



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:49 PM UTC

PDB ID : 9QEF / pdb_00009qef
EMDB ID : EMD-53065
Title : Respiratory supercomplex from Mycobacterium smegmatis with decylbiquinone
Authors : Kovalova, T.; Krol, S.; Brzezinski, P.; Hogbom, M.
Deposited on : 2025-03-09
Resolution : 2.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

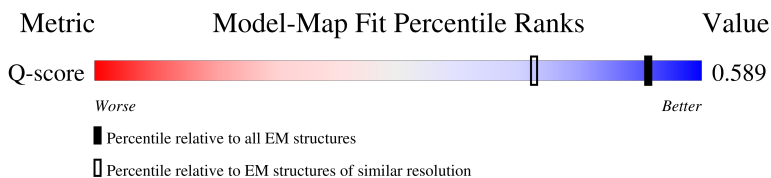
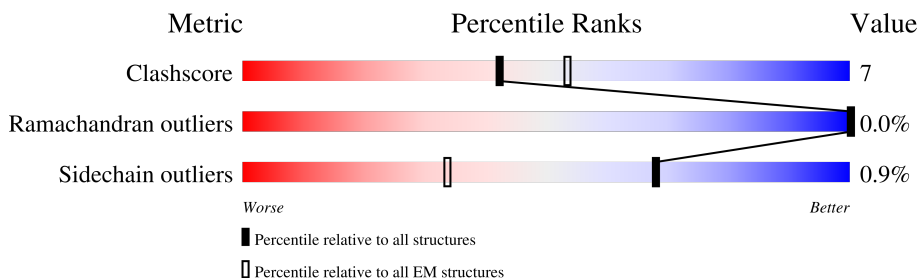
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	C	278	
1	O	278	
2	G	408	
2	M	408	

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Mol	Chain	Length	Quality of chain
3	H	556	
3	N	556	
4	I	100	
4	P	100	
5	J	203	
5	S	203	
6	K	139	
6	T	139	
7	L	575	
7	R	575	
8	Q	341	
8	X	341	
9	U	79	
9	Z	79	
10	V	157	
10	a	157	
11	W	186	
11	b	186	
12	Y	236	
12	c	236	
13	A	123	
13	E	123	
14	B	65	
14	F	65	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	HEA	R	603	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 49157 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 Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	223	Total	C	N	O	S	0	0
			1623	1008	289	314	12		
1	C	223	Total	C	N	O	S	0	0
			1623	1008	289	314	12		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	17	MET	-	initiating methionine	UNP A0R050
O	18	HIS	-	expression tag	UNP A0R050
O	19	HIS	-	expression tag	UNP A0R050
O	20	HIS	-	expression tag	UNP A0R050
O	21	HIS	-	expression tag	UNP A0R050
O	22	HIS	-	expression tag	UNP A0R050
O	23	HIS	-	expression tag	UNP A0R050
O	24	MET	-	expression tag	UNP A0R050
O	25	GLY	-	expression tag	UNP A0R050
O	26	SER	-	expression tag	UNP A0R050
C	17	MET	-	initiating methionine	UNP A0R050
C	18	HIS	-	expression tag	UNP A0R050
C	19	HIS	-	expression tag	UNP A0R050
C	20	HIS	-	expression tag	UNP A0R050
C	21	HIS	-	expression tag	UNP A0R050
C	22	HIS	-	expression tag	UNP A0R050
C	23	HIS	-	expression tag	UNP A0R050
C	24	MET	-	expression tag	UNP A0R050
C	25	GLY	-	expression tag	UNP A0R050
C	26	SER	-	expression tag	UNP A0R050

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	380	Total	C	N	O	S	0	0
			2967	1919	502	535	11		
2	G	380	Total	C	N	O	S	0	0
			2967	1919	502	535	11		

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	533	Total	C	N	O	S	0	0
			4167	2743	707	699	18		
3	H	533	Total	C	N	O	S	0	0
			4167	2743	707	699	18		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	547	LYS	-	expression tag	UNP A0R052
N	548	LEU	-	expression tag	UNP A0R052
N	549	ASP	-	expression tag	UNP A0R052
N	550	TYR	-	expression tag	UNP A0R052
N	551	LYS	-	expression tag	UNP A0R052
N	552	ASP	-	expression tag	UNP A0R052
N	553	ASP	-	expression tag	UNP A0R052
N	554	ASP	-	expression tag	UNP A0R052
N	555	ASP	-	expression tag	UNP A0R052
N	556	LYS	-	expression tag	UNP A0R052
H	547	LYS	-	expression tag	UNP A0R052
H	548	LEU	-	expression tag	UNP A0R052
H	549	ASP	-	expression tag	UNP A0R052
H	550	TYR	-	expression tag	UNP A0R052
H	551	LYS	-	expression tag	UNP A0R052
H	552	ASP	-	expression tag	UNP A0R052
H	553	ASP	-	expression tag	UNP A0R052
H	554	ASP	-	expression tag	UNP A0R052
H	555	ASP	-	expression tag	UNP A0R052
H	556	LYS	-	expression tag	UNP A0R052

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	73	Total	C	N	O	S	0	0
			586	385	107	90	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	73	Total	C	N	O	S	0	0
			586	385	107	90	4		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	initiating methionine	UNP A0QVH4
P	2	SER	-	expression tag	UNP A0QVH4
P	3	SER	-	expression tag	UNP A0QVH4
P	4	THR	-	expression tag	UNP A0QVH4
P	5	GLN	-	expression tag	UNP A0QVH4
P	6	ASP	-	expression tag	UNP A0QVH4
P	7	ARG	-	expression tag	UNP A0QVH4
P	8	SER	-	expression tag	UNP A0QVH4
P	9	GLN	-	expression tag	UNP A0QVH4
P	10	LEU	-	expression tag	UNP A0QVH4
P	11	ASP	-	expression tag	UNP A0QVH4
P	12	PRO	-	expression tag	UNP A0QVH4
P	13	GLU	-	expression tag	UNP A0QVH4
P	14	GLU	-	expression tag	UNP A0QVH4
P	15	GLN	-	expression tag	UNP A0QVH4
P	16	PRO	-	expression tag	UNP A0QVH4
P	17	VAL	-	expression tag	UNP A0QVH4
I	1	MET	-	initiating methionine	UNP A0QVH4
I	2	SER	-	expression tag	UNP A0QVH4
I	3	SER	-	expression tag	UNP A0QVH4
I	4	THR	-	expression tag	UNP A0QVH4
I	5	GLN	-	expression tag	UNP A0QVH4
I	6	ASP	-	expression tag	UNP A0QVH4
I	7	ARG	-	expression tag	UNP A0QVH4
I	8	SER	-	expression tag	UNP A0QVH4
I	9	GLN	-	expression tag	UNP A0QVH4
I	10	LEU	-	expression tag	UNP A0QVH4
I	11	ASP	-	expression tag	UNP A0QVH4
I	12	PRO	-	expression tag	UNP A0QVH4
I	13	GLU	-	expression tag	UNP A0QVH4
I	14	GLU	-	expression tag	UNP A0QVH4
I	15	GLN	-	expression tag	UNP A0QVH4
I	16	PRO	-	expression tag	UNP A0QVH4
I	17	VAL	-	expression tag	UNP A0QVH4

- Molecule 5 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	187	Total	C	N	O	S	0	0
			1465	982	234	242	7		
5	J	187	Total	C	N	O	S	0	0
			1465	982	234	242	7		

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
6	K	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	551	Total	C	N	O	S	0	0
			4369	2936	694	713	26		
7	L	551	Total	C	N	O	S	0	0
			4369	2936	694	713	26		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP A0A2U9PNL2
R	2	VAL	-	expression tag	UNP A0A2U9PNL2
R	3	ALA	-	expression tag	UNP A0A2U9PNL2
R	4	GLU	-	expression tag	UNP A0A2U9PNL2
R	5	ALA	-	expression tag	UNP A0A2U9PNL2
R	6	PRO	-	expression tag	UNP A0A2U9PNL2
R	7	PRO	-	expression tag	UNP A0A2U9PNL2
R	8	ILE	-	expression tag	UNP A0A2U9PNL2
R	9	GLY	-	expression tag	UNP A0A2U9PNL2
R	10	GLU	-	expression tag	UNP A0A2U9PNL2
R	11	LEU	-	expression tag	UNP A0A2U9PNL2
R	12	GLU	-	expression tag	UNP A0A2U9PNL2
R	13	ALA	-	expression tag	UNP A0A2U9PNL2
R	14	ARG	-	expression tag	UNP A0A2U9PNL2
R	15	ARG	-	expression tag	UNP A0A2U9PNL2
R	16	PRO	-	expression tag	UNP A0A2U9PNL2
R	17	PHE	-	expression tag	UNP A0A2U9PNL2
R	18	PRO	-	expression tag	UNP A0A2U9PNL2
R	19	GLU	-	expression tag	UNP A0A2U9PNL2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	20	ARG	-	expression tag	UNP A0A2U9PNL2
L	1	MET	-	initiating methionine	UNP A0A2U9PNL2
L	2	VAL	-	expression tag	UNP A0A2U9PNL2
L	3	ALA	-	expression tag	UNP A0A2U9PNL2
L	4	GLU	-	expression tag	UNP A0A2U9PNL2
L	5	ALA	-	expression tag	UNP A0A2U9PNL2
L	6	PRO	-	expression tag	UNP A0A2U9PNL2
L	7	PRO	-	expression tag	UNP A0A2U9PNL2
L	8	ILE	-	expression tag	UNP A0A2U9PNL2
L	9	GLY	-	expression tag	UNP A0A2U9PNL2
L	10	GLU	-	expression tag	UNP A0A2U9PNL2
L	11	LEU	-	expression tag	UNP A0A2U9PNL2
L	12	GLU	-	expression tag	UNP A0A2U9PNL2
L	13	ALA	-	expression tag	UNP A0A2U9PNL2
L	14	ARG	-	expression tag	UNP A0A2U9PNL2
L	15	ARG	-	expression tag	UNP A0A2U9PNL2
L	16	PRO	-	expression tag	UNP A0A2U9PNL2
L	17	PHE	-	expression tag	UNP A0A2U9PNL2
L	18	PRO	-	expression tag	UNP A0A2U9PNL2
L	19	GLU	-	expression tag	UNP A0A2U9PNL2
L	20	ARG	-	expression tag	UNP A0A2U9PNL2

- Molecule 8 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	287	Total	C	N	O	S	0	0
			2293	1487	378	419	9		
8	X	292	Total	C	N	O	S	0	0
			2328	1508	383	427	10		

- Molecule 9 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	66	Total	C	N	O	S	0	0
			499	329	84	85	1		
9	Z	67	Total	C	N	O	S	0	0
			507	334	85	86	2		

- Molecule 10 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	143	Total	C	N	O	S	0	0
			1024	647	174	201	2		
10	a	143	Total	C	N	O	S	0	0
			1024	647	174	201	2		

- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	148	Total	C	N	O	S	0	0
			1075	664	180	230	1		
11	b	149	Total	C	N	O	S	0	0
			1083	670	181	231	1		

- Molecule 12 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	25	Total	C	N	O	S	0	0
			168	103	26	38	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

- Molecule 13 is a protein called Co-purified transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	87	Total	C	N	O	S	0	0
			660	427	121	110	2		
13	A	83	Total	C	N	O	S	0	0
			620	404	109	106	1		

There are 2 discrepancies between the modelled and reference sequences:

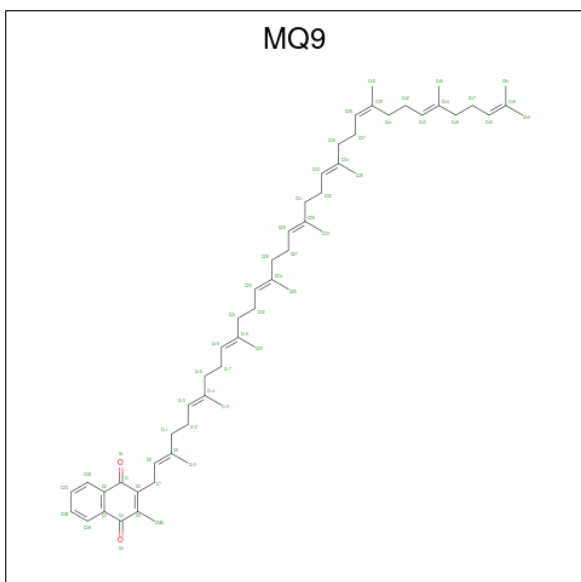
Chain	Residue	Modelled	Actual	Comment	Reference
E	126	ALA	VAL	conflict	UNP A0A653FDI6
A	126	ALA	VAL	conflict	UNP A0A653FDI6

- Molecule 14 is a protein called Co-purified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	F	55	Total	C	N	O	0	0
			417	266	68	83		
14	B	55	Total	C	N	O	0	0
			417	266	68	83		

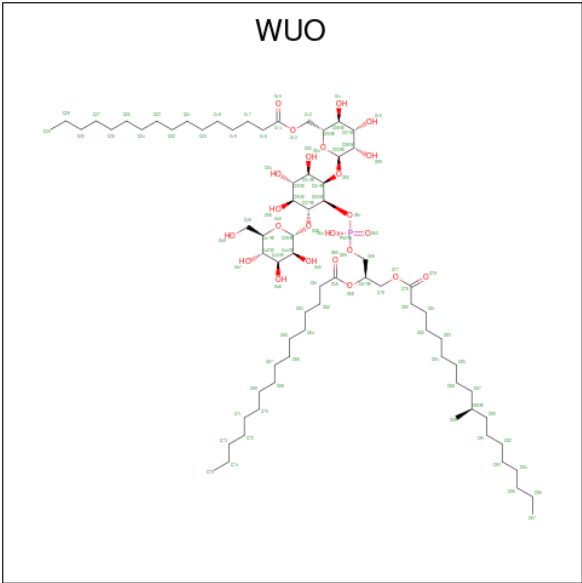
-
- The chemical structure of HEC (Hydroxyethylchlorin) is a complex macrocyclic molecule. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is highly substituted with various side chains and functional groups. Key features include:
- Central Core:** A central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring.
 - Side Chains:** Numerous side chains are attached to the ring, including CMA, C3A, C4A, C1A, C2A, C3B, C4B, C1B, C2B, C3C, C4C, C1C, C2C, C3D, C4D, C1D, C2D, C3E, C4E, C1E, C2E, C3F, C4F, C1F, C2F, C3G, C4G, C1G, C2G, C3H, C4H, C1H, C2H, C3I, C4I, C1I, C2I, C3J, C4J, C1J, C2J, C3K, C4K, C1K, C2K, C3L, C4L, C1L, C2L, C3M, C4M, C1M, C2M, C3N, C4N, C1N, C2N, C3O, C4O, C1O, C2O, C3P, C4P, C1P, C2P, C3Q, C4Q, C1Q, C2Q, C3R, C4R, C1R, C2R, C3S, C4S, C1S, C2S, C3T, C4T, C1T, C2T, C3U, C4U, C1U, C2U, C3V, C4V, C1V, C2V, C3W, C4W, C1W, C2W, C3X, C4X, C1X, C2X, C3Y, C4Y, C1Y, C2Y, C3Z, C4Z, C1Z, C2Z, C3AA, C4AA, C1AA, C2AA, C3AB, C4AB, C1AB, C2AB, C3AC, C4AC, C1AC, C2AC, C3AD, C4AD, C1AD, C2AD, C3AE, C4AE, C1AE, C2AE, C3AF, C4AF, C1AF, C2AF, C3AG, C4AG, C1AG, C2AG, C3AH, C4AH, C1AH, C2AH, C3AI, C4AI, C1AI, C2AI, C3AJ, C4AJ, C1AJ, C2AJ, C3AK, C4AK, C1AK, C2AK, C3AL, C4AL, C1AL, C2AL, C3AM, C4AM, C1AM, C2AM, C3AN, C4AN, C1AN, C2AN, C3AO, C4AO, C1AO, C2AO, C3AP, C4AP, C1AP, C2AP, C3AQ, C4AQ, 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- Molecule 16 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



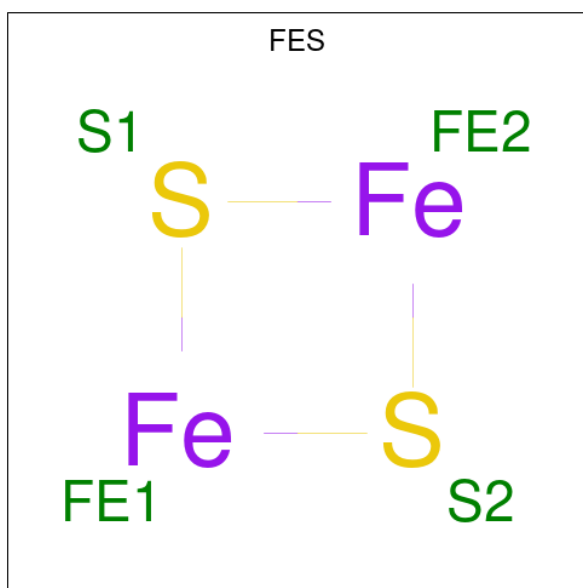
Mol	Chain	Residues	Atoms			AltConf
16	O	1	Total	C	O	0
			58	56	2	
16	N	1	Total	C	O	0
			58	56	2	
16	N	1	Total	C	O	0
			58	56	2	
16	T	1	Total	C	O	0
			58	56	2	
16	C	1	Total	C	O	0
			58	56	2	
16	C	1	Total	C	O	0
			58	56	2	
16	H	1	Total	C	O	0
			58	56	2	

- Molecule 17 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (CCD ID: WUO) (formula: $C_{72}H_{135}O_{24}P$).



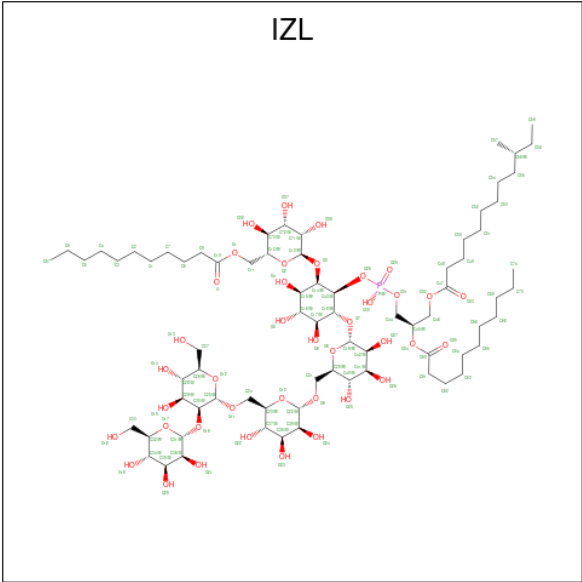
Mol	Chain	Residues	Atoms				AltConf
17	O	1	Total	C	O	P	0
			97	72	24	1	
17	P	1	Total	C	O	P	0
			97	72	24	1	
17	C	1	Total	C	O	P	0
			97	72	24	1	
17	I	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



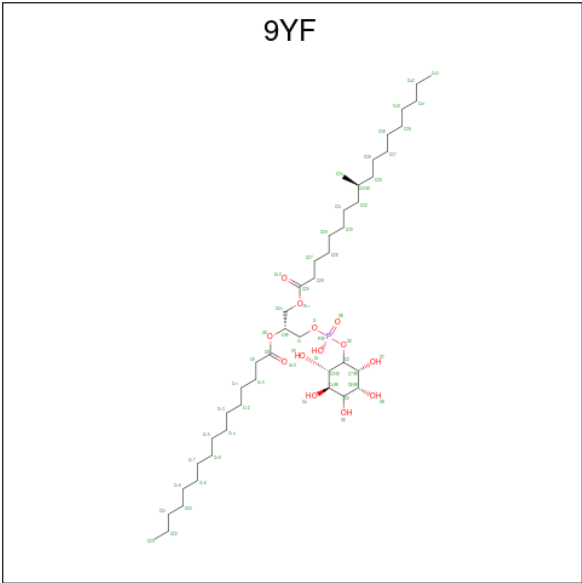
Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	Fe	S	0
			4	2	2	
18	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 19 is [(2 {R})-3-[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (CCD ID: IZL) (formula: $\text{C}_{74}\text{H}_{133}\text{O}_{39}\text{P}$).



Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			114	74	39	1	
19	G	1	Total	C	O	P	0
			114	74	39	1	

- Molecule 20 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: C₄₄H₈₅O₁₃P).



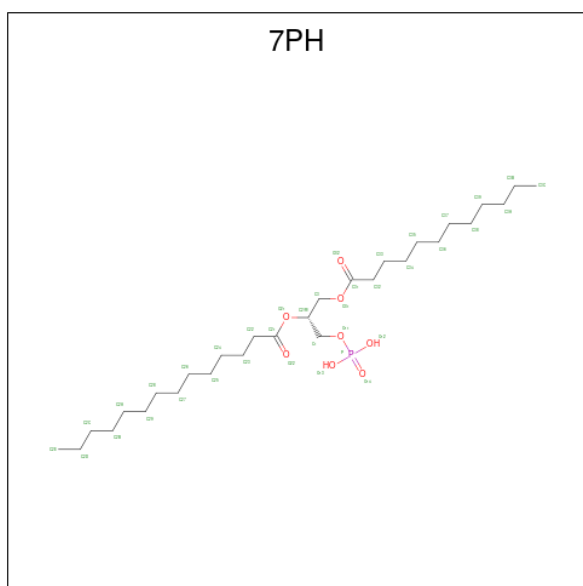
Mol	Chain	Residues	Atoms				AltConf
20	M	1	Total	C	O	P	0
			58	44	13	1	

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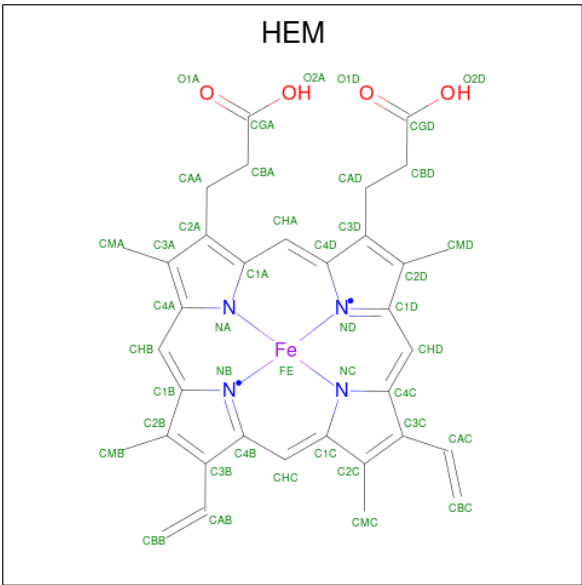
Mol	Chain	Residues	Atoms				AltConf
20	W	1	Total	C	O	P	0
			58	44	13	1	
20	G	1	Total	C	O	P	0
			58	44	13	1	
20	b	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 21 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: $C_{29}H_{57}O_8P$).



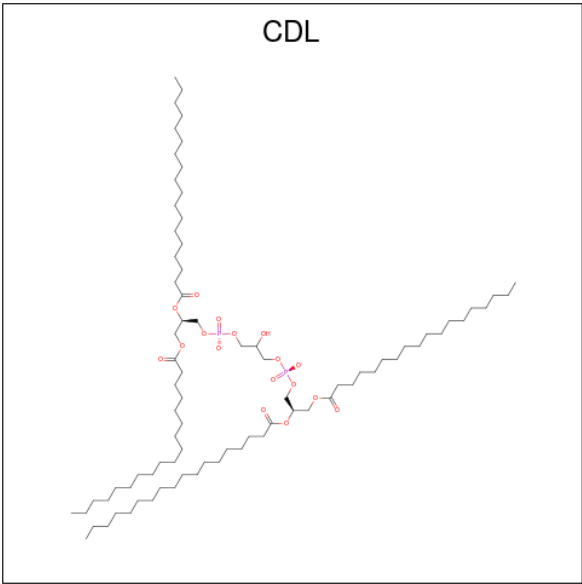
Mol	Chain	Residues	Atoms				AltConf
21	M	1	Total	C	O	P	0
			38	29	8	1	
21	S	1	Total	C	O	P	0
			38	29	8	1	
21	G	1	Total	C	O	P	0
			38	29	8	1	
21	G	1	Total	C	O	P	0
			38	29	8	1	
21	H	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 22 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



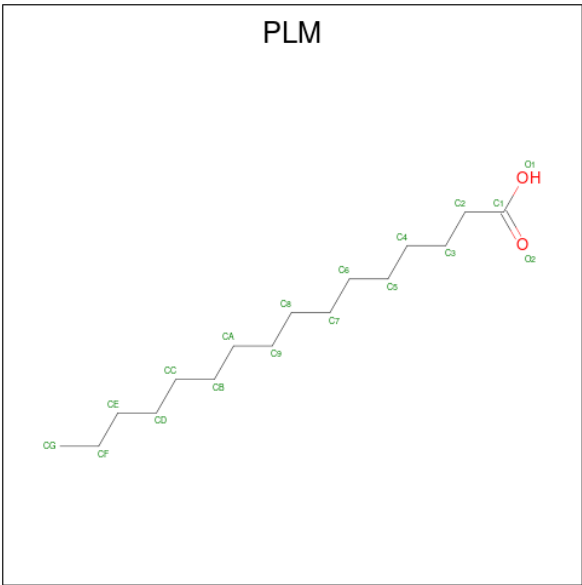
Mol	Chain	Residues	Atoms					AltConf
22	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 23 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



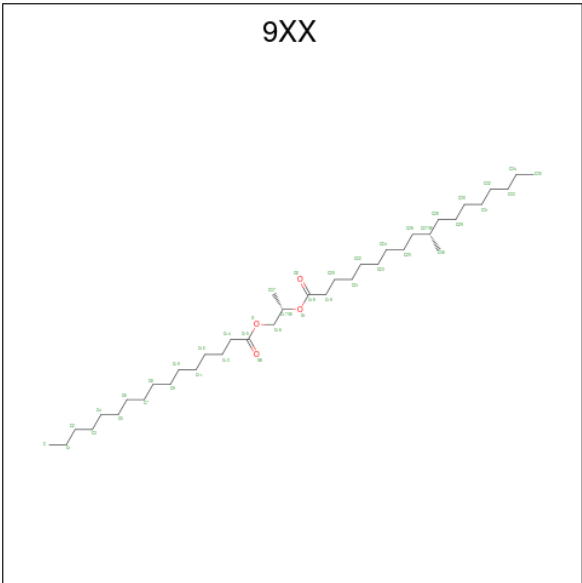
Mol	Chain	Residues	Atoms				AltConf
23	N	1	Total	C	O	P	0
			74	55	17	2	
23	N	1	Total	C	O	P	0
			77	58	17	2	
23	N	1	Total	C	O	P	0
			79	60	17	2	
23	P	1	Total	C	O	P	0
			77	58	17	2	
23	P	1	Total	C	O	P	0
			77	58	17	2	
23	T	1	Total	C	O	P	0
			79	60	17	2	
23	R	1	Total	C	O	P	0
			77	58	17	2	
23	R	1	Total	C	O	P	0
			77	58	17	2	
23	G	1	Total	C	O	P	0
			79	60	17	2	
23	H	1	Total	C	O	P	0
			74	55	17	2	
23	H	1	Total	C	O	P	0
			77	58	17	2	
23	H	1	Total	C	O	P	0
			79	60	17	2	
23	I	1	Total	C	O	P	0
			77	58	17	2	
23	I	1	Total	C	O	P	0
			77	58	17	2	
23	K	1	Total	C	O	P	0
			79	60	17	2	
23	L	1	Total	C	O	P	0
			79	60	17	2	
23	L	1	Total	C	O	P	0
			77	58	17	2	

- Molecule 24 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



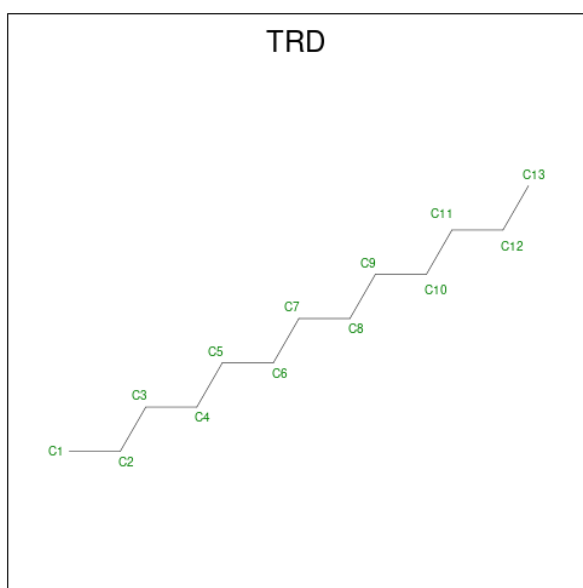
Mol	Chain	Residues	Atoms			AltConf
24	N	1	Total	C	O	0
			11	10	1	
24	W	1	Total	C	O	0
			11	10	1	
24	L	1	Total	C	O	0
			11	10	1	
24	c	1	Total	C	O	0
			11	10	1	

- Molecule 25 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C₃₈H₇₄O₄).



Mol	Chain	Residues	Atoms			AltConf
25	N	1	Total	C	O	0
			32	28	4	
25	W	1	Total	C	O	0
			42	38	4	
25	b	1	Total	C	O	0
			32	28	4	
25	c	1	Total	C	O	0
			32	28	4	

- Molecule 26 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



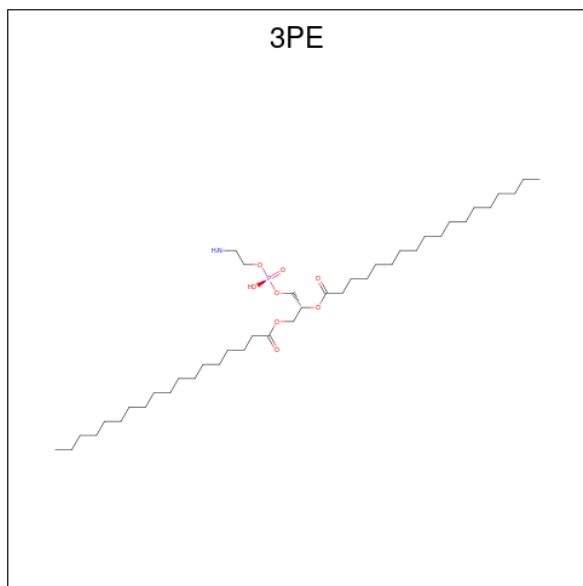
Mol	Chain	Residues	Atoms		AltConf
26	S	1	Total	C	0
			13	13	
26	T	1	Total	C	0
			13	13	
26	R	1	Total	C	0
			13	13	
26	R	1	Total	C	0
			13	13	
26	Q	1	Total	C	0
			13	13	
26	J	1	Total	C	0
			13	13	
26	K	1	Total	C	0
			13	13	
26	L	1	Total	C	0
			13	13	

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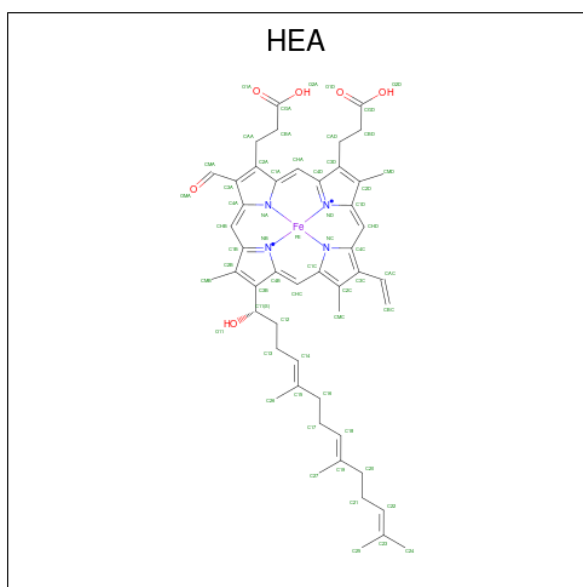
Mol	Chain	Residues	Atoms		AltConf
26	L	1	Total	C	0
			13	13	
26	X	1	Total	C	0
			13	13	

- Molecule 27 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
27	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	J	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 28 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
28	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
28	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
28	L	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
28	L	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 29 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
29	R	1	Total	Cu	0
			1	1	
29	Q	2	Total	Cu	0
			2	2	
29	L	1	Total	Cu	0
			1	1	
29	X	2	Total	Cu	0
			2	2	

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	R	1	Total	Mg	0
			1	1	

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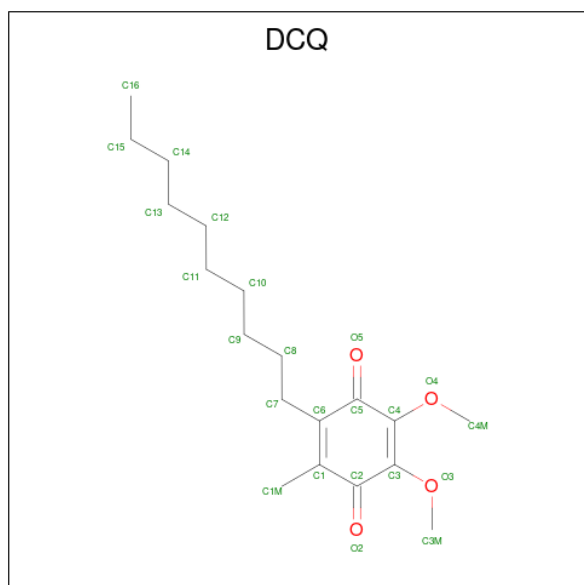
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Mol	Chain	Residues	Atoms		AltConf
30	L	1	Total	Mg	0
			1	1	

- Molecule 31 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
31	R	1	Total	Ca	0
			1	1	
31	L	1	Total	Ca	0
			1	1	

- Molecule 32 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: C₁₉H₃₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	H	1	Total	C	O	0
			23	19	4	

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	O	46	Total	O	0
			46	46	
33	M	54	Total	O	0
			54	54	

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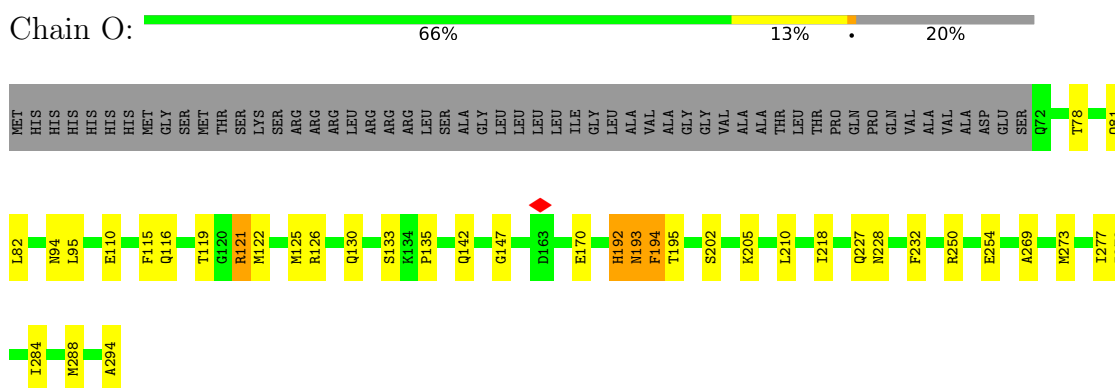
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Mol	Chain	Residues	Atoms		AltConf
33	N	75	Total 75	O 75	0
33	P	6	Total 6	O 6	0
33	S	3	Total 3	O 3	0
33	T	10	Total 10	O 10	0
33	R	51	Total 51	O 51	0
33	Q	23	Total 23	O 23	0
33	W	6	Total 6	O 6	0
33	C	54	Total 54	O 54	0
33	G	61	Total 61	O 61	0
33	H	90	Total 90	O 90	0
33	I	6	Total 6	O 6	0
33	J	4	Total 4	O 4	0
33	K	9	Total 9	O 9	0
33	L	52	Total 52	O 52	0
33	X	29	Total 29	O 29	0
33	Z	2	Total 2	O 2	0
33	a	2	Total 2	O 2	0
33	b	10	Total 10	O 10	0
33	c	1	Total 1	O 1	0
33	F	6	Total 6	O 6	0
33	B	6	Total 6	O 6	0

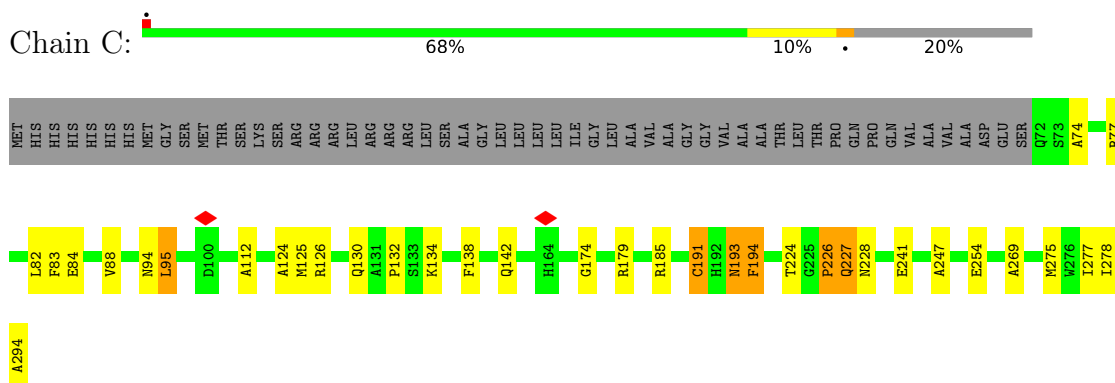
3 Residue-property plots

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.

