



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 01:07 AM JST

PDB ID : 6ADQ / pdb_00006adq
EMDB ID : EMD-9610
Title : Respiratory Complex CIII2CIV2SOD2 from Mycobacterium smegmatis
Authors : Gong, H.R.; Xu, A.; Gao, R.G.; Ji, W.X.; Wang, S.H.; Wang, Q.; Li, J.; Rao, Z.H.
Deposited on : 2018-08-01
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

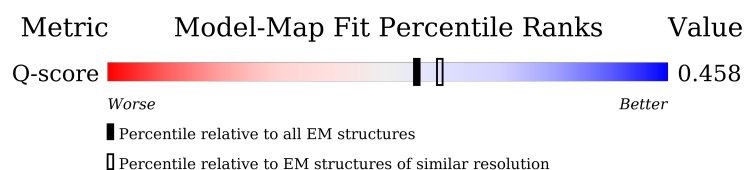
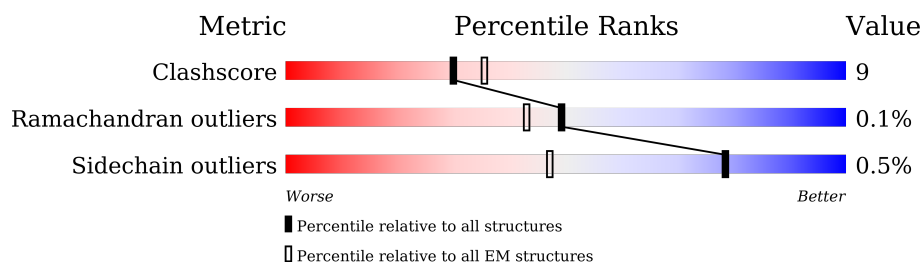
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



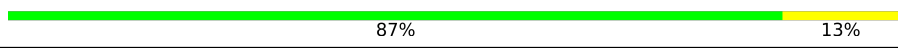
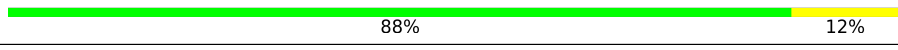
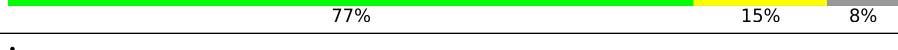
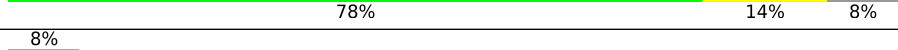
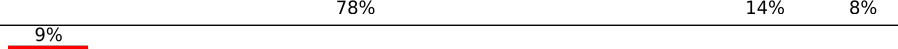
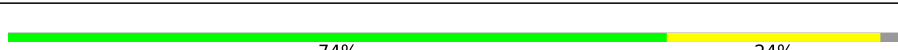
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	341	
1	Q	341	
2	F	575	
2	R	575	

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Mol	Chain	Length	Quality of chain
3	G	203	
3	S	203	
4	H	139	
4	T	139	
5	I	79	
5	U	79	
6	J	157	
6	V	157	
7	D	100	
7	P	100	
8	Y	236	
8	Z	236	
9	K	186	
9	W	186	
10	B	546	
10	N	546	
11	C	294	
11	O	294	
12	A	421	
12	M	421	

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
22	HEC	C	302	X	-	-	-
22	HEC	O	302	X	-	-	-
23	FES	M	502	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48946 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	312	Total	C	N	O	S	0	0
			2465	1592	412	451	10		
1	Q	312	Total	C	N	O	S	0	0
			2465	1592	412	451	10		

- 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	203	Total	C	N	O	S	0	0
			1560	1039	253	260	8		
3	S	203	Total	C	N	O	S	0	0
			1560	1039	253	260	8		

- 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
			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	92	Total	C	N	O	S	0	0
			736	471	136	124	5		
7	P	92	Total	C	N	O	S	0	0
			736	471	136	124	5		

- Molecule 8 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	216	Total	C	N	O	S	0	0
			1092	645	217	229	1		
8	Z	216	Total	C	N	O	S	0	0
			1092	645	217	229	1		

- Molecule 9 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	147	Total	C	N	O	S	0	0
			1072	664	180	227	1		
9	W	147	Total	C	N	O	S	0	0
			1072	664	180	227	1		

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	535	Total	C	N	O	S	0	0
			4181	2751	711	701	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	535	Total	C	N	O	S	0	0
			4181	2751	711	701	18		

- Molecule 11 is a protein called Cytochrome bc1 complex cytochrome c subunit.

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

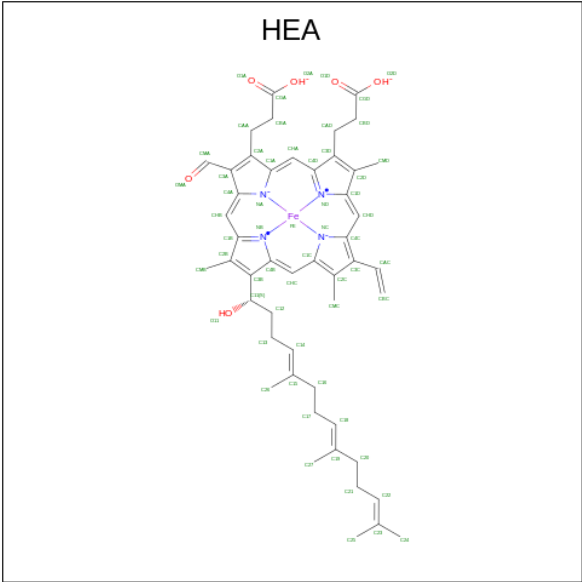
- Molecule 12 is a protein called Rieske iron-sulfur protein QcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	382	Total	C	N	O	S	0	0
			2977	1924	504	538	11		
12	M	382	Total	C	N	O	S	0	0
			2977	1924	504	538	11		

- Molecule 13 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

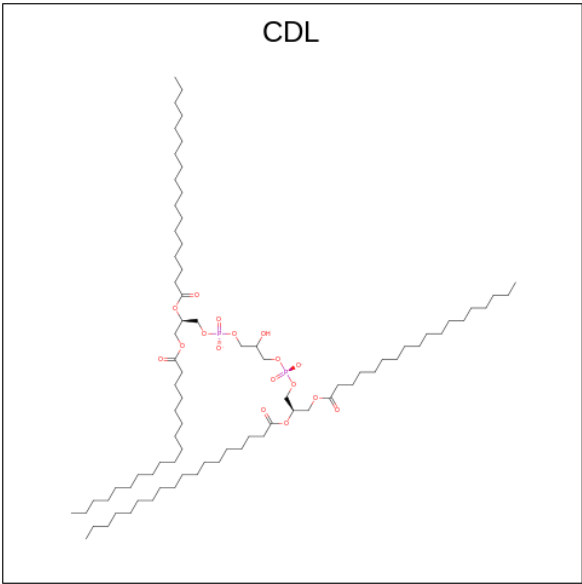
Mol	Chain	Residues	Atoms		AltConf
13	E	2	Total	Cu	0
			2	2	
13	F	2	Total	Cu	0
			2	2	
13	Q	2	Total	Cu	0
			2	2	
13	R	2	Total	Cu	0
			2	2	

