



## wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 03:33 AM JST

PDB ID : 7E1X  
EMDB ID : EMD-30945  
Title : Cryo-EM structure of hybrid respiratory supercomplex consisting of Mycobacterium tuberculosis complexIII and Mycobacterium smegmatis complexIV in presence of TB47  
Authors : Zhou, S.; Wang, W.; Gao, Y.; Gong, H.; Rao, Z.  
Deposited on : 2021-02-03  
Resolution : 2.93 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

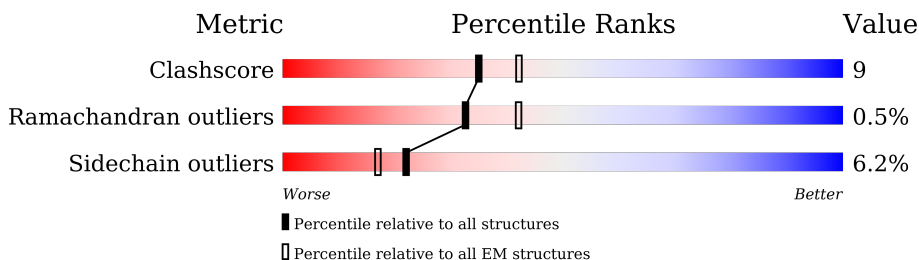
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.93 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	

*Continued on next page...*

Continued from previous page...

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
14	HEA	F	606	X	-	-	-
14	HEA	F	607	X	-	-	-
14	HEA	R	606	X	-	-	-
14	HEA	R	607	X	-	-	-
19	FES	A	501	-	-	X	-
19	FES	M	501	-	-	X	-

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 42679 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
			Total	C	N	O	S		
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
			2242	1459	370	405	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
4	H	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
4	T	139	Total	C	N	O	S	0	0
			1077	719	167	188	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
			507	334	85	86	2		
5	U	67	Total	C	N	O	S	0	0
			507	334	85	86	2		

- 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
			1041	658	176	205	2		
6	V	145	Total	C	N	O	S	0	0
			1041	658	176	205	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
			605	395	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
			4140	2734	707	682	17		
8	B	524	Total	C	N	O	S	0	0
			4140	2734	707	682	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
			2943	1900	501	531	11		
9	A	378	Total	C	N	O	S	0	0
			2943	1900	501	531	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	223	Total	C	N	O	S	0	0
			1621	1015	291	304	11		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	218	1584	995	283	297	9	0	0

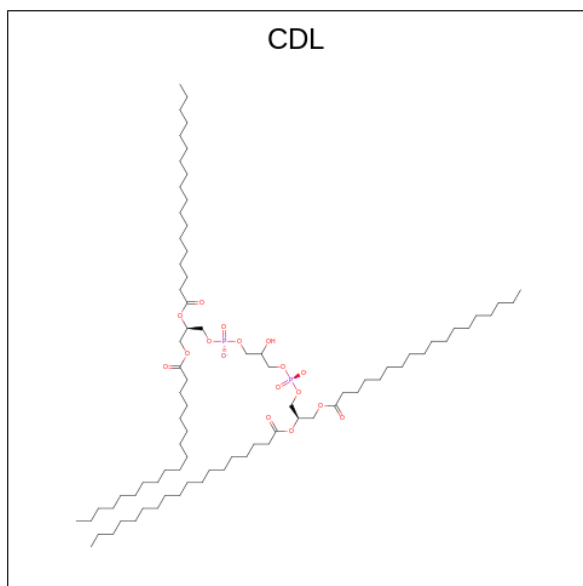
There are 2 discrepancies between the modelled and reference sequences:

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 (three-letter code: CU) (formula: Cu).

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

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



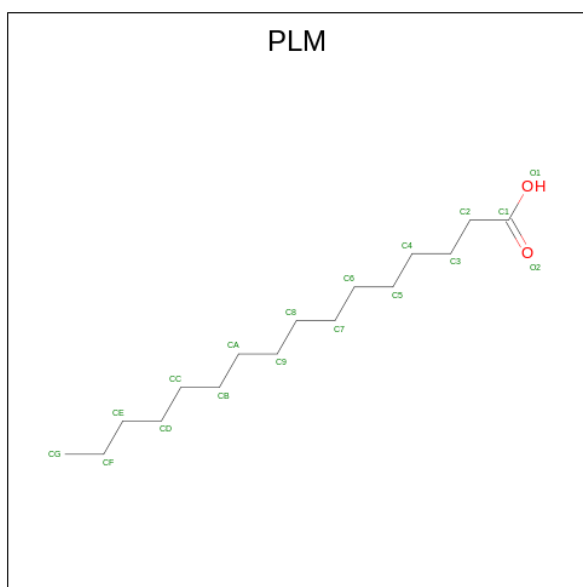
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	F	1	157	119	34	4	0

Continued on next page...

*Continued from previous page...*

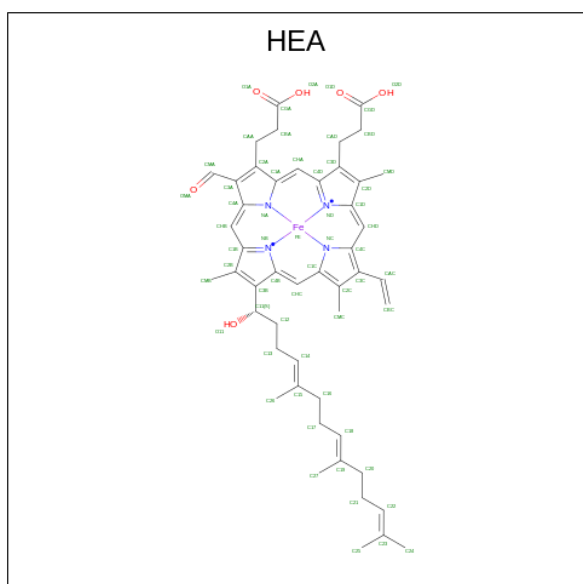
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	F	1	157	119	34	4	0
12	D	1	88	69	17	2	0
12	R	1	157	119	34	4	0
12	R	1	157	119	34	4	0
12	P	1	88	69	17	2	0
12	N	1	230	173	51	6	0
12	N	1	230	173	51	6	0
12	N	1	230	173	51	6	0
12	M	1	95	76	17	2	0
12	O	1	79	60	17	2	0
12	B	1	375	280	85	10	0
12	B	1	375	280	85	10	0
12	B	1	375	280	85	10	0
12	B	1	375	280	85	10	0
12	B	1	375	280	85	10	0
12	A	1	95	76	17	2	0

- Molecule 13 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>) (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	

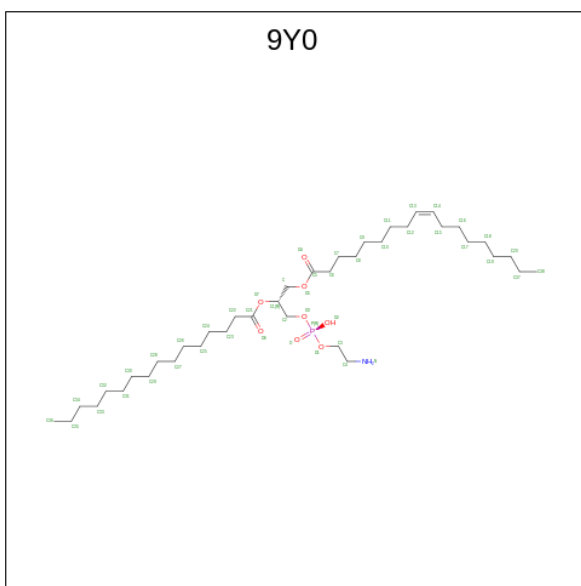
- Molecule 14 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf	
14	F	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
14	F	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
14	R	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
14	R	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 15 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (three-letter code: 9Y0) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



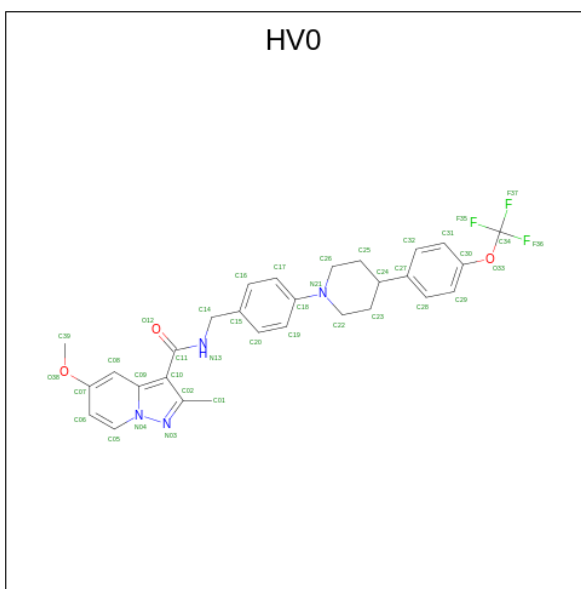
Mol	Chain	Residues	Atoms				AltConf	
15	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	S	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



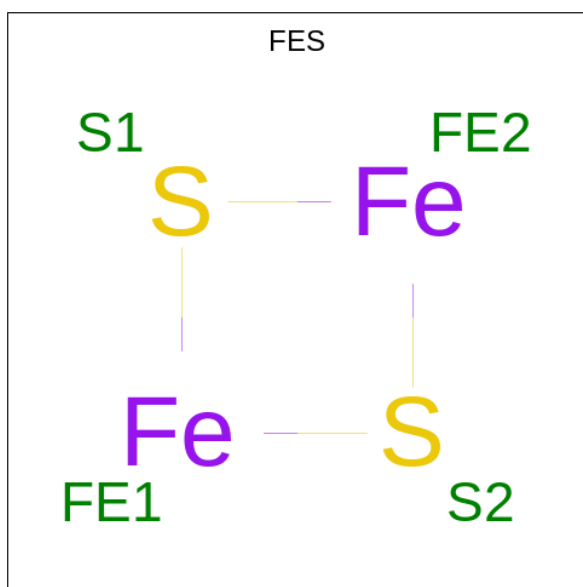
Mol	Chain	Residues	Atoms			AltConf
17	N	1	Total	C	O	0
			116	112	4	
17	N	1	Total	C	O	0
			116	112	4	
17	O	1	Total	C	O	0
			106	102	4	
17	O	1	Total	C	O	0
			106	102	4	
17	B	1	Total	C	O	0
			101	97	4	
17	B	1	Total	C	O	0
			101	97	4	
17	A	1	Total	C	O	0
			43	41	2	
17	C	1	Total	C	O	0
			48	46	2	

- Molecule 18 is 5-methoxy-2-methyl- {N}-[[4-[4-(trifluoromethoxy)phenyl]piperidin-1-yl]phenyl)methyl]pyrazolo[1,5-a]pyridine-3-carboxamide (three-letter code: HV0) (formula: C<sub>29</sub>H<sub>29</sub>F<sub>3</sub>N<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



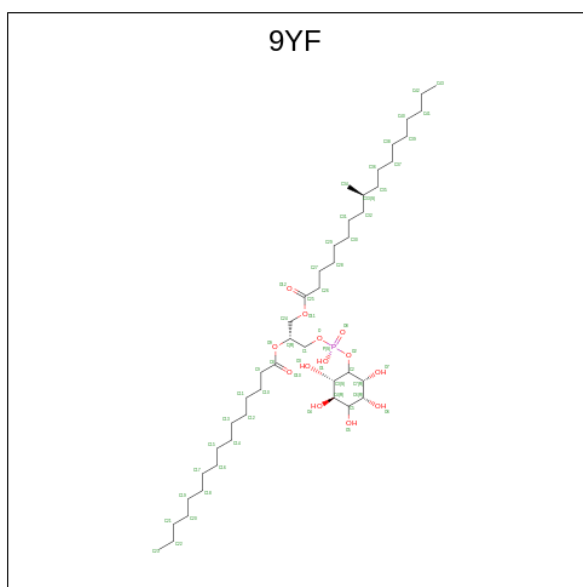
Mol	Chain	Residues	Atoms					AltConf
18	N	1	Total	C	F	N	O	0
			39	29	3	4	3	
18	B	1	Total	C	F	N	O	0
			39	29	3	4	3	

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
19	M	1	4	2	2	0
19	A	1	4	2	2	0

- 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 (three-letter code: 9YF) (formula: C<sub>44</sub>H<sub>85</sub>O<sub>13</sub>P).



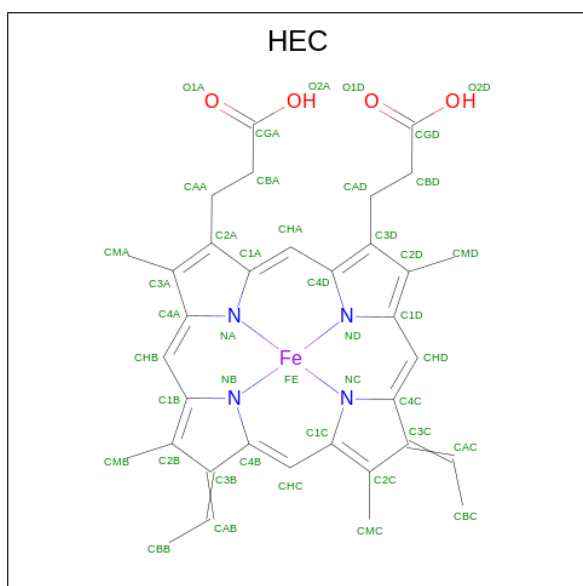
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	M	1	84	56	26	2	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	M	1	Total 84	C 56	O 26	P 2	0
20	A	1	Total 93	C 65	O 26	P 2	0
20	A	1	Total 93	C 65	O 26	P 2	0

- Molecule 21 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).

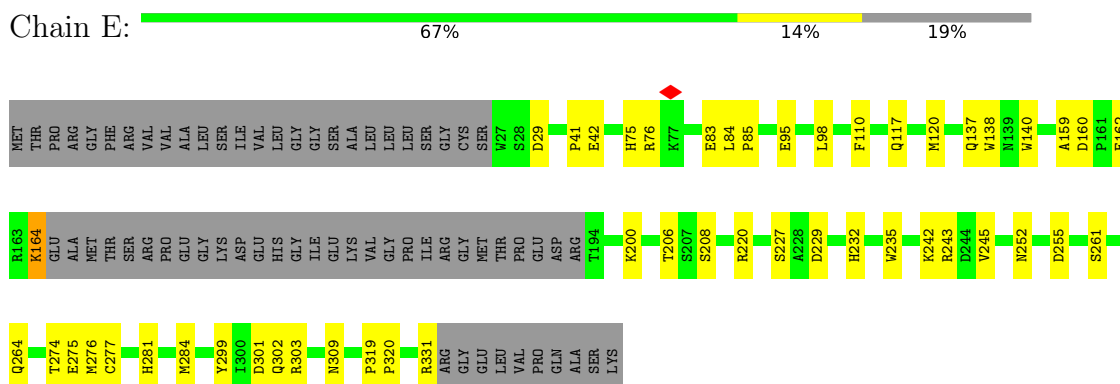


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
21	O	1	Total 86	C 68	Fe 2	N 8	O 8	0
21	O	1	Total 86	C 68	Fe 2	N 8	O 8	0
21	C	1	Total 86	C 68	Fe 2	N 8	O 8	0
21	C	1	Total 86	C 68	Fe 2	N 8	O 8	0

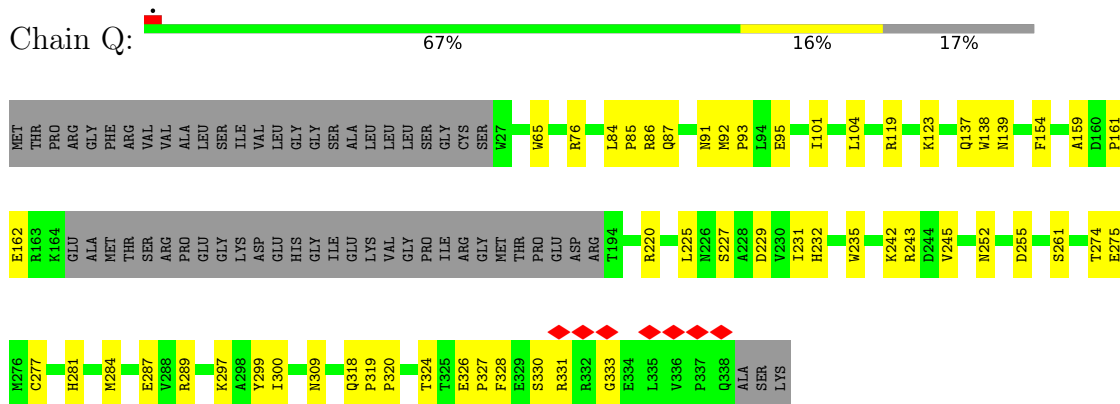
### 3 Residue-property plots [i](#)

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

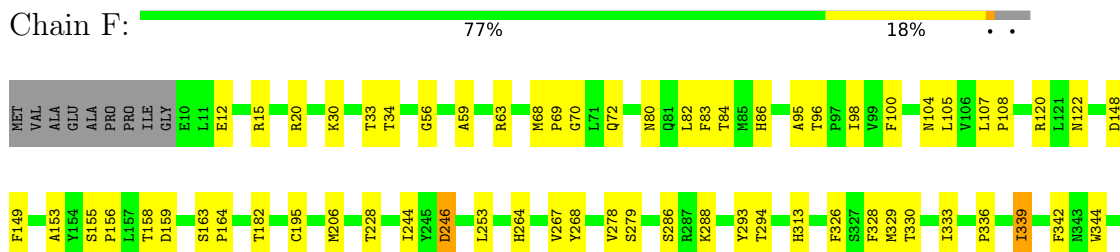
- Molecule 1: Cytochrome c oxidase subunit 2

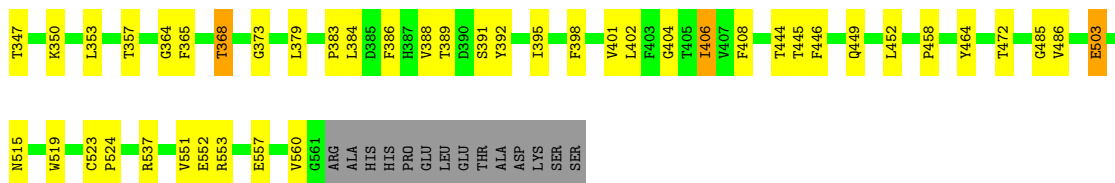


- Molecule 1: Cytochrome c oxidase subunit 2

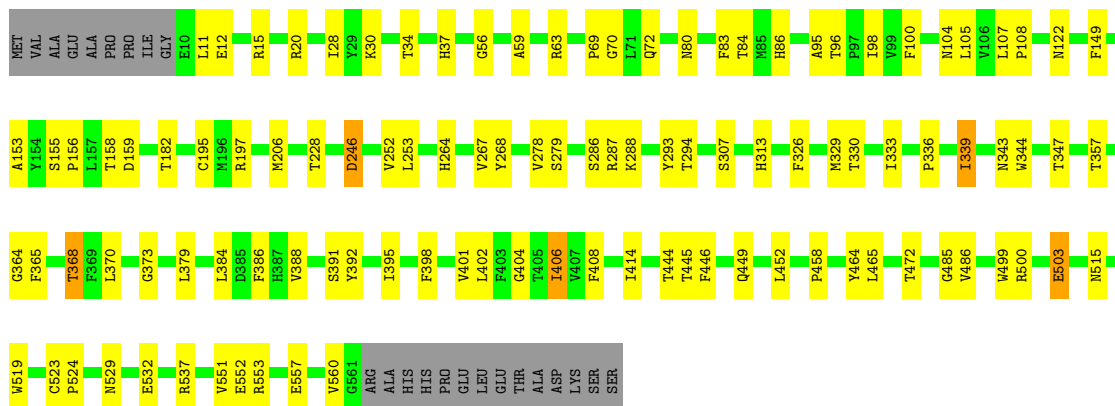
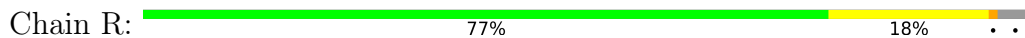


- Molecule 2: Cytochrome c oxidase subunit 1

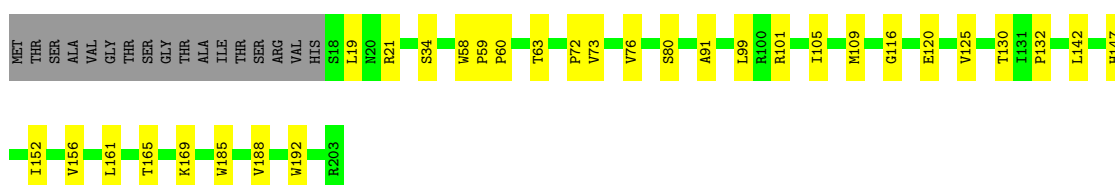
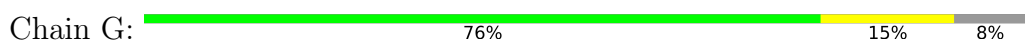




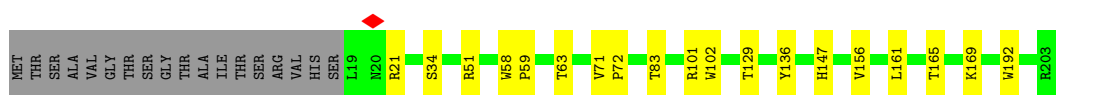
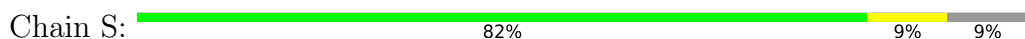
• Molecule 2: Cytochrome c oxidase subunit 1



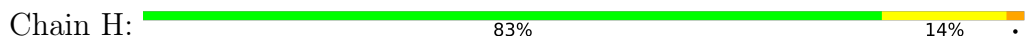
• Molecule 3: Cytochrome c oxidase subunit 3




• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 4: Cytochrome c oxidase polypeptide 4



• Molecule 4: Cytochrome c oxidase polypeptide 4

Chain T:  82% 16%



- Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain I:  53% 29% 15%



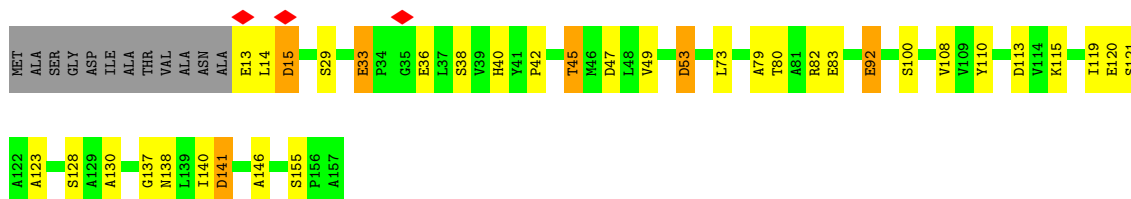
- Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain U:  54% 29% 15%



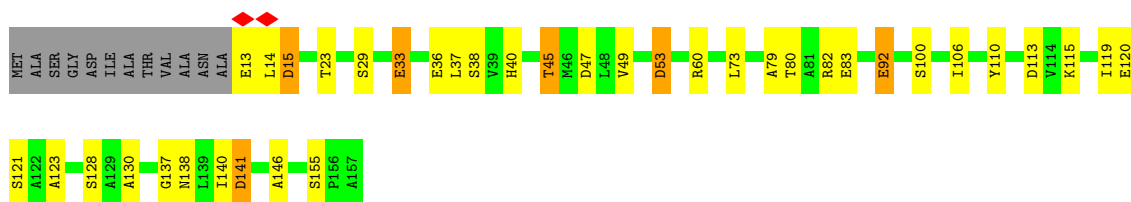
- Molecule 6: Uncharacterized protein MSMEG\_4692/MSMEI\_4575

Chain J:  69% 19% 8%



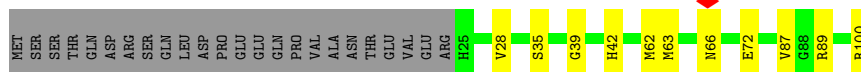
- Molecule 6: Uncharacterized protein MSMEG\_4692/MSMEI\_4575

Chain V:  68% 20% 8%



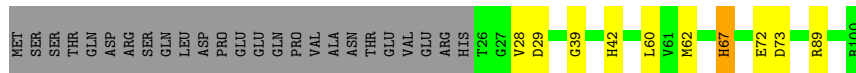
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain D:  65% 11% 24%