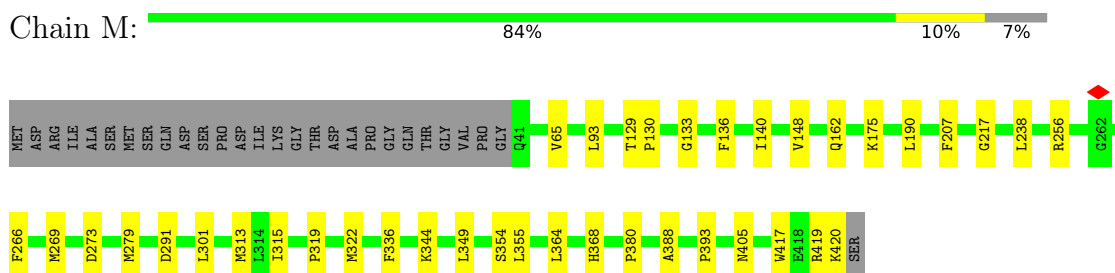
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit



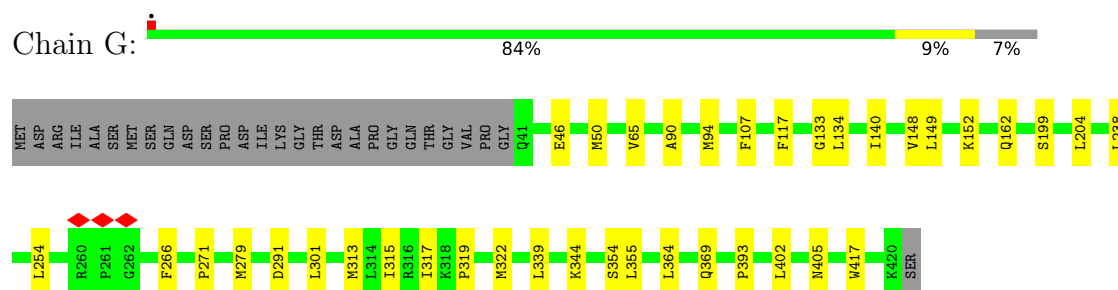
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit



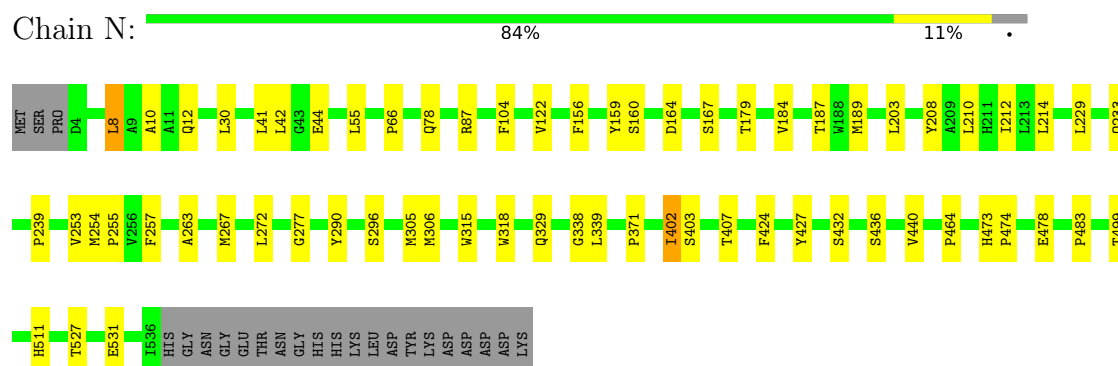
- Molecule 2: Cytochrome bc1 complex cytochrome c subunit



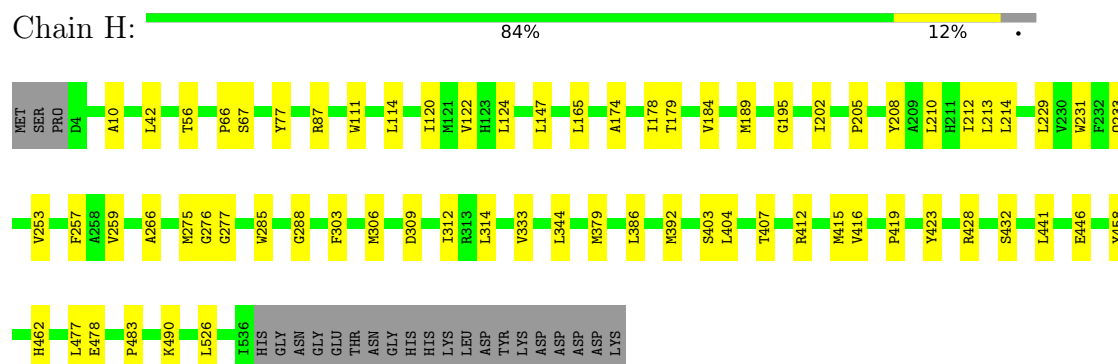
- Molecule 2: Cytochrome bc1 complex cytochrome c subunit



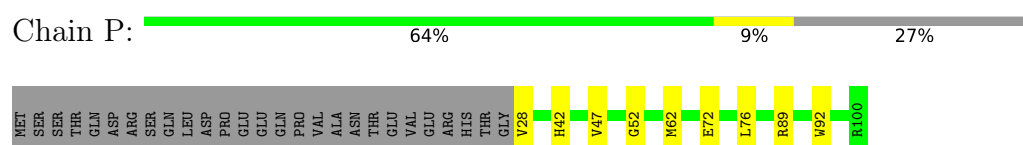
- Molecule 3: Cytochrome bc1 complex cytochrome b subunit



- Molecule 3: Cytochrome bc1 complex cytochrome b subunit

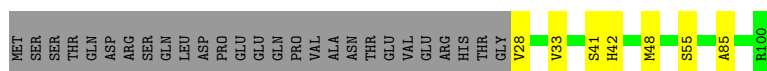


- Molecule 4: Transmembrane protein

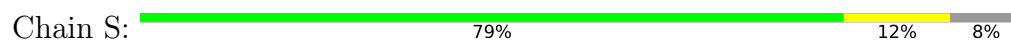


- Molecule 4: Transmembrane protein

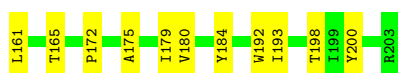




- Molecule 5: Probable cytochrome c oxidase subunit 3



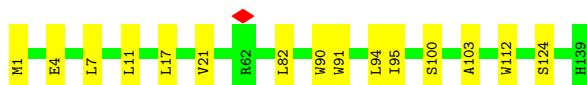
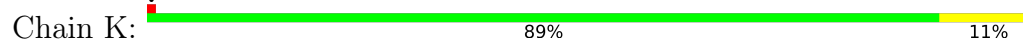
- Molecule 5: Probable cytochrome c oxidase subunit 3



- Molecule 6: Cytochrome c oxidase polypeptide 4



- Molecule 6: Cytochrome c oxidase polypeptide 4



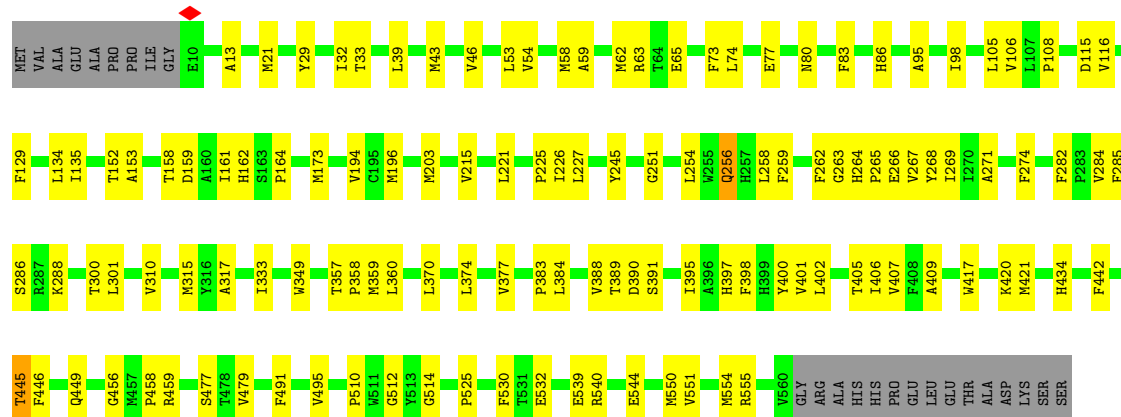
- Molecule 7: Cytochrome c oxidase subunit 1





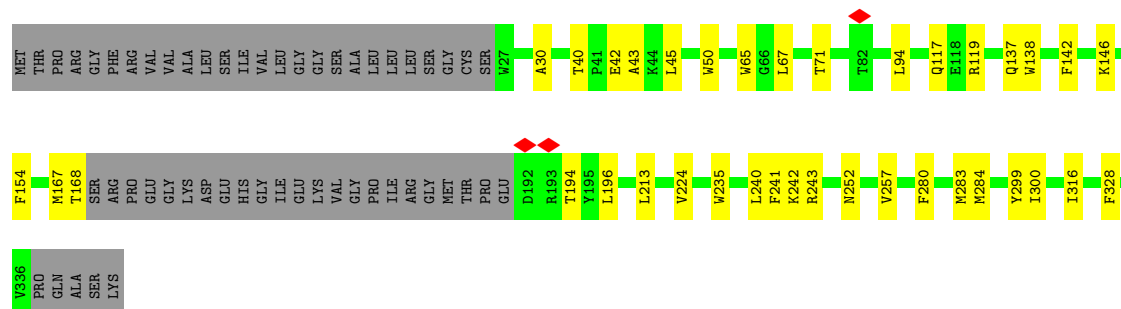
• Molecule 7: Cytochrome c oxidase subunit 1

Chain L: 74% 22%



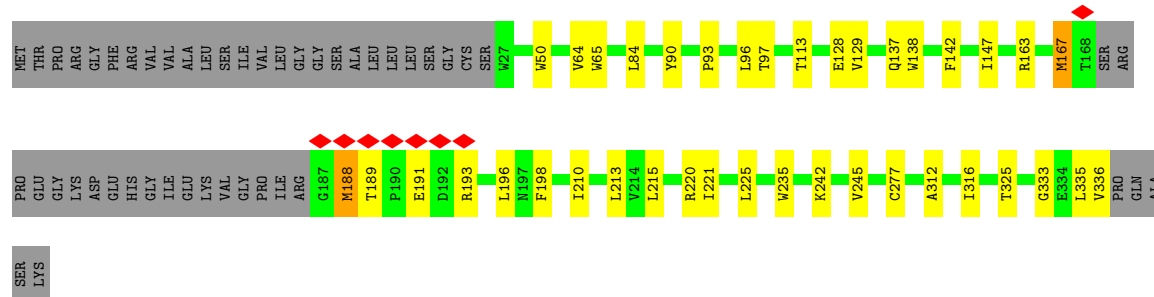
• Molecule 8: cytochrome-c oxidase

Chain Q: 73% 11% 16%

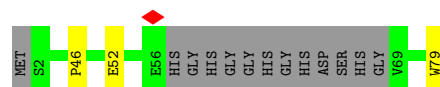
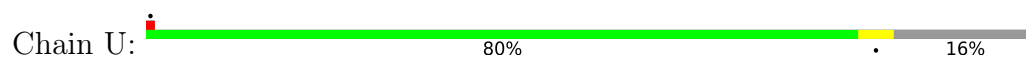


• Molecule 8: cytochrome-c oxidase

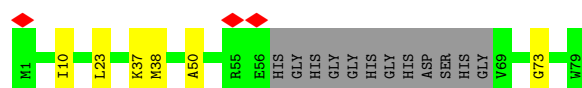
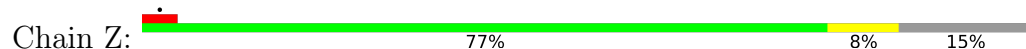
Chain X: 74% 11% 14%



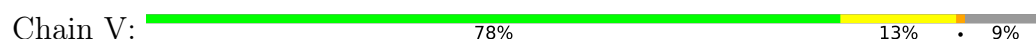
• Molecule 9: Cytochrome c oxidase subunit



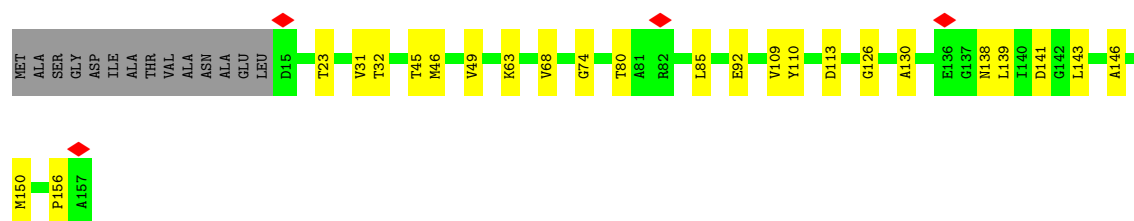
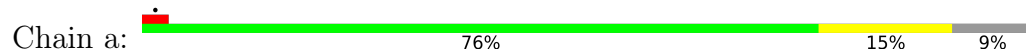
- Molecule 9: Cytochrome c oxidase subunit



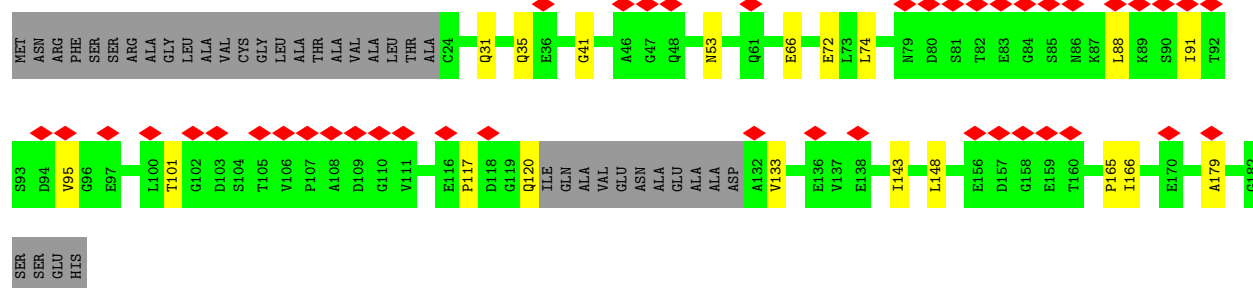
- Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575



- Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575



- Molecule 11: LpqE protein



- Molecule 11: LpqE protein



-
- Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis lists amino acids: MET, TRP, GLY, VAL, ALA, ASP, LYS, LYS, LYS, LYS, Q11, L20, S21, G22, D23, D24, D25, T29, E30, L39, A51, L54, and R65. The LYS residues at positions 8, 9, and 10 show the highest information content, with LYS at position 9 being the most conserved. Red diamonds are placed above the LYS residues at positions 8, 9, 10, 11, and 12.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.831	Depositor
Minimum map value	-0.397	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.129	Depositor
Map size (Å)	445.5, 445.5, 445.5	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WUO, 7PH, DCQ, CU, IZL, HEA, MG, HEC, TRD, MQ9, CA, FES, CDL, HEM, 9YF, 3PE, 9XX, PLM

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	C	0.34	2/1660 (0.1%)	0.49	3/2250 (0.1%)
1	O	0.44	3/1660 (0.2%)	0.62	5/2250 (0.2%)
2	G	0.19	0/3046	0.32	0/4129
2	M	0.14	0/3046	0.27	0/4129
3	H	0.24	0/4299	0.32	0/5862
3	N	0.20	0/4299	0.32	2/5862 (0.0%)
4	I	0.13	0/606	0.25	0/825
4	P	0.12	0/606	0.21	0/825
5	J	0.19	0/1513	0.29	0/2066
5	S	0.20	0/1513	0.33	0/2066
6	K	0.15	0/1112	0.28	0/1524
6	T	0.18	0/1112	0.31	0/1524
7	L	0.21	0/4529	0.38	0/6187
7	R	0.21	0/4529	0.36	0/6187
8	Q	0.14	0/2356	0.27	0/3207
8	X	0.15	0/2392	0.33	0/3256
9	U	0.11	0/515	0.20	0/704
9	Z	0.11	0/523	0.25	0/714
10	V	0.23	0/1042	0.34	0/1423
10	a	0.14	0/1042	0.28	0/1423
11	W	0.14	0/1092	0.31	0/1497
11	b	0.12	0/1100	0.32	0/1508
12	Y	0.12	0/175	0.26	0/244
12	c	0.14	0/175	0.35	0/244
13	A	0.10	0/632	0.33	0/859
13	E	0.13	0/673	0.34	0/912
14	B	0.14	0/429	0.34	0/592
14	F	0.33	0/429	0.57	0/592
All	All	0.21	5/46105 (0.0%)	0.35	10/62861 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	194	PHE	C-N	6.10	1.41	1.33
1	C	95	LEU	C-N	-5.98	1.24	1.33
1	O	228	ASN	C-N	-5.16	1.23	1.33
1	C	228	ASN	C-N	-5.14	1.23	1.33
1	O	192	HIS	CE1-NE2	-5.07	1.27	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	192	HIS	CA-C-O	-7.91	109.70	119.28
1	C	228	ASN	N-CA-C	7.24	121.71	113.02
3	N	187	THR	CA-C-N	-6.72	110.75	120.29
3	N	187	THR	C-N-CA	-6.72	110.75	120.29
1	C	227	GLN	N-CA-C	-6.08	98.53	108.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1623	0	1561	31	0
1	O	1623	0	1560	32	0
2	G	2967	0	2976	27	0
2	M	2967	0	2976	30	0
3	H	4167	0	4192	53	0
3	N	4167	0	4192	44	0
4	I	586	0	578	5	0
4	P	586	0	578	6	0
5	J	1465	0	1462	25	0
5	S	1465	0	1462	31	0
6	K	1077	0	1058	14	0
6	T	1077	0	1058	15	0
7	L	4369	0	4346	107	0
7	R	4369	0	4346	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Q	2293	0	2242	26	0
8	X	2328	0	2274	30	0
9	U	499	0	504	3	0
9	Z	507	0	516	5	0
10	V	1024	0	1035	14	0
10	a	1024	0	1035	16	0
11	W	1075	0	1044	14	0
11	b	1083	0	1055	12	0
12	Y	168	0	151	1	0
12	c	168	0	151	1	0
13	A	620	0	640	3	0
13	E	660	0	685	7	0
14	B	417	0	393	4	0
14	F	417	0	393	17	0
15	C	86	0	61	6	0
15	O	86	0	60	4	0
16	C	116	0	160	4	0
16	H	58	0	80	10	0
16	N	116	0	160	8	0
16	O	58	0	80	3	0
16	T	58	0	80	7	0
17	C	97	0	0	0	0
17	I	97	0	0	0	0
17	O	97	0	0	0	0
17	P	97	0	0	0	0
18	G	4	0	0	0	0
18	M	4	0	0	0	0
19	G	114	0	0	0	0
19	M	114	0	0	0	0
20	G	58	0	0	0	0
20	M	58	0	0	0	0
20	W	58	0	0	0	0
20	b	58	0	0	0	0
21	G	76	0	110	3	0
21	H	38	0	55	1	0
21	M	38	0	55	3	0
21	S	38	0	55	2	0
22	H	86	0	60	6	0
22	N	86	0	60	5	0
23	G	79	0	105	1	0
23	H	230	0	295	6	0
23	I	154	0	196	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K	79	0	105	2	0
23	L	156	0	203	6	0
23	N	230	0	295	9	0
23	P	154	0	196	13	0
23	R	154	0	196	6	0
23	T	79	0	105	5	0
24	L	11	0	16	0	0
24	N	11	0	16	1	0
24	W	11	0	16	0	0
24	c	11	0	16	0	0
25	N	32	0	0	0	0
25	W	42	0	0	0	0
25	b	32	0	0	0	0
25	c	32	0	0	0	0
26	J	13	0	28	1	0
26	K	13	0	28	0	0
26	L	26	0	56	0	0
26	Q	13	0	28	1	0
26	R	26	0	56	0	0
26	S	13	0	28	0	0
26	T	13	0	28	0	0
26	X	13	0	28	0	0
27	J	32	0	38	0	0
27	S	32	0	38	0	0
28	L	120	0	108	12	0
28	R	120	0	108	38	0
29	L	1	0	0	0	0
29	Q	2	0	0	0	0
29	R	1	0	0	0	0
29	X	2	0	0	1	0
30	L	1	0	0	0	0
30	R	1	0	0	0	0
31	L	1	0	0	0	0
31	R	1	0	0	0	0
32	H	23	0	30	0	0
33	B	6	0	0	0	0
33	C	54	0	0	0	0
33	F	6	0	0	0	0
33	G	61	0	0	0	0
33	H	90	0	0	0	0
33	I	6	0	0	0	0
33	J	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	K	9	0	0	0	0
33	L	52	0	0	0	0
33	M	54	0	0	0	0
33	N	75	0	0	0	0
33	O	46	0	0	0	0
33	P	6	0	0	0	0
33	Q	23	0	0	0	0
33	R	51	0	0	0	0
33	S	3	0	0	0	0
33	T	10	0	0	0	0
33	W	6	0	0	0	0
33	X	29	0	0	0	0
33	Z	2	0	0	0	0
33	a	2	0	0	0	0
33	b	10	0	0	0	0
33	c	1	0	0	0	0
All	All	49157	0	47901	646	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 7.

The worst 5 of 646 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)
7:R:264:HIS:CE1	7:R:268:TYR:HE2	1.42	1.35
7:L:264:HIS:NE2	7:L:268:TYR:HE2	1.31	1.28
7:L:264:HIS:CE1	7:L:268:TYR:HE2	1.54	1.25
7:R:264:HIS:NE2	7:R:268:TYR:HE2	1.39	1.19
7:R:264:HIS:CE1	7:R:268:TYR:CE2	2.31	1.19

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	C	221/278 (80%)	214 (97%)	6 (3%)	1 (0%)	24	43
1	O	221/278 (80%)	210 (95%)	11 (5%)	0	100	100
2	G	378/408 (93%)	366 (97%)	12 (3%)	0	100	100
2	M	378/408 (93%)	368 (97%)	10 (3%)	0	100	100
3	H	531/556 (96%)	519 (98%)	12 (2%)	0	100	100
3	N	531/556 (96%)	521 (98%)	10 (2%)	0	100	100
4	I	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
4	P	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
5	J	185/203 (91%)	183 (99%)	2 (1%)	0	100	100
5	S	185/203 (91%)	183 (99%)	2 (1%)	0	100	100
6	K	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
6	T	137/139 (99%)	134 (98%)	3 (2%)	0	100	100
7	L	549/575 (96%)	534 (97%)	15 (3%)	0	100	100
7	R	549/575 (96%)	535 (97%)	14 (3%)	0	100	100
8	Q	283/341 (83%)	274 (97%)	9 (3%)	0	100	100
8	X	288/341 (84%)	277 (96%)	11 (4%)	0	100	100
9	U	62/79 (78%)	61 (98%)	1 (2%)	0	100	100
9	Z	63/79 (80%)	62 (98%)	1 (2%)	0	100	100
10	V	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
10	a	141/157 (90%)	139 (99%)	2 (1%)	0	100	100
11	W	144/186 (77%)	138 (96%)	6 (4%)	0	100	100
11	b	145/186 (78%)	143 (99%)	2 (1%)	0	100	100
12	Y	23/236 (10%)	21 (91%)	2 (9%)	0	100	100
12	c	23/236 (10%)	22 (96%)	1 (4%)	0	100	100
13	A	79/123 (64%)	76 (96%)	3 (4%)	0	100	100
13	E	83/123 (68%)	78 (94%)	5 (6%)	0	100	100
14	B	53/65 (82%)	50 (94%)	3 (6%)	0	100	100
14	F	53/65 (82%)	48 (91%)	5 (9%)	0	100	100
All	All	5725/6892 (83%)	5569 (97%)	155 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	194	PHE

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	C	163/206 (79%)	161 (99%)	2 (1%)	63	83
1	O	163/206 (79%)	159 (98%)	4 (2%)	42	69
2	G	311/333 (93%)	310 (100%)	1 (0%)	86	94
2	M	311/333 (93%)	310 (100%)	1 (0%)	86	94
3	H	428/448 (96%)	427 (100%)	1 (0%)	87	95
3	N	428/448 (96%)	422 (99%)	6 (1%)	59	81
4	I	58/83 (70%)	58 (100%)	0	100	100
4	P	58/83 (70%)	56 (97%)	2 (3%)	32	60
5	J	149/161 (92%)	148 (99%)	1 (1%)	76	89
5	S	149/161 (92%)	147 (99%)	2 (1%)	61	82
6	K	106/106 (100%)	106 (100%)	0	100	100
6	T	106/106 (100%)	104 (98%)	2 (2%)	50	76
7	L	453/471 (96%)	449 (99%)	4 (1%)	70	87
7	R	453/471 (96%)	449 (99%)	4 (1%)	70	87
8	Q	245/288 (85%)	242 (99%)	3 (1%)	63	83
8	X	249/288 (86%)	246 (99%)	3 (1%)	63	83
9	U	51/59 (86%)	51 (100%)	0	100	100
9	Z	52/59 (88%)	51 (98%)	1 (2%)	50	76
10	V	105/114 (92%)	103 (98%)	2 (2%)	50	76
10	a	105/114 (92%)	105 (100%)	0	100	100
11	W	120/146 (82%)	120 (100%)	0	100	100
11	b	121/146 (83%)	121 (100%)	0	100	100
12	Y	20/167 (12%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c	20/167 (12%)	20 (100%)	0	100	100
13	A	60/86 (70%)	60 (100%)	0	100	100
13	E	64/86 (74%)	64 (100%)	0	100	100
14	B	46/54 (85%)	46 (100%)	0	100	100
14	F	46/54 (85%)	44 (96%)	2 (4%)	26	51
All	All	4640/5444 (85%)	4599 (99%)	41 (1%)	68	87

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	134	LEU
8	X	96	LEU
3	H	386	LEU
7	L	256	GLN
8	X	188	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
8	Q	226	ASN
11	b	35	GLN
1	C	228	ASN
14	F	26	HIS
8	X	232	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 84 ligands modelled in this entry, 10 are monoatomic - leaving 74 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	$\# Z > 2$
27	3PE	J	602	-	31,31,50	1.08	4 (12%)	34,36,55	1.20	2 (5%)
21	7PH	S	501	-	37,37,37	0.97	4 (10%)	40,42,42	1.16	2 (5%)
23	CDL	P	303	-	76,76,99	1.41	10 (13%)	82,88,111	1.13	4 (4%)
23	CDL	H	1003	-	73,73,99	1.42	10 (13%)	79,85,111	1.19	4 (5%)
17	WUO	P	302	-	99,99,99	1.56	8 (8%)	122,125,125	1.30	14 (11%)
23	CDL	T	1302	-	78,78,99	1.38	10 (12%)	84,90,111	1.18	5 (5%)
23	CDL	K	201	-	78,78,99	1.39	11 (14%)	84,90,111	1.16	4 (4%)
19	IZL	M	502	-	119,119,119	1.73	21 (17%)	160,163,163	1.18	14 (8%)
16	MQ9	C	303	-	59,59,59	1.21	2 (3%)	73,75,75	1.75	20 (27%)
23	CDL	R	605	-	76,76,99	1.41	11 (14%)	82,88,111	1.15	4 (4%)
21	7PH	G	505	-	37,37,37	0.97	4 (10%)	40,42,42	1.11	2 (5%)
24	PLM	L	610	-	9,10,17	0.37	0	8,9,17	0.68	0
22	HEM	N	601	3	50,50,50	1.44	8 (16%)	67,82,82	1.04	3 (4%)
24	PLM	N	608	-	9,10,17	0.37	0	8,9,17	0.44	0
28	HEA	R	603	7	67,67,67	2.23	25 (37%)	81,103,103	2.65	32 (39%)
26	TRD	R	608	-	12,12,12	0.28	0	11,11,11	0.85	0
26	TRD	K	202	-	12,12,12	0.29	0	11,11,11	0.86	0
21	7PH	H	1001	-	37,37,37	0.96	4 (10%)	40,42,42	1.14	2 (5%)
20	9YF	b	201	-	58,58,58	1.32	5 (8%)	68,71,71	1.14	3 (4%)
16	MQ9	O	303	-	59,59,59	1.56	5 (8%)	73,75,75	1.67	20 (27%)
16	MQ9	N	605	-	59,59,59	1.61	5 (8%)	73,75,75	1.62	18 (24%)
23	CDL	L	609	-	76,76,99	1.41	11 (14%)	82,88,111	1.14	4 (4%)
23	CDL	N	603	-	76,76,99	1.40	10 (13%)	82,88,111	1.16	4 (4%)
26	TRD	S	502	-	12,12,12	0.29	0	11,11,11	0.85	0
26	TRD	L	608	-	12,12,12	0.28	0	11,11,11	0.84	0
26	TRD	T	1303	-	12,12,12	0.29	0	11,11,11	0.85	0
22	HEM	N	606	3	50,50,50	1.42	8 (16%)	67,82,82	1.02	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CDL	N	602	-	73,73,99	1.41	11 (15%)	79,85,111	1.19	4 (5%)
23	CDL	N	604	-	78,78,99	1.36	10 (12%)	84,90,111	1.19	4 (4%)
22	HEM	H	1007	3	50,50,50	1.66	10 (20%)	67,82,82	1.60	16 (23%)
32	DCQ	H	1008	-	23,23,23	0.60	0	27,29,29	0.47	0
15	HEC	C	302	1	46,50,50	2.04	8 (17%)	58,82,82	1.74	7 (12%)
16	MQ9	H	1006	-	59,59,59	1.57	5 (8%)	73,75,75	1.70	19 (26%)
17	WUO	I	303	-	99,99,99	1.53	8 (8%)	122,125,125	1.29	15 (12%)
21	7PH	G	504	-	37,37,37	0.95	4 (10%)	40,42,42	1.16	2 (5%)
23	CDL	I	301	-	76,76,99	1.41	11 (14%)	82,88,111	1.14	4 (4%)
26	TRD	X	403	-	12,12,12	0.28	0	11,11,11	0.86	0
24	PLM	c	301	-	9,10,17	0.37	0	8,9,17	0.44	0
17	WUO	C	304	-	99,99,99	1.53	8 (8%)	122,125,125	1.27	12 (9%)
26	TRD	Q	403	-	12,12,12	0.28	0	11,11,11	0.86	0
15	HEC	O	302	1	46,50,50	2.04	9 (19%)	58,82,82	1.74	7 (12%)
26	TRD	L	607	-	12,12,12	0.29	0	11,11,11	0.83	0
19	IZL	G	502	-	119,119,119	1.72	21 (17%)	160,163,163	1.26	16 (10%)
27	3PE	S	503	-	31,31,50	1.10	4 (12%)	34,36,55	1.14	2 (5%)
18	FES	M	501	2	0,4,4	-	-	-	-	-
23	CDL	H	1004	-	76,76,99	1.39	10 (13%)	82,88,111	1.18	5 (6%)
20	9YF	W	201	-	58,58,58	1.35	4 (6%)	68,71,71	1.16	3 (4%)
23	CDL	H	1005	-	78,78,99	1.37	10 (12%)	84,90,111	1.18	4 (4%)
17	WUO	O	304	-	99,99,99	1.54	8 (8%)	122,125,125	1.29	14 (11%)
23	CDL	L	601	-	78,78,99	1.38	10 (12%)	84,90,111	1.15	4 (4%)
25	9XX	N	609	-	31,31,41	1.11	4 (12%)	34,34,44	1.37	3 (8%)
25	9XX	b	202	-	31,31,41	1.08	4 (12%)	34,34,44	1.30	3 (8%)
25	9XX	c	302	-	31,31,41	1.10	4 (12%)	34,34,44	1.36	3 (8%)
23	CDL	G	506	-	78,78,99	1.39	10 (12%)	84,90,111	1.11	4 (4%)
28	HEA	L	602	7	67,67,67	2.45	29 (43%)	81,103,103	2.52	35 (43%)
15	HEC	O	301	1	46,50,50	1.98	6 (13%)	58,82,82	1.61	6 (10%)
23	CDL	P	301	-	76,76,99	1.42	11 (14%)	82,88,111	1.17	4 (4%)
28	HEA	L	603	7	67,67,67	2.46	27 (40%)	81,103,103	2.42	36 (44%)
24	PLM	W	203	-	9,10,17	0.38	0	8,9,17	0.43	0
16	MQ9	T	1301	-	59,59,59	1.55	5 (8%)	73,75,75	1.71	19 (26%)
23	CDL	I	302	-	76,76,99	1.40	11 (14%)	82,88,111	1.12	4 (4%)
16	MQ9	N	607	-	59,59,59	1.66	5 (8%)	73,75,75	1.55	19 (26%)
28	HEA	R	602	7	67,67,67	2.45	27 (40%)	81,103,103	2.47	33 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	9XX	W	202	-	41,41,41	0.98	4 (9%)	44,44,44	1.26	4 (9%)
23	CDL	R	601	-	76,76,99	1.40	10 (13%)	82,88,111	1.16	4 (4%)
18	FES	G	501	2	0,4,4	-	-	-		
15	HEC	C	301	1	46,50,50	1.97	7 (15%)	58,82,82	1.61	5 (8%)
26	TRD	R	609	-	12,12,12	0.28	0	11,11,11	0.85	0
16	MQ9	C	305	-	59,59,59	1.55	5 (8%)	73,75,75	1.73	21 (28%)
20	9YF	G	503	-	58,58,58	1.33	6 (10%)	68,71,71	1.18	5 (7%)
22	HEM	H	1002	3	50,50,50	1.41	9 (18%)	67,82,82	1.17	5 (7%)
21	7PH	M	504	-	37,37,37	0.96	4 (10%)	40,42,42	1.15	2 (5%)
26	TRD	J	601	-	12,12,12	0.29	0	11,11,11	0.86	0
20	9YF	M	503	-	58,58,58	1.32	6 (10%)	68,71,71	1.26	5 (7%)