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



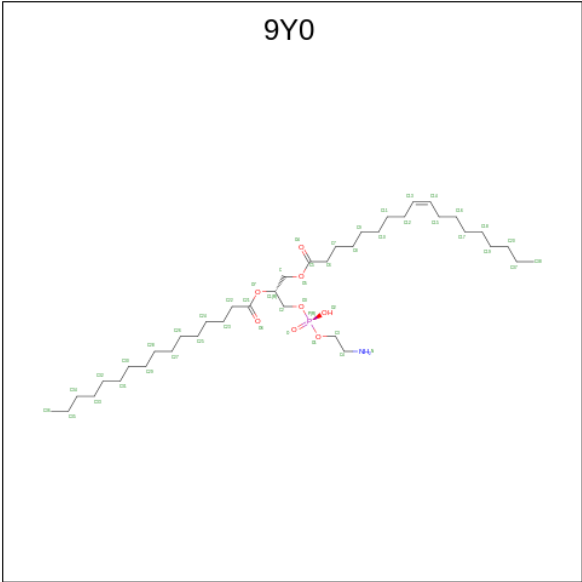
Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



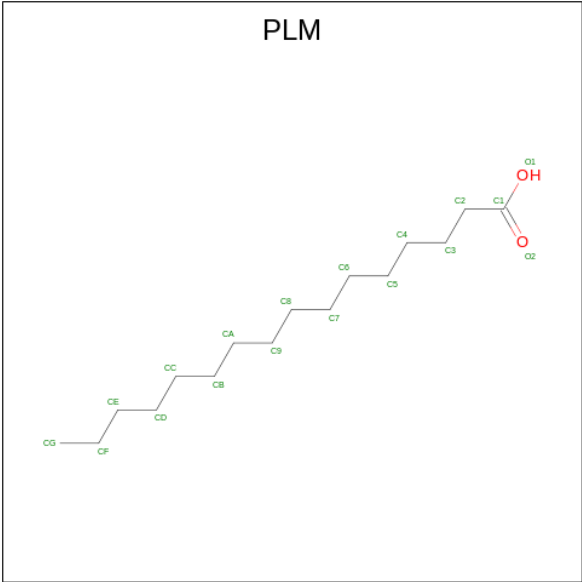
Mol	Chain	Residues	Atoms				AltConf
15	F	1	Total	C	O	P	0
			76	57	17	2	
15	F	1	Total	C	O	P	0
			81	62	17	2	
15	H	1	Total	C	O	P	0
			79	60	17	2	
15	D	1	Total	C	O	P	0
			88	69	17	2	
15	B	1	Total	C	O	P	0
			74	55	17	2	
15	B	1	Total	C	O	P	0
			77	58	17	2	
15	B	1	Total	C	O	P	0
			79	60	17	2	
15	B	1	Total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

- Molecule 16 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: C₃₉H₇₆NO₈P).



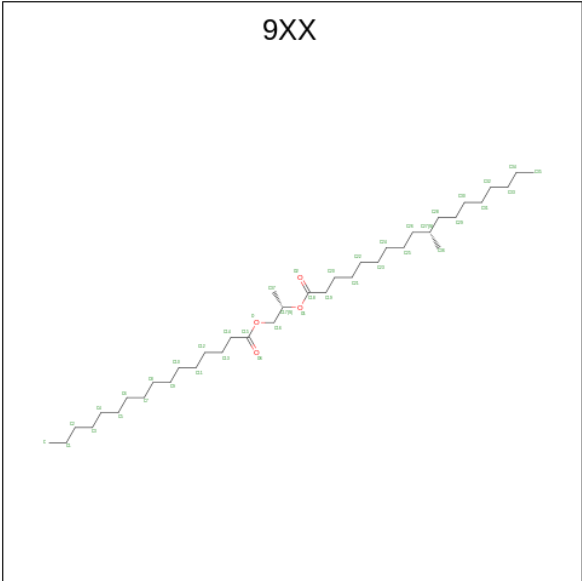
Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
16	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
16	K	1	Total	C	N	O	P	0
			38	28	1	8	1	
16	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
16	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
16	S	1	Total	C	N	O	P	0
			43	33	1	8	1	
16	P	1	Total	C	N	O	P	0
			41	31	1	8	1	
16	W	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 17 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



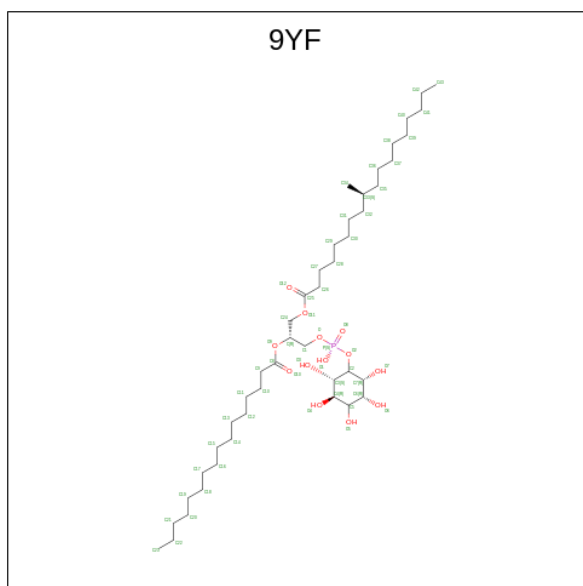
Mol	Chain	Residues	Atoms			AltConf
17	Y	1	Total	C	O	0
			11	10	1	
17	K	1	Total	C	O	0
			17	16	1	
17	Z	1	Total	C	O	0
			11	10	1	
17	W	1	Total	C	O	0
			17	16	1	

- Molecule 18 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C₃₈H₇₄O₄).



Mol	Chain	Residues	Atoms			AltConf
18	Y	1	Total	C	O	0
			32	28	4	
18	K	1	Total	C	O	0
			42	38	4	
18	Z	1	Total	C	O	0
			32	28	4	
18	W	1	Total	C	O	0
			42	38	4	

- 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: C₄₄H₈₅O₁₃P).



