



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2025 – 06:24 PM JST

PDB ID : 7E1V / pdb_00007e1v
EMDB ID : EMD-30943
Title : Cryo-EM structure of apo hybrid respiratory supercomplex consisting of Mycobacterium tuberculosis complexIII and Mycobacterium smegmatis complexIV
Authors : Zhou, S.; Wang, W.; Gao, Y.; Gong, H.; Rao, Z.
Deposited on : 2021-02-03
Resolution : 2.68 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

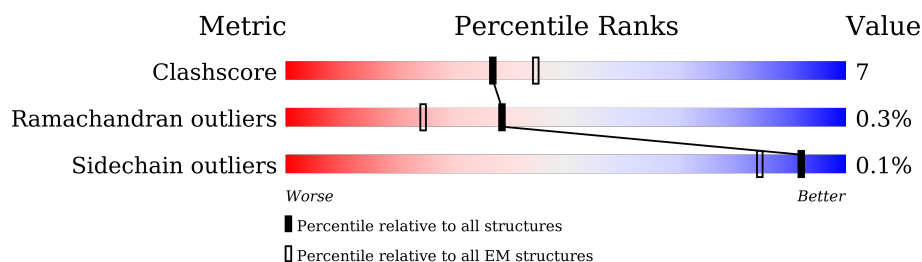
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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.











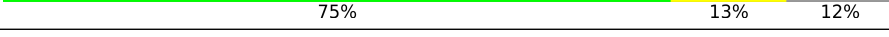

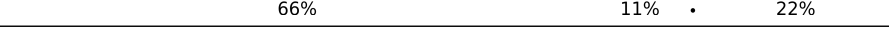

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	E	341	
1	Q	341	
2	F	575	
2	R	575	
3	G	203	
3	S	203	
4	H	139	
4	T	139	

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Mol	Chain	Length	Quality of chain
5	I	79	
5	U	79	
6	J	157	
6	V	157	
7	D	100	
7	P	100	
8	B	549	
8	N	549	
9	A	429	
9	M	429	
10	C	280	
10	O	280	

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
17	MQ9	N	609	-	X	-	-
18	FES	A	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 42279 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 c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	276	Total	C	N	O	S	0	0
			2191	1428	360	395	8		
1	Q	283	Total	C	N	O	S	0	0
			2236	1456	367	405	8		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	552	Total	C	N	O	S	0	0
			4373	2938	695	714	26		
2	R	552	Total	C	N	O	S	0	0
			4373	2938	695	714	26		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	186	Total	C	N	O	S	0	0
			1455	976	231	241	7		
3	S	185	Total	C	N	O	S	0	0
			1449	973	230	239	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	139	Total	C	N	O	S	0	0
			1071	716	164	188	3		
4	T	139	Total	C	N	O	S	0	0
			1068	715	164	186	3		

- Molecule 5 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	67	Total	C	N	O	S	0	0
			500	330	85	84	1		
5	U	67	Total	C	N	O	S	0	0
			499	330	85	83	1		

- Molecule 6 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	145	Total	C	N	O	S	0	0
			1026	651	176	197	2		
6	V	145	Total	C	N	O	S	0	0
			1029	652	176	199	2		

- Molecule 7 is a protein called Prokaryotic respiratory supercomplex associate factor 1 PRSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	76	Total	C	N	O	S	0	0
			607	397	112	94	4		
7	P	75	Total	C	N	O	S	0	0
			597	391	109	93	4		

- Molecule 8 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	524	Total	C	N	O	S	0	0
			4118	2723	701	677	17		
8	B	524	Total	C	N	O	S	0	0
			4130	2729	703	681	17		

- Molecule 9 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	378	Total	C	N	O	S	0	0
			2924	1890	500	523	11		
9	A	378	Total	C	N	O	S	0	0
			2912	1884	499	518	11		

- Molecule 10 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	213	Total	C	N	O	S	0	0
			1458	921	261	268	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	218	Total	C	N	O	S	0	0
			1487	930	274	274	9		

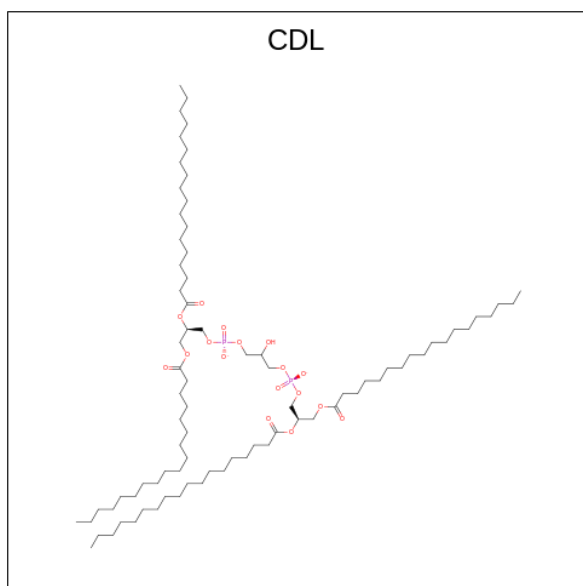
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1	LEU	-	expression tag	UNP P9WP35
C	1	LEU	-	expression tag	UNP P9WP35

- Molecule 11 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

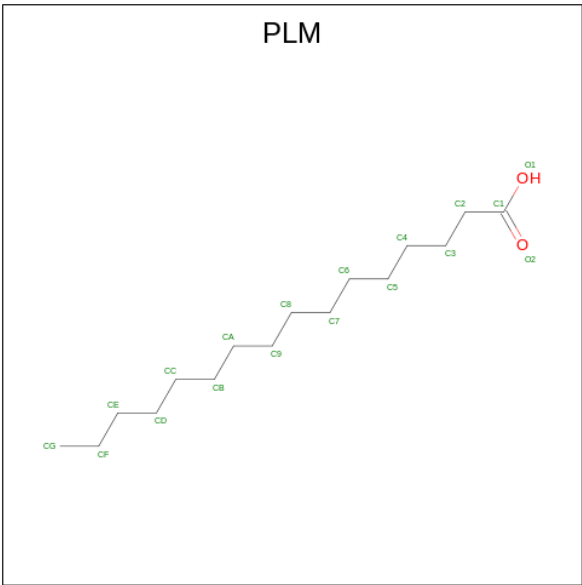
Mol	Chain	Residues	Atoms		AltConf
11	E	2	Total	Cu	0
			2	2	
11	F	2	Total	Cu	0
			2	2	
11	Q	3	Total	Cu	0
			3	3	
11	R	1	Total	Cu	0
			1	1	

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



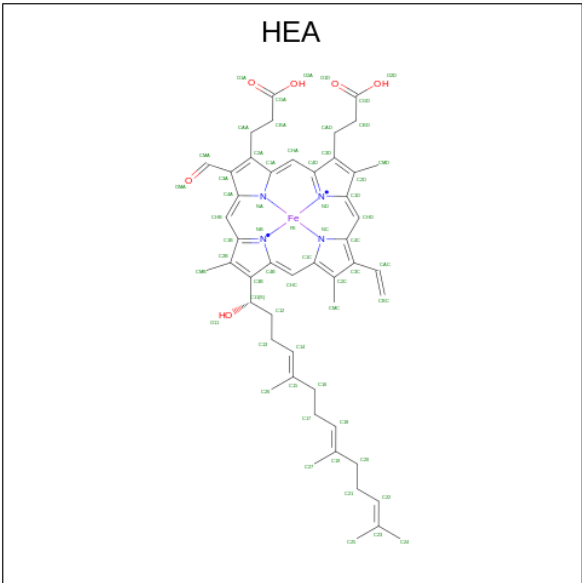
Mol	Chain	Residues	Atoms				AltConf
12	F	1	Total	C	O	P	0
			76	57	17	2	
12	F	1	Total	C	O	P	0
			81	62	17	2	
12	D	1	Total	C	O	P	0
			88	69	17	2	
12	R	1	Total	C	O	P	0
			76	57	17	2	
12	R	1	Total	C	O	P	0
			81	62	17	2	
12	P	1	Total	C	O	P	0
			88	69	17	2	
12	N	1	Total	C	O	P	0
			79	60	17	2	
12	N	1	Total	C	O	P	0
			74	55	17	2	
12	N	1	Total	C	O	P	0
			77	58	17	2	
12	N	1	Total	C	O	P	0
			79	60	17	2	
12	M	1	Total	C	O	P	0
			95	76	17	2	
12	B	1	Total	C	O	P	0
			66	47	17	2	
12	B	1	Total	C	O	P	0
			74	55	17	2	
12	B	1	Total	C	O	P	0
			77	58	17	2	
12	B	1	Total	C	O	P	0
			79	60	17	2	
12	C	1	Total	C	O	P	0
			79	60	17	2	
12	C	1	Total	C	O	P	0
			95	76	17	2	

- Molecule 13 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



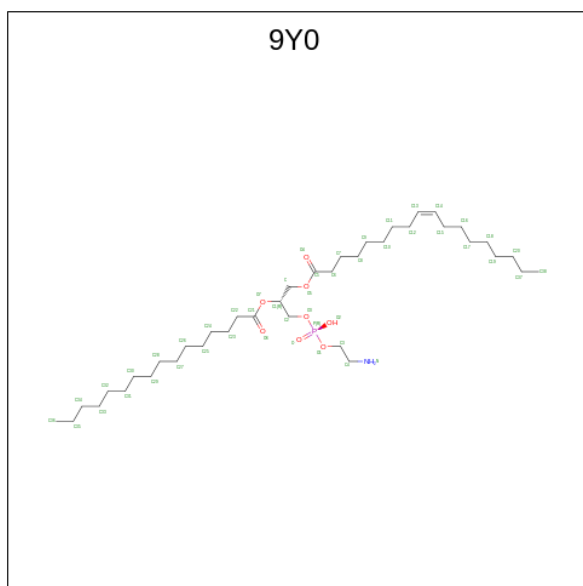
Mol	Chain	Residues	Atoms			AltConf
13	F	1	Total	C	O	0
			17	16	1	
13	R	1	Total	C	O	0
			17	16	1	
13	N	1	Total	C	O	0
			11	10	1	
13	B	1	Total	C	O	0
			11	10	1	

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



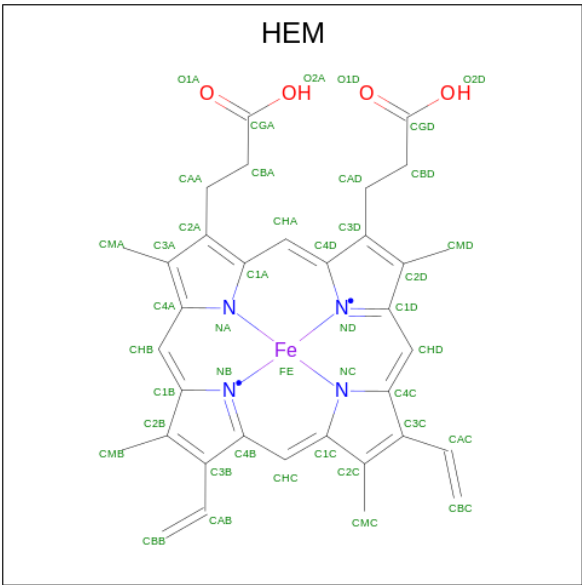
Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 15 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: C₃₉H₇₆NO₈P) (labeled as "Ligand of Interest" by depositor).



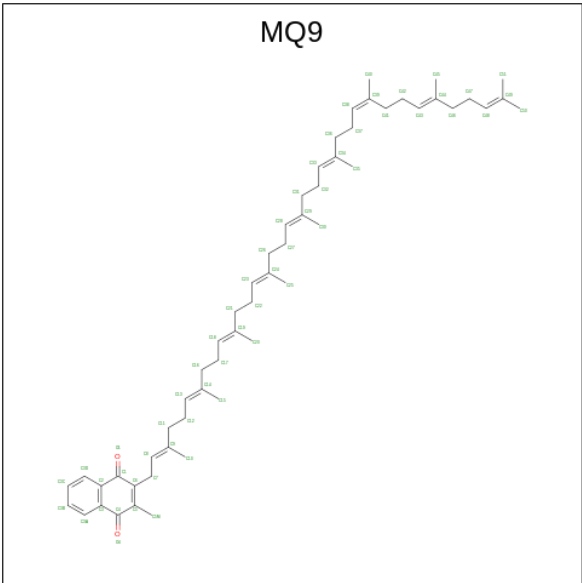
Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	S	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



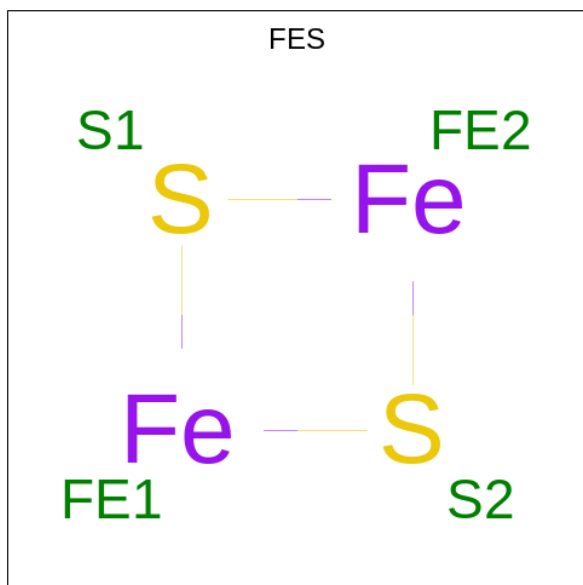
Mol	Chain	Residues	Atoms					AltConf
16	N	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
16	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	B	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
16	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



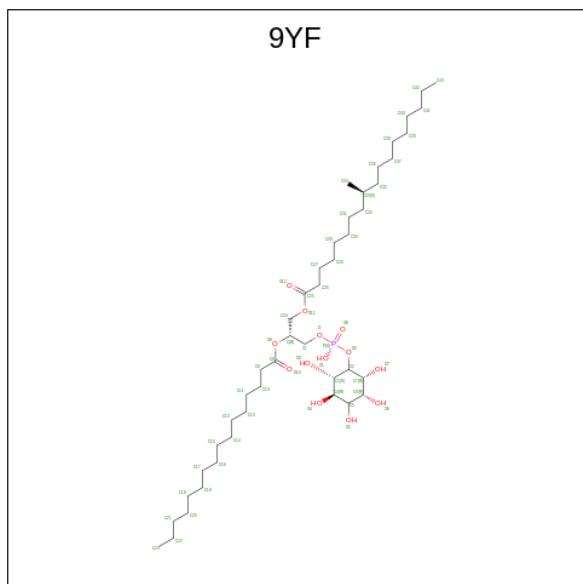
Mol	Chain	Residues	Atoms			AltConf
17	N	1	Total	C	O	0
			58	56	2	
17	N	1	Total	C	O	0
			58	56	2	
17	N	1	Total	C	O	0
			43	41	2	
17	N	1	Total	C	O	0
			43	41	2	
17	O	1	Total	C	O	0
			48	46	2	
17	O	1	Total	C	O	0
			58	56	2	
17	B	1	Total	C	O	0
			43	41	2	
17	B	1	Total	C	O	0
			38	36	2	
17	C	1	Total	C	O	0
			48	46	2	
17	C	1	Total	C	O	0
			58	56	2	

- 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	A	1	Total	Fe	S	0
			4	2	2	

- Molecule 19 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: $C_{44}H_{85}O_{13}P$).

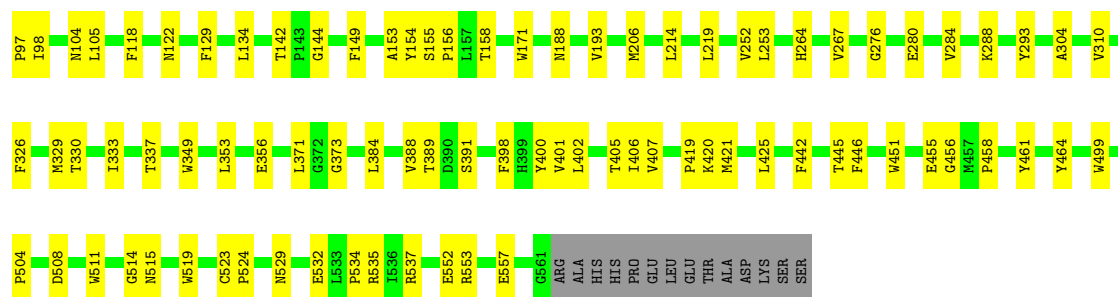


Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			44	30	13	1	
19	M	1	Total	C	O	P	0
			40	26	13	1	
19	A	1	Total	C	O	P	0
			51	37	13	1	
19	A	1	Total	C	O	P	0
			42	28	13	1	

- Molecule 20 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

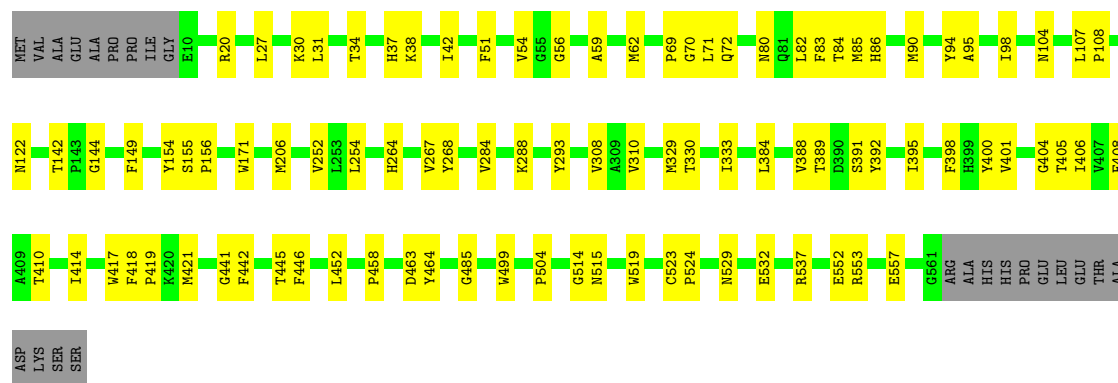


Mol	Chain	Residues	Atoms					AltConf
20	O	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	O	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	C	1	Total 43	C 34	Fe 1	N 4	O 4	0



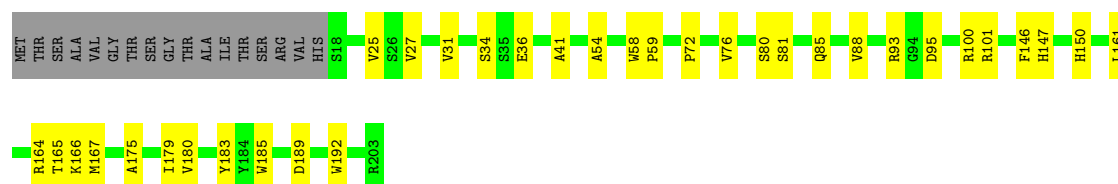
- Molecule 2: Cytochrome c oxidase subunit 1

Chain R: 80% 16%



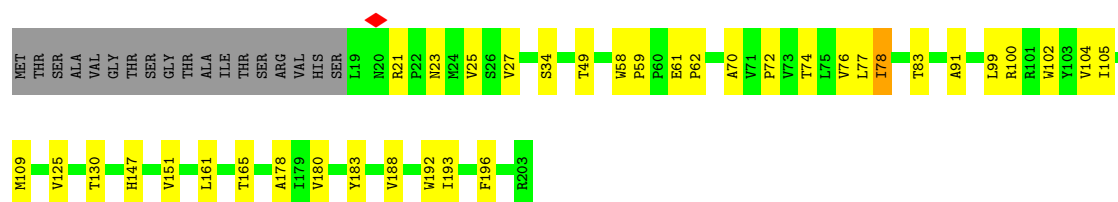
- Molecule 3: Cytochrome c oxidase subunit 3

Chain G: 75% 17% 8%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain S: 73% 18% 9%



- Molecule 4: Cytochrome c oxidase polypeptide 4

Chain H: 95% 5%



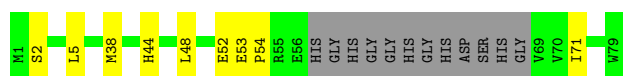
- Molecule 4: Cytochrome c oxidase polypeptide 4

Chain T: 96% .



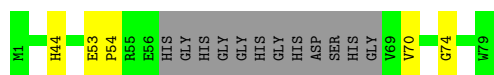
- Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain I: 73% 11% 15%



- Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain U: 78% 6% 15%



- Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain J: 79% 13% 8%



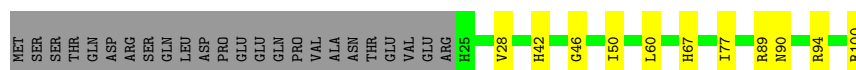
- Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V: 74% 18% 8%



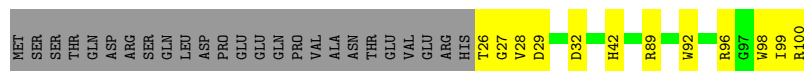
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain D: 65% 11% 24%




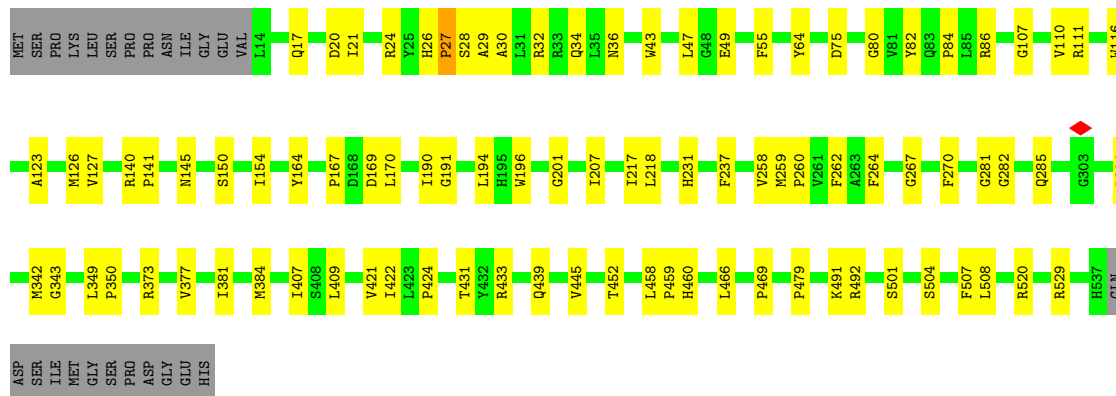
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain P: 




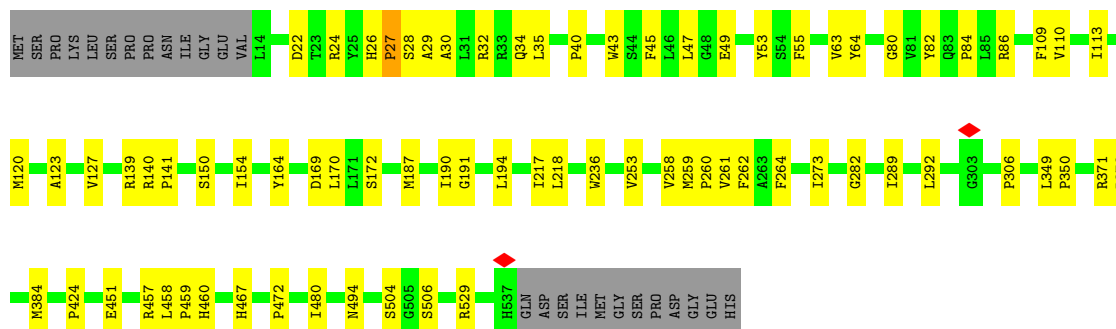
- Molecule 8: Cytochrome bc1 complex cytochrome b subunit

Chain N: 



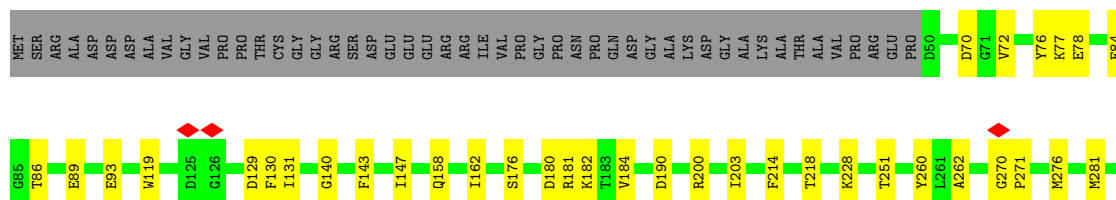
- Molecule 8: Cytochrome bc1 complex cytochrome b subunit