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
27	3PE	J	602	-	-	14/35/35/54	-
21	7PH	S	501	-	-	15/39/39/39	-
23	CDL	P	303	-	-	58/87/87/110	-
23	CDL	H	1003	-	-	40/84/84/110	-
17	WUO	P	302	-	-	44/84/148/148	0/3/3/3
23	CDL	T	1302	-	-	56/89/89/110	-
23	CDL	K	201	-	-	54/89/89/110	-
19	IZL	M	502	-	-	40/84/208/208	0/6/6/6
16	MQ9	C	303	-	-	7/53/73/73	0/2/2/2
23	CDL	R	605	-	-	58/87/87/110	-
21	7PH	G	505	-	-	12/39/39/39	-
24	PLM	L	610	-	-	5/8/8/15	-
22	HEM	N	601	3	-	1/14/54/54	-
24	PLM	N	608	-	-	0/8/8/15	-
28	HEA	R	603	7	-	13/36/76/76	-
26	TRD	R	608	-	-	0/10/10/10	-
26	TRD	K	202	-	-	0/10/10/10	-
21	7PH	H	1001	-	-	13/39/39/39	-
20	9YF	b	201	-	-	32/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MQ9	O	303	-	-	10/53/73/73	0/2/2/2
16	MQ9	N	605	-	-	20/53/73/73	0/2/2/2
23	CDL	L	609	-	-	51/87/87/110	-
23	CDL	N	603	-	-	48/87/87/110	-
26	TRD	S	502	-	-	1/10/10/10	-
26	TRD	L	608	-	-	0/10/10/10	-
26	TRD	T	1303	-	-	2/10/10/10	-
22	HEM	N	606	3	-	4/14/54/54	-
23	CDL	N	602	-	-	52/84/84/110	-
23	CDL	N	604	-	-	50/89/89/110	-
22	HEM	H	1007	3	-	5/14/54/54	-
32	DCQ	H	1008	-	-	4/14/38/38	0/1/1/1
15	HEC	C	302	1	-	7/14/54/54	-
16	MQ9	H	1006	-	-	18/53/73/73	0/2/2/2
17	WUO	I	303	-	-	36/84/148/148	0/3/3/3
21	7PH	G	504	-	-	15/39/39/39	-
23	CDL	I	301	-	-	48/87/87/110	-
26	TRD	X	403	-	-	1/10/10/10	-
24	PLM	c	301	-	-	0/8/8/15	-
17	WUO	C	304	-	-	46/84/148/148	0/3/3/3
26	TRD	Q	403	-	-	0/10/10/10	-
15	HEC	O	302	1	-	7/14/54/54	-
26	TRD	L	607	-	-	1/10/10/10	-
19	IZL	G	502	-	-	29/84/208/208	0/6/6/6
27	3PE	S	503	-	-	18/35/35/54	-
18	FES	M	501	2	-	-	0/1/1/1
23	CDL	H	1004	-	-	44/87/87/110	-
20	9YF	W	201	-	-	25/54/78/78	0/1/1/1
23	CDL	H	1005	-	-	47/89/89/110	-
17	WUO	O	304	-	-	35/84/148/148	0/3/3/3
23	CDL	L	601	-	-	44/89/89/110	-
25	9XX	N	609	-	-	12/33/33/43	-
25	9XX	b	202	-	-	13/33/33/43	-
25	9XX	c	302	-	-	8/33/33/43	-
23	CDL	G	506	-	-	54/89/89/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	HEA	L	602	7	-	12/36/76/76	-
15	HEC	O	301	1	-	9/14/54/54	-
23	CDL	P	301	-	-	50/87/87/110	-
28	HEA	L	603	7	-	11/36/76/76	-
24	PLM	W	203	-	-	2/8/8/15	-
16	MQ9	T	1301	-	-	11/53/73/73	0/2/2/2
23	CDL	I	302	-	-	54/87/87/110	-
16	MQ9	N	607	-	-	20/53/73/73	0/2/2/2
28	HEA	R	602	7	-	15/36/76/76	-
25	9XX	W	202	-	-	20/43/43/43	-
23	CDL	R	601	-	-	43/87/87/110	-
26	TRD	R	609	-	-	1/10/10/10	-
15	HEC	C	301	1	-	9/14/54/54	-
26	TRD	J	601	-	-	1/10/10/10	-
16	MQ9	C	305	-	-	15/53/73/73	0/2/2/2
20	9YF	G	503	-	-	38/54/78/78	0/1/1/1
22	HEM	H	1002	3	-	3/14/54/54	-
21	7PH	M	504	-	-	15/39/39/39	-
18	FES	G	501	2	-	-	0/1/1/1
20	9YF	M	503	-	-	33/54/78/78	0/1/1/1

The worst 5 of 521 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	607	MQ9	C6-C5	8.16	1.49	1.35
16	N	605	MQ9	C6-C5	7.87	1.49	1.35
15	O	302	HEC	CAC-C3C	7.59	1.59	1.35
15	C	302	HEC	CAC-C3C	7.58	1.59	1.35
15	O	301	HEC	CAC-C3C	7.55	1.59	1.35

The worst 5 of 522 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	R	603	HEA	C12-C11-C3B	-8.87	98.26	112.12
15	C	302	HEC	CBB-CAB-C3B	-8.76	109.92	127.43
15	O	302	HEC	CBB-CAB-C3B	-8.75	109.95	127.43
15	C	301	HEC	CBB-CAB-C3B	-8.35	110.74	127.43
15	O	301	HEC	CBB-CAB-C3B	-8.35	110.75	127.43

There are no chirality outliers.

5 of 1579 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	O	301	HEC	C2B-C3B-CAB-CBB
15	O	301	HEC	C4B-C3B-CAB-CBB
15	O	301	HEC	C2C-C3C-CAC-CBC
15	O	301	HEC	C4C-C3C-CAC-CBC
15	O	302	HEC	C2C-C3C-CAC-CBC

There are no ring outliers.

41 monomers are involved in 164 short contacts:

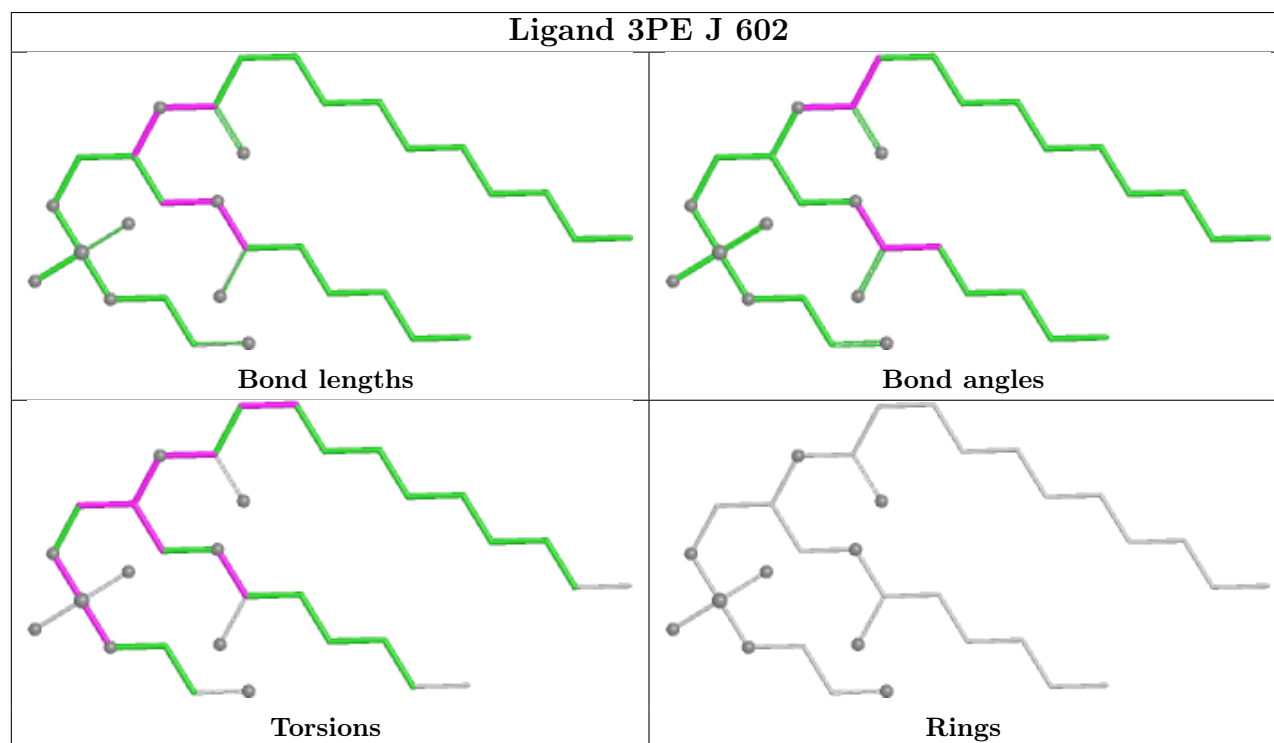
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	S	501	7PH	2	0
23	P	303	CDL	7	0
23	H	1003	CDL	1	0
23	T	1302	CDL	5	0
23	K	201	CDL	2	0
16	C	303	MQ9	1	0
23	R	605	CDL	4	0
22	N	601	HEM	3	0
24	N	608	PLM	1	0
28	R	603	HEA	31	0
21	H	1001	7PH	1	0
16	O	303	MQ9	3	0
16	N	605	MQ9	3	0
23	L	609	CDL	3	0
23	N	603	CDL	5	0
22	N	606	HEM	2	0
23	N	604	CDL	5	0
22	H	1007	HEM	4	0
15	C	302	HEC	5	0
16	H	1006	MQ9	10	0
21	G	504	7PH	3	0
23	I	301	CDL	5	0
26	Q	403	TRD	1	0
15	O	302	HEC	4	0
23	H	1004	CDL	1	0
23	H	1005	CDL	5	0
23	L	601	CDL	3	0
23	G	506	CDL	1	0
28	L	602	HEA	10	0
23	P	301	CDL	6	0

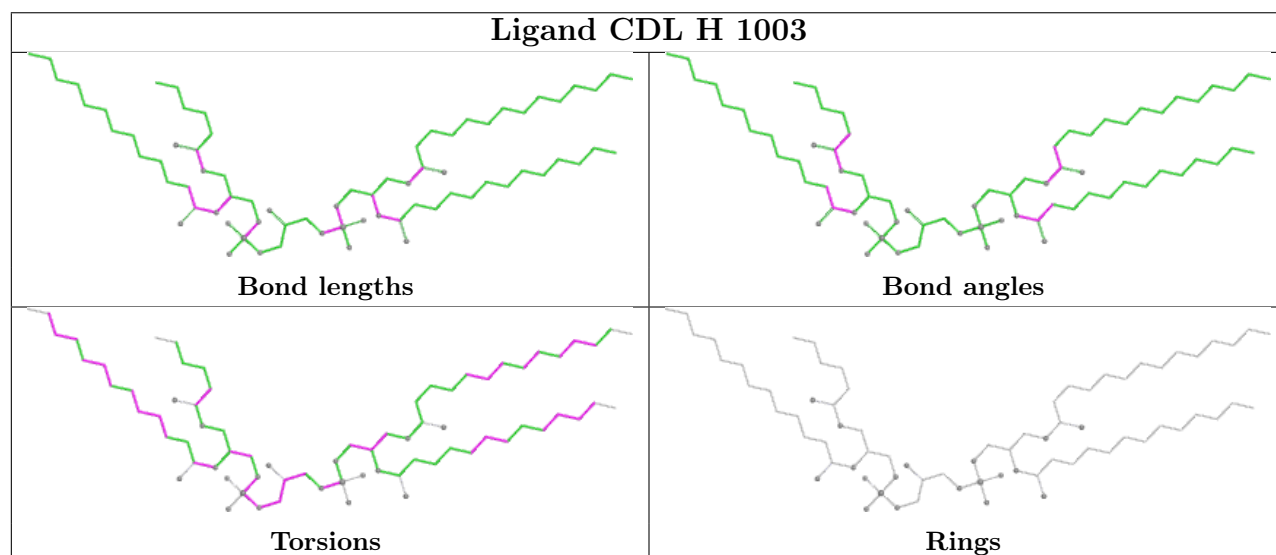
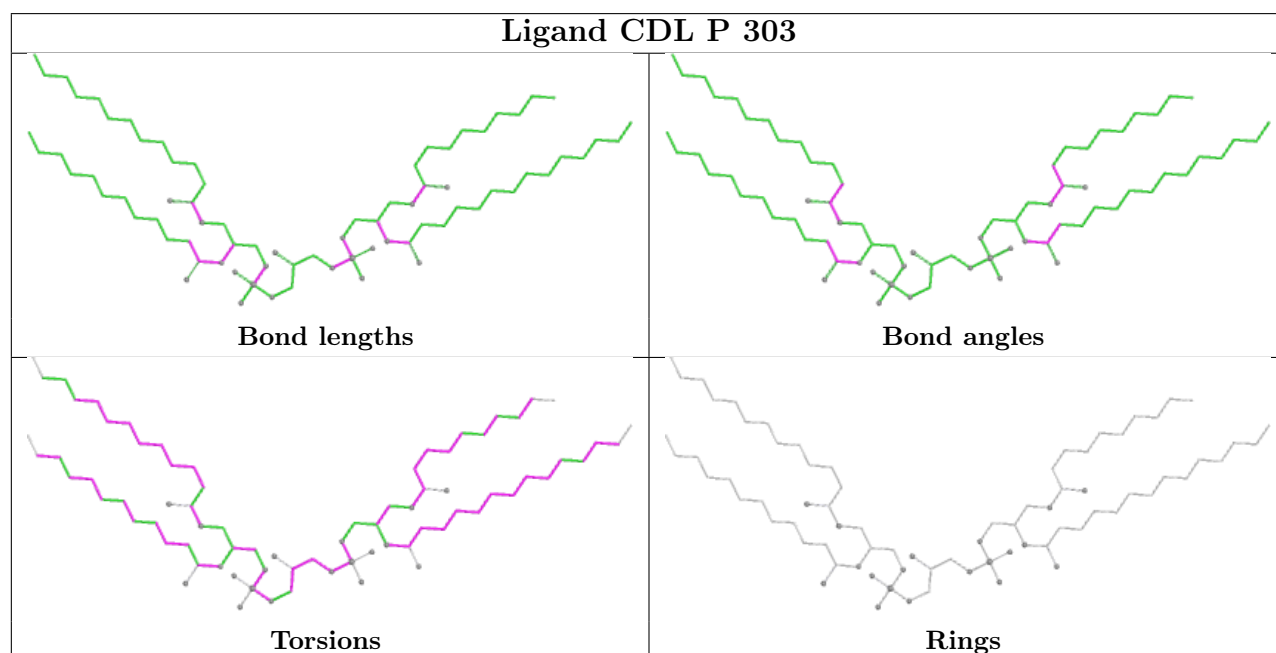
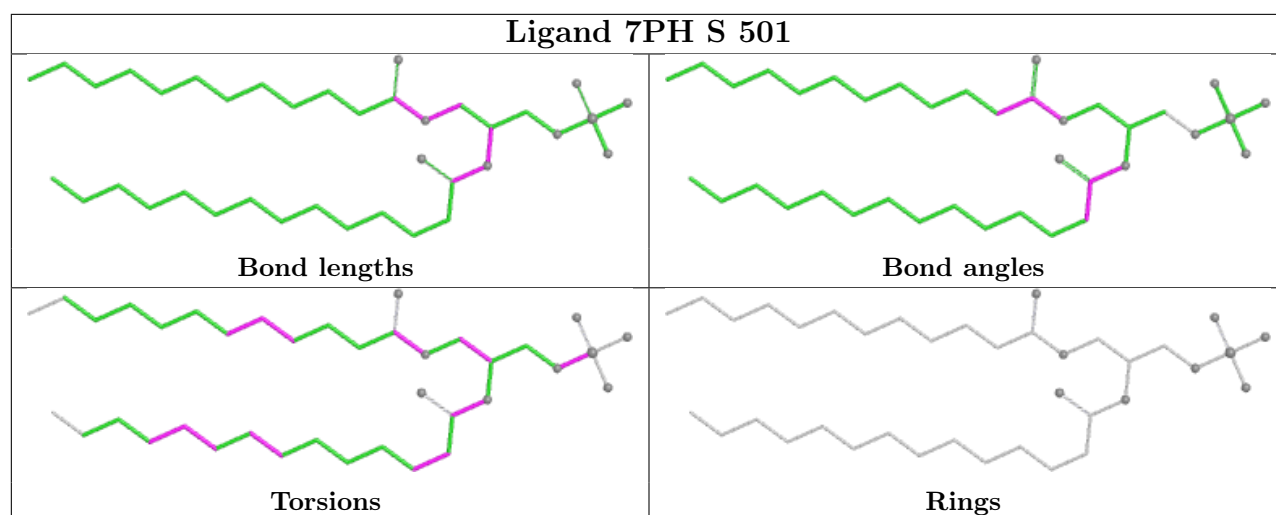
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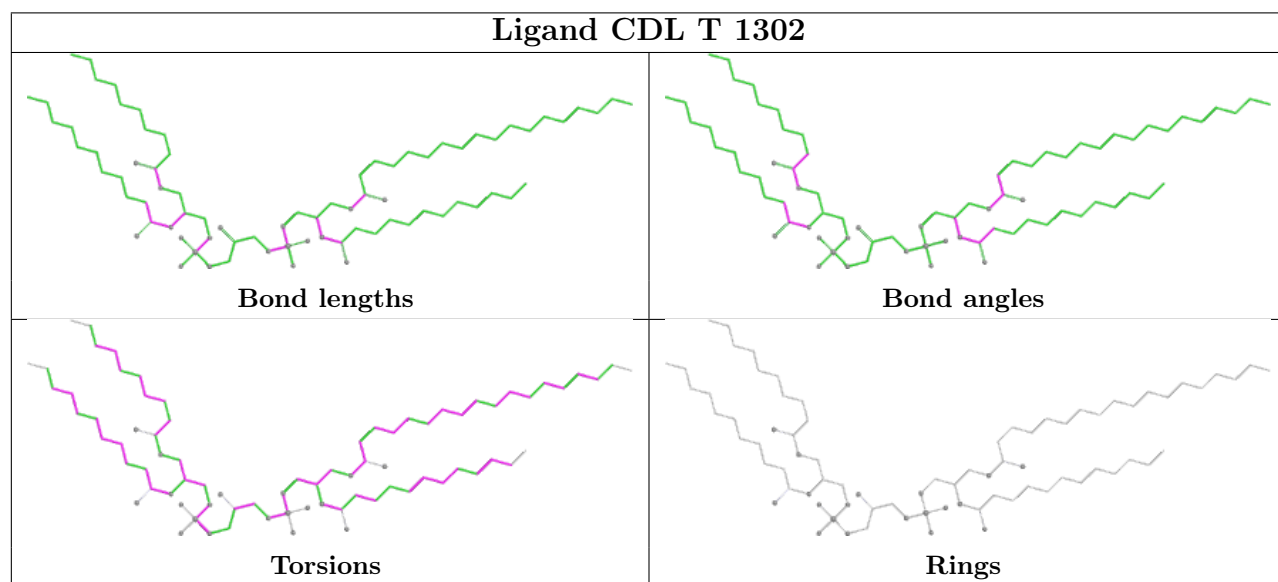
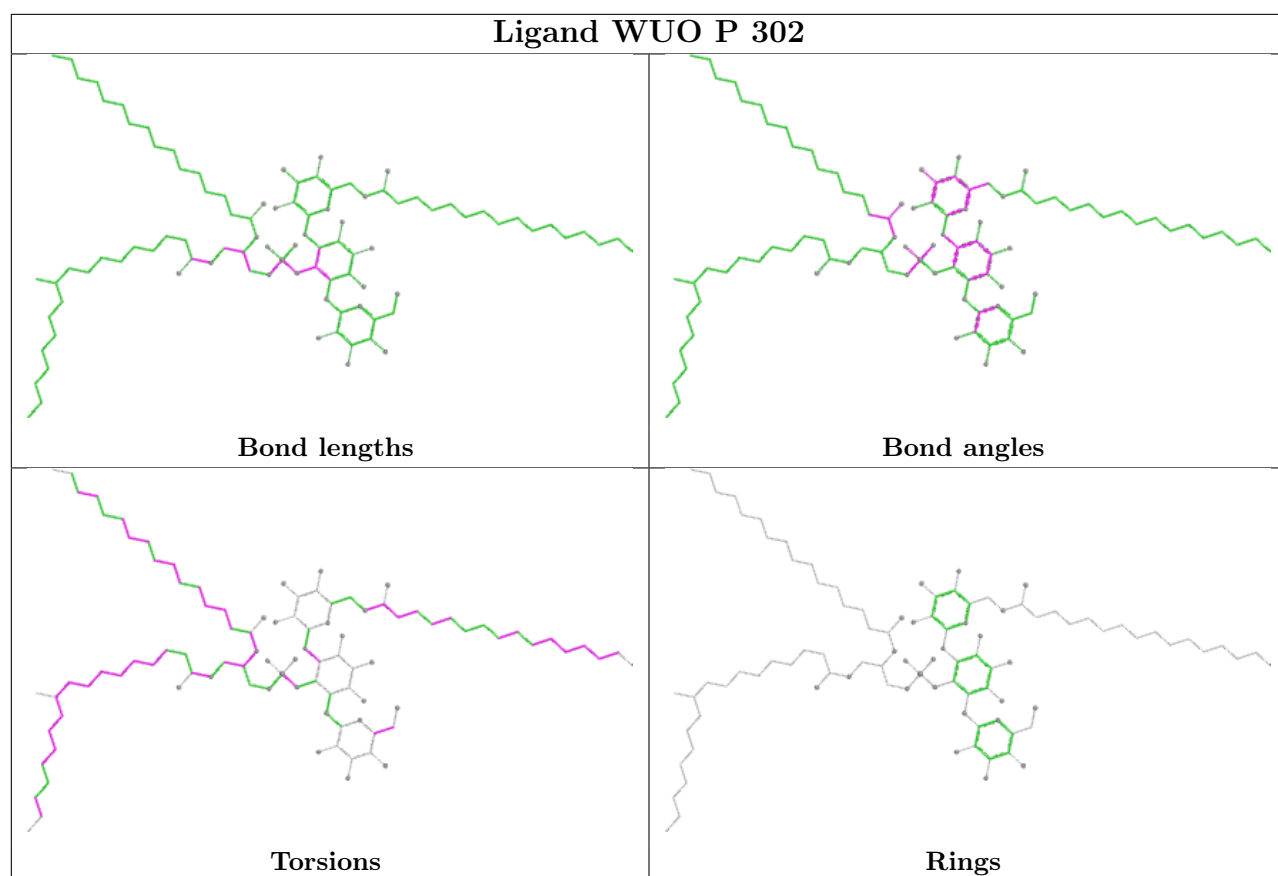
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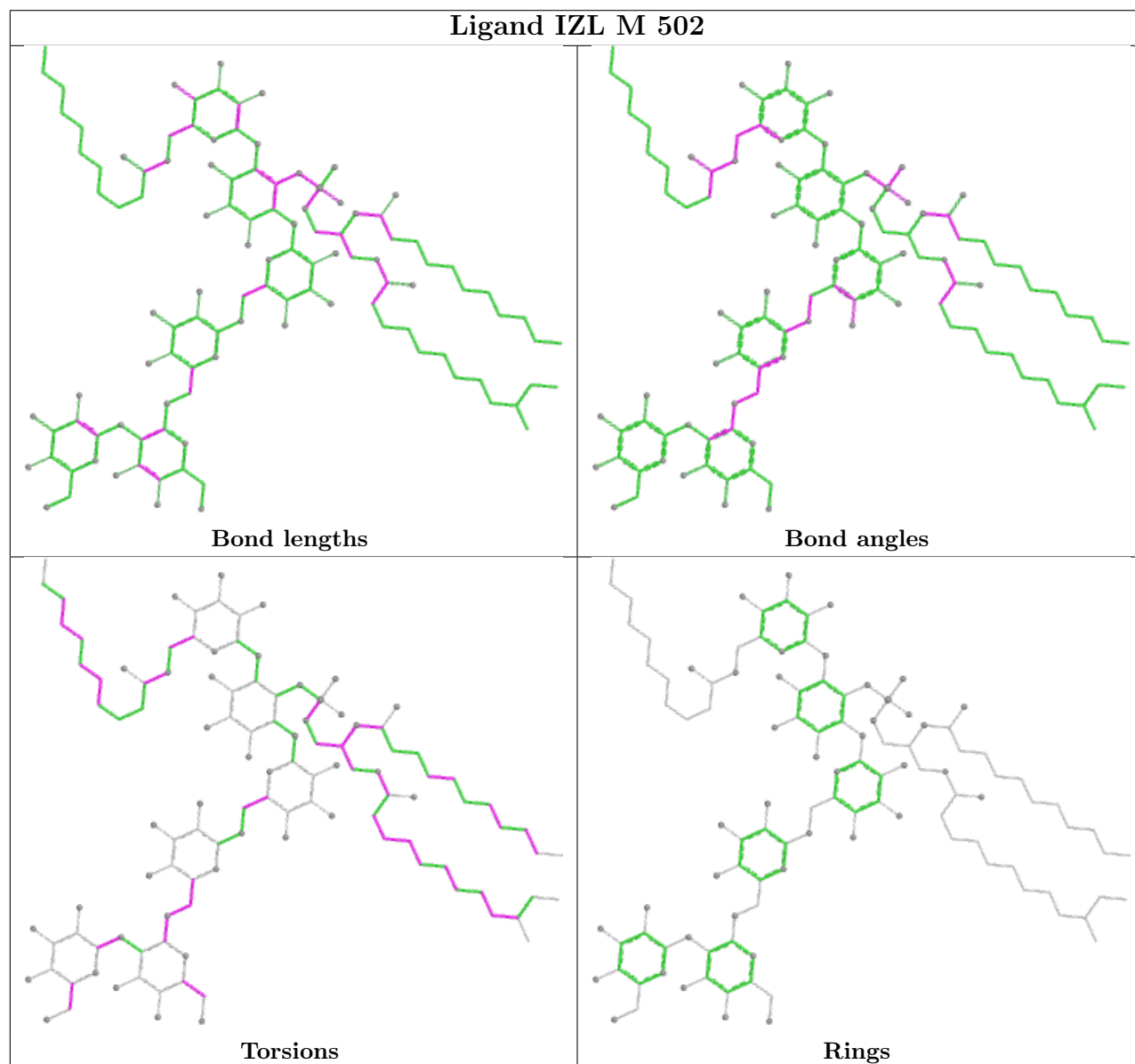
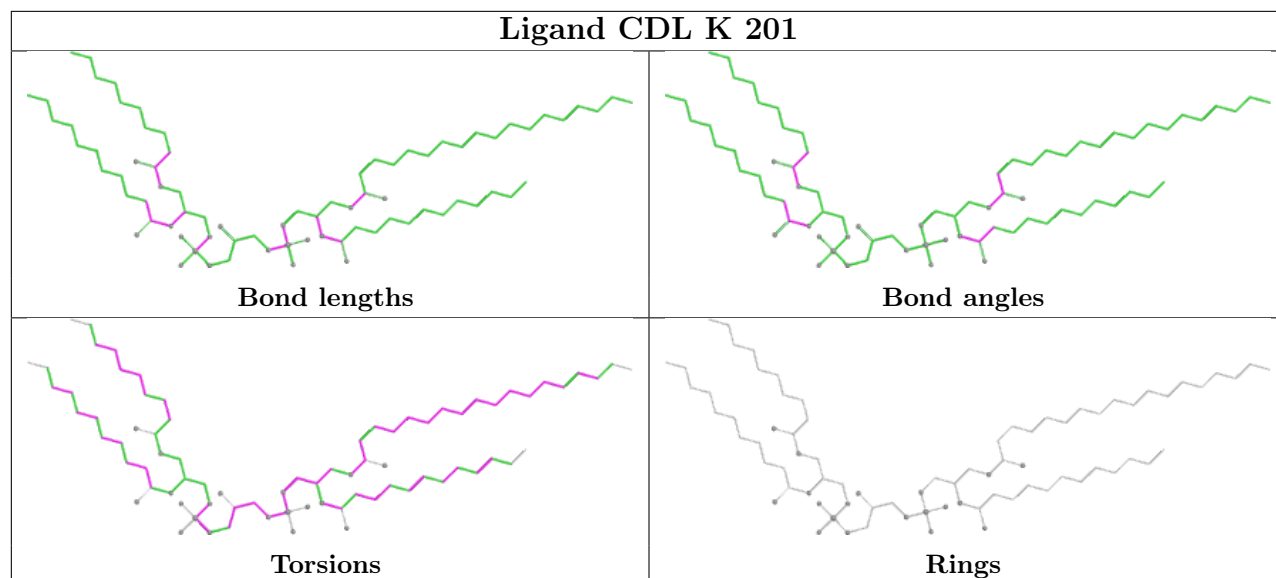
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	L	603	HEA	2	0
16	T	1301	MQ9	7	0
23	I	302	CDL	2	0
16	N	607	MQ9	5	0
28	R	602	HEA	7	0
23	R	601	CDL	2	0
15	C	301	HEC	1	0
16	C	305	MQ9	3	0
22	H	1002	HEM	2	0
21	M	504	7PH	3	0
26	J	601	TRD	1	0

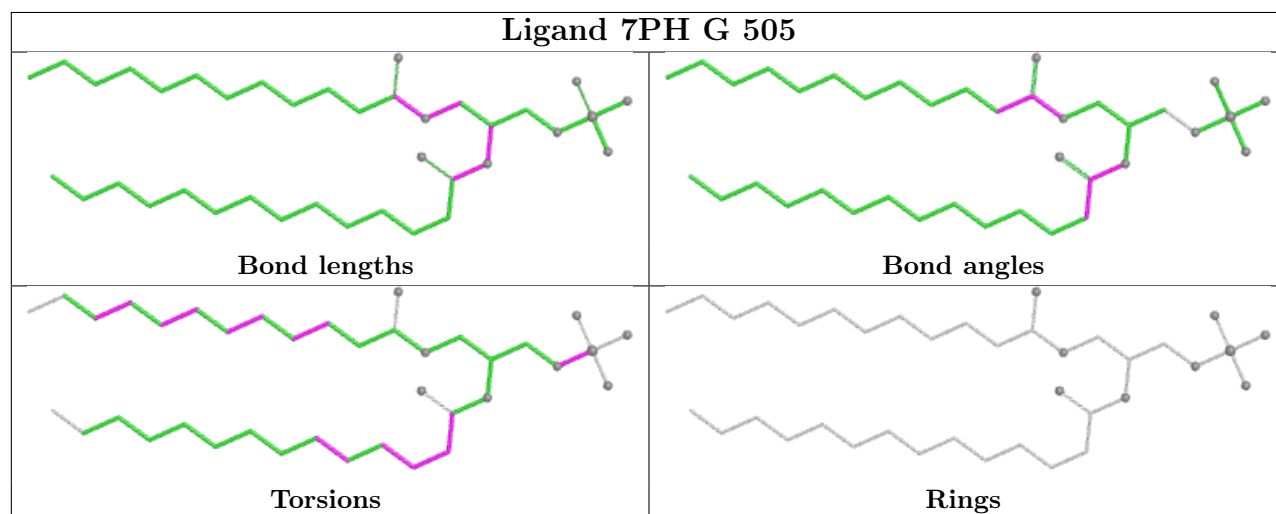
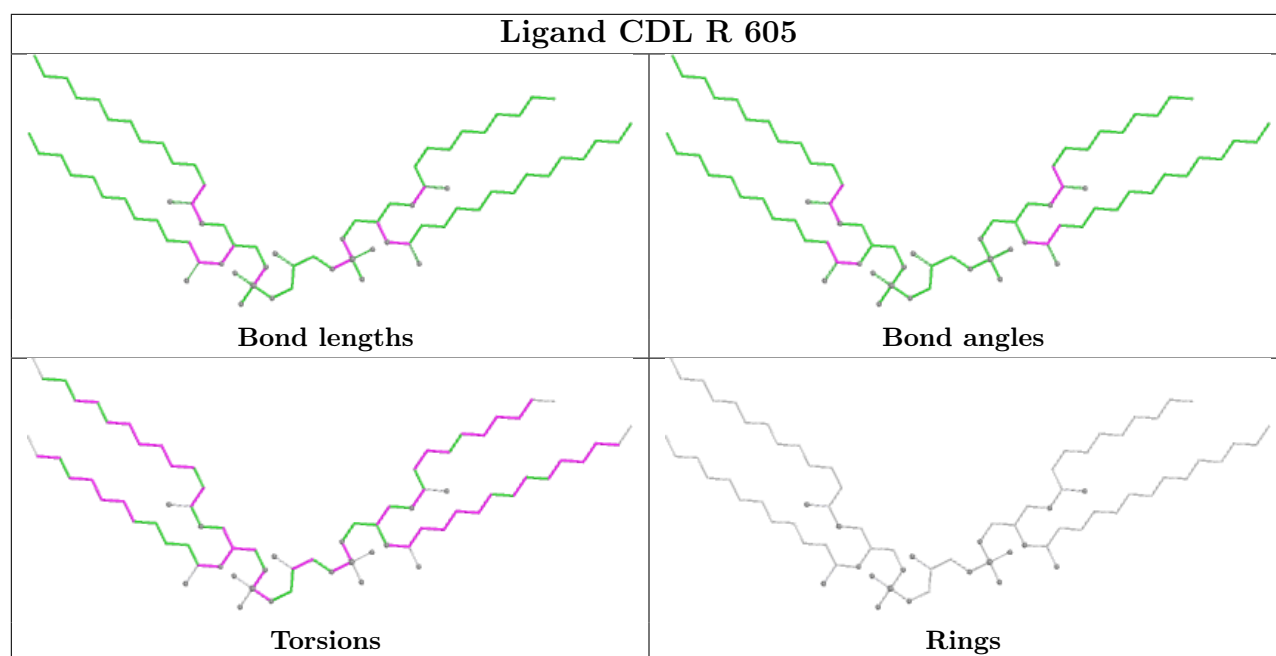
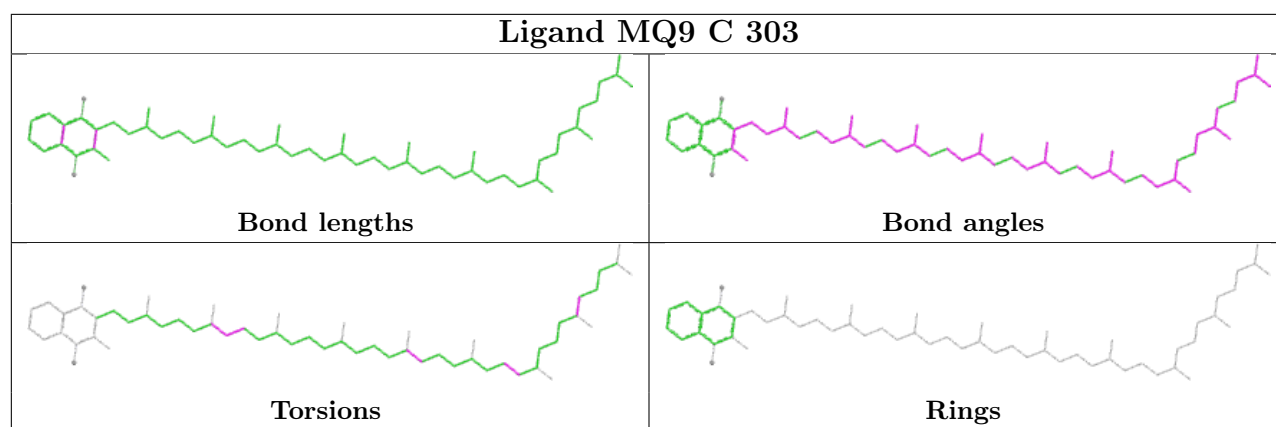
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

