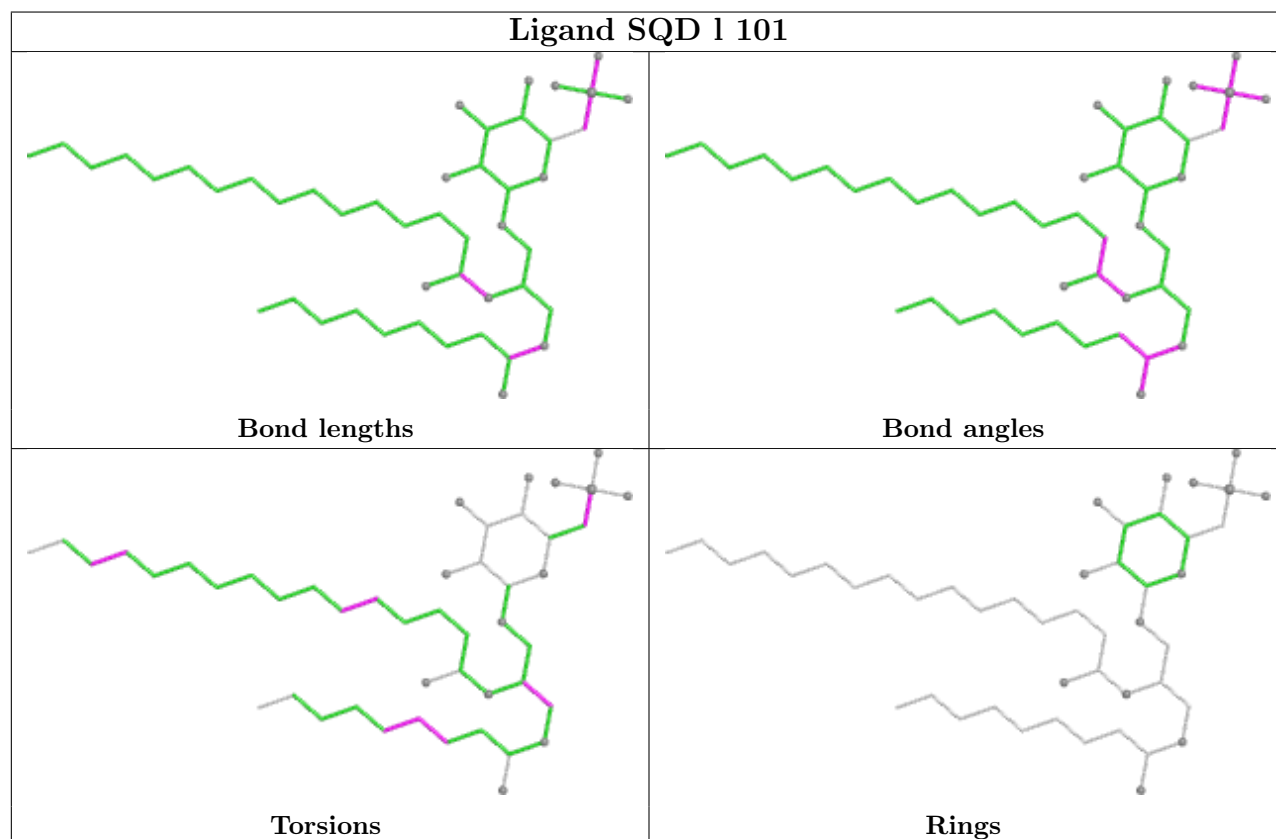
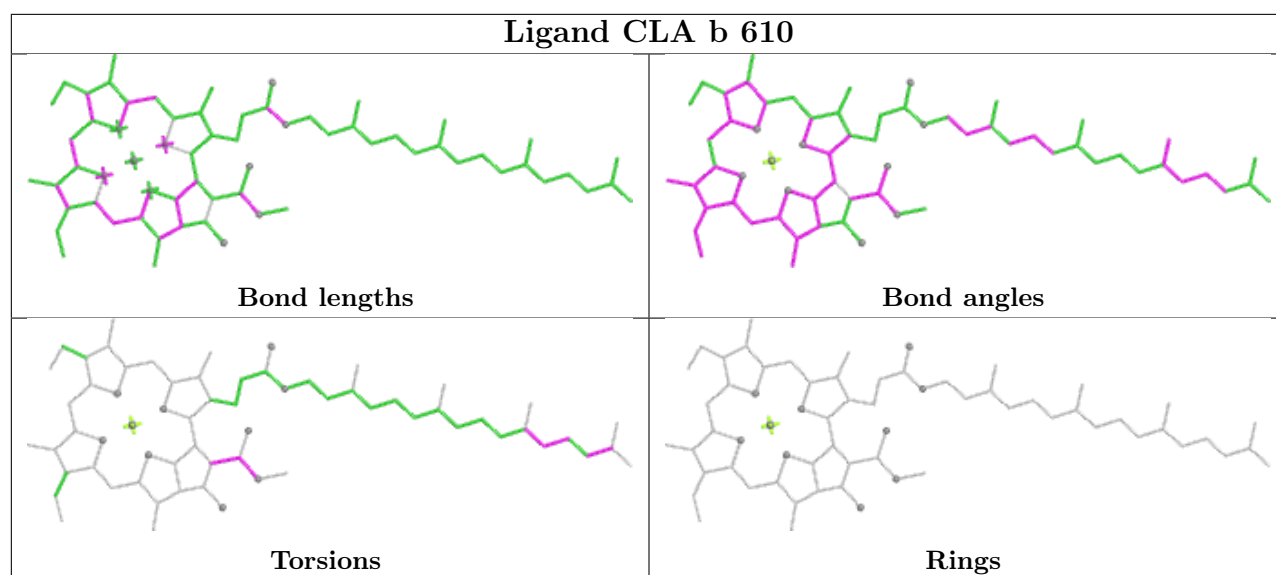
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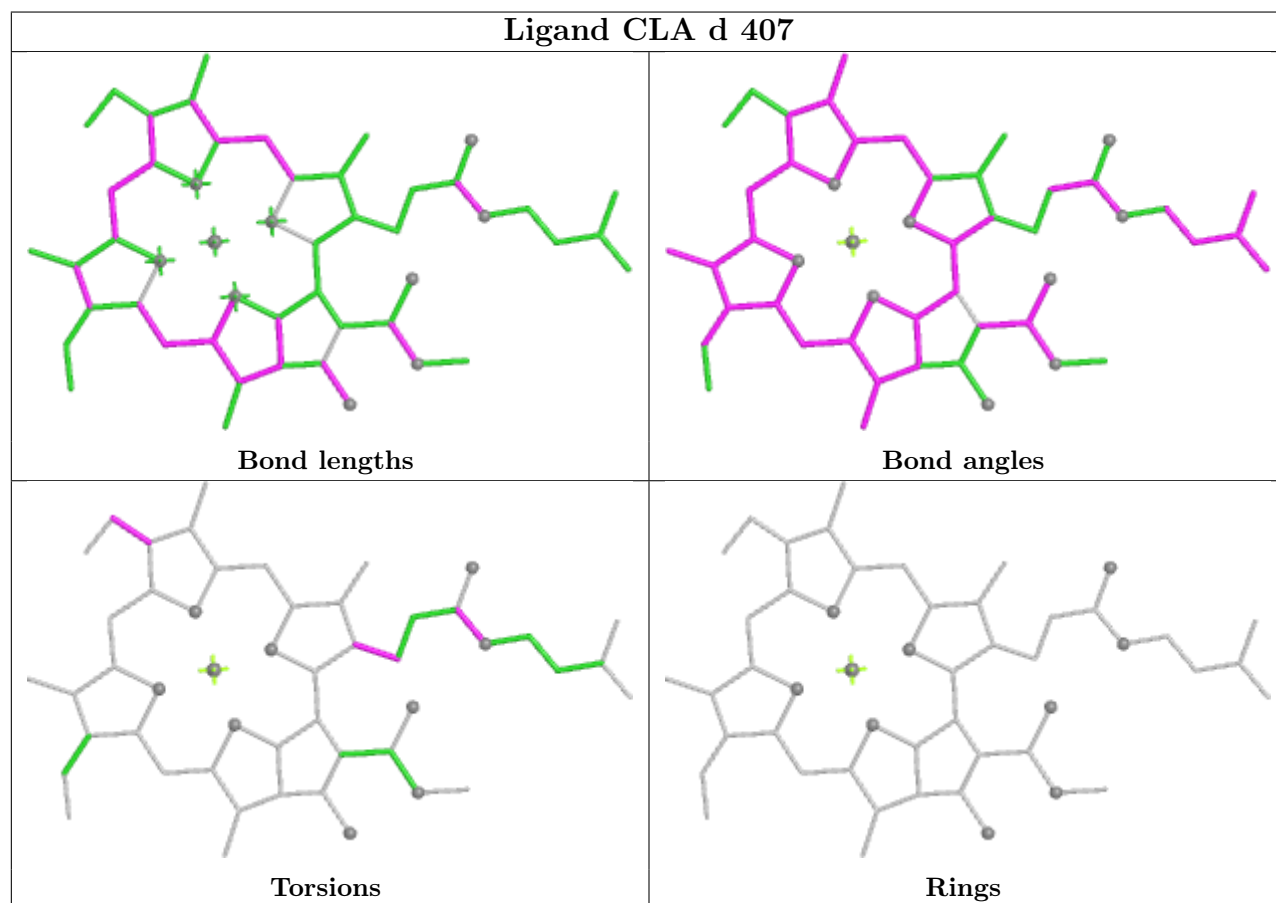
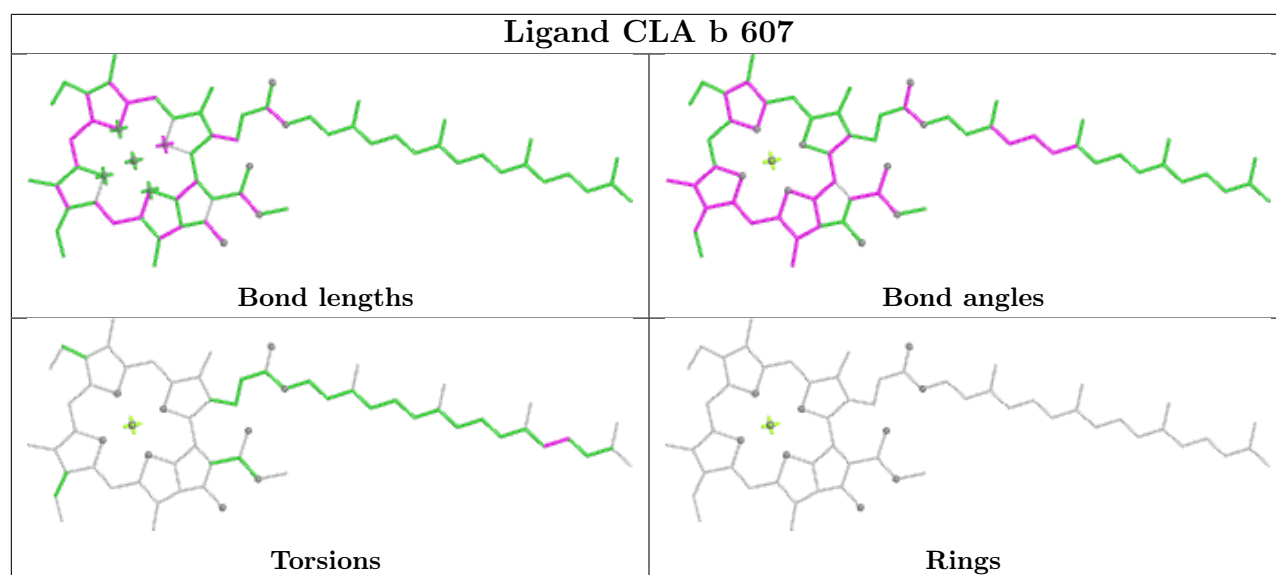
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	c	503	CLA	33	0
21	b	601	CLA	2	0
25	d	401	PHO	4	0

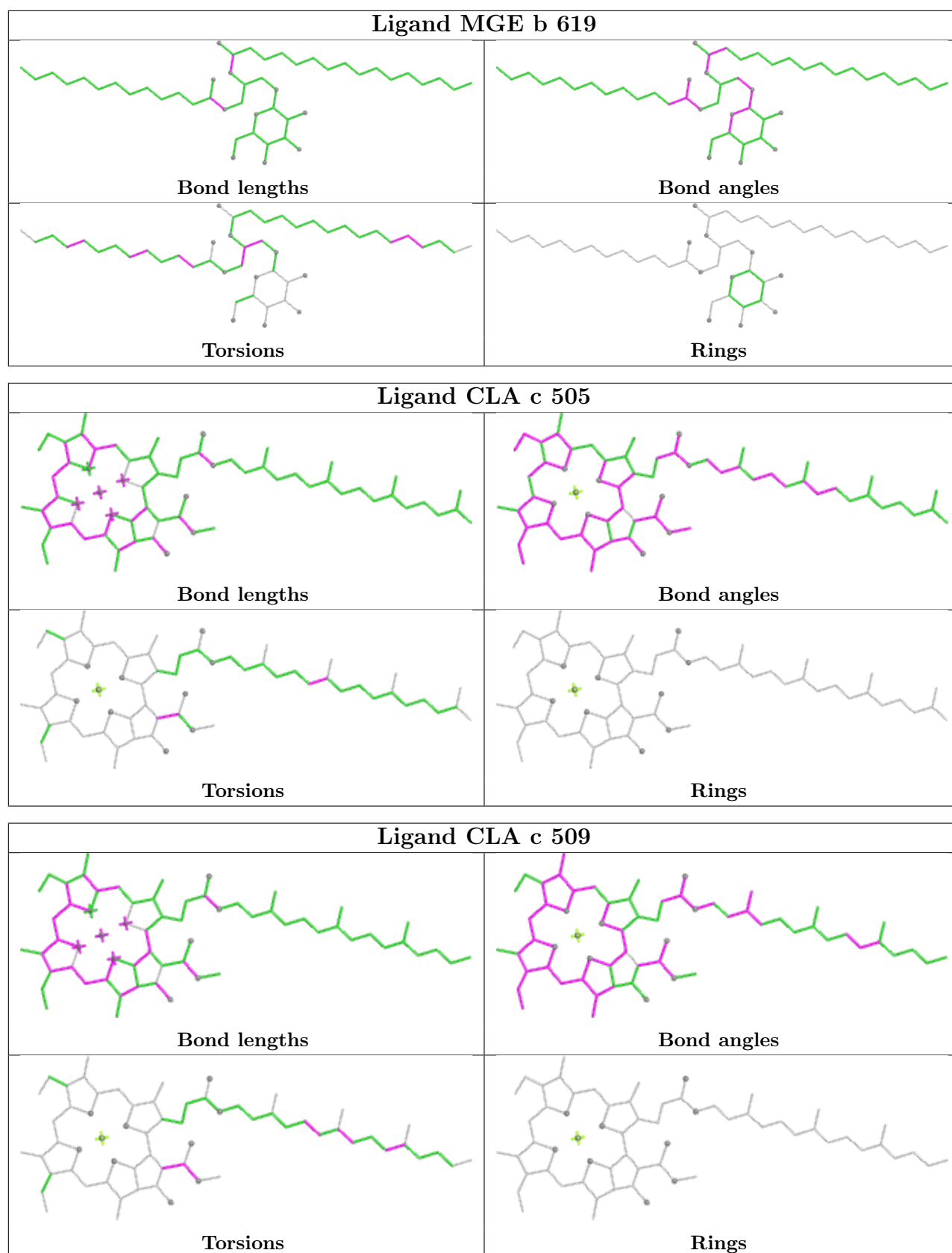
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

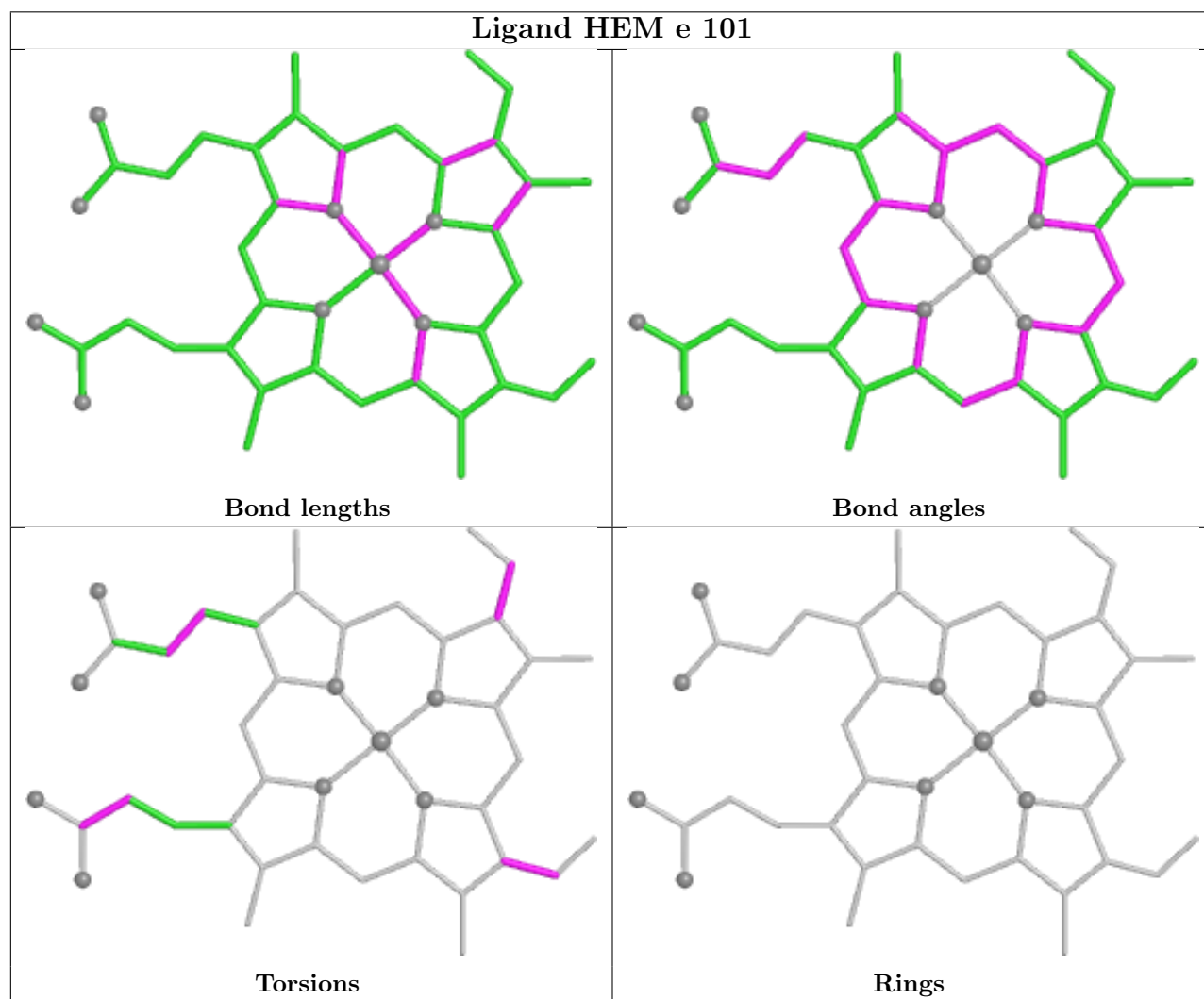
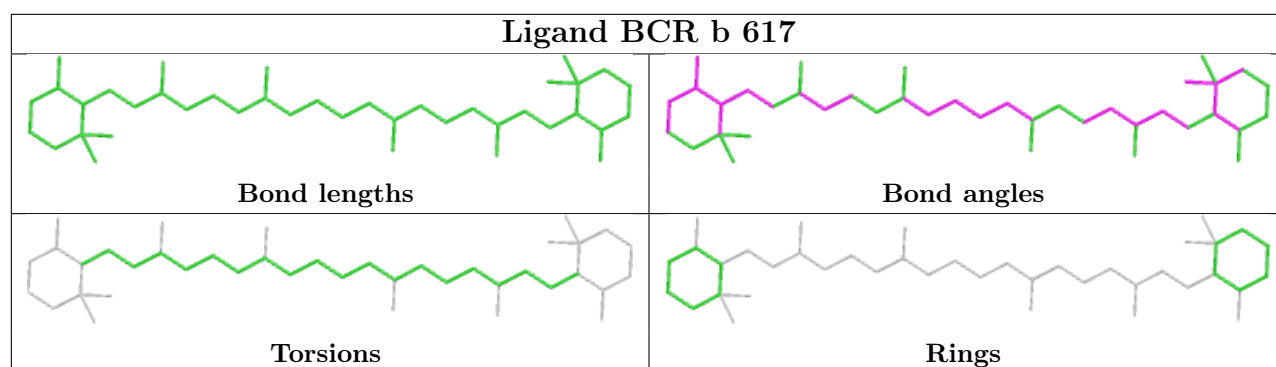