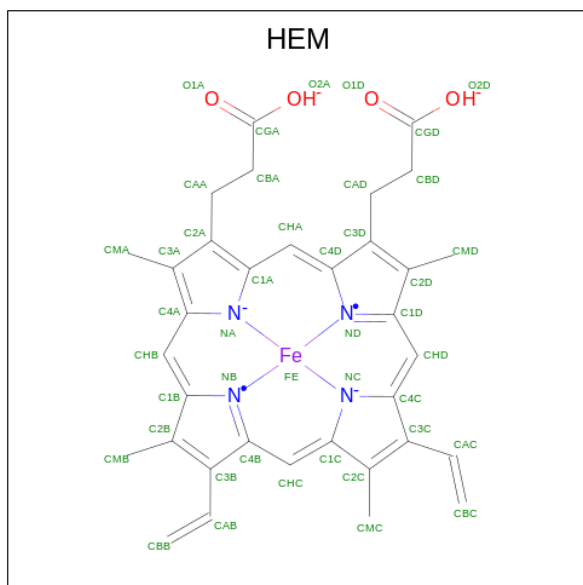
Mol	Chain	Residues	Atoms				AltConf
19	K	1	Total	C	O	P	0
			58	44	13	1	
19	C	1	Total	C	O	P	0
			58	44	13	1	
19	A	1	Total	C	O	P	0
			58	44	13	1	
19	A	1	Total	C	O	P	0
			58	44	13	1	
19	W	1	Total	C	O	P	0
			58	44	13	1	
19	O	1	Total	C	O	P	0
			58	44	13	1	
19	M	1	Total	C	O	P	0
			58	44	13	1	

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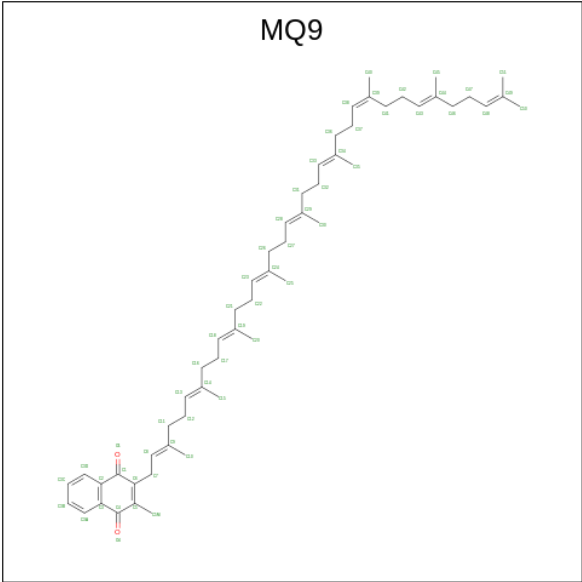
Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



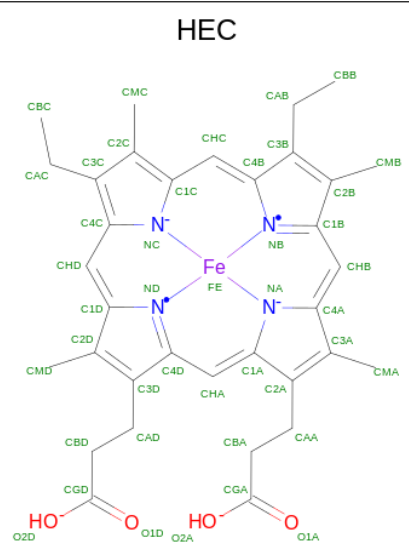
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
20	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	N	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
20	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 21 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



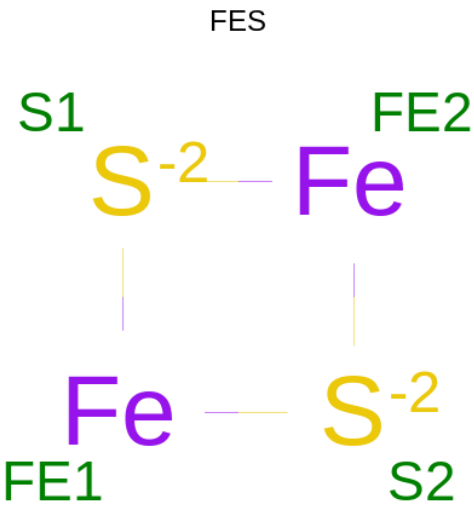
Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	C	O	0
			43	41	2	
21	B	1	Total	C	O	0
			48	46	2	
21	B	1	Total	C	O	0
			58	56	2	
21	B	1	Total	C	O	0
			43	41	2	
21	C	1	Total	C	O	0
			58	56	2	
21	N	1	Total	C	O	0
			43	41	2	
21	N	1	Total	C	O	0
			48	46	2	
21	N	1	Total	C	O	0
			58	56	2	
21	N	1	Total	C	O	0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

- Molecule 22 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

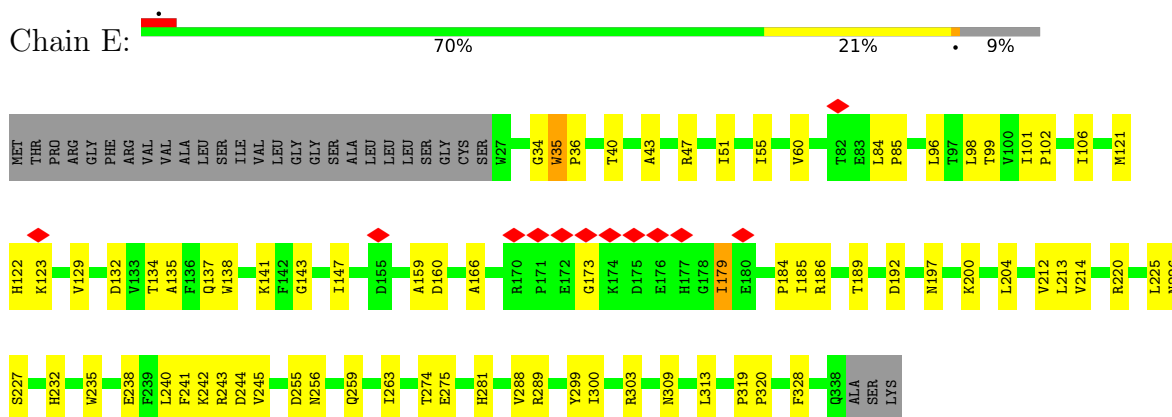


Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total 4	Fe 2	S 2	0
23	M	1	Total 4	Fe 2	S 2	0