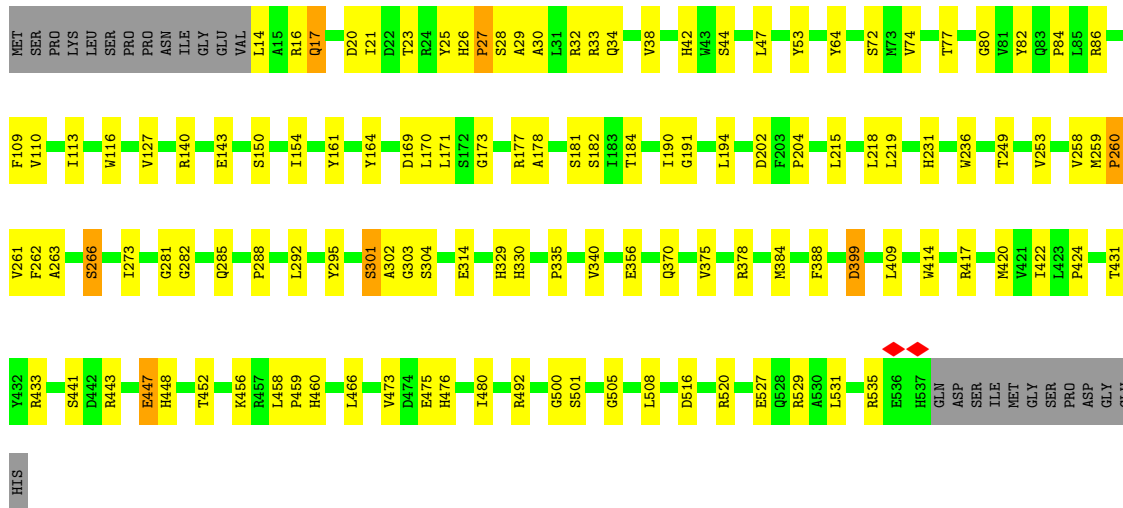


- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

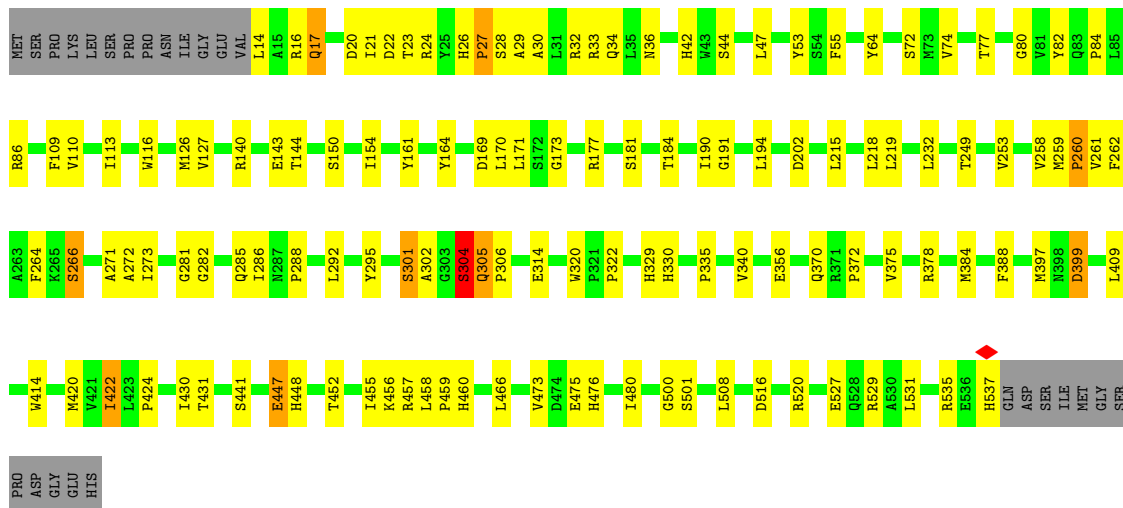




• Molecule 8: Cytochrome bc1 complex cytochrome b subunit

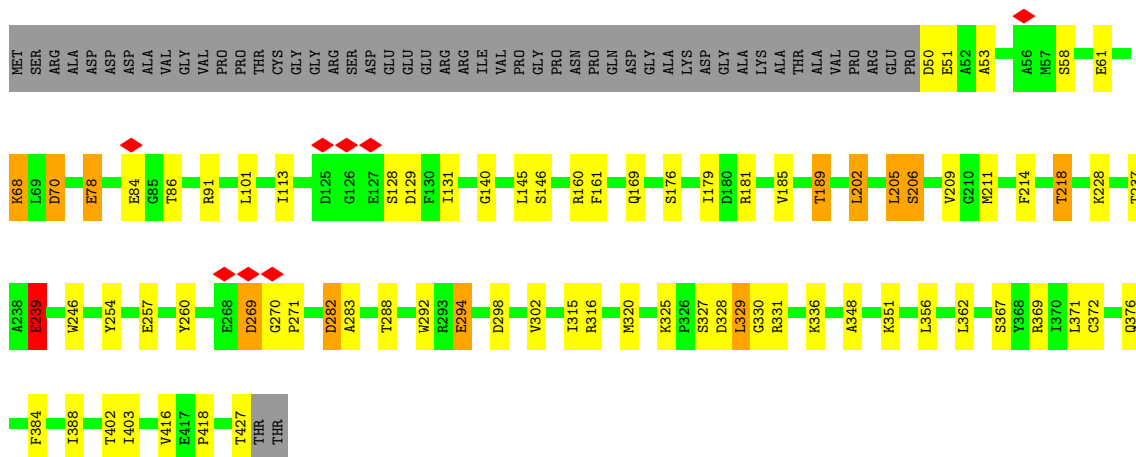


• Molecule 8: Cytochrome bc1 complex cytochrome b subunit

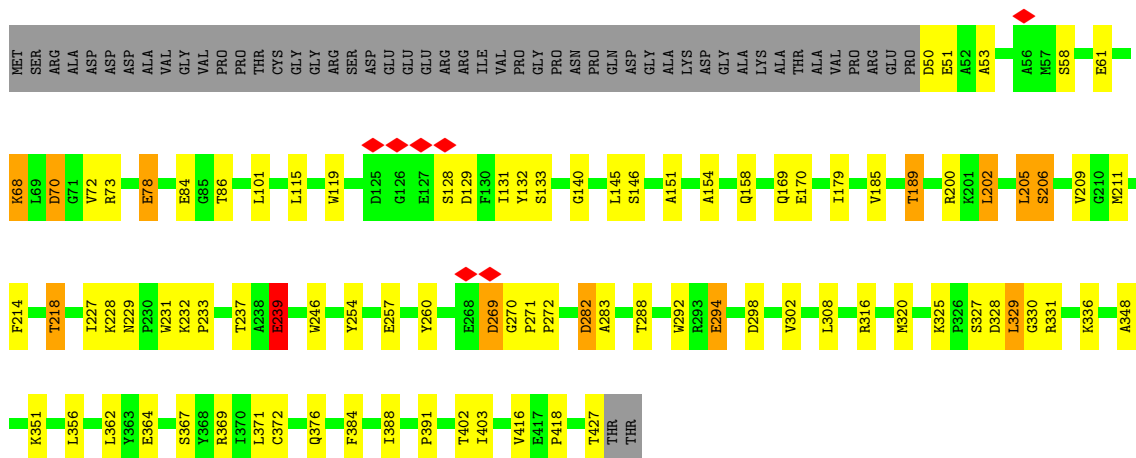


• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit





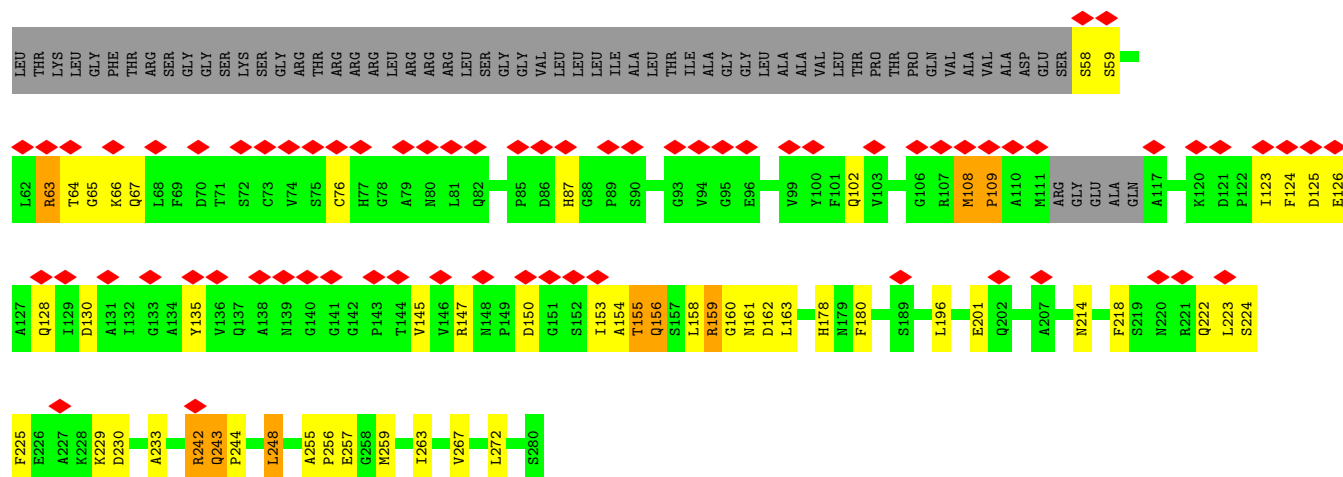
• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit



• 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	169988	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	3.778	Depositor
Minimum map value	-2.364	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, FES, HV0, HEC, MQ9, 9Y0, CDL, 9YF, CU, PLM, 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	0.30	0/2254	0.46	0/3072
1	Q	0.32	0/2306	0.47	0/3144
2	F	0.34	0/4533	0.48	0/6192
2	R	0.34	0/4533	0.48	0/6192
3	G	0.34	0/1502	0.49	0/2051
3	S	0.35	0/1496	0.48	0/2043
4	H	0.33	0/1112	0.47	0/1524
4	T	0.33	0/1112	0.47	0/1524
5	I	0.29	0/523	0.58	0/714
5	U	0.29	0/523	0.58	0/714
6	J	0.36	0/1059	0.56	0/1446
6	V	0.36	0/1059	0.56	0/1446
7	D	0.27	0/626	0.43	0/852
7	P	0.29	0/617	0.50	1/840 (0.1%)
8	B	0.34	0/4276	0.57	3/5833 (0.1%)
8	N	0.34	0/4276	0.50	2/5833 (0.0%)
9	A	0.33	0/3020	0.51	1/4094 (0.0%)
9	M	0.33	0/3020	0.51	1/4094 (0.0%)
10	C	0.36	0/1616	0.63	2/2188 (0.1%)
10	O	0.35	0/1654	0.59	0/2239
All	All	0.34	0/41117	0.51	10/56035 (0.0%)

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
10	C	0	1
10	O	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	304	SER	CB-CA-C	19.74	147.60	110.10
8	B	305	GLN	N-CA-CB	11.54	131.37	110.60
8	N	304	SER	N-CA-CB	-8.57	97.65	110.50
8	N	303	GLY	N-CA-C	-8.45	91.98	113.10
8	B	304	SER	N-CA-C	-6.65	93.05	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	C	108	MET	Peptide
10	O	108	MET	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	40	0
1	Q	2242	0	2175	43	0
2	F	4373	0	4347	68	0
2	R	4373	0	4347	84	0
3	G	1455	0	1455	21	0
3	S	1449	0	1450	15	0
4	H	1077	0	1058	12	0
4	T	1077	0	1058	14	0
5	I	507	0	516	11	0
5	U	507	0	516	11	0
6	J	1041	0	1052	21	0
6	V	1041	0	1052	23	0
7	D	605	0	587	9	0
7	P	597	0	586	9	0
8	B	4140	0	4163	85	0
8	N	4140	0	4165	72	0
9	A	2943	0	2931	83	0
9	M	2943	0	2931	60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	1584	0	1562	49	0
10	O	1621	0	1598	40	0
11	E	2	0	0	0	0
11	F	2	0	0	0	0
11	Q	2	0	0	0	0
11	R	2	0	0	0	0
12	A	95	0	143	5	0
12	B	375	0	476	13	0
12	D	88	0	126	6	0
12	F	157	0	208	3	0
12	M	95	0	143	1	0
12	N	230	0	295	9	0
12	O	79	0	105	2	0
12	P	88	0	126	7	0
12	R	157	0	208	5	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	104	14	0
14	R	120	0	104	14	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	A	43	0	53	6	0
17	B	101	0	133	14	0
17	C	48	0	61	5	0
17	N	116	0	158	8	0
17	O	106	0	141	8	0
18	B	39	0	0	0	0
18	N	39	0	0	0	0
19	A	4	0	0	3	0
19	M	4	0	0	2	0
20	A	93	0	0	24	0
20	M	84	0	0	10	0
21	C	86	0	62	3	0
21	O	86	0	58	1	0
All	All	42679	0	42590	742	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 9.

The worst 5 of 742 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)
10:C:76:CYS:CB	21:C:301:HEC:HBC2	1.30	1.54
2:R:264:HIS:NE2	2:R:268:TYR:CE2	2.06	1.24
10:C:76:CYS:CB	21:C:301:HEC:CBC	2.18	1.20
2:R:268:TYR:OH	2:R:333:ILE:HD13	1.38	1.17
2:R:268:TYR:CD2	2:R:307:SER:HB2	1.82	1.15

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%)	243 (89%)	28 (10%)	1 (0%)	34	64
1	Q	279/341 (82%)	246 (88%)	33 (12%)	0	100	100
2	F	550/575 (96%)	517 (94%)	33 (6%)	0	100	100
2	R	550/575 (96%)	518 (94%)	32 (6%)	0	100	100
3	G	184/203 (91%)	177 (96%)	7 (4%)	0	100	100
3	S	183/203 (90%)	176 (96%)	7 (4%)	0	100	100
4	H	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
4	T	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
5	I	63/79 (80%)	59 (94%)	4 (6%)	0	100	100
5	U	63/79 (80%)	59 (94%)	4 (6%)	0	100	100
6	J	143/157 (91%)	134 (94%)	9 (6%)	0	100	100
6	V	143/157 (91%)	134 (94%)	9 (6%)	0	100	100
7	D	74/100 (74%)	71 (96%)	3 (4%)	0	100	100
7	P	73/100 (73%)	71 (97%)	2 (3%)	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	B	522/549 (95%)	475 (91%)	41 (8%)	6 (1%)	14	40
8	N	522/549 (95%)	477 (91%)	41 (8%)	4 (1%)	19	49
9	A	376/429 (88%)	334 (89%)	39 (10%)	3 (1%)	19	49
9	M	376/429 (88%)	336 (89%)	37 (10%)	3 (1%)	19	49
10	C	214/280 (76%)	182 (85%)	29 (14%)	3 (1%)	11	34
10	O	221/280 (79%)	186 (84%)	30 (14%)	5 (2%)	6	22
All	All	5082/5704 (89%)	4655 (92%)	402 (8%)	25 (0%)	32	60

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	N	28	SER
9	M	329	LEU
8	B	28	SER
9	A	329	LEU
10	C	155	THR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	231/288 (80%)	230 (100%)	1 (0%)	91	97
1	Q	236/288 (82%)	235 (100%)	1 (0%)	91	97
2	F	453/471 (96%)	432 (95%)	21 (5%)	27	57
2	R	453/471 (96%)	432 (95%)	21 (5%)	27	57
3	G	148/161 (92%)	148 (100%)	0	100	100
3	S	147/161 (91%)	147 (100%)	0	100	100
4	H	106/106 (100%)	94 (89%)	12 (11%)	6	17
4	T	106/106 (100%)	94 (89%)	12 (11%)	6	17
5	I	52/59 (88%)	37 (71%)	15 (29%)	0	1
5	U	52/59 (88%)	37 (71%)	15 (29%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	107/114 (94%)	90 (84%)	17 (16%)	2	7
6	V	107/114 (94%)	90 (84%)	17 (16%)	2	7
7	D	59/83 (71%)	58 (98%)	1 (2%)	60	83
7	P	59/83 (71%)	59 (100%)	0	100	100
8	B	424/446 (95%)	401 (95%)	23 (5%)	22	51
8	N	424/446 (95%)	401 (95%)	23 (5%)	22	51
9	A	304/343 (89%)	279 (92%)	25 (8%)	11	31
9	M	304/343 (89%)	280 (92%)	24 (8%)	12	32
10	C	158/207 (76%)	146 (92%)	12 (8%)	13	35
10	O	162/207 (78%)	150 (93%)	12 (7%)	13	36
All	All	4092/4556 (90%)	3840 (94%)	252 (6%)	22	45

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	U	78	LYS
9	A	101	LEU
8	N	301	SER
9	A	84	GLU
9	A	288	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	104	ASN
10	C	87	HIS
3	S	186	HIS
10	C	67	GLN
8	B	36	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	9YF	M	504	-	40,40,58	1.01	3 (7%)	50,52,71	1.38	7 (14%)
14	HEA	R	606	2	57,67,67	2.53	30 (52%)	61,103,103	3.10	31 (50%)
16	HEM	N	602	8	41,50,50	1.47	4 (9%)	45,82,82	1.40	6 (13%)
12	CDL	P	201	-	87,87,99	1.07	6 (6%)	93,99,111	0.94	4 (4%)
12	CDL	N	605	-	76,76,99	1.13	7 (9%)	82,88,111	0.98	4 (4%)
14	HEA	F	607	2	57,67,67	2.56	30 (52%)	61,103,103	3.00	32 (52%)
16	HEM	B	602	8	41,50,50	1.46	4 (9%)	45,82,82	1.40	7 (15%)
20	9YF	A	503	-	51,51,58	0.95	5 (9%)	62,64,71	1.01	4 (6%)
21	HEC	C	302	10	32,50,50	2.22	3 (9%)	24,82,82	1.51	4 (16%)
12	CDL	B	603	-	78,78,99	1.14	8 (10%)	84,90,111	0.99	4 (4%)
17	MQ9	O	303	-	59,59,59	3.87	18 (30%)	72,75,75	3.38	33 (45%)
12	CDL	D	201	-	87,87,99	1.07	6 (6%)	93,99,111	0.96	4 (4%)
17	MQ9	A	502	-	44,44,59	3.90	15 (34%)	54,57,75	3.22	24 (44%)
17	MQ9	N	607	-	59,59,59	3.94	18 (30%)	72,75,75	3.30	31 (43%)
17	MQ9	C	303	-	49,49,59	3.96	16 (32%)	60,63,75	3.16	26 (43%)
19	FES	A	501	9	0,4,4	-	-	-	-	-
20	9YF	M	503	-	44,44,58	0.99	4 (9%)	55,57,71	1.10	5 (9%)
12	CDL	B	606	-	73,73,99	1.16	7 (9%)	79,85,111	1.01	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CDL	R	602	-	80,80,99	1.11	7 (8%)	86,92,111	0.97	4 (4%)
12	CDL	F	602	-	80,80,99	1.11	7 (8%)	86,92,111	0.97	4 (4%)
13	PLM	B	604	-	10,10,17	0.62	0	9,9,17	0.55	0
16	HEM	B	601	8	41,49,50	1.24	2 (4%)	46,81,82	1.26	4 (8%)
19	FES	M	501	9	0,4,4	-	-	-	-	-
17	MQ9	B	610	-	59,59,59	3.86	18 (30%)	72,75,75	3.40	33 (45%)
18	HV0	B	611	-	39,43,43	2.04	8 (20%)	50,62,62	1.94	5 (10%)
15	9Y0	S	301	-	42,42,48	0.95	4 (9%)	44,47,53	0.91	2 (4%)
12	CDL	B	605	-	65,65,99	1.22	8 (12%)	71,77,111	0.98	4 (5%)
12	CDL	N	606	-	78,78,99	1.11	8 (10%)	84,90,111	0.99	4 (4%)
14	HEA	F	606	2	57,67,67	2.54	30 (52%)	61,103,103	3.10	31 (50%)
14	HEA	R	607	2	57,67,67	2.56	30 (52%)	61,103,103	2.99	32 (52%)
12	CDL	N	604	-	73,73,99	1.16	7 (9%)	79,85,111	1.03	4 (5%)
20	9YF	A	505	-	42,42,58	1.03	4 (9%)	52,54,71	1.27	6 (11%)
12	CDL	A	504	-	94,94,99	1.05	7 (7%)	100,106,111	0.91	4 (4%)
13	PLM	F	603	-	16,16,17	0.56	0	15,15,17	0.42	0
12	CDL	B	608	-	78,78,99	1.12	7 (8%)	84,90,111	1.03	4 (4%)
12	CDL	R	601	-	75,75,99	1.14	7 (9%)	81,87,111	1.00	4 (4%)
17	MQ9	O	302	-	49,49,59	3.90	16 (32%)	60,63,75	3.25	25 (41%)
17	MQ9	N	608	-	59,59,59	3.96	19 (32%)	72,75,75	3.33	33 (45%)
12	CDL	F	601	-	75,75,99	1.14	7 (9%)	81,87,111	1.00	4 (4%)
17	MQ9	B	609	-	44,44,59	3.89	15 (34%)	54,57,75	3.16	22 (40%)
21	HEC	O	304	10	32,50,50	2.27	3 (9%)	24,82,82	1.31	2 (8%)
21	HEC	O	305	10	32,50,50	2.24	3 (9%)	24,82,82	1.53	4 (16%)
13	PLM	R	603	-	16,16,17	0.56	0	15,15,17	0.42	0
12	CDL	B	607	-	76,76,99	1.13	7 (9%)	82,88,111	1.03	4 (4%)
12	CDL	M	502	-	94,94,99	1.05	7 (7%)	100,106,111	0.85	4 (4%)
13	PLM	N	603	-	10,10,17	0.62	0	9,9,17	0.55	0
18	HV0	N	609	-	39,43,43	2.03	8 (20%)	50,62,62	2.07	11 (22%)
21	HEC	C	301	10	32,50,50	2.29	3 (9%)	24,82,82	1.32	2 (8%)
16	HEM	N	601	8	41,49,50	1.23	2 (4%)	46,81,82	1.25	4 (8%)
15	9Y0	G	301	-	42,42,48	0.94	4 (9%)	44,47,53	0.91	2 (4%)
12	CDL	O	301	-	78,78,99	1.12	7 (8%)	84,90,111	0.97	5 (5%)

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	9YF	M	504	-	-	18/35/59/78	0/1/1/1
14	HEA	R	606	2	3/3/7/16	14/32/76/76	-
16	HEM	N	602	8	-	2/12/54/54	-
14	HEA	F	607	2	3/3/7/16	16/32/76/76	-
12	CDL	P	201	-	-	63/98/98/110	-
12	CDL	N	605	-	-	40/87/87/110	-
16	HEM	B	602	8	-	2/12/54/54	-
20	9YF	A	503	-	-	30/47/71/78	0/1/1/1
21	HEC	C	302	10	-	0/10/54/54	-
12	CDL	B	603	-	-	53/89/89/110	-
17	MQ9	O	303	-	-	26/53/73/73	0/2/2/2
12	CDL	D	201	-	-	49/98/98/110	-
17	MQ9	A	502	-	-	21/35/55/73	0/2/2/2
17	MQ9	N	607	-	-	30/53/73/73	0/2/2/2
17	MQ9	C	303	-	-	24/41/61/73	0/2/2/2
19	FES	A	501	9	-	-	0/1/1/1
20	9YF	M	503	-	-	19/39/63/78	0/1/1/1
12	CDL	B	606	-	-	39/84/84/110	-
12	CDL	R	602	-	-	58/91/91/110	-
12	CDL	F	602	-	-	58/91/91/110	-
13	PLM	B	604	-	-	1/7/8/15	-
16	HEM	B	601	8	-	2/12/52/54	-
19	FES	M	501	9	-	-	0/1/1/1
17	MQ9	B	610	-	-	24/53/73/73	0/2/2/2
18	HV0	B	611	-	-	4/20/34/34	0/5/5/5
15	9Y0	S	301	-	-	29/46/46/52	-
12	CDL	B	605	-	-	48/76/76/110	-
14	HEA	R	607	2	3/3/7/16	16/32/76/76	-
14	HEA	F	606	2	3/3/7/16	14/32/76/76	-
12	CDL	N	606	-	-	46/89/89/110	-
12	CDL	N	604	-	-	51/84/84/110	-
20	9YF	A	505	-	-	15/37/61/78	0/1/1/1
12	CDL	A	504	-	-	57/105/105/110	-
13	PLM	F	603	-	-	5/13/14/15	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CDL	B	608	-	-	45/89/89/110	-
12	CDL	R	601	-	-	42/86/86/110	-
17	MQ9	O	302	-	-	26/41/61/73	0/2/2/2
17	MQ9	N	608	-	-	30/53/73/73	0/2/2/2
12	CDL	F	601	-	-	42/86/86/110	-
17	MQ9	B	609	-	-	20/35/55/73	0/2/2/2
21	HEC	O	304	10	-	7/10/54/54	-
21	HEC	O	305	10	-	0/10/54/54	-
13	PLM	R	603	-	-	4/13/14/15	-
12	CDL	B	607	-	-	38/87/87/110	-
12	CDL	M	502	-	-	65/105/105/110	-
13	PLM	N	603	-	-	1/7/8/15	-
18	HV0	N	609	-	-	4/20/34/34	0/5/5/5
21	HEC	C	301	10	-	7/10/54/54	-
16	HEM	N	601	8	-	1/12/52/54	-
15	9Y0	G	301	-	-	29/46/46/52	-
12	CDL	O	301	-	-	47/89/89/110	-

The worst 5 of 439 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	607	MQ9	C18-C19	9.34	1.55	1.33
17	C	303	MQ9	C23-C24	9.34	1.55	1.33
17	N	608	MQ9	C18-C19	9.29	1.55	1.33
17	N	608	MQ9	C33-C34	9.29	1.55	1.33
17	A	502	MQ9	C23-C24	9.28	1.55	1.33

The worst 5 of 497 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	608	MQ9	C7-C8-C9	-10.15	109.89	126.79
18	B	611	HV0	C25-C24-C27	-9.96	89.45	112.79
17	O	303	MQ9	C7-C8-C9	-9.88	110.34	126.79
17	B	610	MQ9	C7-C8-C9	-9.82	110.44	126.79
17	O	302	MQ9	C7-C8-C9	-9.82	110.45	126.79

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	F	606	HEA	ND
14	F	606	HEA	NA
14	F	606	HEA	NB
14	F	607	HEA	ND
14	F	607	HEA	NA

5 of 1282 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	601	CDL	CB2-OB2-PB2-OB3
12	F	601	CDL	OB5-CB3-CB4-OB6
12	F	602	CDL	CA3-OA5-PA1-OA4
12	F	602	CDL	CB3-OB5-PB2-OB3
12	F	602	CDL	CB3-OB5-PB2-OB4

There are no ring outliers.