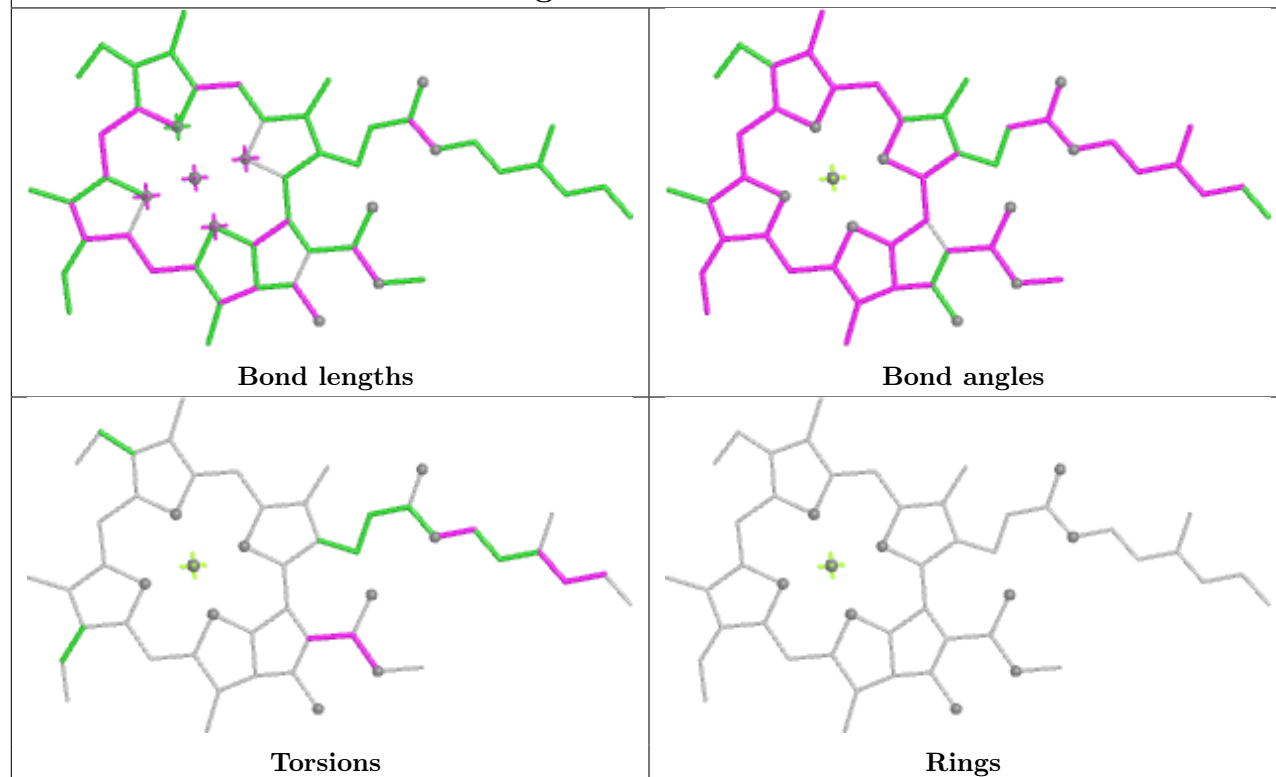




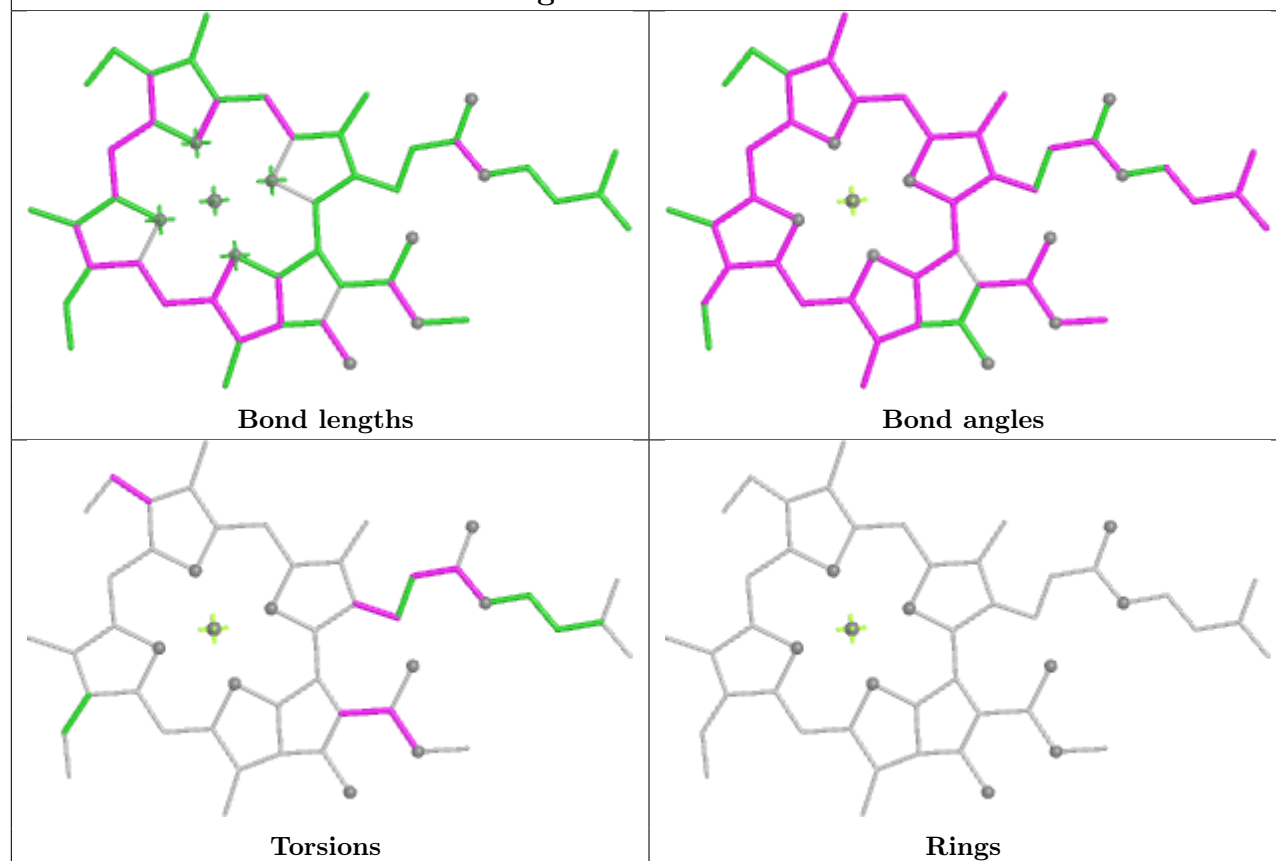


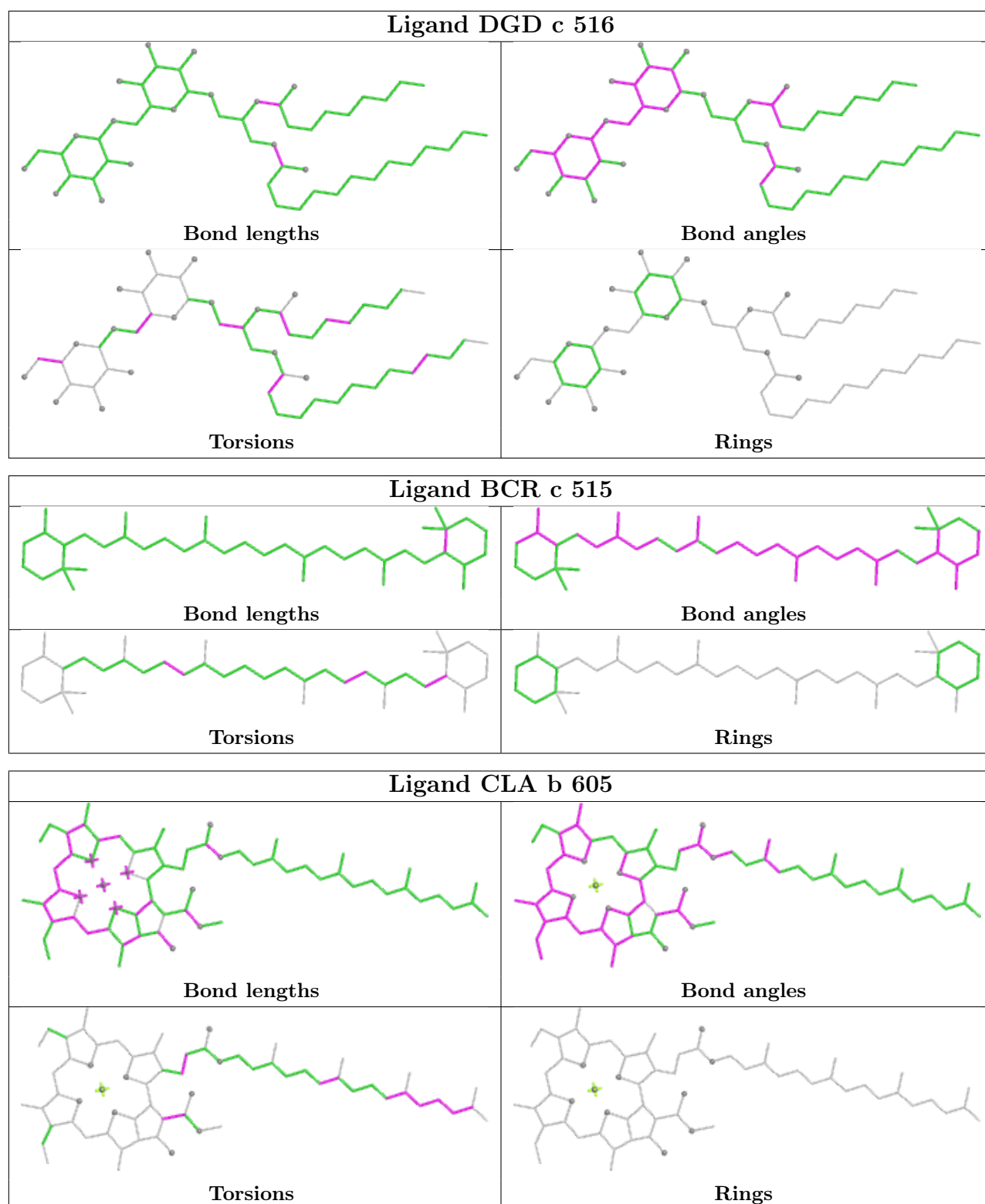


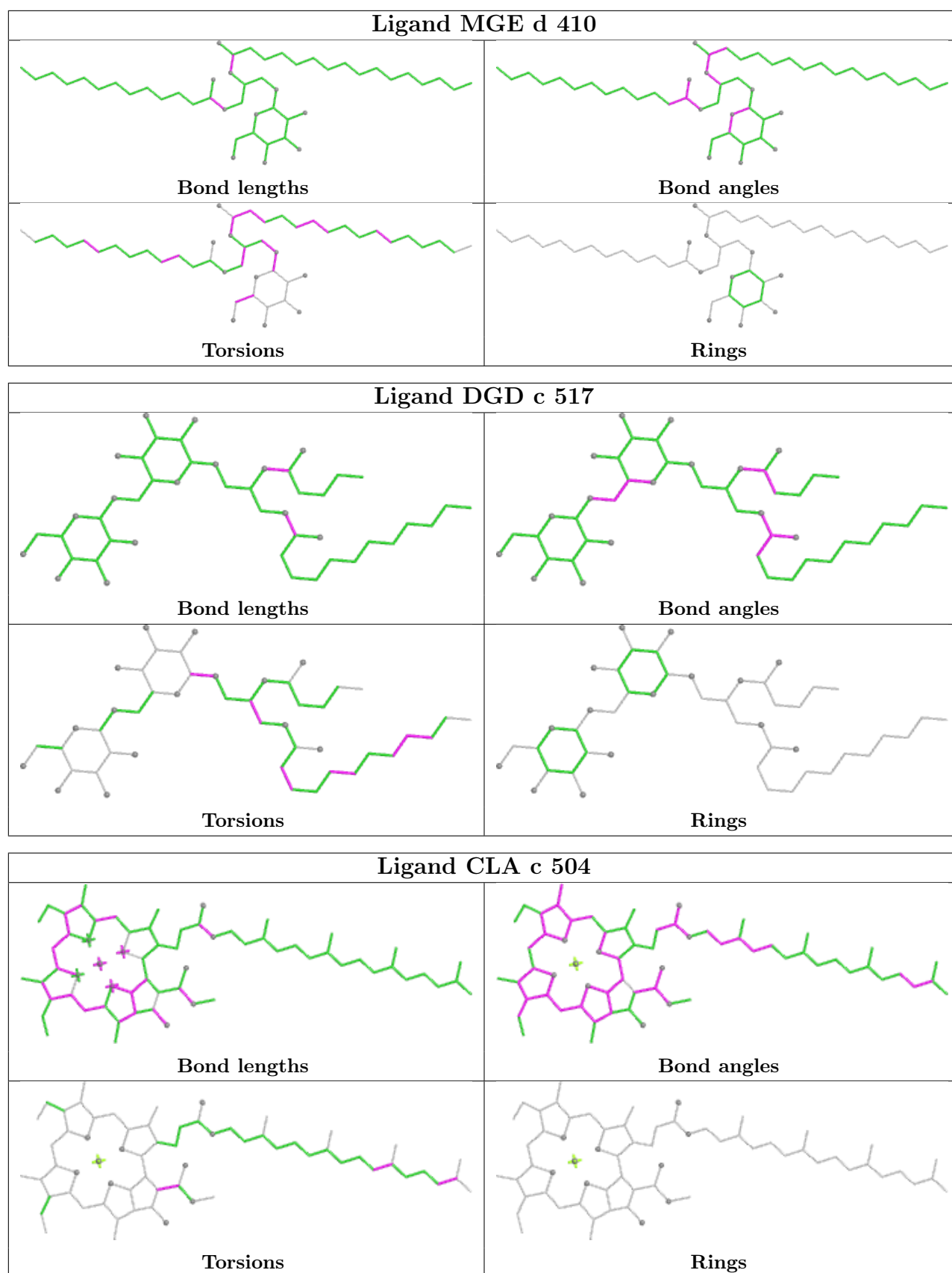
Ligand CLA b 613

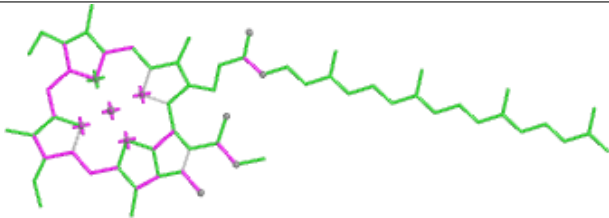
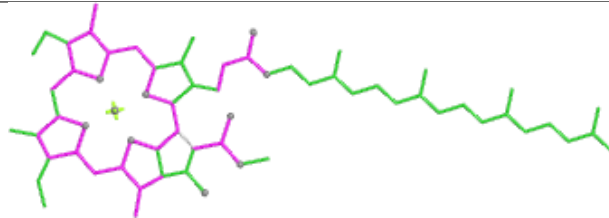
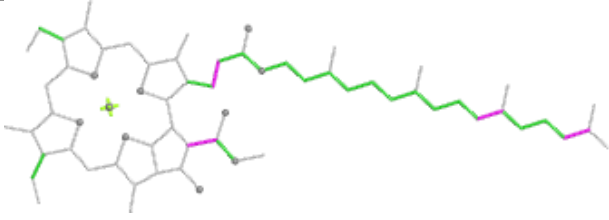
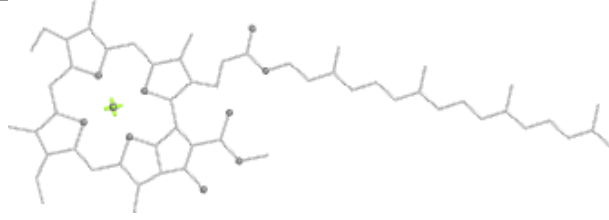


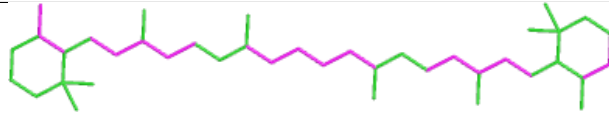
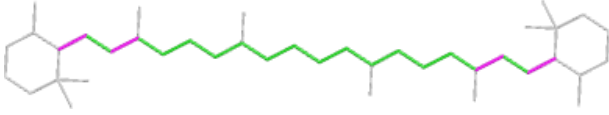
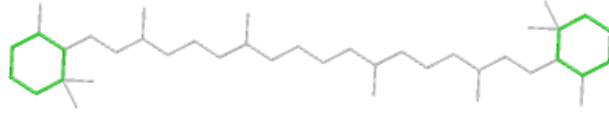
Ligand CLA c 513

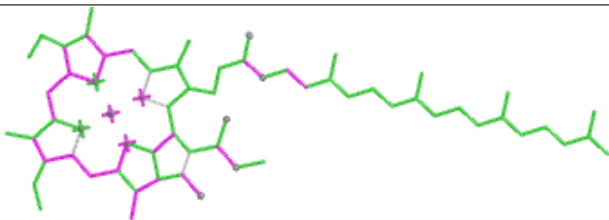
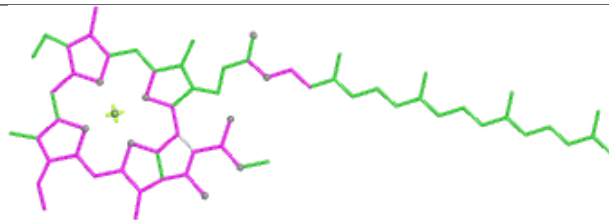
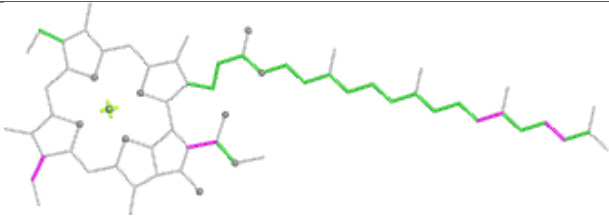
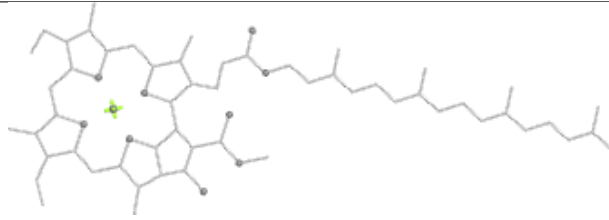