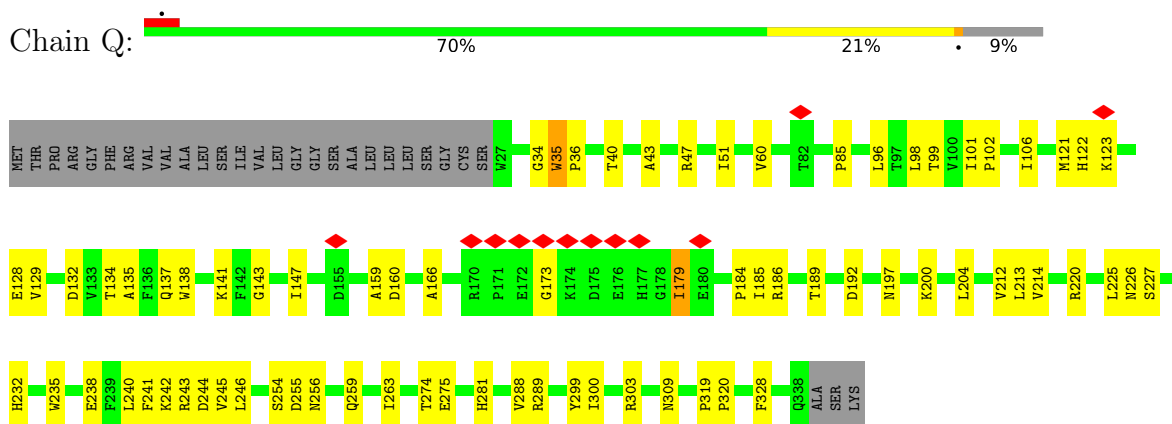
3 Residue-property plots

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

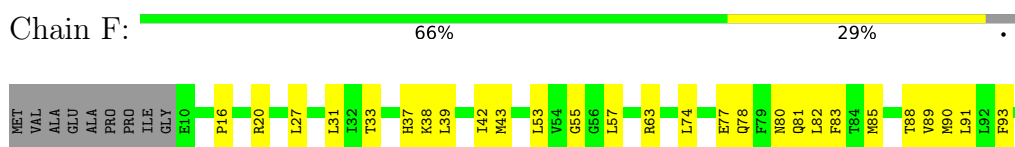
• Molecule 1: Cytochrome c oxidase subunit 2

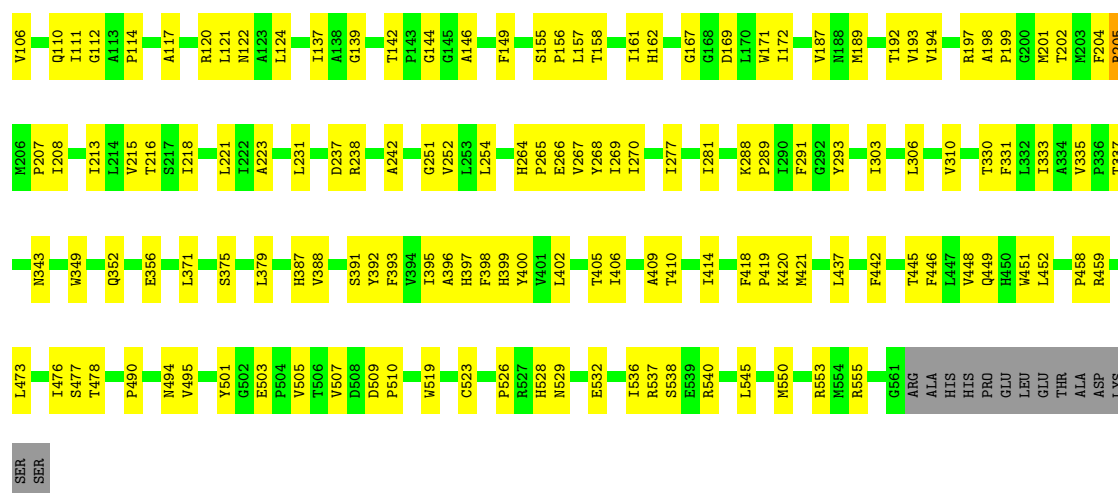


• Molecule 1: Cytochrome c oxidase subunit 2



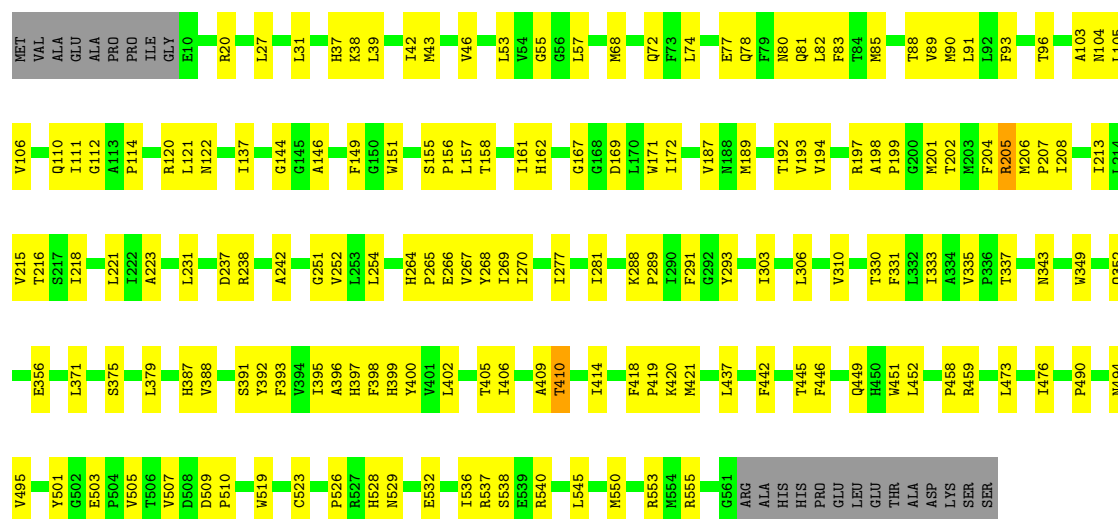
• Molecule 2: Cytochrome c oxidase subunit 1