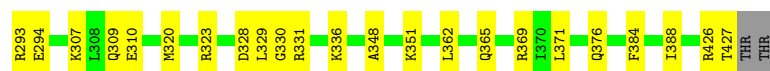
Chain B: 



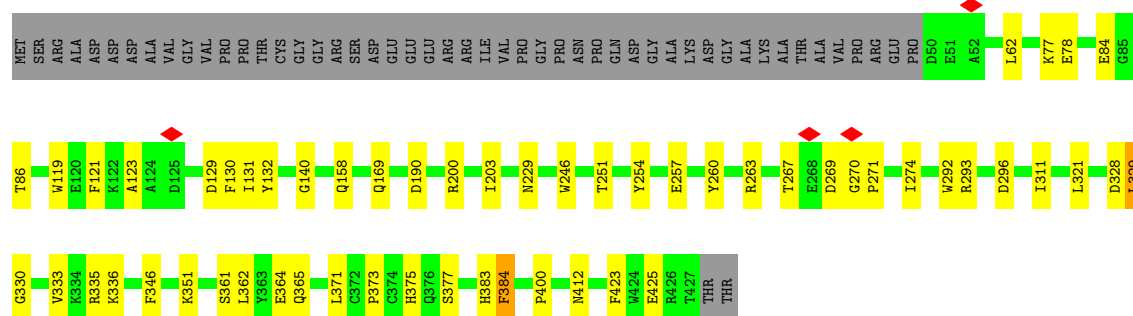
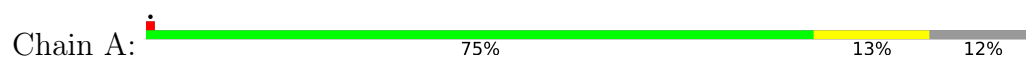
- Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain M: 

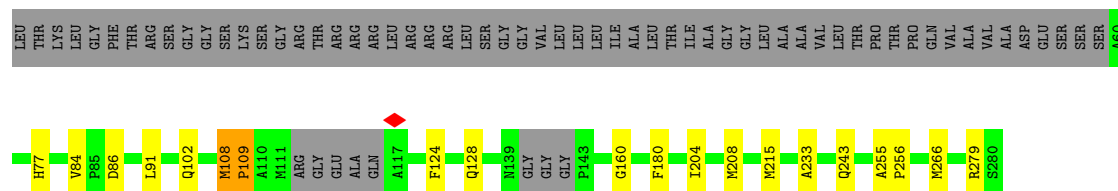




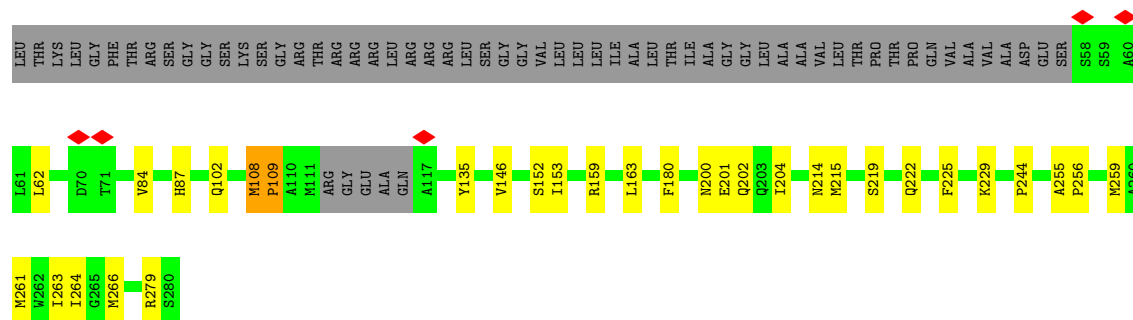
• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit



• Molecule 10: Cytochrome bc1 complex cytochrome c subunit



• Molecule 10: Cytochrome bc1 complex cytochrome c subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112804	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.664	Depositor
Minimum map value	-1.439	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, MQ9, FES, HEA, 9YF, PLM, 9Y0, CU, HEC, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.18	0/2254	0.42	0/3072
1	Q	0.18	0/2300	0.45	0/3137
2	F	0.21	0/4533	0.45	0/6192
2	R	0.20	0/4533	0.44	0/6192
3	G	0.21	0/1502	0.44	0/2051
3	S	0.21	0/1496	0.45	0/2043
4	H	0.18	0/1106	0.38	0/1517
4	T	0.16	0/1103	0.37	0/1513
5	I	0.15	0/516	0.35	0/706
5	U	0.14	0/515	0.34	0/705
6	J	0.17	0/1044	0.40	0/1427
6	V	0.17	0/1047	0.44	0/1431
7	D	0.15	0/628	0.38	0/855
7	P	0.16	0/617	0.35	0/840
8	B	0.19	0/4266	0.43	0/5821
8	N	0.20	0/4253	0.43	0/5804
9	A	0.19	0/2989	0.43	0/4056
9	M	0.19	0/3001	0.44	0/4071
10	C	0.16	0/1516	0.44	0/2061
10	O	0.16	0/1487	0.42	0/2022
All	All	0.19	0/40706	0.43	0/55516

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	R	0	1
8	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	C	0	1
10	O	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	B	139	ARG	Peptide
10	C	108	MET	Peptide
2	F	154	TYR	Peptide
10	O	108	MET	Peptide
2	R	154	TYR	Peptide

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	E	2191	0	2129	30	0
1	Q	2236	0	2164	46	0
2	F	4373	0	4347	84	0
2	R	4373	0	4347	66	0
3	G	1455	0	1455	24	0
3	S	1449	0	1450	29	0
4	H	1071	0	1047	8	0
4	T	1068	0	1045	5	0
5	I	500	0	505	8	0
5	U	499	0	502	6	0
6	J	1026	0	1038	17	0
6	V	1029	0	1040	22	0
7	D	607	0	594	7	0
7	P	597	0	586	7	0
8	B	4130	0	4145	60	0
8	N	4118	0	4137	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	2912	0	2893	42	0
9	M	2924	0	2907	44	0
10	C	1487	0	1396	22	0
10	O	1458	0	1365	14	0
11	E	2	0	0	0	0
11	F	2	0	0	0	0
11	Q	3	0	0	0	0
11	R	1	0	0	0	0
12	B	296	0	371	13	0
12	C	174	0	248	9	0
12	D	88	0	126	6	0
12	F	157	0	208	5	0
12	M	95	0	143	5	0
12	N	309	0	400	16	0
12	P	88	0	126	5	0
12	R	157	0	208	6	0
13	B	11	0	16	0	0
13	F	17	0	31	0	0
13	N	11	0	16	0	0
13	R	17	0	31	0	0
14	F	120	0	108	12	0
14	R	120	0	108	8	0
15	G	43	0	0	0	0
15	S	43	0	0	0	0
16	B	85	0	57	6	0
16	N	85	0	57	5	0
17	B	81	0	98	2	0
17	C	106	0	141	11	0
17	N	202	0	264	17	0
17	O	106	0	141	10	0
18	A	4	0	0	2	0
18	M	4	0	0	0	0
19	A	93	0	0	8	0
19	M	84	0	0	6	0
20	C	86	0	61	2	0
20	O	86	0	62	4	0
All	All	42279	0	42113	621	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 621 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)
19:M:504:9YF:O4	9:A:119:TRP:HZ2	1.36	1.05
19:M:504:9YF:O4	9:A:119:TRP:CZ2	2.13	1.00
1:E:303:ARG:HH12	1:E:309:ASN:HA	1.34	0.92
8:N:267:GLY:HA3	17:N:611:MQ9:H111	1.50	0.90
9:M:228:LYS:HG2	19:M:504:9YF:O7	1.75	0.85

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	E	272/341 (80%)	247 (91%)	24 (9%)	1 (0%)	30	52
1	Q	279/341 (82%)	248 (89%)	31 (11%)	0	100	100
2	F	550/575 (96%)	517 (94%)	33 (6%)	0	100	100
2	R	550/575 (96%)	522 (95%)	28 (5%)	0	100	100
3	G	184/203 (91%)	176 (96%)	8 (4%)	0	100	100
3	S	183/203 (90%)	174 (95%)	9 (5%)	0	100	100
4	H	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
4	T	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
5	I	63/79 (80%)	60 (95%)	3 (5%)	0	100	100
5	U	63/79 (80%)	60 (95%)	3 (5%)	0	100	100
6	J	143/157 (91%)	134 (94%)	9 (6%)	0	100	100
6	V	143/157 (91%)	136 (95%)	7 (5%)	0	100	100
7	D	74/100 (74%)	71 (96%)	3 (4%)	0	100	100
7	P	73/100 (73%)	67 (92%)	6 (8%)	0	100	100
8	B	522/549 (95%)	478 (92%)	41 (8%)	3 (1%)	22	42
8	N	522/549 (95%)	480 (92%)	39 (8%)	3 (1%)	22	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	A	376/429 (88%)	342 (91%)	32 (8%)	2 (0%)	25	46
9	M	376/429 (88%)	343 (91%)	30 (8%)	3 (1%)	16	35
10	C	214/280 (76%)	192 (90%)	21 (10%)	1 (0%)	25	46
10	O	207/280 (74%)	191 (92%)	15 (7%)	1 (0%)	25	46
All	All	5068/5704 (89%)	4701 (93%)	353 (7%)	14 (0%)	38	59

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	M	329	LEU
9	A	329	LEU
8	N	28	SER
9	M	384	PHE
8	B	28	SER

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	E	231/288 (80%)	231 (100%)	0	100	100
1	Q	235/288 (82%)	235 (100%)	0	100	100
2	F	453/471 (96%)	453 (100%)	0	100	100
2	R	453/471 (96%)	453 (100%)	0	100	100
3	G	148/161 (92%)	148 (100%)	0	100	100
3	S	147/161 (91%)	146 (99%)	1 (1%)	81	92
4	H	105/106 (99%)	105 (100%)	0	100	100
4	T	104/106 (98%)	104 (100%)	0	100	100
5	I	50/59 (85%)	50 (100%)	0	100	100
5	U	49/59 (83%)	49 (100%)	0	100	100
6	J	103/114 (90%)	103 (100%)	0	100	100
6	V	104/114 (91%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	60/83 (72%)	59 (98%)	1 (2%)	56	79
7	P	59/83 (71%)	59 (100%)	0	100	100
8	B	422/446 (95%)	422 (100%)	0	100	100
8	N	419/446 (94%)	419 (100%)	0	100	100
9	A	296/343 (86%)	296 (100%)	0	100	100
9	M	299/343 (87%)	299 (100%)	0	100	100
10	C	131/207 (63%)	131 (100%)	0	100	100
10	O	128/207 (62%)	128 (100%)	0	100	100
All	All	3996/4556 (88%)	3994 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	D	77	ILE
3	S	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
8	B	367	ASN
8	B	467	HIS
9	A	375	HIS
1	Q	259	GLN
1	Q	252	ASN

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 59 ligands modelled in this entry, 8 are monoatomic - leaving 51 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
20	HEC	O	303	-	32,50,50	2.26	4 (12%)	24,82,82	1.29	1 (4%)
17	MQ9	O	302	-	59,59,59	3.87	17 (28%)	72,75,75	3.31	31 (43%)
14	HEA	R	605	-	57,67,67	2.02	14 (24%)	61,103,103	2.38	22 (36%)
14	HEA	F	606	2	57,67,67	2.02	14 (24%)	61,103,103	2.36	23 (37%)
16	HEM	B	602	8	41,49,50	1.26	3 (7%)	46,81,82	1.30	6 (13%)
12	CDL	B	607	-	78,78,99	1.17	6 (7%)	84,90,111	1.10	5 (5%)
14	HEA	R	606	2	57,67,67	2.01	14 (24%)	61,103,103	2.32	27 (44%)
16	HEM	B	603	8	41,50,50	1.48	4 (9%)	45,82,82	1.47	7 (15%)
13	PLM	B	601	-	10,10,17	0.64	0	9,9,17	0.54	0
12	CDL	C	303	-	78,78,99	1.20	7 (8%)	84,90,111	0.99	5 (5%)
15	9Y0	G	301	-	42,42,48	0.94	4 (9%)	44,47,53	0.93	2 (4%)
17	MQ9	N	610	-	44,44,59	3.92	15 (34%)	54,57,75	3.10	20 (37%)
18	FES	A	501	9	0,4,4	-	-	-	-	-
15	9Y0	S	301	-	42,42,48	0.94	4 (9%)	44,47,53	0.95	2 (4%)
12	CDL	N	603	-	78,78,99	1.19	7 (8%)	84,90,111	0.94	4 (4%)
12	CDL	B	606	-	76,76,99	1.19	7 (9%)	82,88,111	1.02	4 (4%)
17	MQ9	N	611	-	44,44,59	3.89	15 (34%)	54,57,75	3.09	22 (40%)
19	9YF	A	502	-	51,51,58	0.95	5 (9%)	62,64,71	1.02	4 (6%)
12	CDL	P	201	-	87,87,99	1.15	7 (8%)	93,99,111	1.01	5 (5%)
17	MQ9	C	304	-	49,49,59	3.98	15 (30%)	60,63,75	3.05	23 (38%)
17	MQ9	O	301	-	49,49,59	3.92	15 (30%)	60,63,75	3.19	23 (38%)
17	MQ9	B	609	-	39,39,59	3.87	14 (35%)	48,51,75	3.00	17 (35%)
14	HEA	F	607	2	57,67,67	2.02	13 (22%)	61,103,103	2.31	25 (40%)
13	PLM	F	603	-	16,16,17	0.52	0	15,15,17	0.43	0
20	HEC	O	304	10	32,50,50	2.19	3 (9%)	24,82,82	1.44	3 (12%)
17	MQ9	C	305	-	59,59,59	3.89	17 (28%)	72,75,75	3.32	31 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CDL	D	201	-	87,87,99	1.16	7 (8%)	93,99,111	1.04	5 (5%)
20	HEC	C	302	10	32,50,50	2.18	3 (9%)	24,82,82	1.41	3 (12%)
17	MQ9	N	608	-	59,59,59	3.93	18 (30%)	72,75,75	3.28	31 (43%)
19	9YF	M	504	-	40,40,58	1.01	3 (7%)	50,52,71	1.38	7 (14%)
17	MQ9	N	609	-	59,59,59	3.94	18 (30%)	72,75,75	3.27	32 (44%)
18	FES	M	501	9	0,4,4	-	-	-	-	-
19	9YF	A	503	-	42,42,58	1.02	4 (9%)	52,54,71	1.27	6 (11%)
20	HEC	C	301	10	32,50,50	2.17	3 (9%)	24,82,82	1.49	3 (12%)
12	CDL	B	604	-	65,65,99	1.27	7 (10%)	71,77,111	1.02	4 (5%)
12	CDL	B	605	-	73,73,99	1.23	8 (10%)	79,85,111	0.99	4 (5%)
13	PLM	N	604	-	10,10,17	0.59	0	9,9,17	0.55	0
13	PLM	R	603	-	16,16,17	0.56	0	15,15,17	0.42	0
12	CDL	F	601	-	75,75,99	1.21	7 (9%)	81,87,111	0.96	4 (4%)
12	CDL	N	607	-	78,78,99	1.18	6 (7%)	84,90,111	1.09	5 (5%)
12	CDL	M	502	-	94,94,99	1.12	7 (7%)	100,106,111	0.97	5 (5%)
12	CDL	N	605	-	73,73,99	1.24	7 (9%)	79,85,111	1.03	4 (5%)
12	CDL	R	601	-	75,75,99	1.20	7 (9%)	81,87,111	0.98	4 (4%)
12	CDL	C	306	-	94,94,99	1.12	7 (7%)	100,106,111	1.01	5 (5%)
17	MQ9	B	608	-	44,44,59	3.88	15 (34%)	54,57,75	3.13	21 (38%)
12	CDL	F	602	-	80,80,99	1.17	7 (8%)	86,92,111	0.96	4 (4%)
16	HEM	N	601	8	41,49,50	1.26	3 (7%)	46,81,82	1.32	5 (10%)
19	9YF	M	503	-	44,44,58	0.99	4 (9%)	55,57,71	1.10	5 (9%)
12	CDL	N	606	-	76,76,99	1.20	7 (9%)	82,88,111	0.97	4 (4%)
12	CDL	R	602	-	80,80,99	1.16	6 (7%)	86,92,111	1.00	5 (5%)
16	HEM	N	602	8	41,50,50	1.48	3 (7%)	45,82,82	1.50	8 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	HEC	O	303	-	-	2/10/54/54	-
17	MQ9	O	302	-	-	26/53/73/73	0/2/2/2
14	HEA	R	605	-	-	9/32/76/76	-
14	HEA	F	606	2	-	17/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEM	B	602	8	-	2/12/52/54	-
12	CDL	B	607	-	-	53/89/89/110	-
14	HEA	R	606	2	-	13/32/76/76	-
16	HEM	B	603	8	-	4/12/54/54	-
13	PLM	B	601	-	-	0/7/8/15	-
12	CDL	C	303	-	-	54/89/89/110	-
15	9Y0	G	301	-	-	24/46/46/52	-
17	MQ9	N	610	-	-	21/35/55/73	0/2/2/2
18	FES	A	501	9	-	-	0/1/1/1
15	9Y0	S	301	-	-	27/46/46/52	-
12	CDL	N	603	-	-	51/89/89/110	-
12	CDL	B	606	-	-	42/87/87/110	-
17	MQ9	N	611	-	-	21/35/55/73	0/2/2/2
19	9YF	A	502	-	-	30/47/71/78	0/1/1/1
12	CDL	P	201	-	-	58/98/98/110	-
17	MQ9	C	304	-	-	22/41/61/73	0/2/2/2
17	MQ9	O	301	-	-	23/41/61/73	0/2/2/2
17	MQ9	B	609	-	-	14/29/49/73	0/2/2/2
14	HEA	F	607	2	-	10/32/76/76	-
13	PLM	F	603	-	-	5/13/14/15	-
20	HEC	O	304	10	-	0/10/54/54	-
17	MQ9	C	305	-	-	25/53/73/73	0/2/2/2
12	CDL	D	201	-	-	53/98/98/110	-
20	HEC	C	302	10	-	0/10/54/54	-
17	MQ9	N	608	-	-	29/53/73/73	0/2/2/2
19	9YF	M	504	-	-	18/35/59/78	0/1/1/1
17	MQ9	N	609	-	-	35/53/73/73	0/2/2/2
20	HEC	C	301	10	-	3/10/54/54	-
19	9YF	A	503	-	-	15/37/61/78	0/1/1/1
18	FES	M	501	9	-	-	0/1/1/1
12	CDL	B	604	-	-	49/76/76/110	-
12	CDL	B	605	-	-	47/84/84/110	-
13	PLM	N	604	-	-	1/7/8/15	-
13	PLM	R	603	-	-	4/13/14/15	-
12	CDL	F	601	-	-	39/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CDL	N	607	-	-	42/89/89/110	-
12	CDL	M	502	-	-	68/105/105/110	-
12	CDL	N	605	-	-	44/84/84/110	-
12	CDL	R	601	-	-	39/86/86/110	-
12	CDL	C	306	-	-	60/105/105/110	-
17	MQ9	B	608	-	-	21/35/55/73	0/2/2/2
12	CDL	F	602	-	-	41/91/91/110	-
16	HEM	N	601	8	-	2/12/52/54	-
19	9YF	M	503	-	-	19/39/63/78	0/1/1/1
12	CDL	N	606	-	-	40/87/87/110	-
12	CDL	R	602	-	-	43/91/91/110	-
16	HEM	N	602	8	-	4/12/54/54	-

The worst 5 of 381 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	608	MQ9	C18-C19	9.58	1.56	1.33
17	C	304	MQ9	C18-C19	9.58	1.56	1.33
17	N	609	MQ9	C18-C19	9.52	1.55	1.33
17	N	610	MQ9	C18-C19	9.52	1.55	1.33
17	N	611	MQ9	C18-C19	9.48	1.55	1.33

The worst 5 of 486 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	O	301	MQ9	C7-C8-C9	-10.86	108.72	126.79
17	C	305	MQ9	C7-C8-C9	-10.67	109.03	126.79
17	N	608	MQ9	C7-C8-C9	-10.58	109.19	126.79
17	N	609	MQ9	C7-C8-C9	-10.40	109.48	126.79
17	N	610	MQ9	C7-C8-C9	-10.14	109.91	126.79

There are no chirality outliers.

5 of 1269 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	601	CDL	CB2-OB2-PB2-OB3
12	F	601	CDL	CB2-OB2-PB2-OB4
12	F	601	CDL	CB3-OB5-PB2-OB3
12	F	601	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
12	F	602	CDL	CB3-OB5-PB2-OB3

There are no ring outliers.