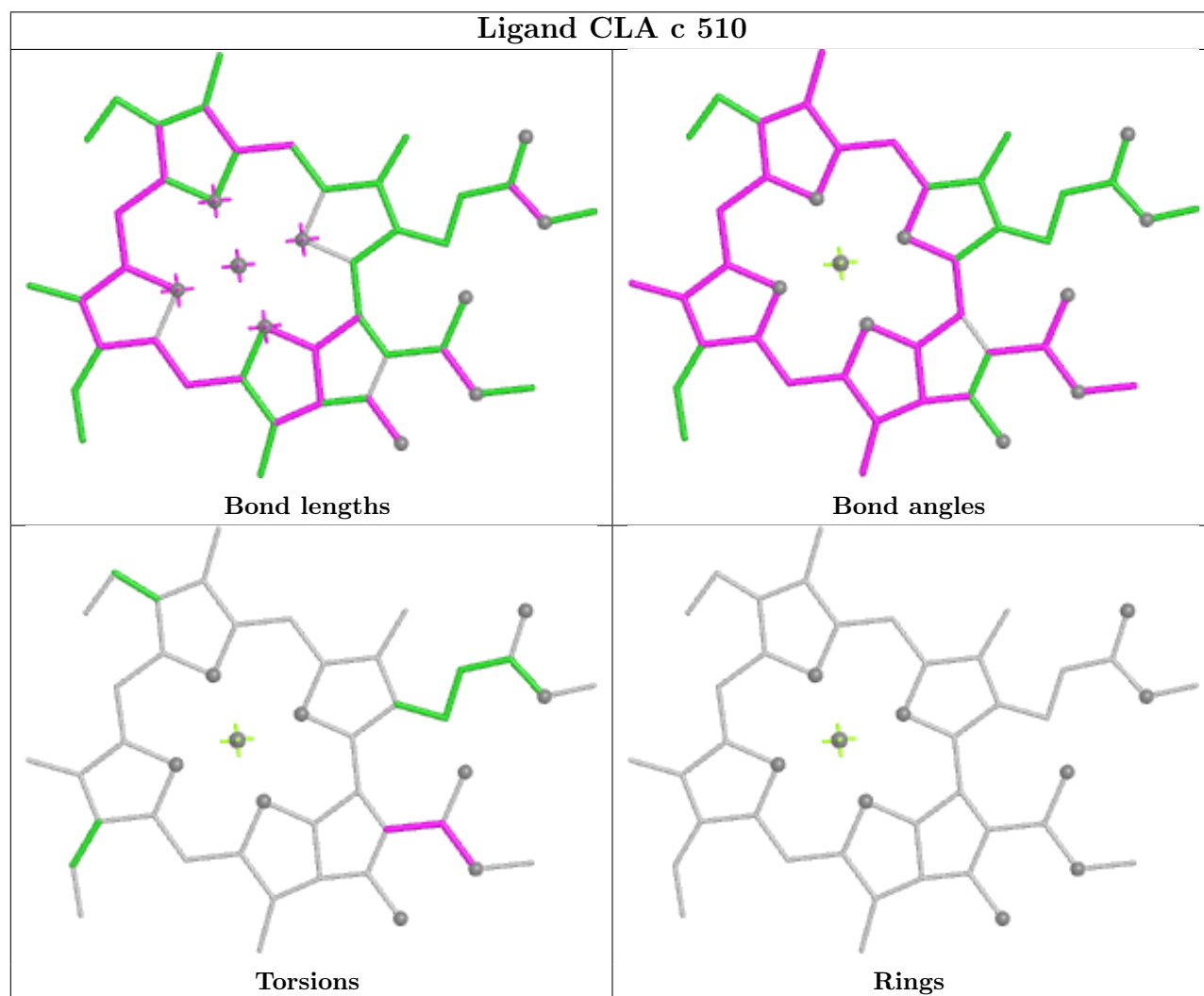
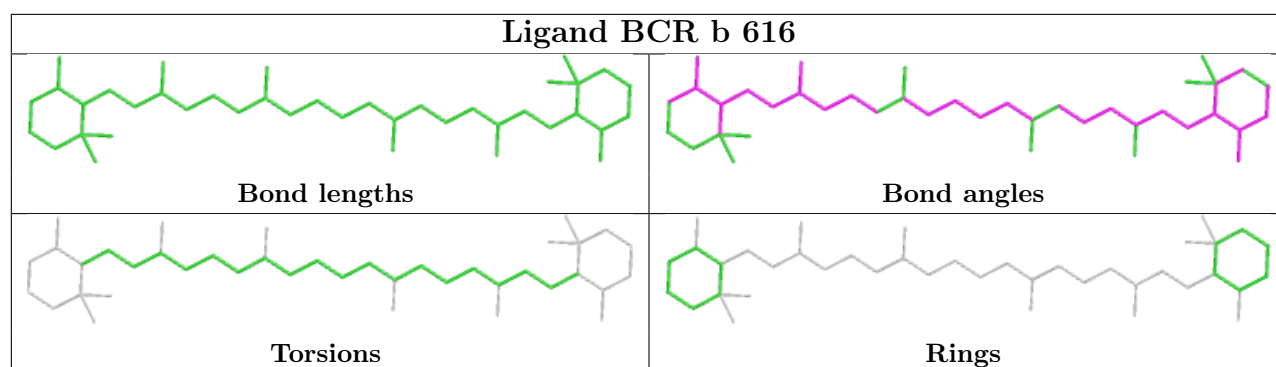


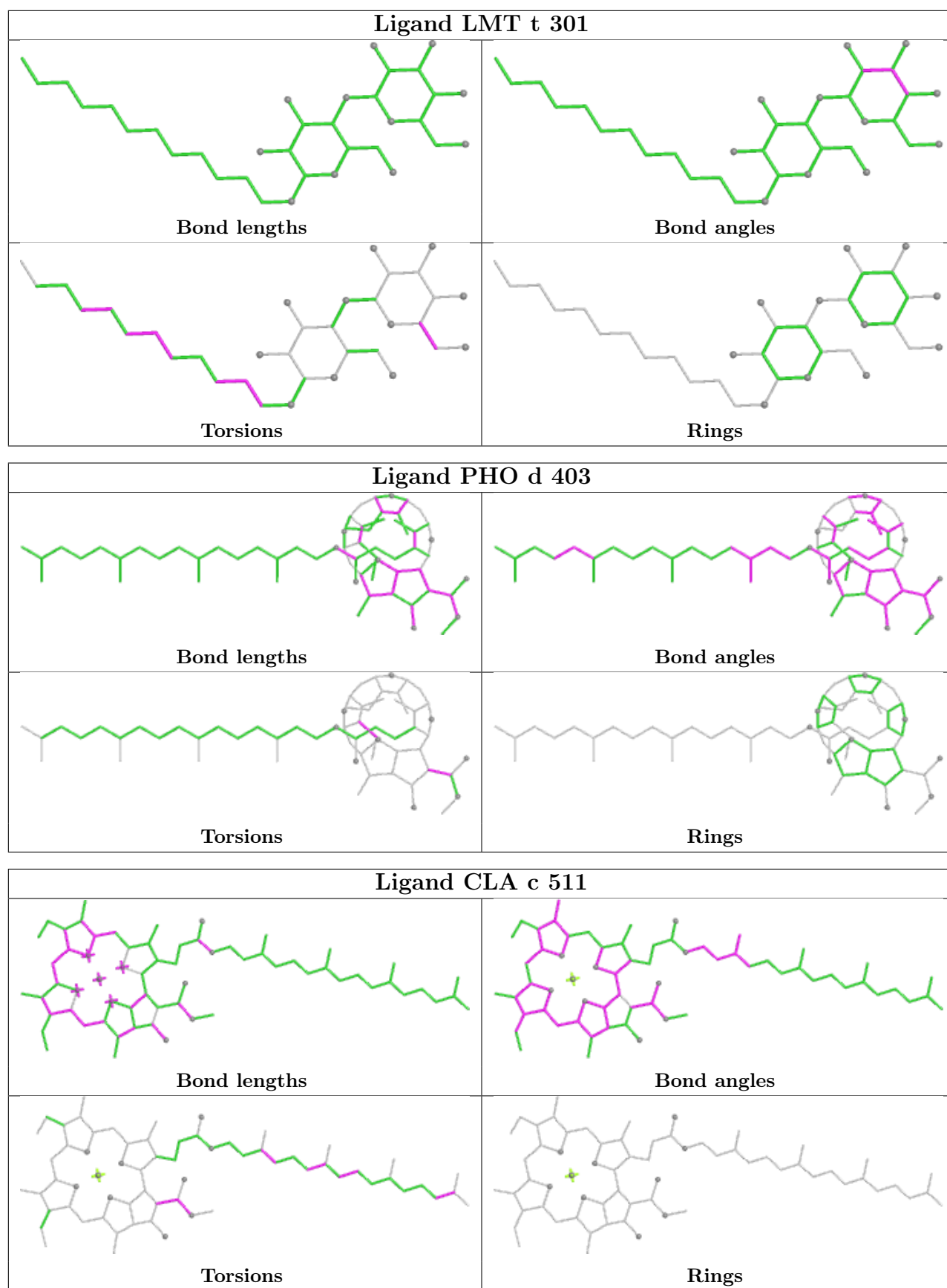


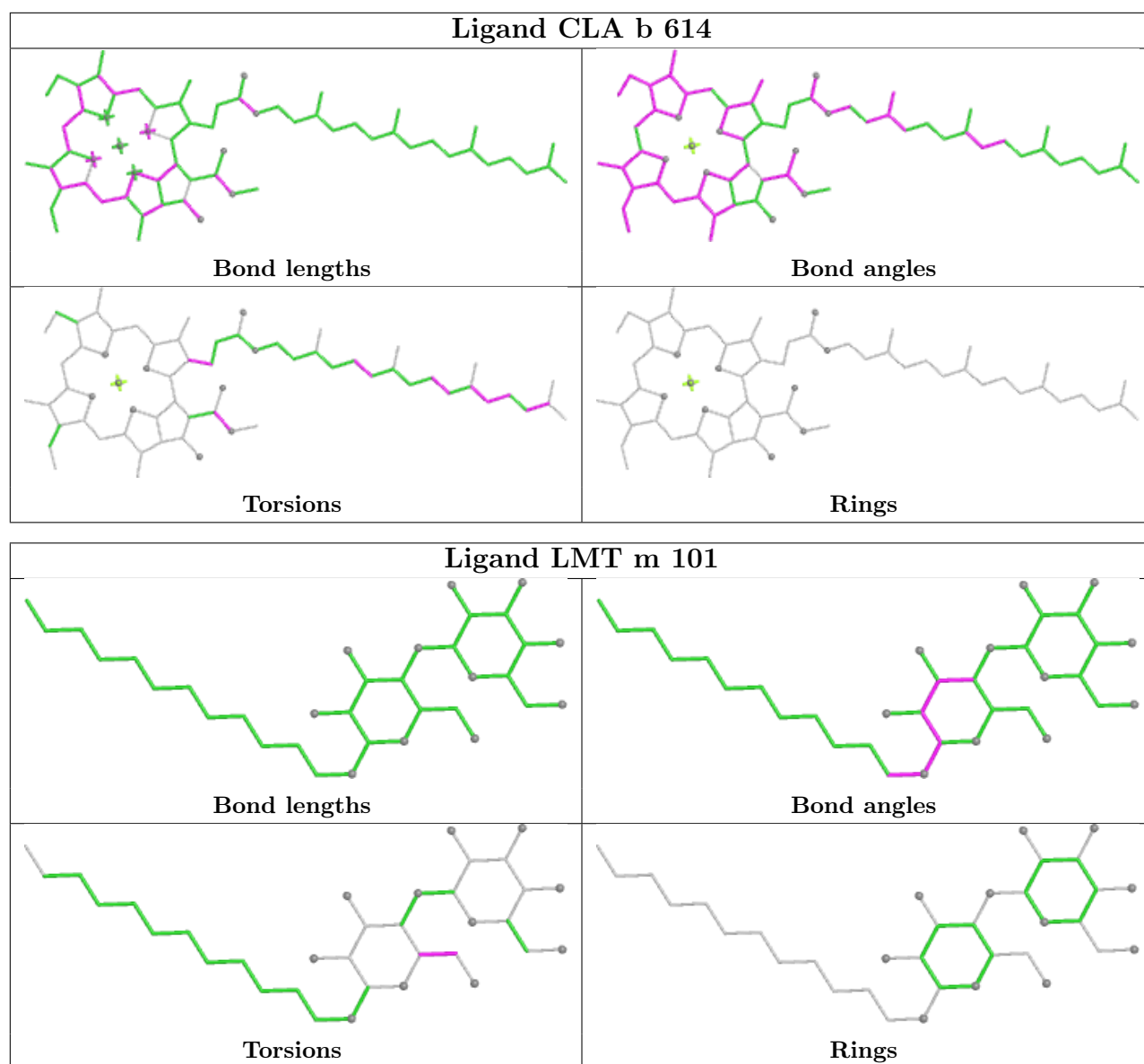
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

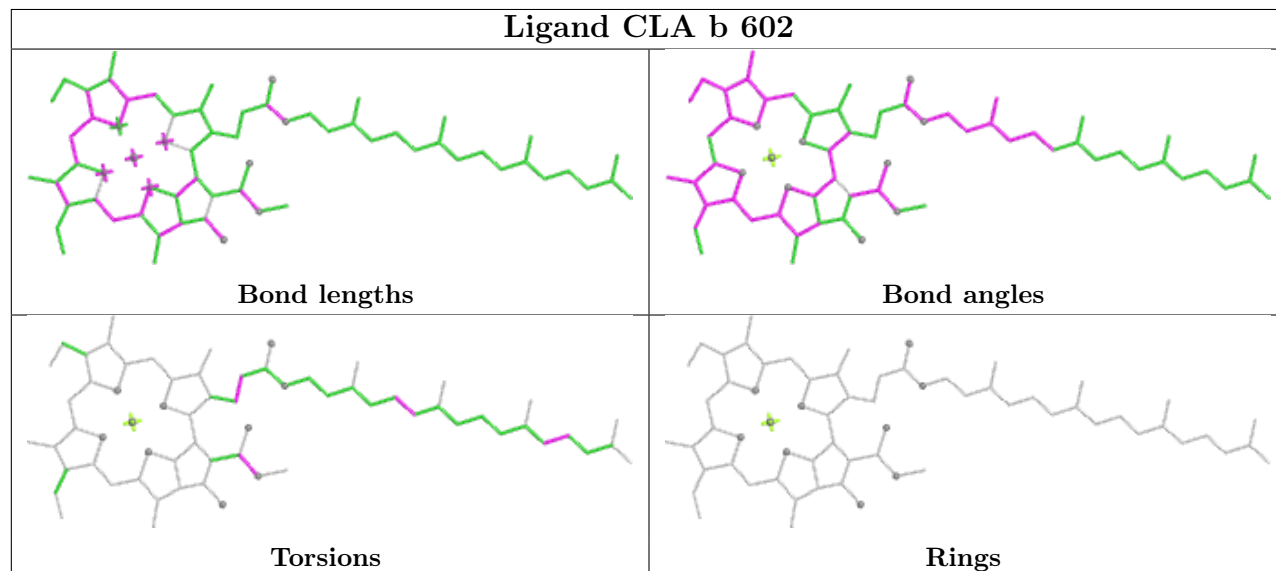
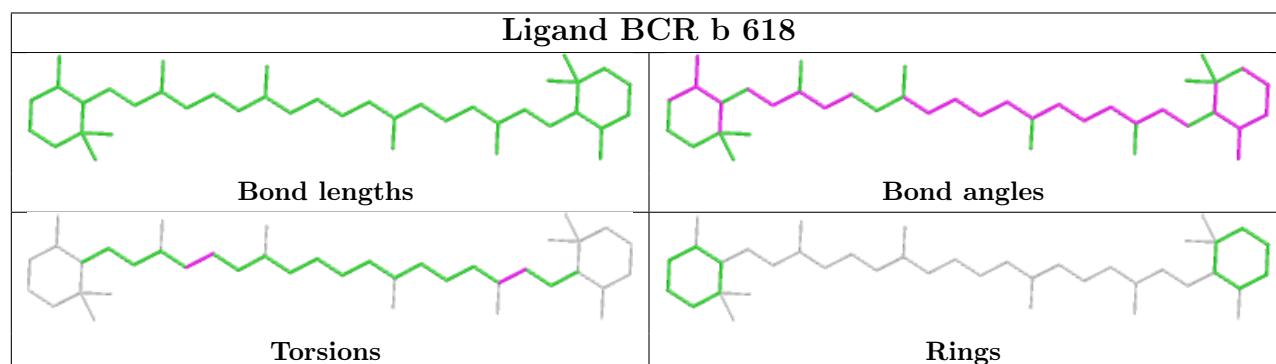
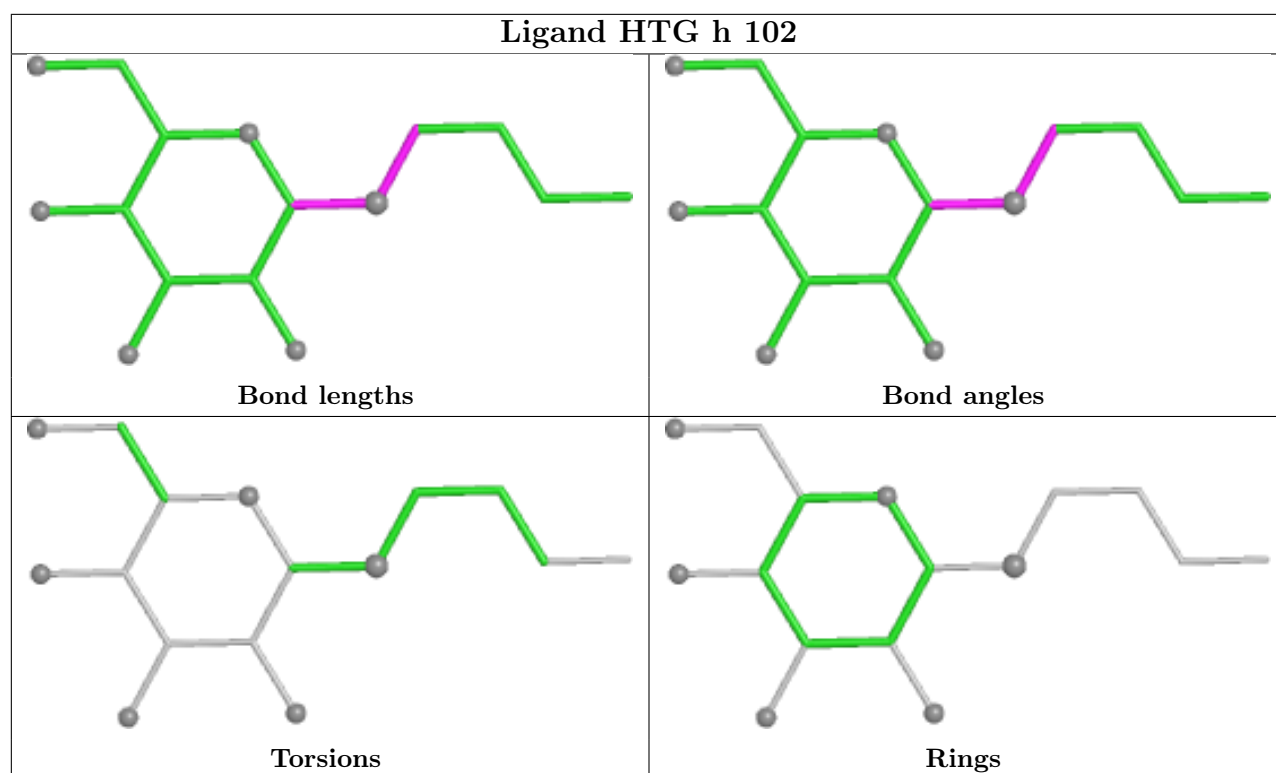
Ligand BCR d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