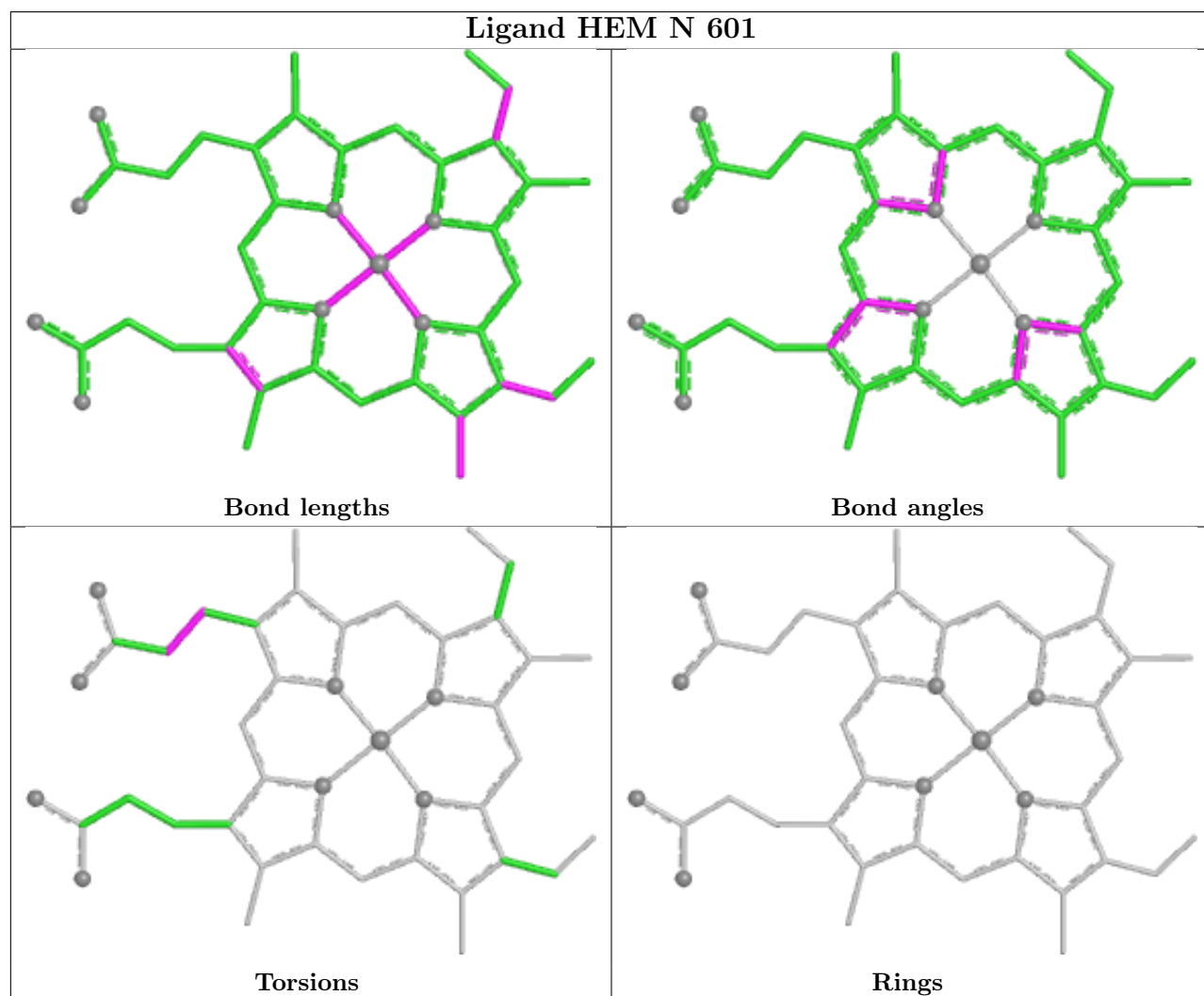
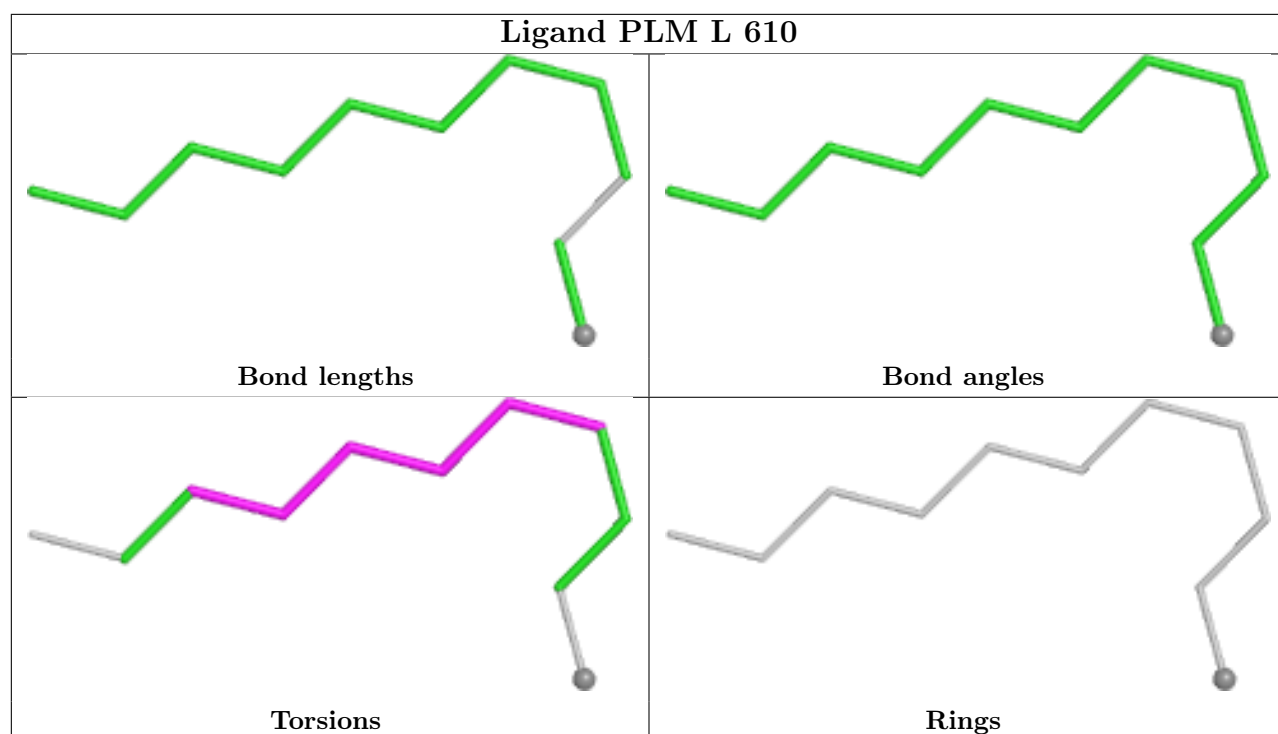


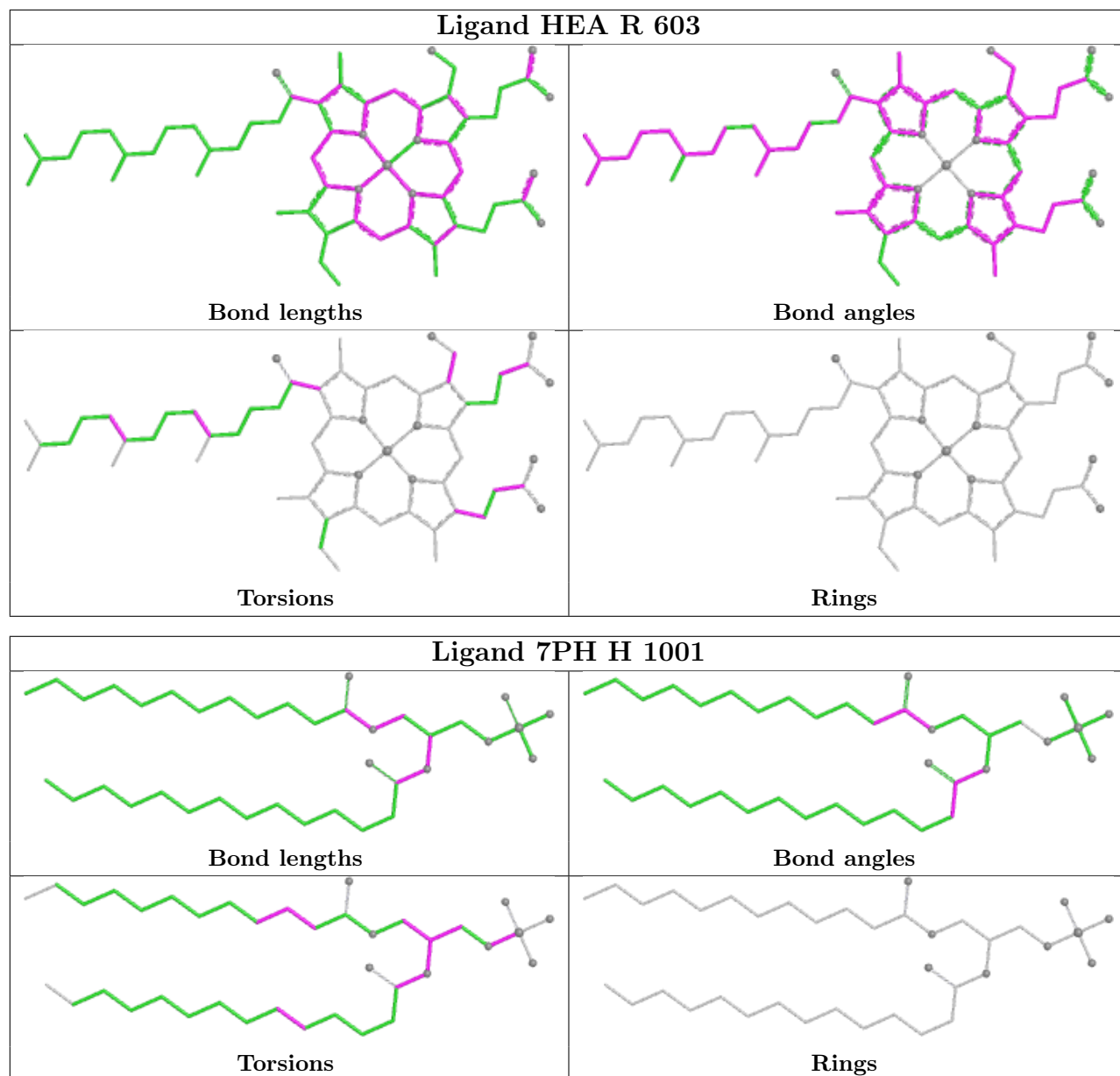


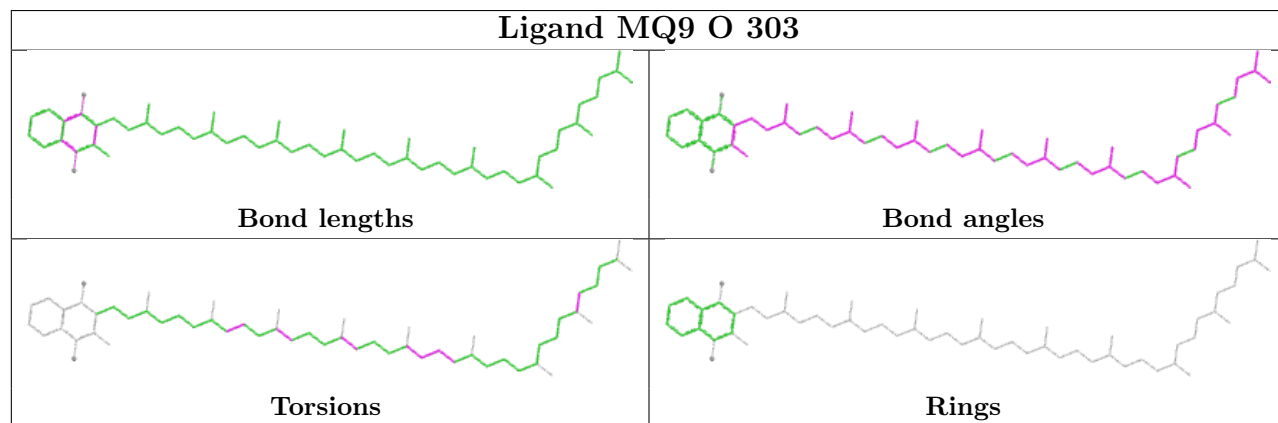
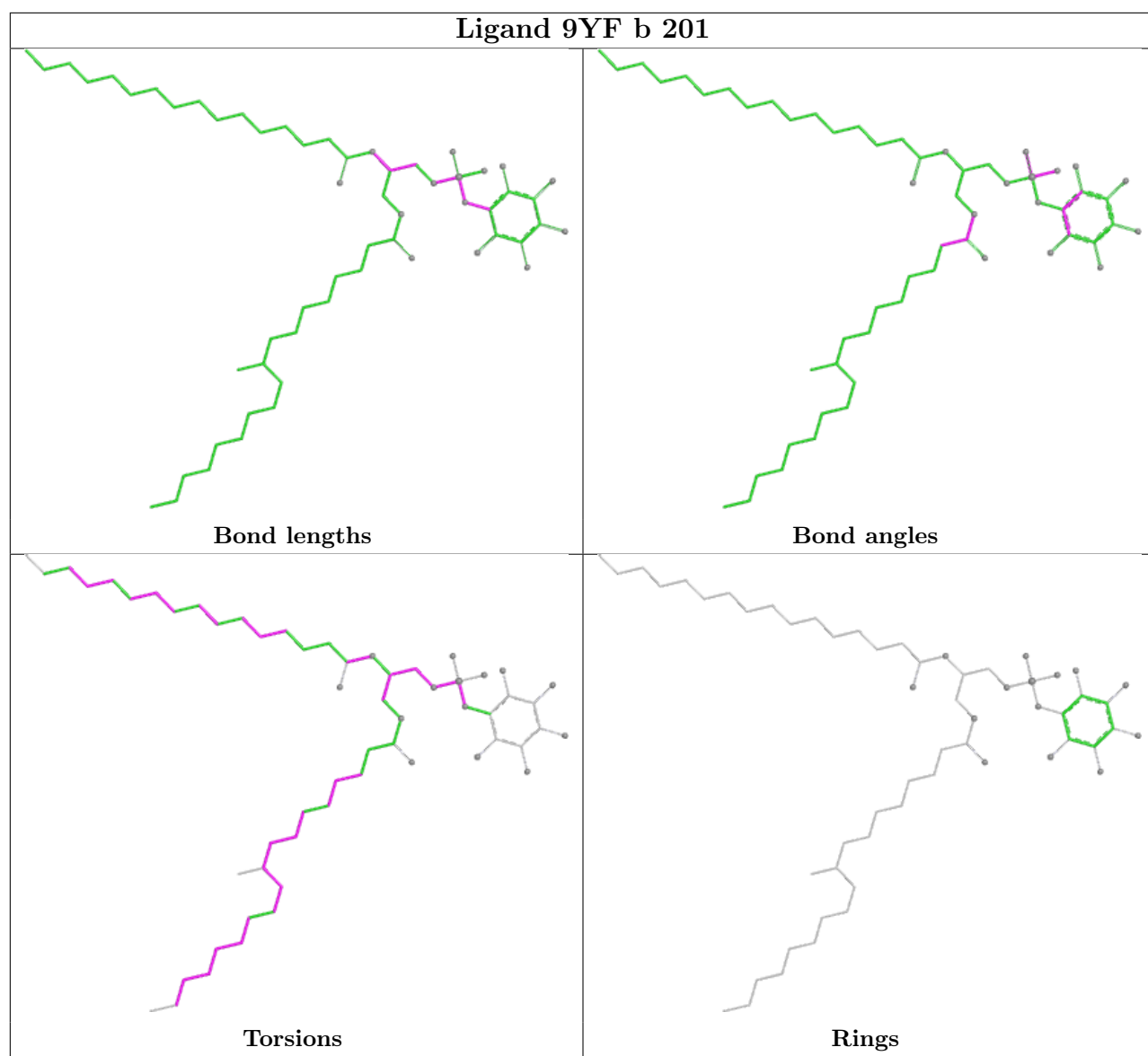


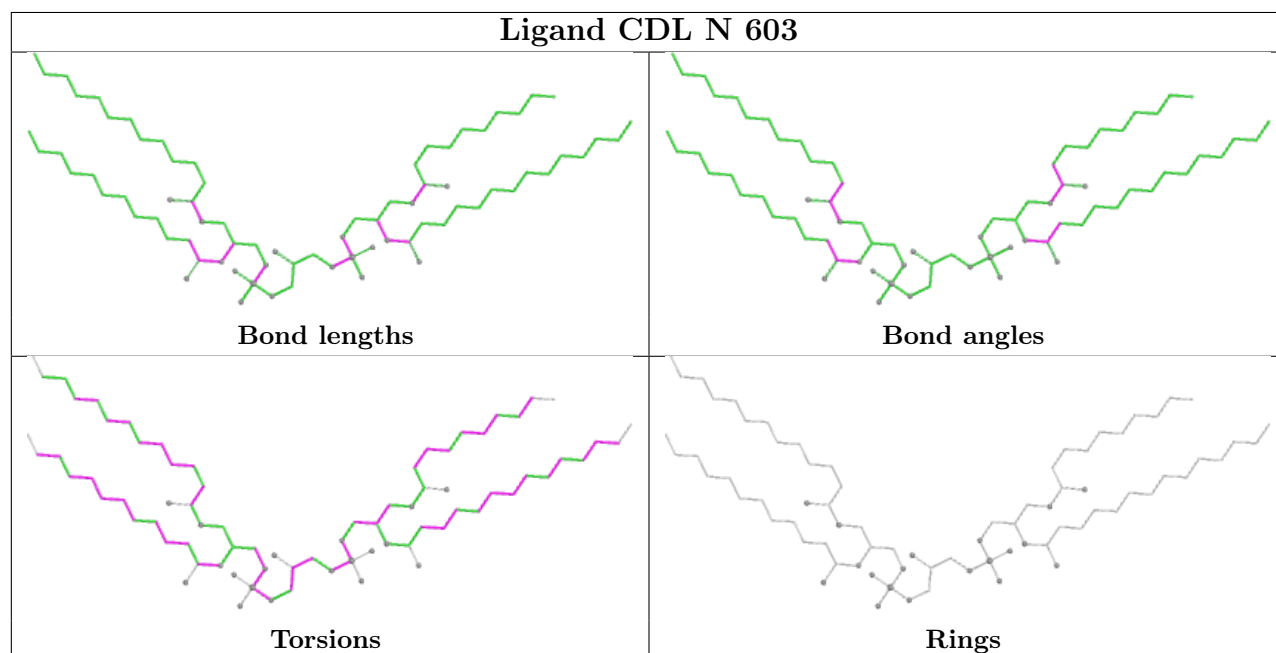
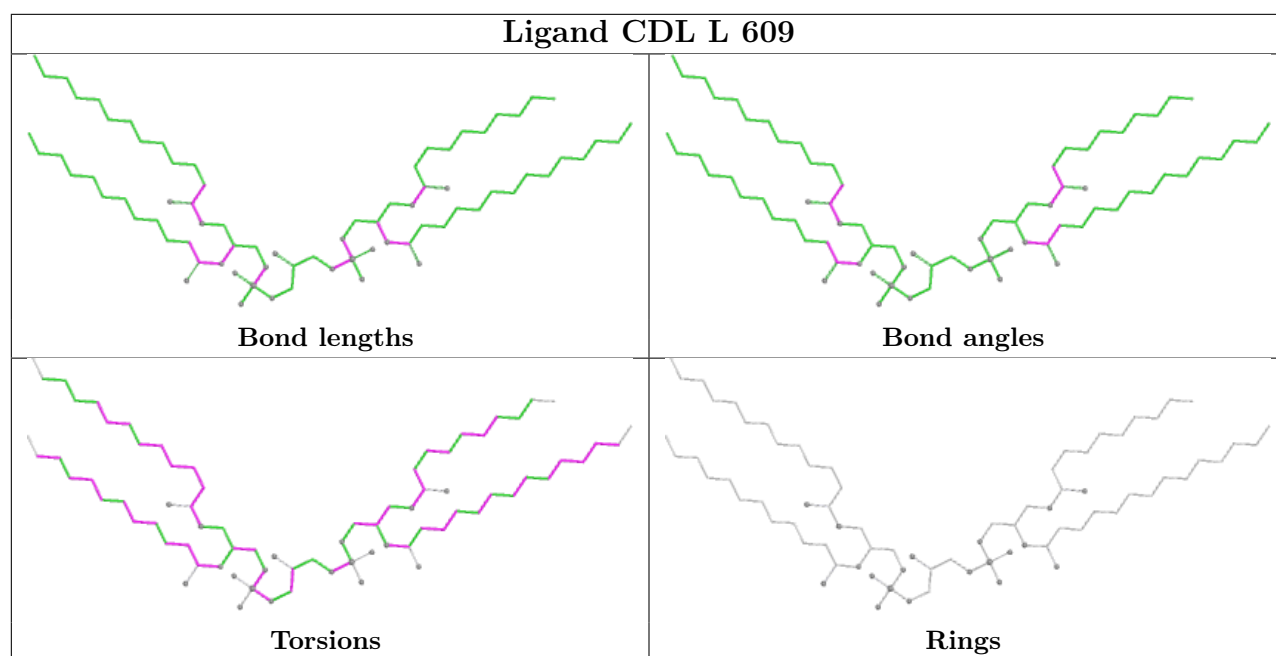
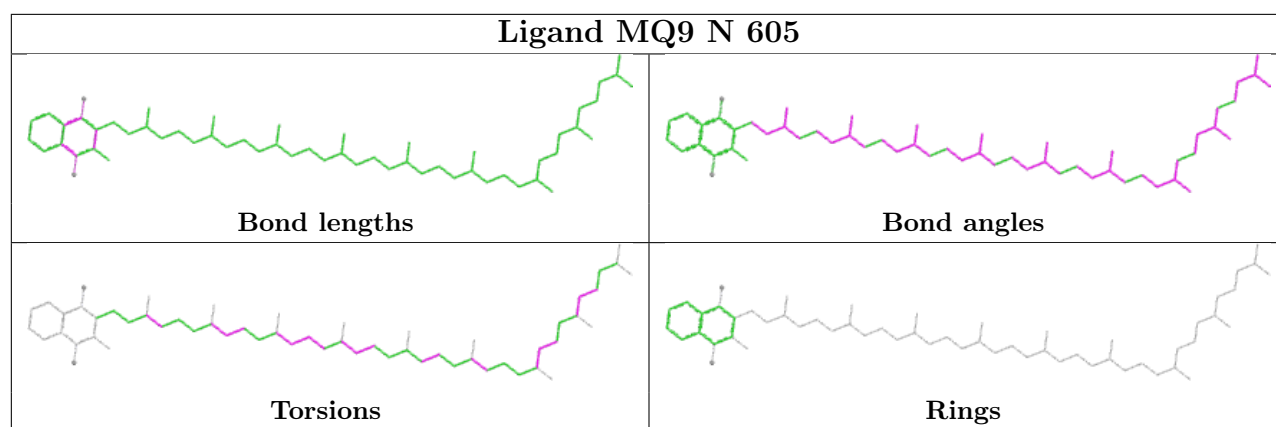


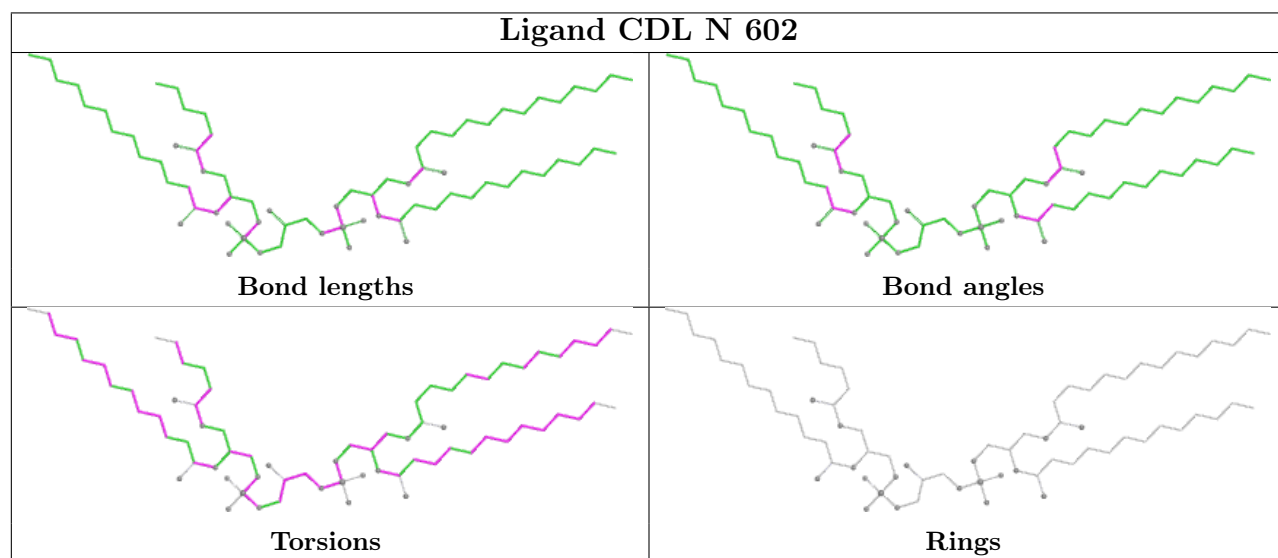
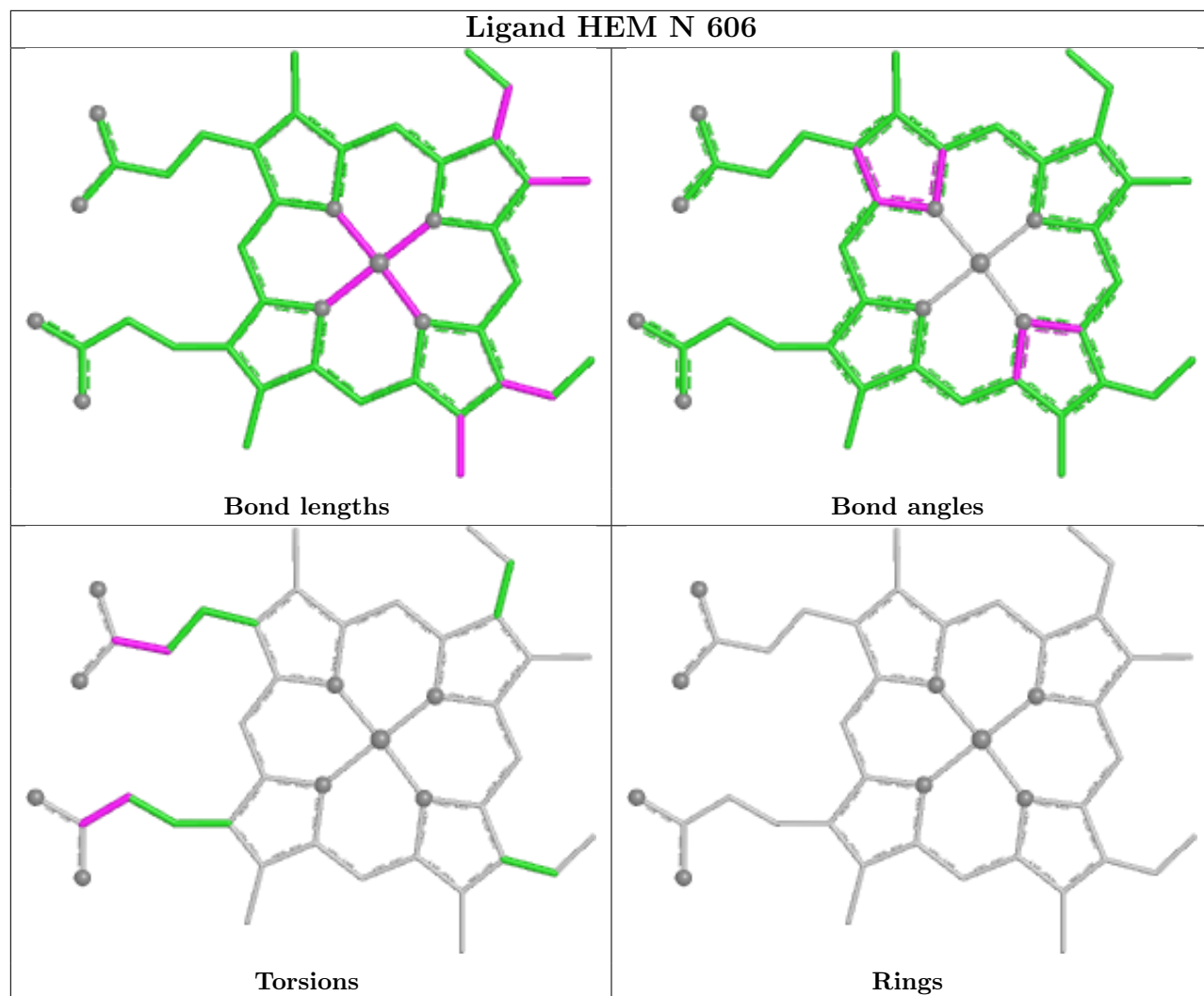


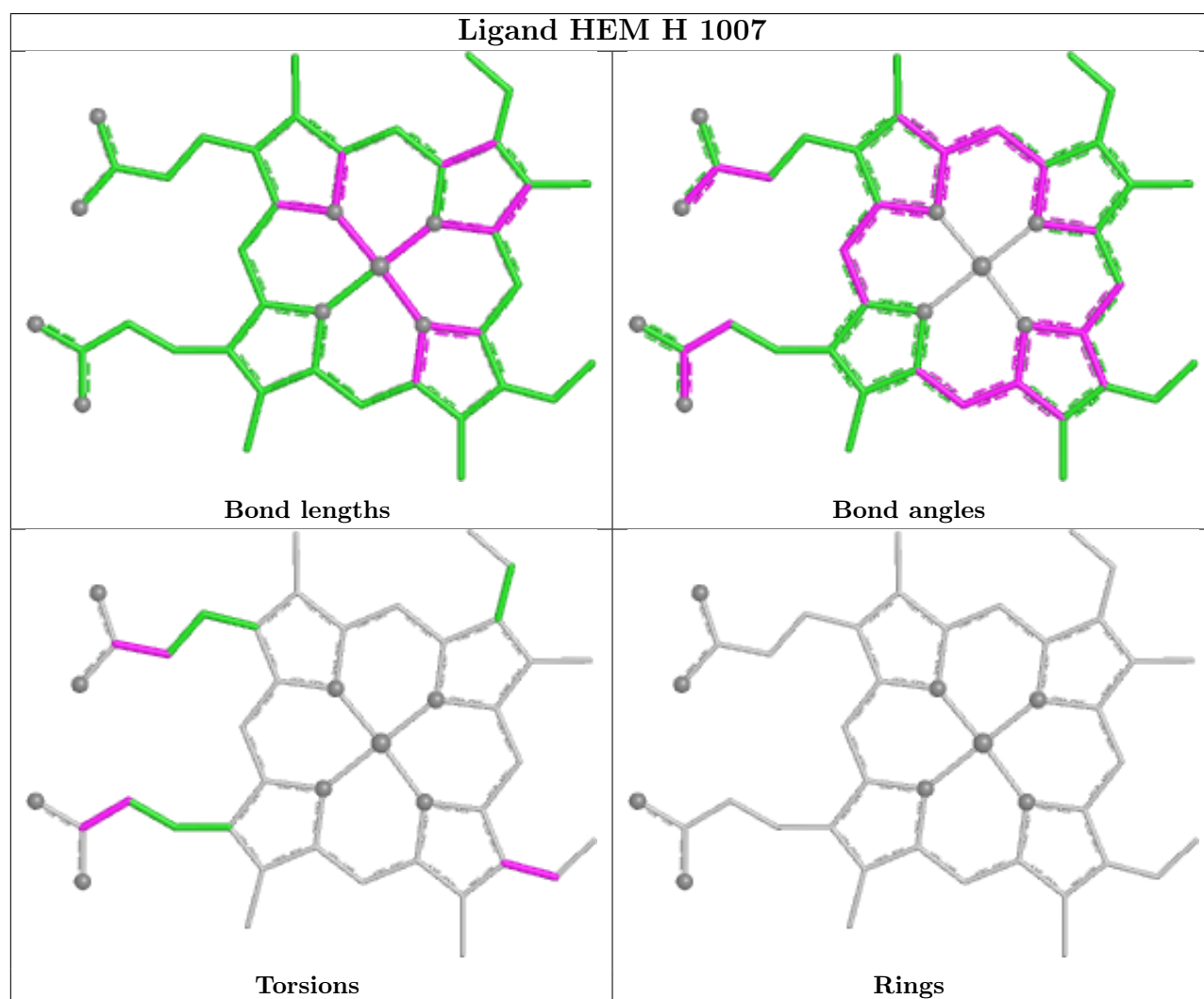
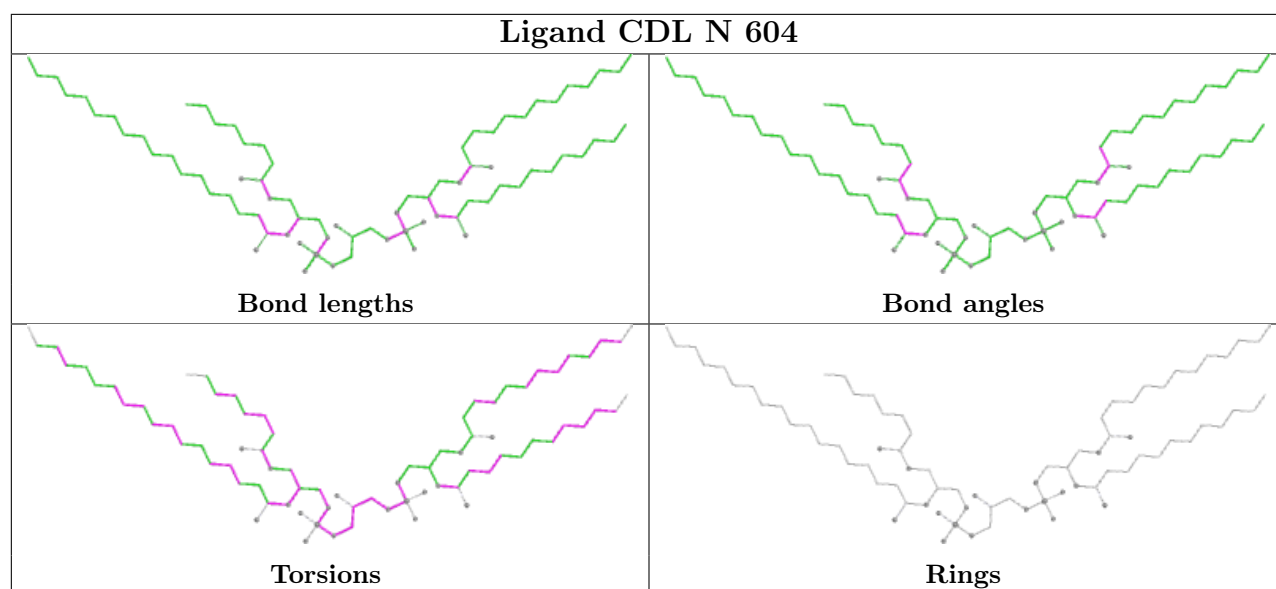