40 monomers are involved in 169 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	M	504	9YF	4	0
14	R	606	HEA	6	0
16	N	602	HEM	3	0
12	P	201	CDL	7	0
12	N	605	CDL	5	0
14	F	607	HEA	8	0
16	B	602	HEM	5	0
20	A	503	9YF	6	0
12	B	603	CDL	4	0
17	O	303	MQ9	2	0
12	D	201	CDL	6	0
17	A	502	MQ9	6	0
17	N	607	MQ9	4	0
17	C	303	MQ9	5	0
19	A	501	FES	3	0
20	M	503	9YF	6	0
12	B	606	CDL	3	0
12	R	602	CDL	5	0
12	F	602	CDL	2	0
16	B	601	HEM	1	0
19	M	501	FES	2	0
17	B	610	MQ9	10	0
12	B	605	CDL	3	0
12	N	606	CDL	4	0

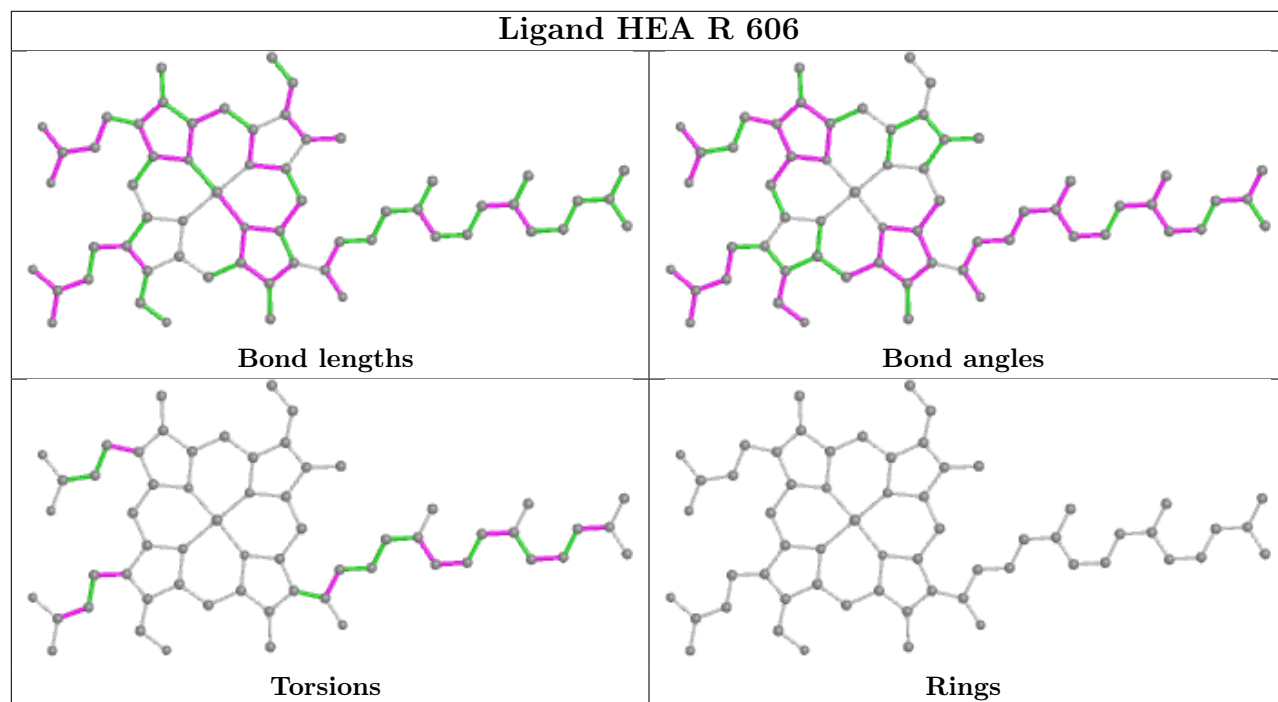
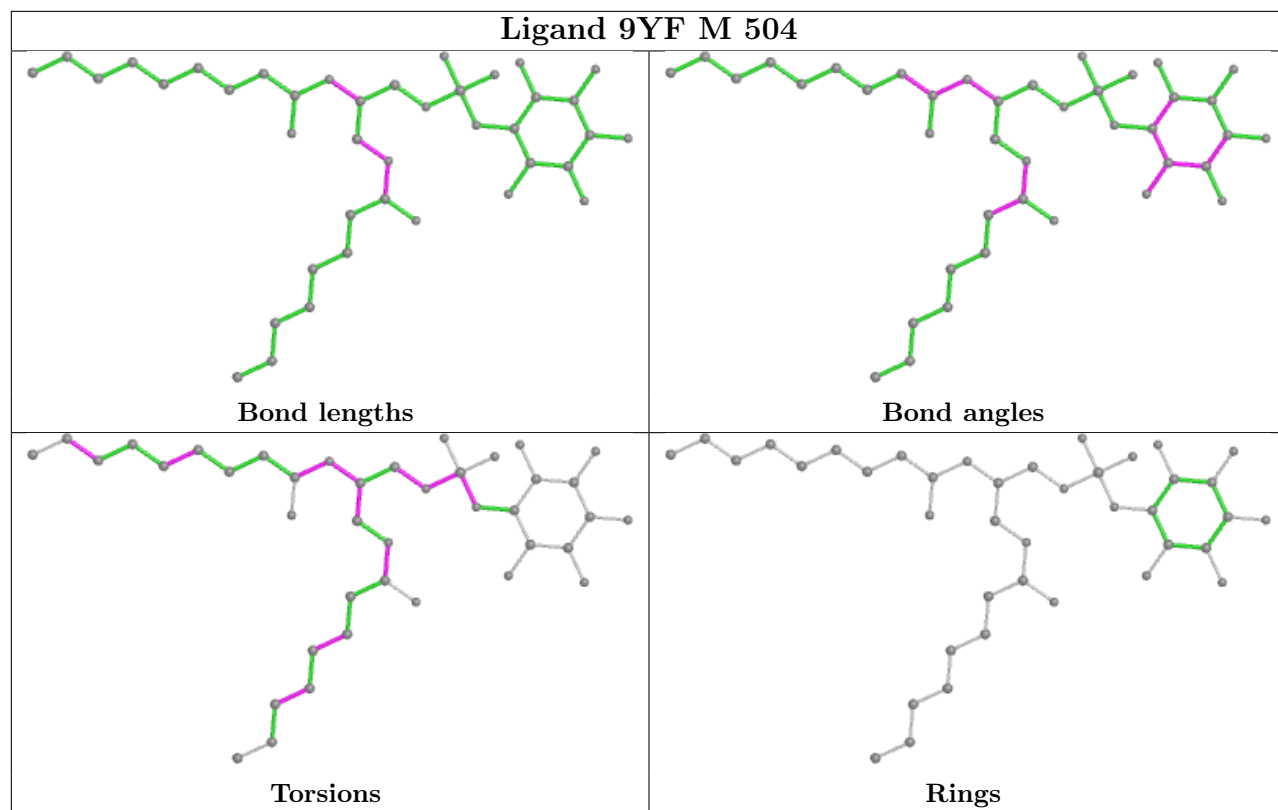
*Continued on next page...*

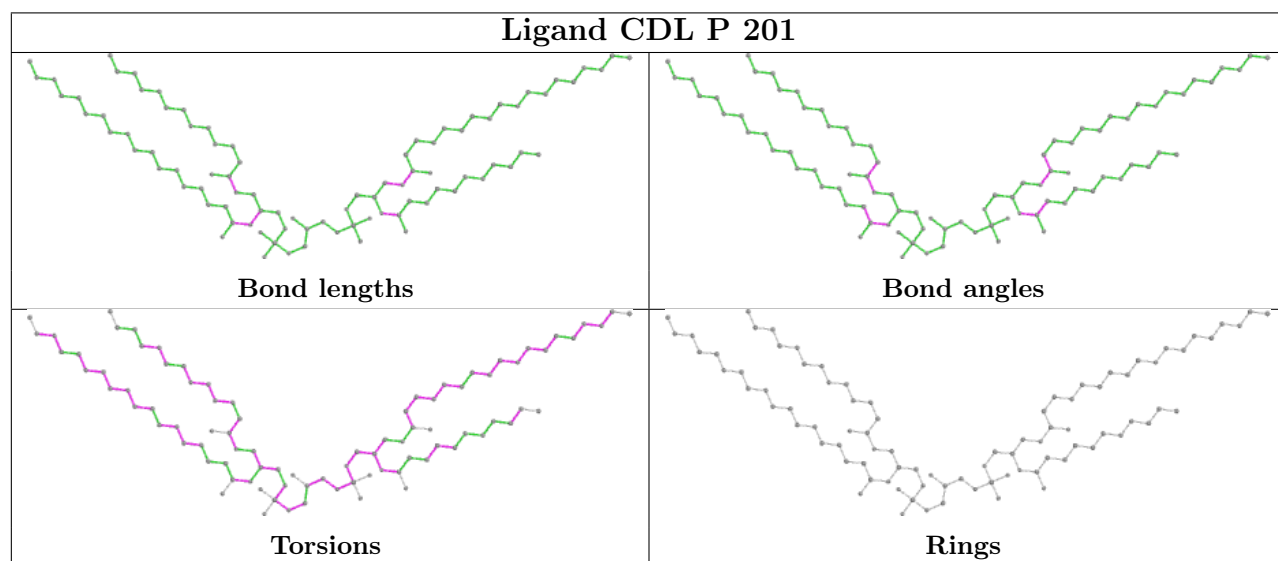
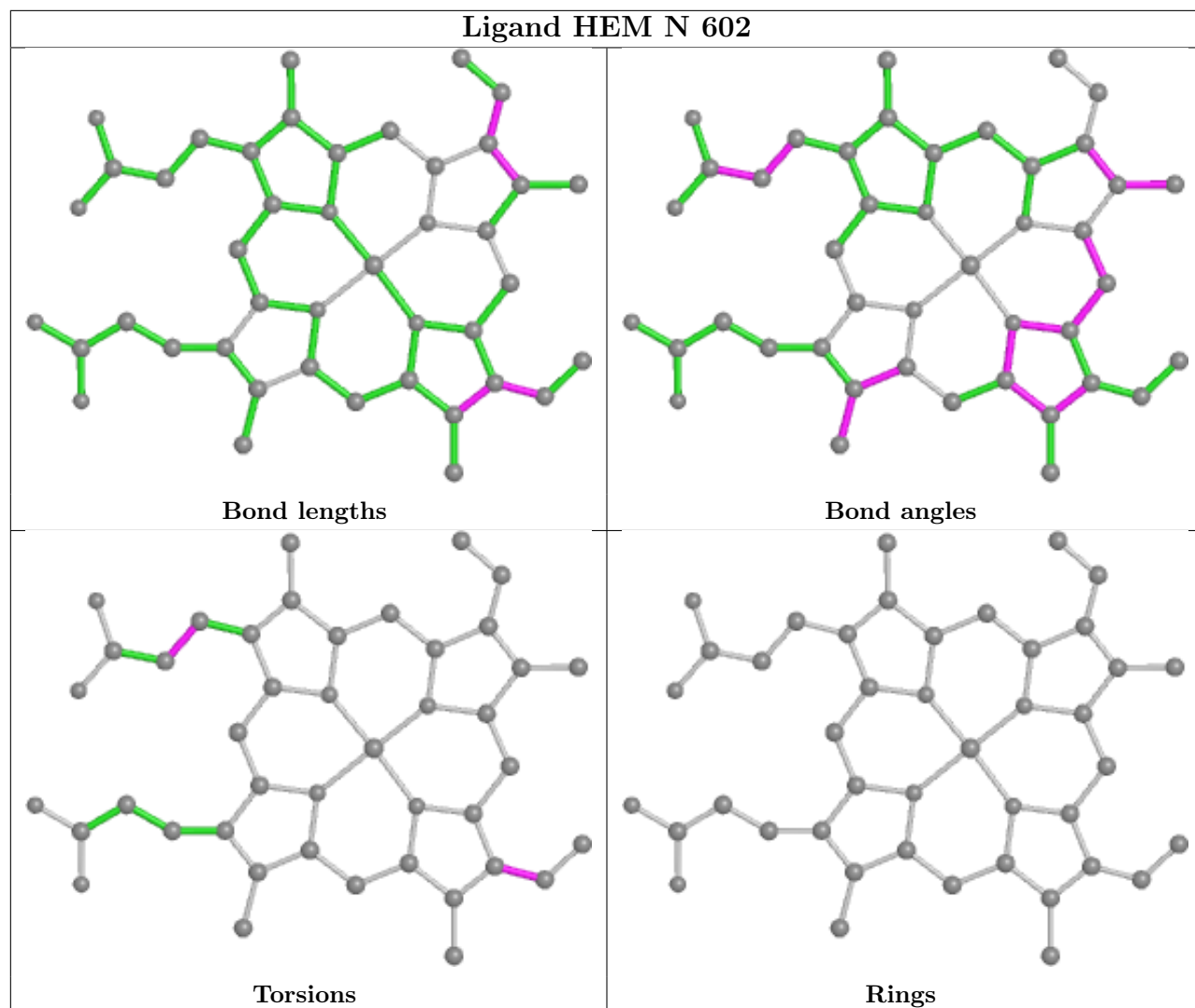
*Continued from previous page...*

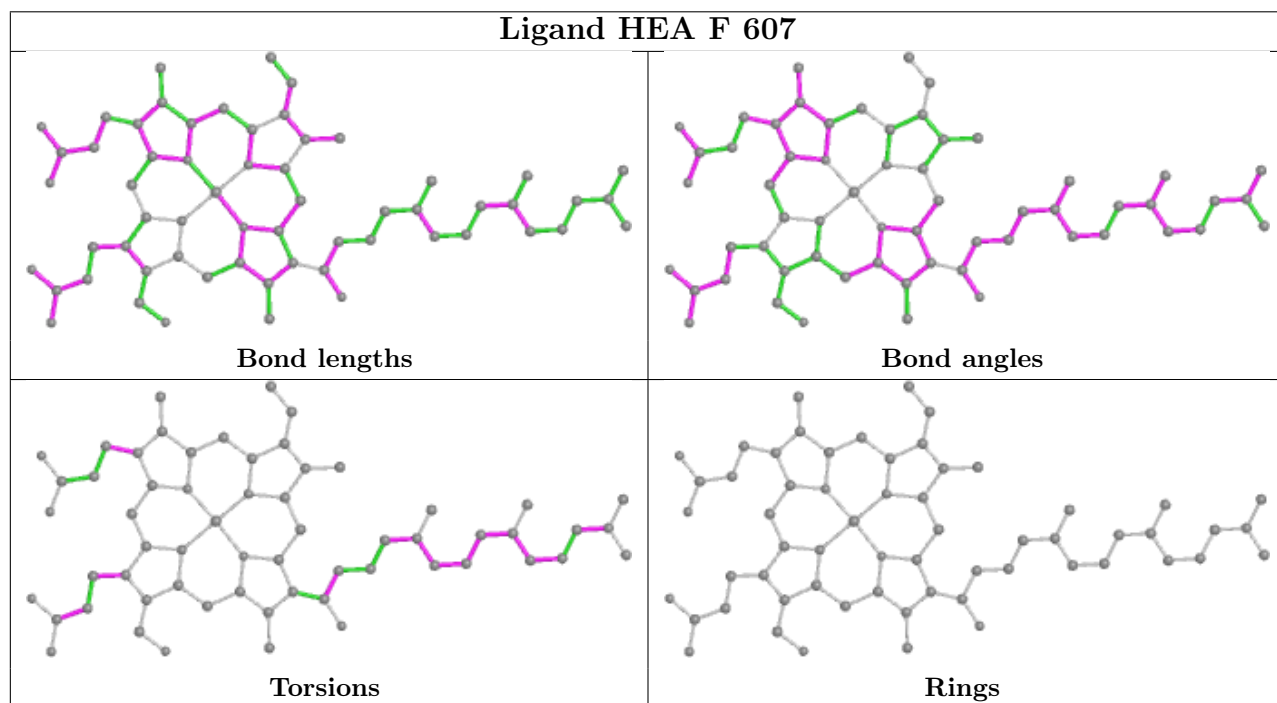
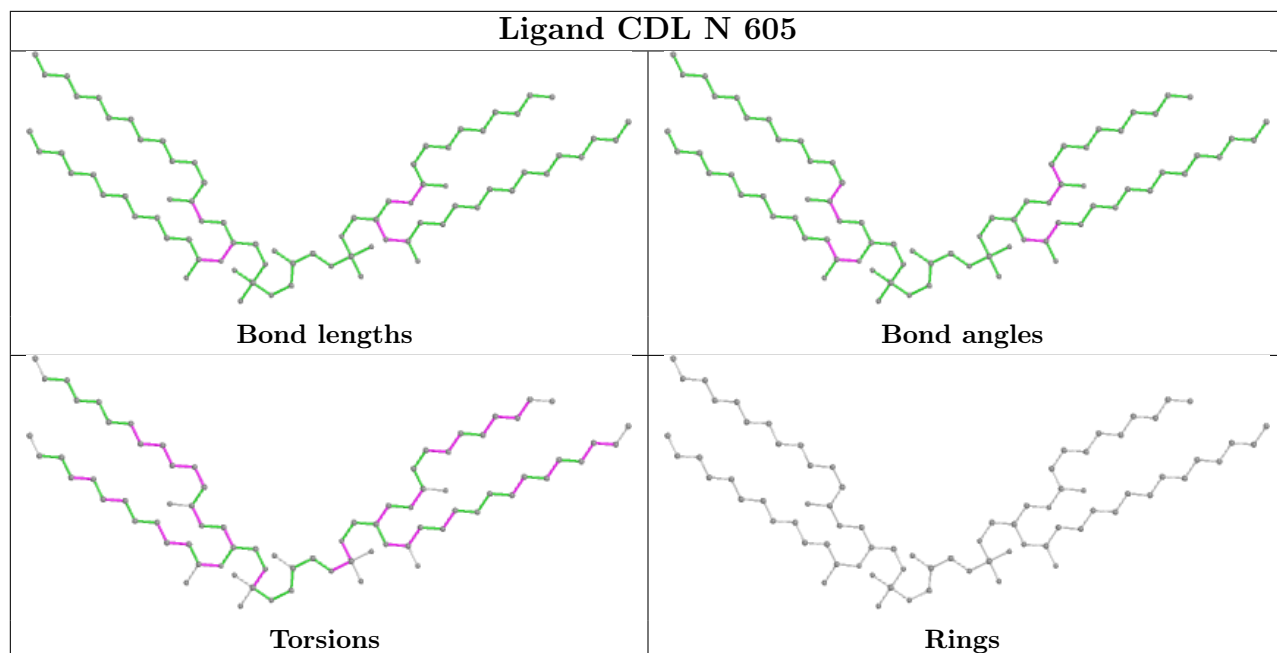
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	606	HEA	6	0
14	R	607	HEA	8	0
12	N	604	CDL	2	0
20	A	505	9YF	18	0
12	A	504	CDL	5	0
12	B	608	CDL	3	0
17	O	302	MQ9	6	0
17	N	608	MQ9	4	0
12	F	601	CDL	1	0
17	B	609	MQ9	4	0
21	O	304	HEC	1	0
12	B	607	CDL	2	0
12	M	502	CDL	1	0
21	C	301	HEC	3	0
16	N	601	HEM	2	0
12	O	301	CDL	2	0

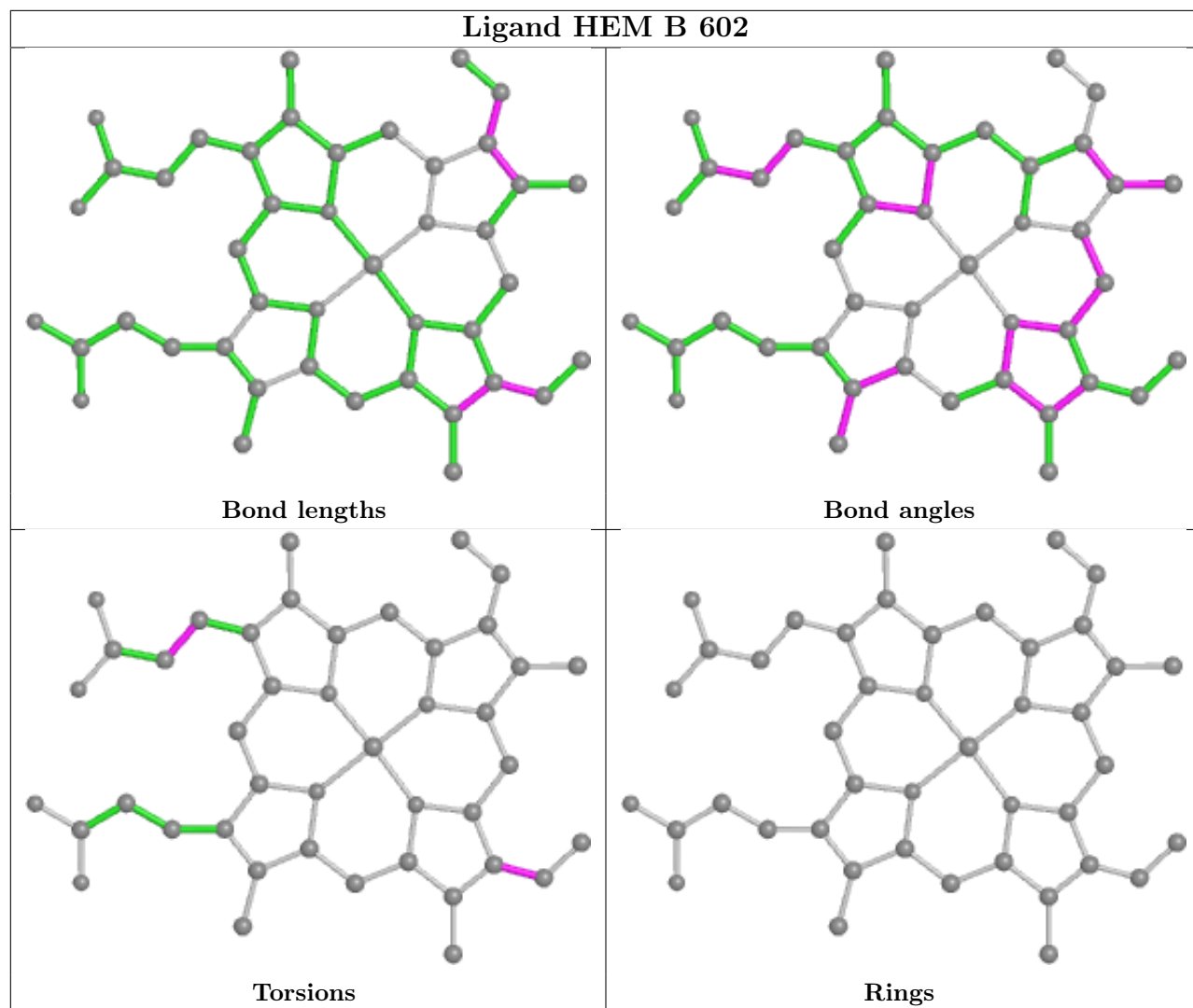
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