42 monomers are involved in 153 short contacts:

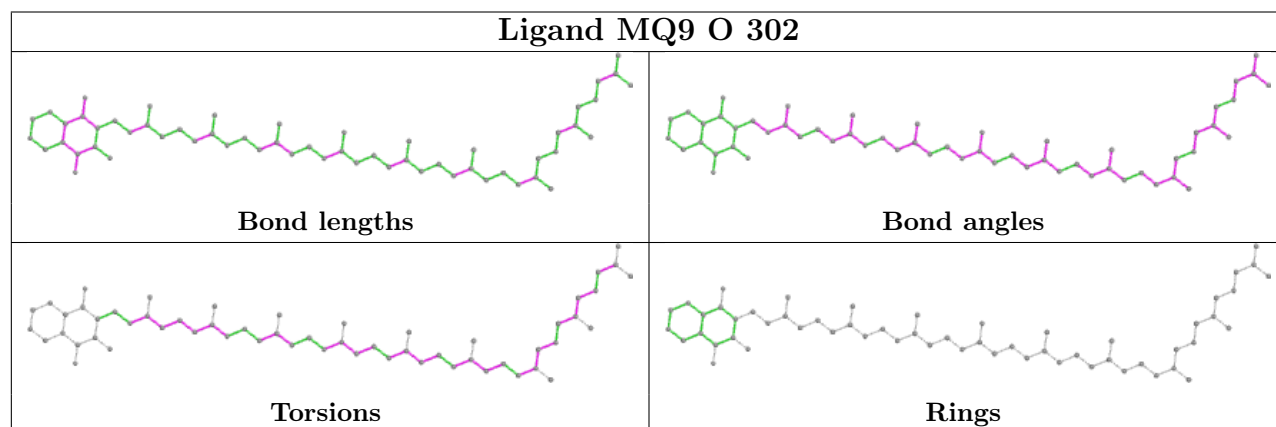
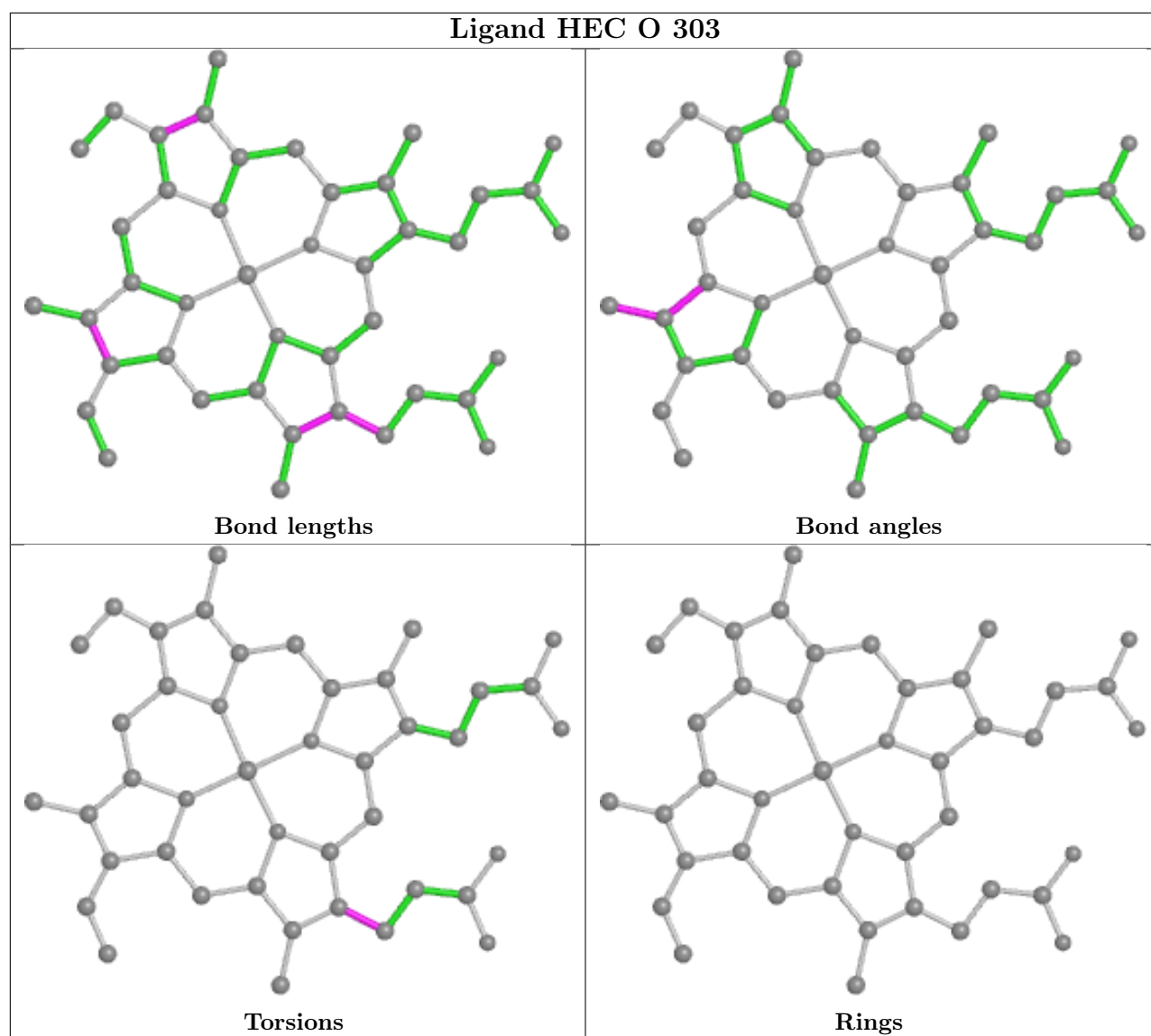
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	O	303	HEC	4	0
17	O	302	MQ9	4	0
14	R	605	HEA	4	0
14	F	606	HEA	5	0
16	B	602	HEM	1	0
12	B	607	CDL	5	0
14	R	606	HEA	4	0
16	B	603	HEM	5	0
12	C	303	CDL	5	0
17	N	610	MQ9	4	0
18	A	501	FES	2	0
12	N	603	CDL	5	0
12	B	606	CDL	5	0
17	N	611	MQ9	6	0
19	A	502	9YF	3	0
12	P	201	CDL	5	0
17	C	304	MQ9	4	0
17	O	301	MQ9	6	0
17	B	609	MQ9	1	0
14	F	607	HEA	7	0
17	C	305	MQ9	7	0
12	D	201	CDL	6	0
17	N	608	MQ9	3	0
19	M	504	9YF	4	0
17	N	609	MQ9	5	0
19	A	503	9YF	5	0
20	C	301	HEC	2	0
12	B	604	CDL	3	0
12	B	605	CDL	2	0
12	F	601	CDL	1	0
12	N	607	CDL	3	0
12	M	502	CDL	5	0
12	N	605	CDL	5	0
12	R	601	CDL	2	0
12	C	306	CDL	4	0
17	B	608	MQ9	1	0

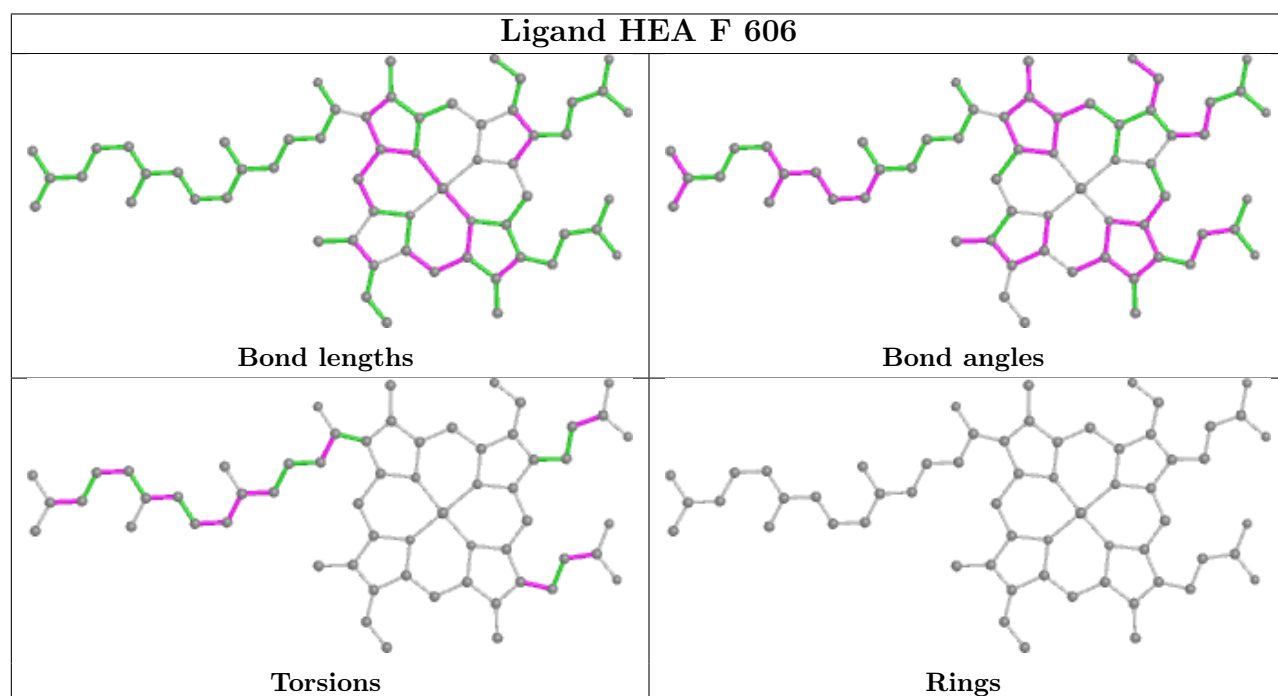
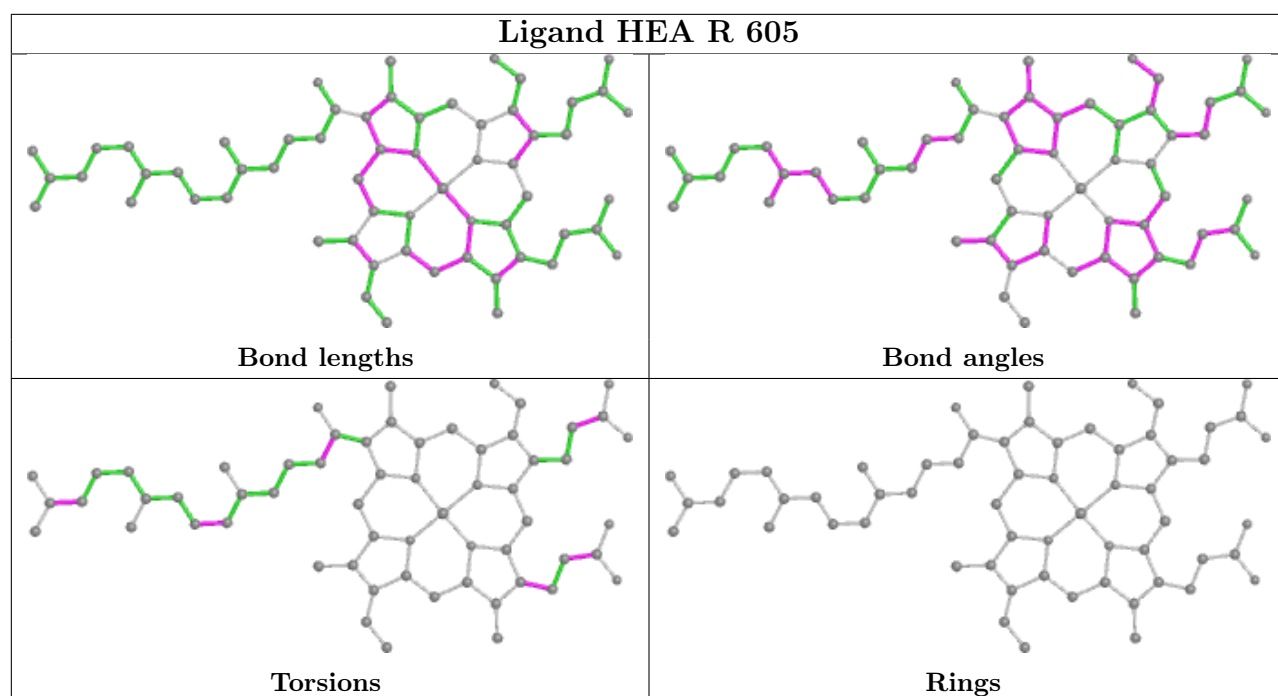
Continued on next page...

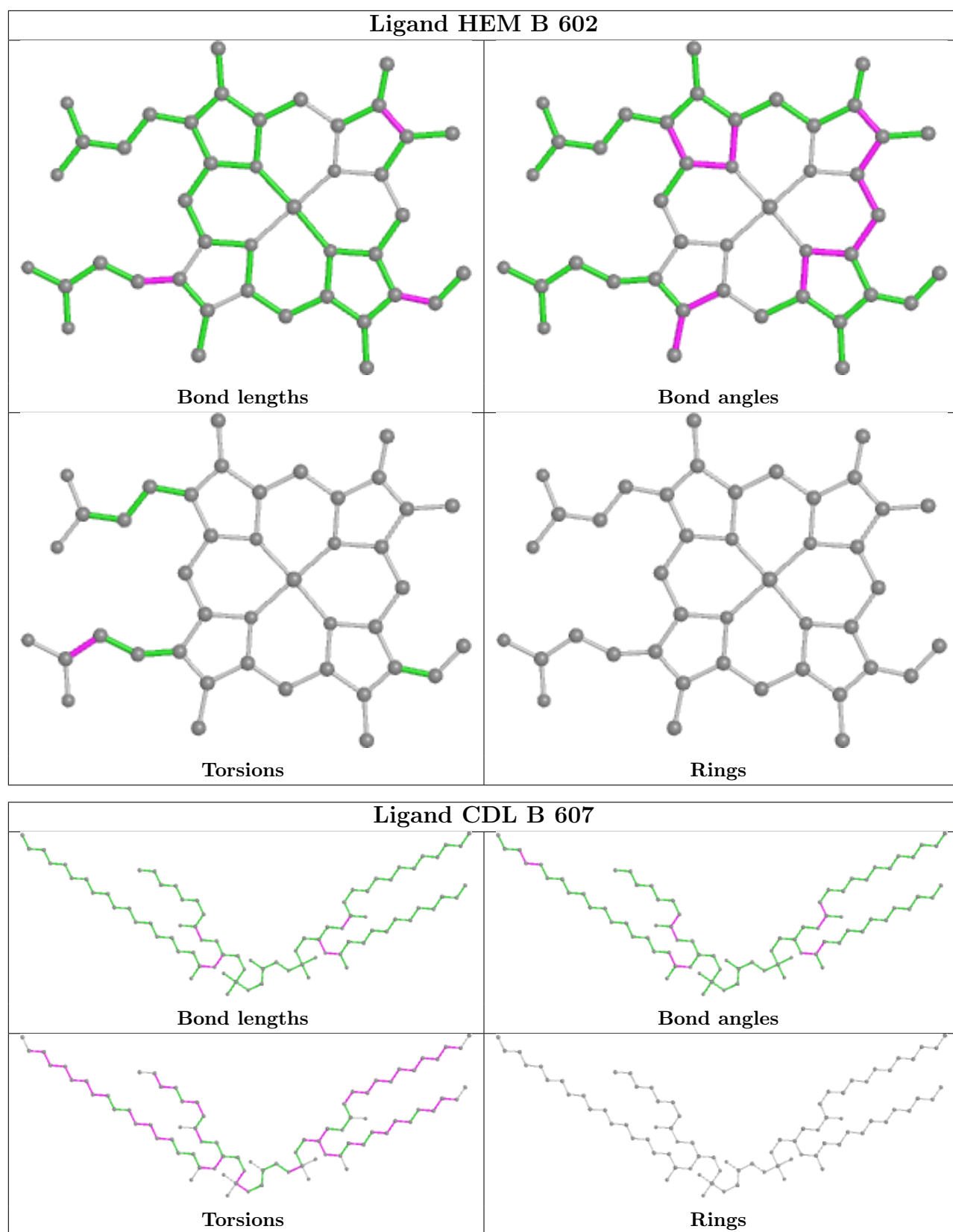
Continued from previous page...

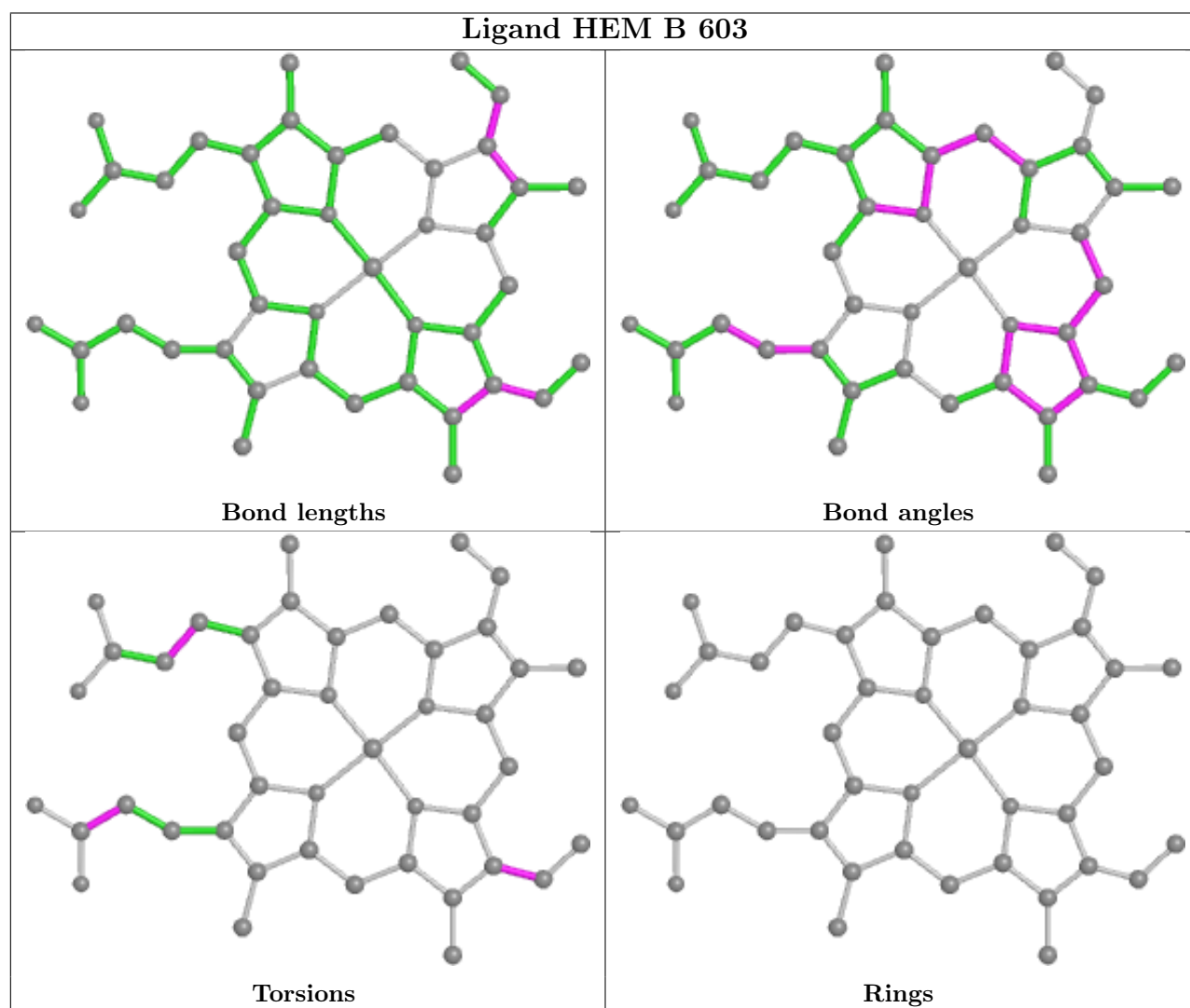
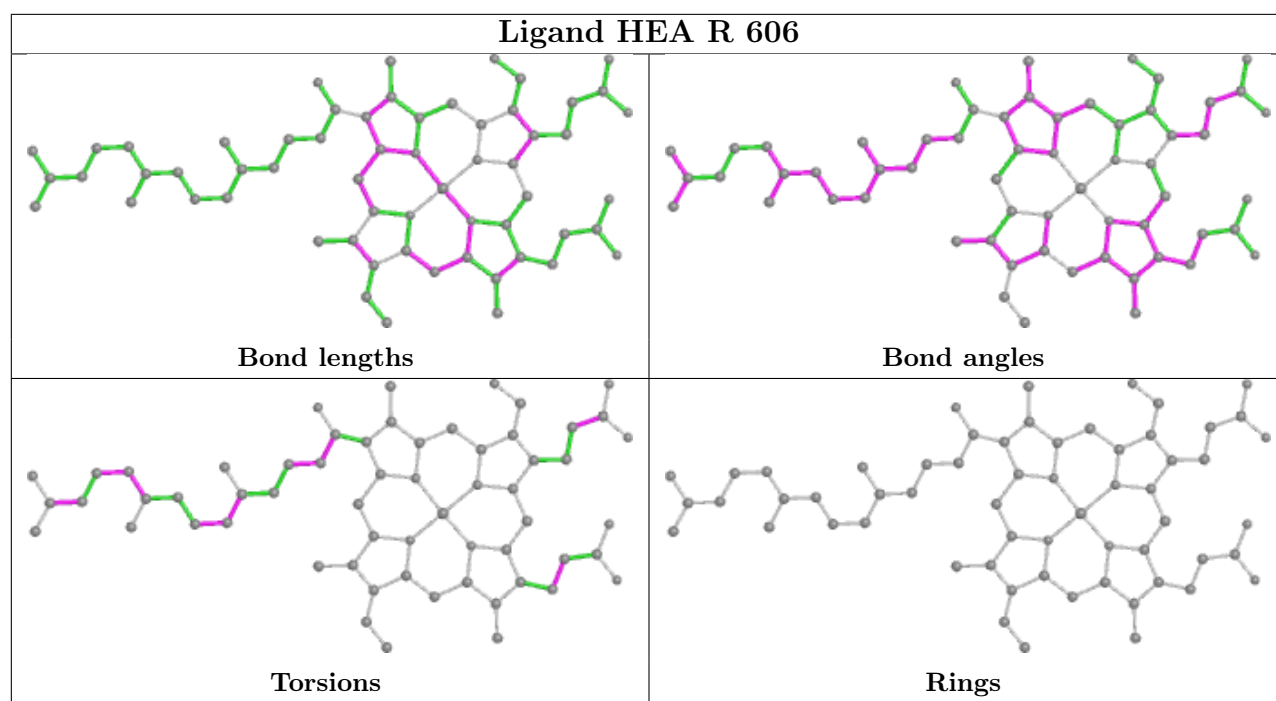
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	602	CDL	4	0
16	N	601	HEM	1	0
19	M	503	9YF	2	0
12	N	606	CDL	4	0
12	R	602	CDL	4	0
16	N	602	HEM	4	0

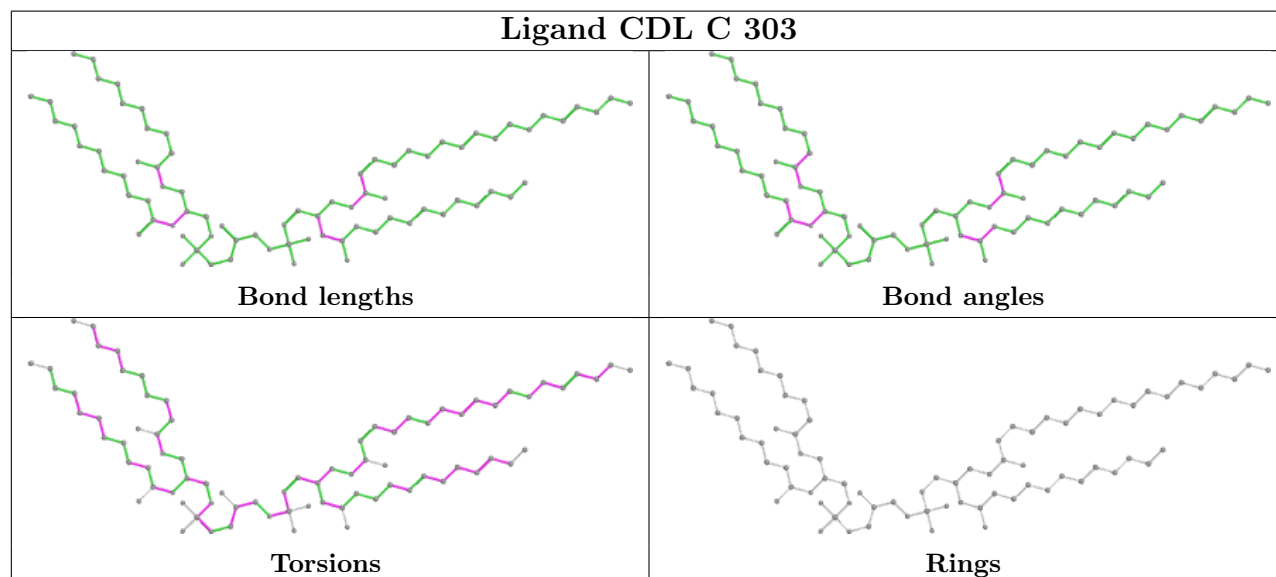
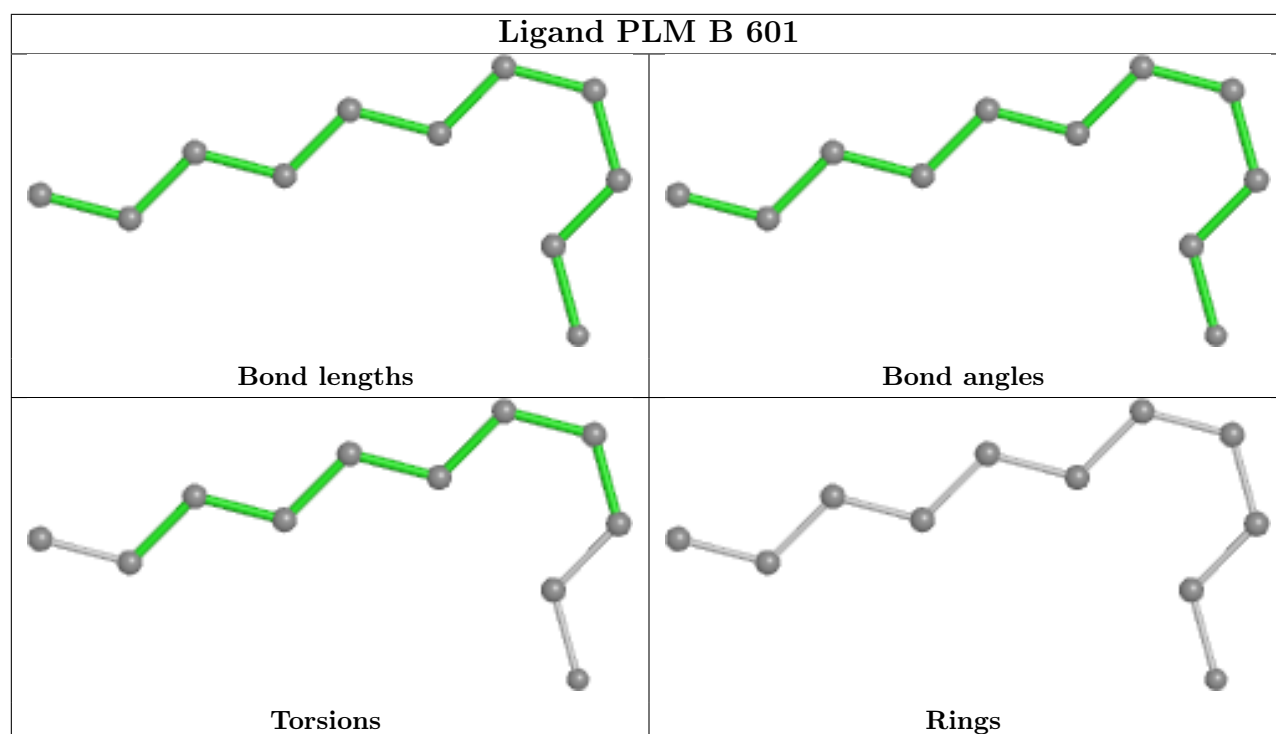
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