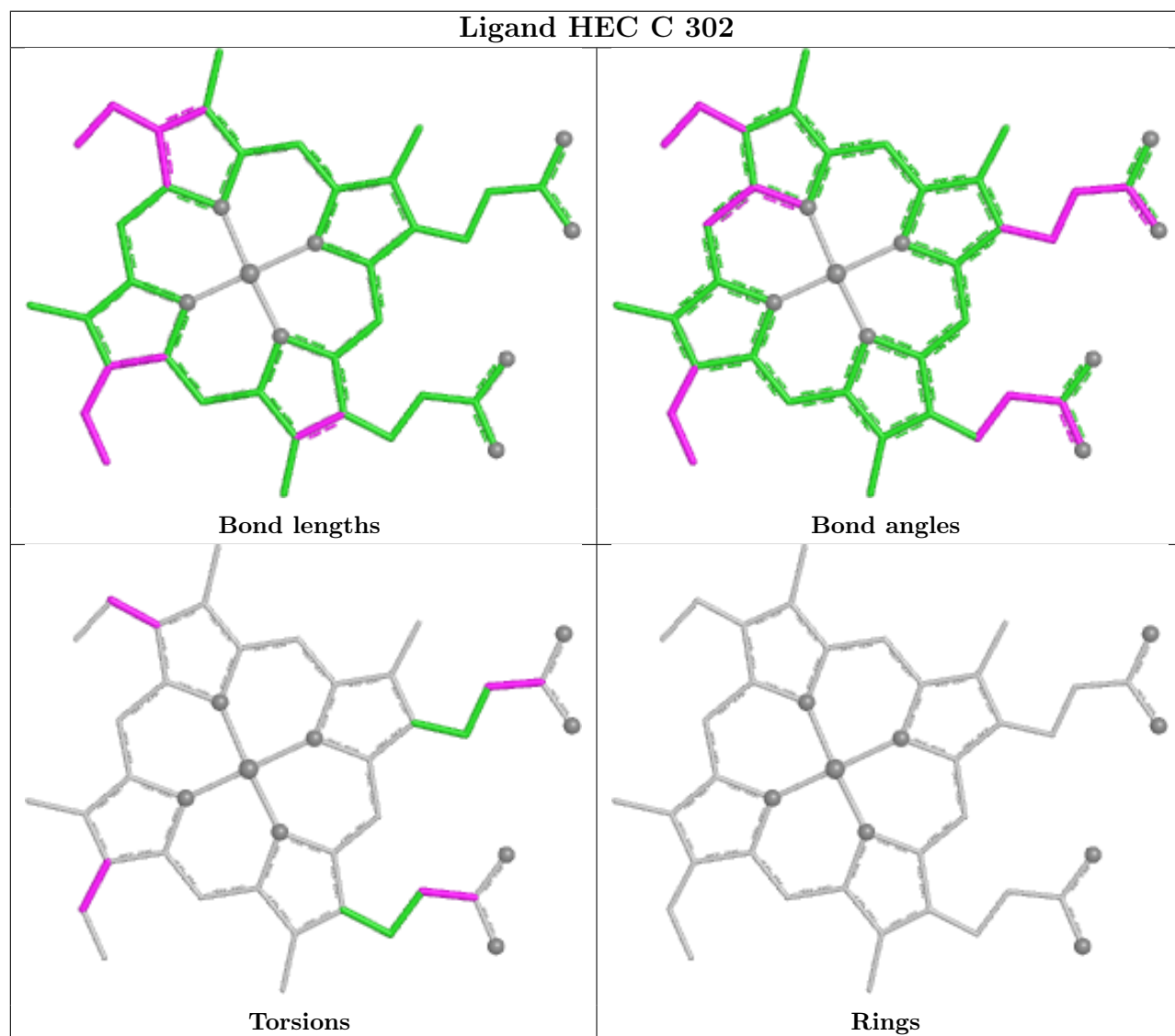
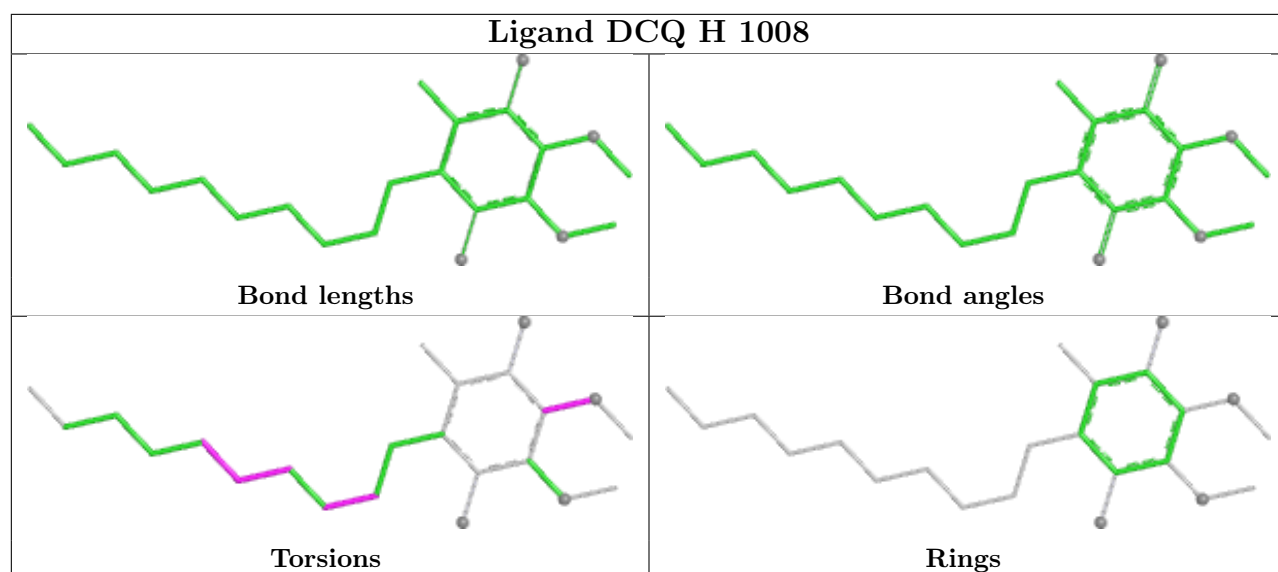


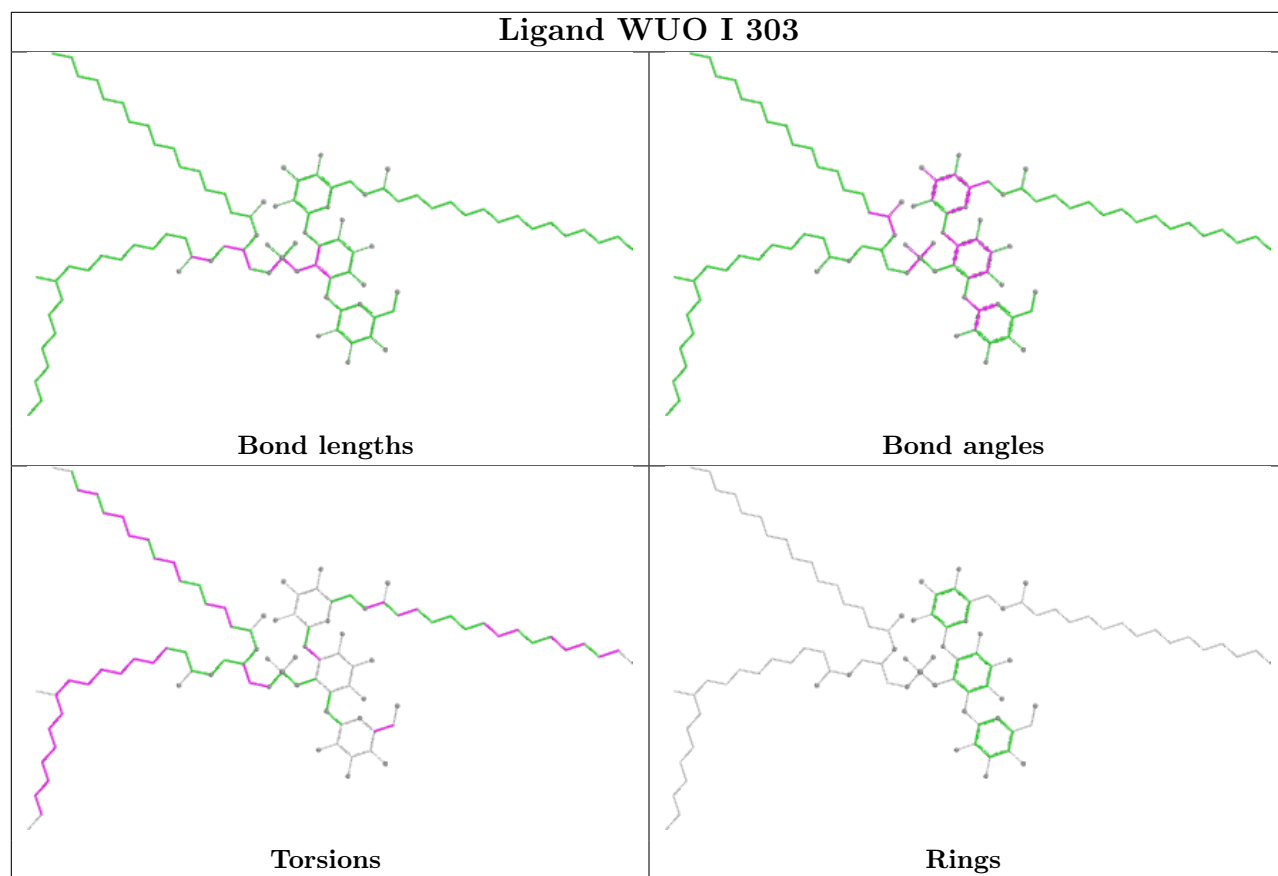
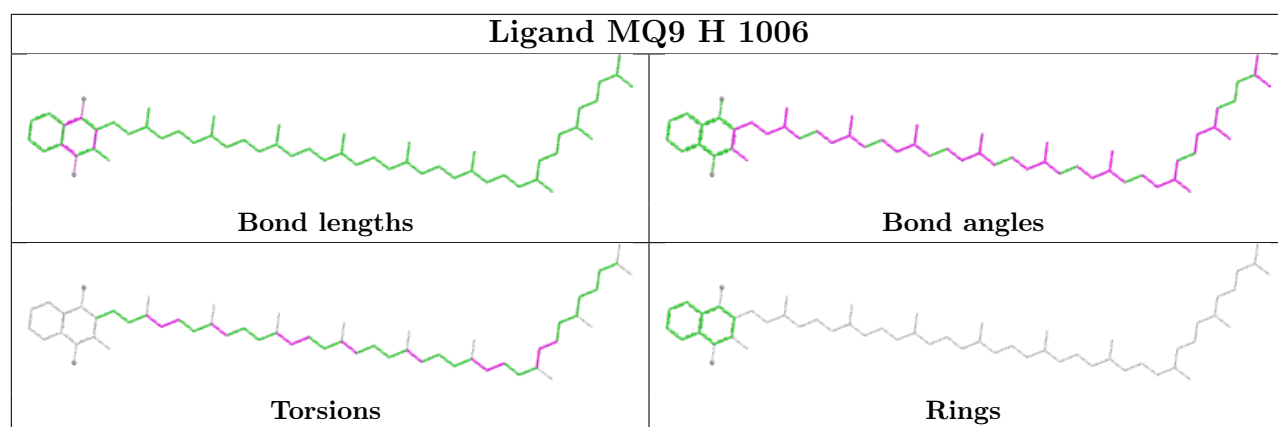


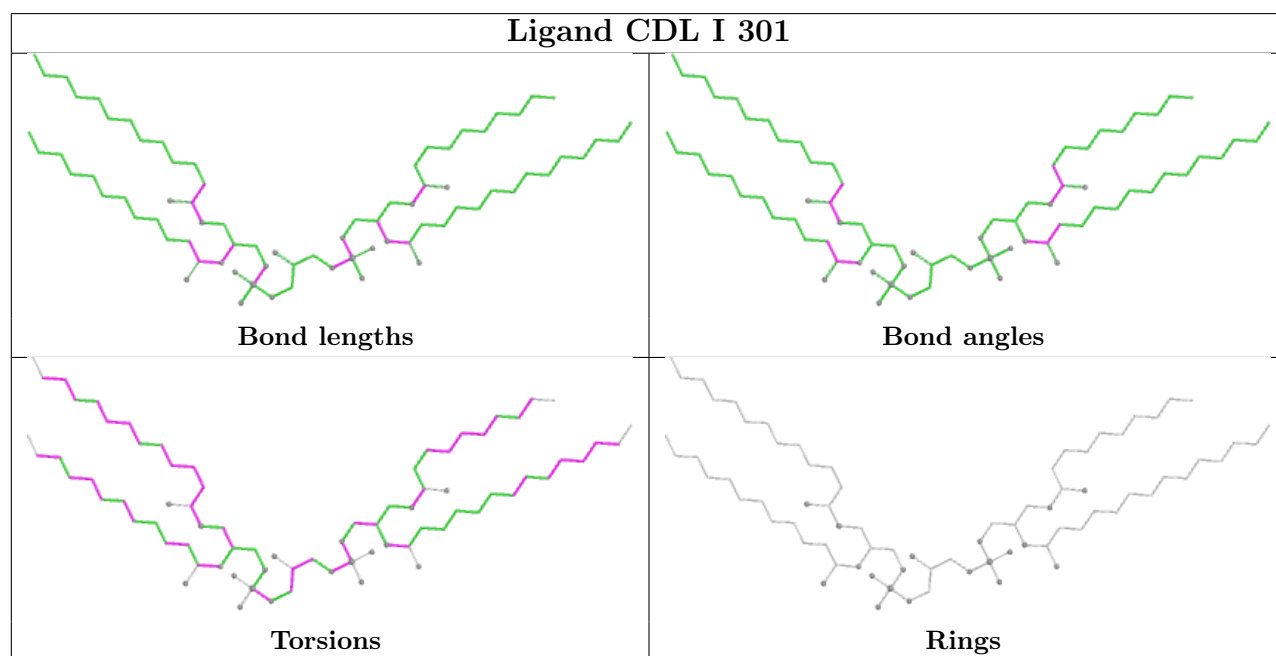
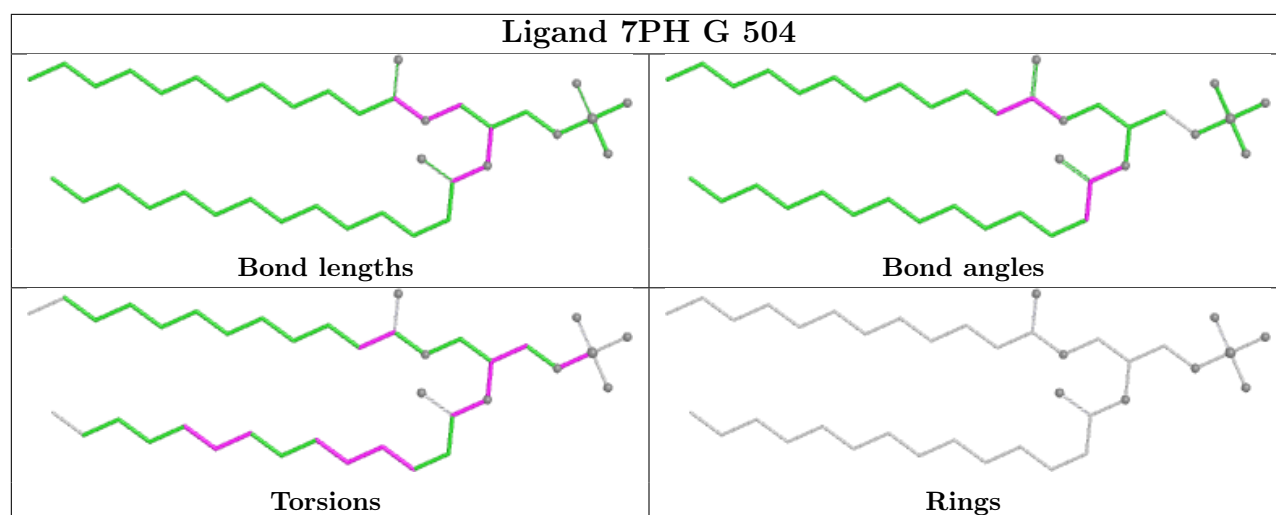


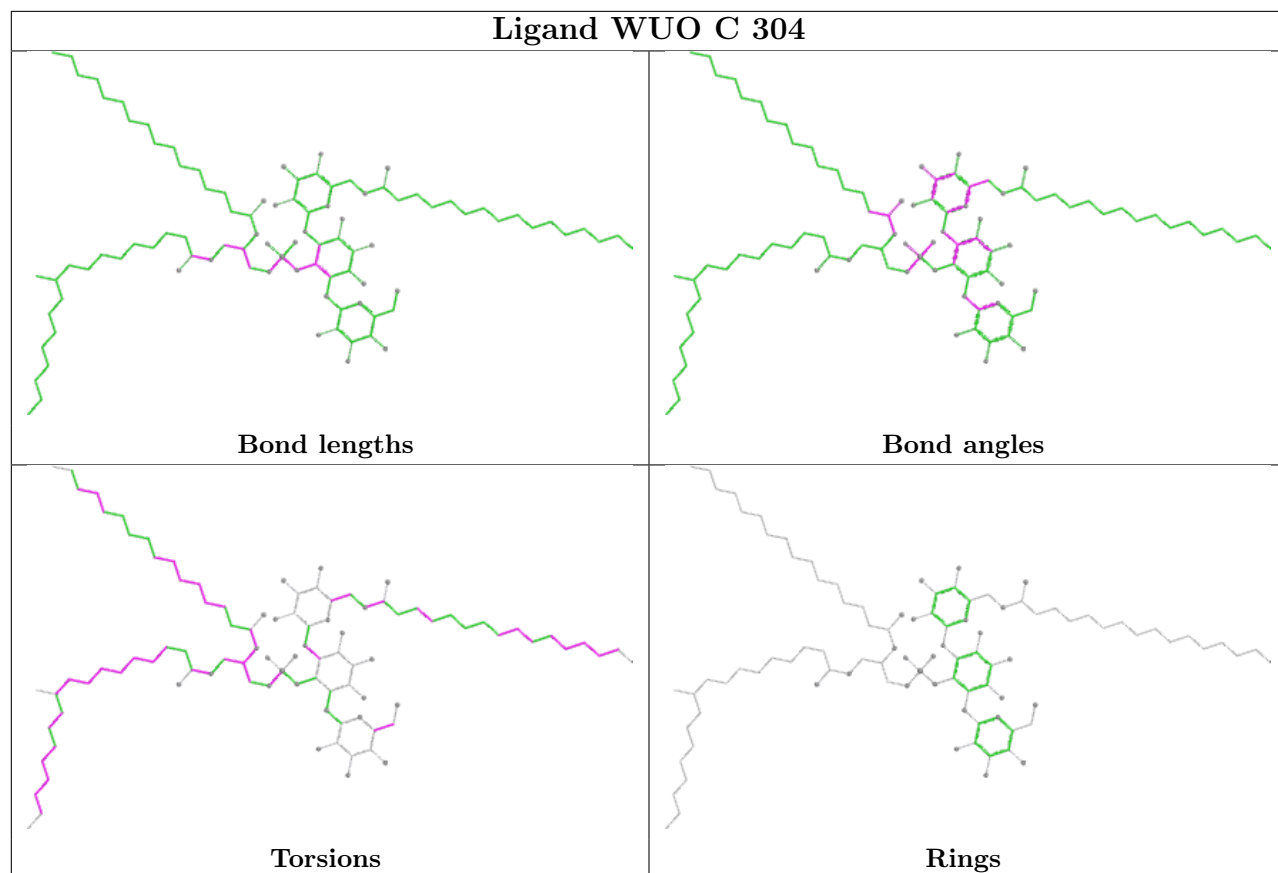


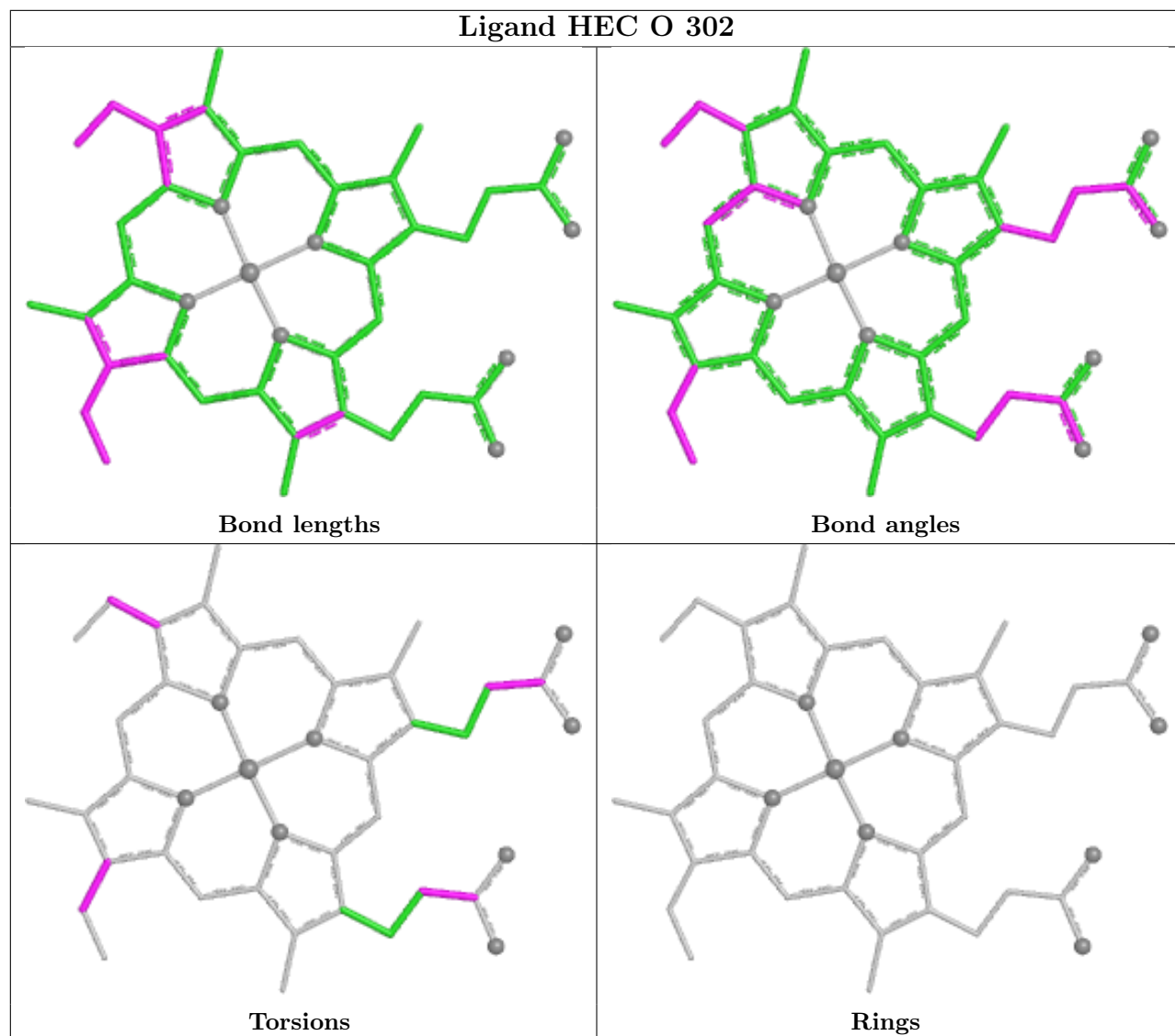




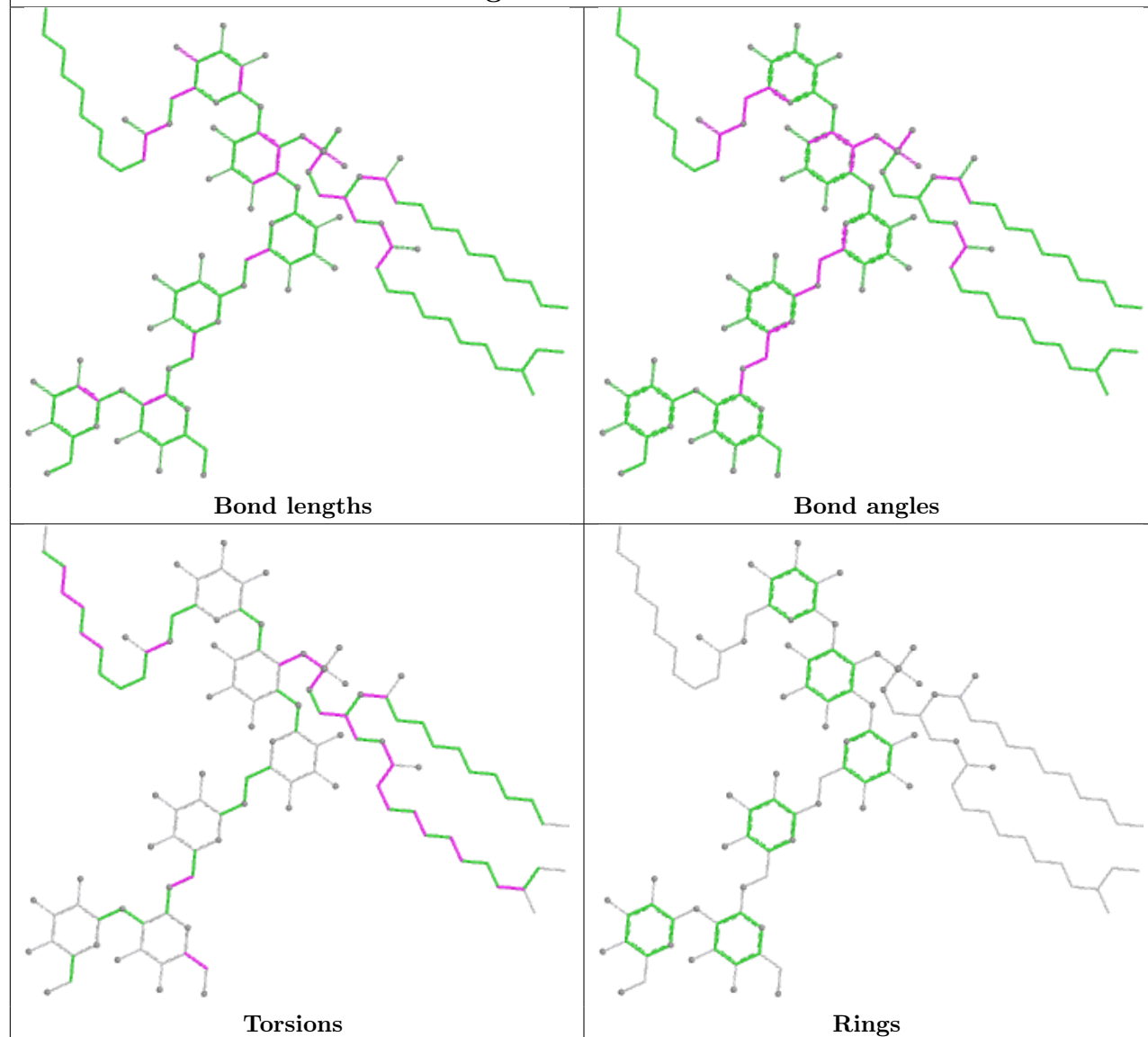


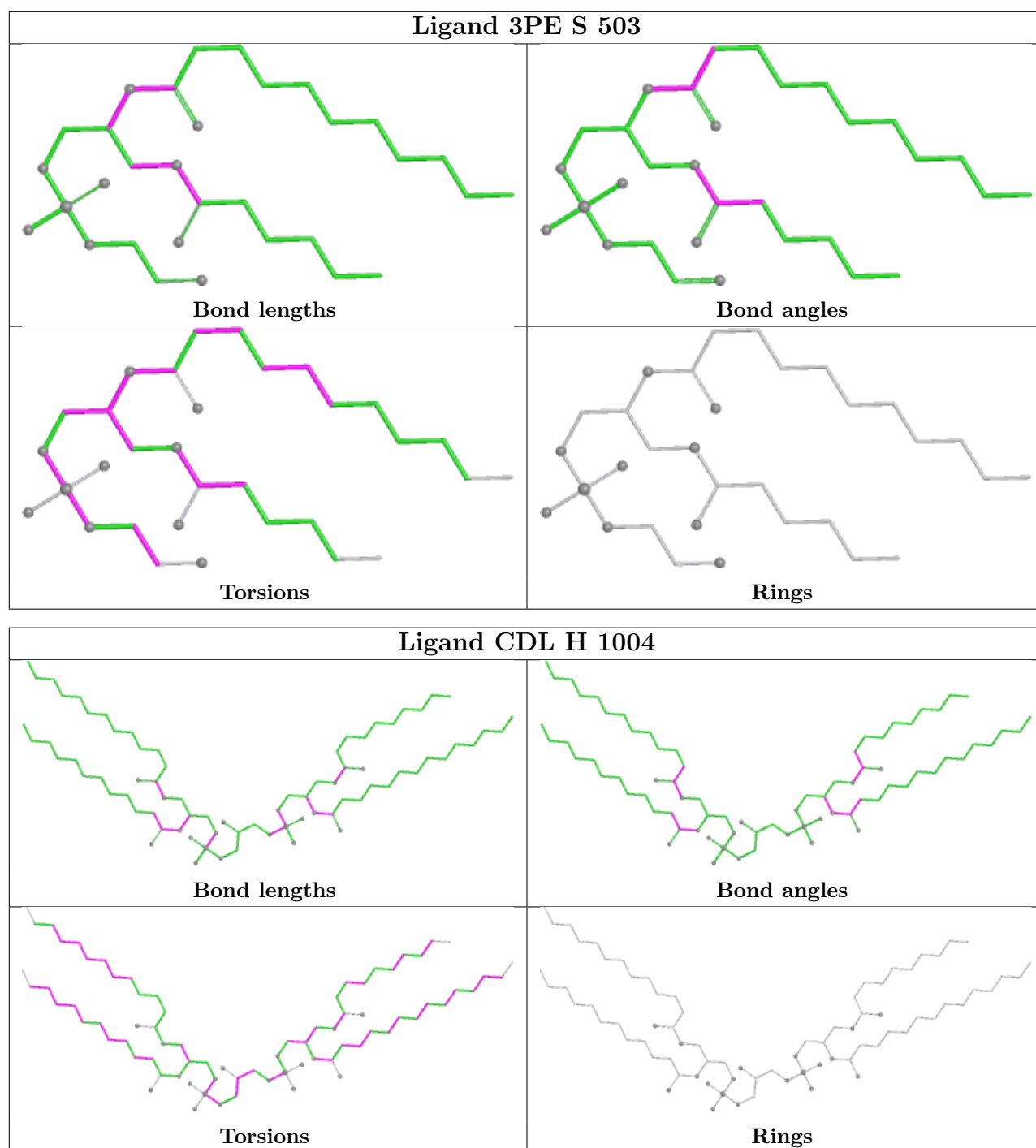


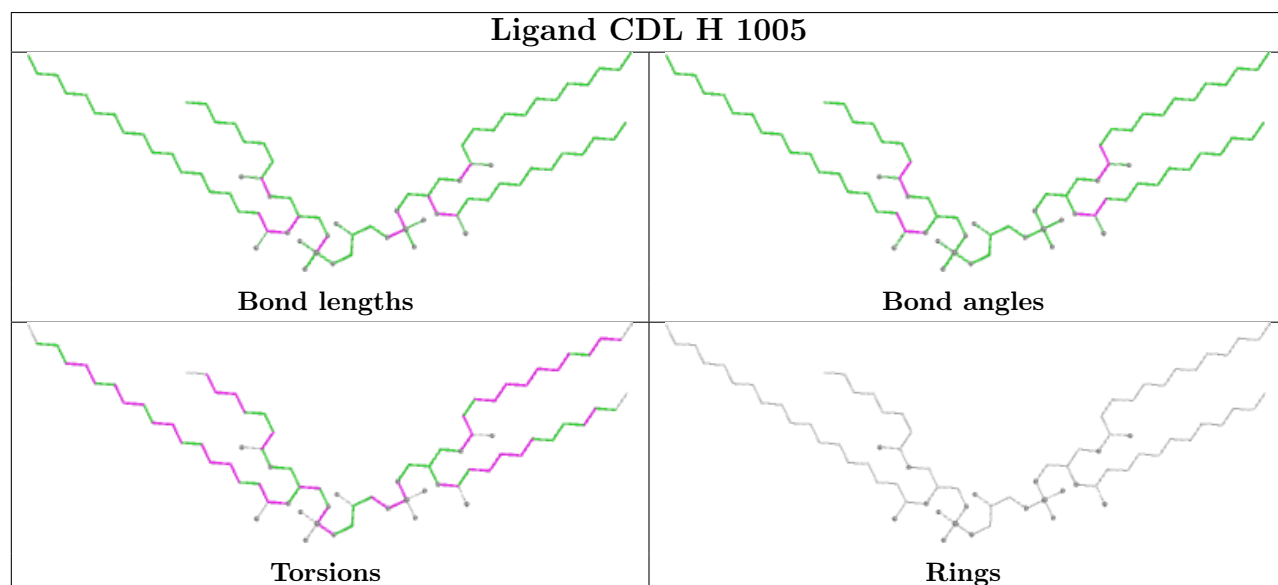
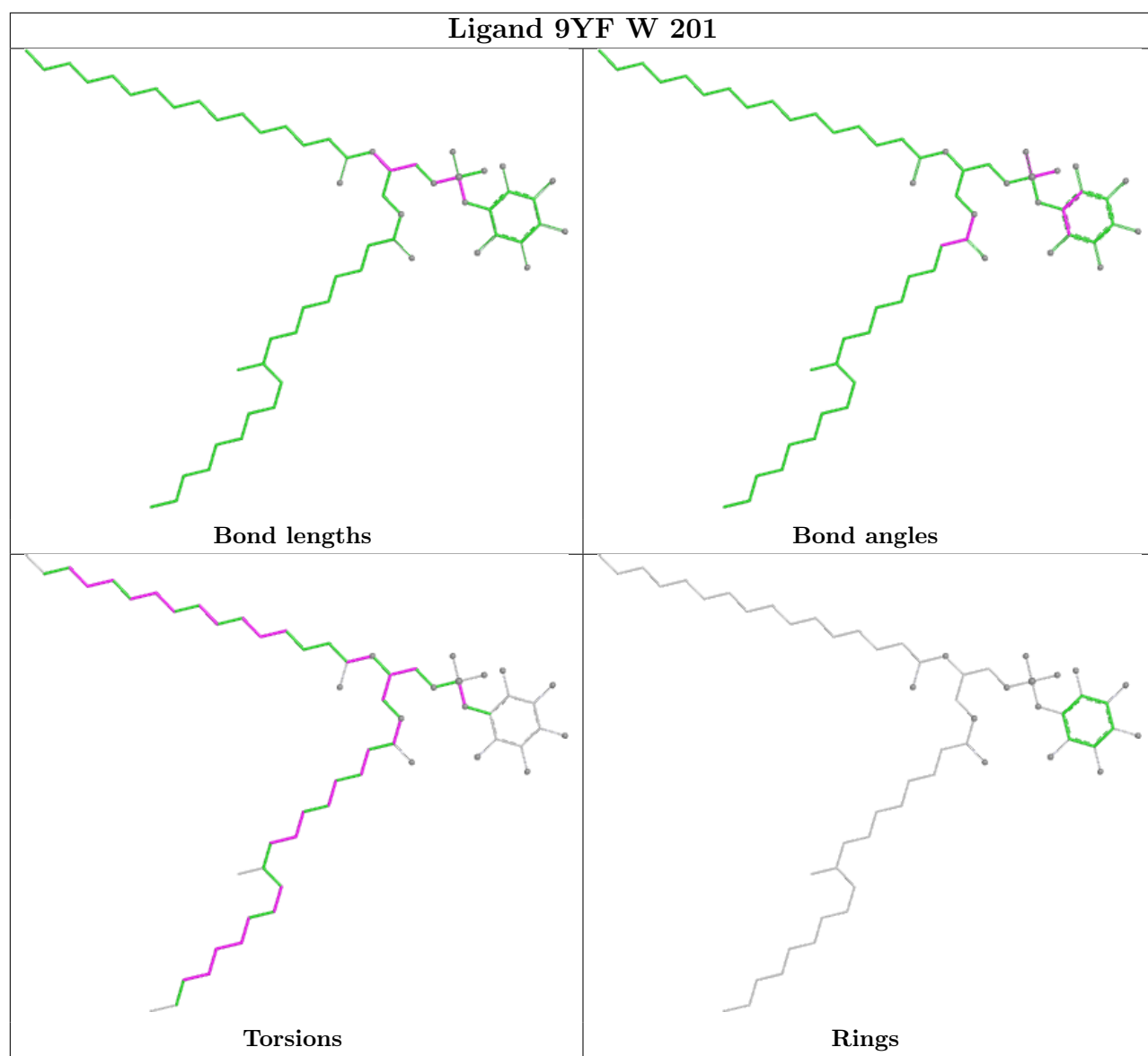