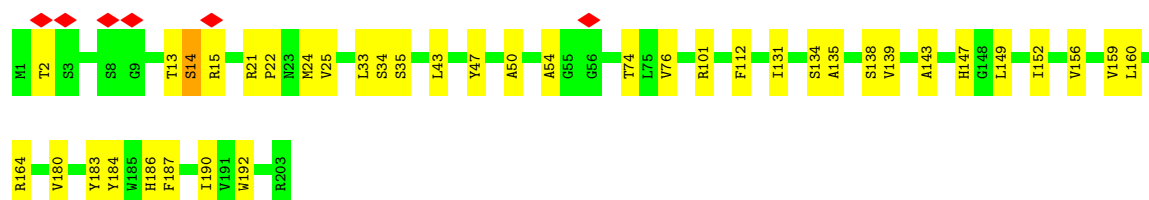
• Molecule 2: Cytochrome c oxidase subunit 1

Chain R: 67% 28%



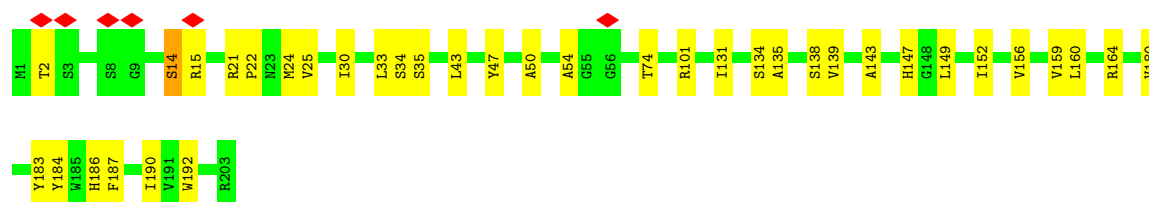
• Molecule 3: Cytochrome c oxidase subunit 3

Chain G: 81% 19%



• Molecule 3: Cytochrome c oxidase subunit 3

Chain S: 82% 18%



- Molecule 4: Cytochrome c oxidase polypeptide 4

Chain H:

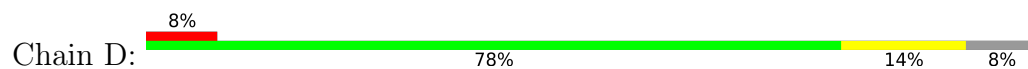


- Molecule 4: Cytochrome c oxidase polypeptide 4

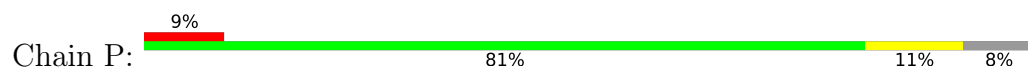
Chain T:



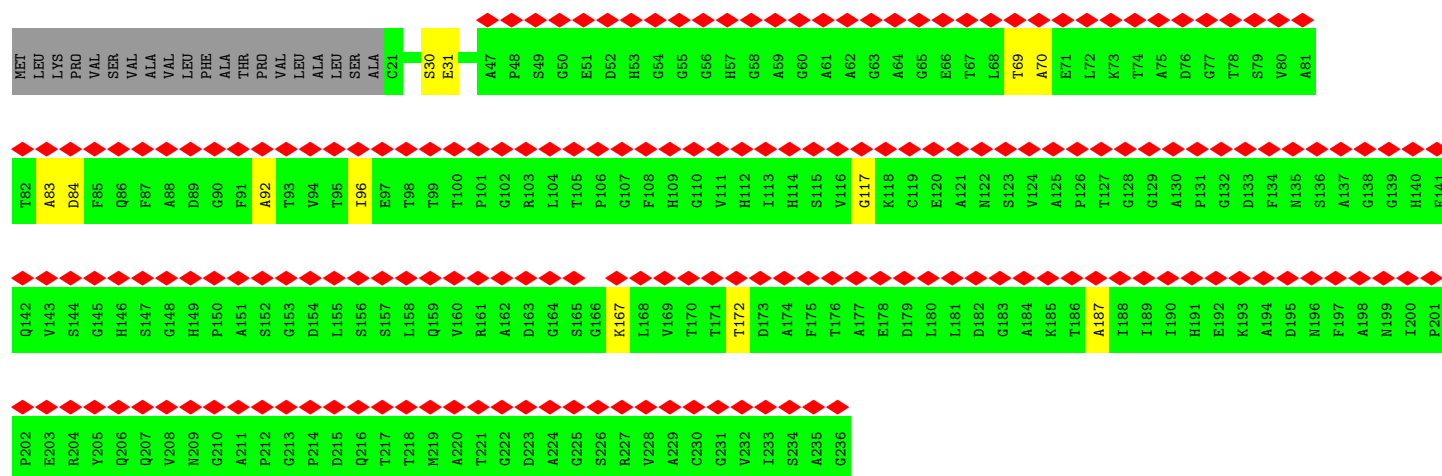
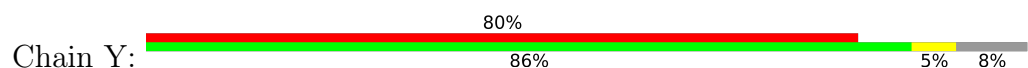
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1



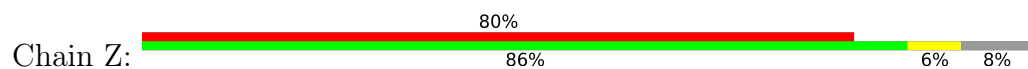
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

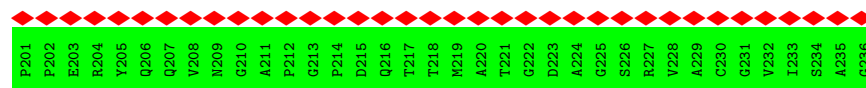


- Molecule 8: Superoxide dismutase [Cu-Zn]

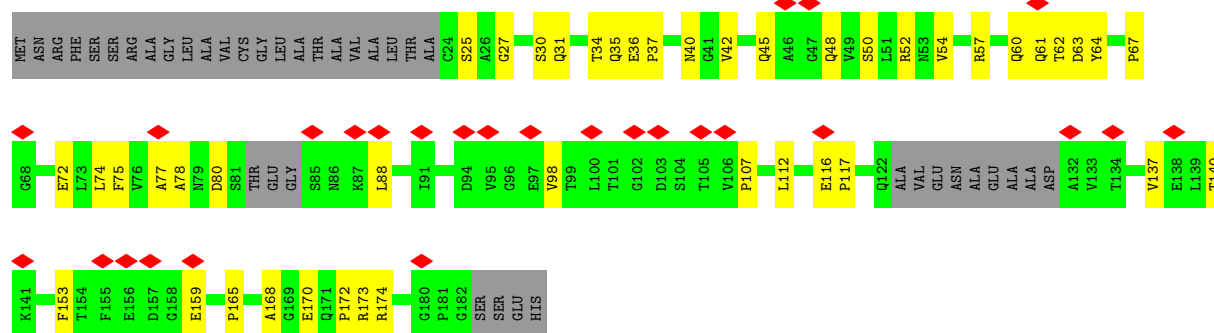


- Molecule 8: Superoxide dismutase [Cu-Zn]