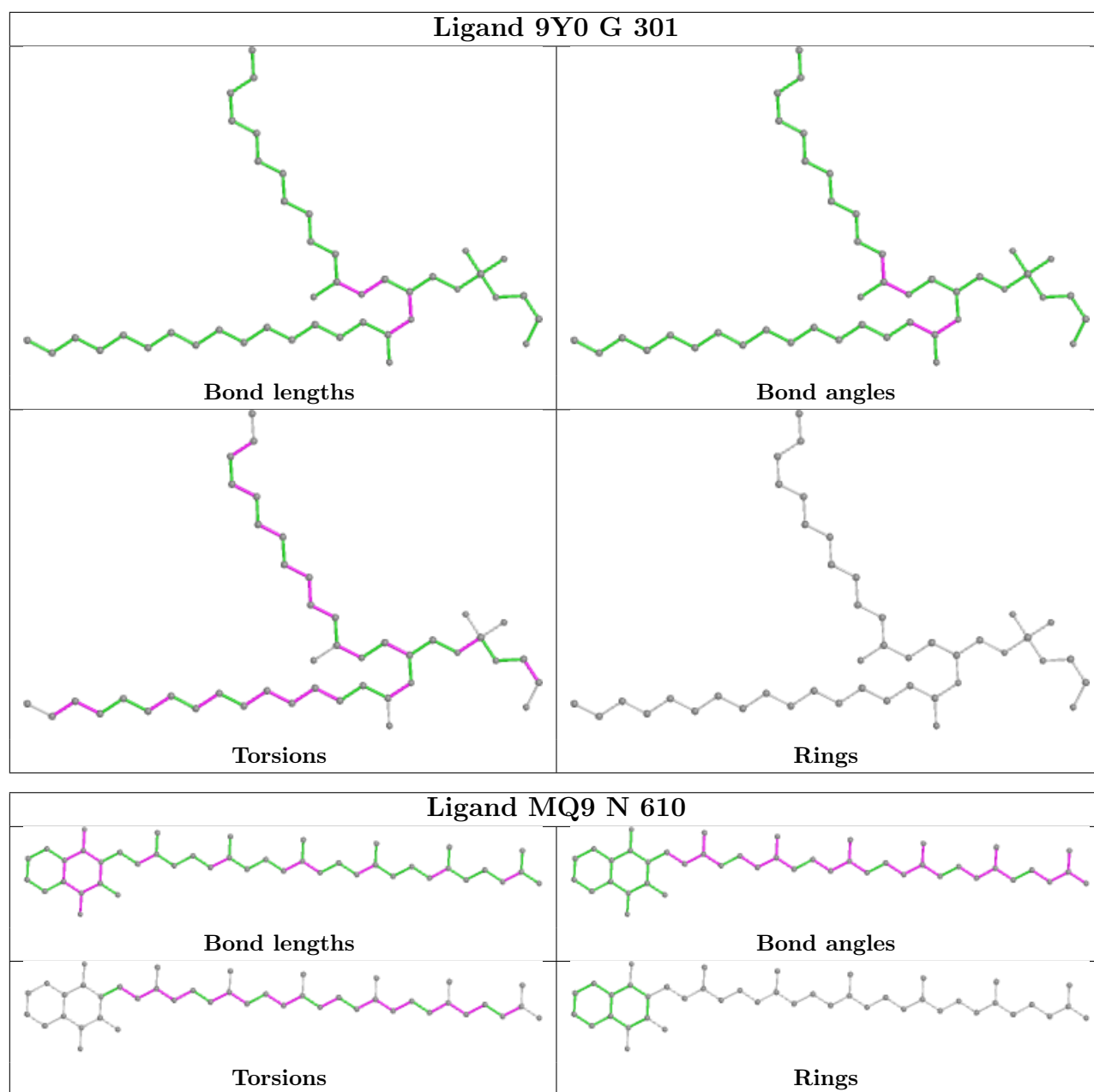


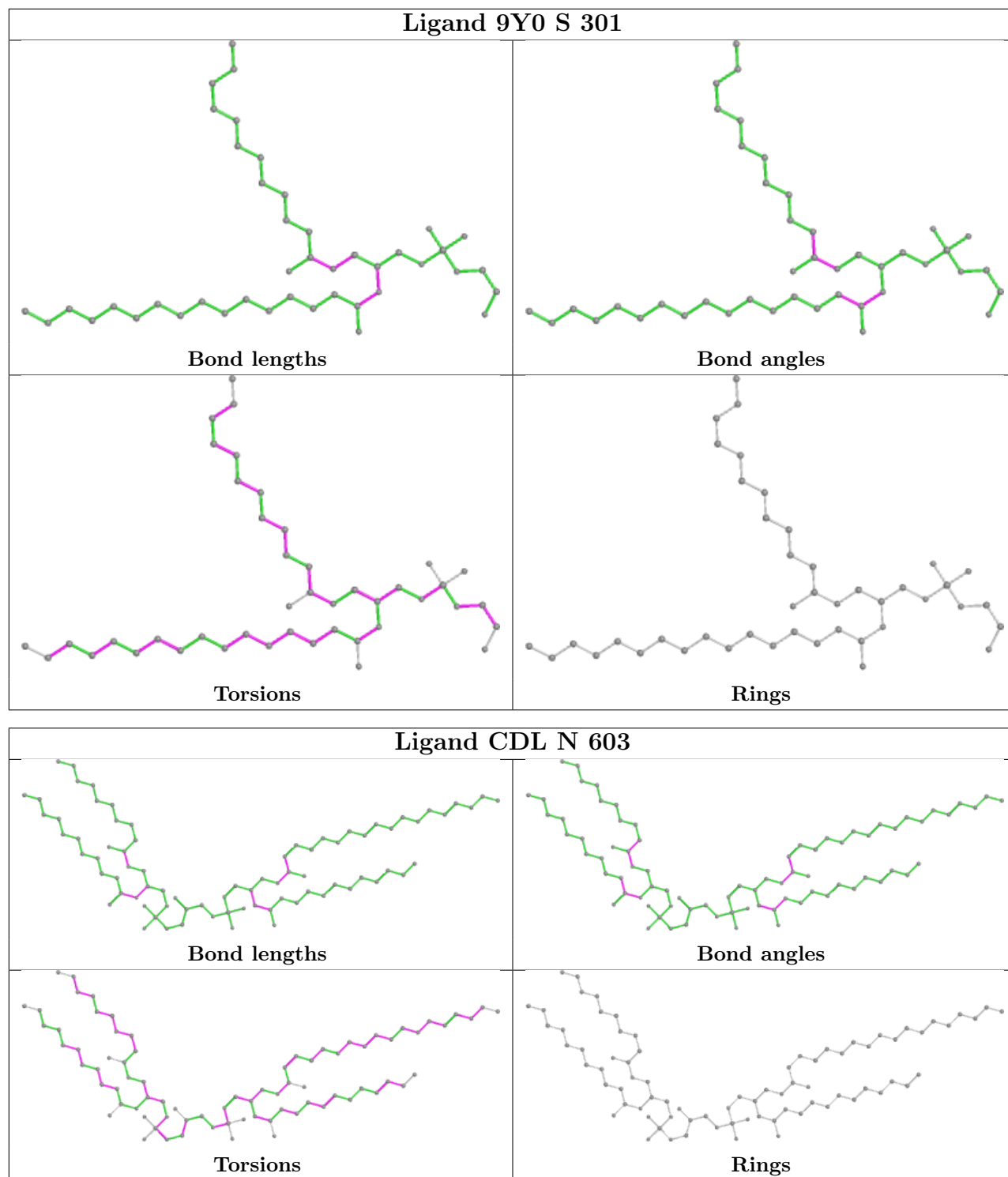


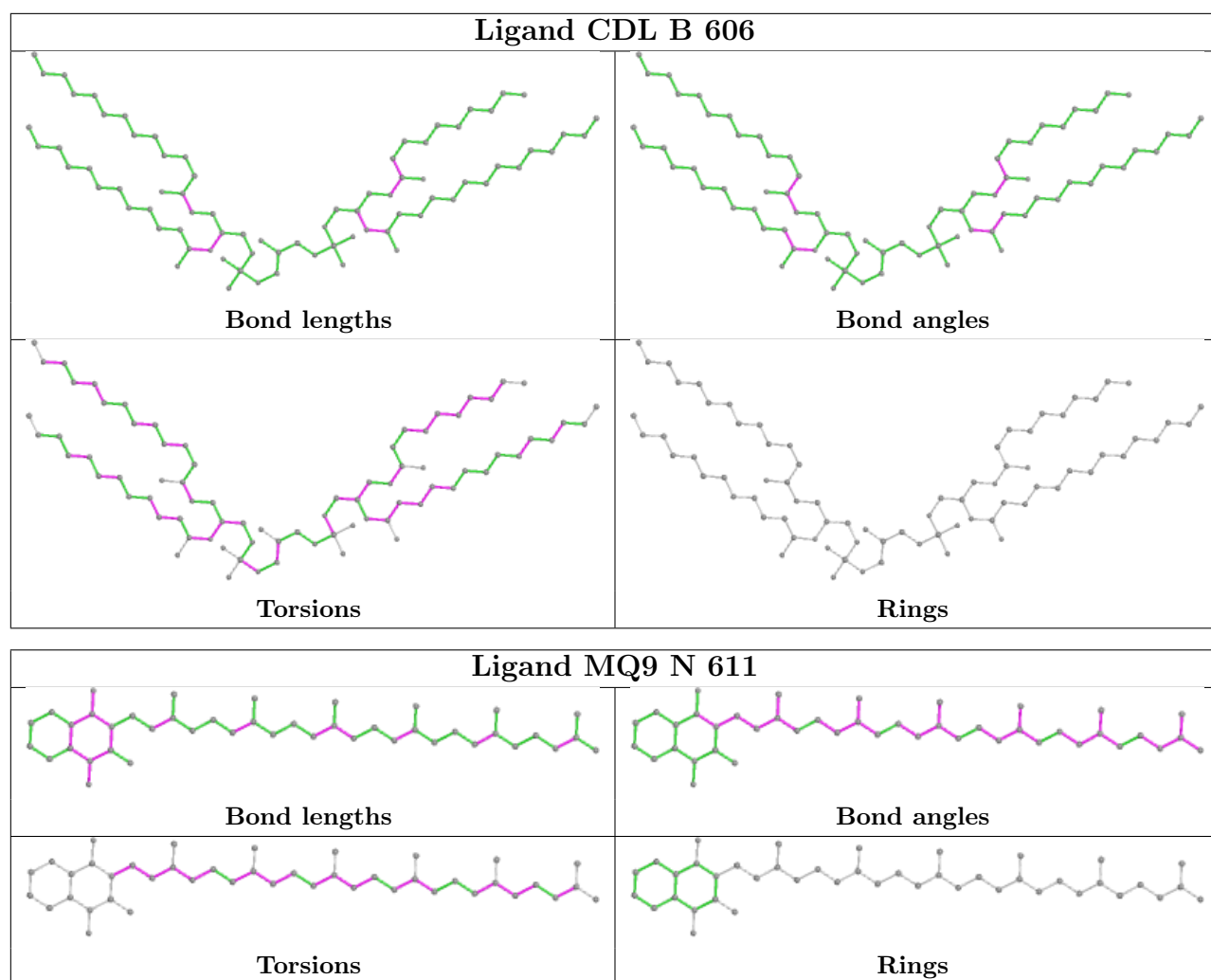




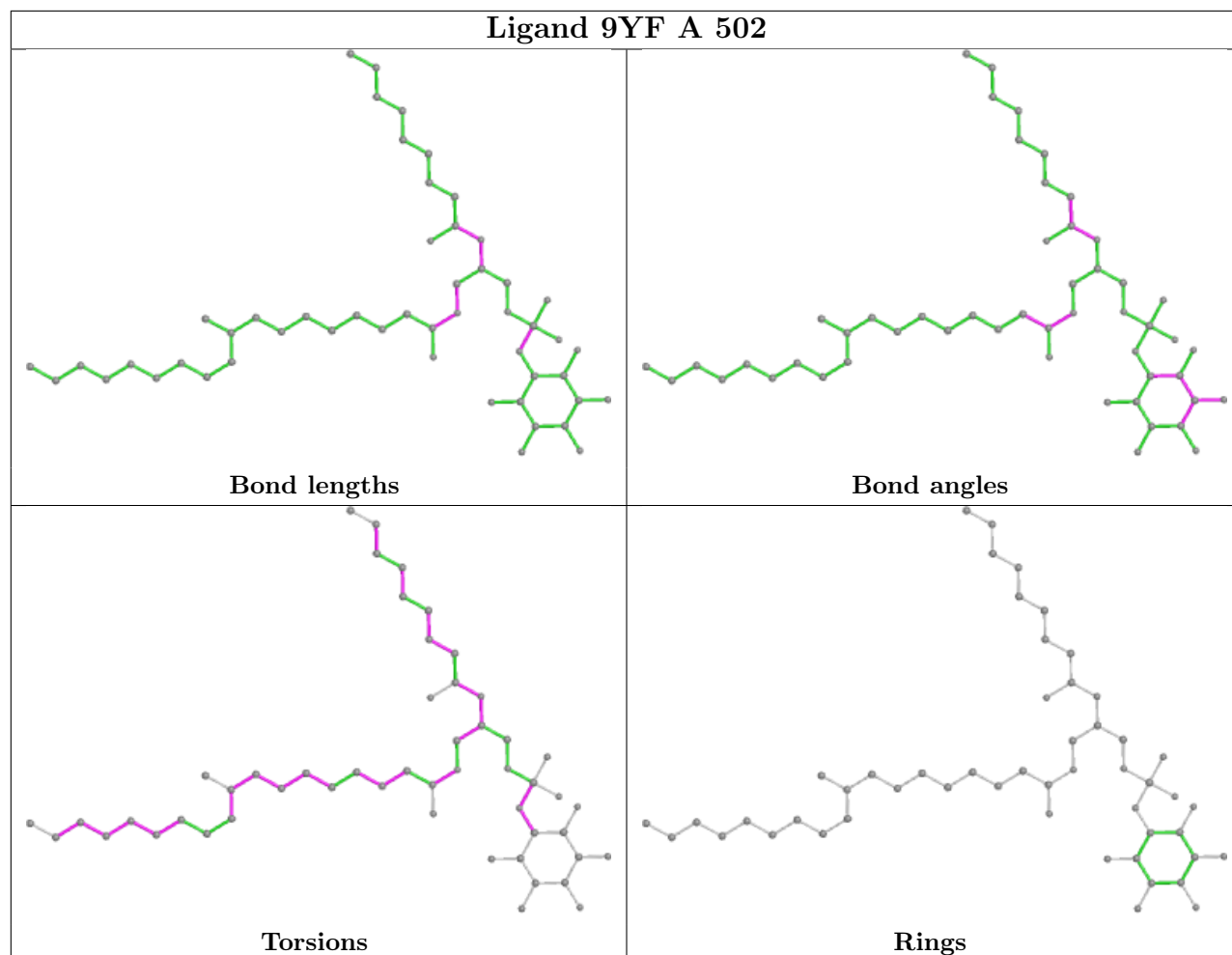




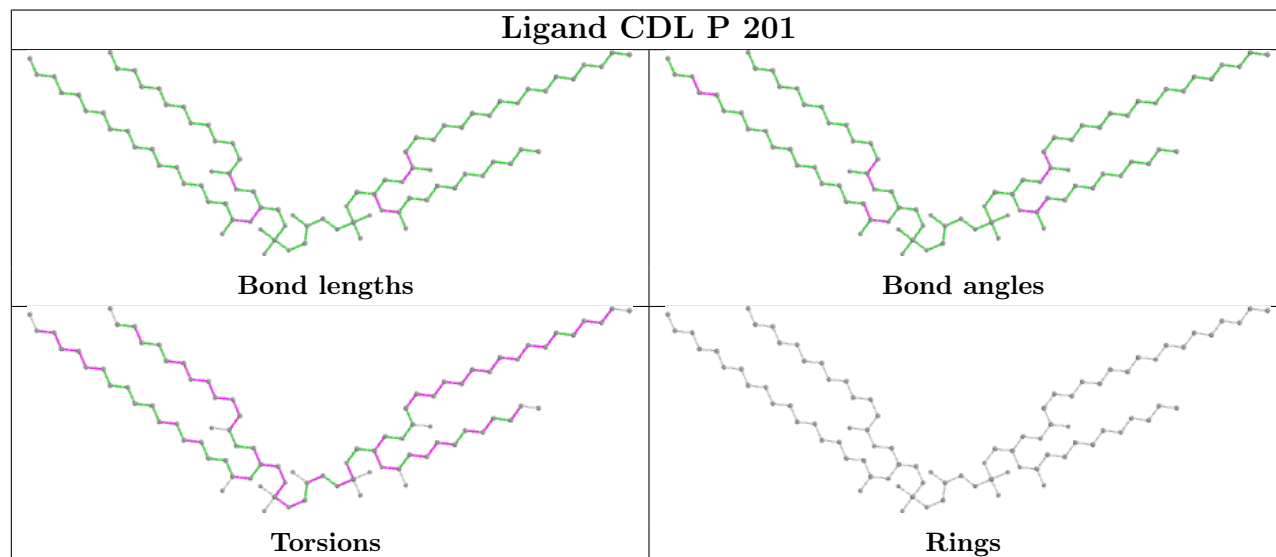


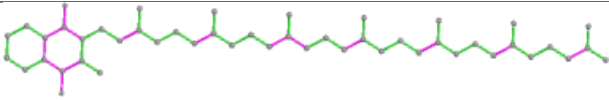
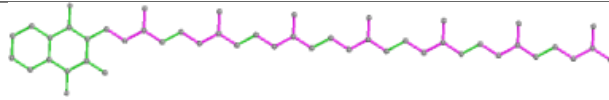
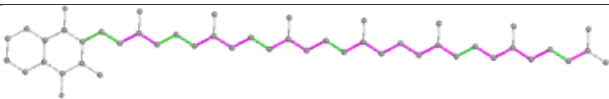
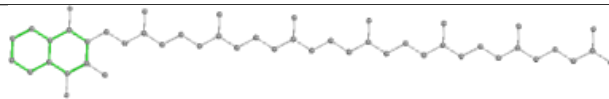


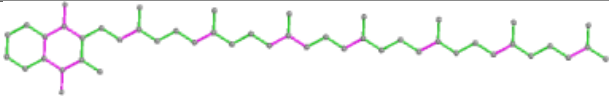
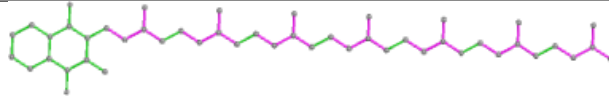
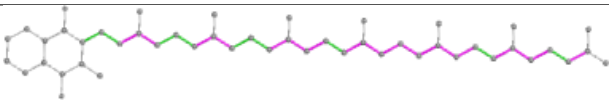
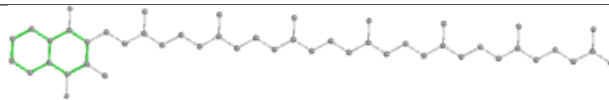
Ligand 9YF A 502

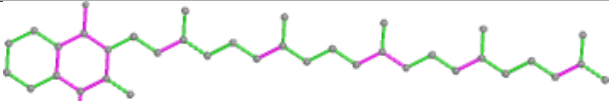
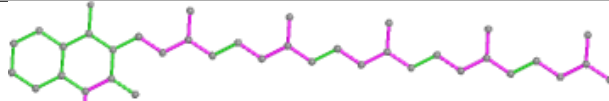
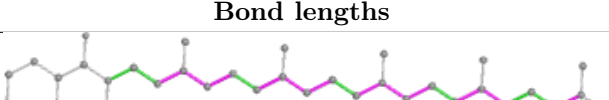
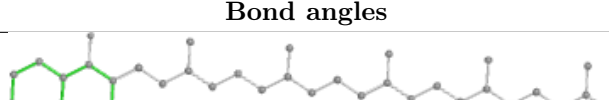


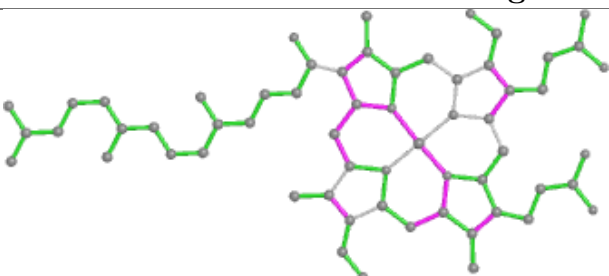
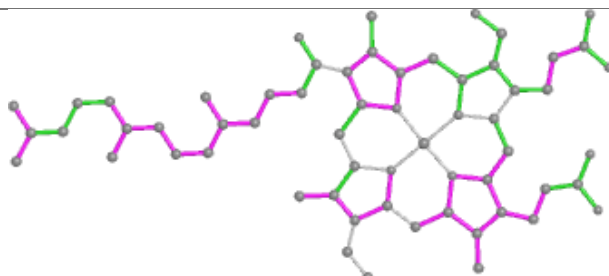
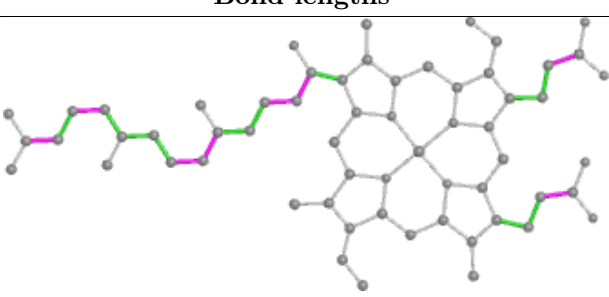
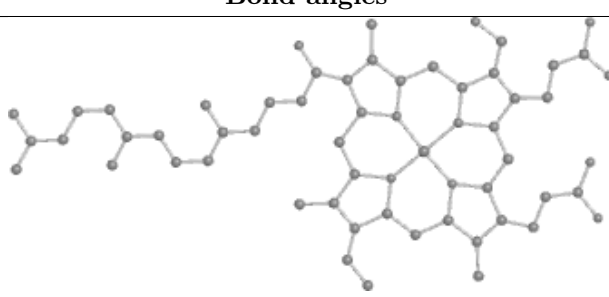
Ligand CDL P 201