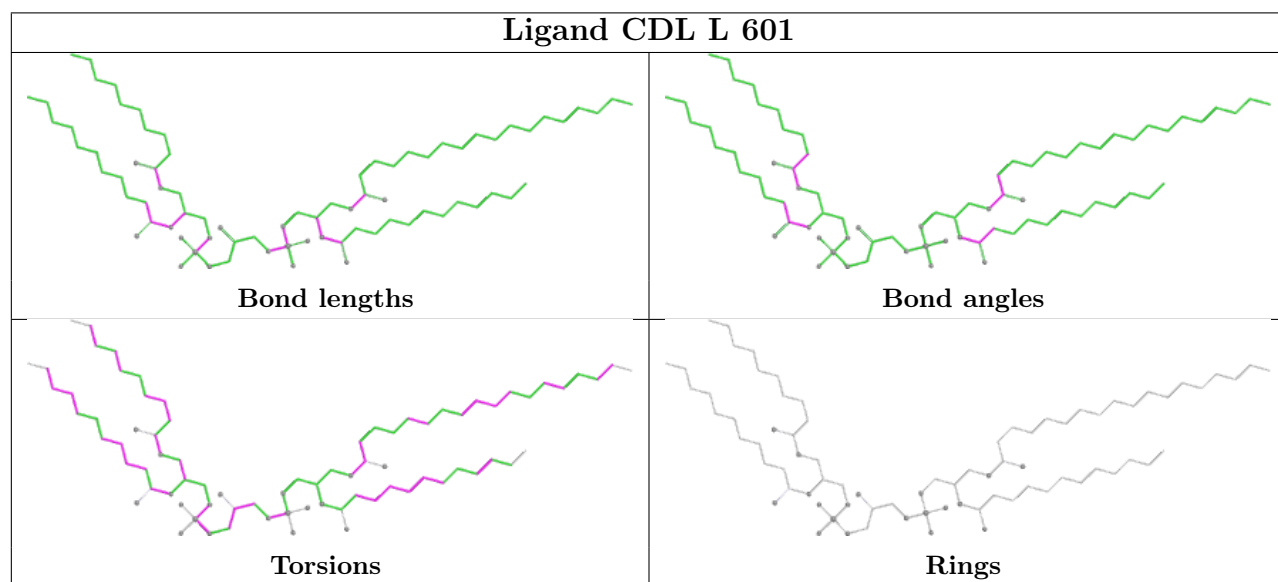
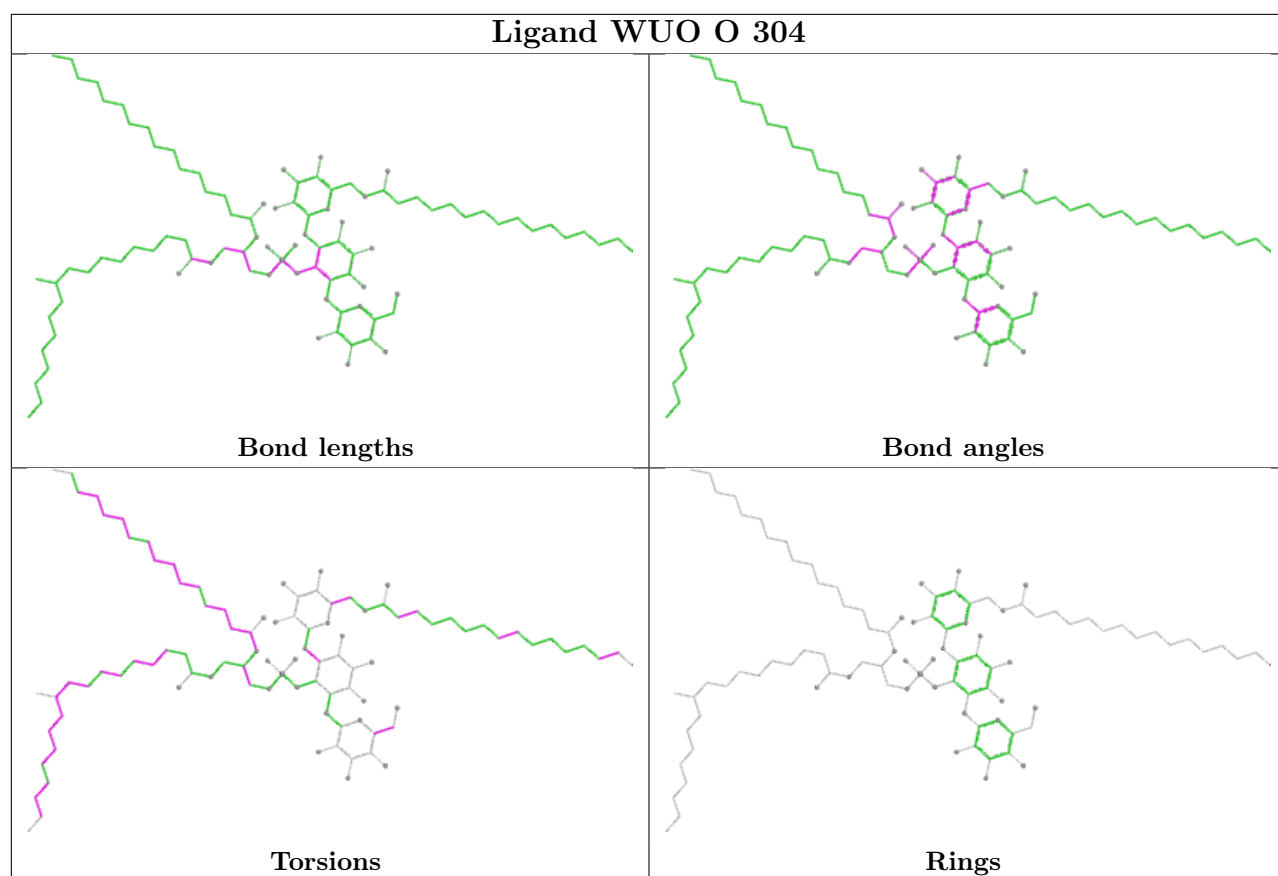


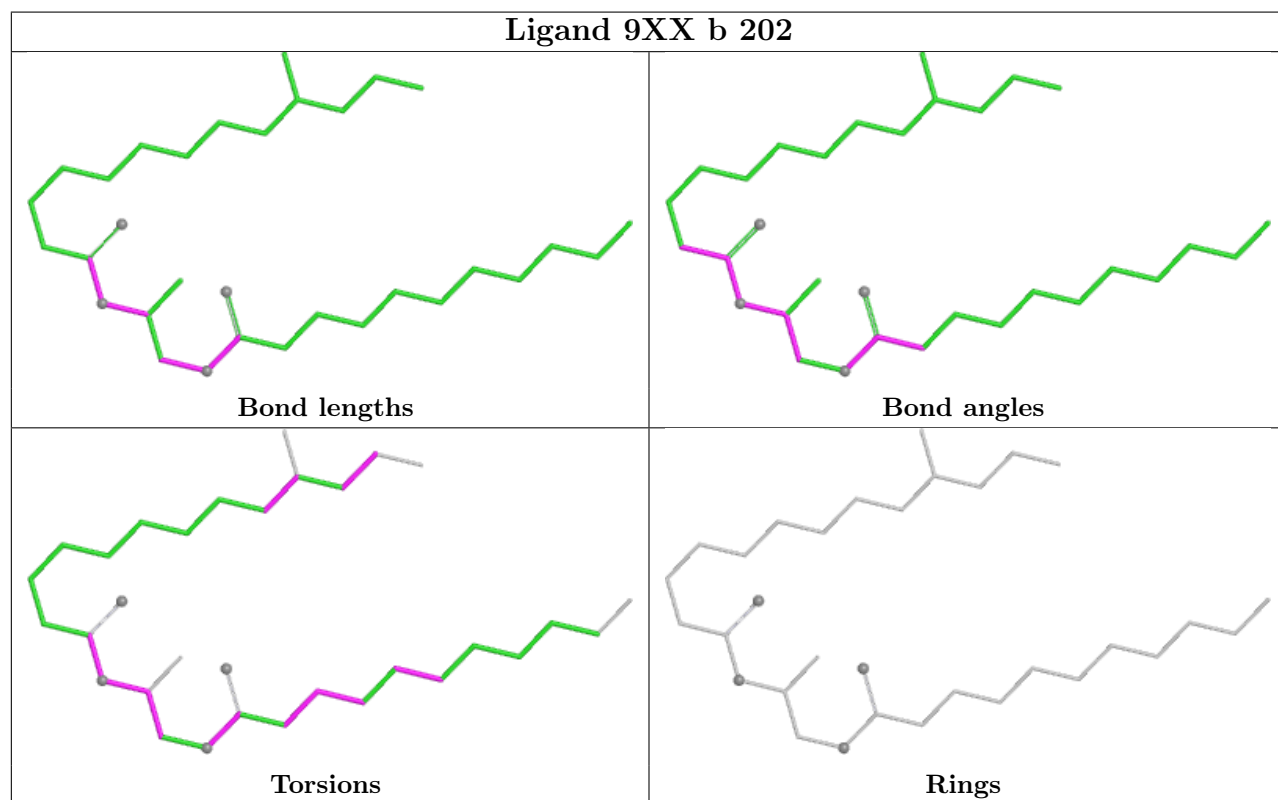
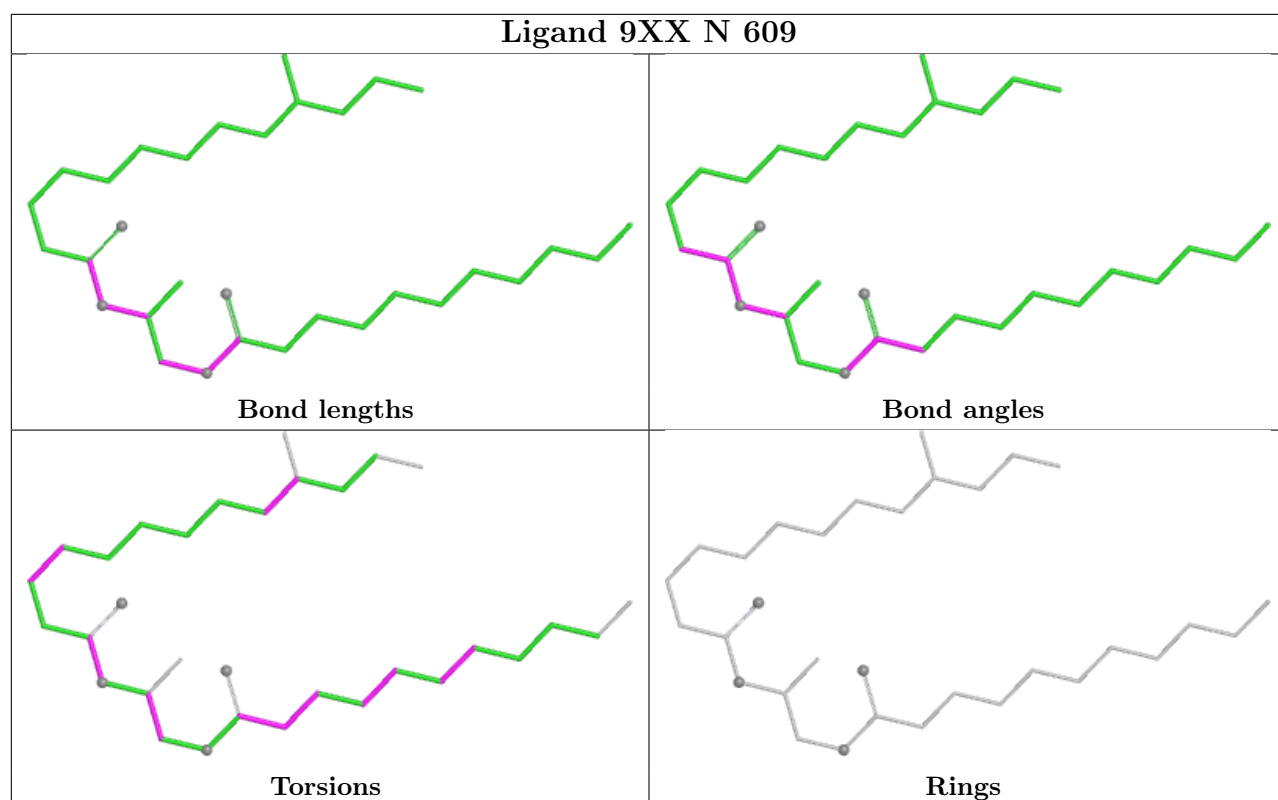
Ligand IZL G 502

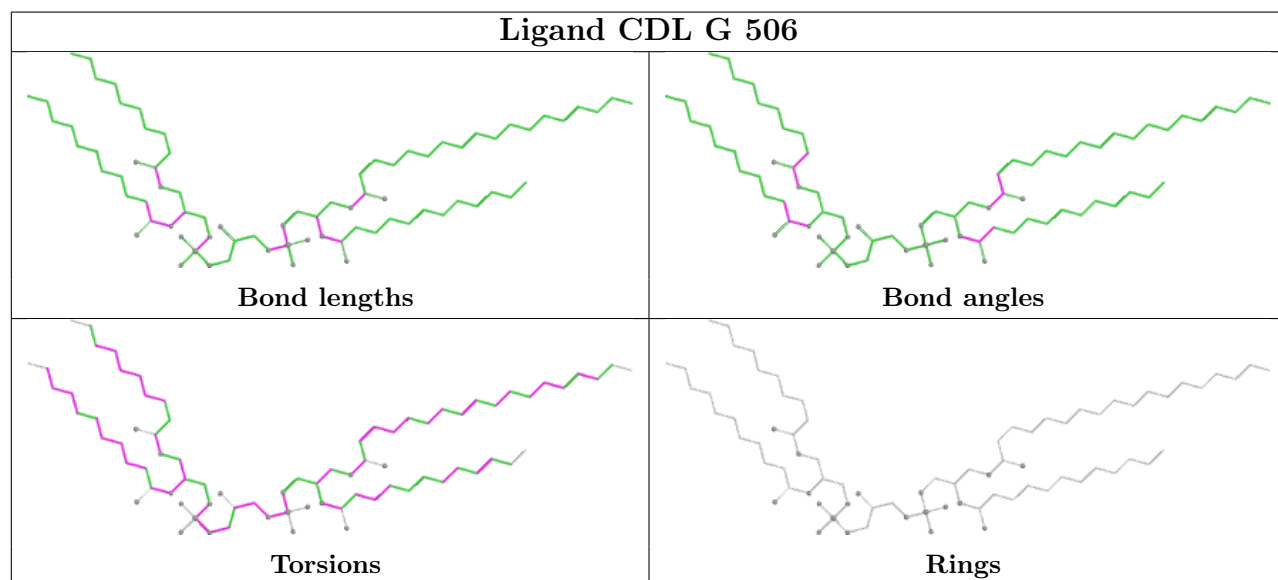
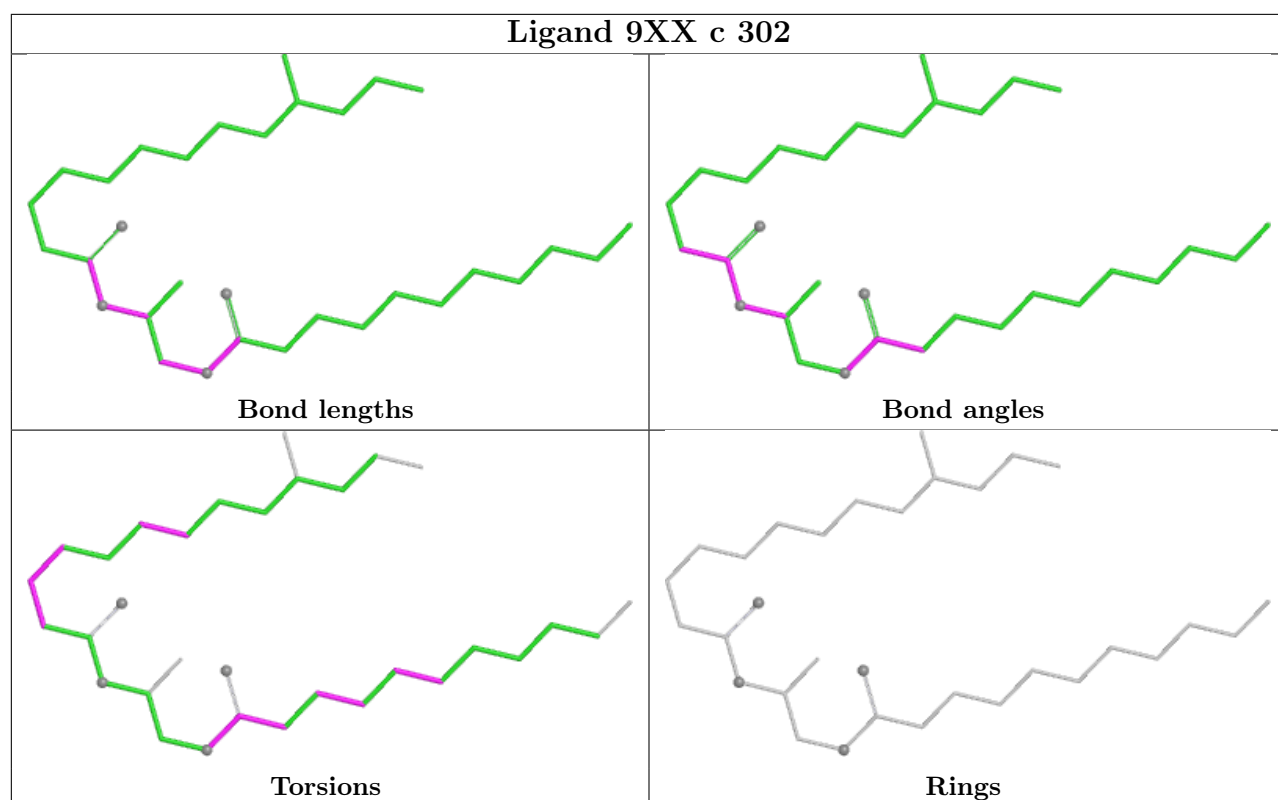


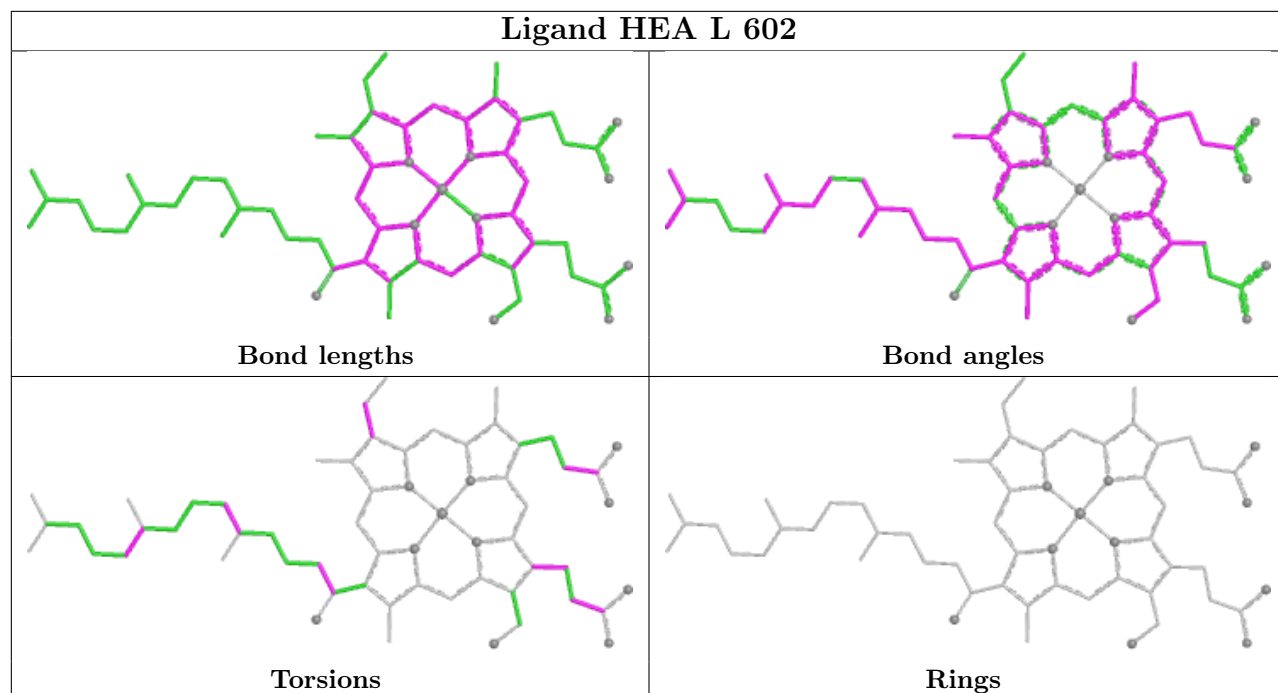


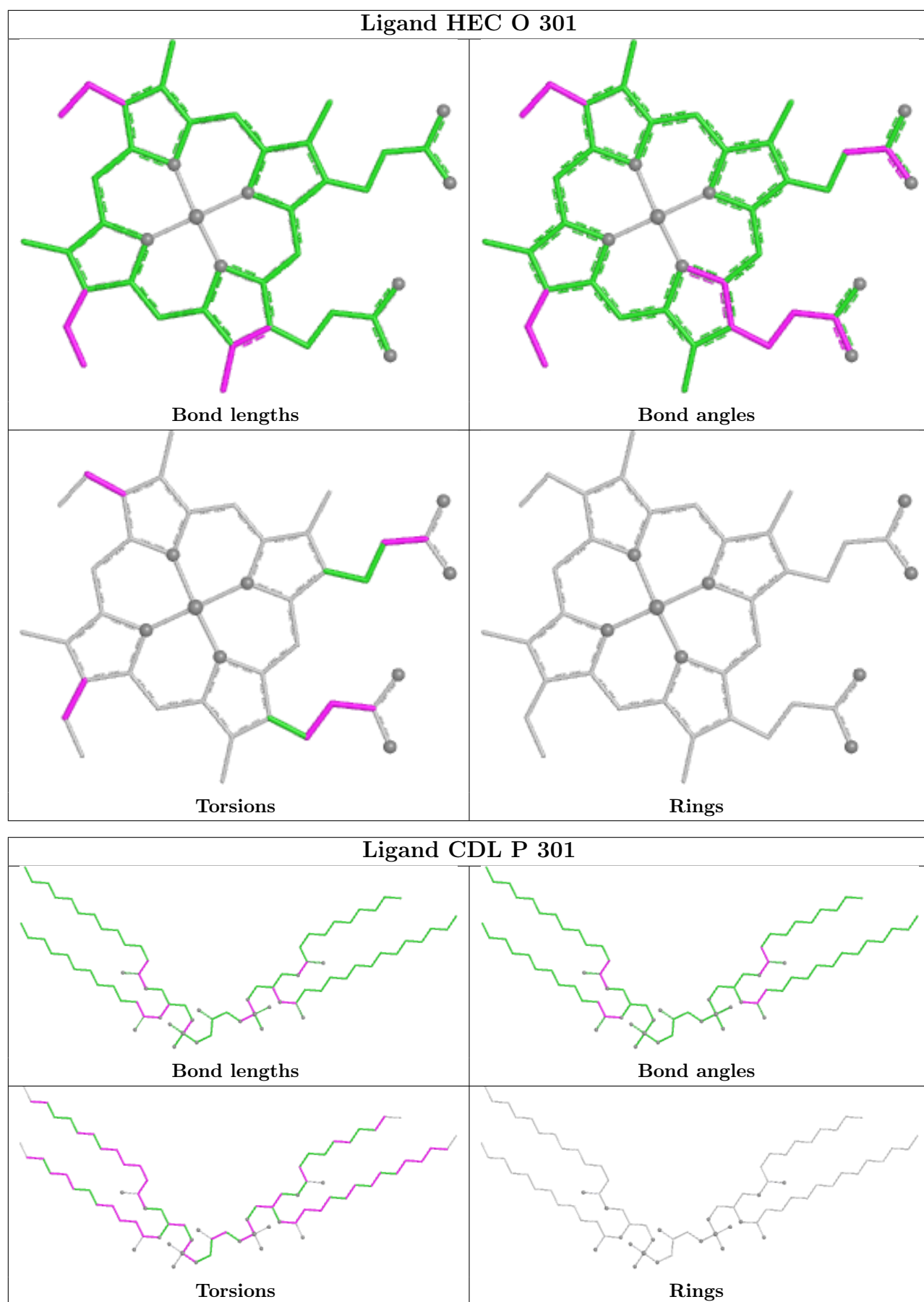


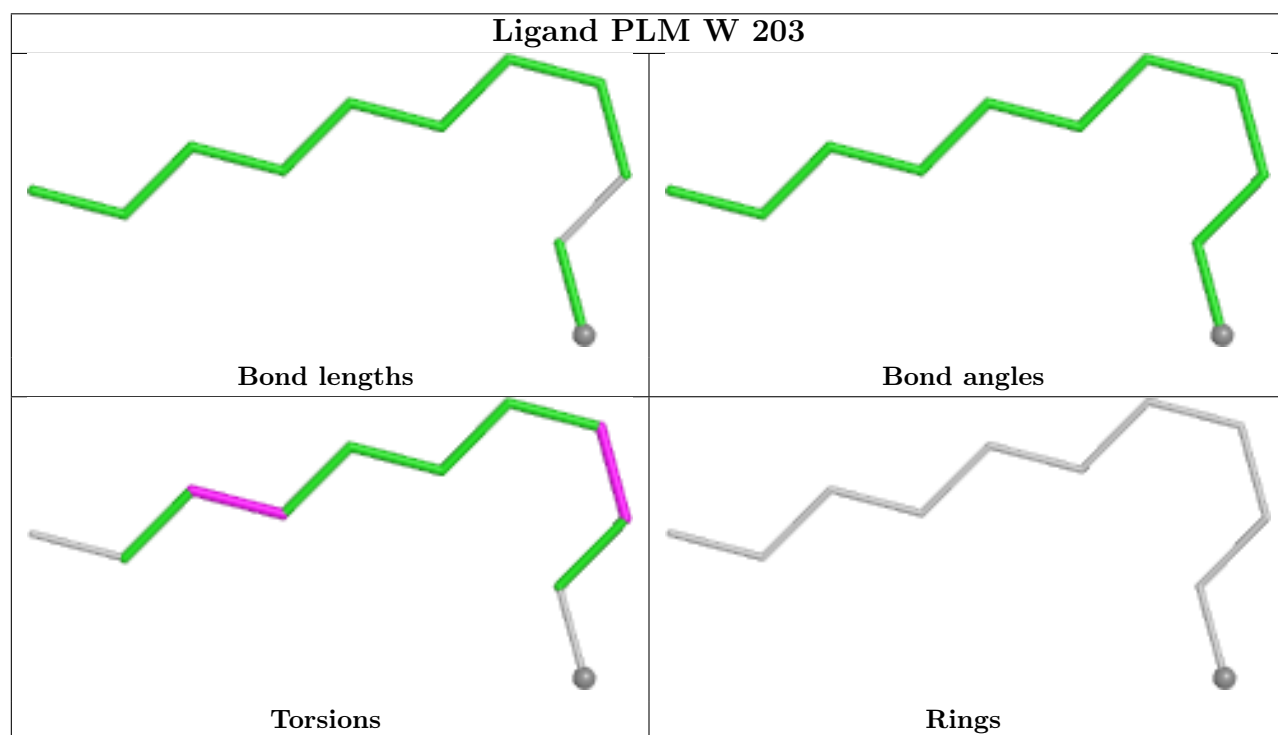
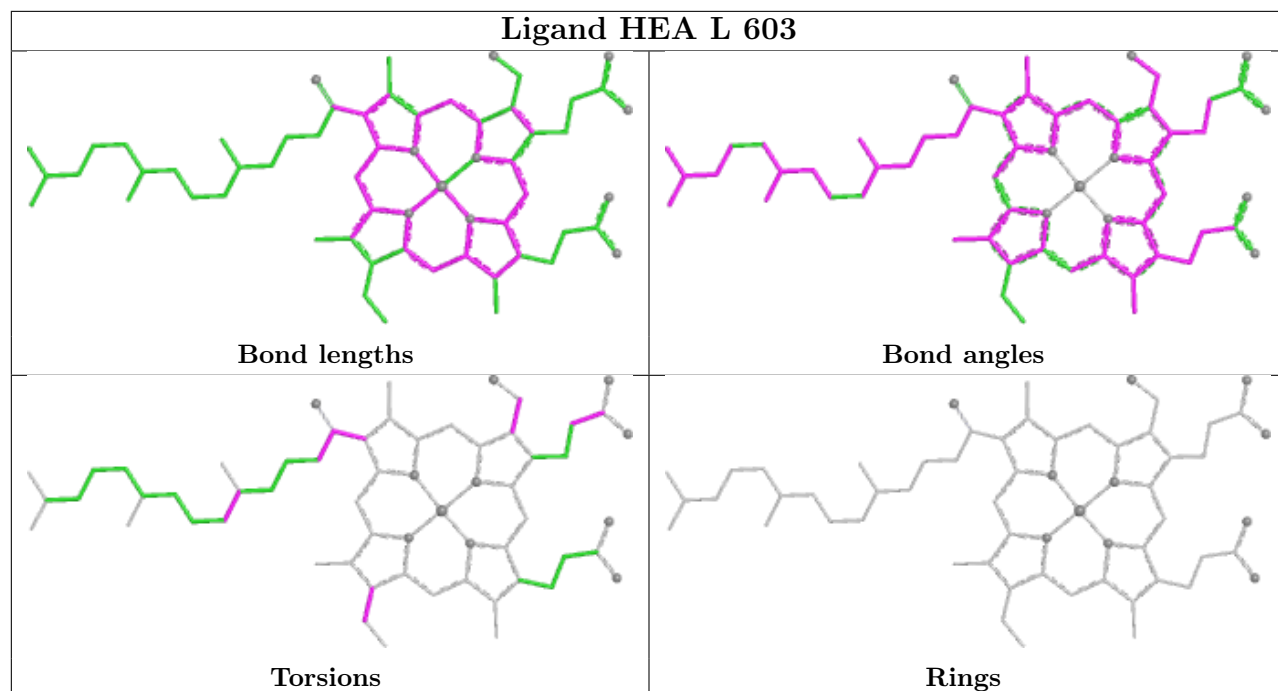