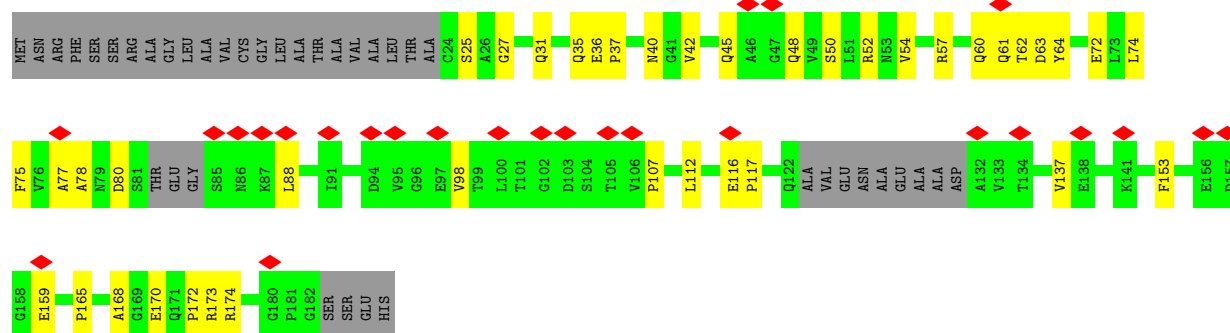




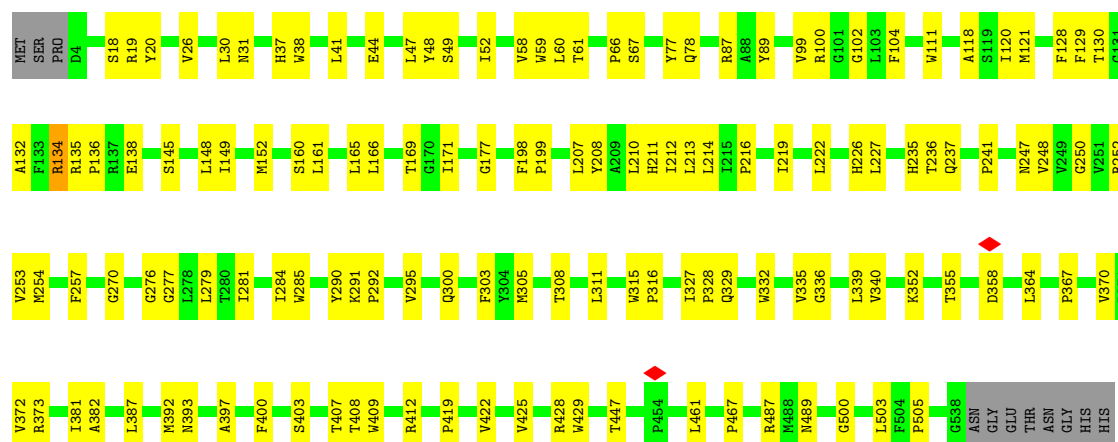
• Molecule 9: LpqE protein

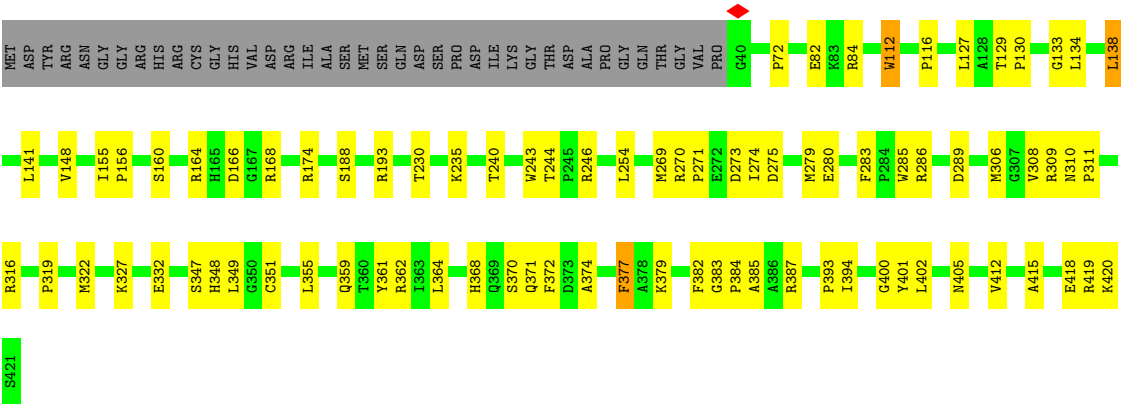


• Molecule 9: LpqE protein

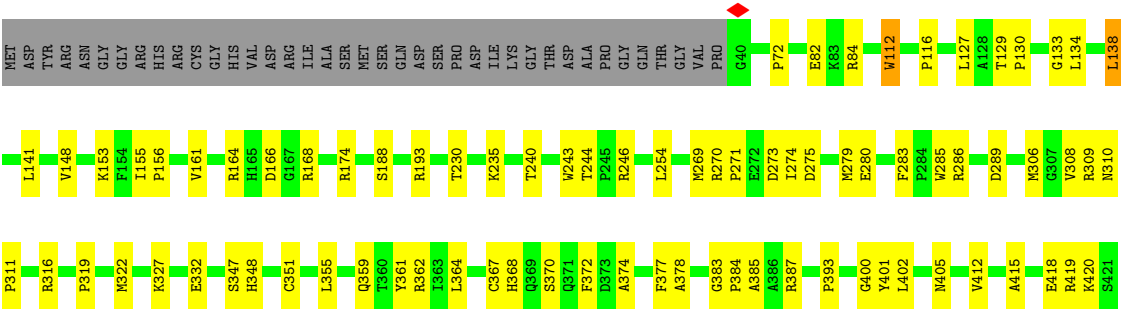


• Molecule 10: Ubiquinol-cytochrome c reductase cytochrome b subunit





• Molecule 12: Rieske iron-sulfur protein QcrA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	202215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.563	Depositor
Minimum map value	-0.271	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0452	Depositor
Map size ($\text{\AA}$)	379.59998, 379.59998, 379.59998	wwPDB
Map dimensions	292, 292, 292	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.36	0/2534	0.67	0/3451
1	Q	0.36	0/2534	0.67	0/3451
2	F	0.48	0/4533	0.78	1/6192 (0.0%)
2	R	0.48	0/4533	0.78	1/6192 (0.0%)
3	G	0.37	0/1608	0.73	0/2195
3	S	0.37	0/1608	0.72	0/2195
4	H	0.34	0/1112	0.62	0/1524
4	T	0.35	0/1112	0.62	0/1524
5	I	0.30	0/523	0.60	0/714
5	U	0.30	0/523	0.60	0/714
6	J	0.28	0/1059	0.58	0/1446
6	V	0.28	0/1059	0.58	0/1446
7	D	0.30	0/757	0.56	0/1027
7	P	0.30	0/757	0.56	0/1027
8	Y	0.18	0/1099	0.44	0/1519
8	Z	0.18	0/1099	0.45	0/1519
9	K	0.30	0/1088	0.65	0/1490
9	W	0.28	0/1088	0.66	0/1490
10	B	0.40	0/4314	0.64	2/5882 (0.0%)
10	N	0.40	0/4314	0.65	2/5882 (0.0%)
11	C	0.39	0/1660	0.67	0/2250
11	O	0.39	0/1660	0.67	0/2250
12	A	0.36	0/3056	0.69	3/4142 (0.1%)
12	M	0.36	0/3056	0.71	5/4142 (0.1%)
All	All	0.38	0/46686	0.68	14/63664 (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
1	E	0	3
1	Q	0	3
2	F	0	4
2	R	0	4
3	G	0	3
3	S	0	3
9	K	0	1
9	W	0	1
10	B	0	1
10	N	0	1
All	All	0	24

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	378	ALA	CA-C-N	7.35	130.93	120.49
12	M	378	ALA	C-N-CA	7.35	130.93	120.49
12	M	377	PHE	N-CA-C	-6.50	98.65	108.52
12	A	377	PHE	N-CA-C	-6.49	97.75	108.07
2	R	155	SER	N-CA-C	6.47	122.50	113.57

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	160	ASP	Peptide
1	E	328	PHE	Peptide
1	E	35	TRP	Peptide
2	F	356	GLU	Peptide
2	F	437	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2465	0	2392	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	2465	0	2392	51	0
2	F	4373	0	4347	118	0
2	R	4373	0	4347	114	0
3	G	1560	0	1547	27	0
3	S	1560	0	1547	25	0
4	H	1077	0	1058	18	0
4	T	1077	0	1058	16	0
5	I	507	0	516	8	0
5	U	507	0	516	6	0
6	J	1041	0	1052	20	0
6	V	1041	0	1052	18	0
7	D	736	0	717	13	0
7	P	736	0	717	11	0
8	Y	1092	0	640	7	0
8	Z	1092	0	640	8	0
9	K	1072	0	1045	29	0
9	W	1072	0	1045	26	0
10	B	4181	0	4201	103	0
10	N	4181	0	4201	102	0
11	C	1623	0	1564	43	0
11	O	1623	0	1564	41	0
12	A	2977	0	2986	76	0
12	M	2977	0	2986	63	0
13	E	2	0	0	0	0