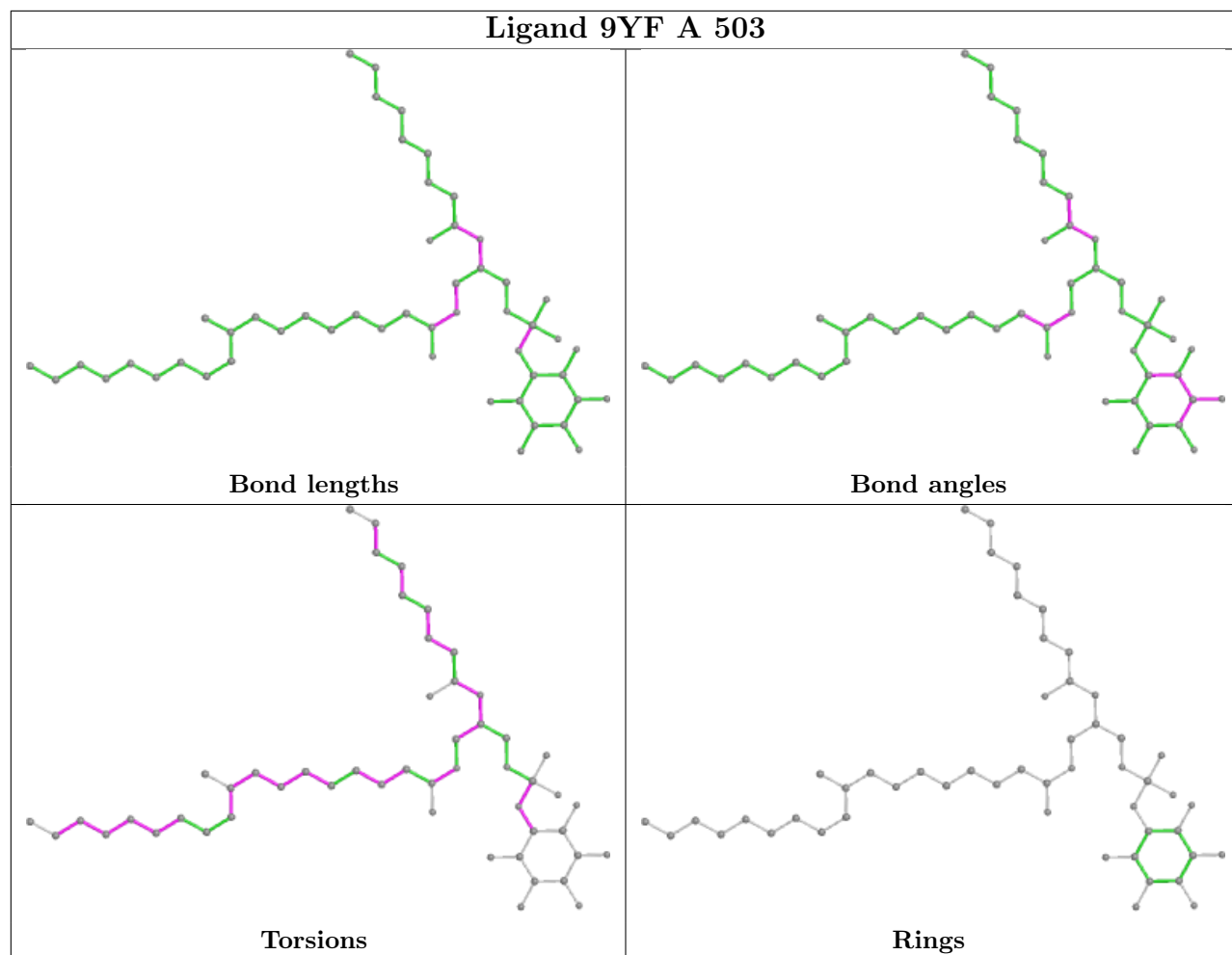


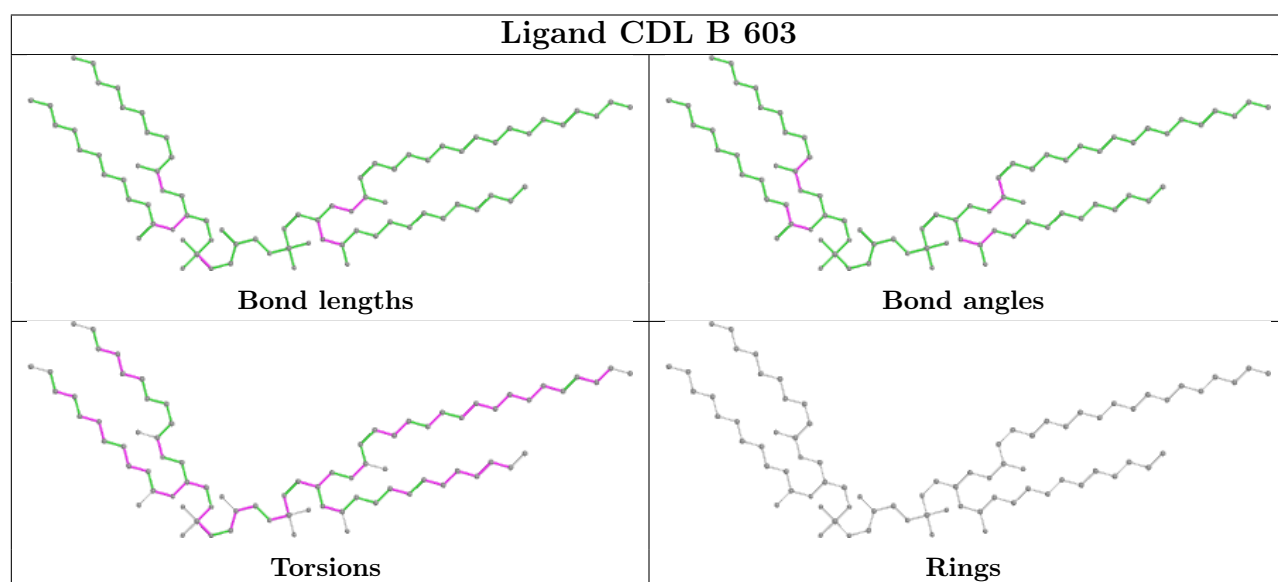
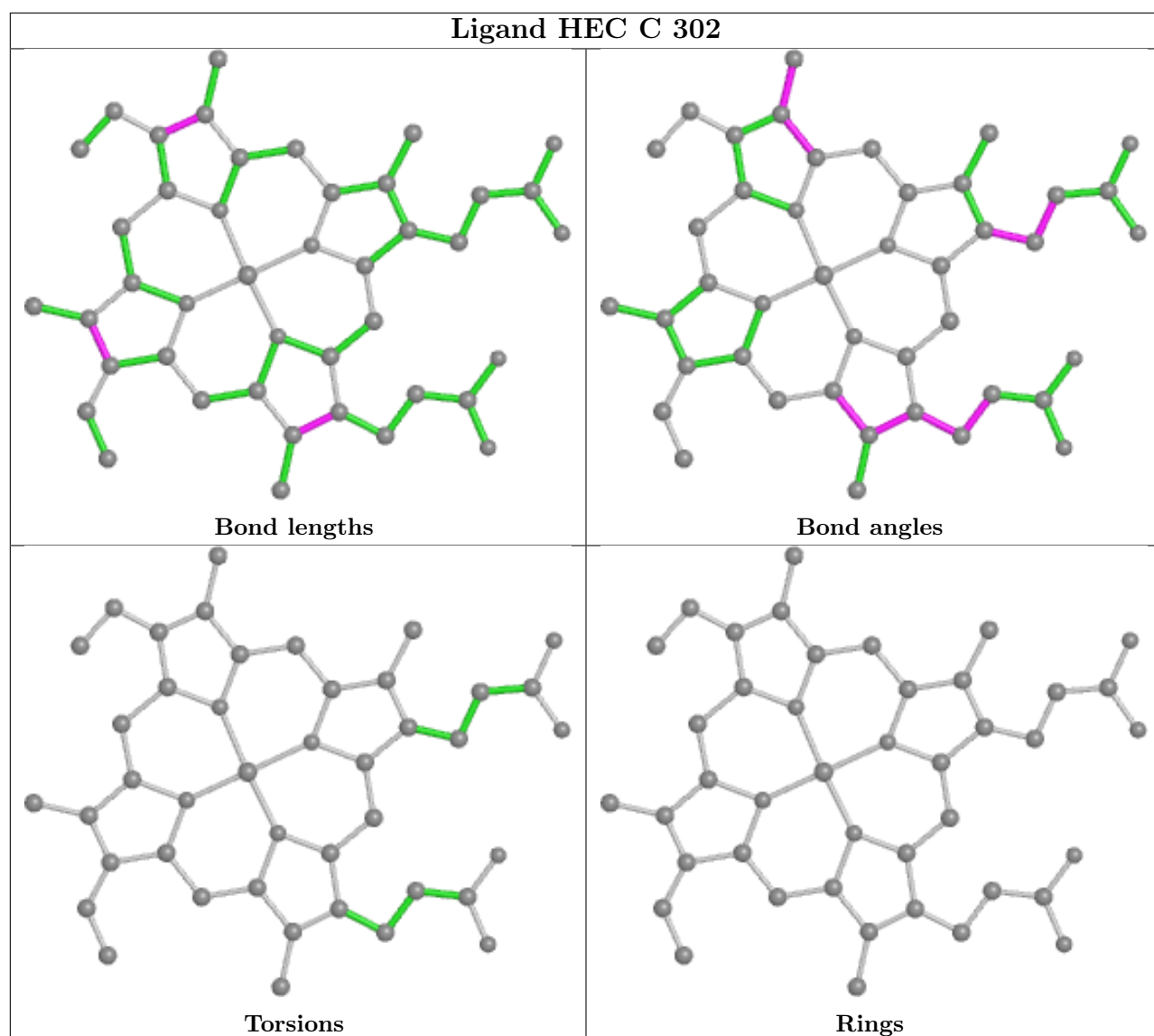