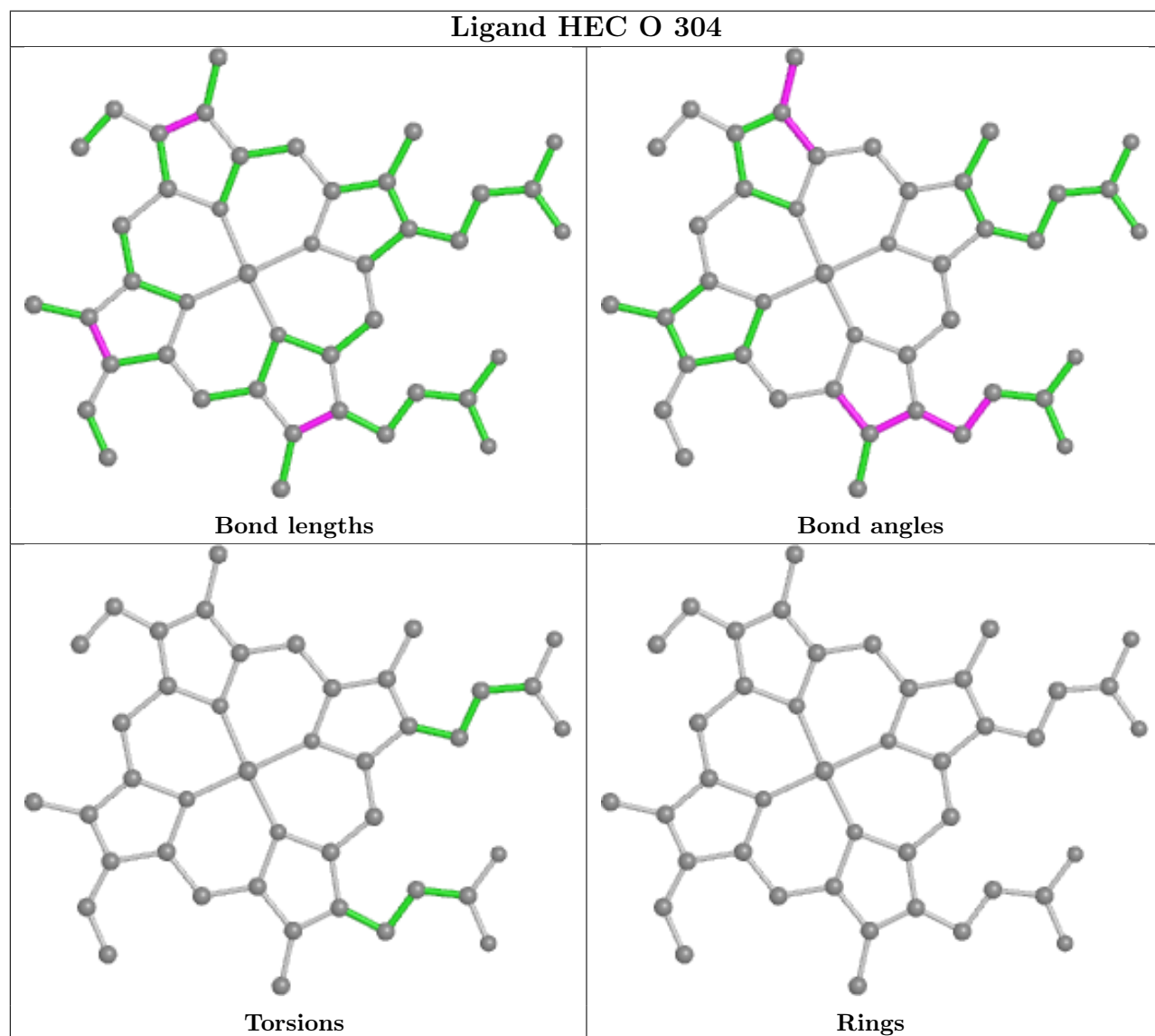
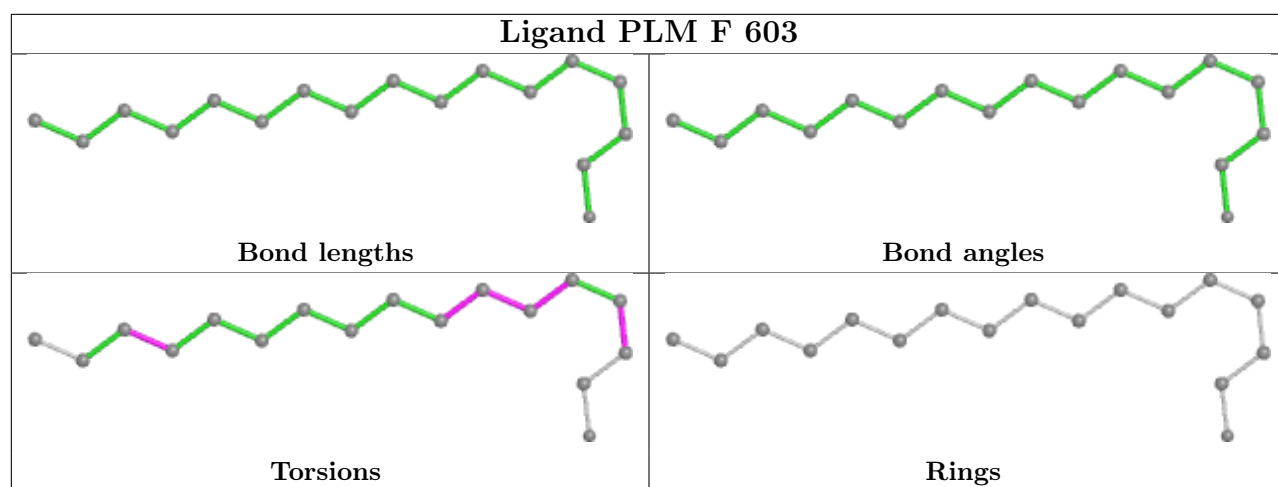


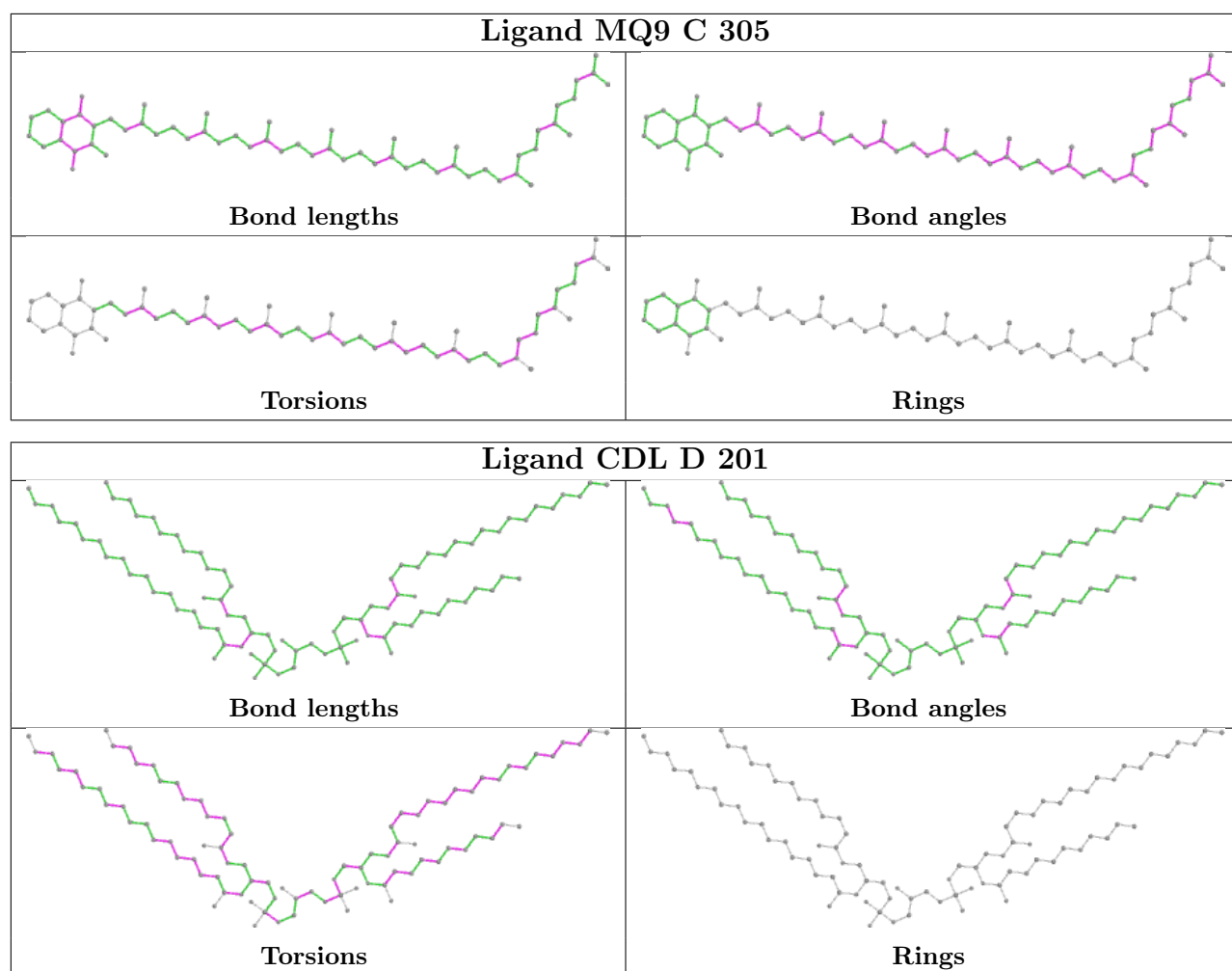
Ligand MQ9 C 304	
	Bond lengths
	Bond angles
	Torsions
	Rings

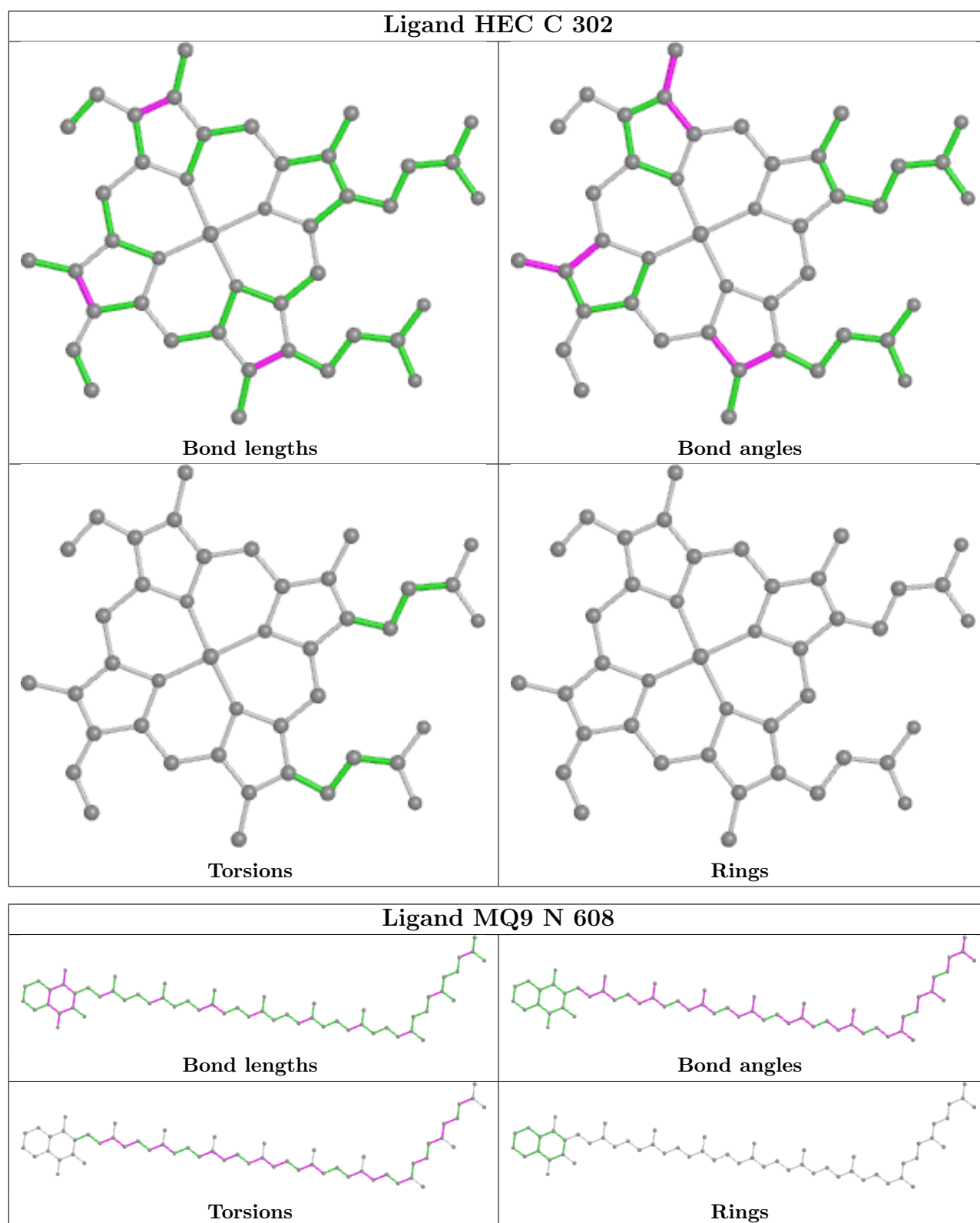
Ligand MQ9 O 301	
	Bond lengths
	Bond angles
	Torsions
	Rings

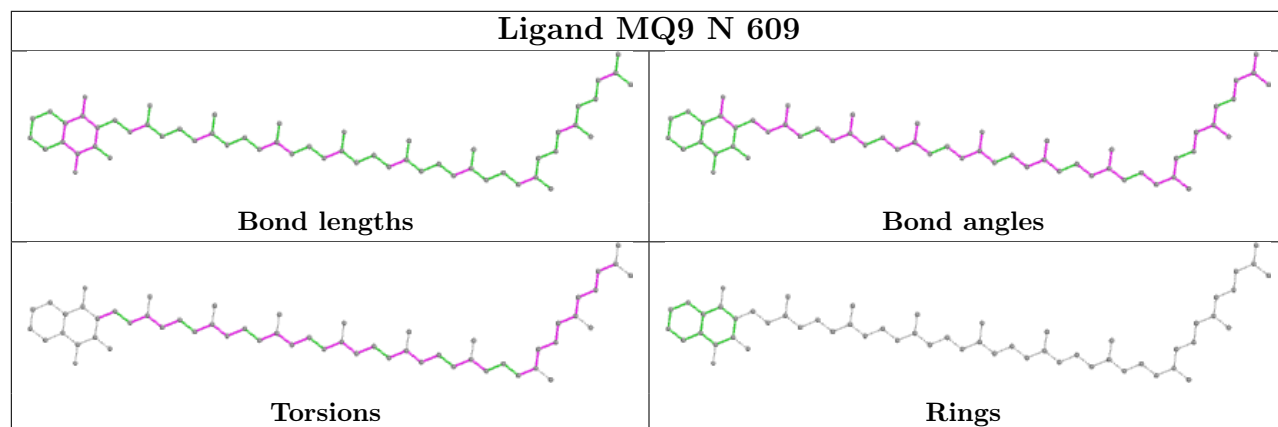
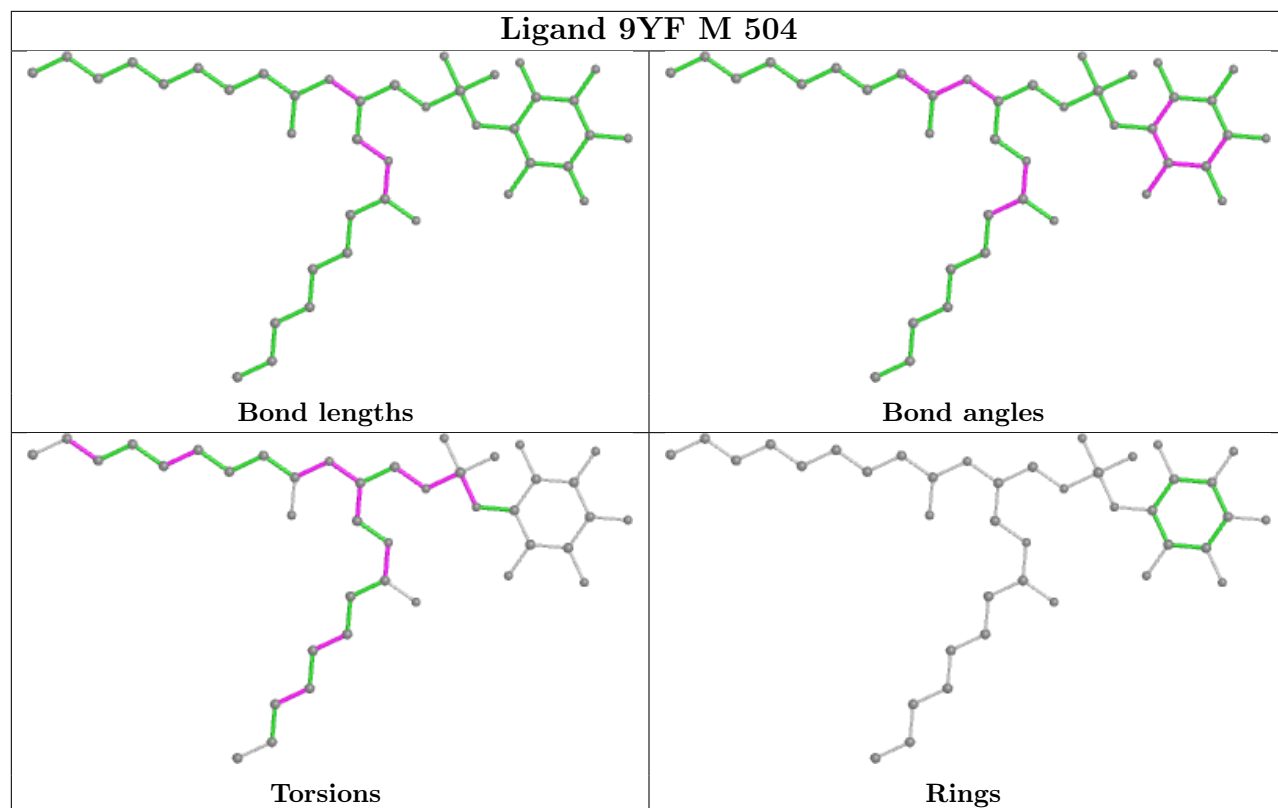
Ligand MQ9 B 609	
	Bond lengths
	Bond angles
	Torsions
	Rings

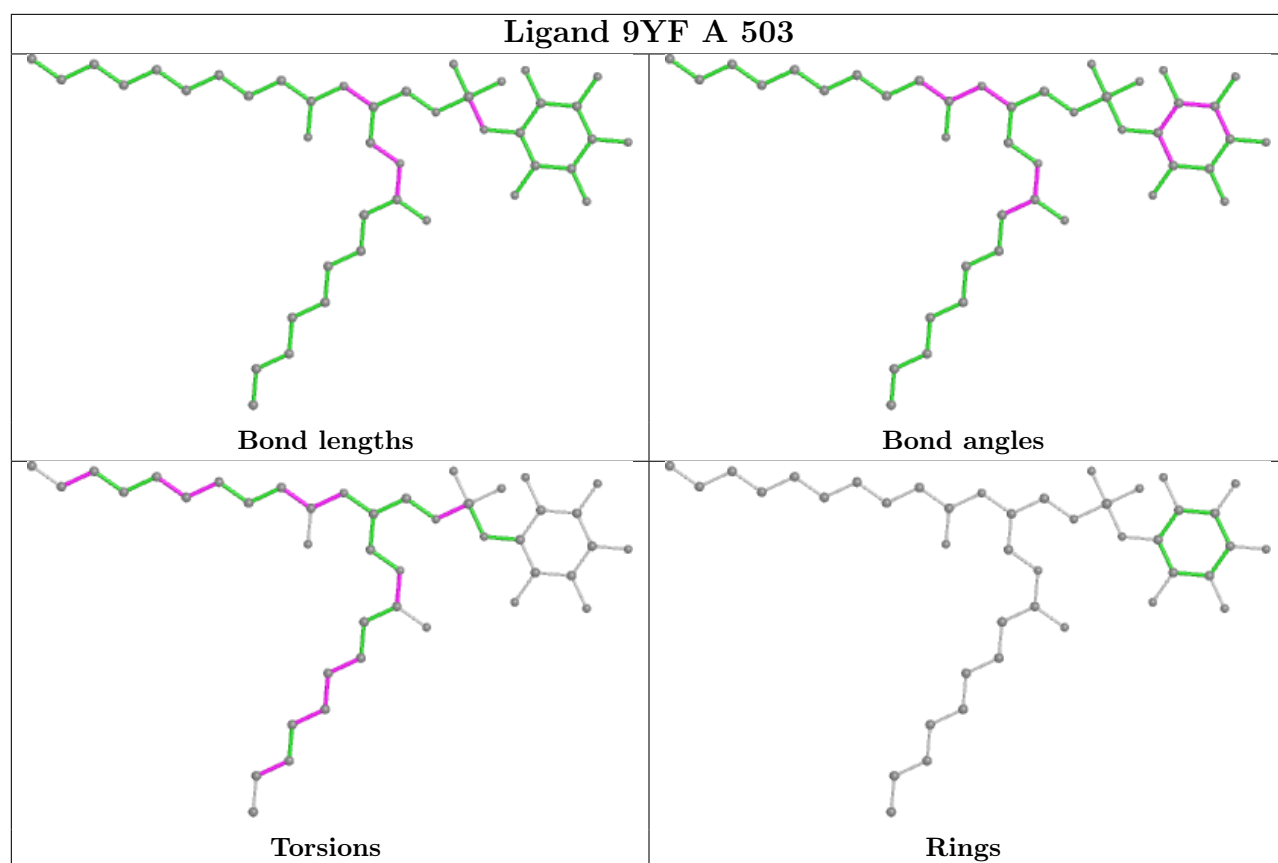
Ligand HEA F 607	
	Bond lengths
	Bond angles
	Torsions
	Rings