13	F	2	0	0	0	0
13	Q	2	0	0	0	0
13	R	2	0	0	0	0
14	F	120	0	107	11	0
14	R	120	0	107	11	0
15	A	95	0	143	3	0
15	B	296	0	371	14	0
15	D	88	0	126	6	0
15	F	157	0	208	6	0
15	H	79	0	105	2	0
15	M	95	0	143	3	0
15	N	296	0	371	16	0
15	P	88	0	126	5	0
15	R	157	0	208	8	0
15	T	79	0	105	2	0
16	B	98	0	0	0	0
16	D	41	0	0	0	0
16	G	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	38	0	0	0	0
16	P	41	0	0	0	0
16	S	43	0	0	0	0
16	W	38	0	0	0	0
17	K	17	0	31	1	0
17	W	17	0	31	0	0
17	Y	11	0	16	0	0
17	Z	11	0	16	0	0
18	K	42	0	0	0	0
18	W	42	0	0	0	0
18	Y	32	0	0	0	0
18	Z	32	0	0	0	0
19	A	116	0	0	17	0
19	C	58	0	0	1	0
19	K	58	0	0	1	0
19	M	116	0	0	6	0
19	O	58	0	0	1	0
19	W	58	0	0	1	0
20	B	85	0	57	3	0
20	N	85	0	57	3	0
21	B	192	0	247	7	0
21	C	58	0	80	7	0
21	N	192	0	247	6	0
21	O	58	0	80	7	0
22	C	86	0	64	5	0
22	O	86	0	64	5	0
23	A	4	0	0	1	0
23	M	4	0	0	2	0
All	All	48946	0	47240	879	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 879 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)
2:F:398:PHE:O	2:F:402:LEU:HB3	1.65	0.96
2:R:398:PHE:O	2:R:402:LEU:HB3	1.66	0.95
12:A:355:LEU:HB2	12:A:364:LEU:O	1.70	0.91
12:M:355:LEU:HB2	12:M:364:LEU:O	1.69	0.90
2:F:88:THR:HG21	2:F:171:TRP:HE1	1.44	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	310/341 (91%)	269 (87%)	41 (13%)	0	100	100
1	Q	310/341 (91%)	268 (86%)	42 (14%)	0	100	100
2	F	550/575 (96%)	506 (92%)	44 (8%)	0	100	100
2	R	550/575 (96%)	507 (92%)	43 (8%)	0	100	100
3	G	201/203 (99%)	187 (93%)	13 (6%)	1 (0%)	24	57
3	S	201/203 (99%)	187 (93%)	13 (6%)	1 (0%)	24	57
4	H	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
4	T	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
5	I	63/79 (80%)	57 (90%)	6 (10%)	0	100	100
5	U	63/79 (80%)	57 (90%)	6 (10%)	0	100	100
6	J	143/157 (91%)	129 (90%)	14 (10%)	0	100	100
6	V	143/157 (91%)	129 (90%)	14 (10%)	0	100	100
7	D	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
7	P	88/100 (88%)	83 (94%)	5 (6%)	0	100	100
8	Y	214/236 (91%)	185 (86%)	29 (14%)	0	100	100
8	Z	214/236 (91%)	188 (88%)	26 (12%)	0	100	100
9	K	141/186 (76%)	118 (84%)	22 (16%)	1 (1%)	18	51
9	W	141/186 (76%)	116 (82%)	24 (17%)	1 (1%)	18	51
10	B	533/546 (98%)	492 (92%)	40 (8%)	1 (0%)	43	74
10	N	533/546 (98%)	492 (92%)	40 (8%)	1 (0%)	43	74
11	C	221/294 (75%)	197 (89%)	23 (10%)	1 (0%)	24	57
11	O	221/294 (75%)	196 (89%)	24 (11%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	A	380/421 (90%)	337 (89%)	43 (11%)	0	100	100
12	M	380/421 (90%)	336 (88%)	44 (12%)	0	100	100
All	All	5962/6554 (91%)	5370 (90%)	584 (10%)	8 (0%)	49	79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	14	SER
3	S	14	SER
11	C	226	PRO
11	O	226	PRO
9	K	117	PRO