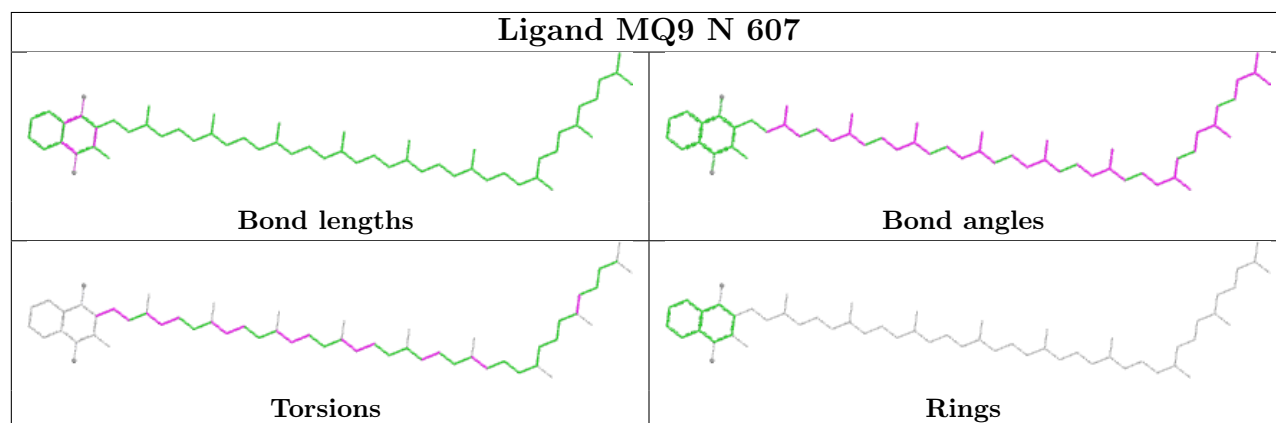
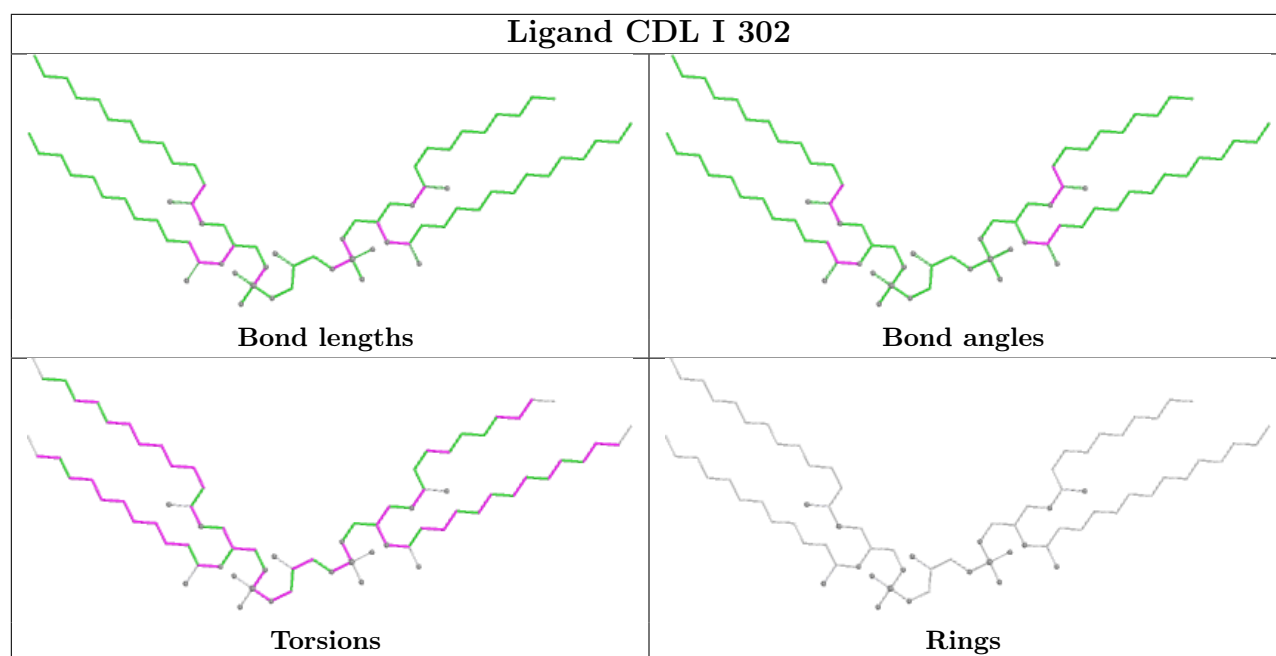
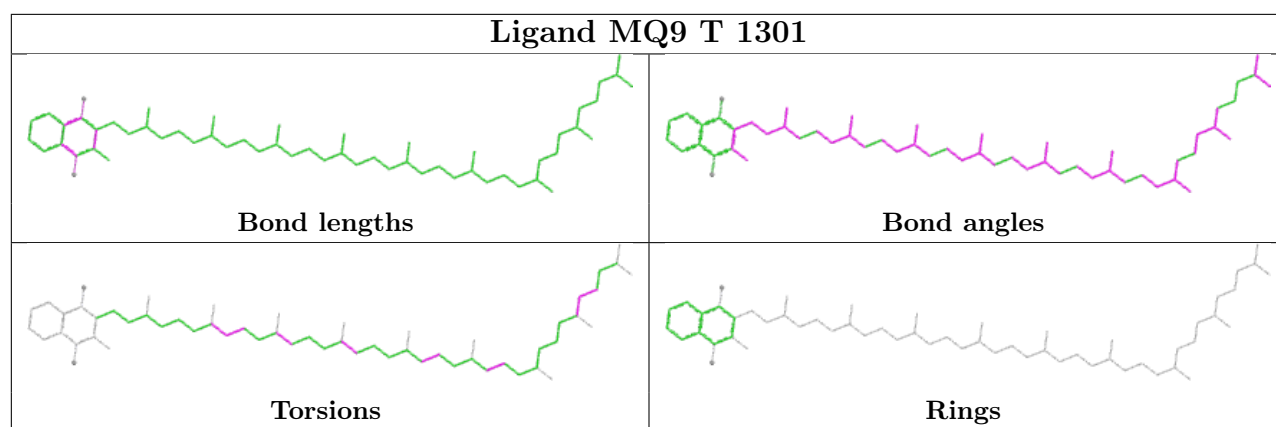


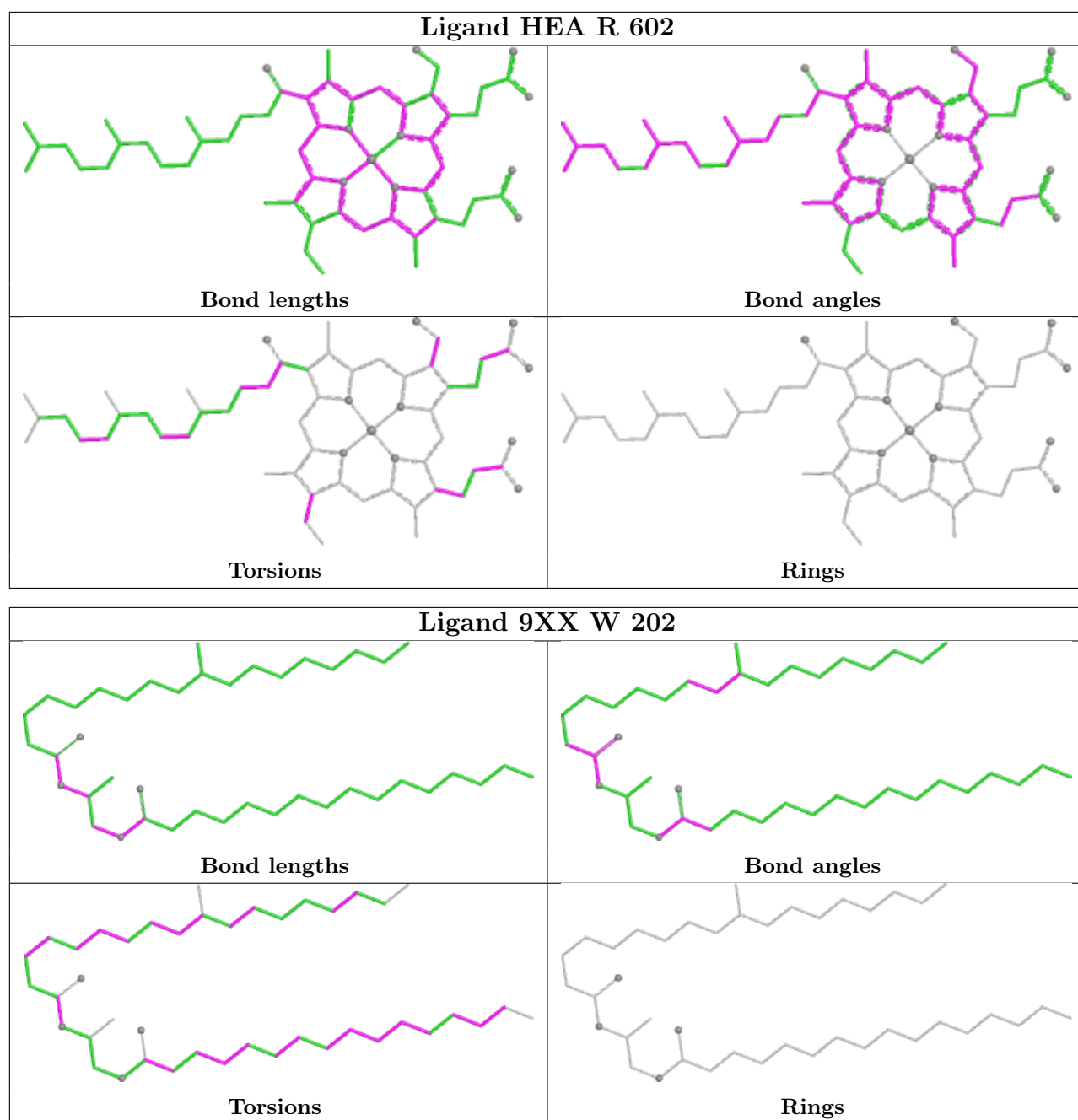


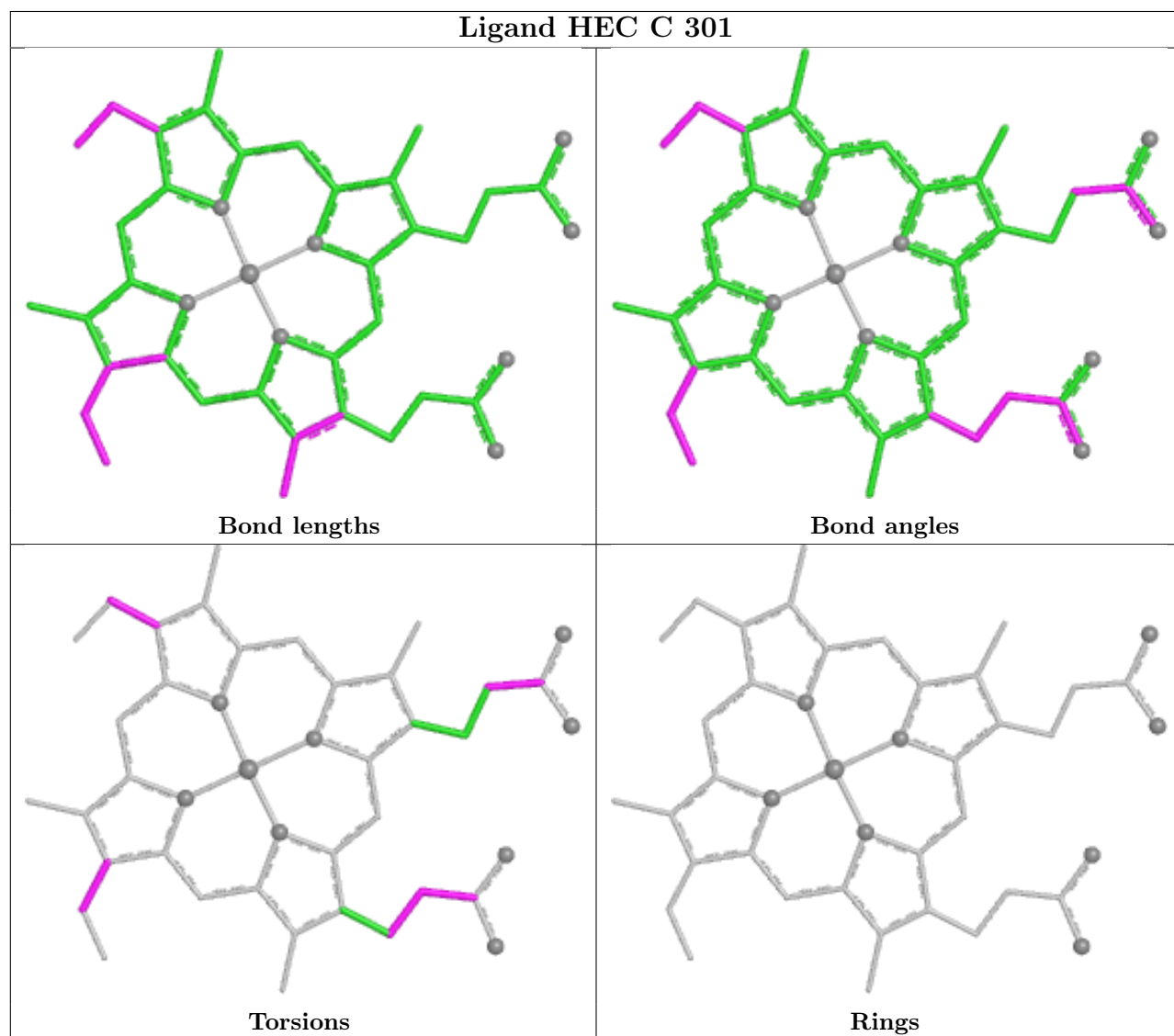
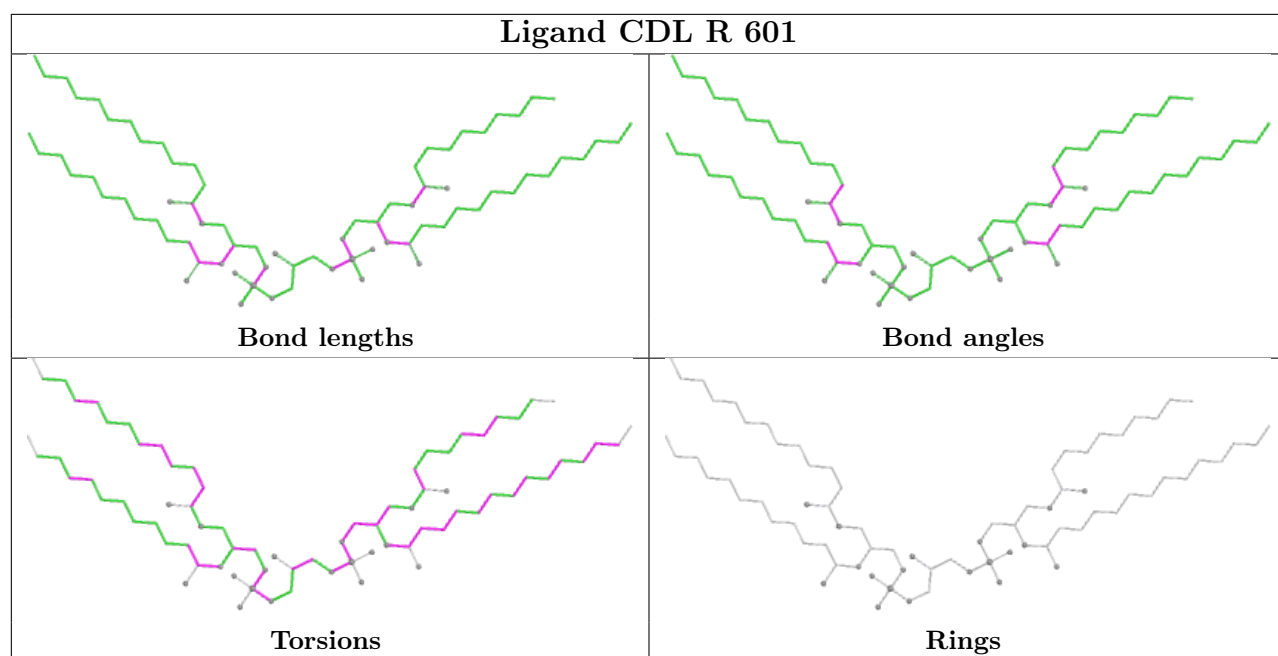


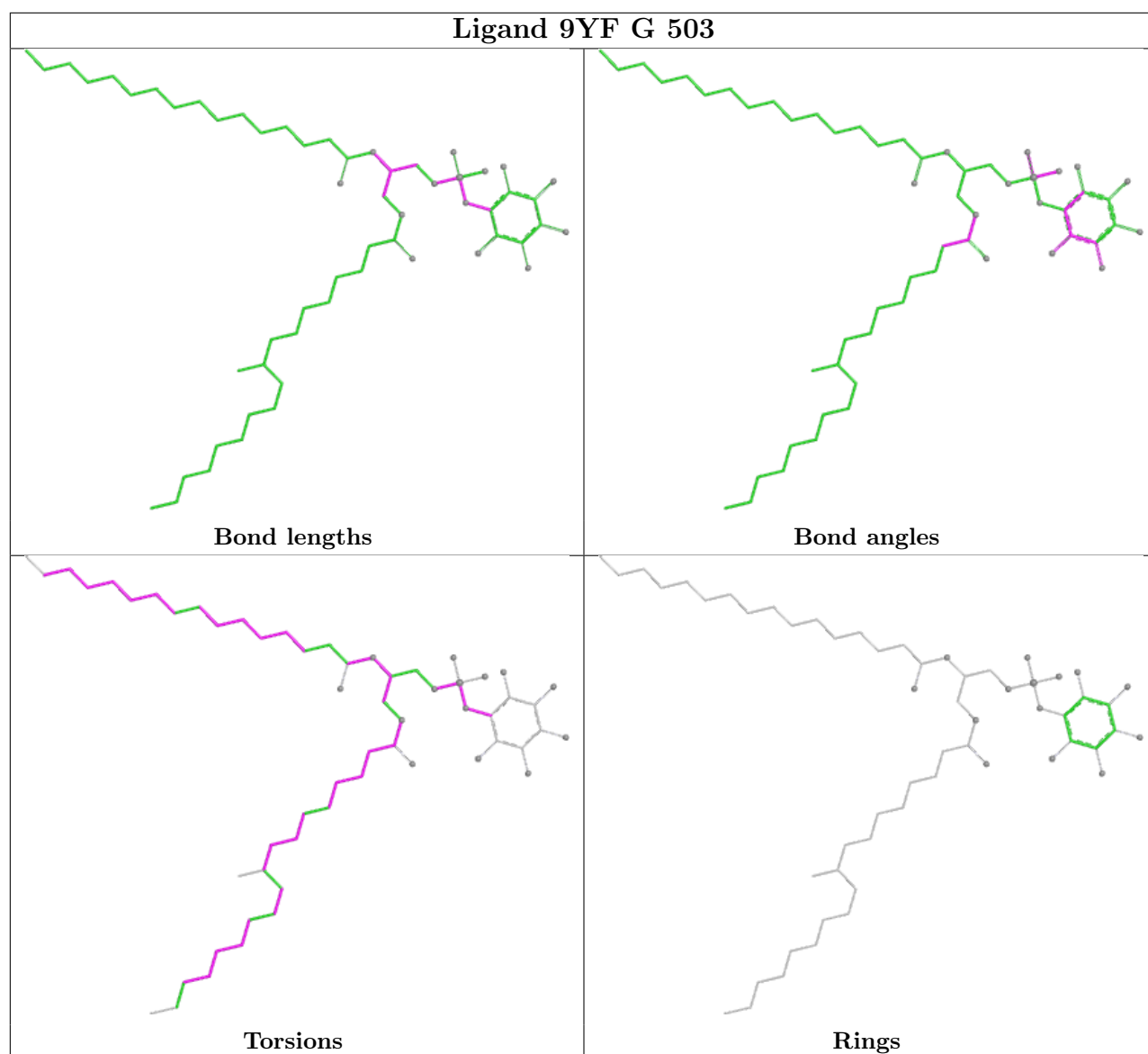
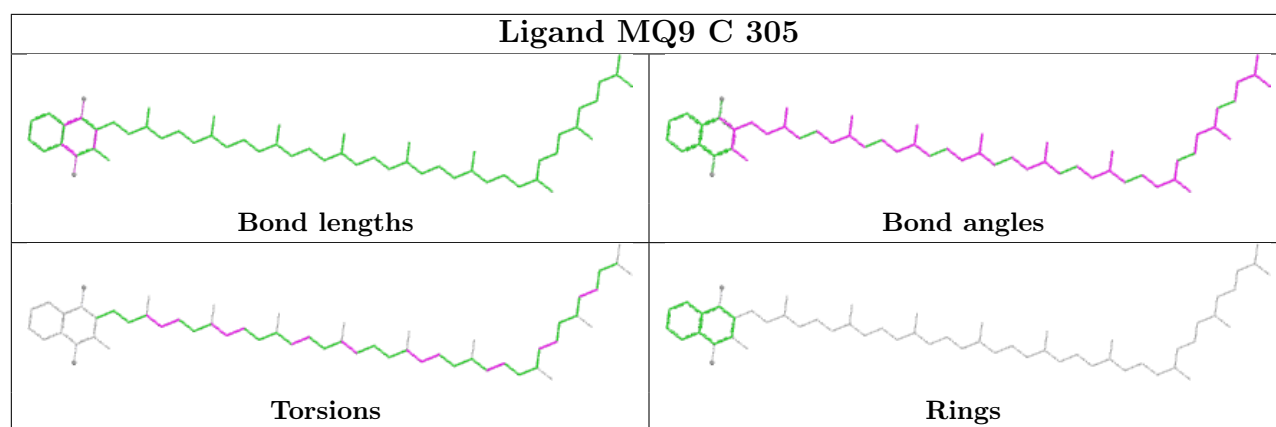




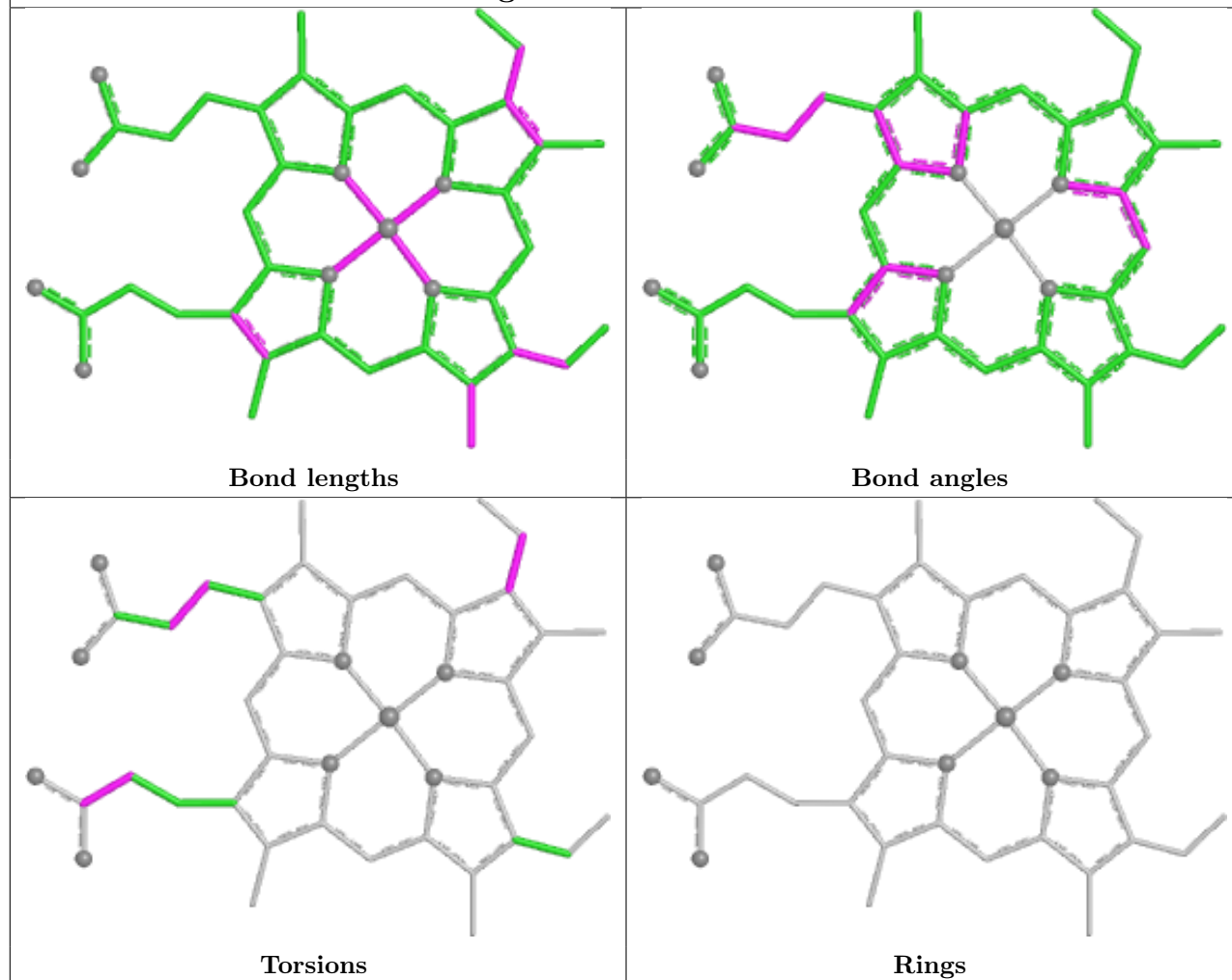




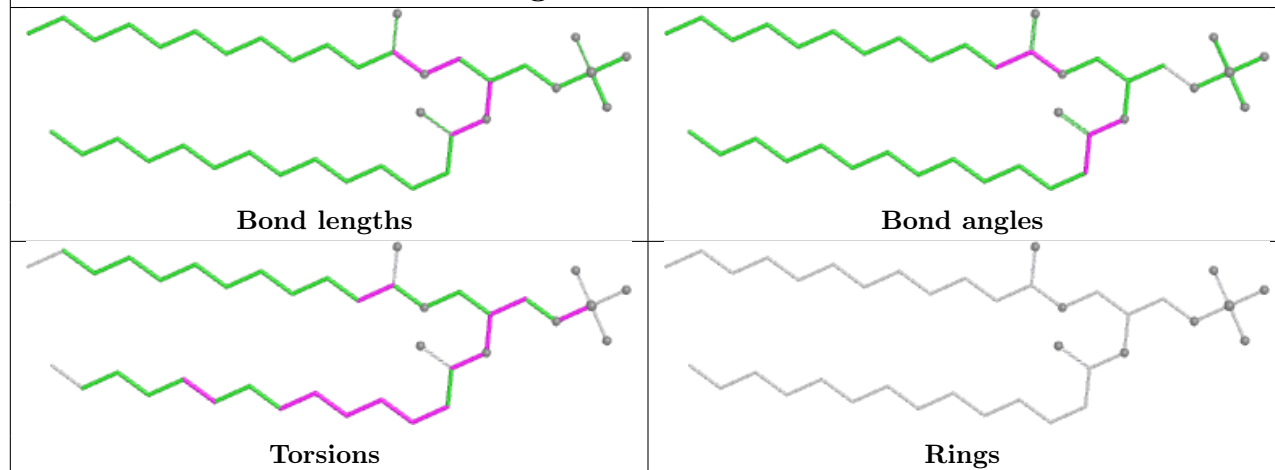


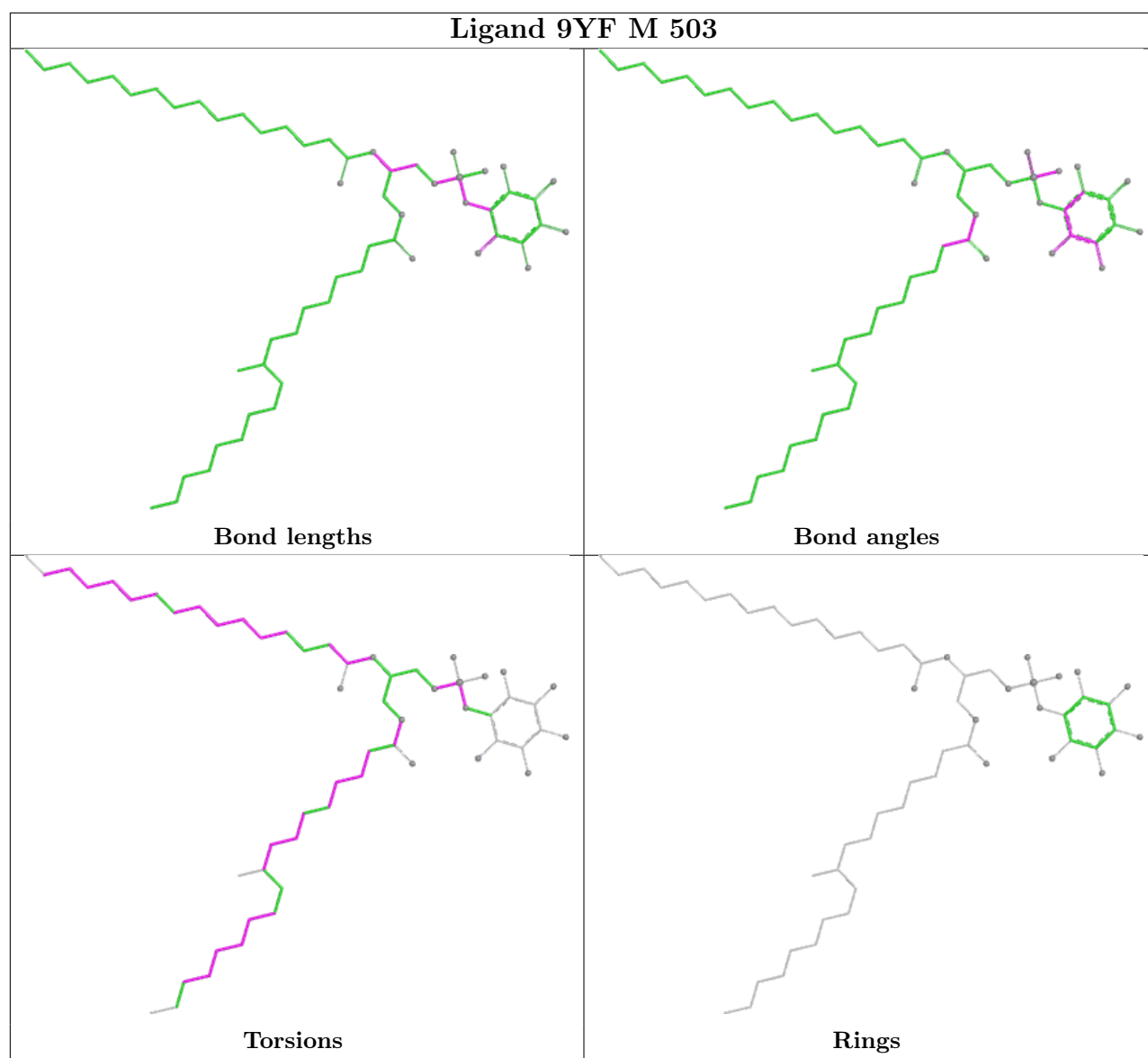


Ligand HEM H 1002



Ligand 7PH M 504





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.

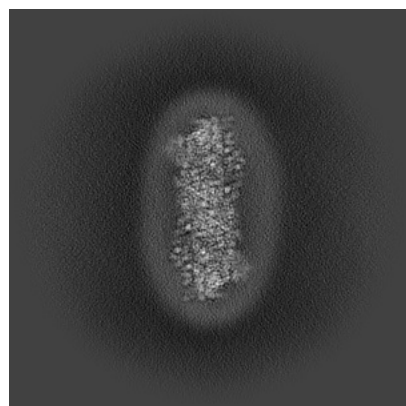
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53065. These allow visual inspection of the internal detail of the map and identification of artifacts.

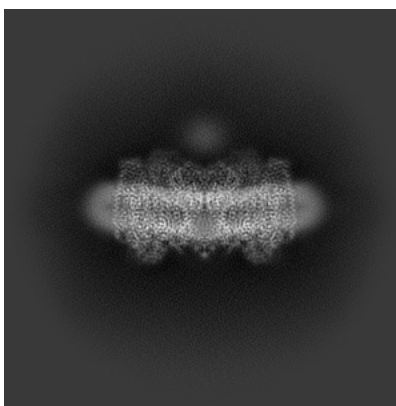
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

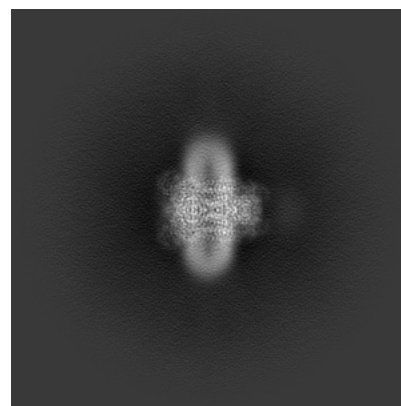
6.1.1 Primary map



X

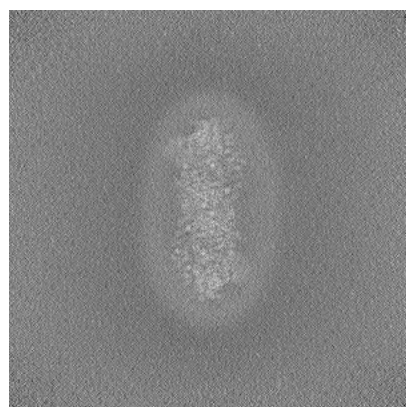


Y

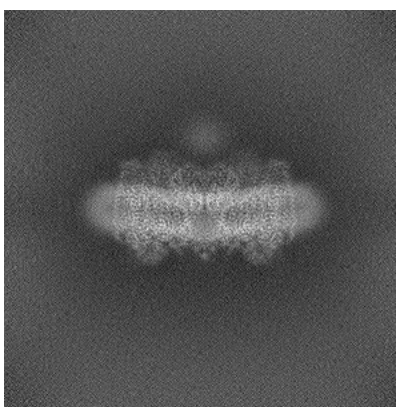


Z

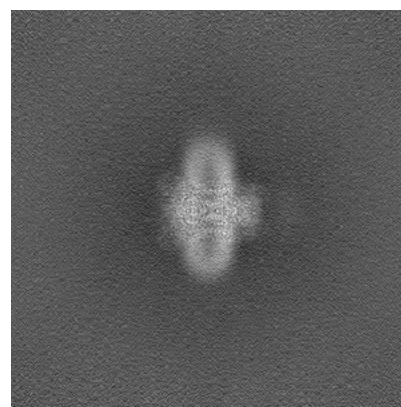
6.1.2 Raw map



X



Y

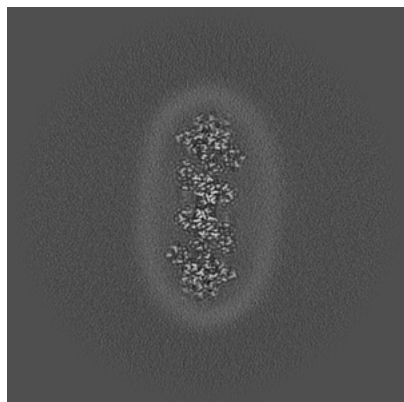


Z

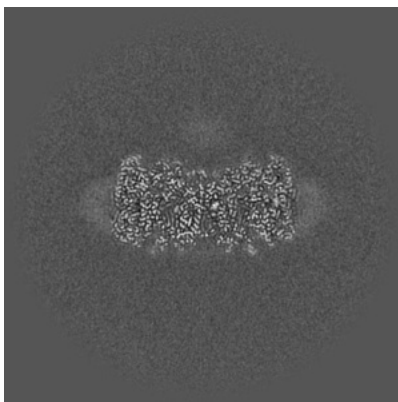
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

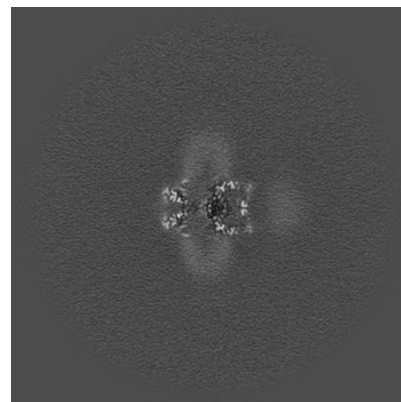
6.2.1 Primary map



X Index: 270

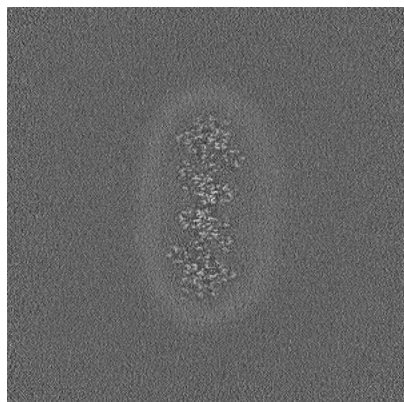


Y Index: 270

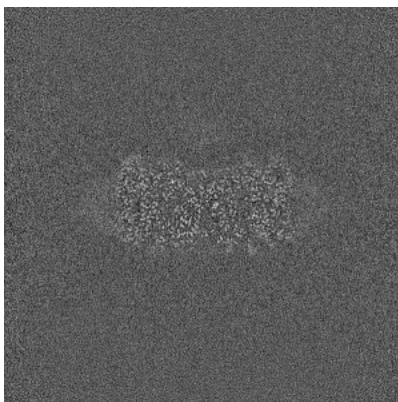


Z Index: 270

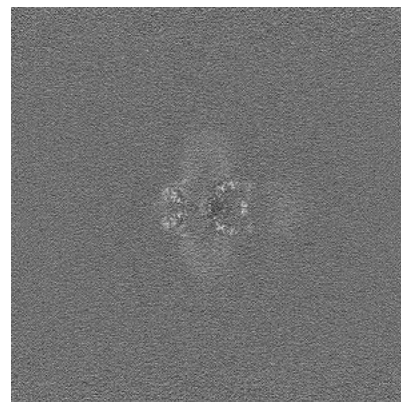
6.2.2 Raw map



X Index: 270



Y Index: 270

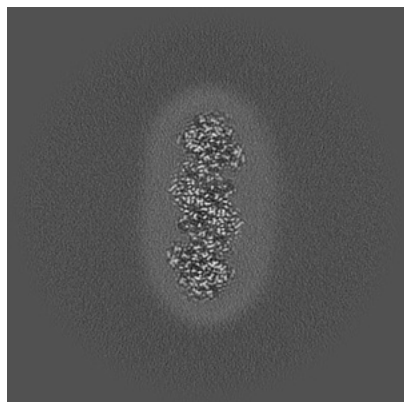


Z Index: 270

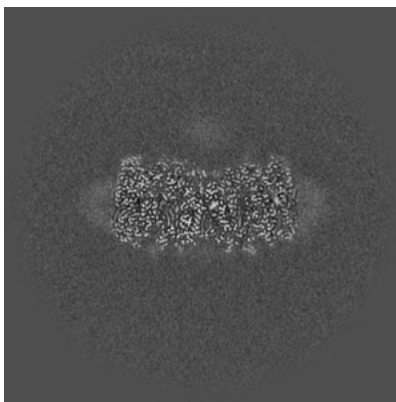
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

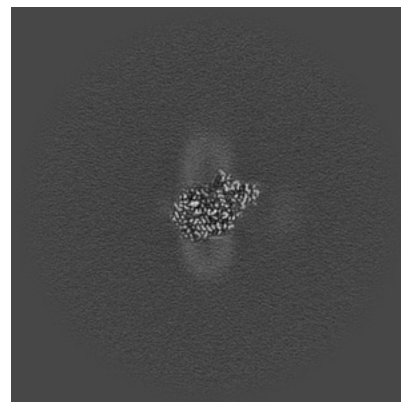
6.3.1 Primary map



X Index: 284

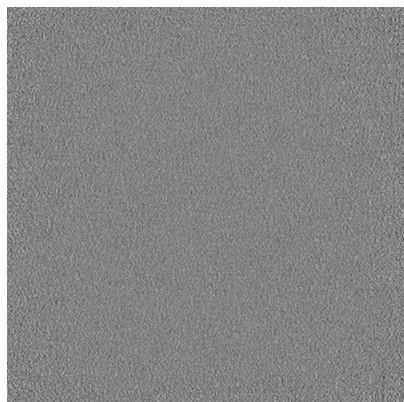


Y Index: 271

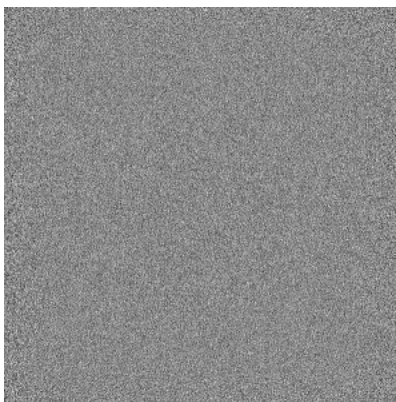


Z Index: 248

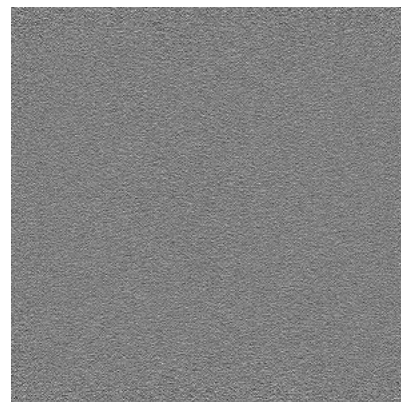
6.3.2 Raw map



X Index: 0



Y Index: 0

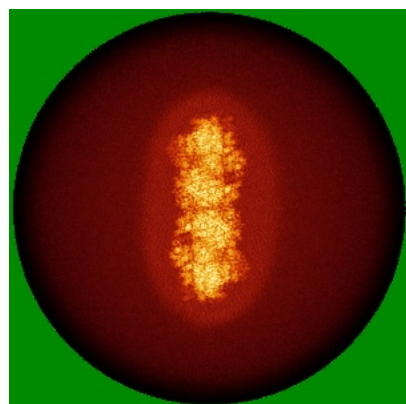


Z Index: 0

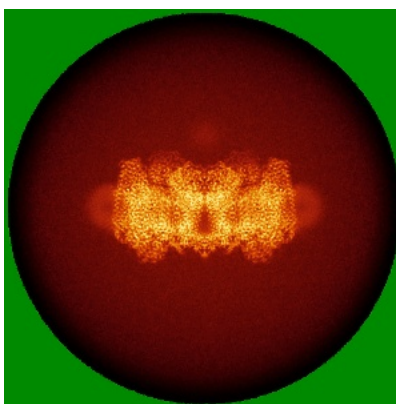
The images above show the largest variance slices of the map in three orthogonal directions.