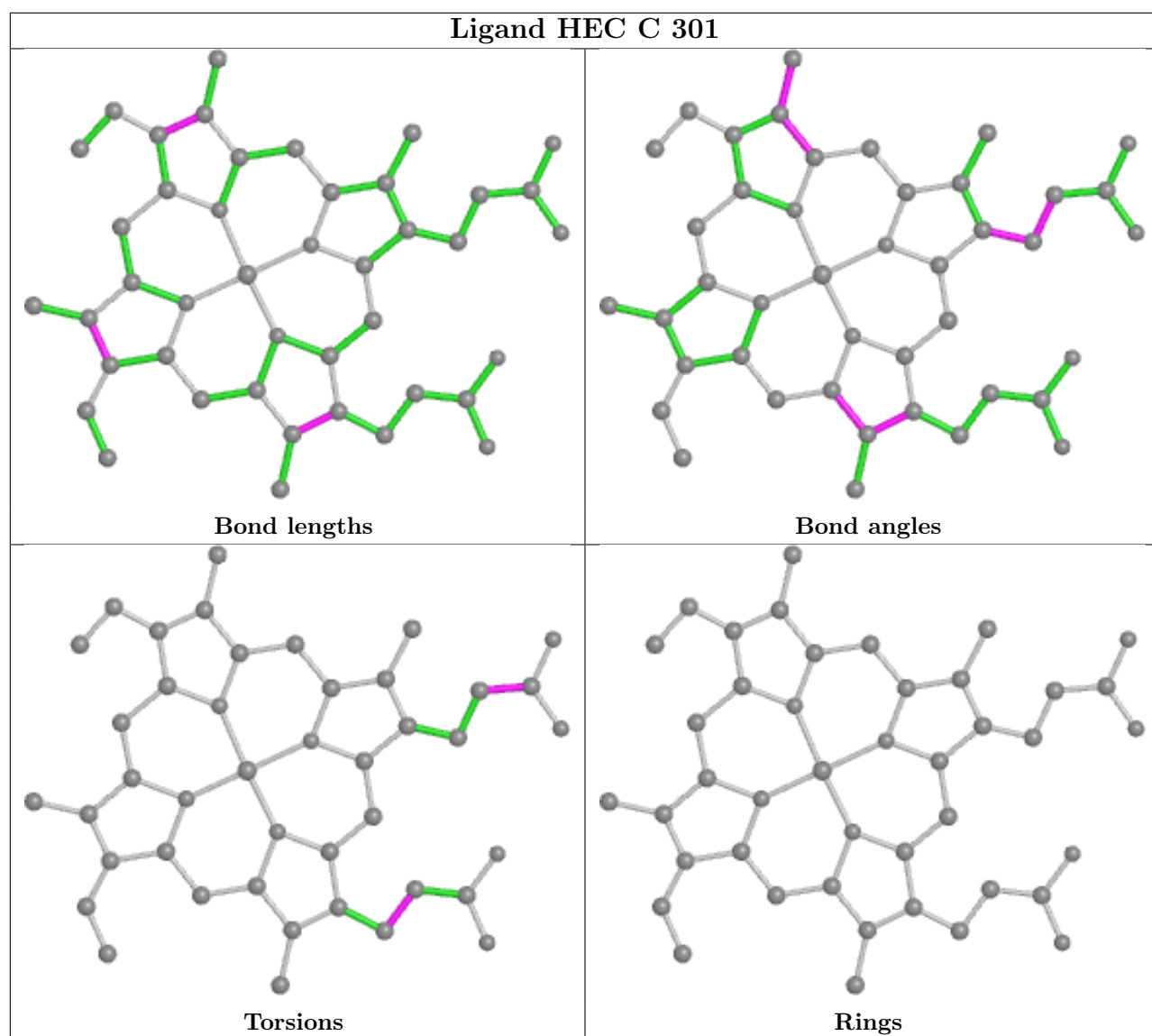


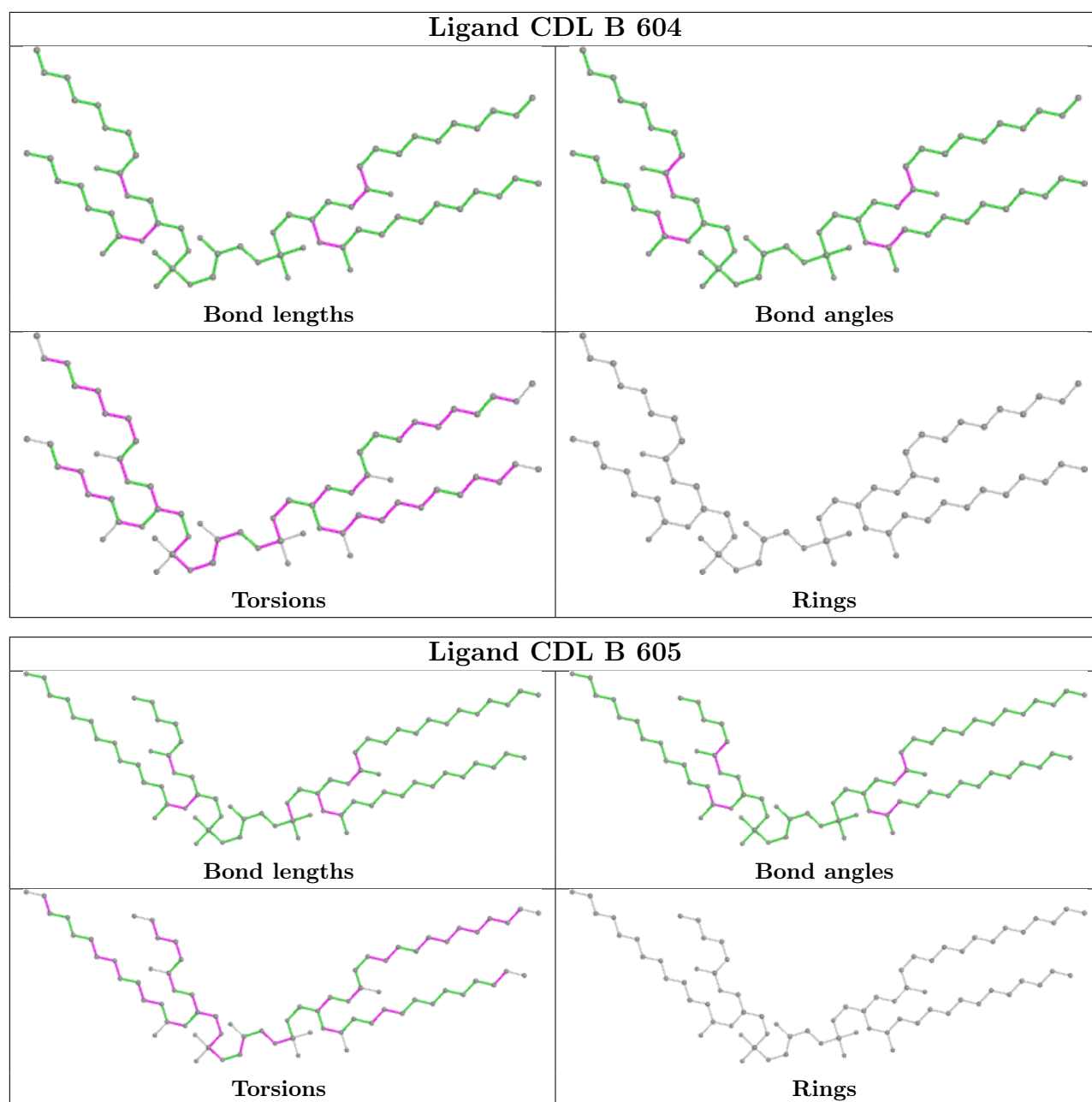


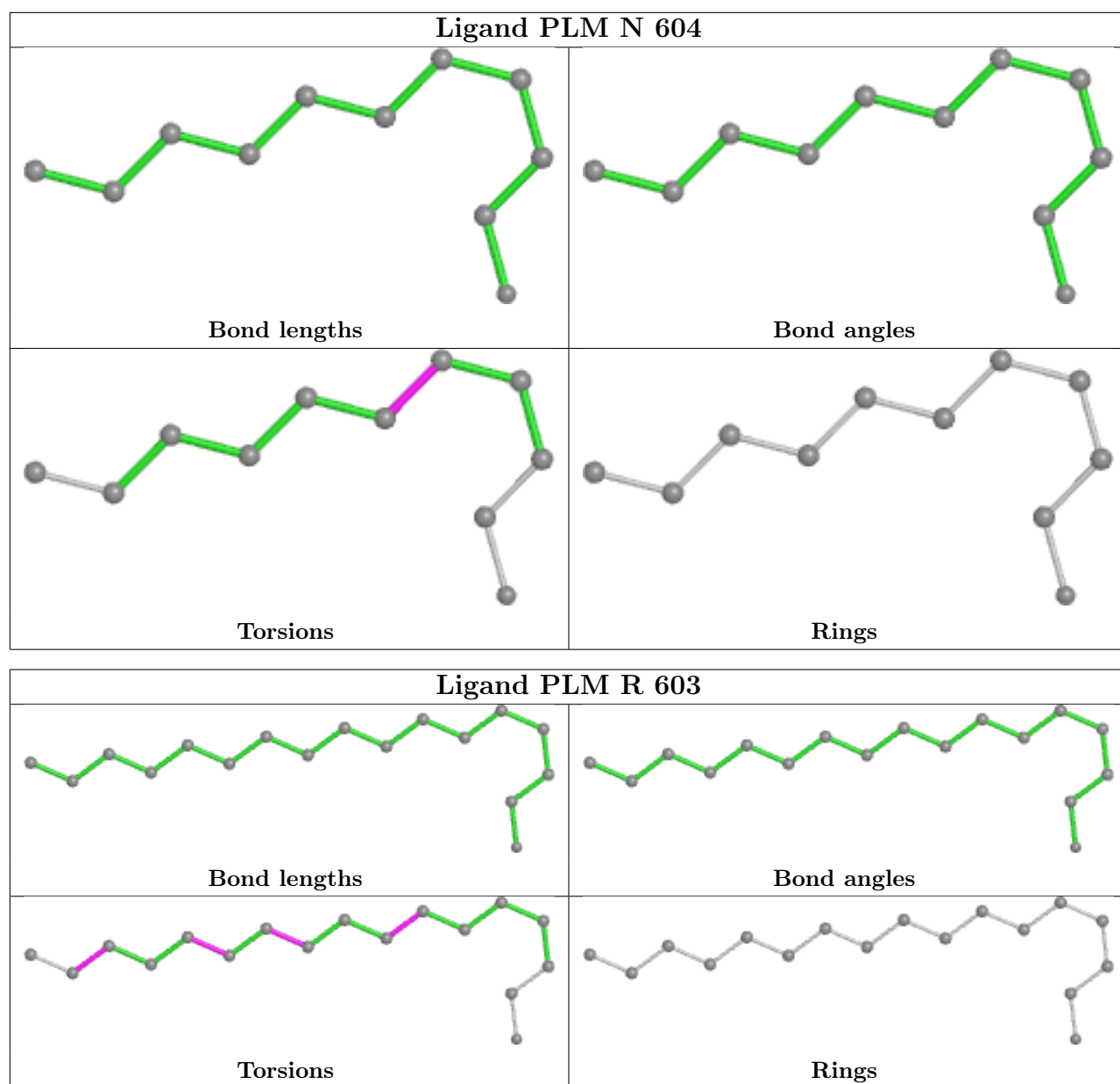


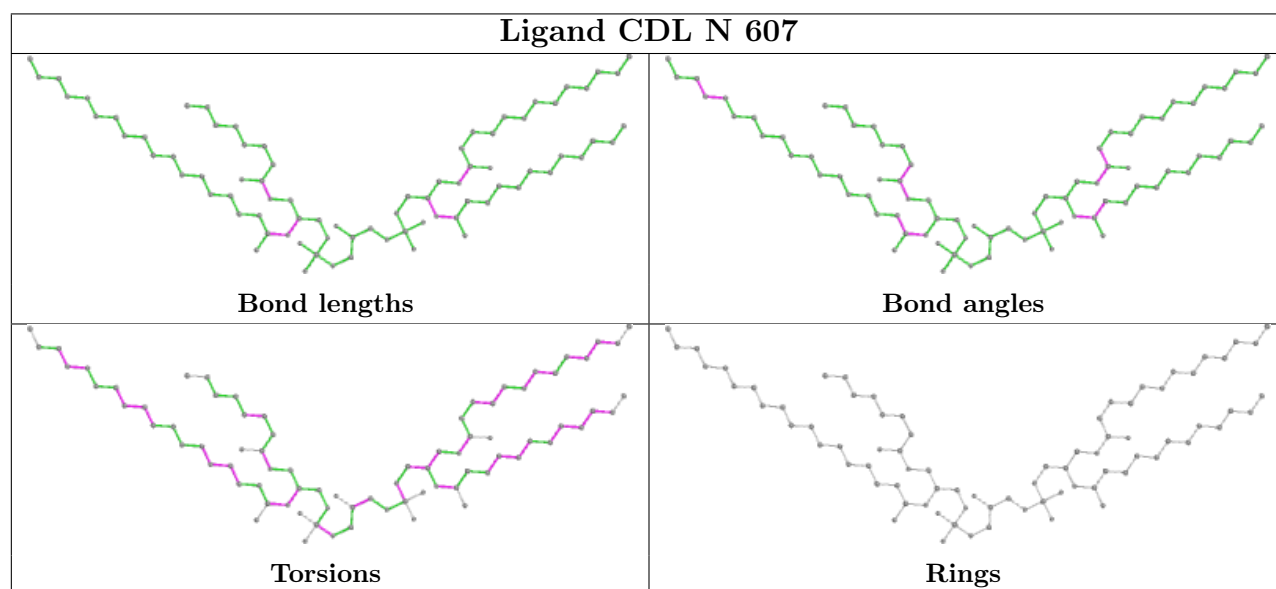
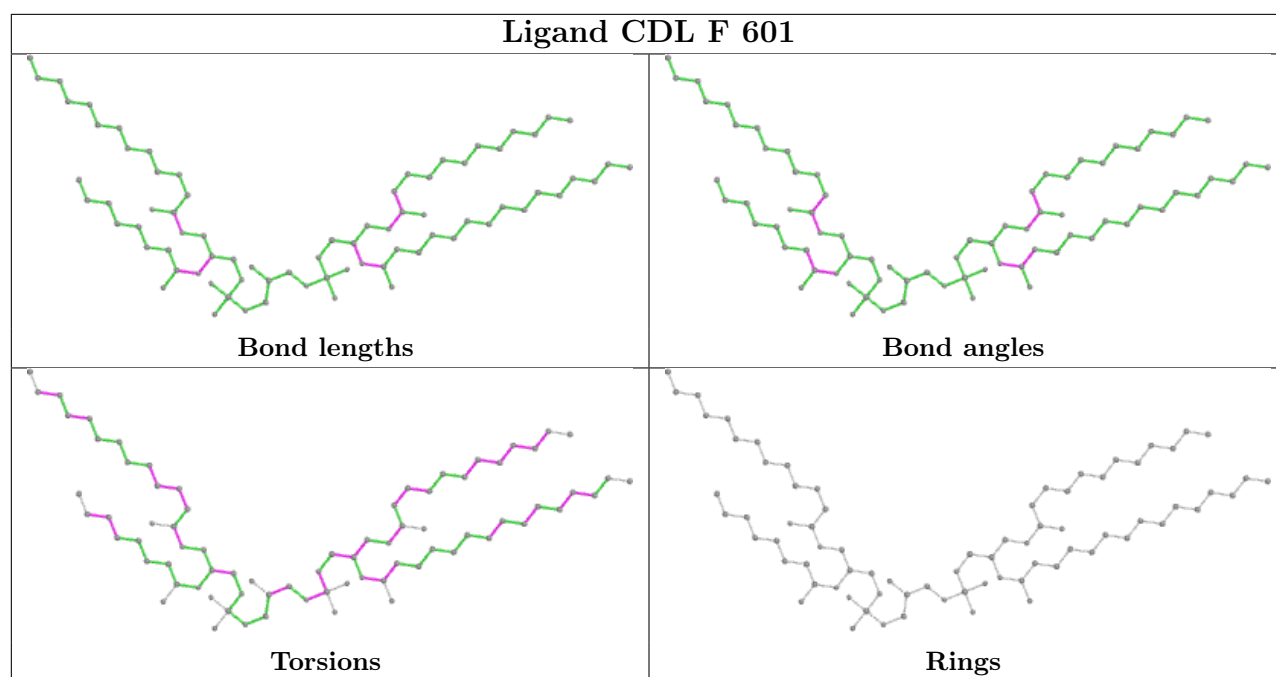


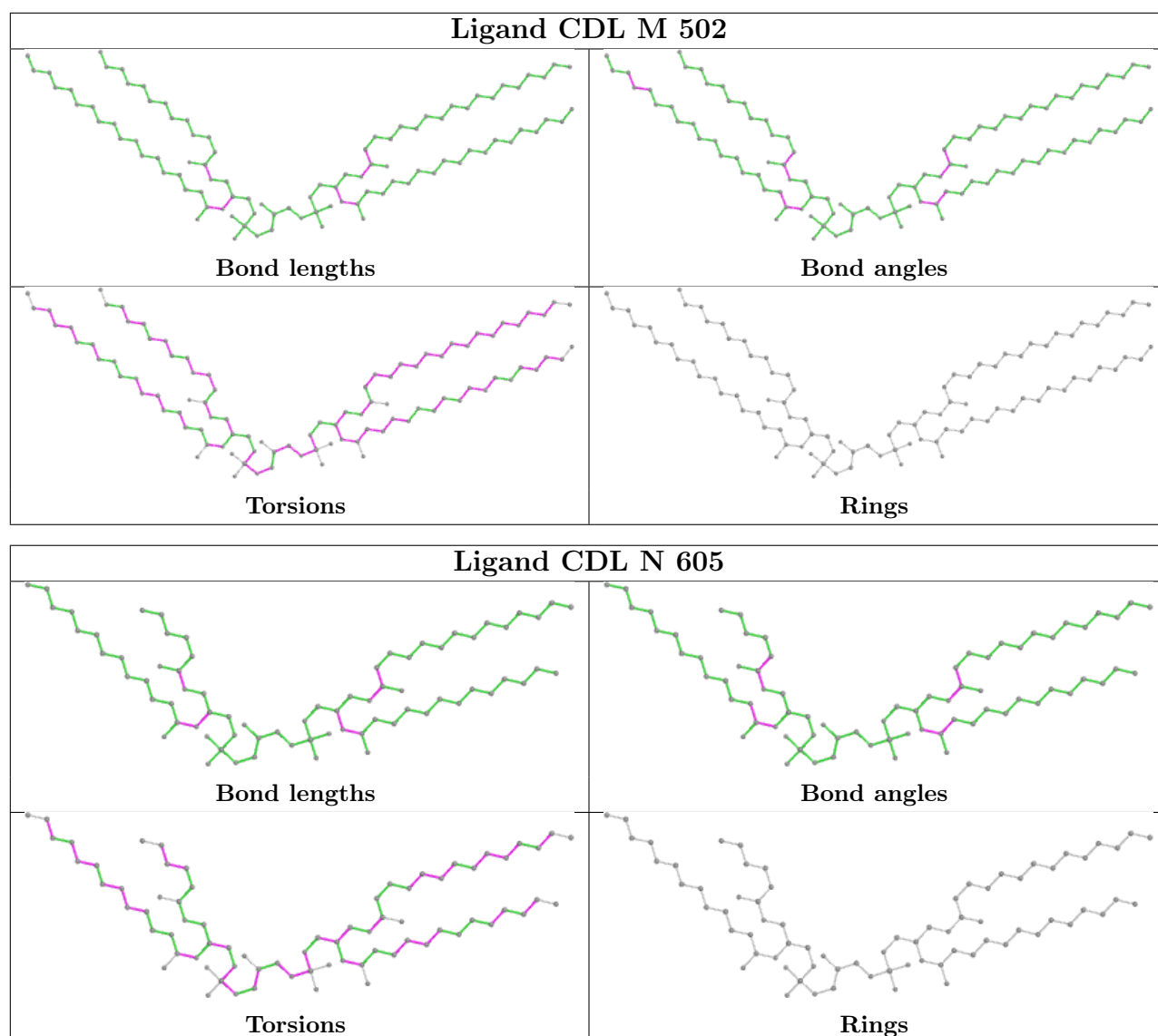


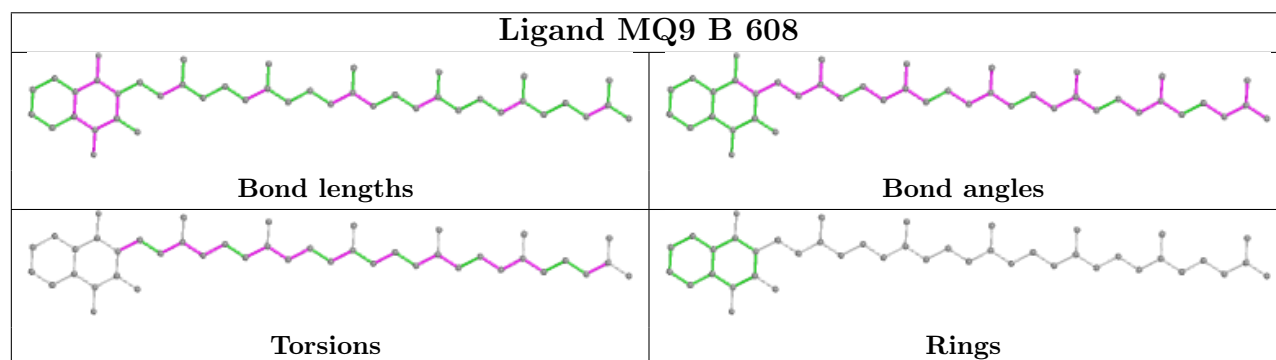
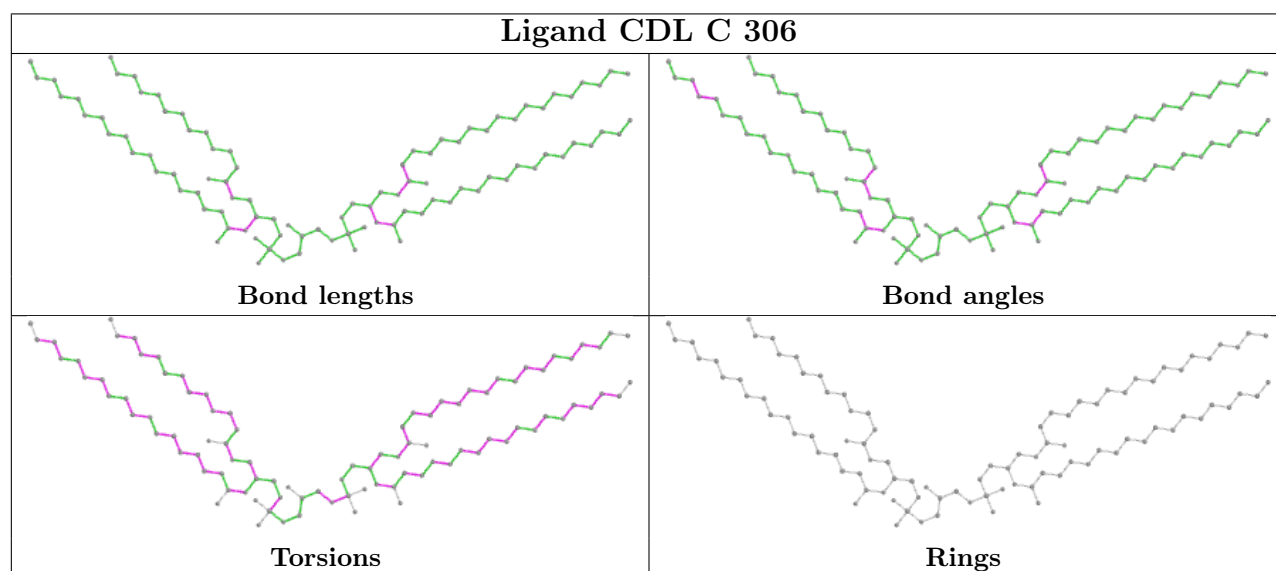
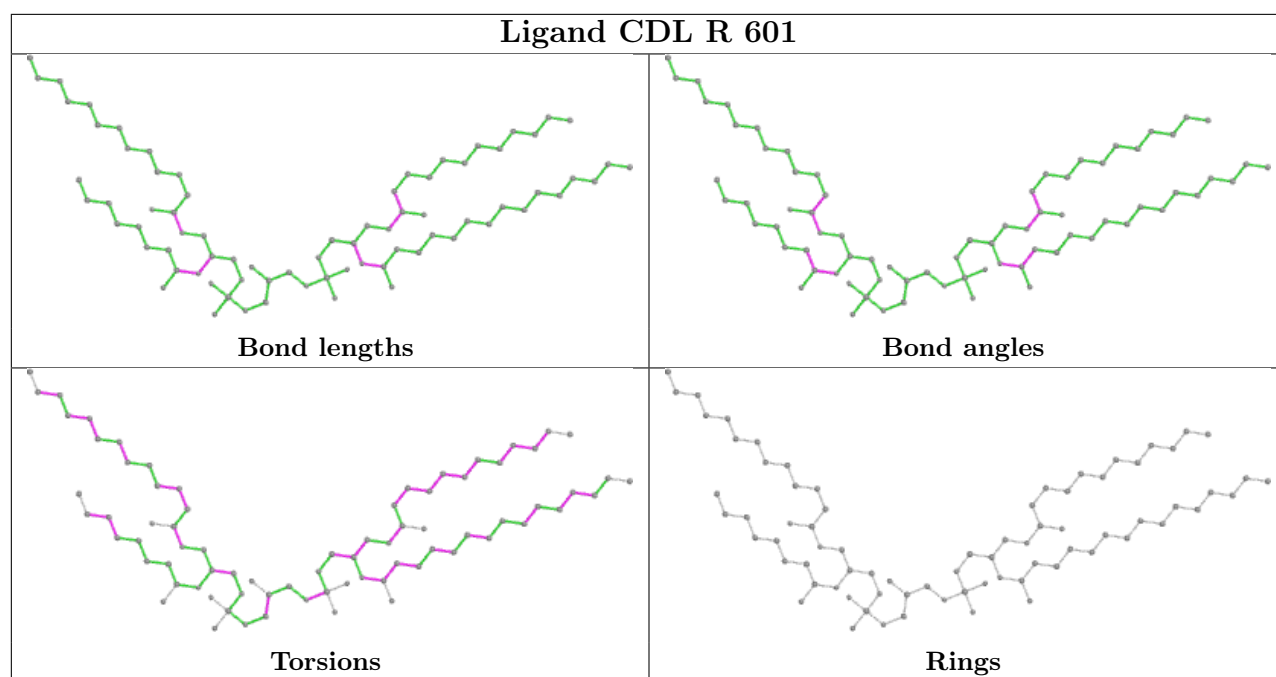