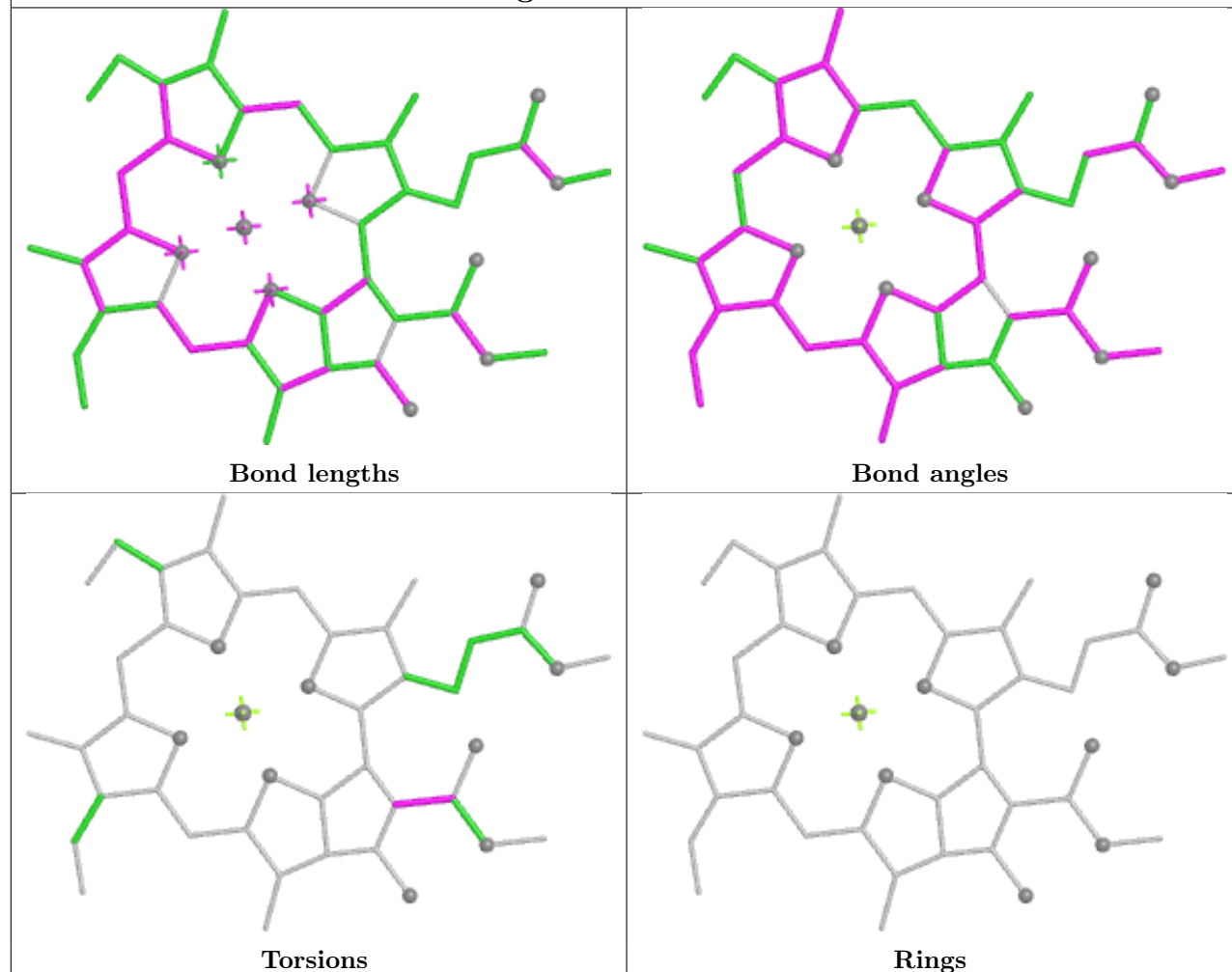




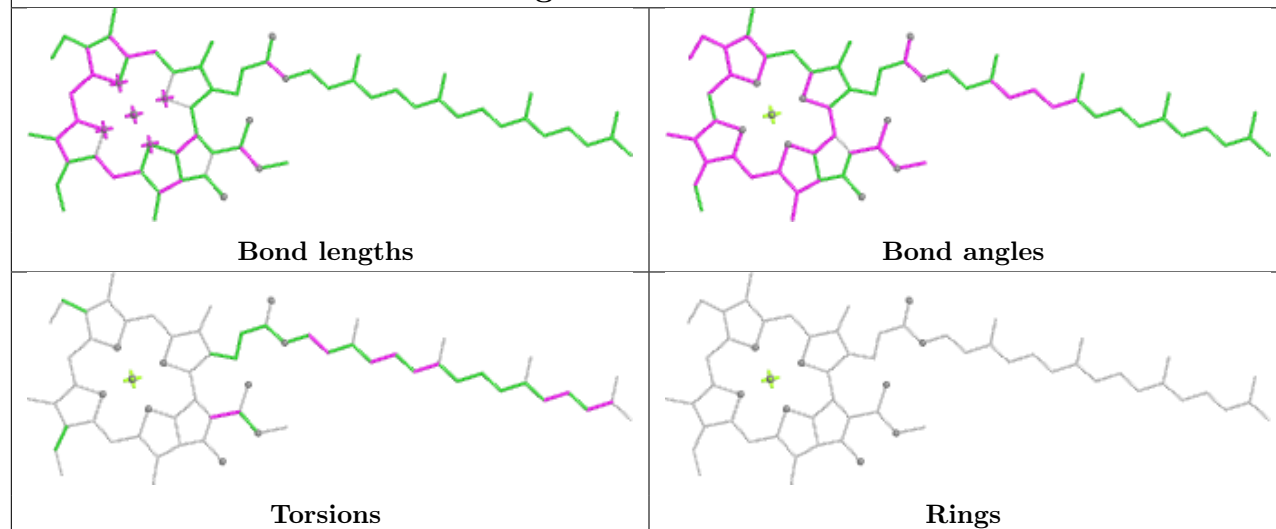


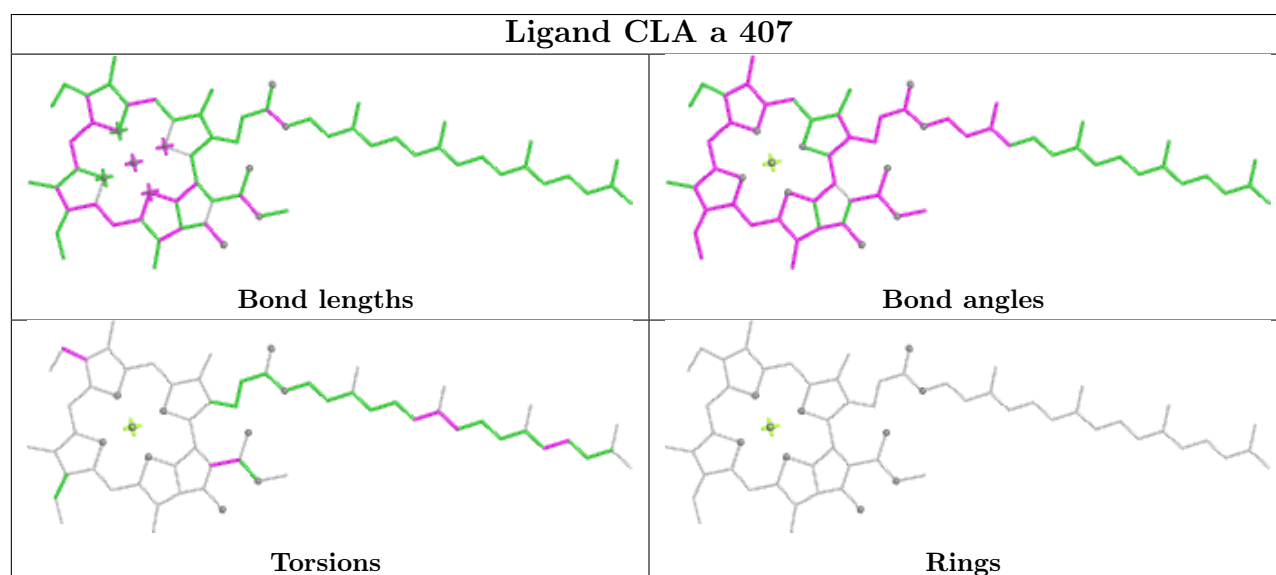
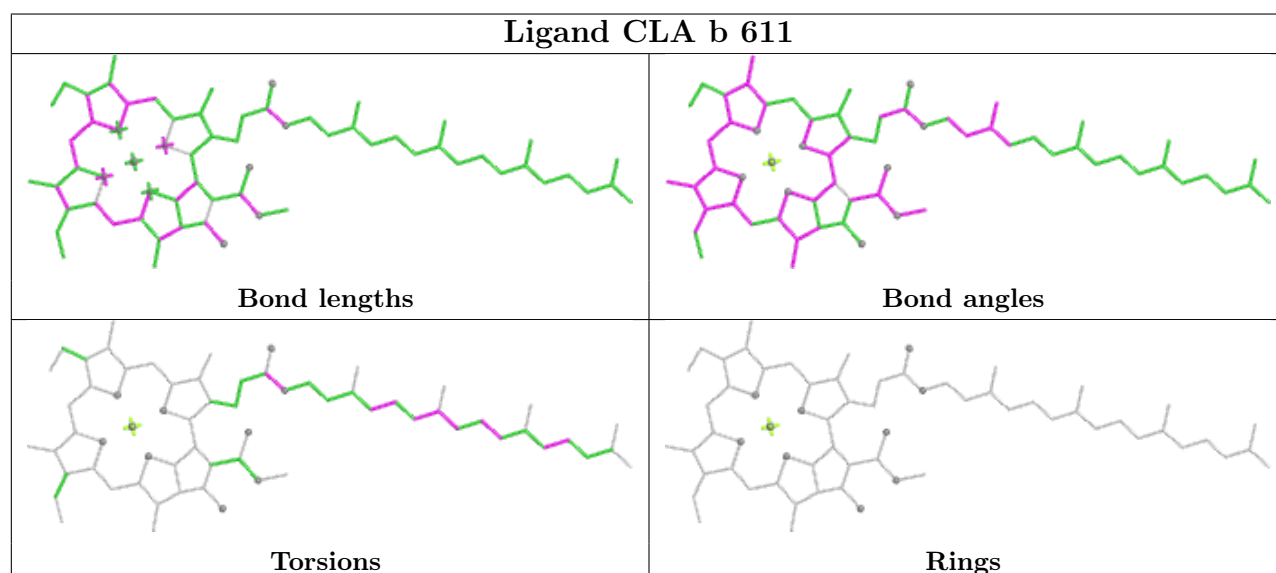
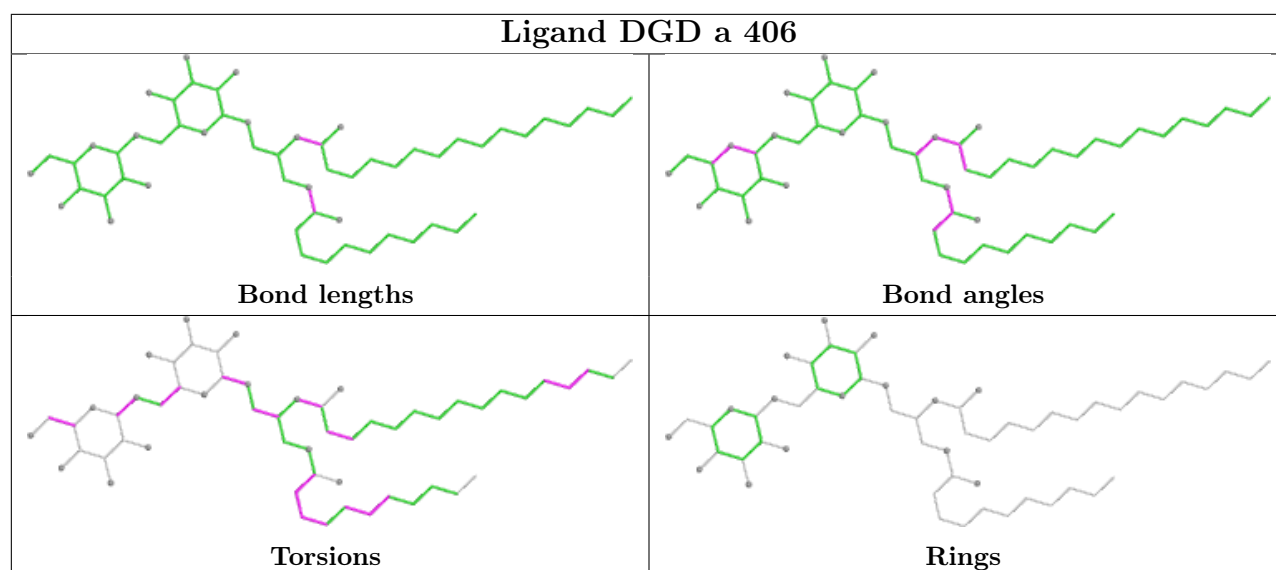


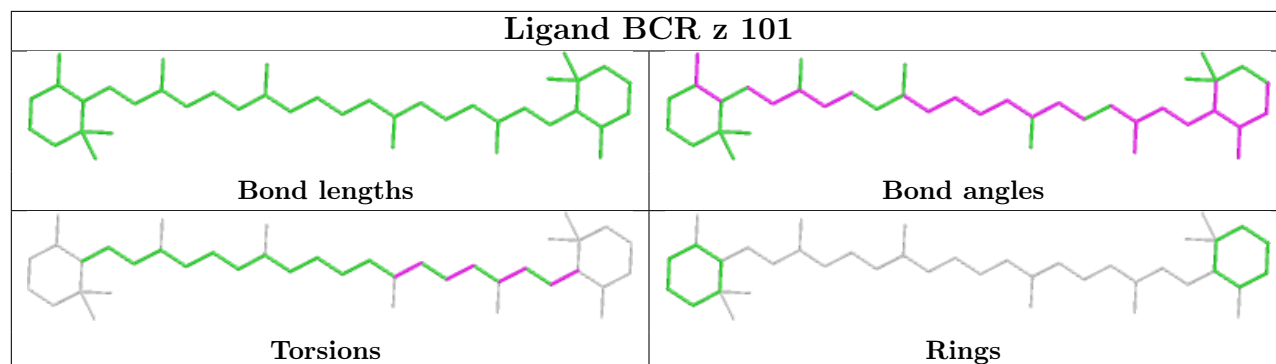
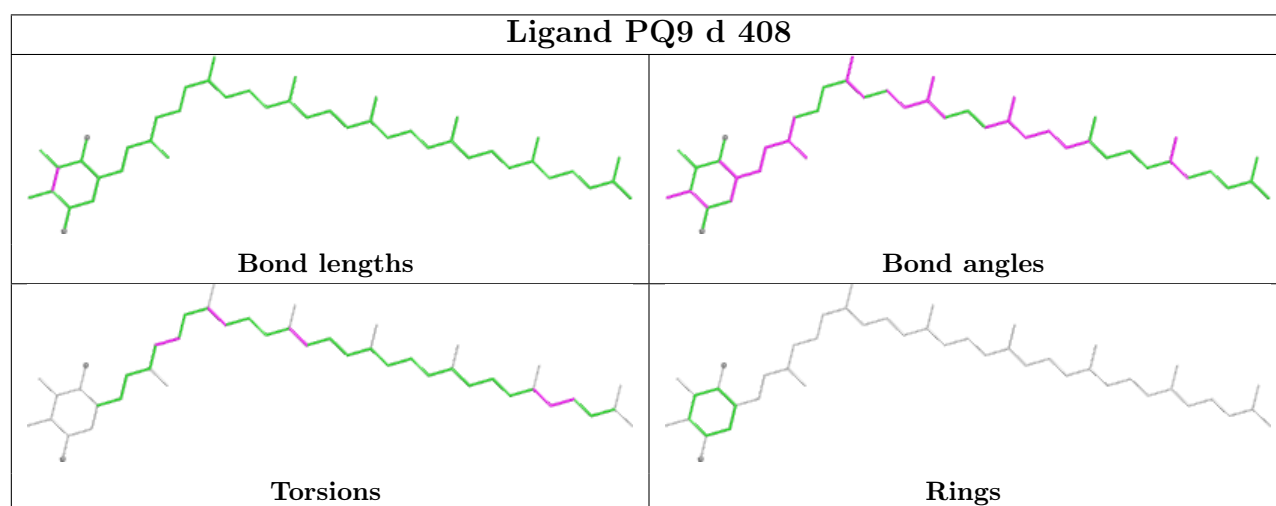
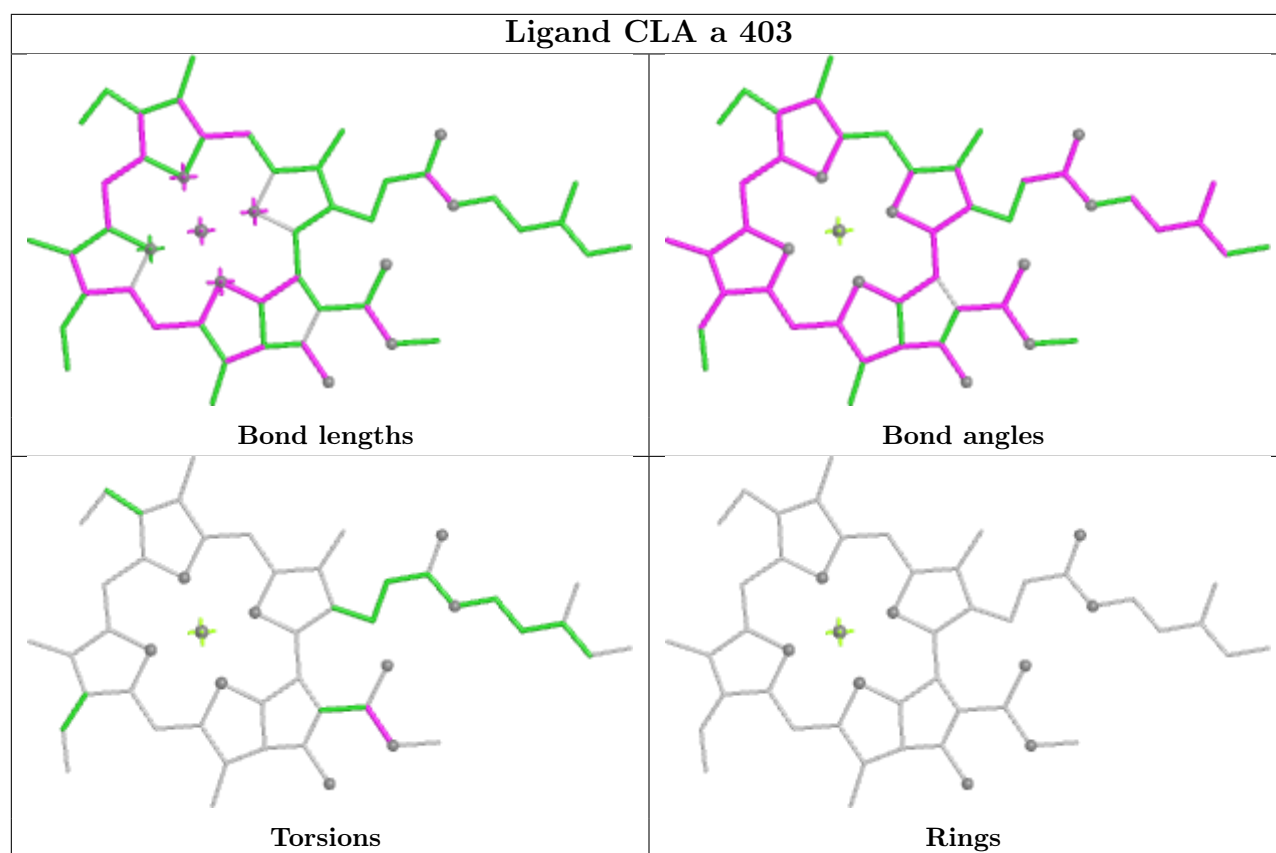
Ligand CLA b 615