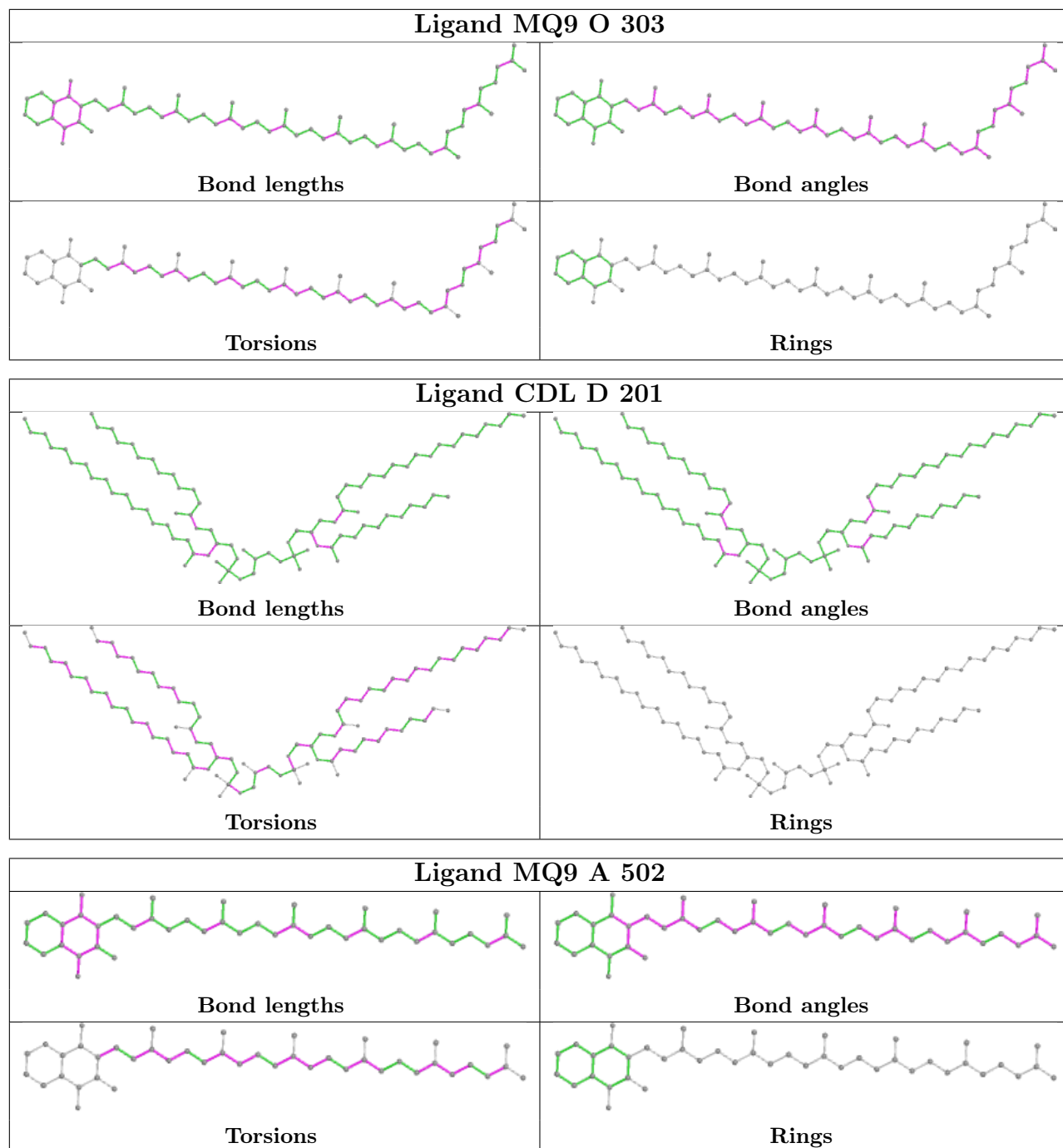


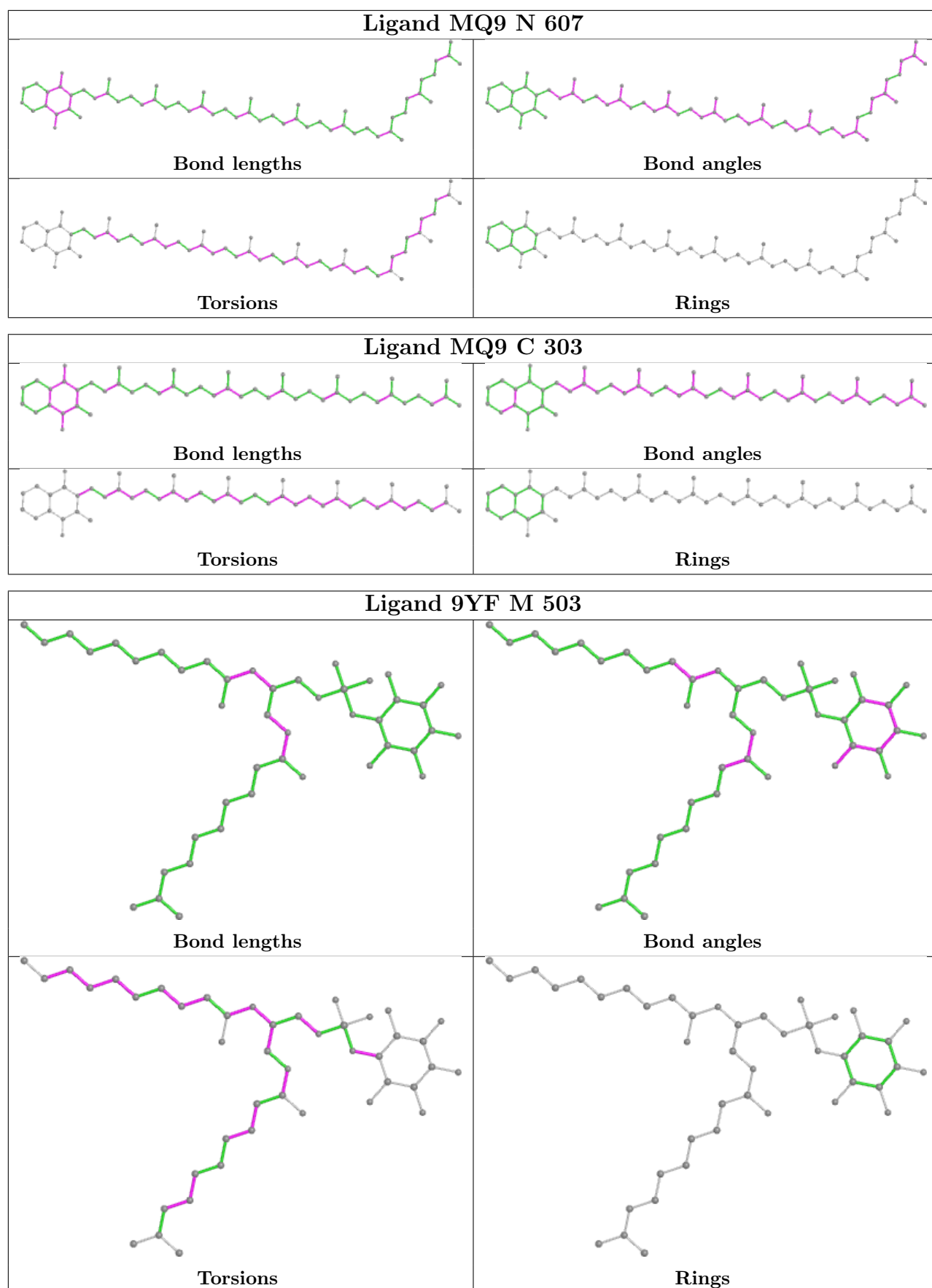




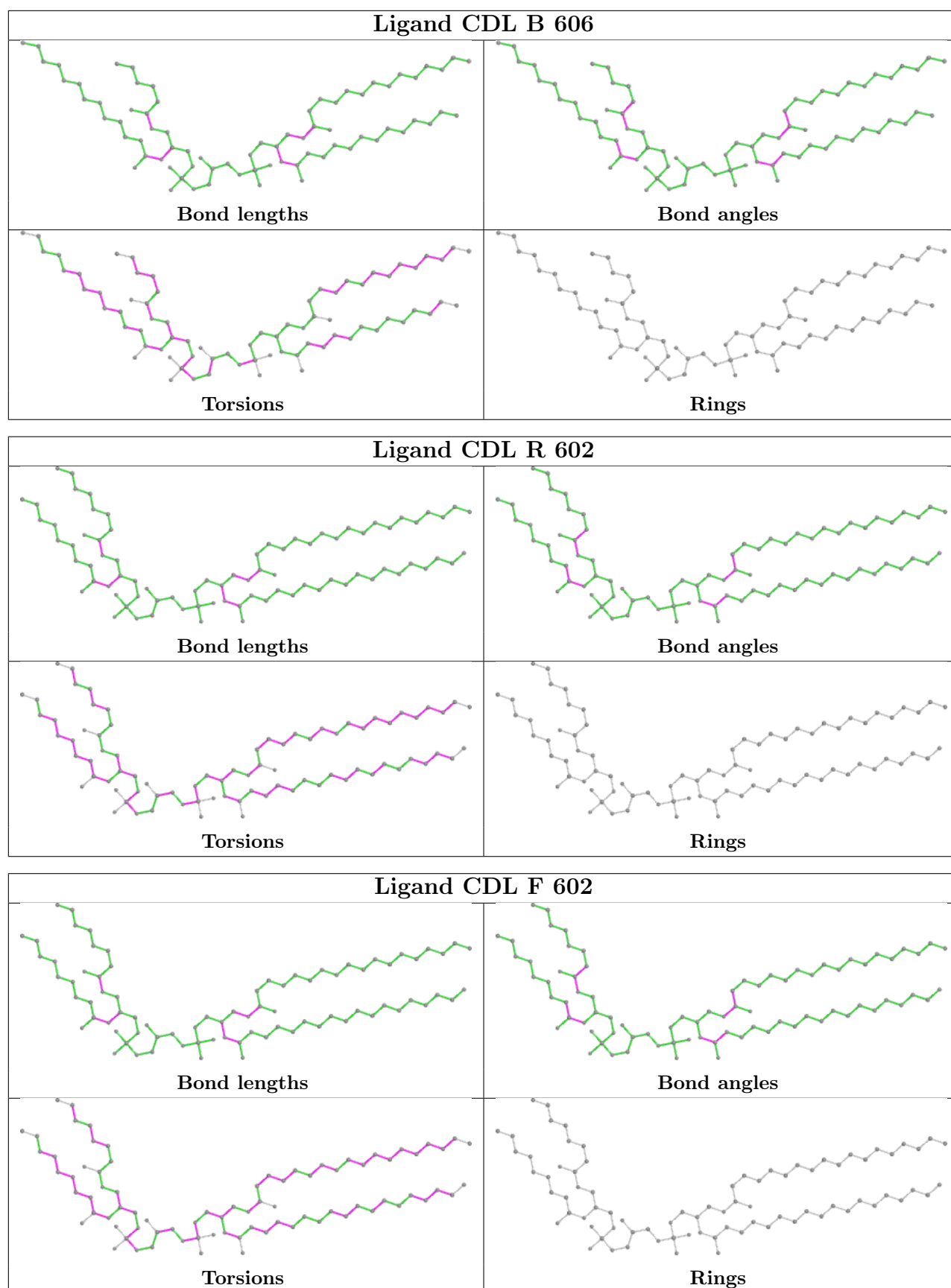


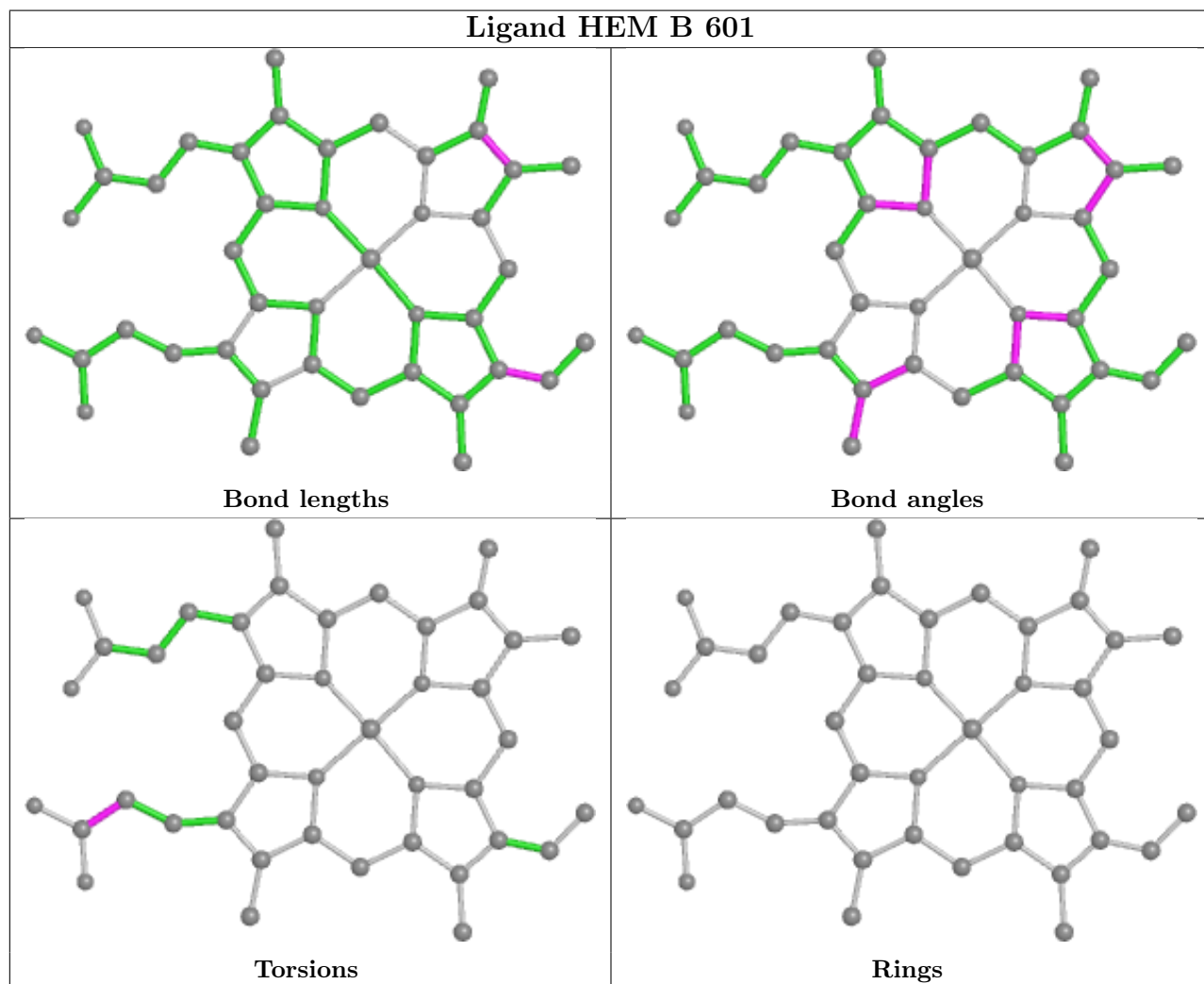
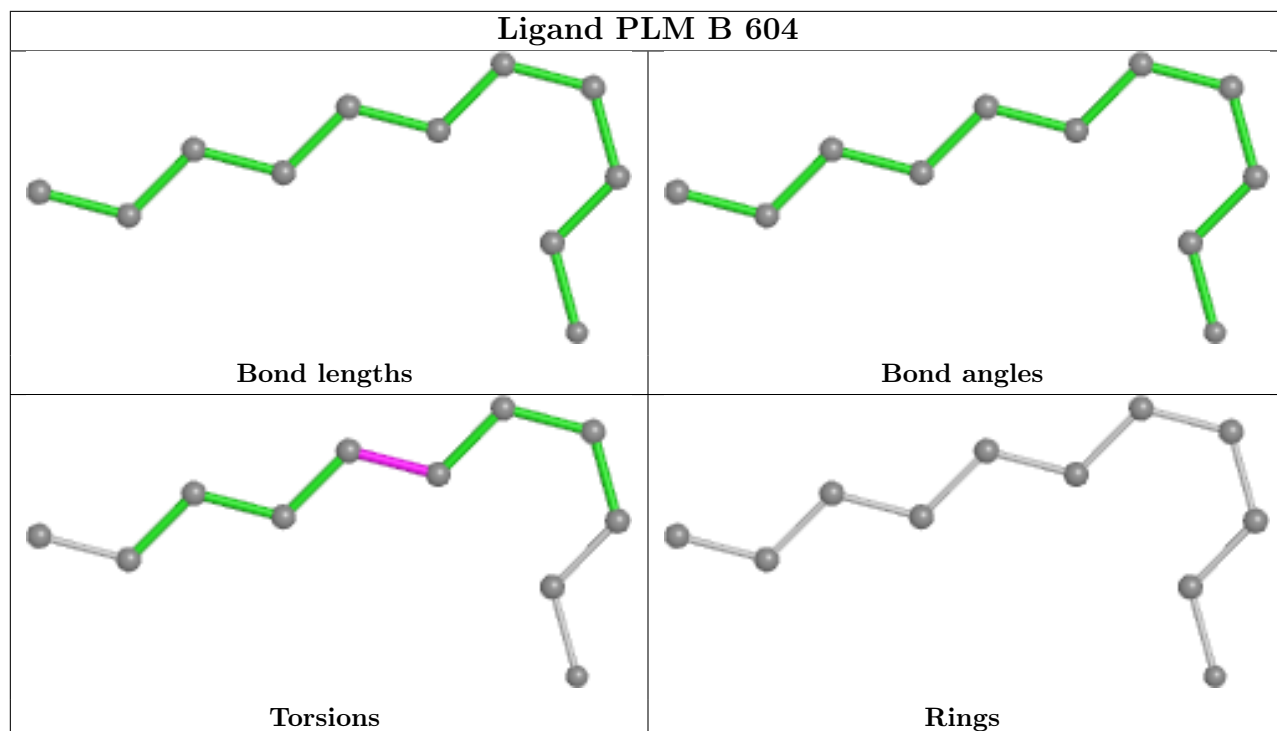


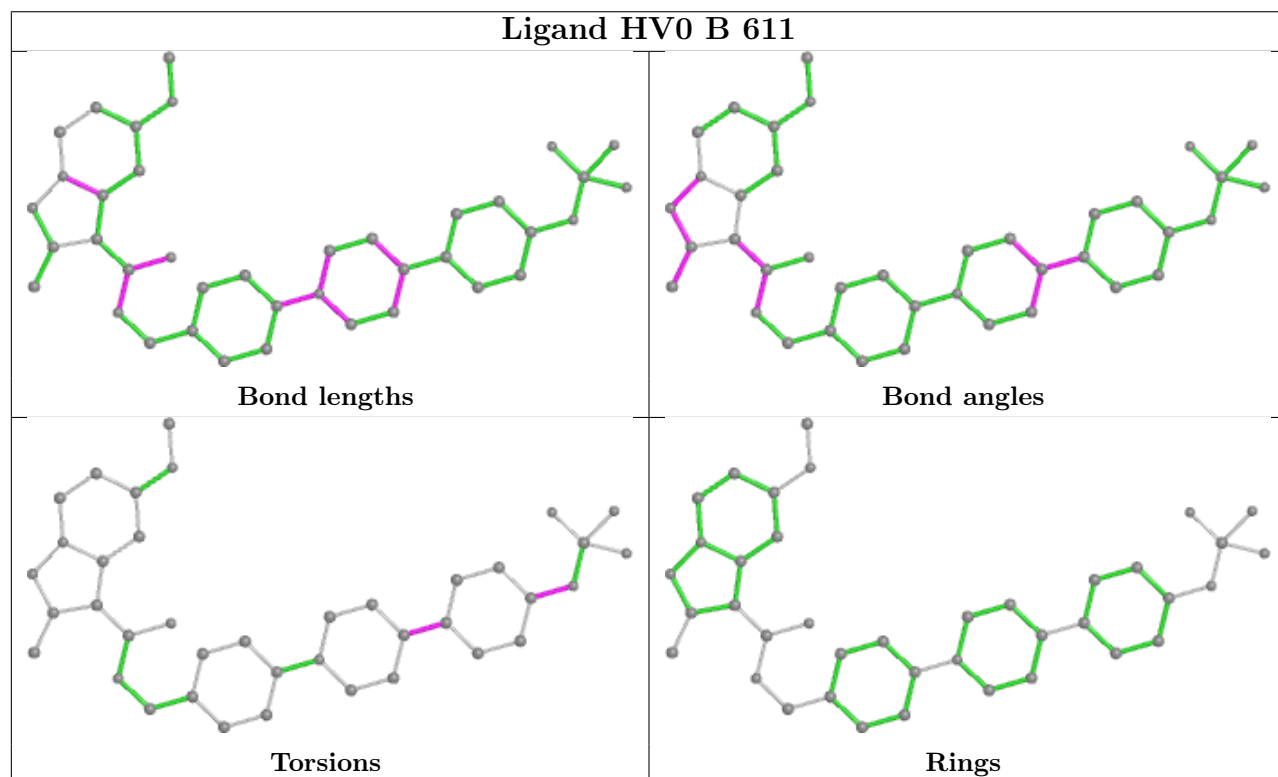
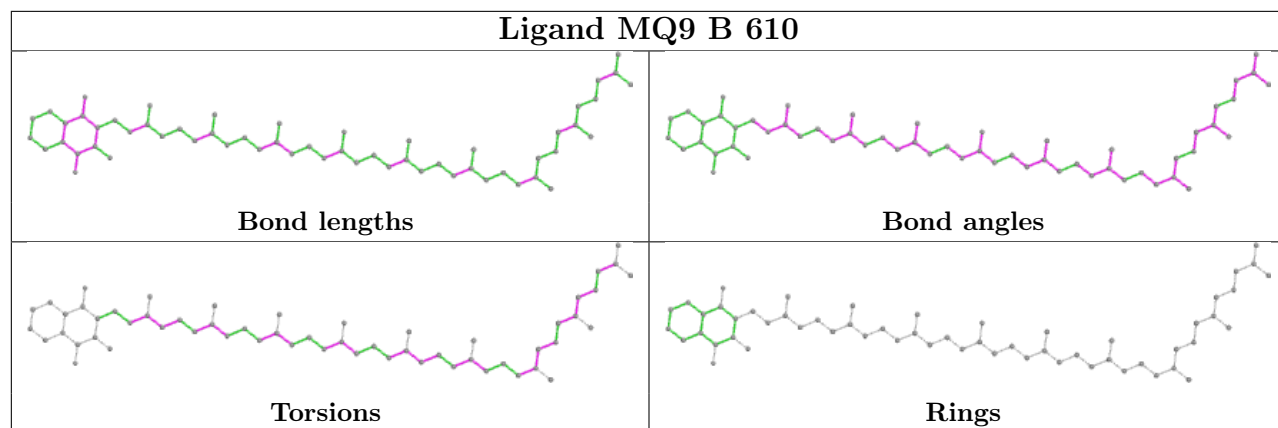


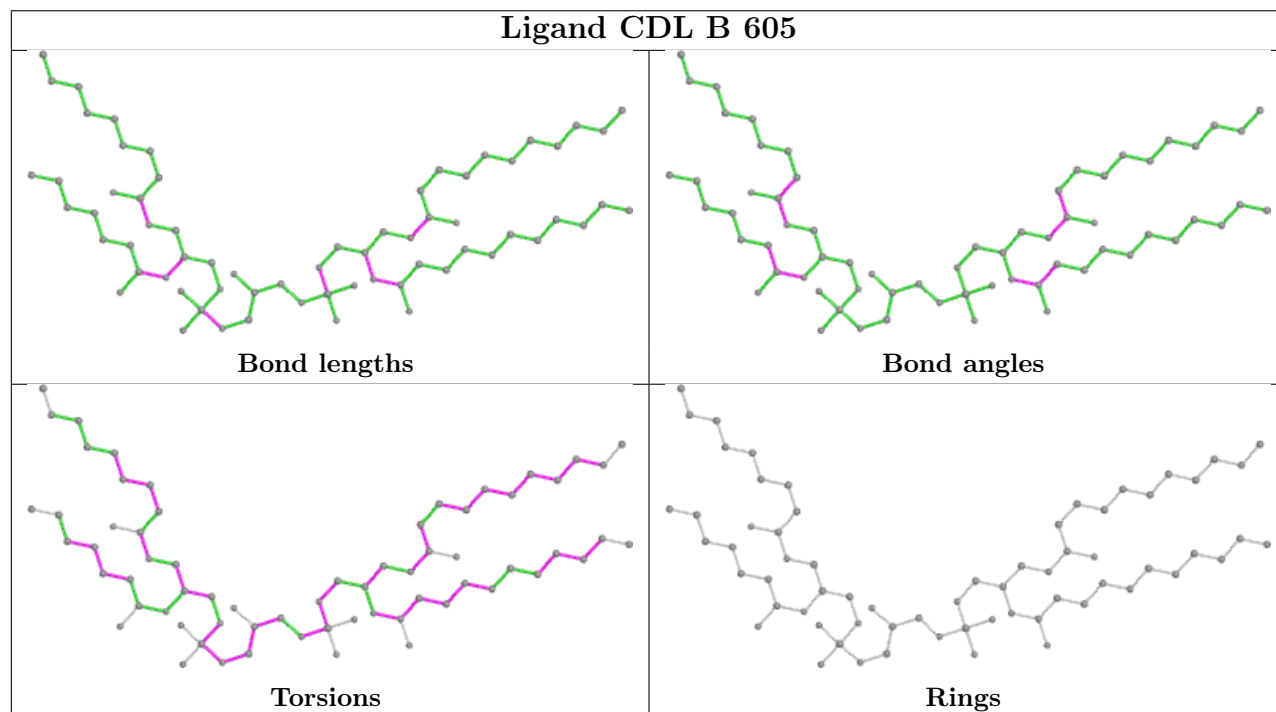
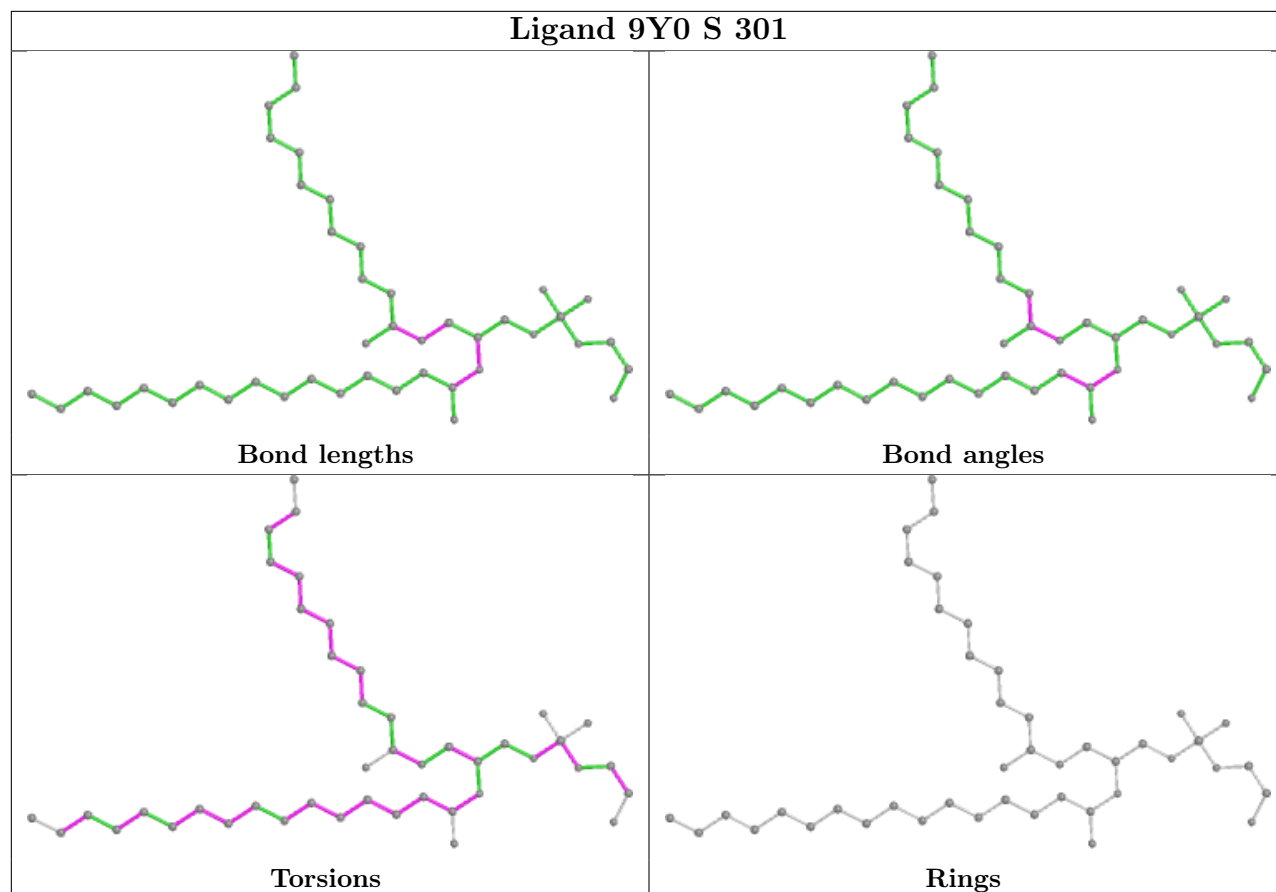


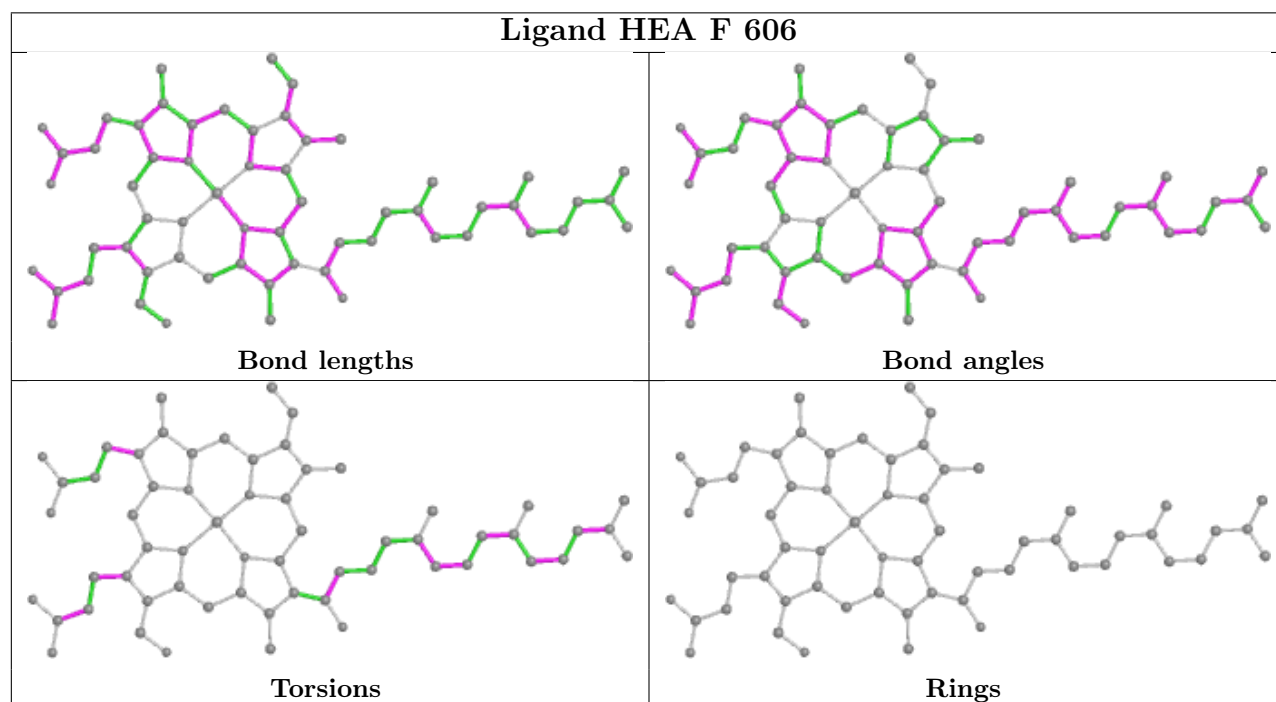
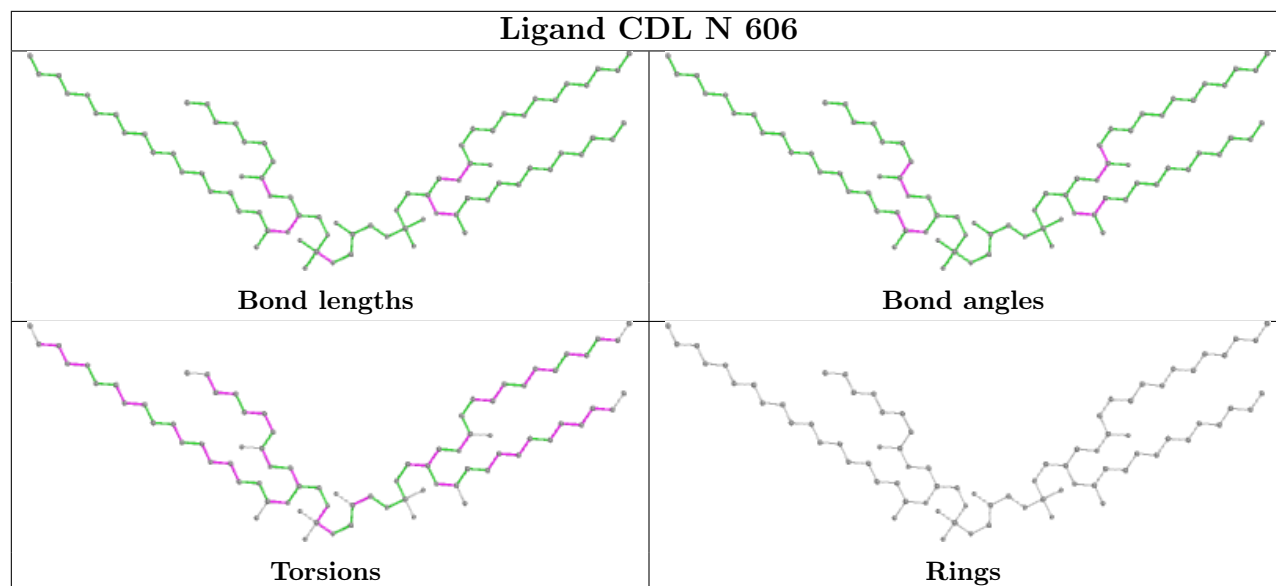