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

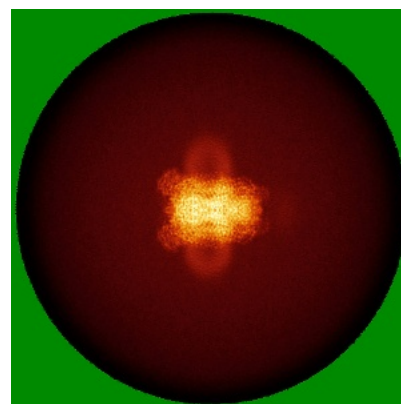
6.4.1 Primary map



X

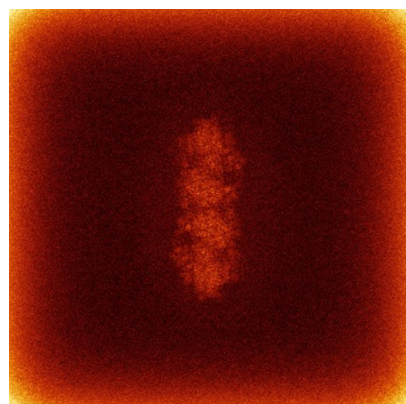


Y

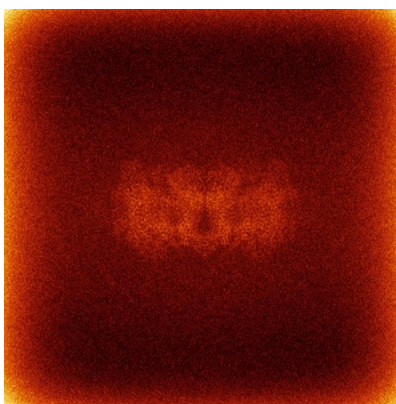


Z

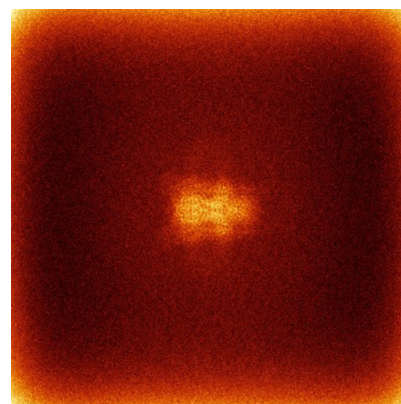
6.4.2 Raw map



X



Y

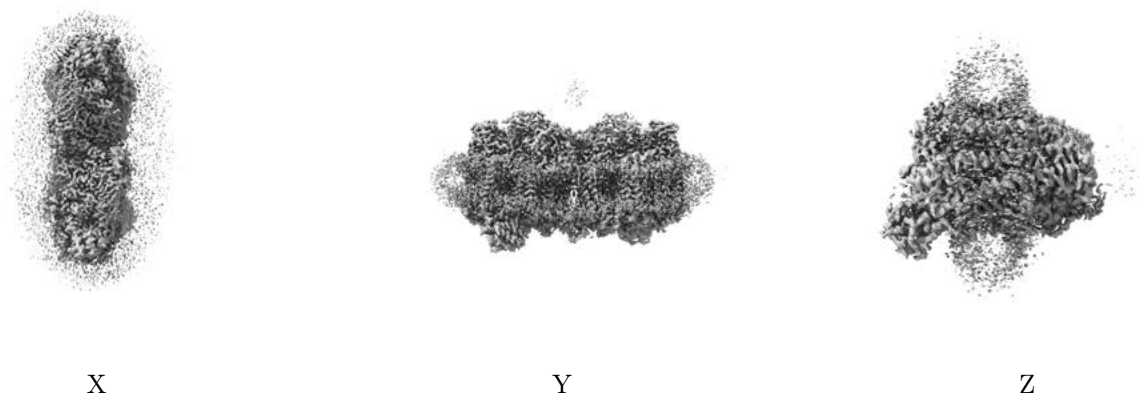


Z

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

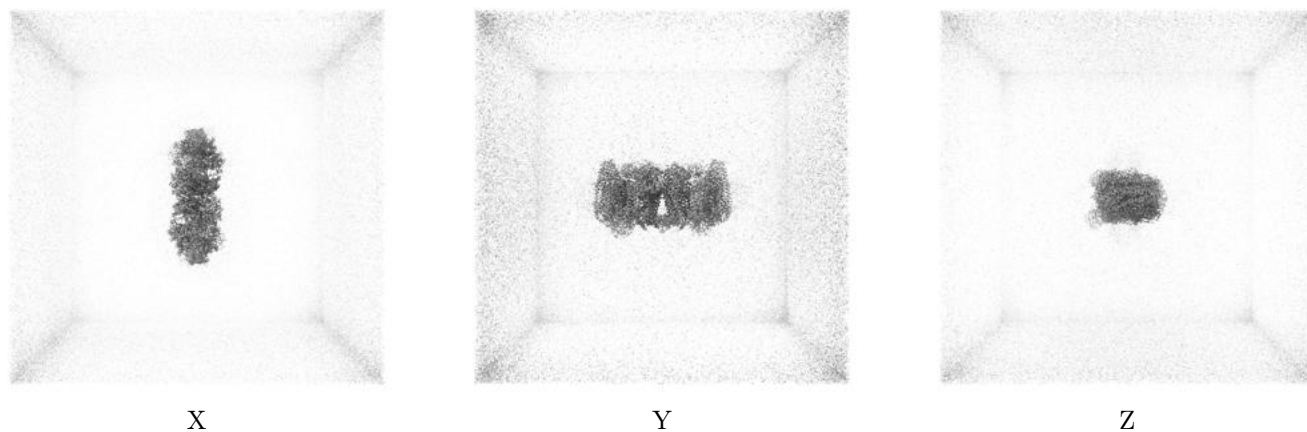
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

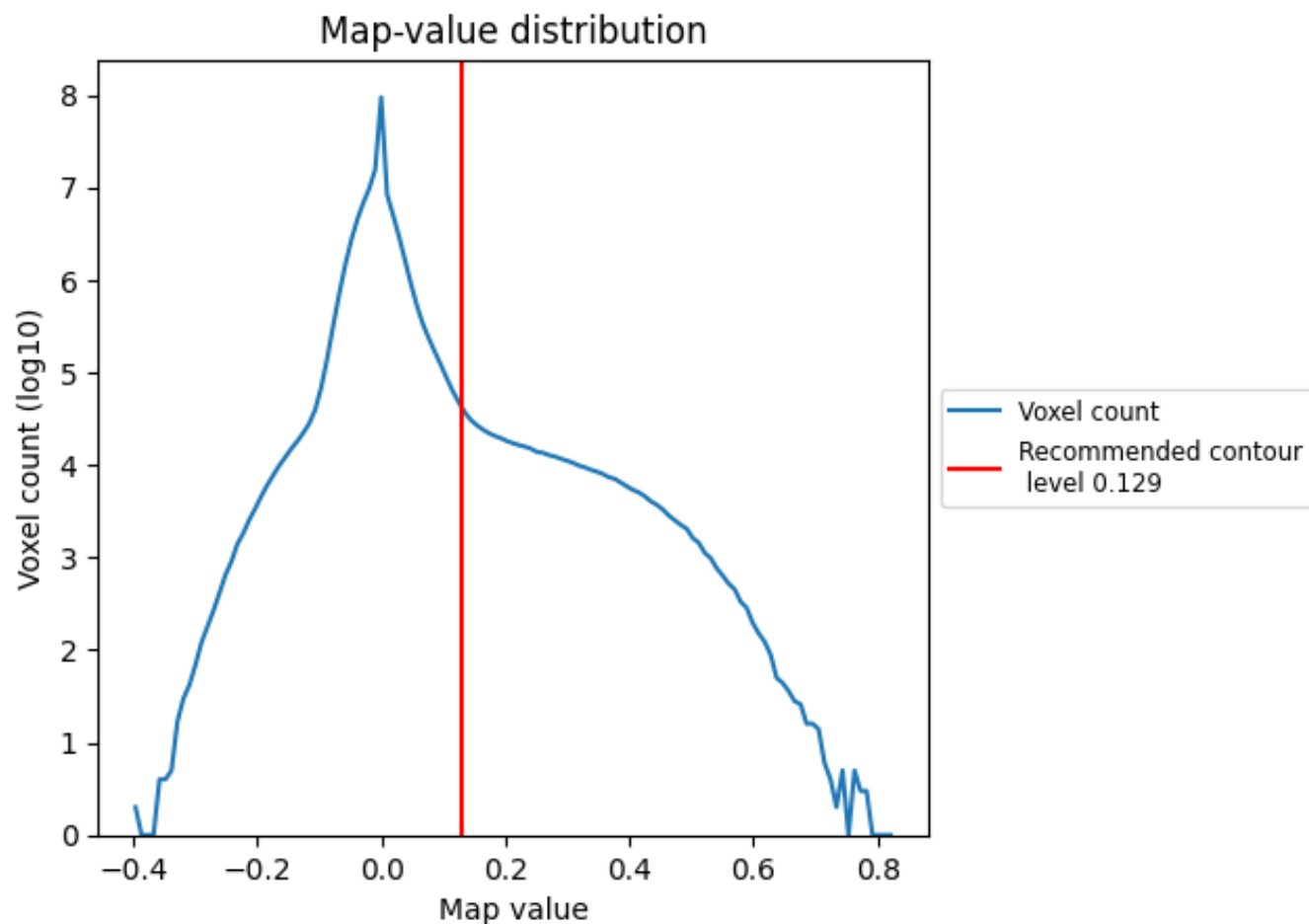
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

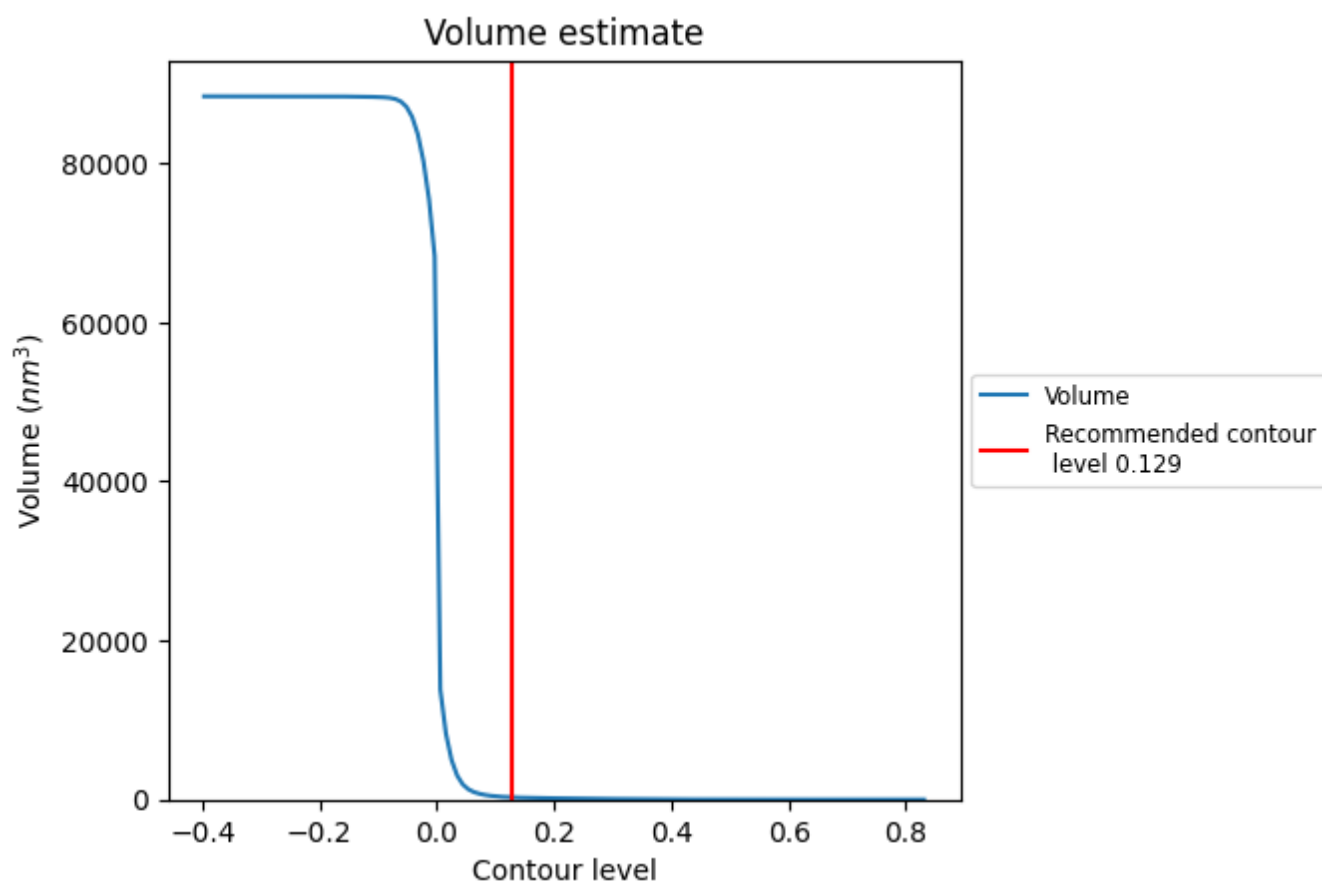
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

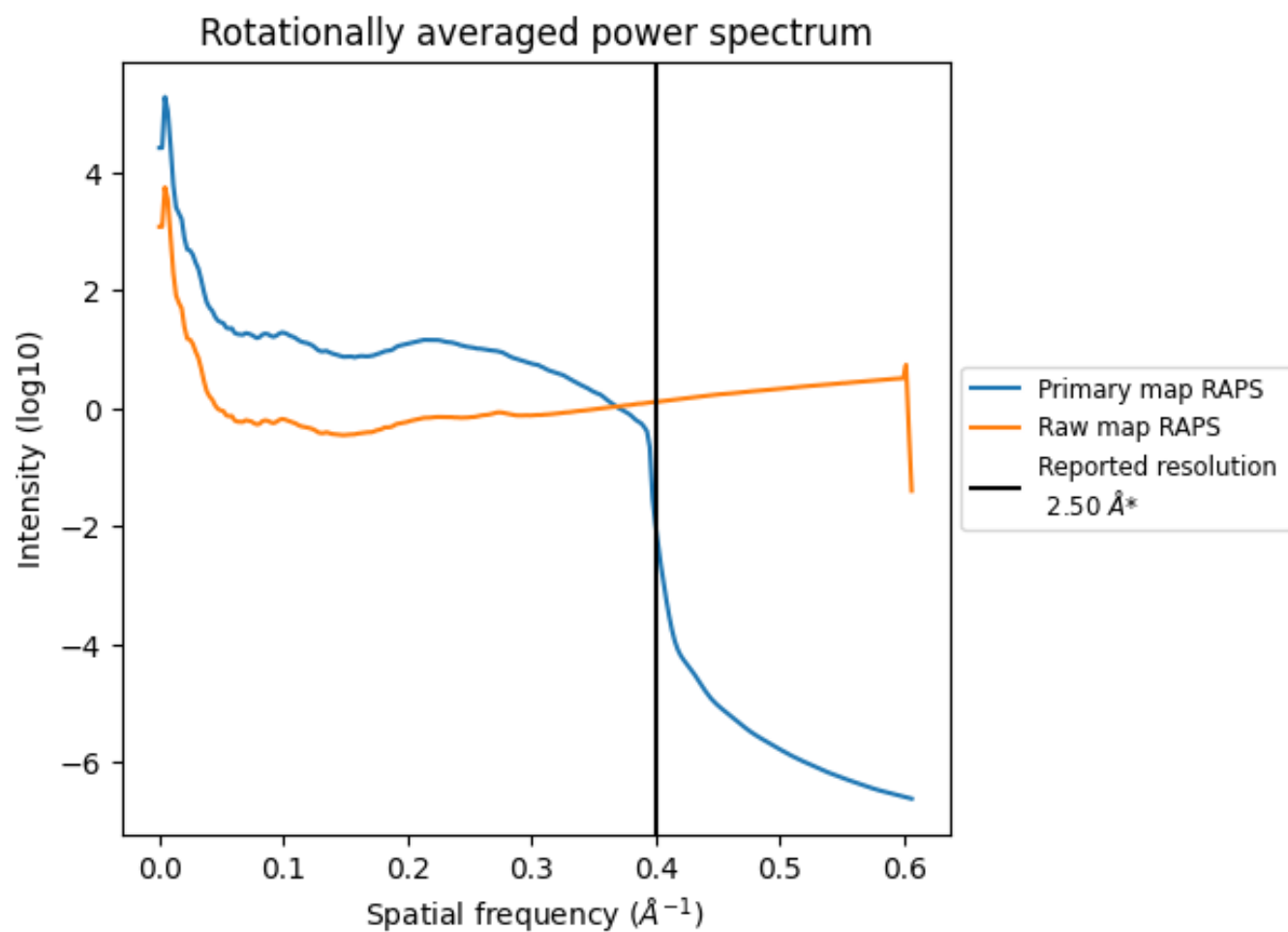
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm³; this corresponds to an approximate mass of 250 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 ⓘ

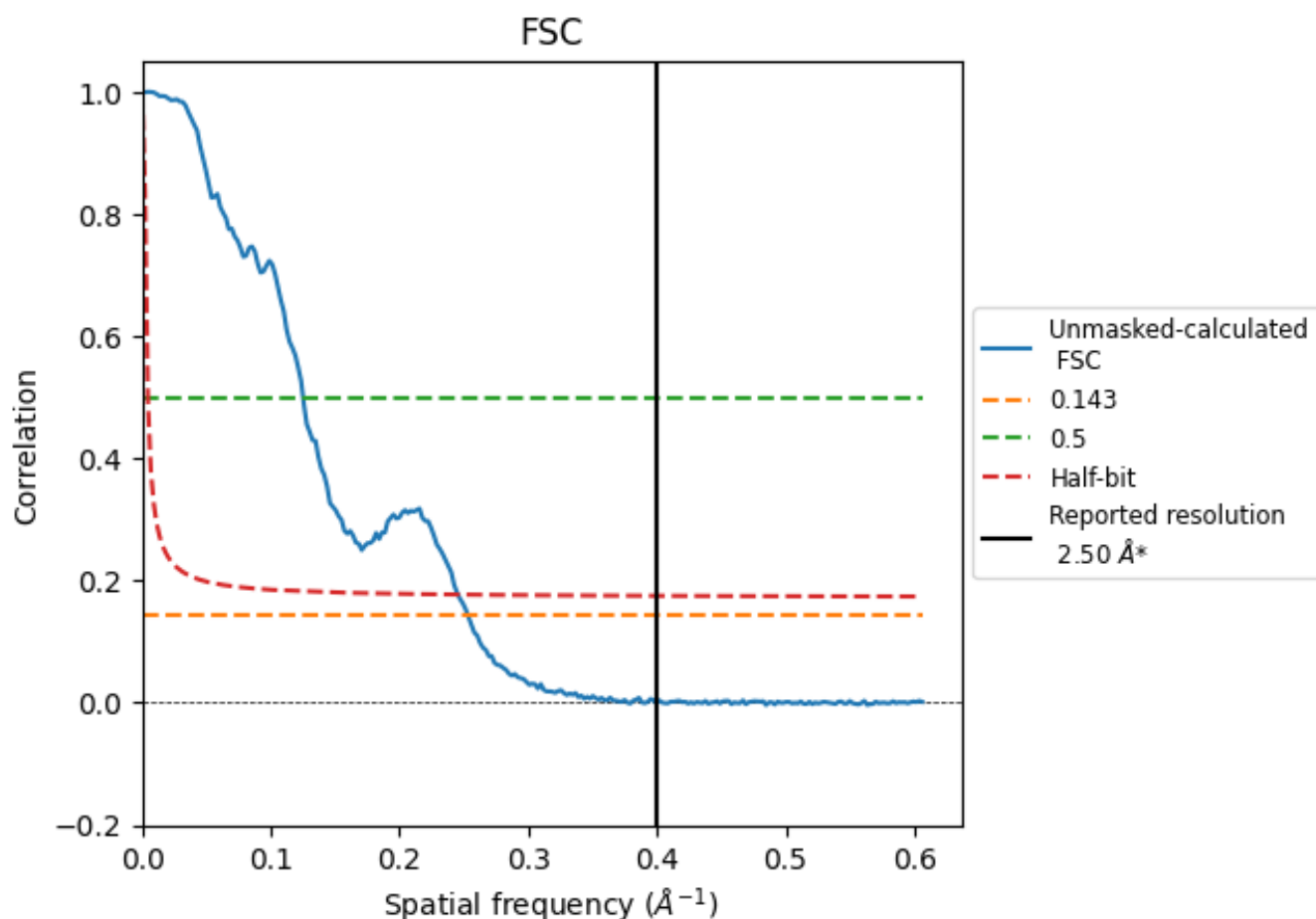


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

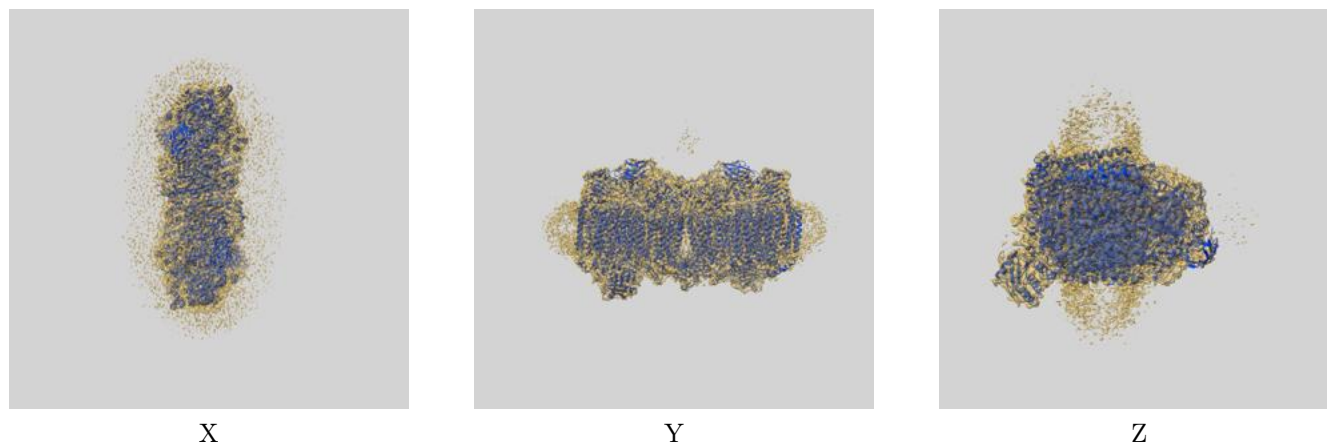
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	8.00	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

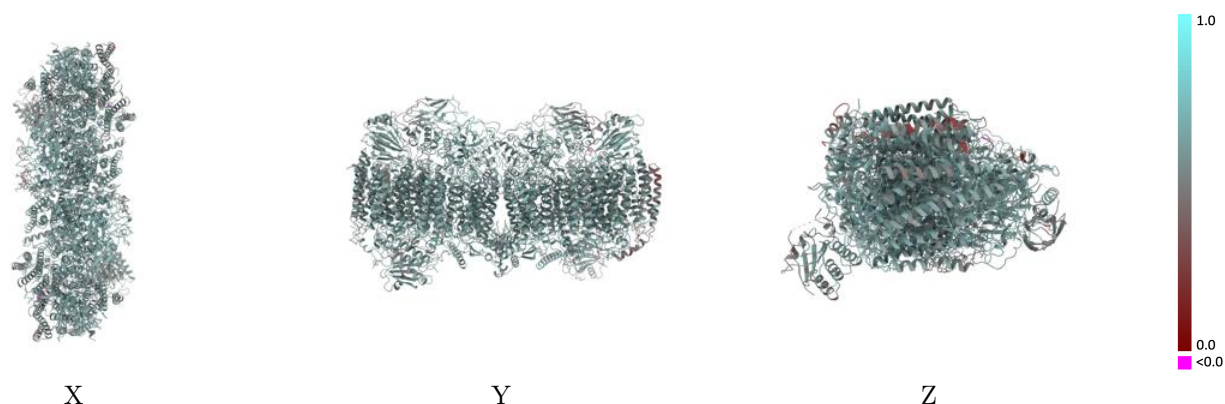
This section contains information regarding the fit between EMDB map EMD-53065 and PDB model 9QEF. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



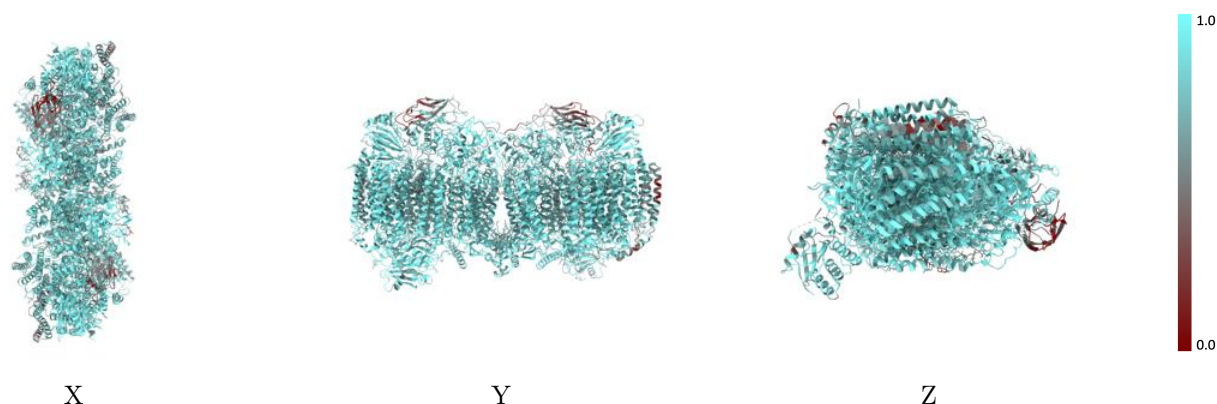
The images above show the 3D surface view of the map at the recommended contour level 0.129 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



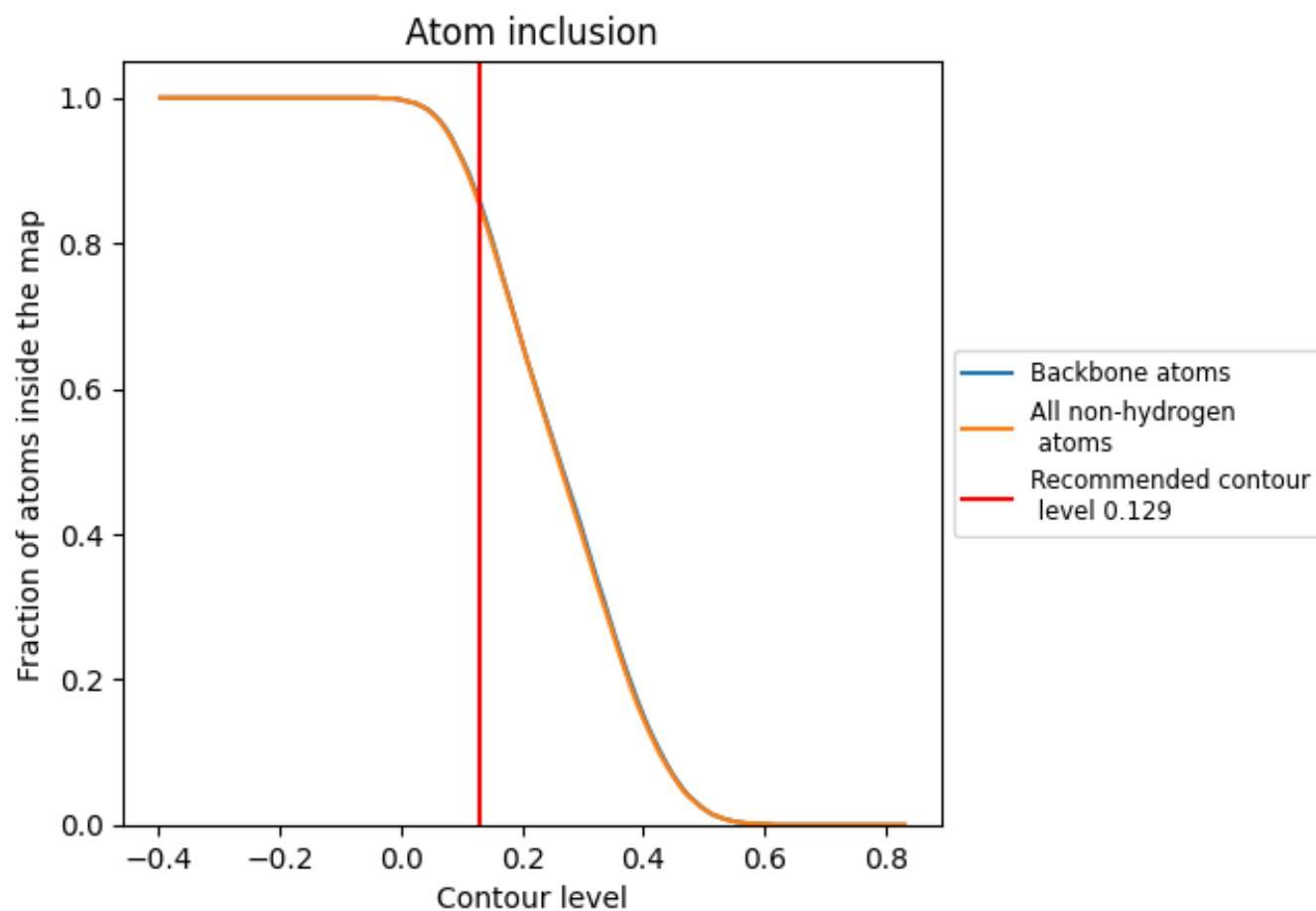
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.129).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8540	 0.5890
A	 0.5220	 0.4510
B	 0.7760	 0.5530
C	 0.8540	 0.6060
E	 0.5720	 0.4720
F	 0.8370	 0.5770
G	 0.8840	 0.6010
H	 0.9270	 0.6190
I	 0.8030	 0.5890
J	 0.8580	 0.5810
K	 0.8880	 0.5970
L	 0.9080	 0.5970
M	 0.8990	 0.6080
N	 0.9260	 0.6210
O	 0.8870	 0.6050
P	 0.8080	 0.5870
Q	 0.8520	 0.5670
R	 0.9250	 0.6040
S	 0.8960	 0.5900
T	 0.8960	 0.5990
U	 0.8190	 0.5560
V	 0.8590	 0.5600
W	 0.5290	 0.5440
X	 0.8260	 0.5640
Y	 0.8800	 0.5710
Z	 0.7760	 0.5440
a	 0.8070	 0.5480
b	 0.4120	 0.5220
c	 0.7860	 0.5480