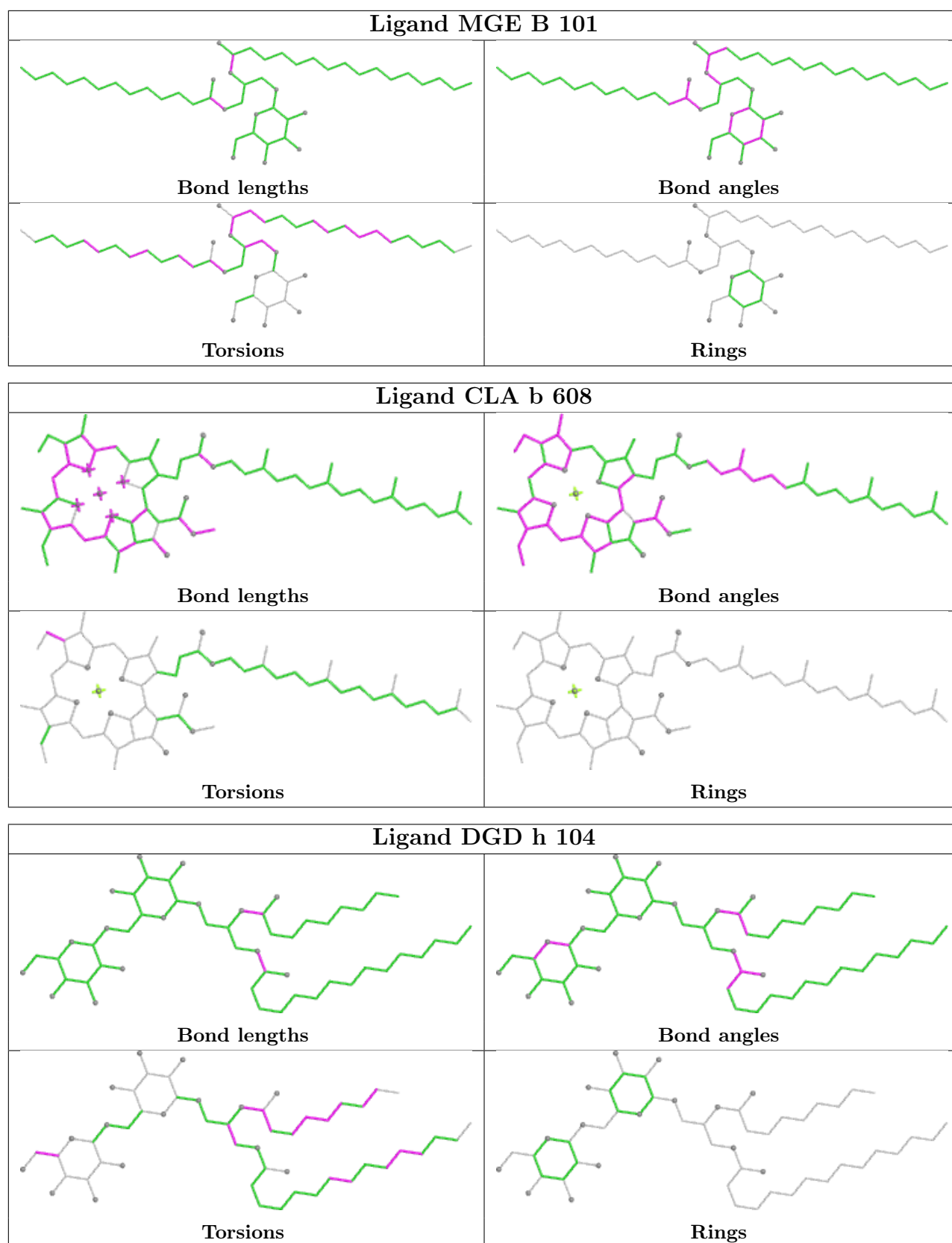


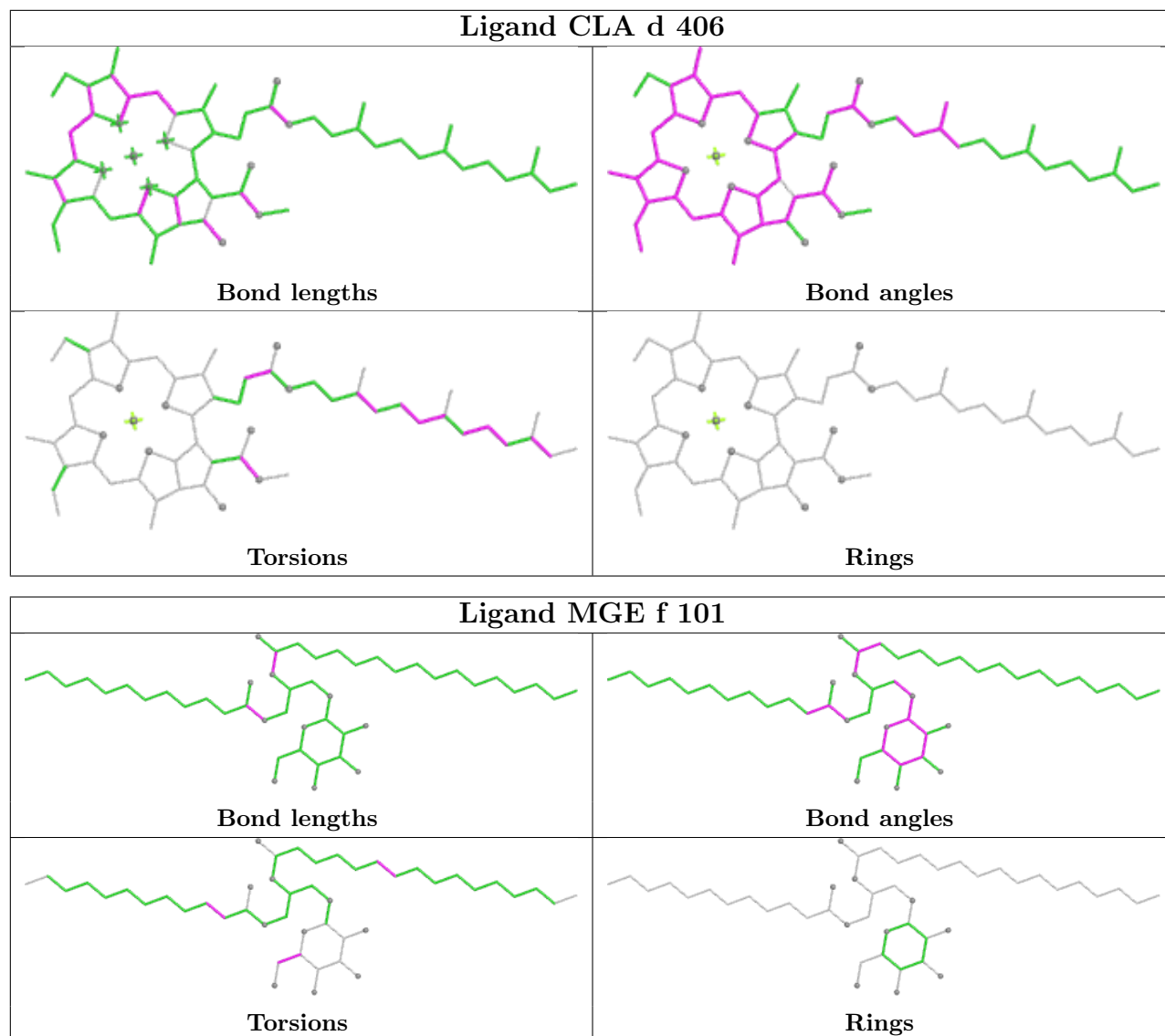
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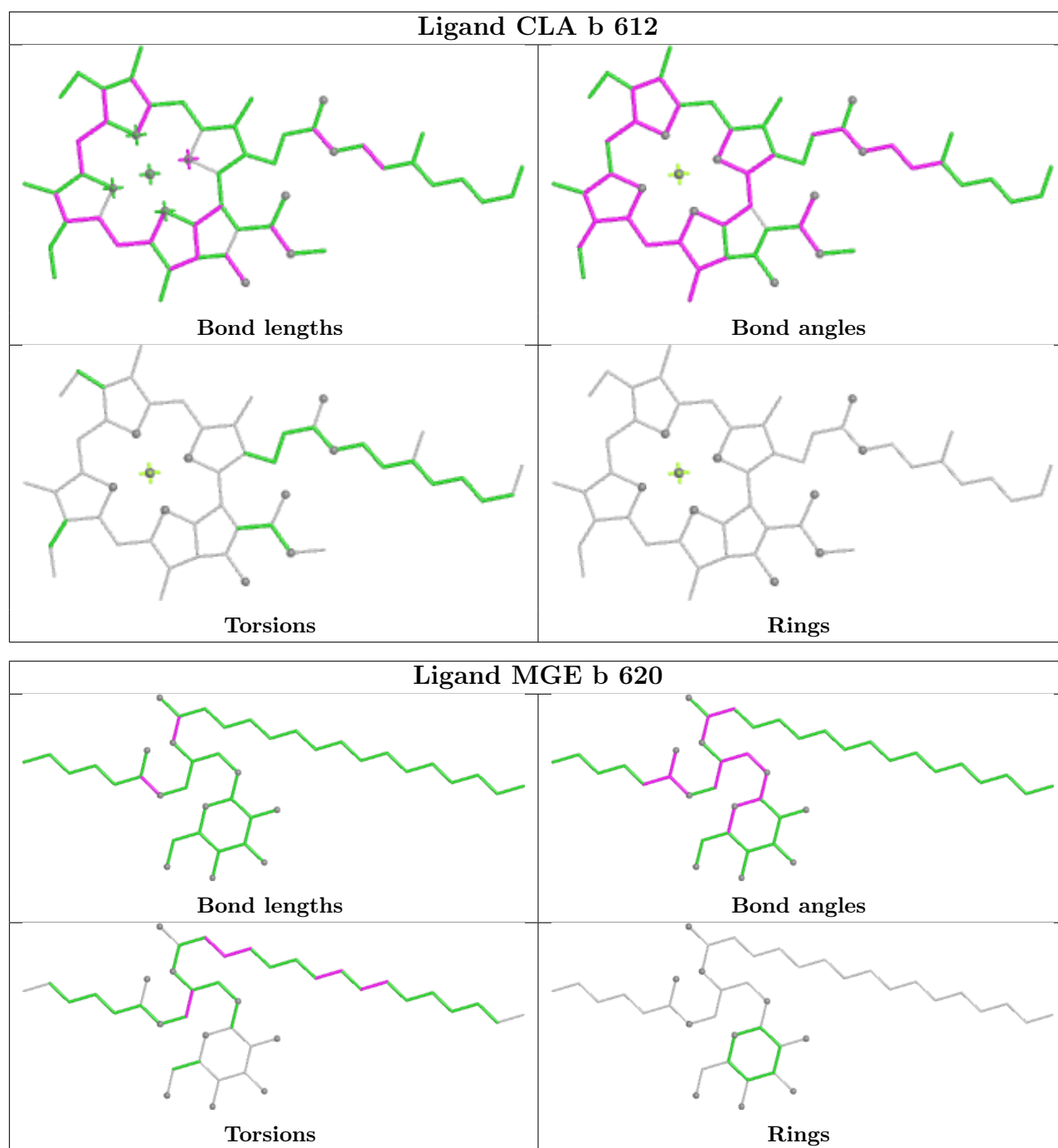