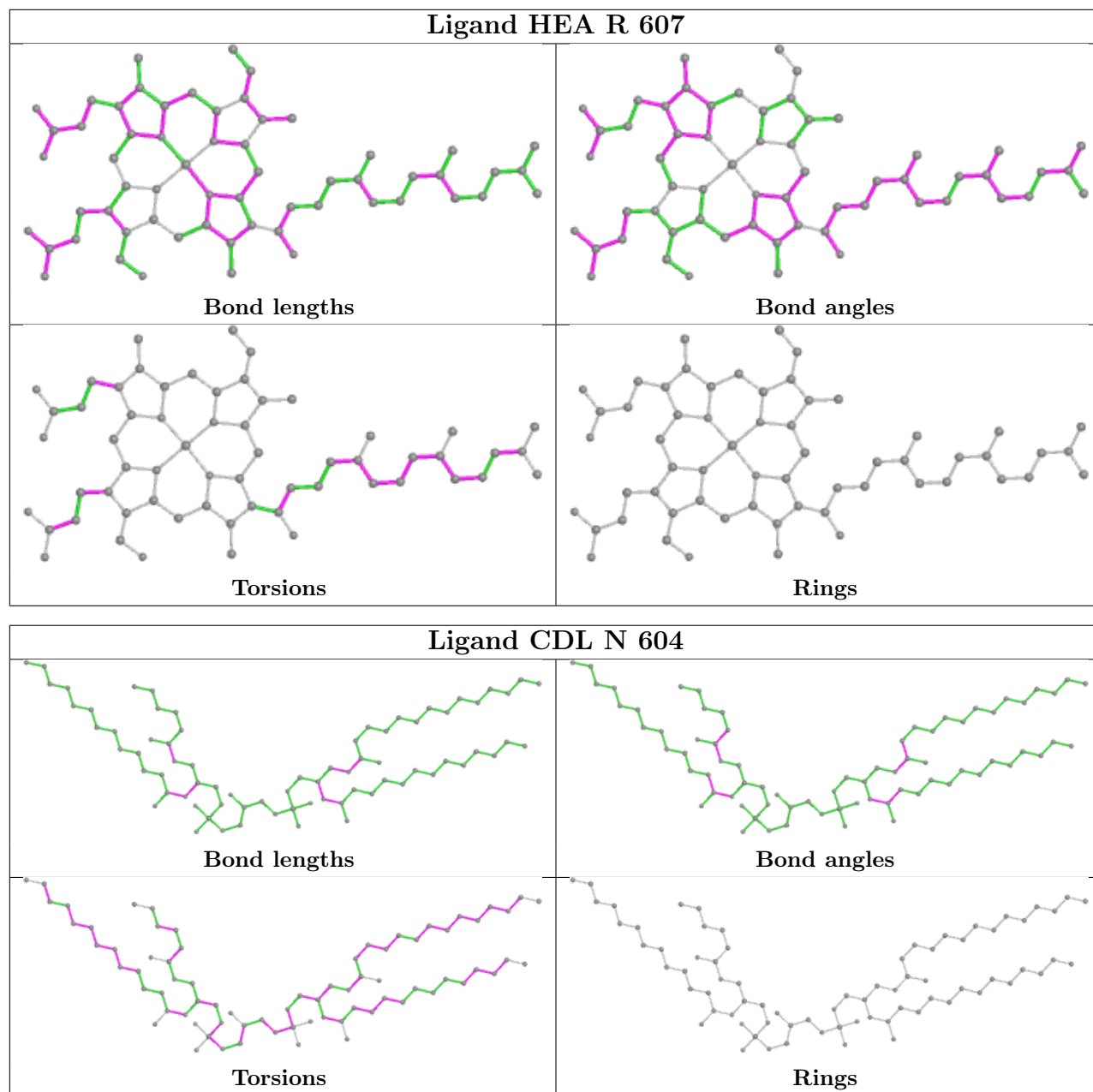


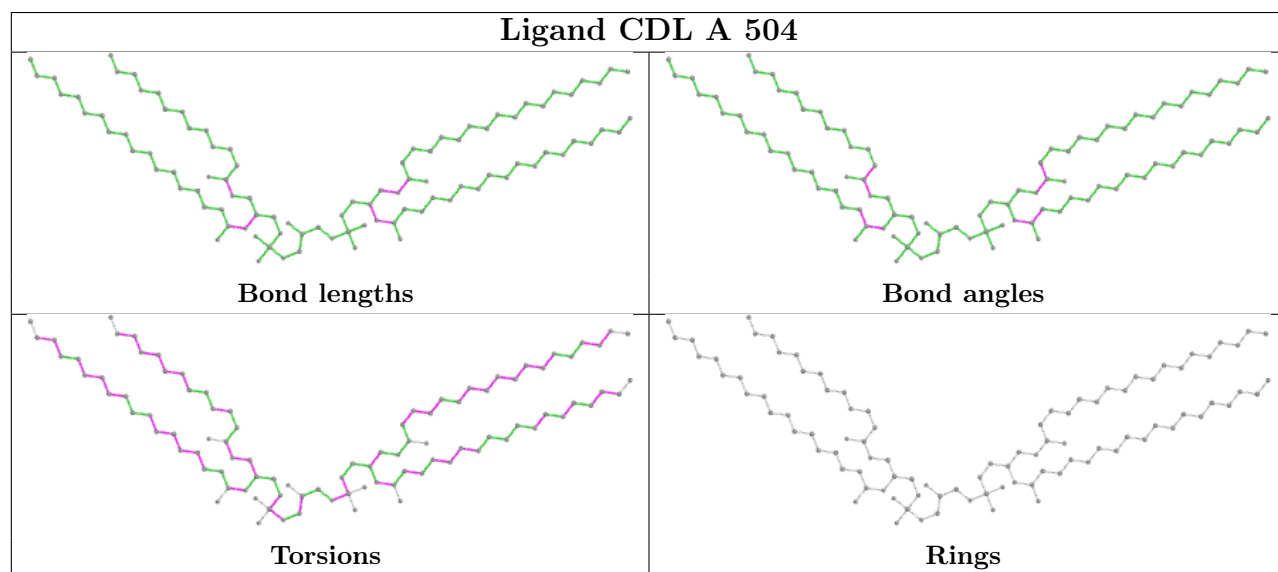
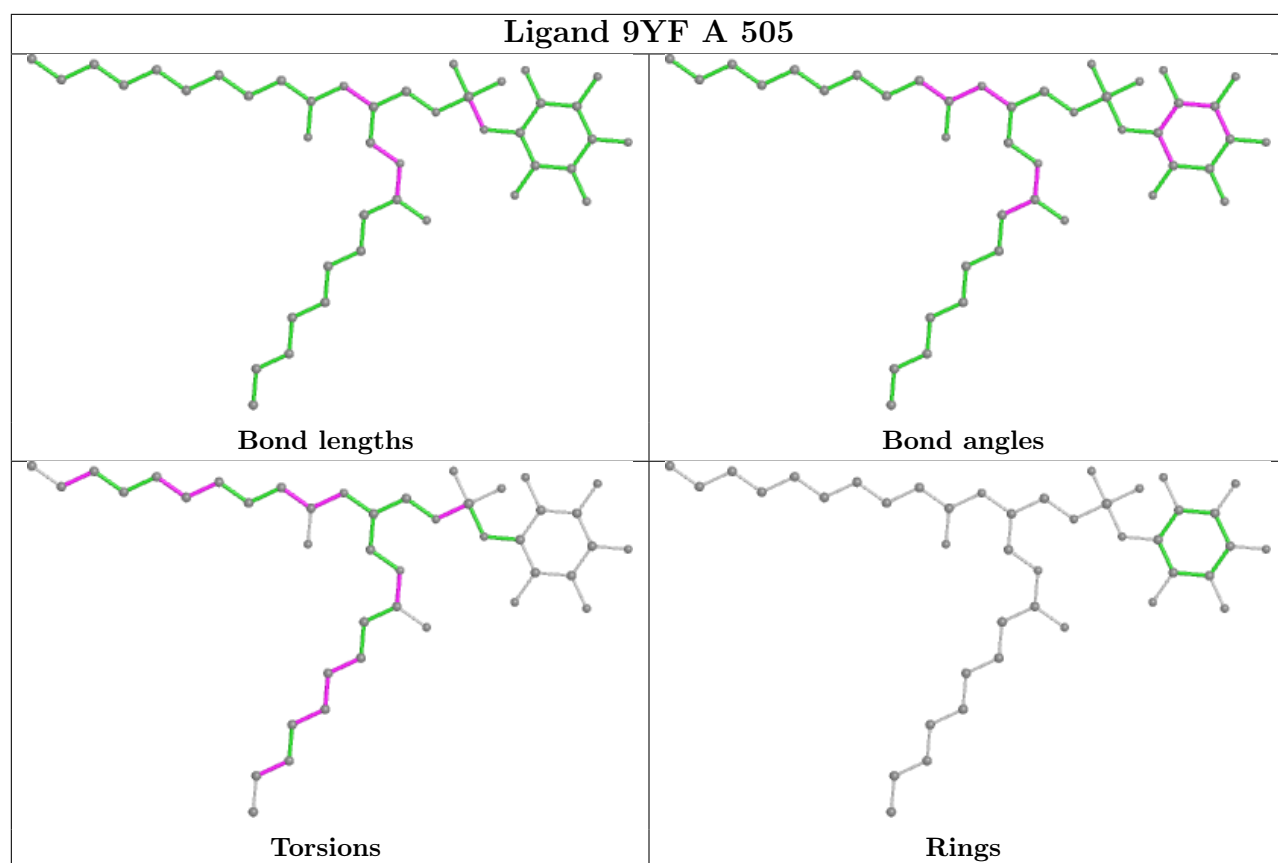


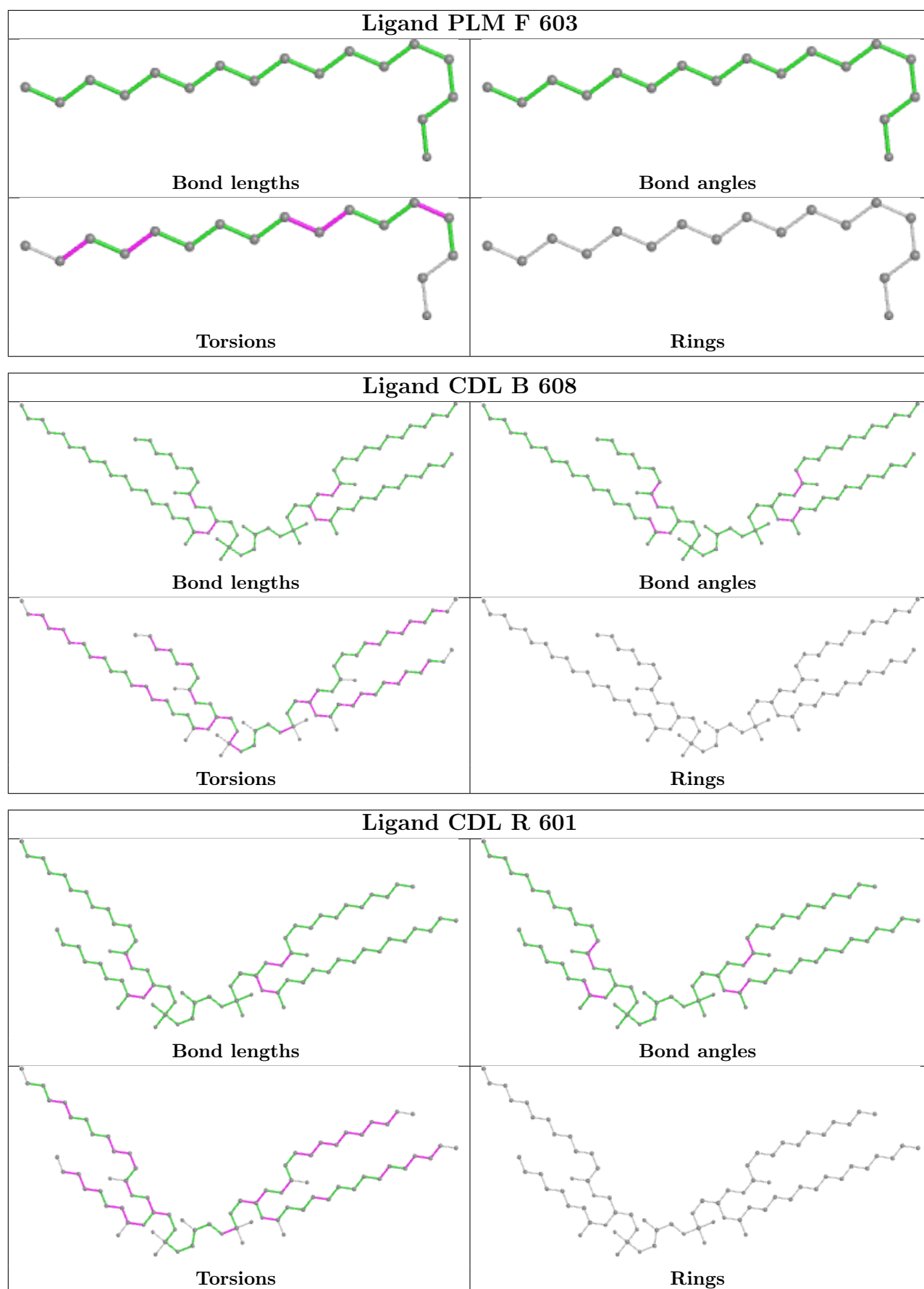




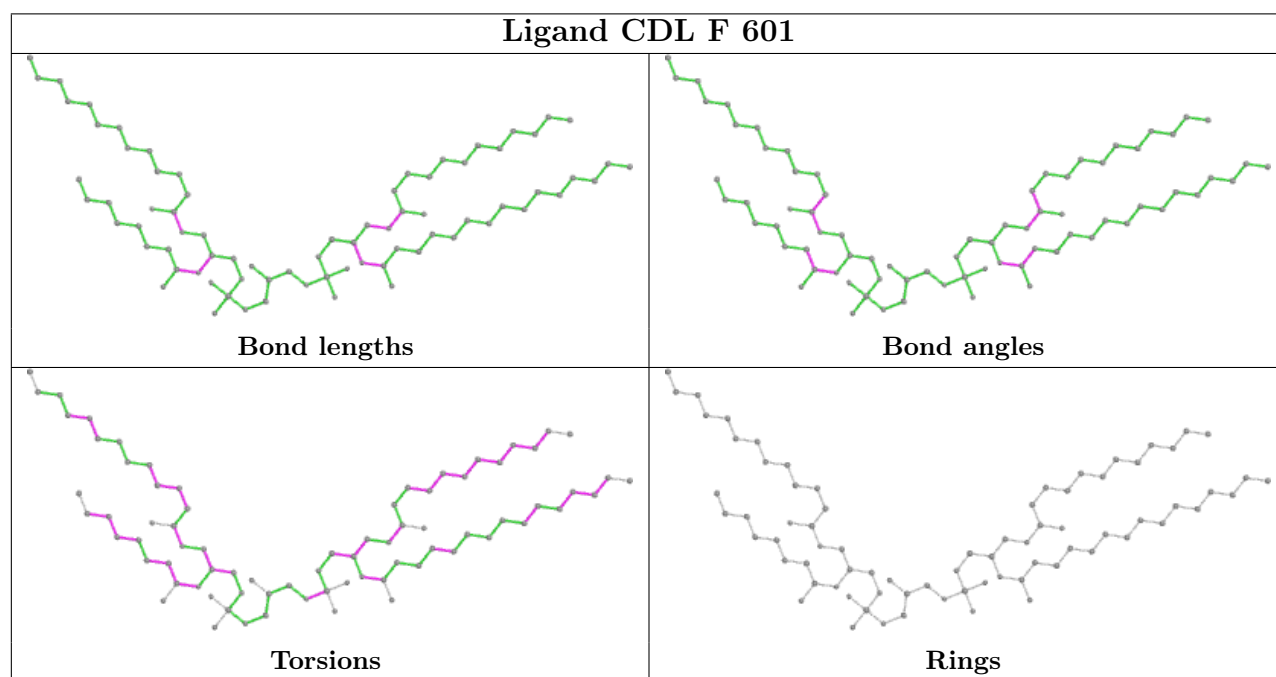
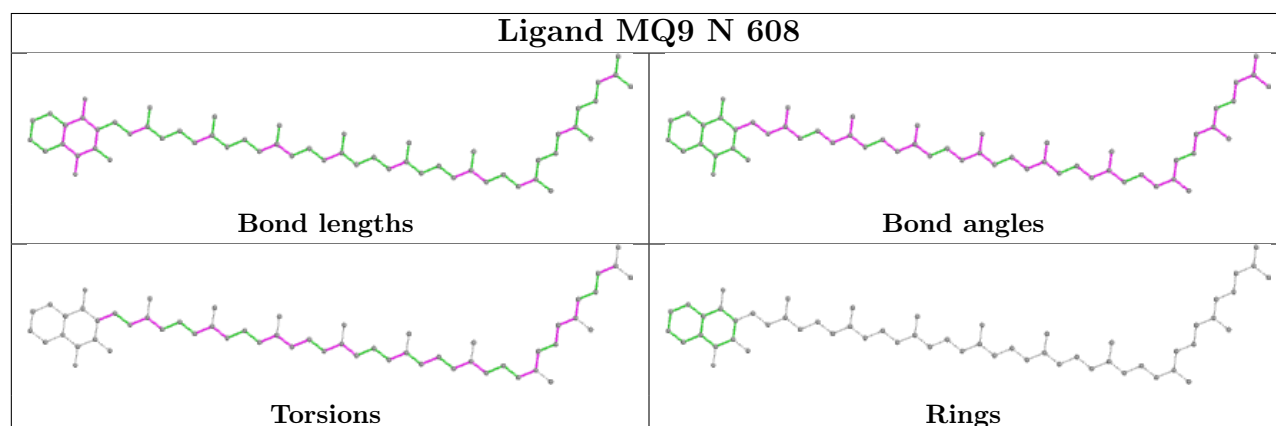
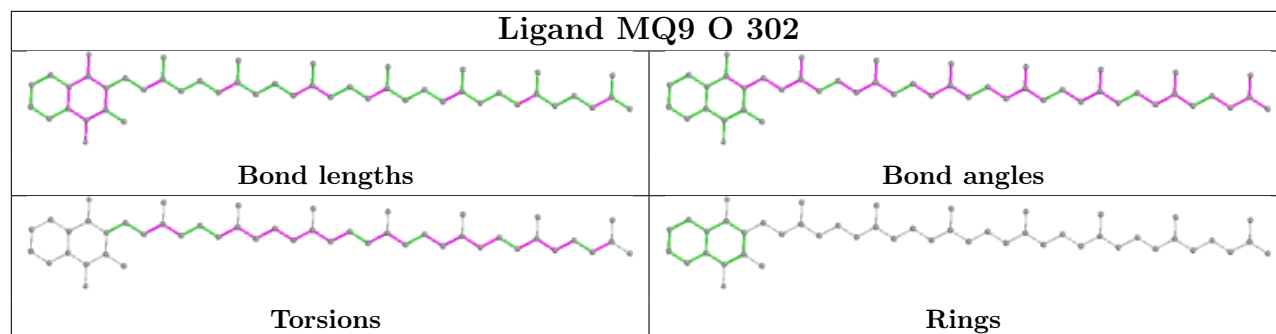


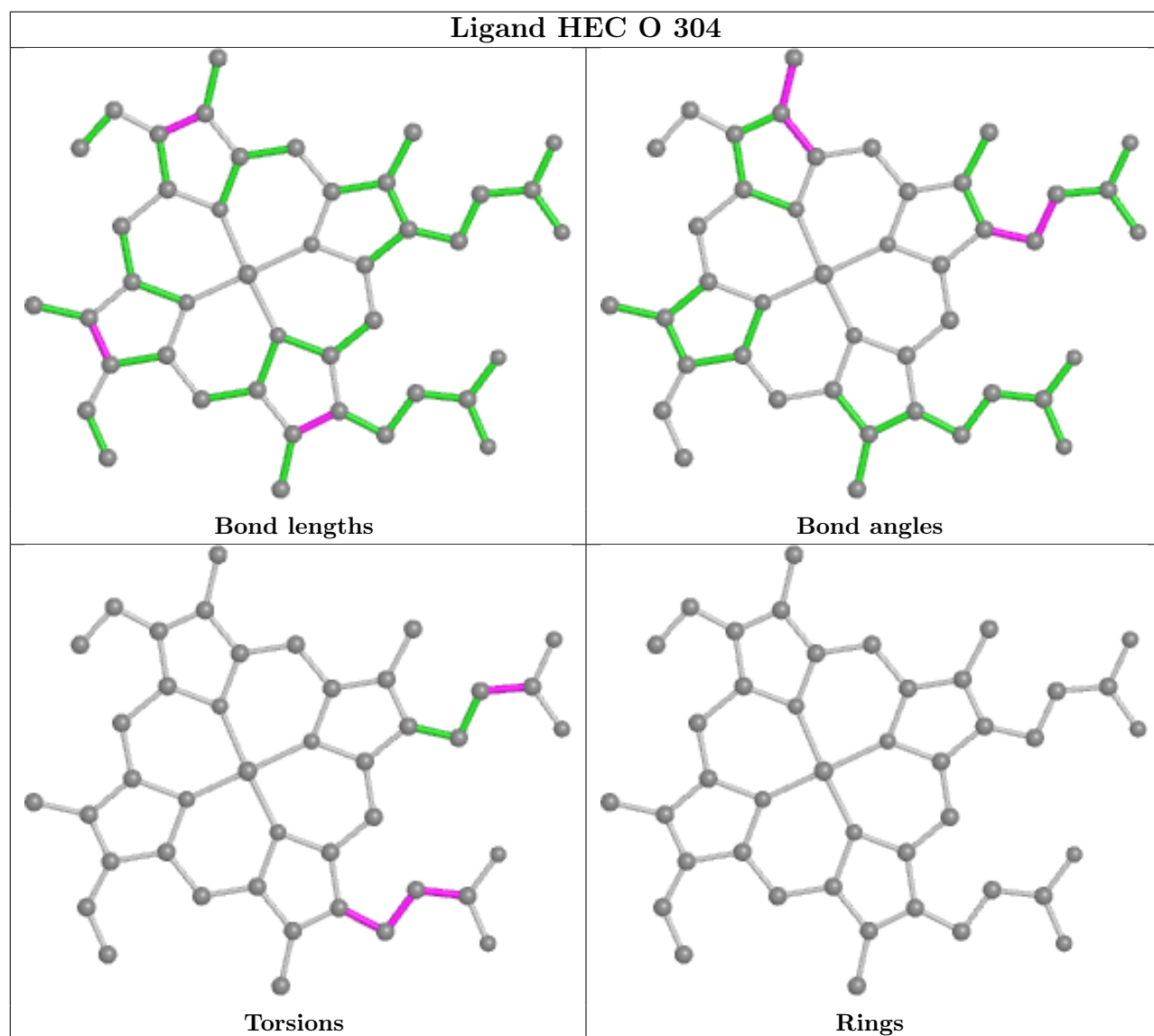
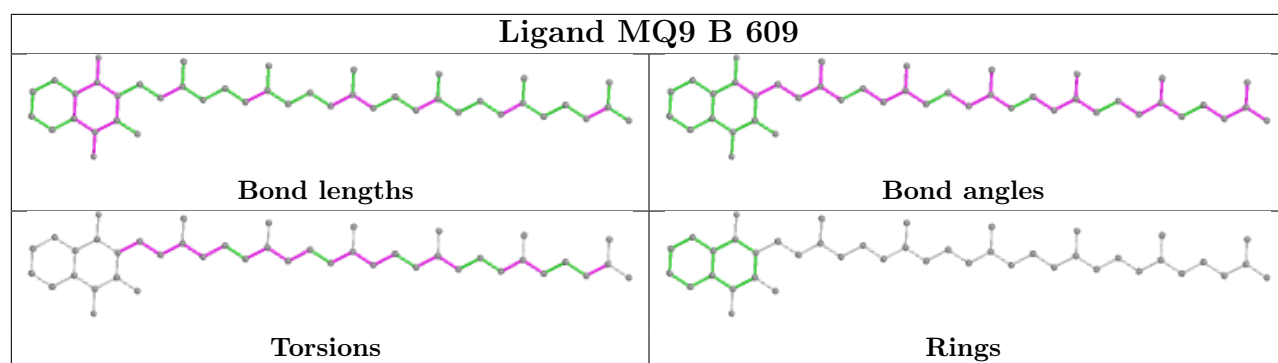