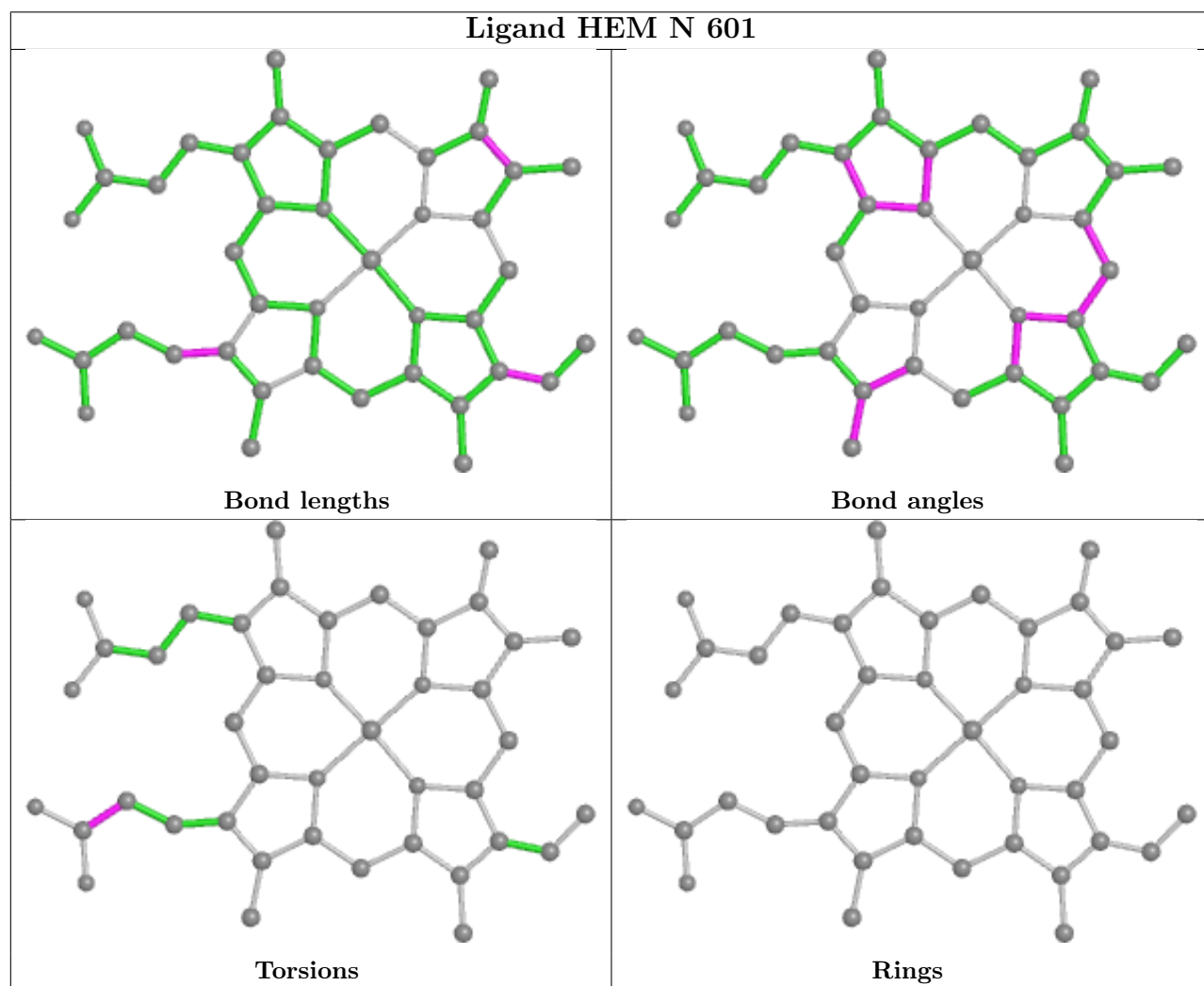
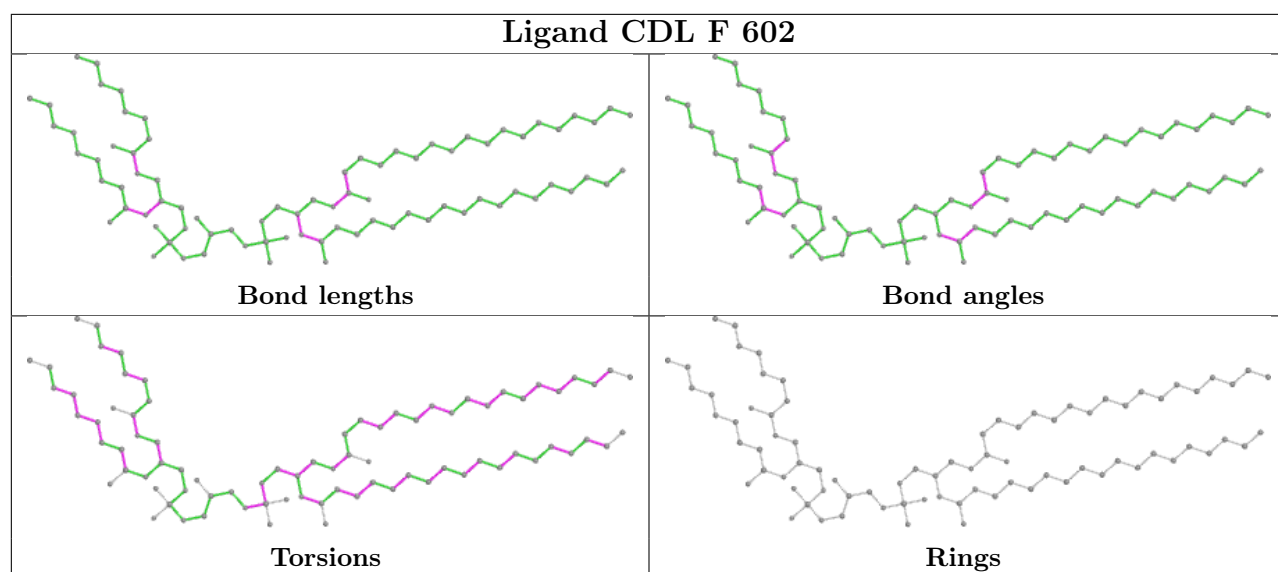


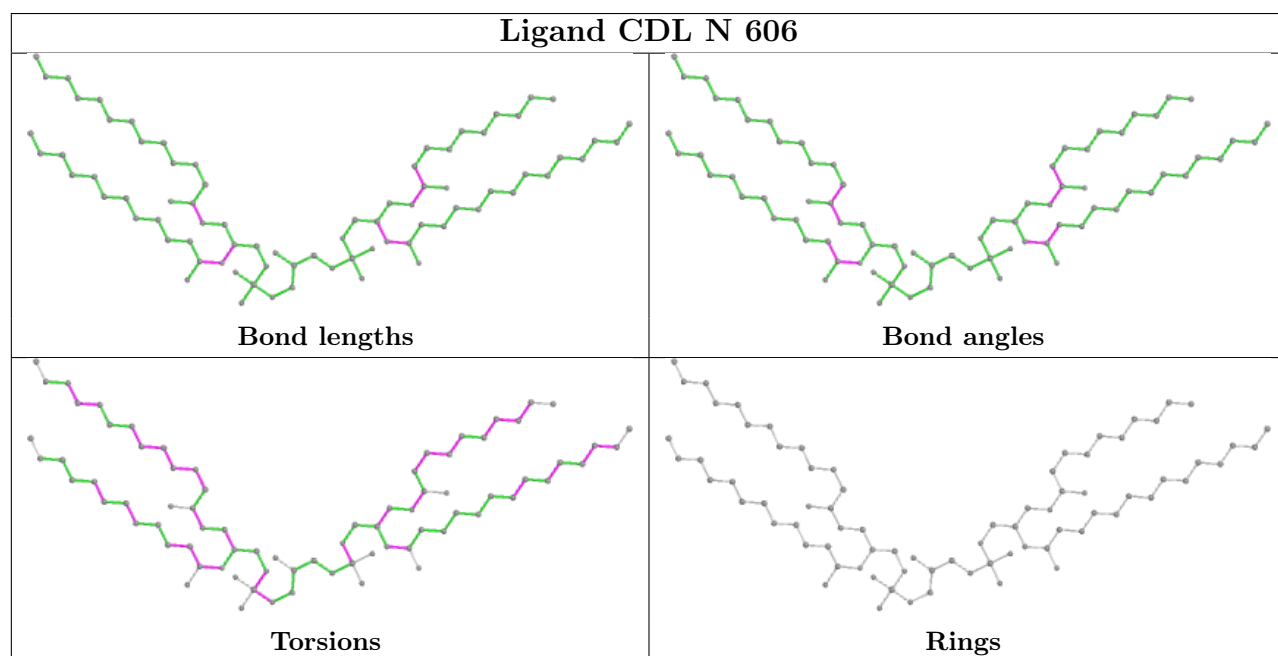
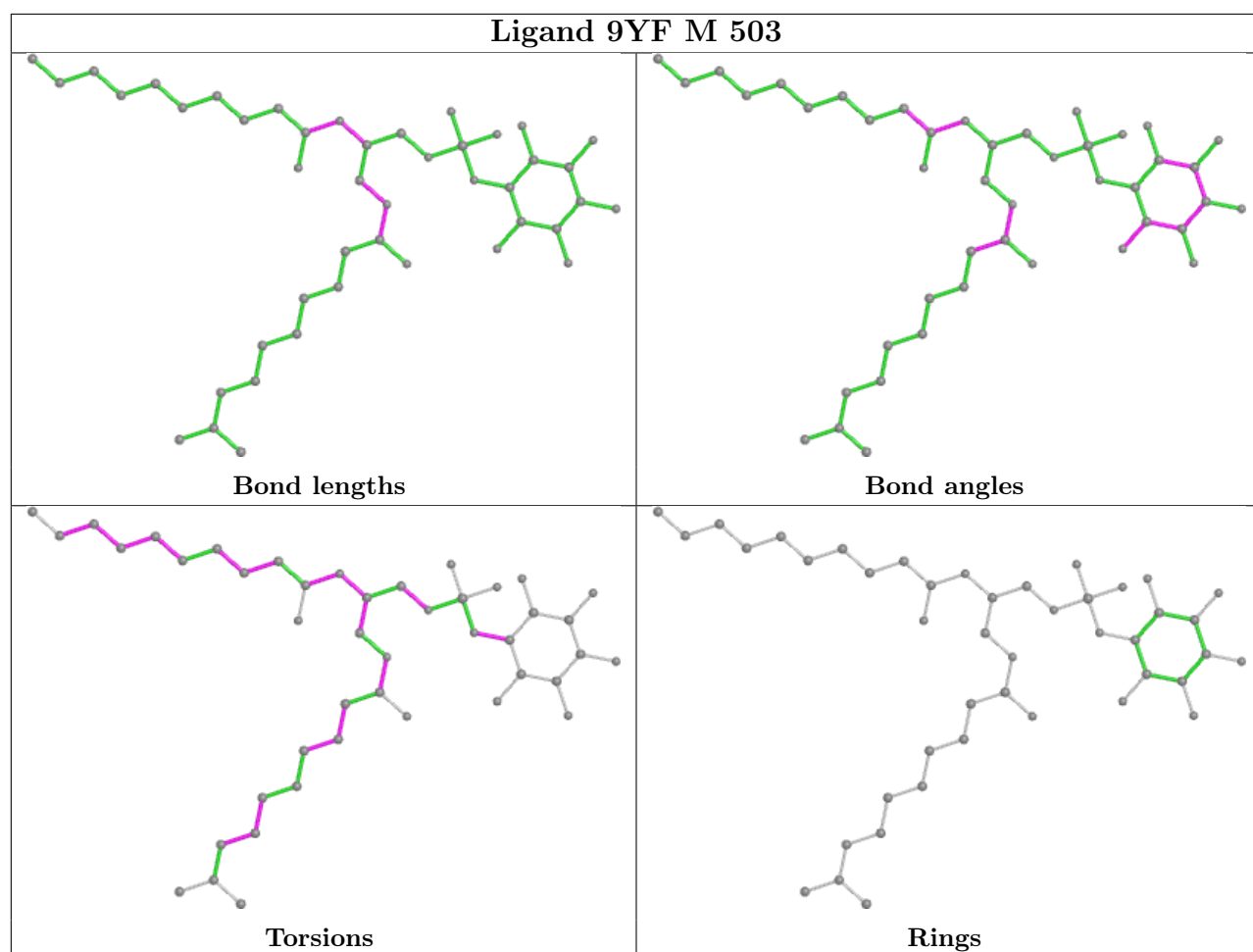


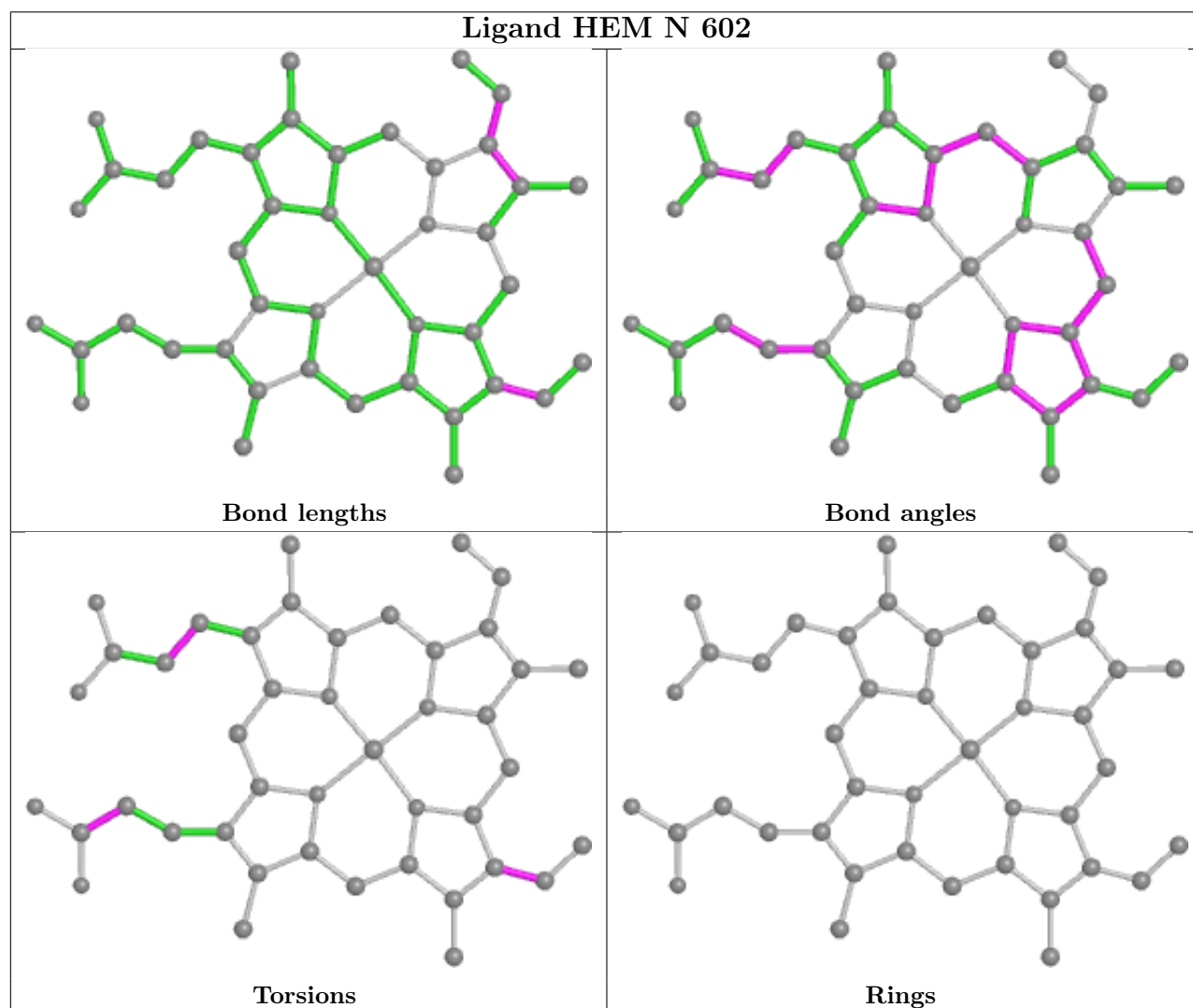
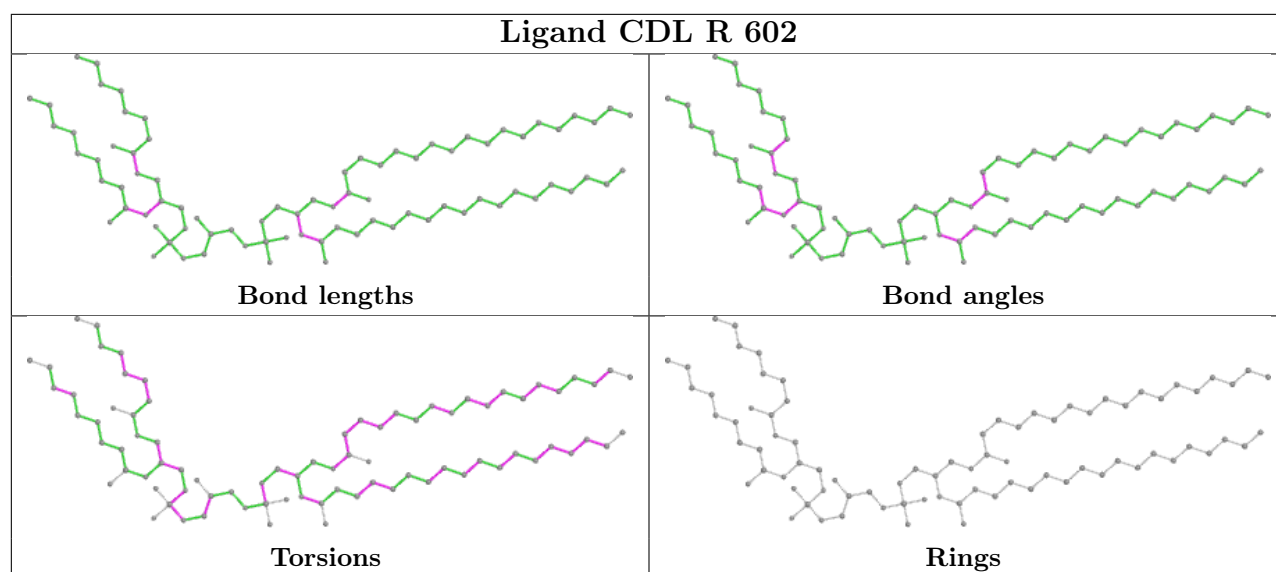












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

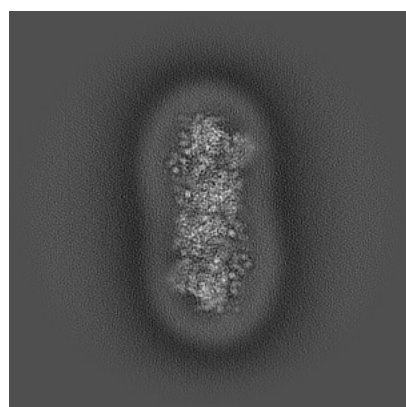
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30943. These allow visual inspection of the internal detail of the map and identification of artifacts.

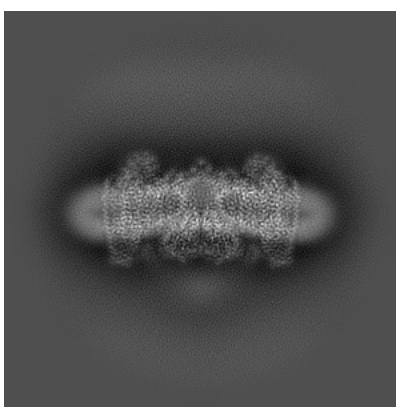
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

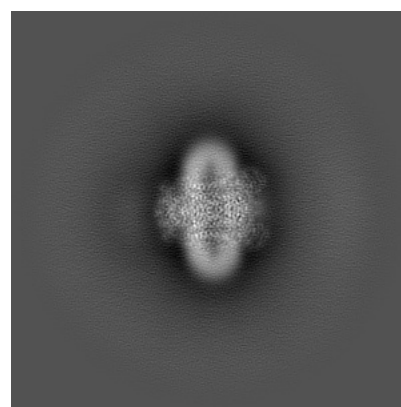
6.1.1 Primary map



X



Y

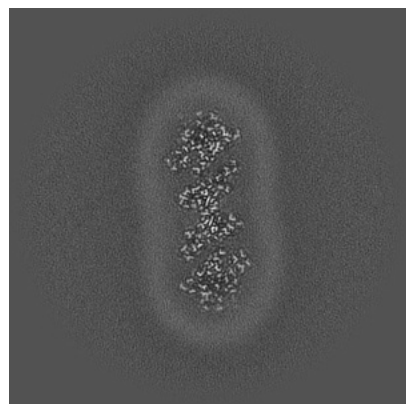


Z

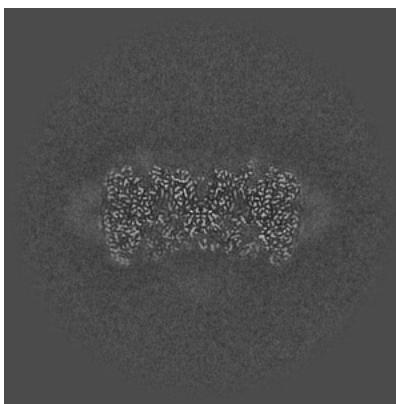
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

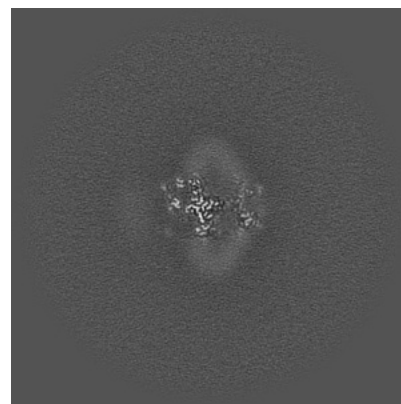
6.2.1 Primary map



X Index: 256



Y Index: 256

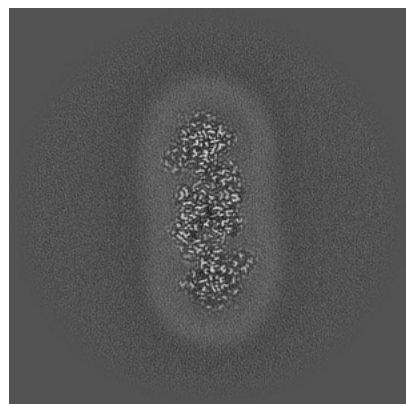


Z Index: 256

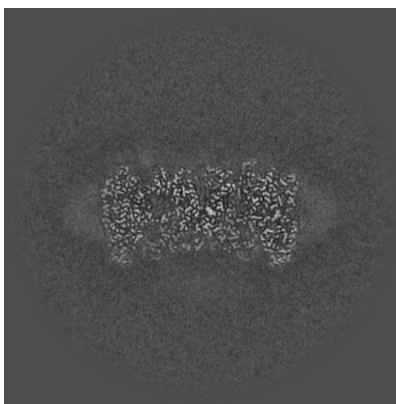
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

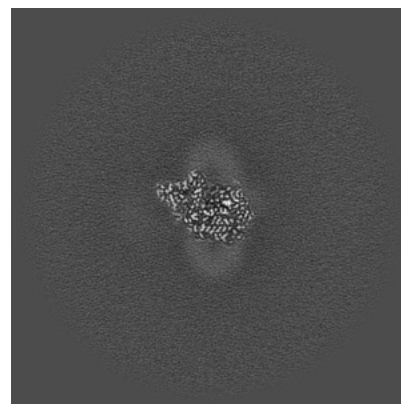
6.3.1 Primary map



X Index: 243



Y Index: 252

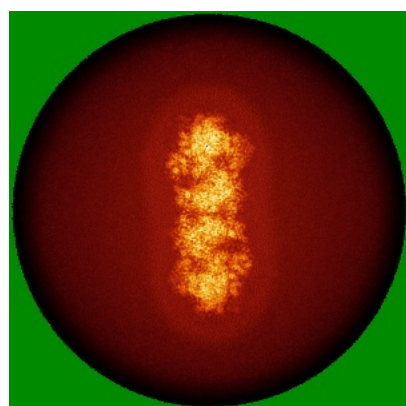


Z Index: 274

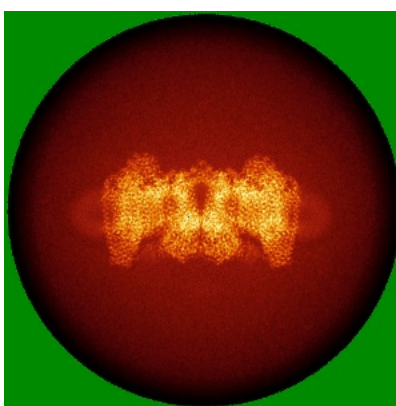
The images above show the largest variance slices of the map in three orthogonal directions.