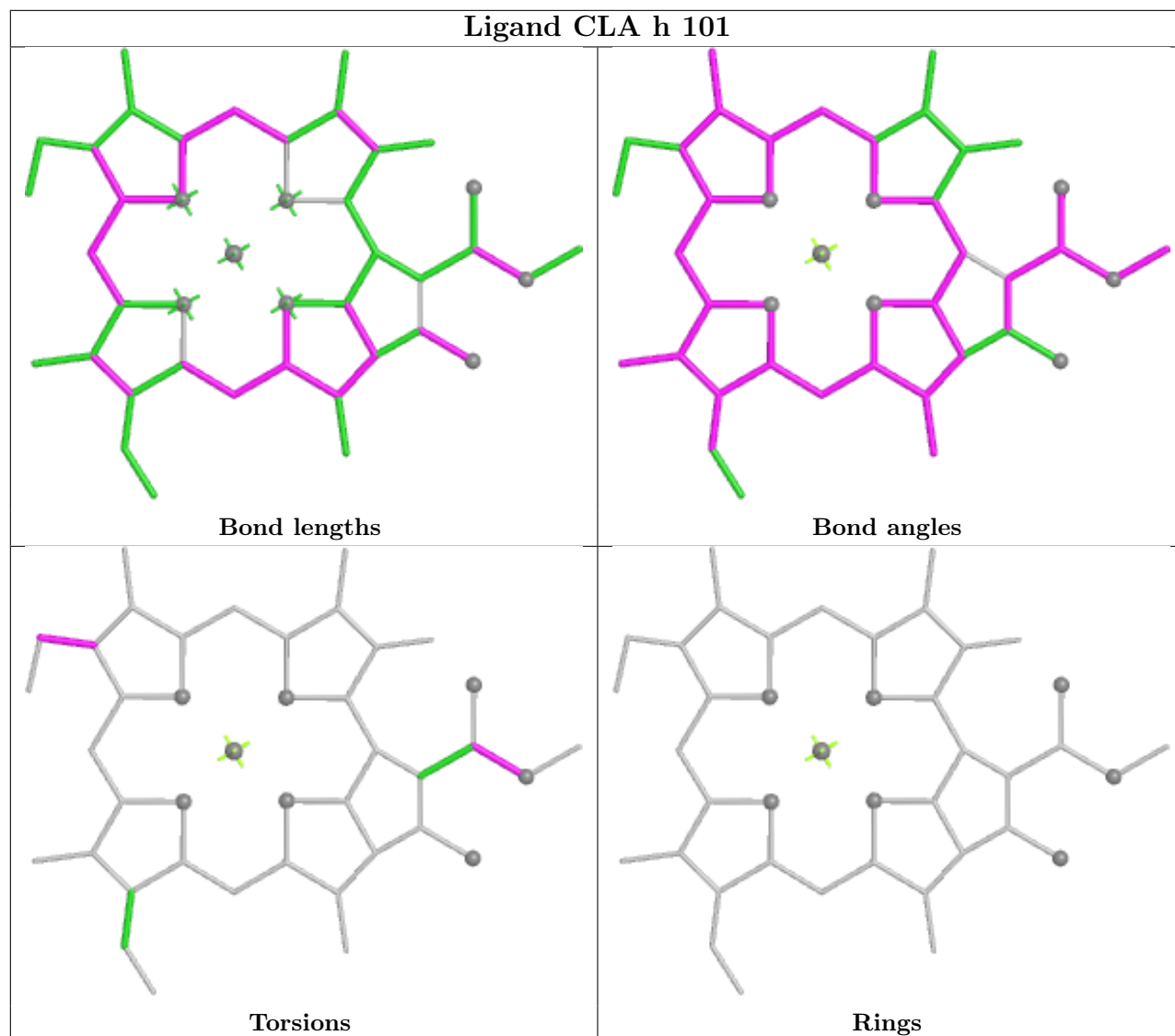




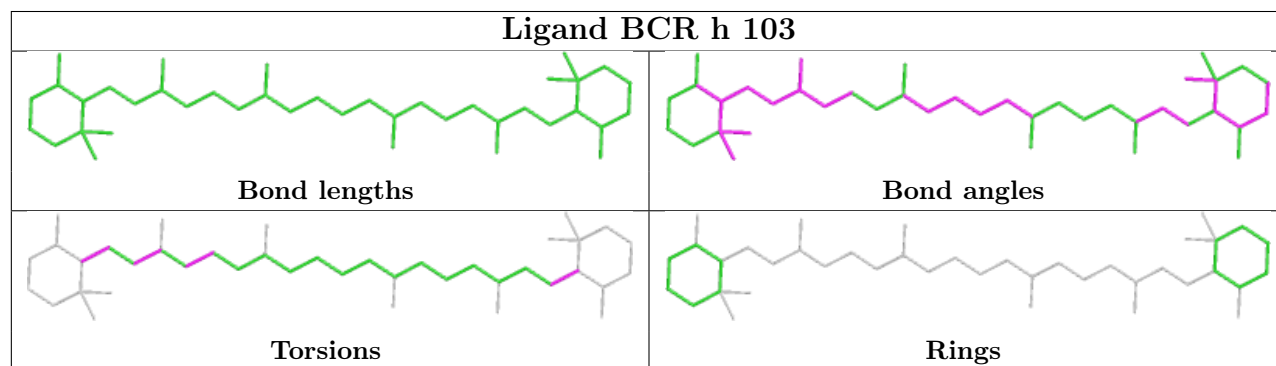


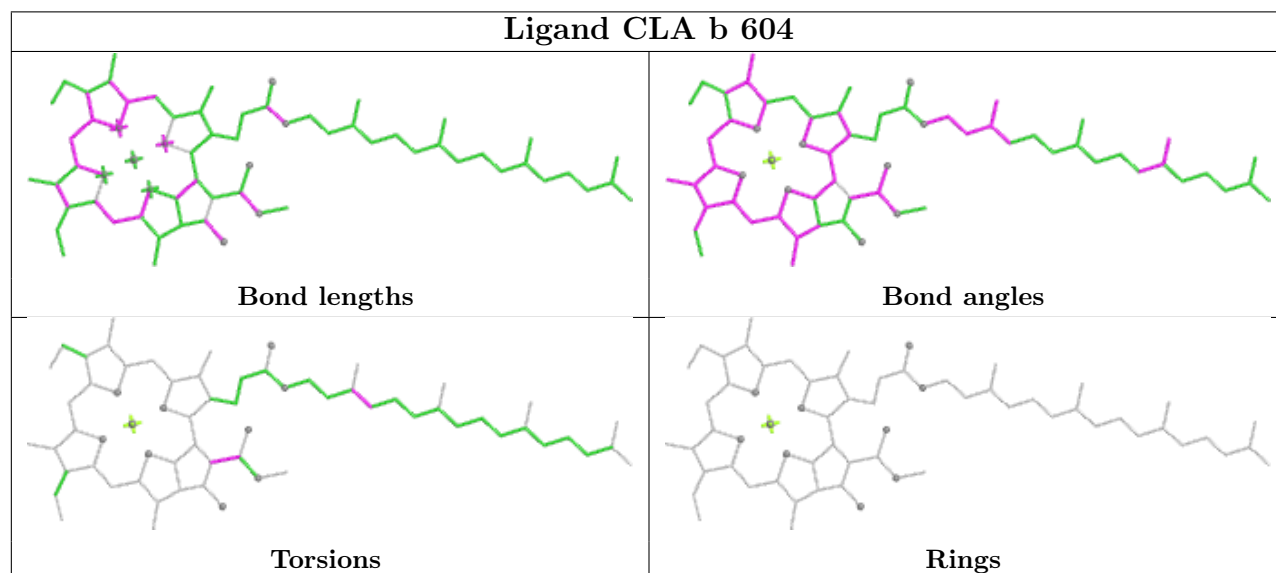
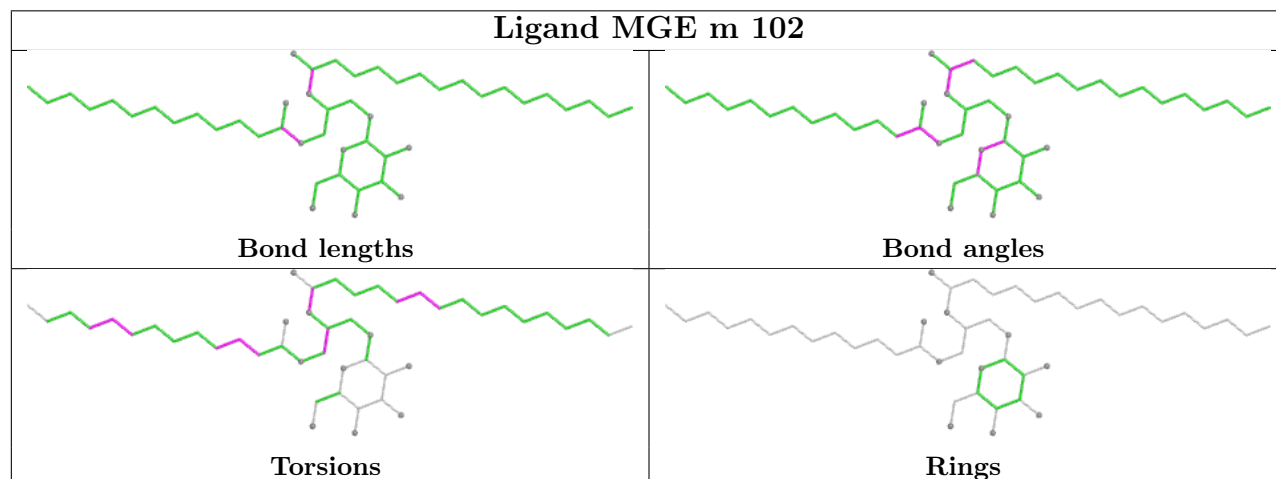
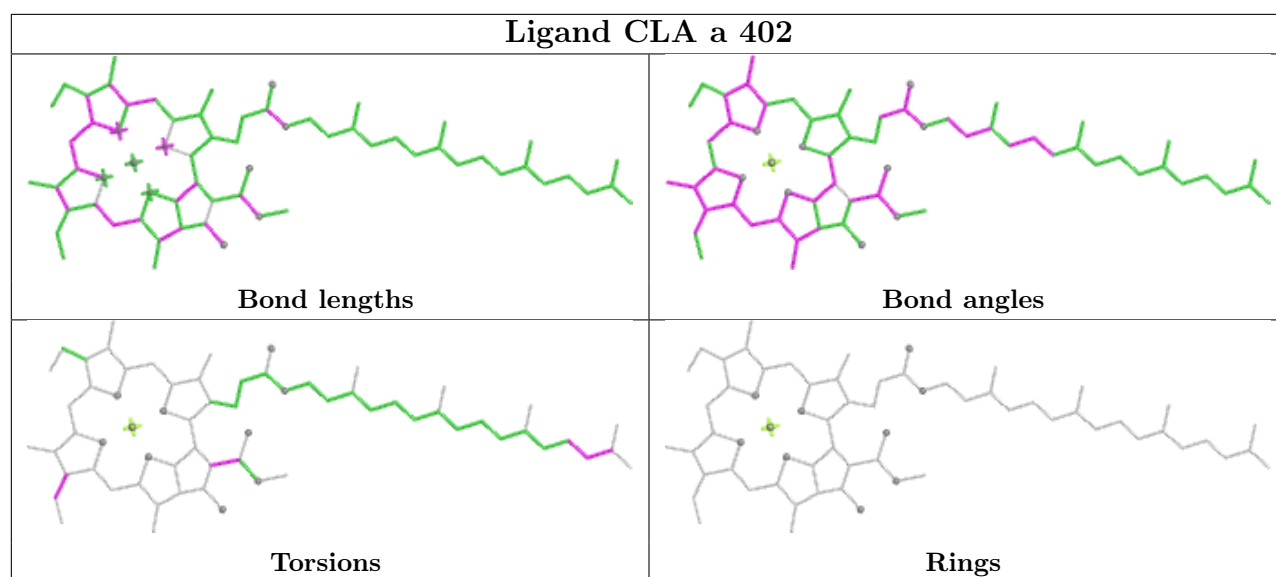


Ligand CLA h 101

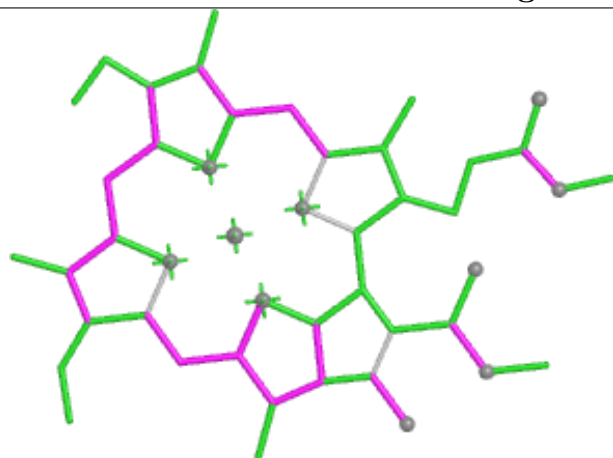


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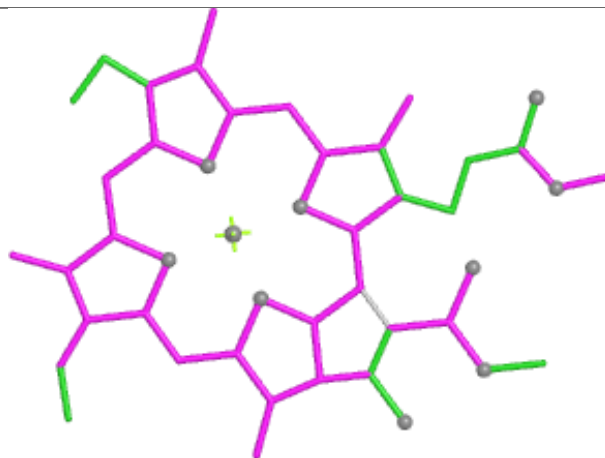




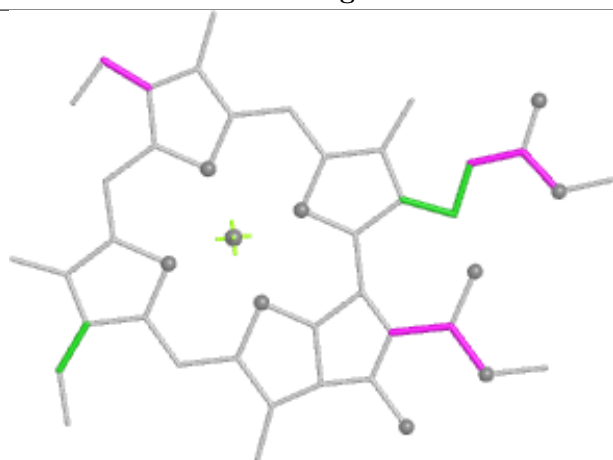
Ligand CLA k 501



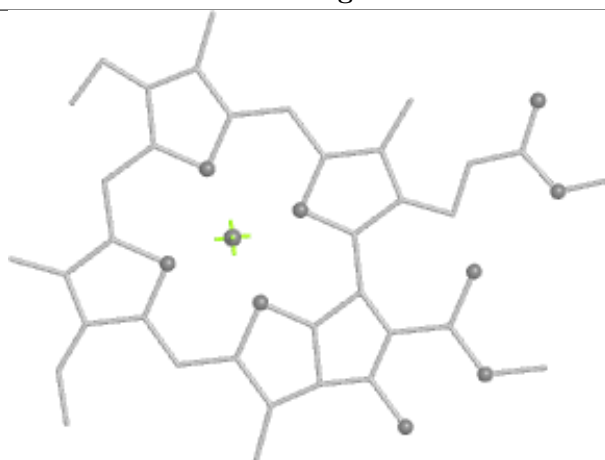
Bond lengths



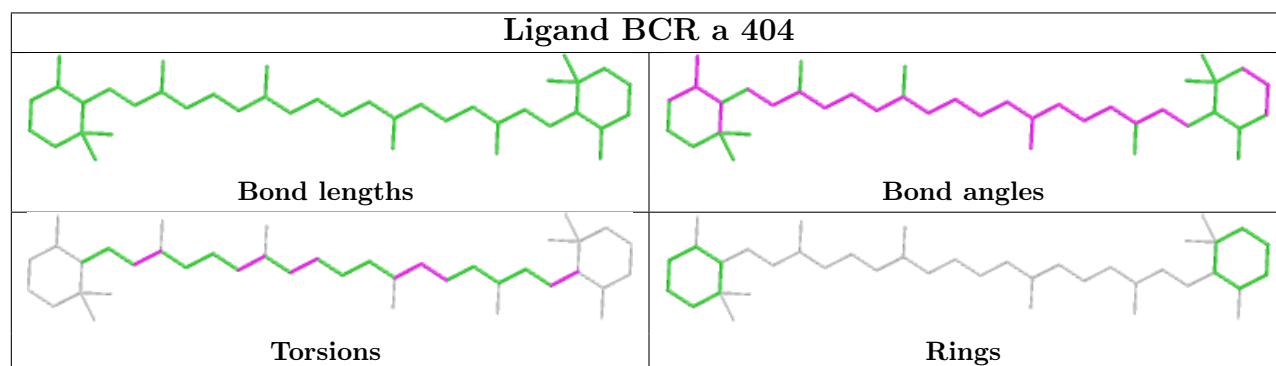
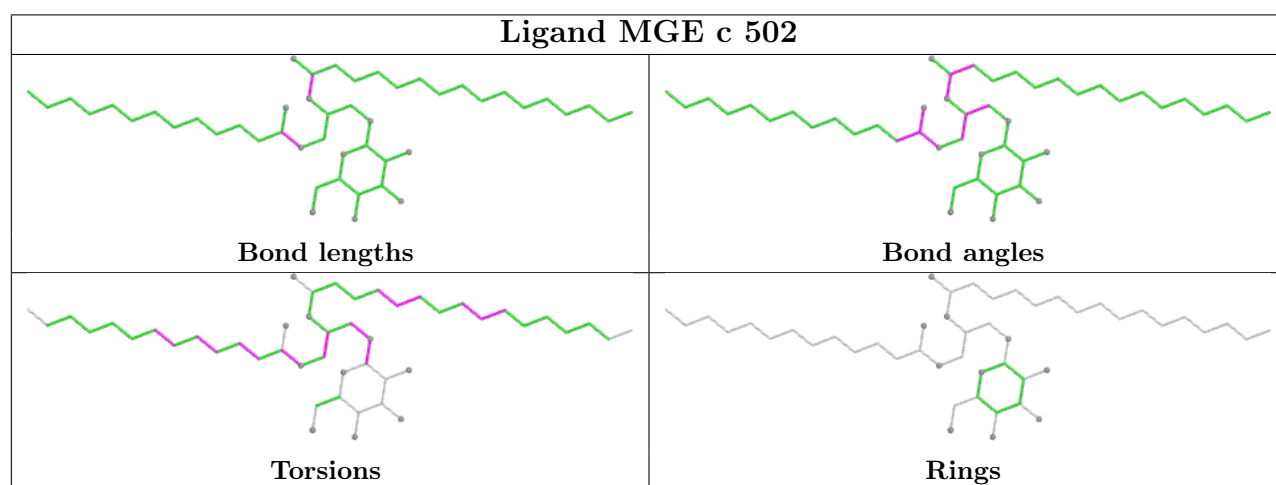
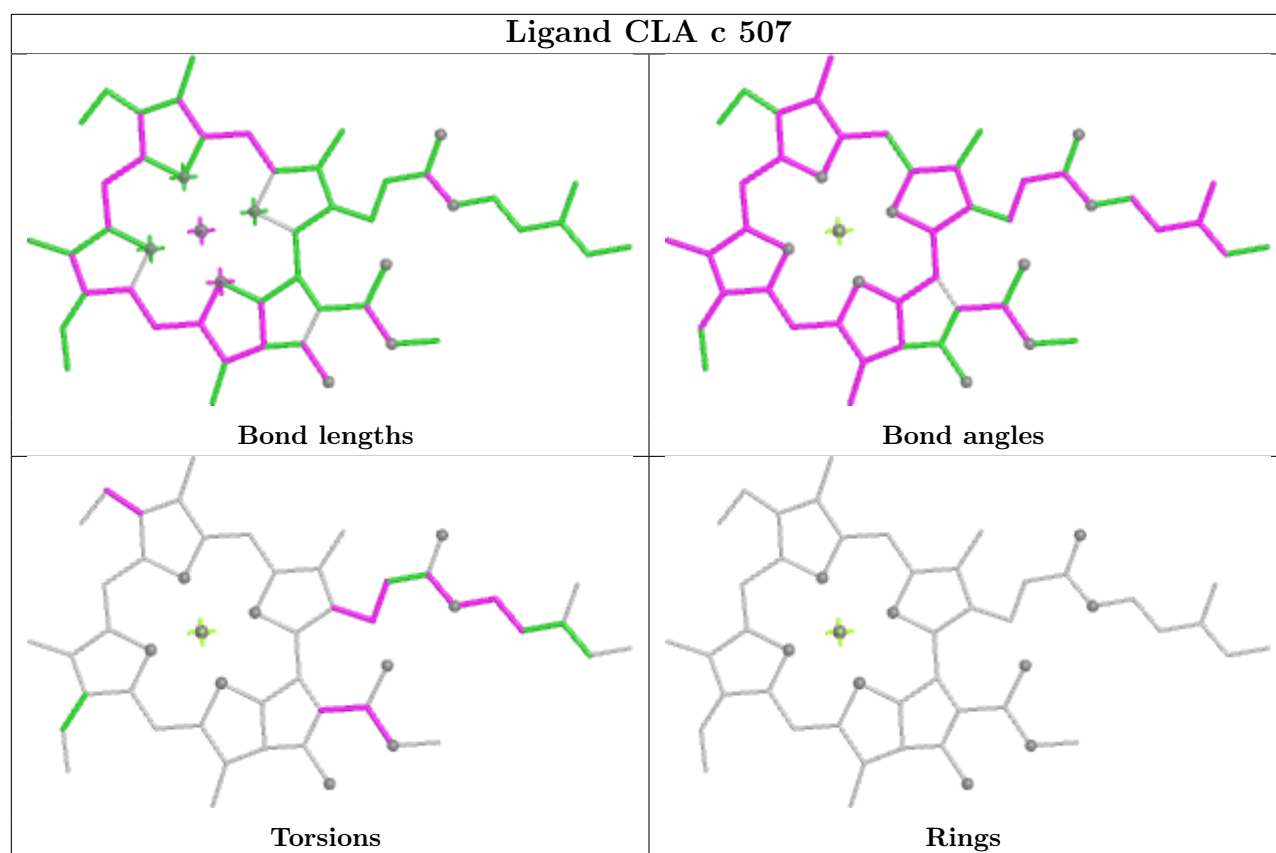
Bond angles

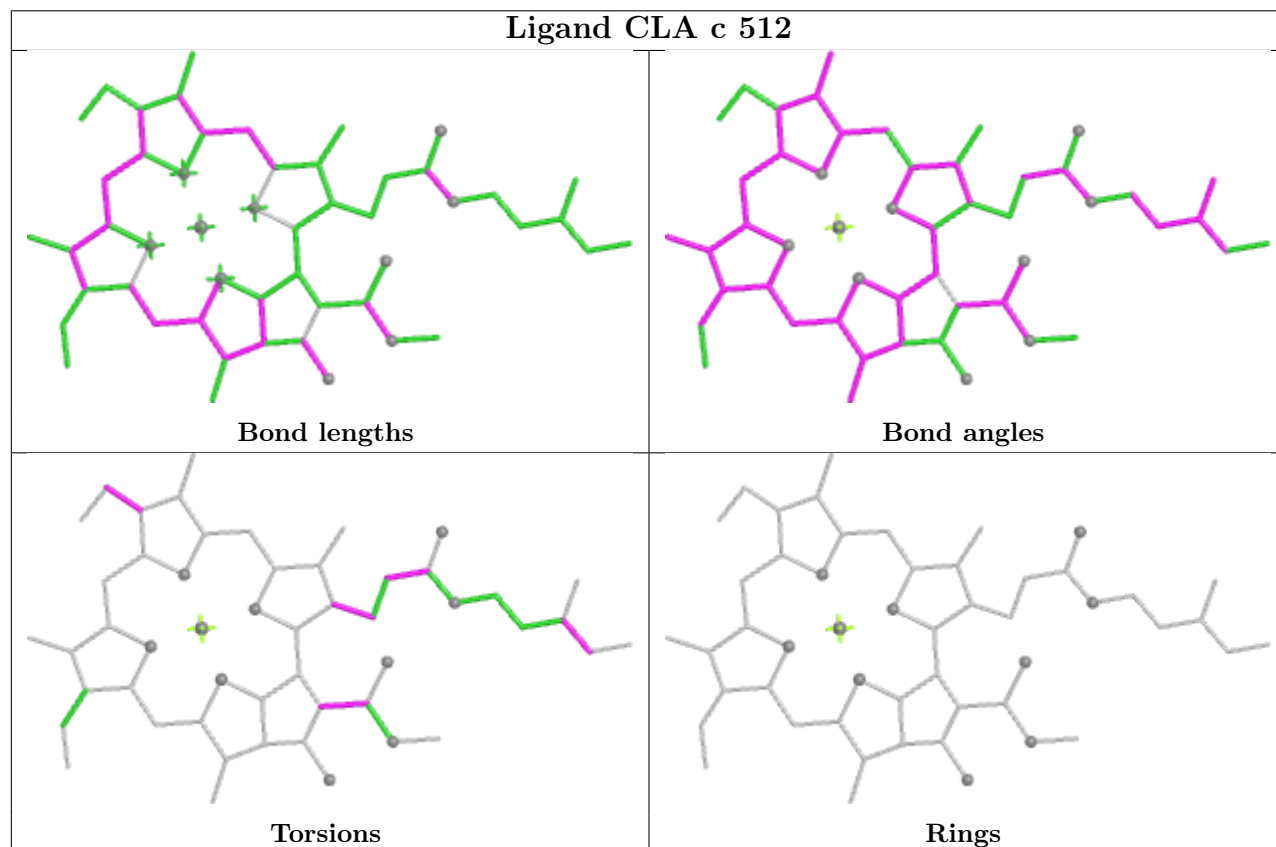
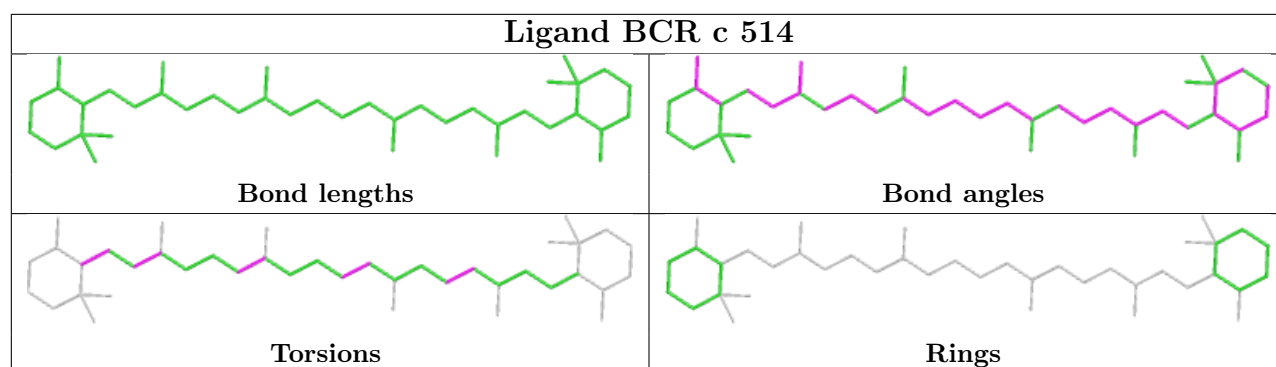