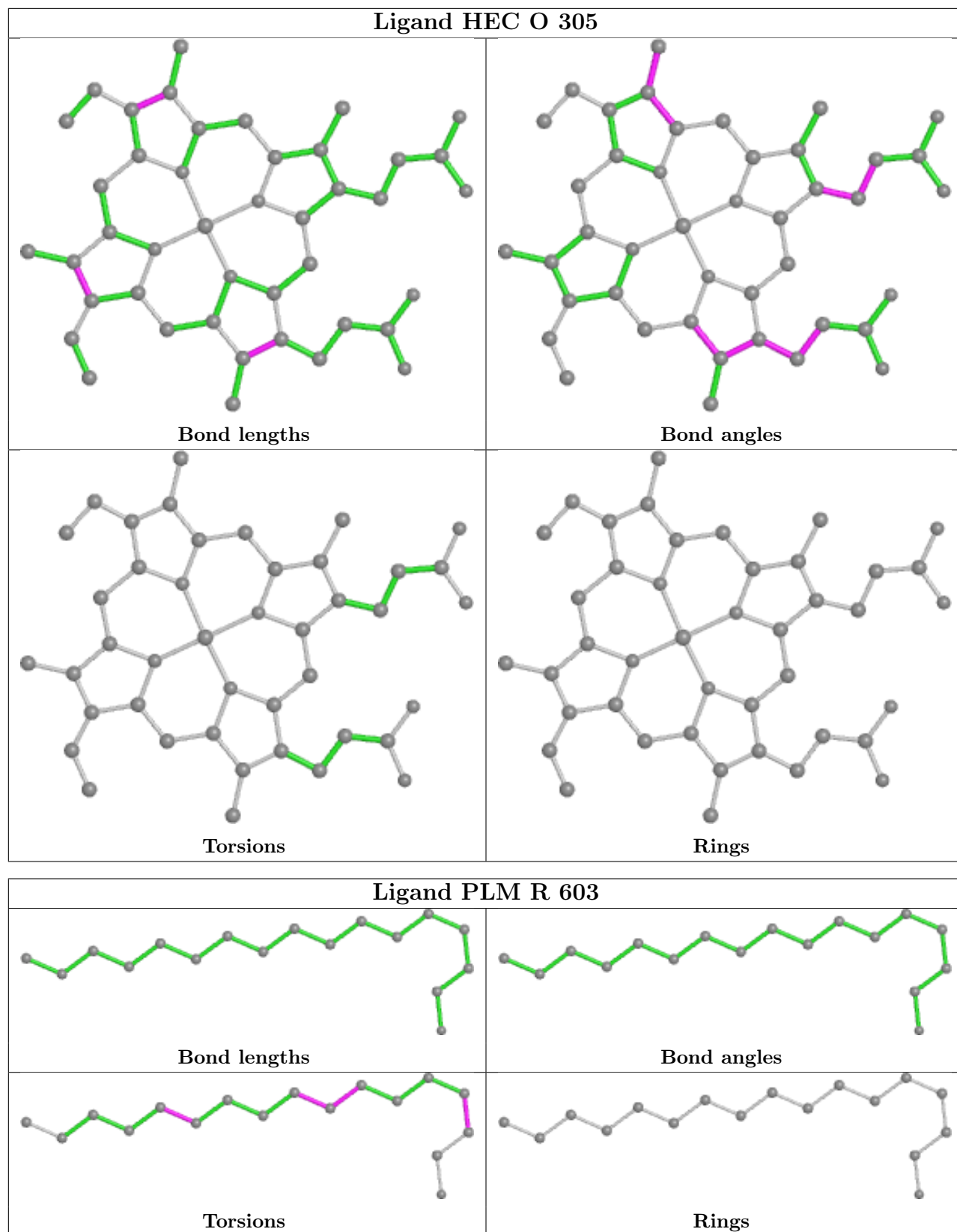


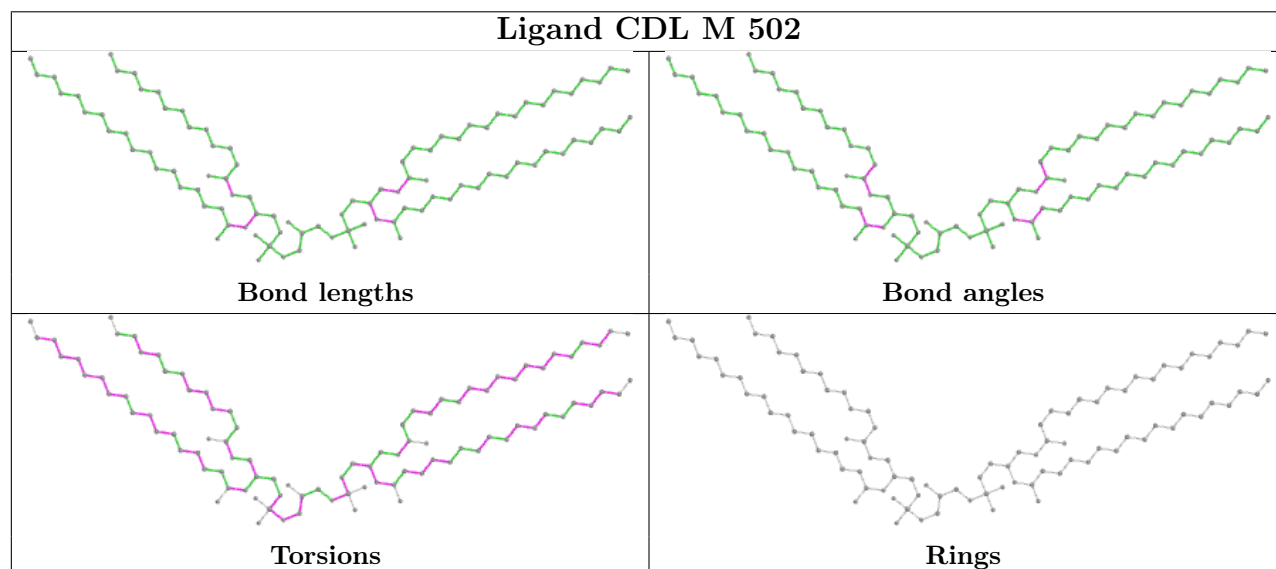
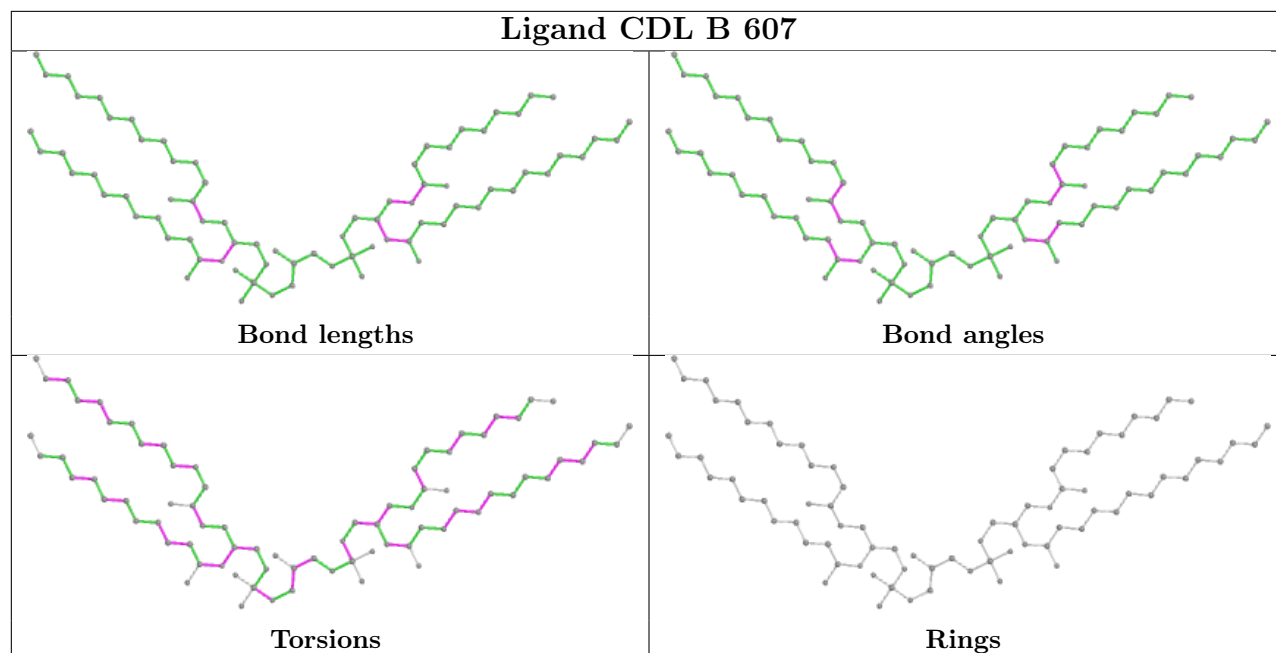


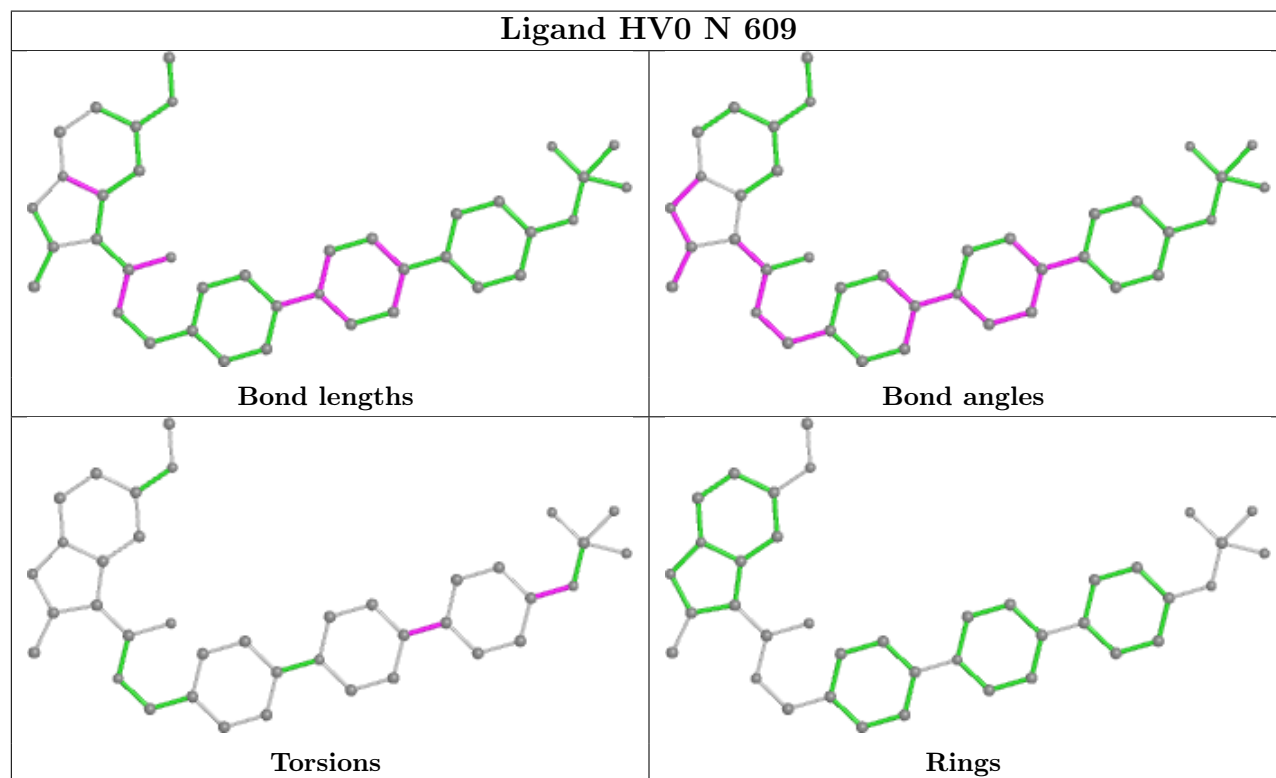
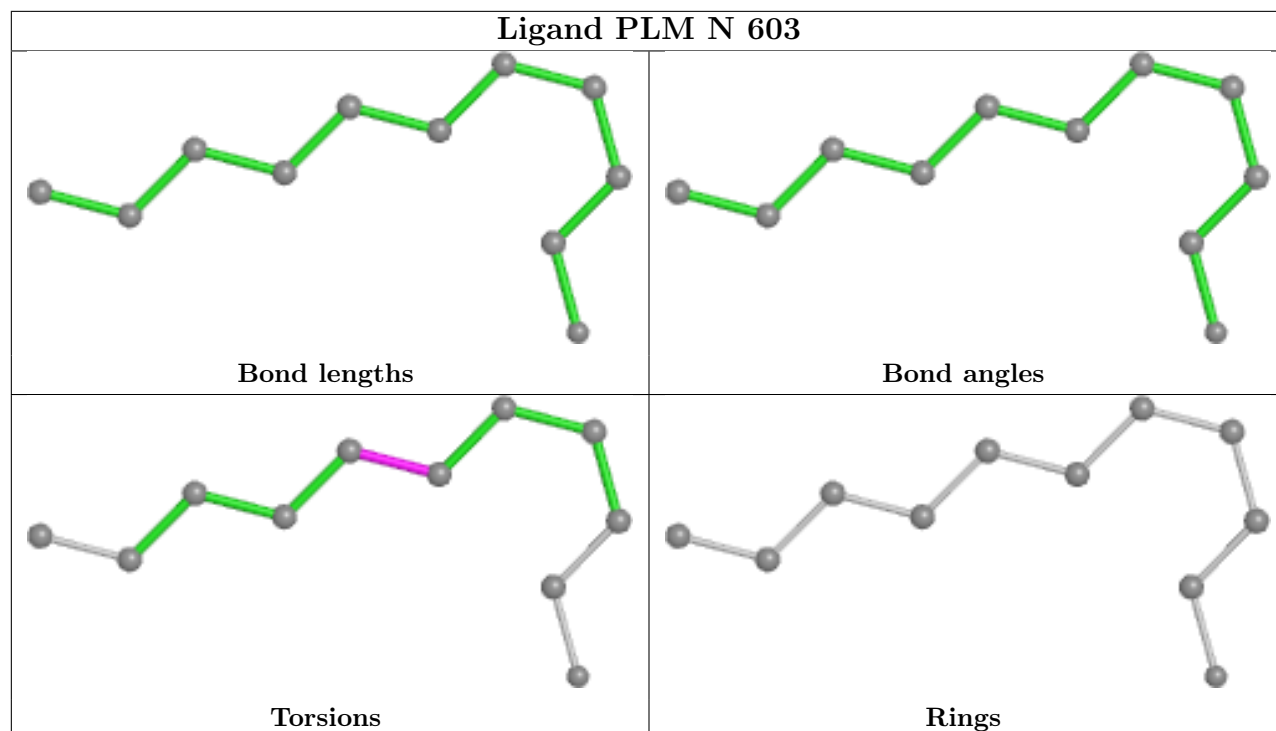


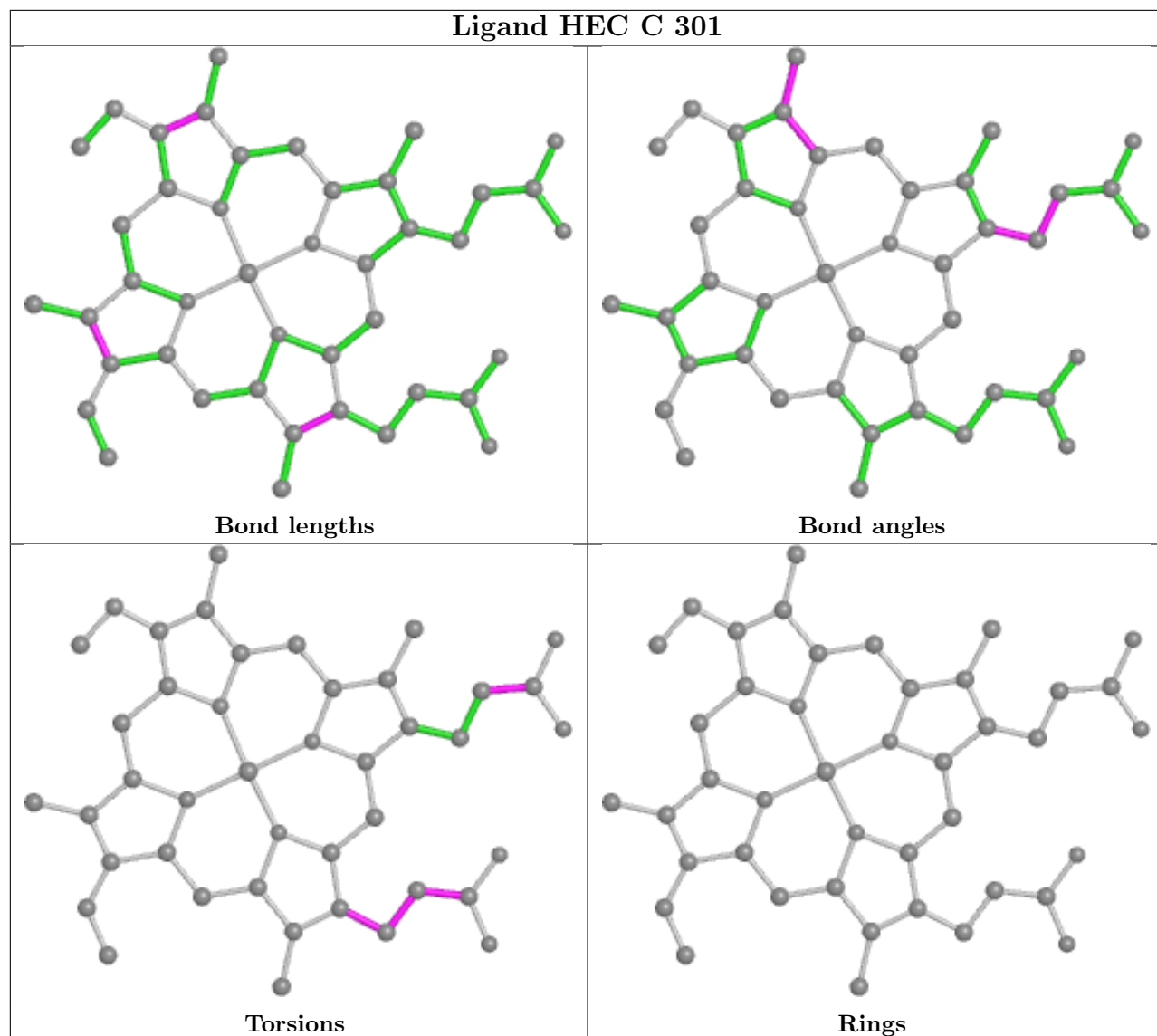


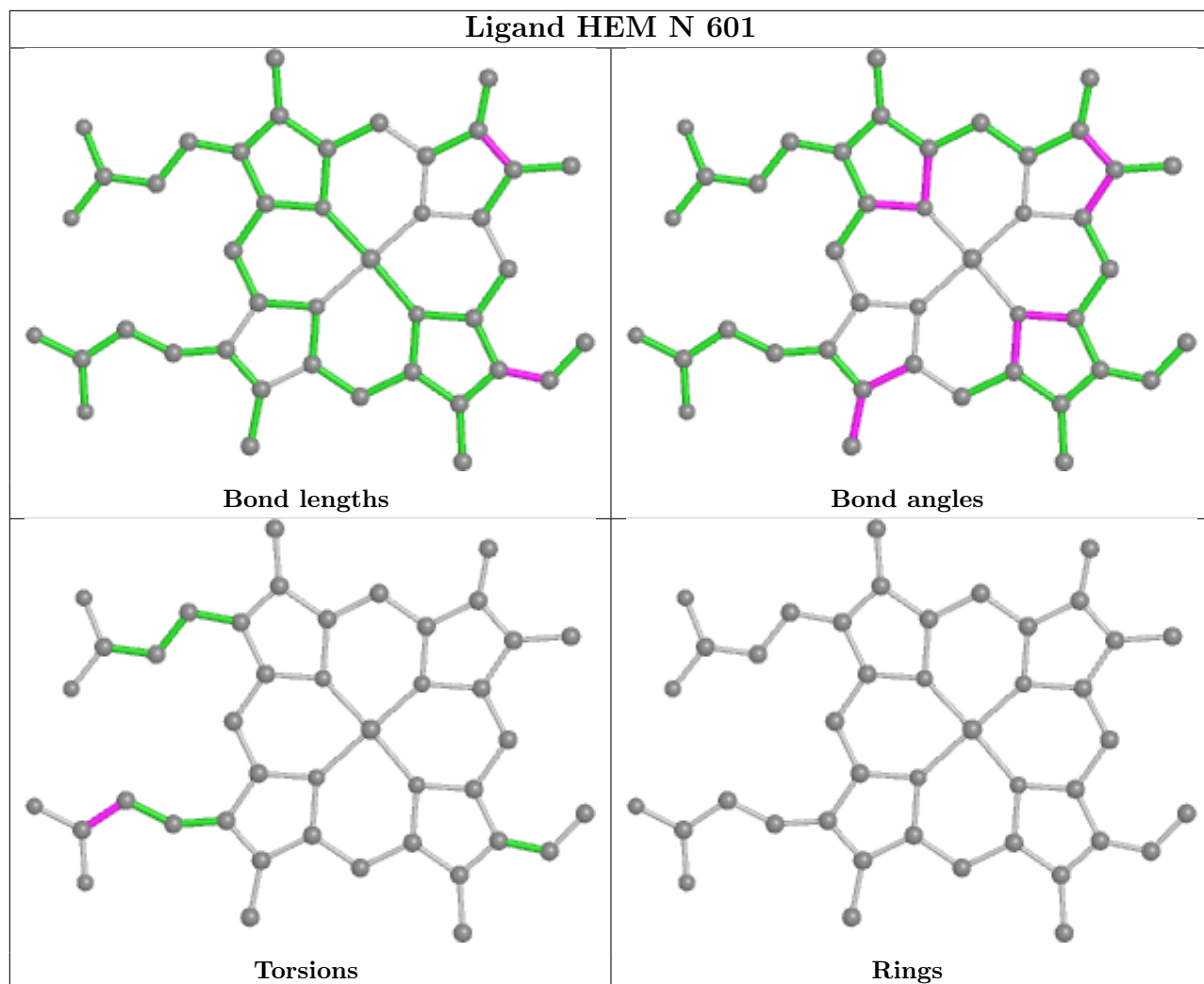


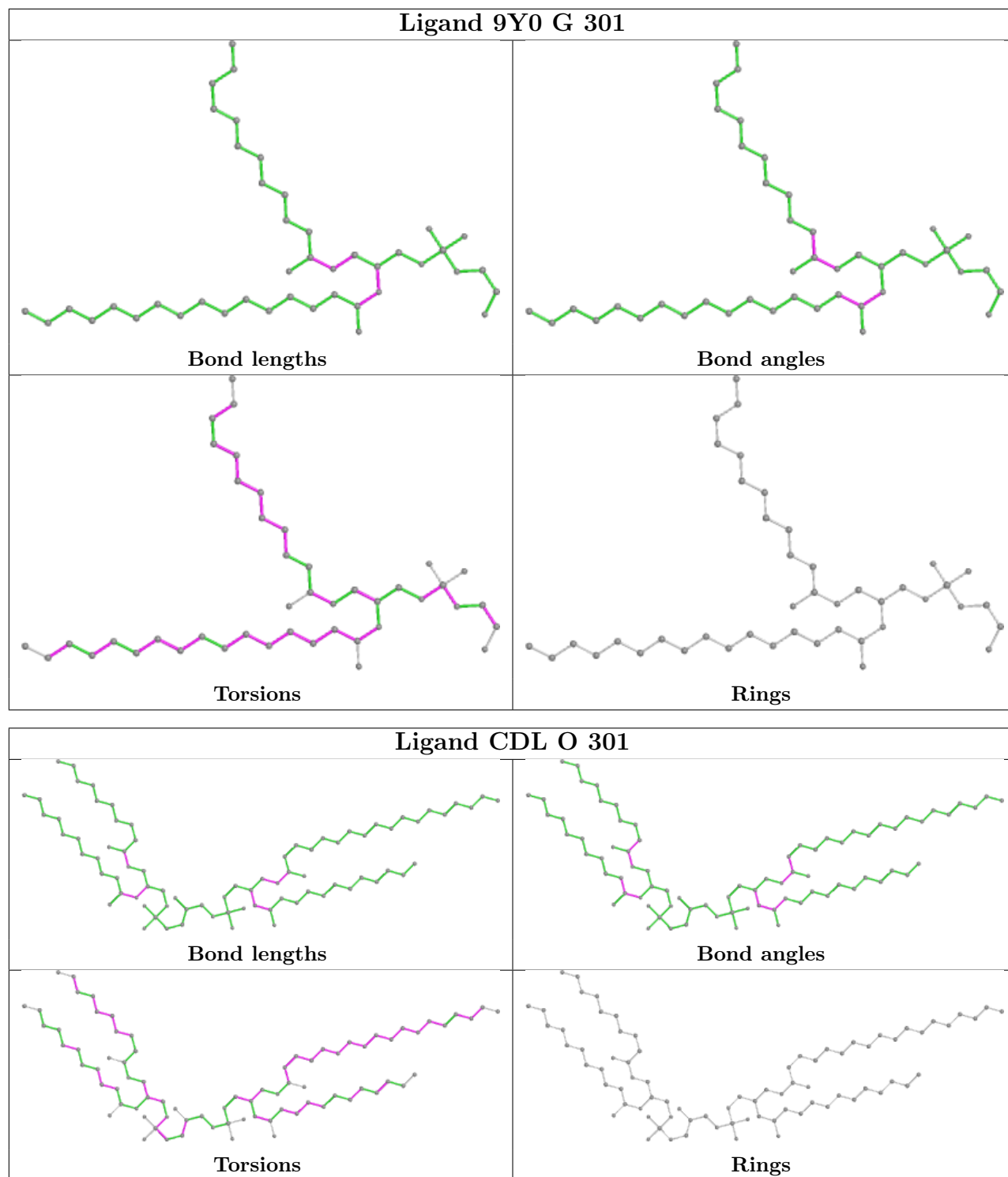












## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

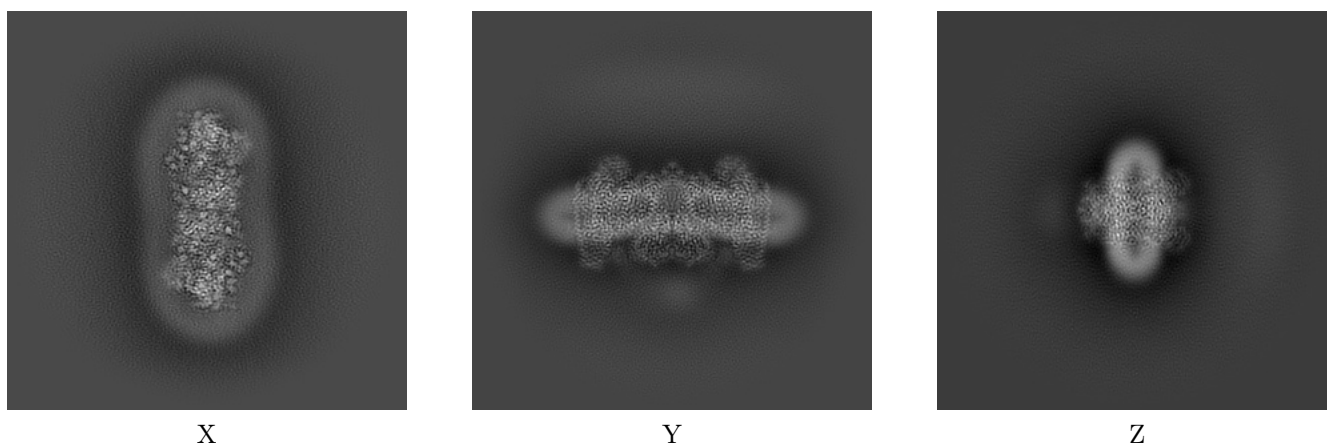
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30945. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