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

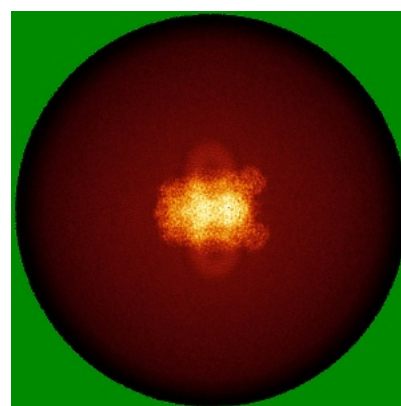
6.4.1 Primary map



X



Y

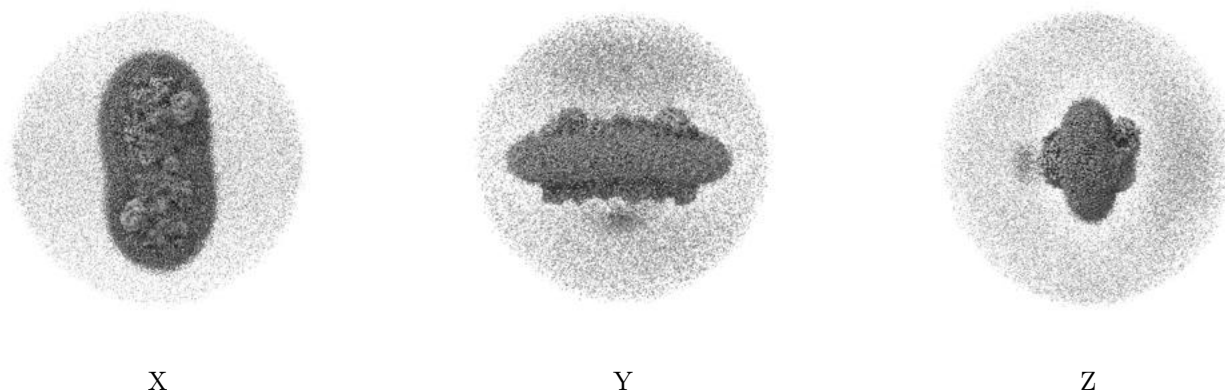


Z

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

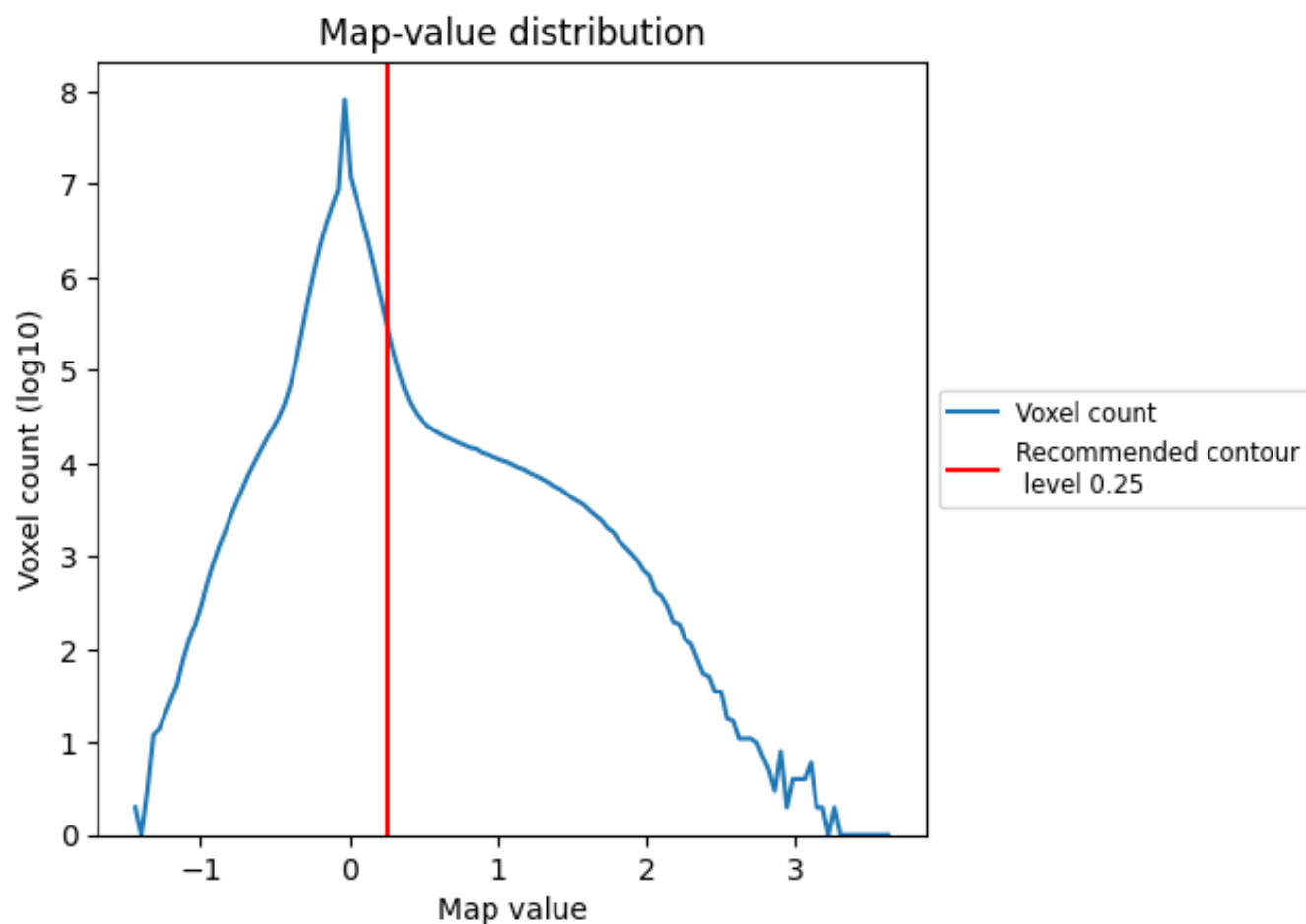
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

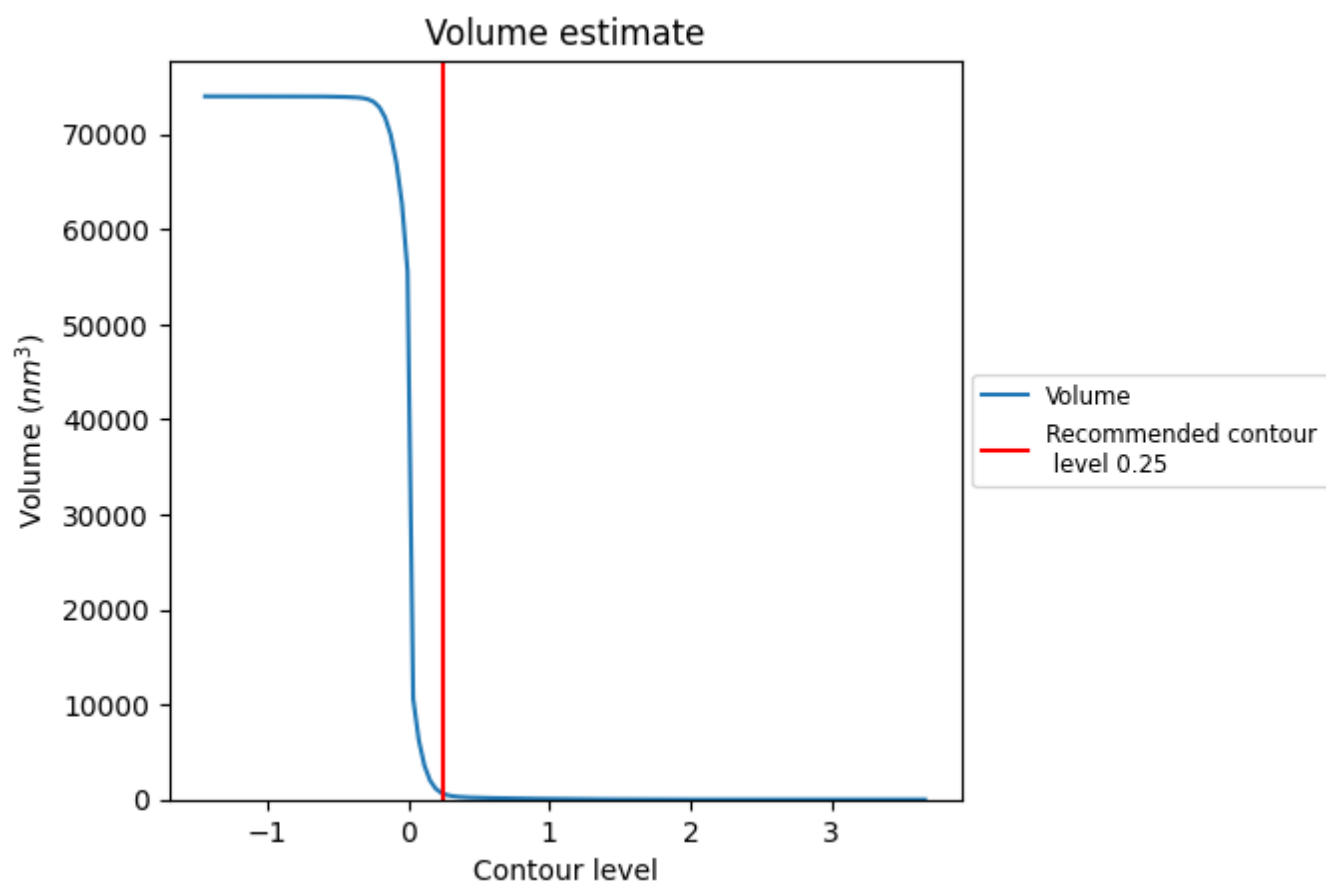
This section contains the results of statistical analysis of the map.

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.

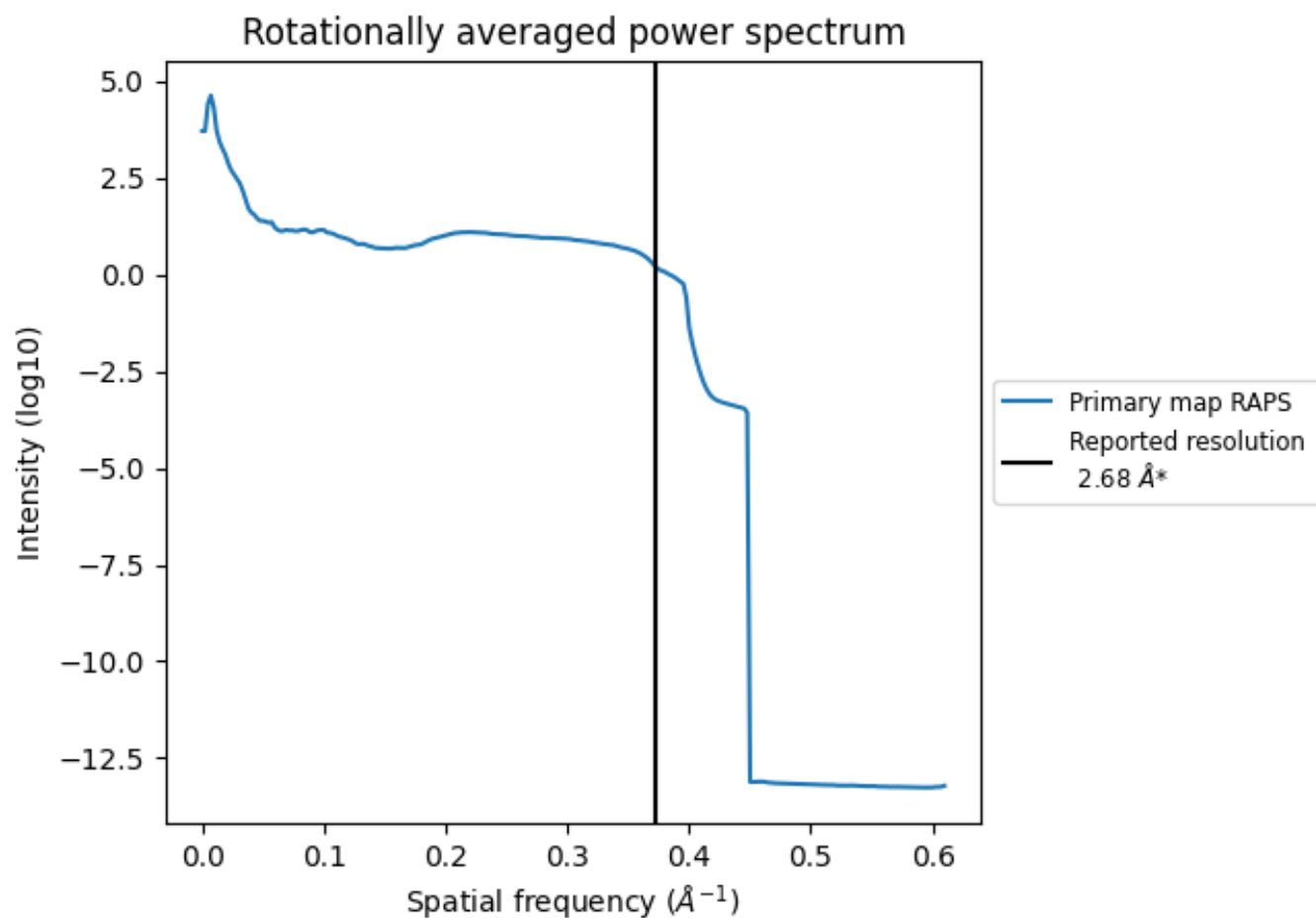
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 620 nm^3 ; this corresponds to an approximate mass of 560 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 0.373 Å⁻¹

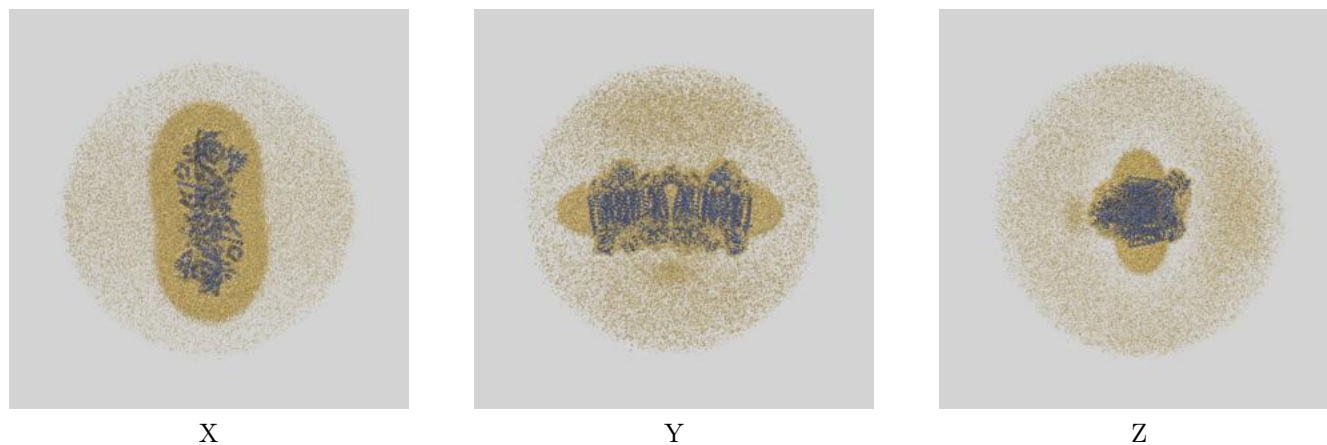
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

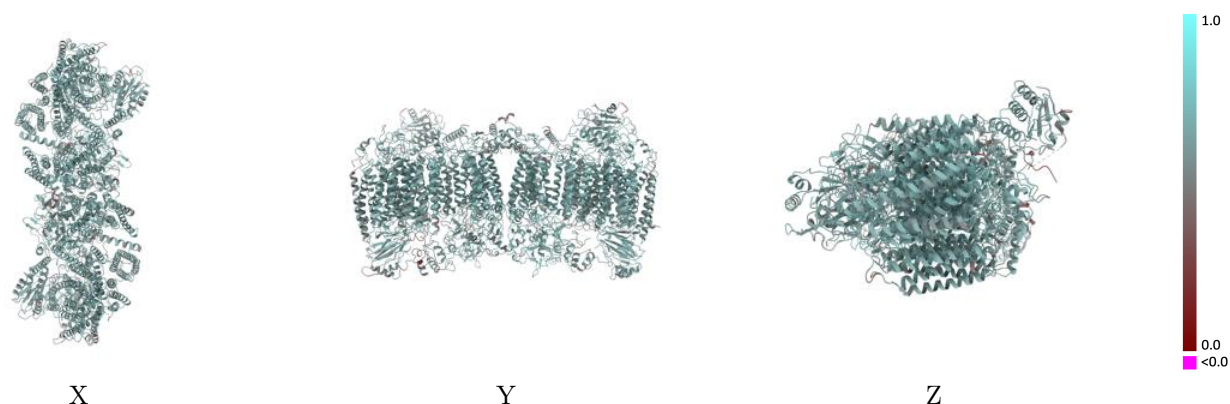
This section contains information regarding the fit between EMDB map EMD-30943 and PDB model 7E1V. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



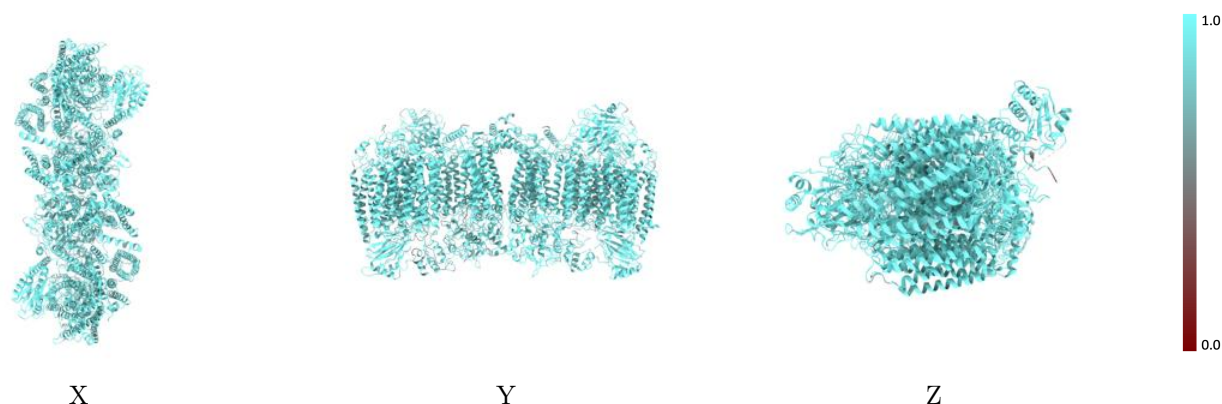
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



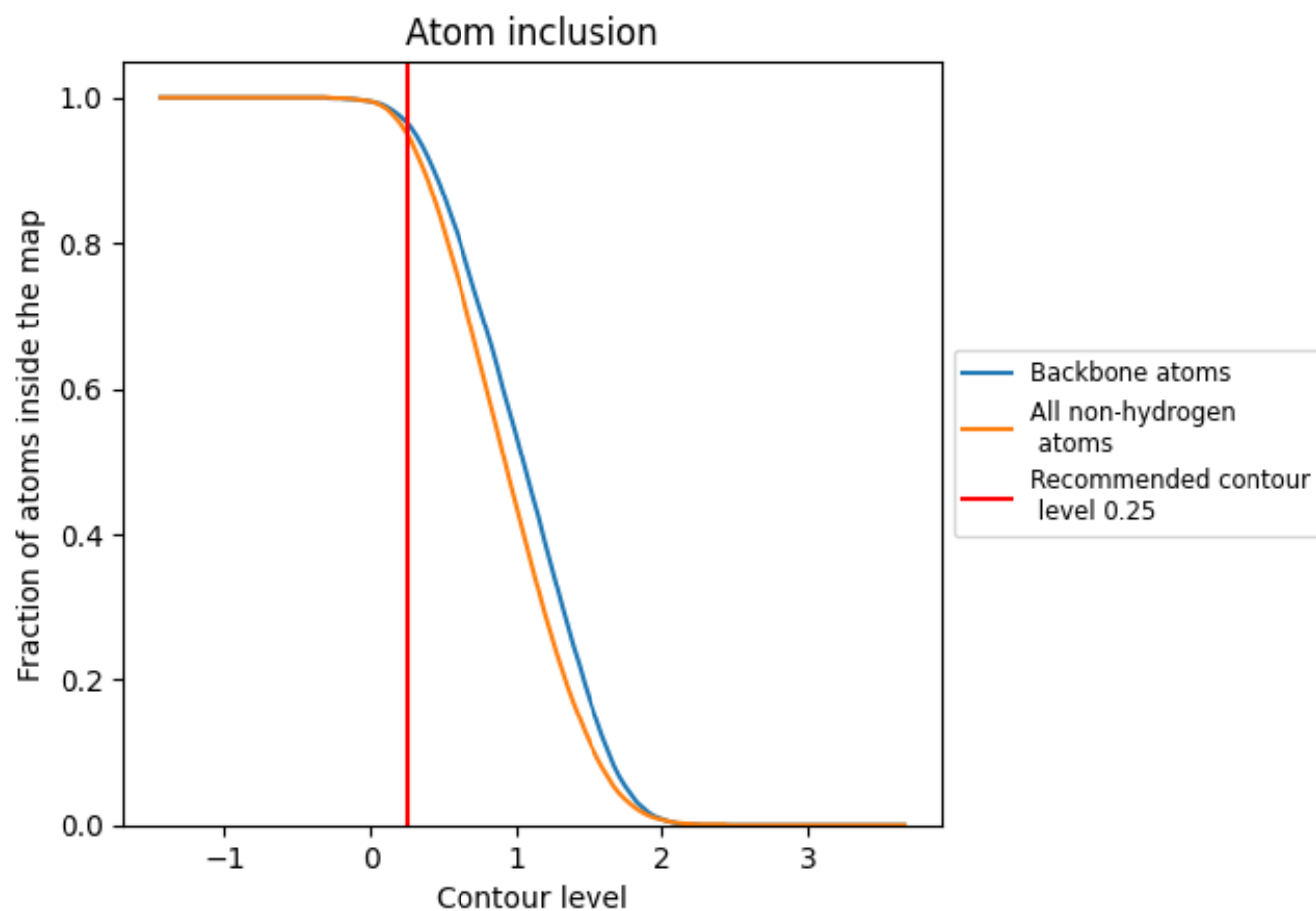
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9510	 0.6140
A	 0.9560	 0.6130
B	 0.9590	 0.6310
C	 0.8700	 0.5840
D	 0.9530	 0.6060
E	 0.9500	 0.5980
F	 0.9780	 0.6410
G	 0.9500	 0.6020
H	 0.9620	 0.6210
I	 0.9490	 0.5830
J	 0.9460	 0.5790
M	 0.9510	 0.6140
N	 0.9580	 0.6330
O	 0.9290	 0.6060
P	 0.9450	 0.6030
Q	 0.9120	 0.5590
R	 0.9690	 0.6340
S	 0.9390	 0.5940
T	 0.9610	 0.6180
U	 0.9230	 0.5700
V	 0.9360	 0.5660