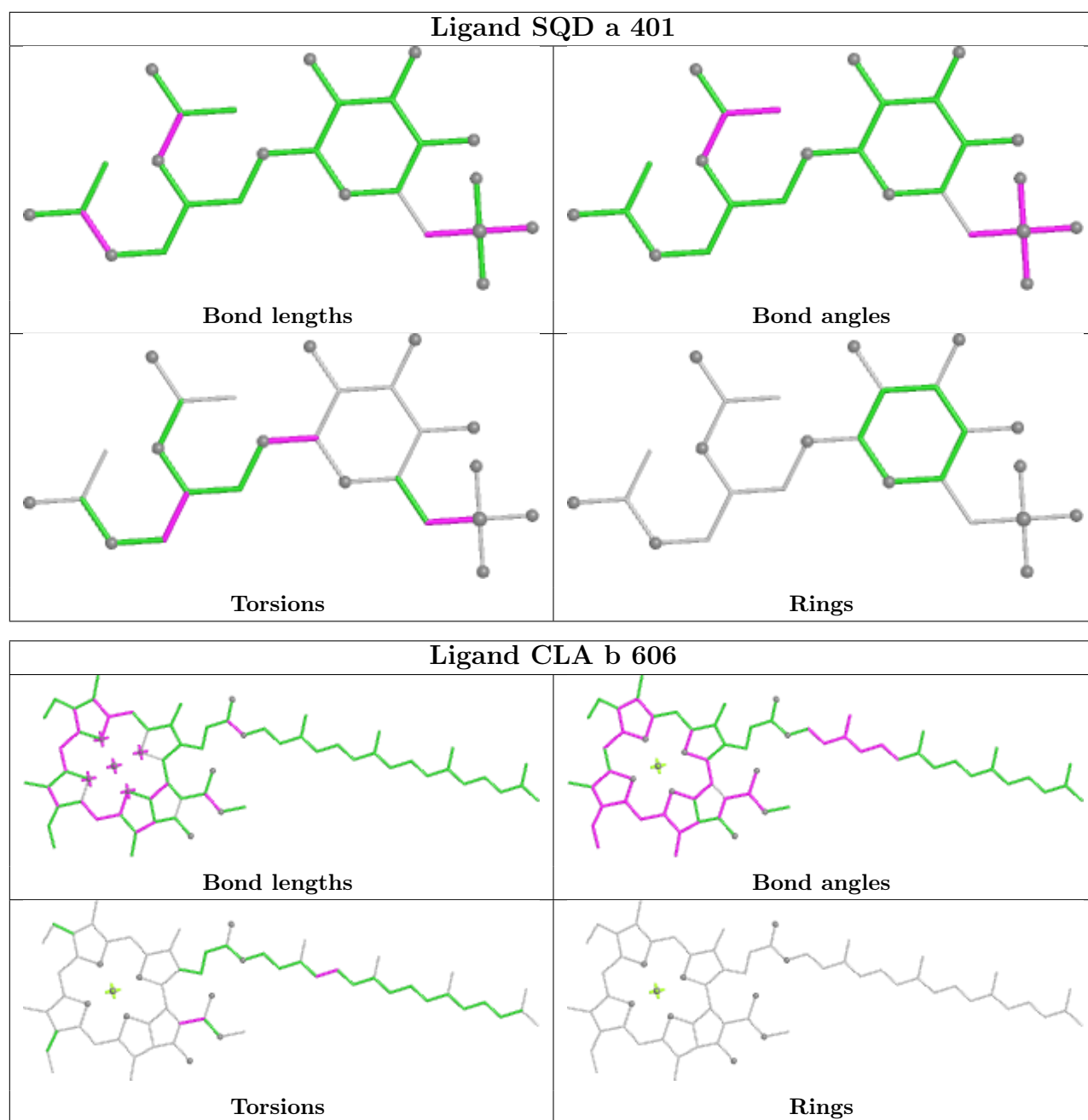
Torsions

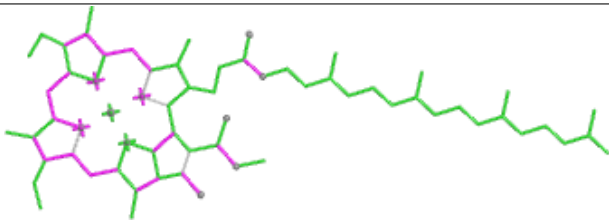
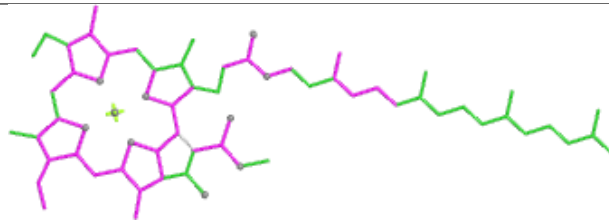
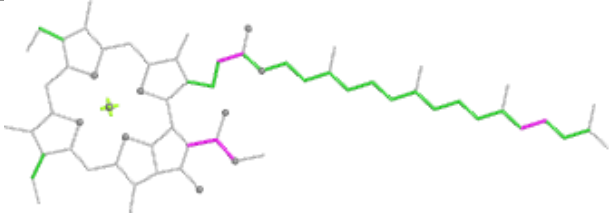
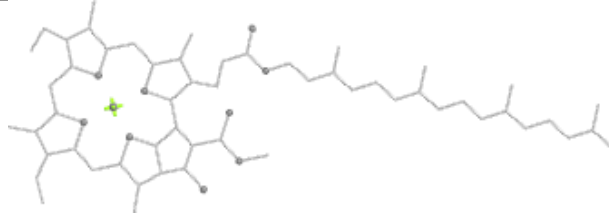


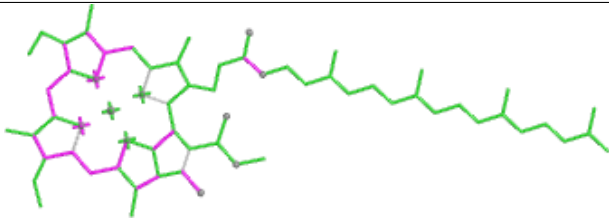
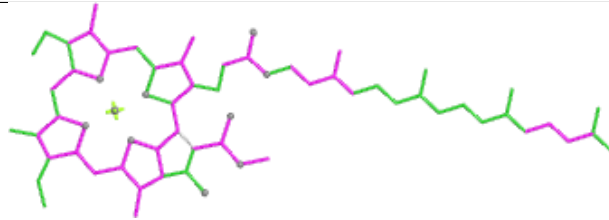
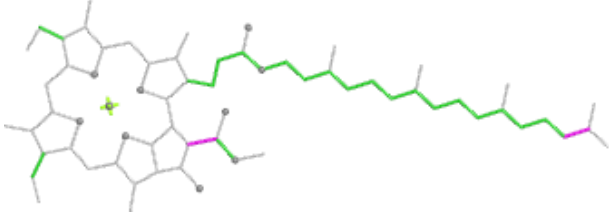
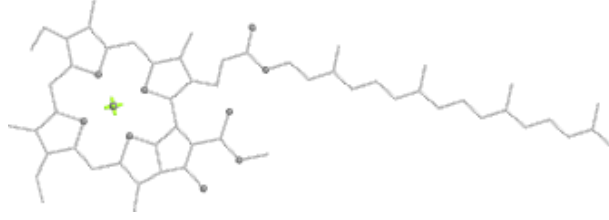
Rings

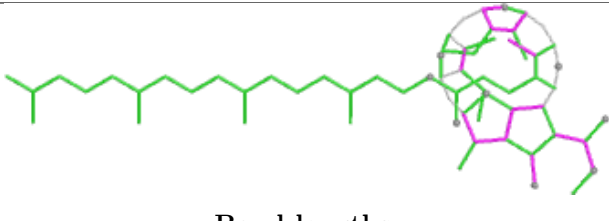
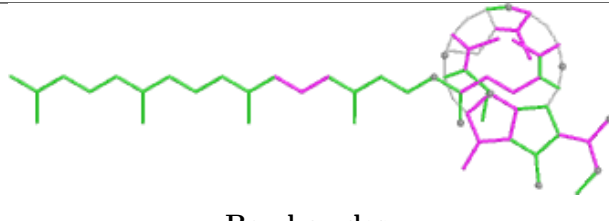
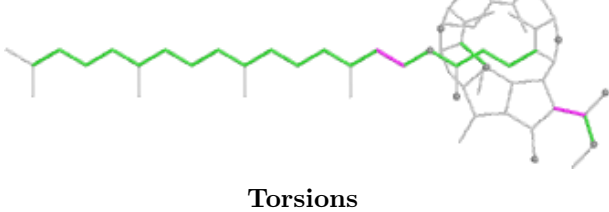
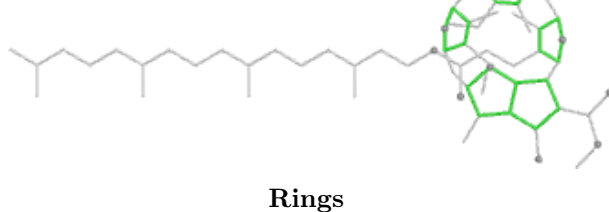






Ligand CLA c 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

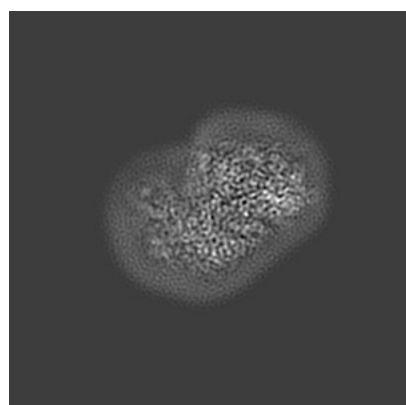
6 Map visualisation [i](#)

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

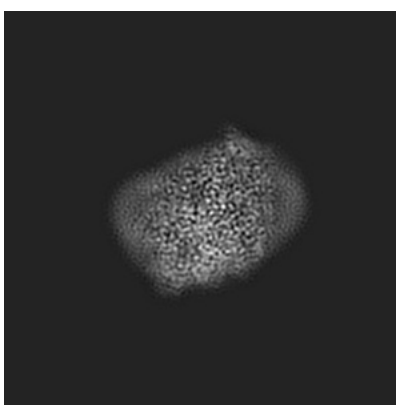
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

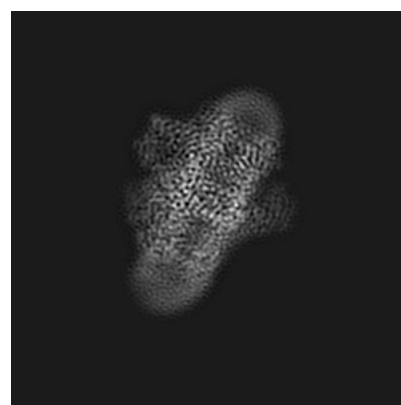
6.1.1 Primary map



X



Y

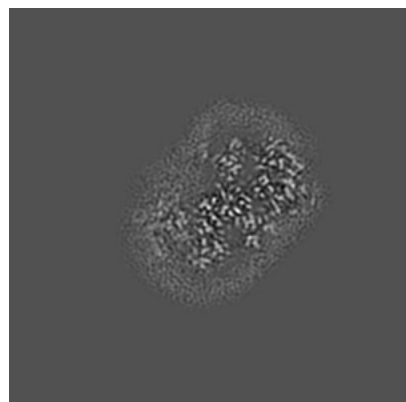


Z

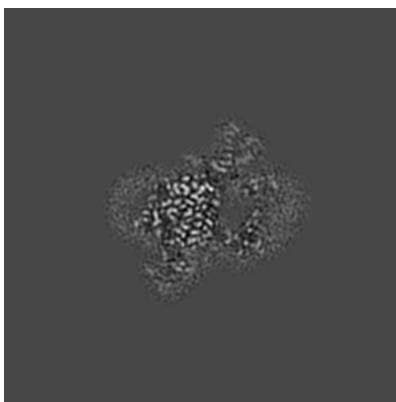
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

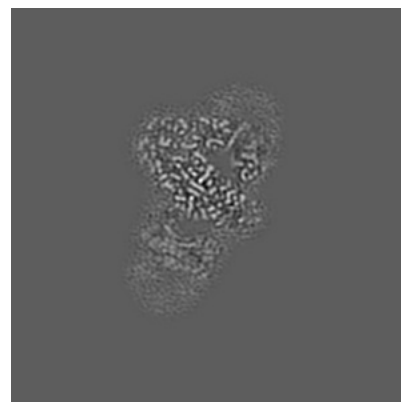
6.2.1 Primary map



X Index: 100



Y Index: 100

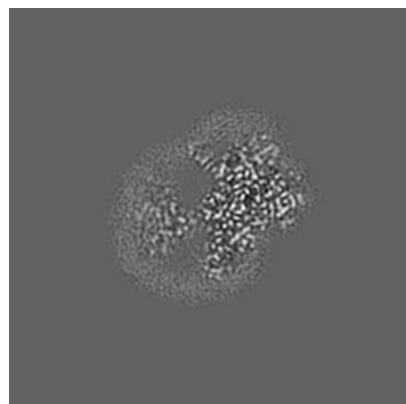


Z Index: 100

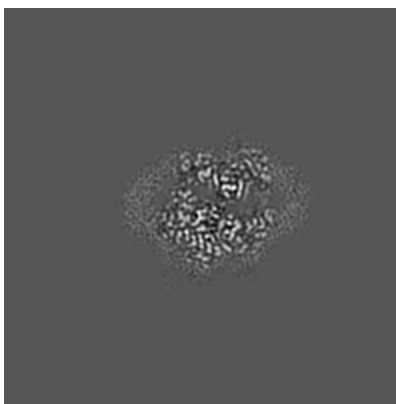
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

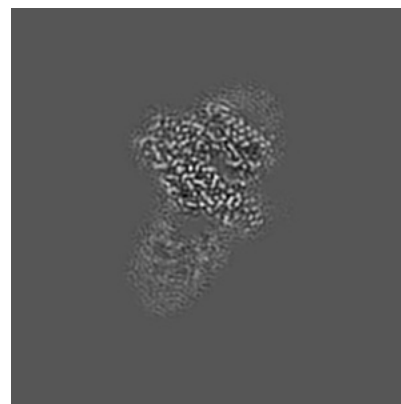
6.3.1 Primary map



X Index: 91



Y Index: 118

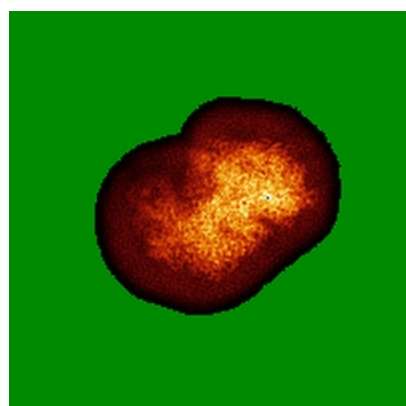


Z Index: 104

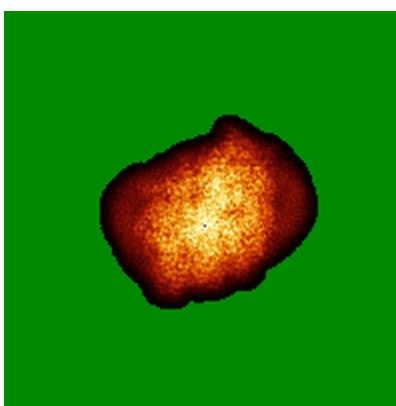
The images above show the largest variance slices of the map in three orthogonal directions.

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

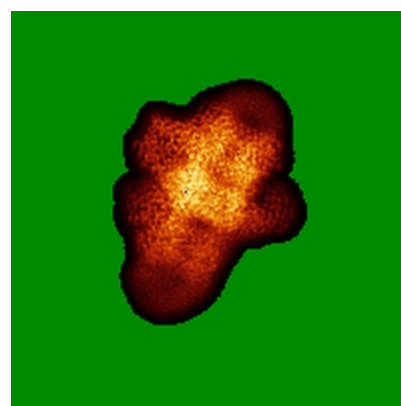
6.4.1 Primary map



X



Y

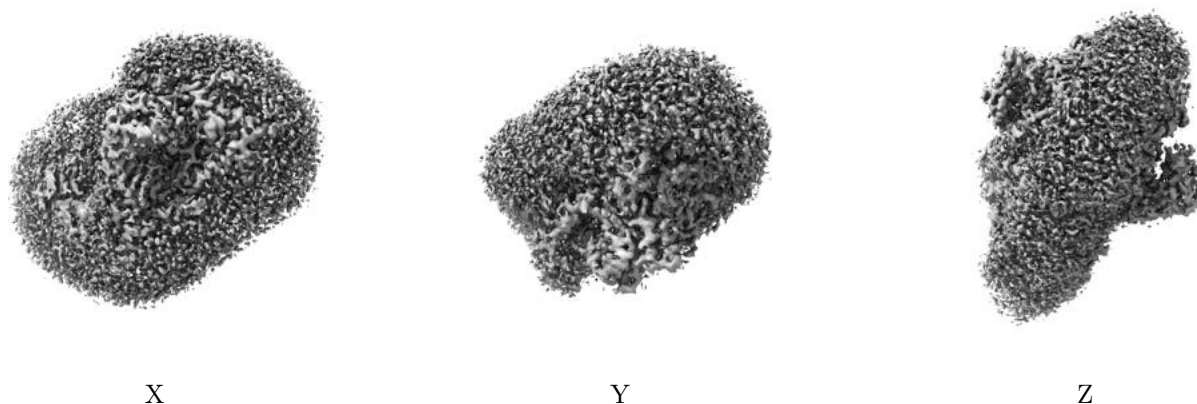


Z

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 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