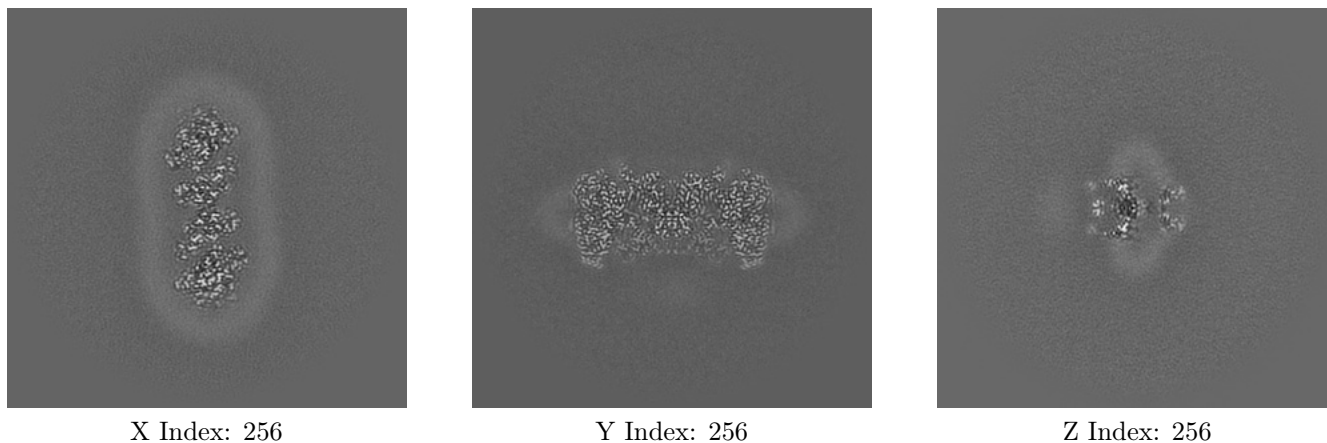
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

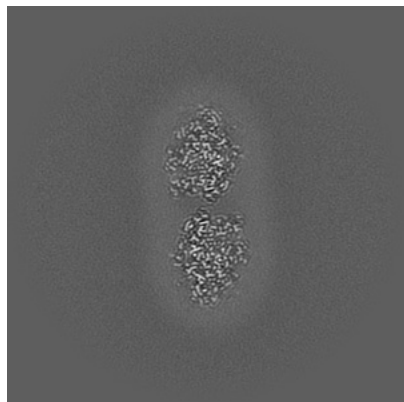
#### 6.2.1 Primary map



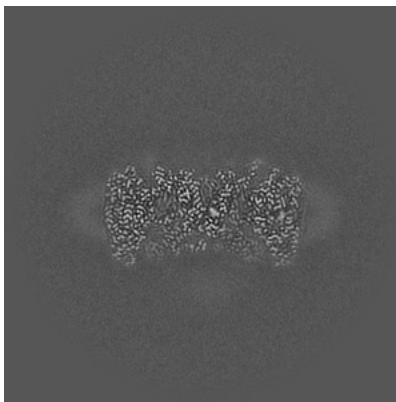
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

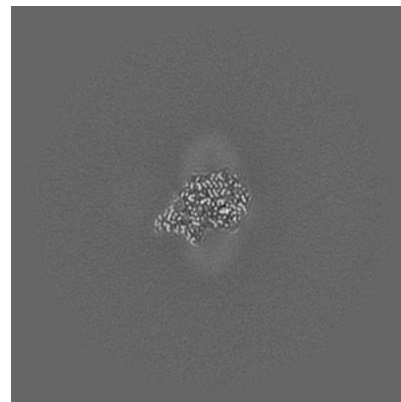
### 6.3.1 Primary map



X Index: 275



Y Index: 252



Z Index: 233

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

## 6.4 Orthogonal surface views [i](#)

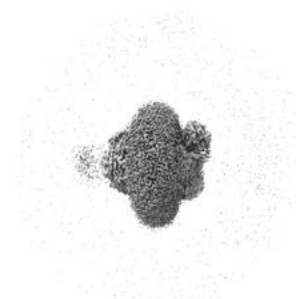
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

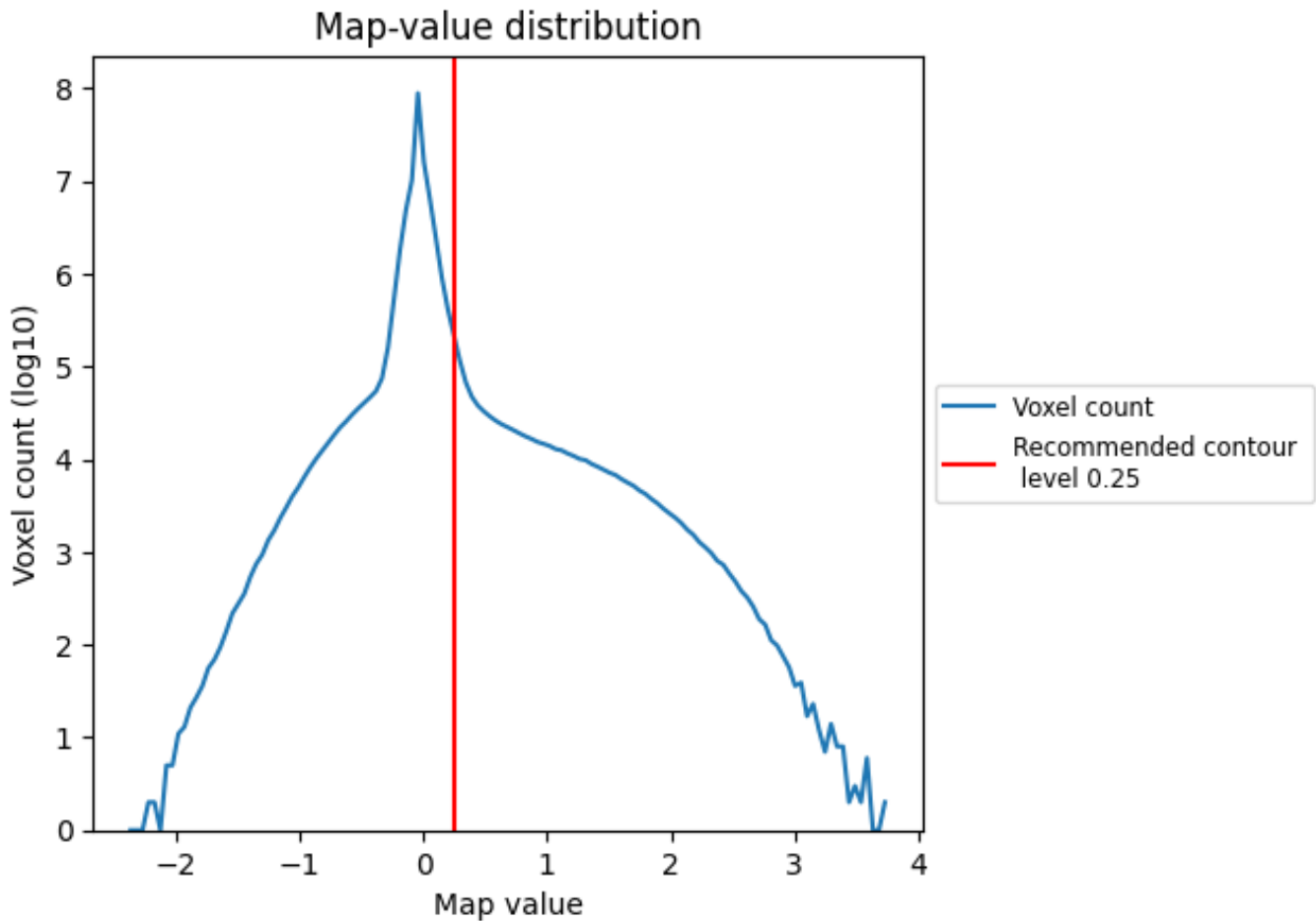
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

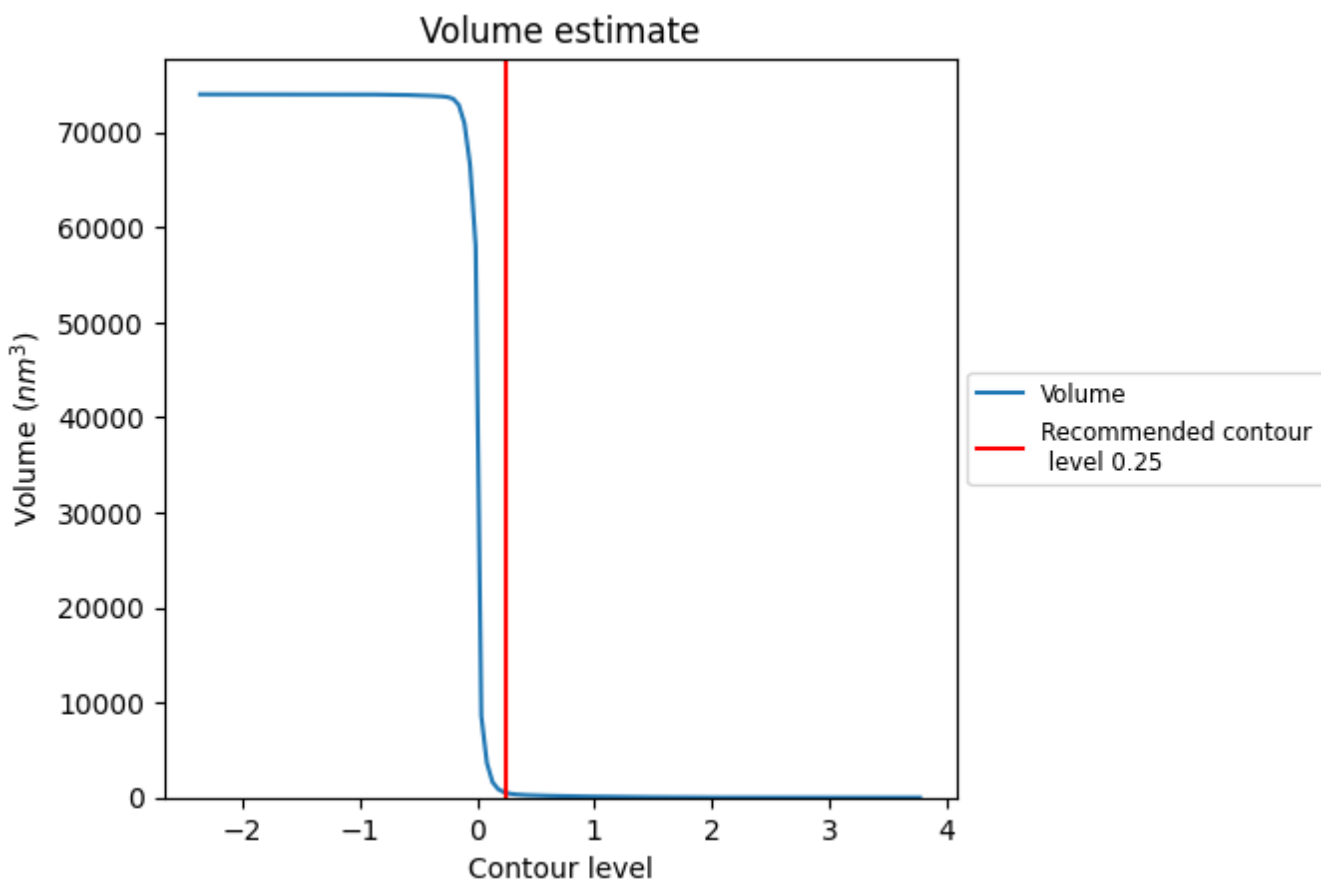
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

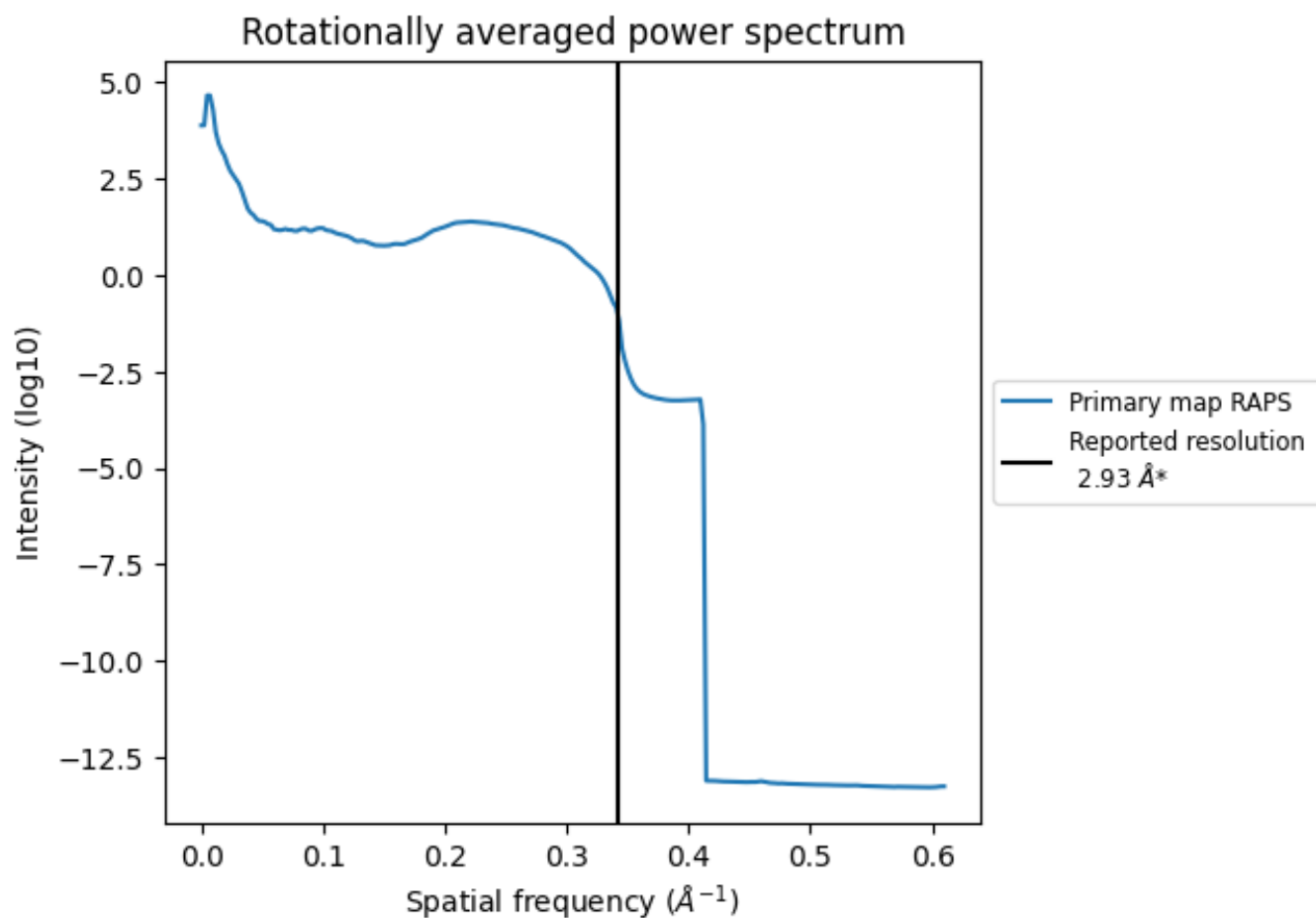
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 502 nm<sup>3</sup>; this corresponds to an approximate mass of 453 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.341 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

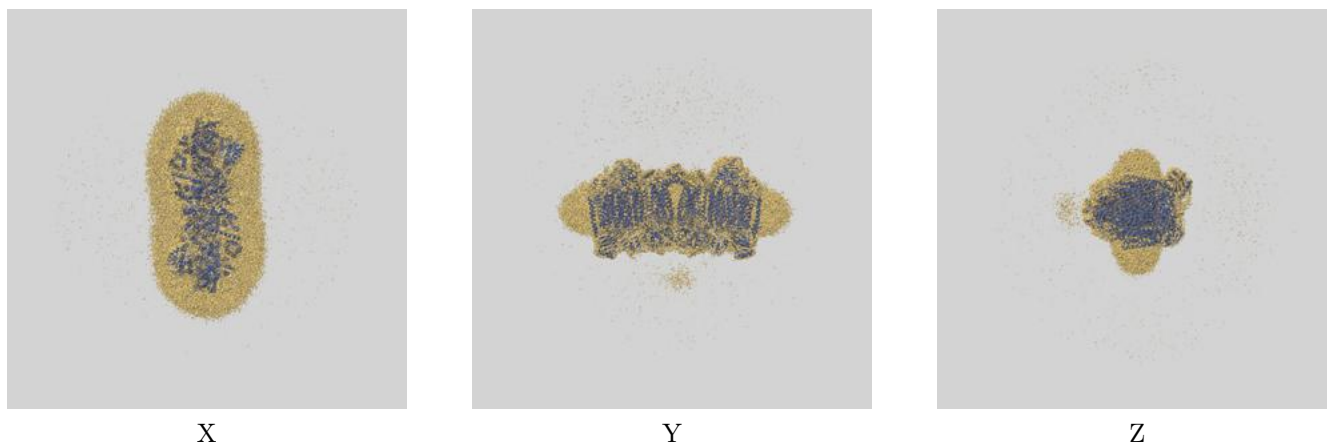
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

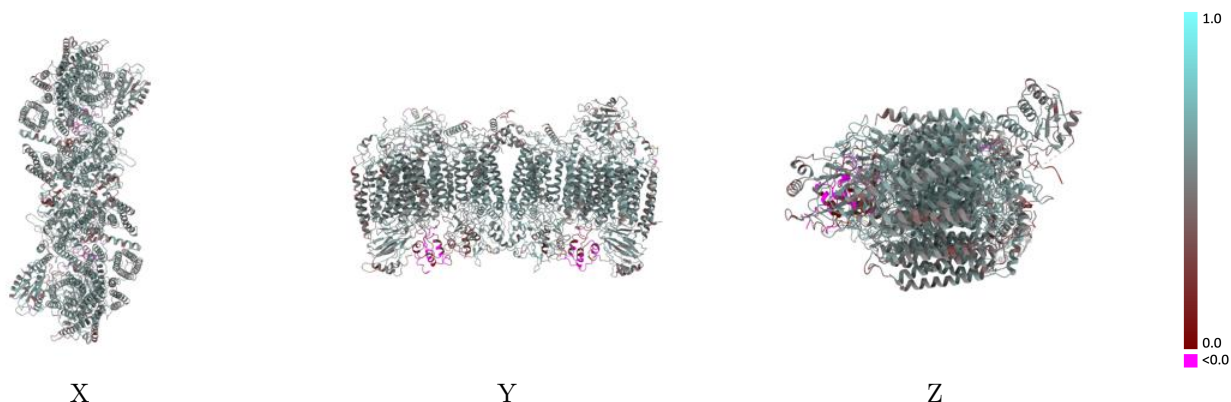
This section contains information regarding the fit between EMDB map EMD-30945 and PDB model 7E1X. Per-residue inclusion information can be found in section [3](#) on page [14](#).

### 9.1 Map-model overlay [i](#)



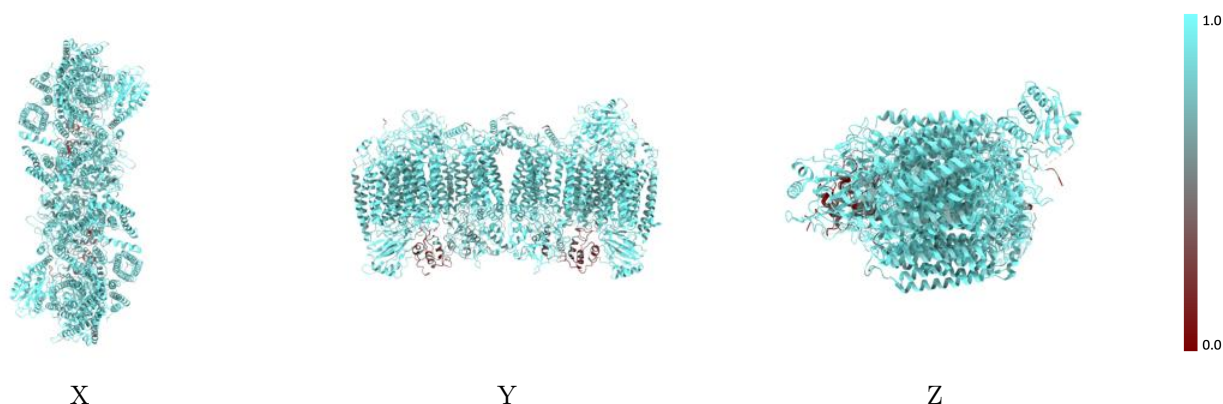
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



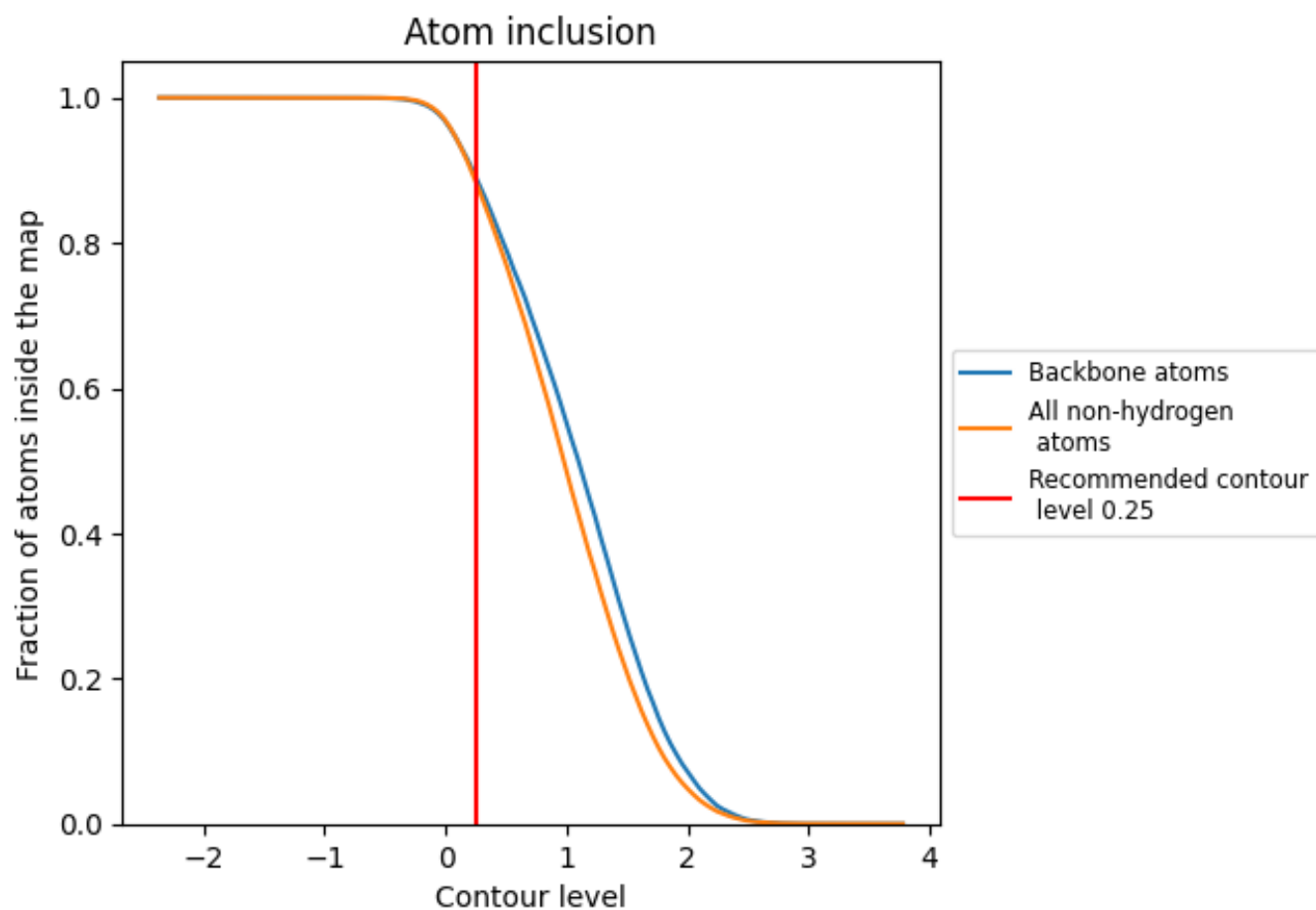
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 89% of all backbone atoms, 88% 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	 0.8842	 0.5130
A	 0.8979	 0.5180
B	 0.9239	 0.5540
C	 0.5865	 0.2820
D	 0.8963	 0.5370
E	 0.9003	 0.4980
F	 0.9357	 0.5570
G	 0.9000	 0.5120
H	 0.8903	 0.5050
I	 0.8858	 0.4890
J	 0.9002	 0.4820
M	 0.8962	 0.5280
N	 0.9274	 0.5680
O	 0.5558	 0.2890
P	 0.9190	 0.5490
Q	 0.8749	 0.4790
R	 0.9379	 0.5610
S	 0.8996	 0.5020
T	 0.9082	 0.5330
U	 0.8878	 0.5010
V	 0.9080	 0.5080