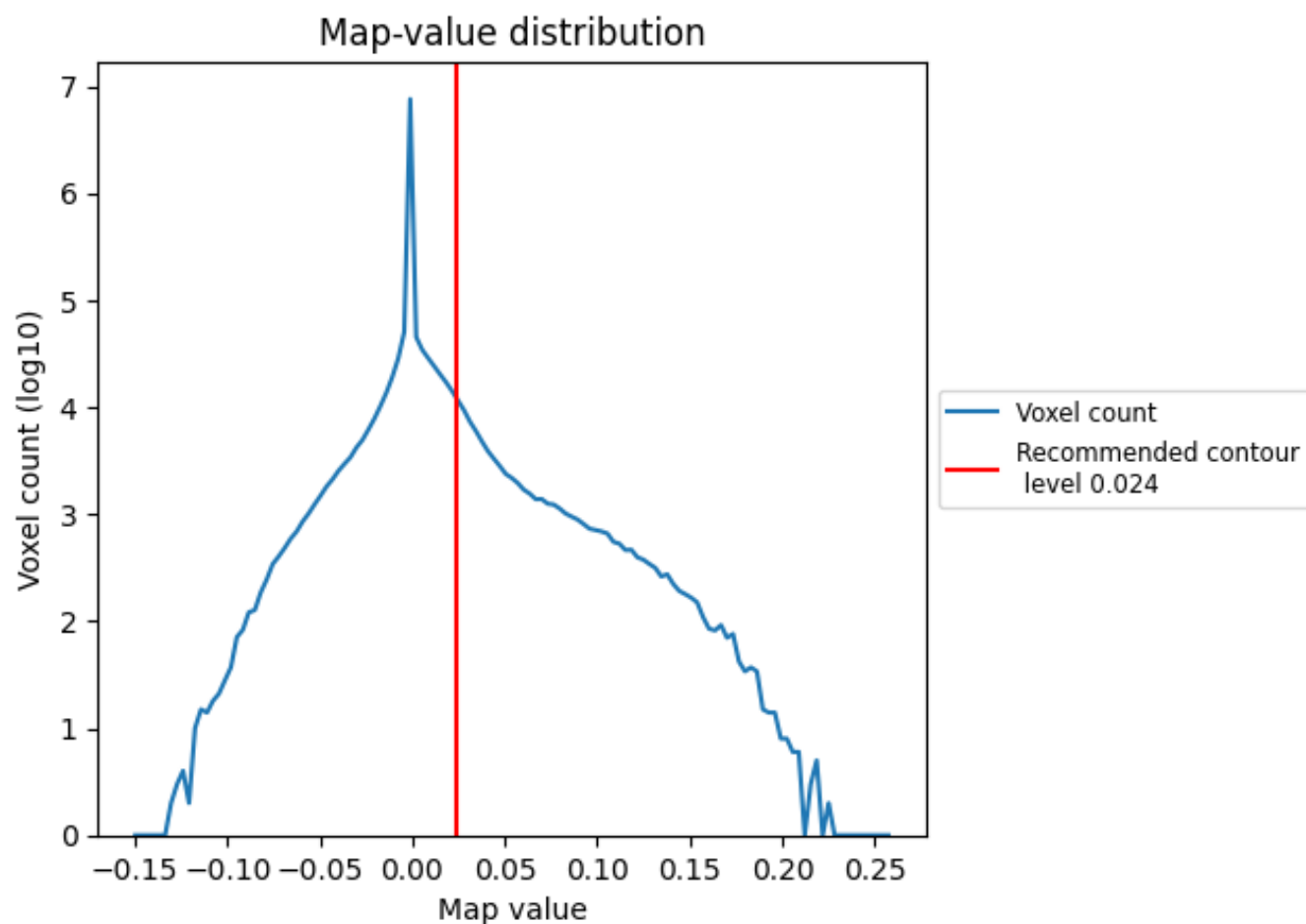
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

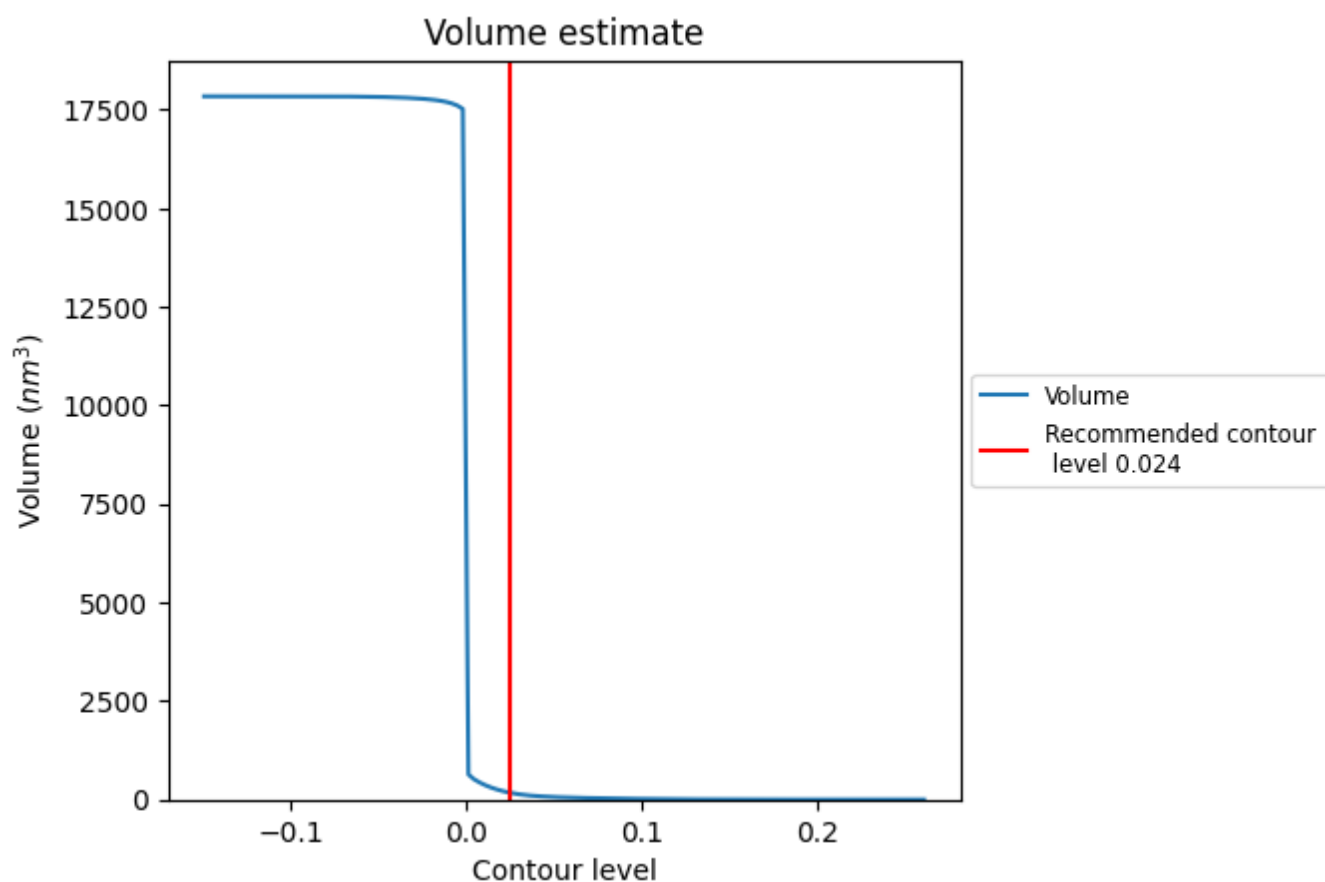
This section contains the results of statistical analysis of the map.

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.

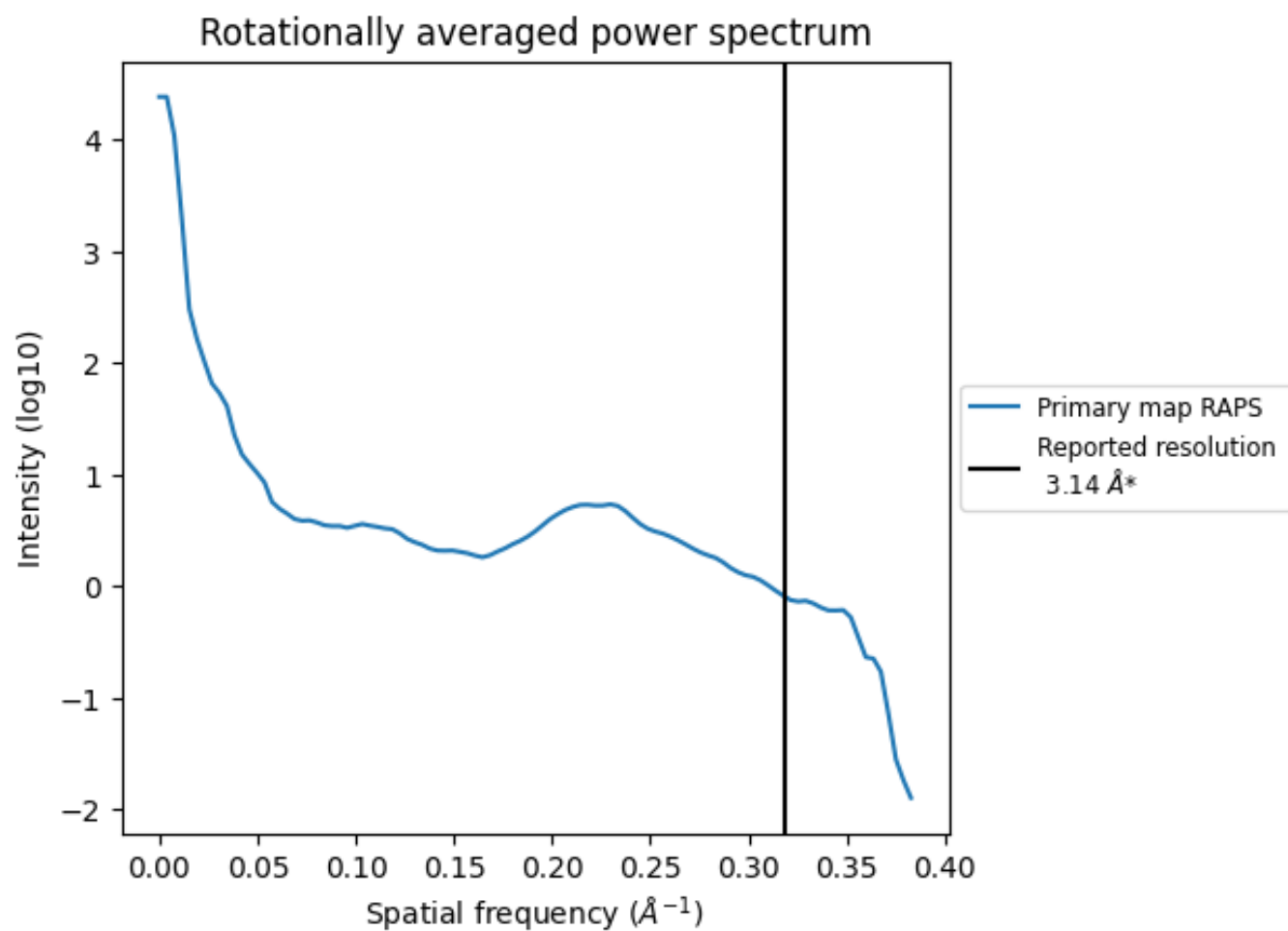
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



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

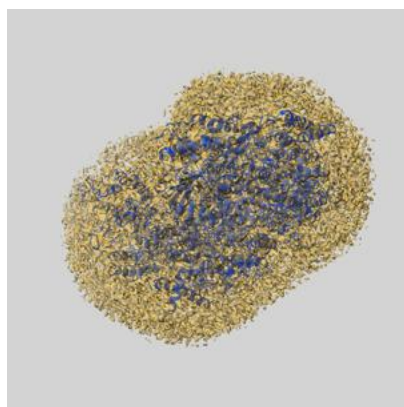
8 Fourier-Shell correlation

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

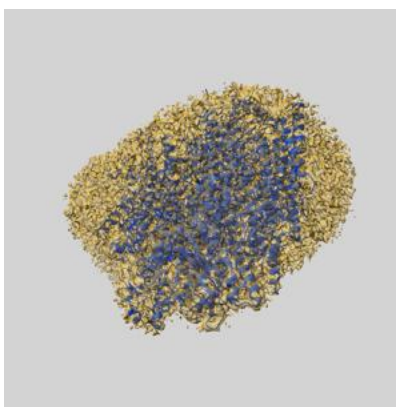
9 Map-model fit [i](#)

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](#).

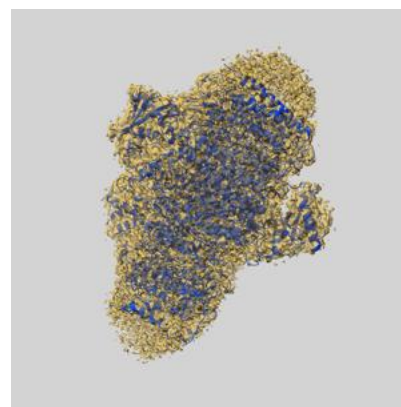
9.1 Map-model overlay [i](#)



X



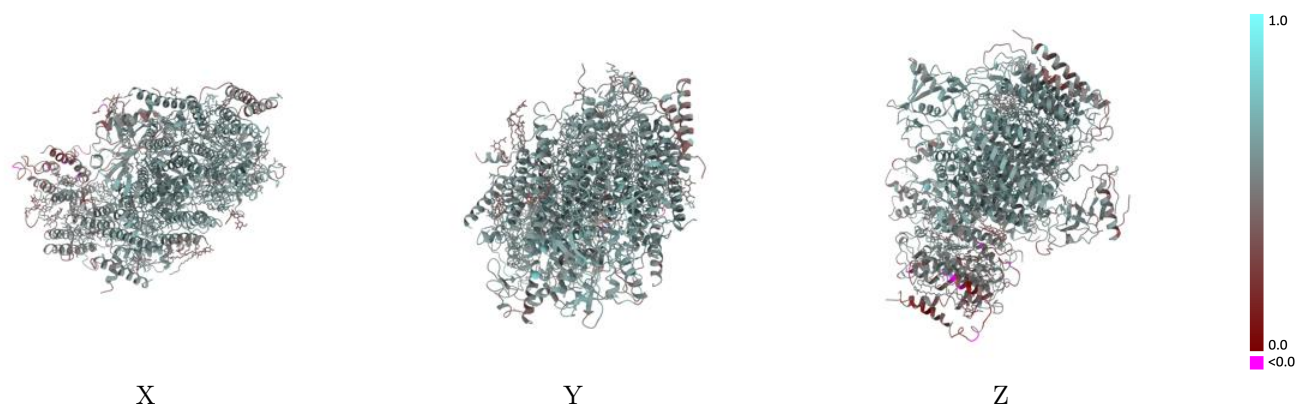
Y



Z

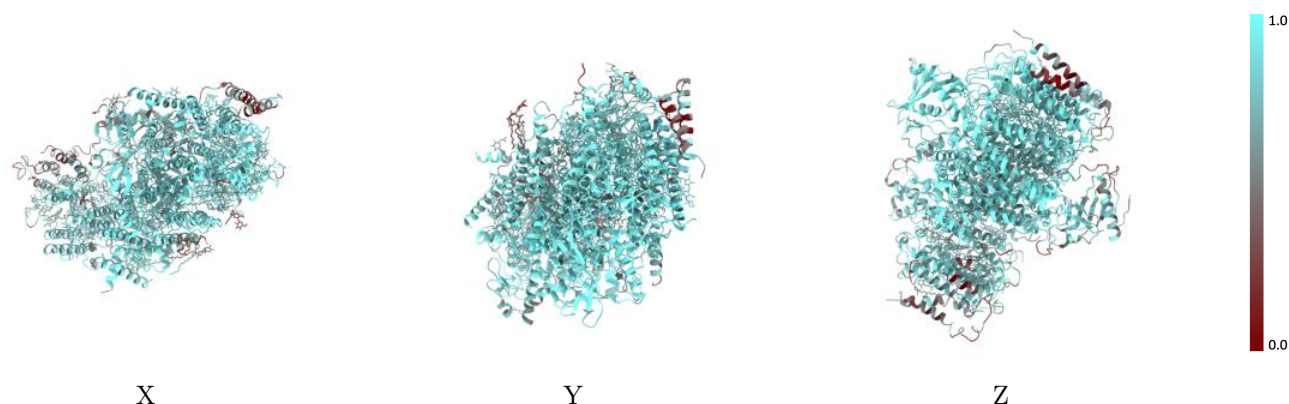
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



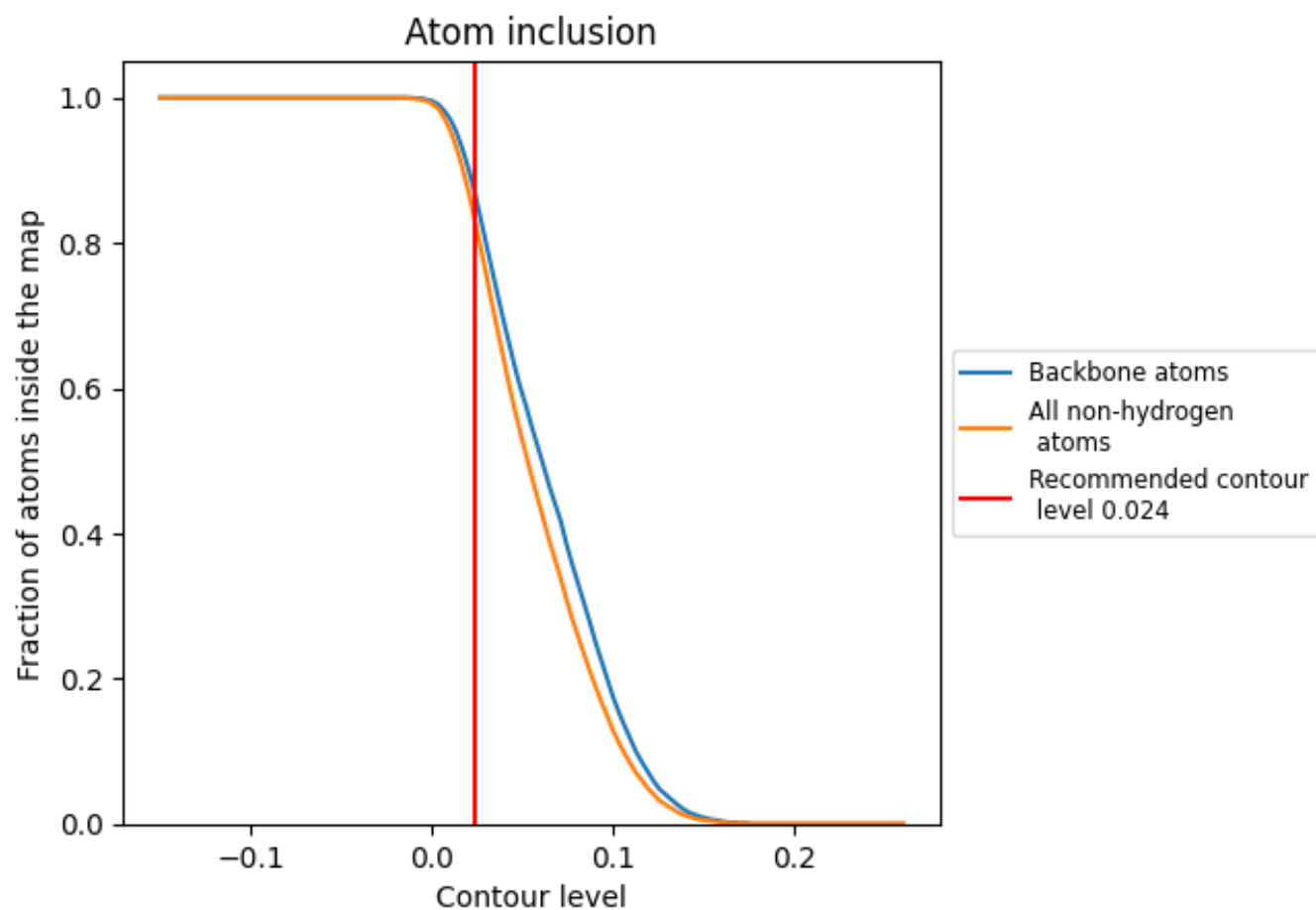
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	 0.8310	 0.5420
A	 0.6930	 0.4890
B	 0.5420	 0.4840
C	 0.4350	 0.4330
a	 0.8940	 0.5730
b	 0.8880	 0.5800
c	 0.8260	 0.5060
d	 0.9100	 0.5950
e	 0.7530	 0.4920
f	 0.8100	 0.5430
h	 0.8920	 0.5710
i	 0.8130	 0.5100
k	 0.6910	 0.4490
l	 0.7740	 0.5510
m	 0.6660	 0.5040
t	 0.7710	 0.5220
x	 0.8310	 0.5580
y	 0.3360	 0.2240
z	 0.4530	 0.3120