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	260/288 (90%)	258 (99%)	2 (1%)	73	77
1	Q	260/288 (90%)	258 (99%)	2 (1%)	73	77
2	F	453/471 (96%)	450 (99%)	3 (1%)	76	78
2	R	453/471 (96%)	449 (99%)	4 (1%)	70	76
3	G	155/161 (96%)	155 (100%)	0	100	100
3	S	155/161 (96%)	155 (100%)	0	100	100
4	H	106/106 (100%)	106 (100%)	0	100	100
4	T	106/106 (100%)	106 (100%)	0	100	100
5	I	52/59 (88%)	52 (100%)	0	100	100
5	U	52/59 (88%)	52 (100%)	0	100	100
6	J	107/114 (94%)	106 (99%)	1 (1%)	70	76
6	V	107/114 (94%)	106 (99%)	1 (1%)	70	76
7	D	76/83 (92%)	76 (100%)	0	100	100
7	P	76/83 (92%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Y	20/167 (12%)	20 (100%)	0	100	100
8	Z	20/167 (12%)	20 (100%)	0	100	100
9	K	120/146 (82%)	119 (99%)	1 (1%)	73	77
9	W	120/146 (82%)	119 (99%)	1 (1%)	73	77
10	B	429/438 (98%)	426 (99%)	3 (1%)	76	78
10	N	429/438 (98%)	426 (99%)	3 (1%)	76	78
11	C	163/220 (74%)	163 (100%)	0	100	100
11	O	163/220 (74%)	163 (100%)	0	100	100
12	A	312/343 (91%)	311 (100%)	1 (0%)	86	83
12	M	312/343 (91%)	311 (100%)	1 (0%)	86	83
All	All	4506/5192 (87%)	4483 (100%)	23 (0%)	78	80

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	205	ARG
6	V	73	LEU
2	R	452	LEU
9	W	88	LEU
9	K	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
11	O	153	ASN
11	O	169	GLN
12	M	369	GLN
11	C	153	ASN
11	C	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 8 are monoatomic - leaving 66 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	$\# Z > 2$
19	9YF	C	303	-	58,58,58	0.85	4 (6%)	69,71,71	0.94	3 (4%)
15	CDL	F	606	-	80,80,99	1.23	6 (7%)	86,92,111	1.00	5 (5%)
22	HEC	O	302	11	50,50,50	1.70	6 (12%)	68,82,82	2.11	18 (26%)
15	CDL	B	611	-	65,65,99	1.35	8 (12%)	71,77,111	1.15	4 (5%)
15	CDL	N	606	-	78,78,99	1.25	7 (8%)	84,90,111	0.98	5 (5%)
16	9Y0	B	606	15	48,48,48	1.30	5 (10%)	51,53,53	0.89	2 (3%)
19	9YF	M	504	-	58,58,58	1.16	4 (6%)	69,71,71	1.11	5 (7%)
21	MQ9	N	607	-	44,44,59	3.93	15 (34%)	54,57,75	3.23	23 (42%)
18	9XX	K	204	9	41,41,41	1.16	3 (7%)	44,44,44	1.15	3 (6%)
16	9Y0	S	301	-	42,42,48	1.35	5 (11%)	44,47,53	0.85	2 (4%)
17	PLM	Y	301	8	10,10,17	0.56	0	9,9,17	0.56	0
16	9Y0	G	301	-	42,42,48	1.35	5 (11%)	44,47,53	0.85	2 (4%)
15	CDL	F	605	-	75,75,99	1.25	7 (9%)	81,87,111	1.04	4 (4%)
15	CDL	N	601	-	65,65,99	1.35	7 (10%)	71,77,111	1.15	4 (5%)
16	9Y0	B	612	15	48,48,48	1.30	5 (10%)	51,53,53	0.89	2 (3%)
21	MQ9	N	609	-	59,59,59	3.97	19 (32%)	72,75,75	3.44	35 (48%)
19	9YF	W	202	-	58,58,58	0.88	4 (6%)	69,71,71	0.96	3 (4%)
15	CDL	R	606	-	80,80,99	1.22	6 (7%)	86,92,111	1.00	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CDL	B	605	-	78,78,99	1.25	7 (8%)	84,90,111	0.98	5 (5%)
20	HEM	B	601	10	49,49,50	1.20	4 (8%)	66,81,82	1.40	9 (13%)
19	9YF	K	202	-	58,58,58	0.88	4 (6%)	69,71,71	0.94	3 (4%)
16	9Y0	W	201	-	37,37,48	1.42	4 (10%)	40,42,53	1.00	2 (5%)
23	FES	M	502	12	0,4,4	-	-	-	-	-
16	9Y0	K	201	-	37,37,48	1.42	3 (8%)	40,42,53	1.02	2 (5%)
14	HEA	R	602	2	66,67,67	5.49	24 (36%)	78,103,103	5.14	56 (71%)
18	9XX	Z	302	8	31,31,41	1.27	3 (9%)	34,34,44	1.13	2 (5%)
17	PLM	Z	301	8	10,10,17	0.57	0	9,9,17	0.56	0
22	HEC	O	301	11	50,50,50	1.78	6 (12%)	68,82,82	1.54	8 (11%)
15	CDL	N	605	-	76,76,99	1.26	7 (9%)	82,88,111	1.08	5 (6%)
21	MQ9	C	304	-	59,59,59	3.89	18 (30%)	72,75,75	3.43	31 (43%)
16	9Y0	D	202	-	40,40,48	1.37	4 (10%)	43,45,53	1.00	2 (4%)
19	9YF	A	504	-	58,58,58	0.87	3 (5%)	69,71,71	0.96	4 (5%)
22	HEC	C	302	11	50,50,50	1.70	6 (12%)	68,82,82	2.11	18 (26%)
20	HEM	B	602	10	50,50,50	1.49	7 (14%)	66,82,82	1.13	7 (10%)
15	CDL	D	201	-	87,87,99	1.20	8 (9%)	93,99,111	0.94	5 (5%)
15	CDL	B	604	-	76,76,99	1.25	7 (9%)	82,88,111	1.08	5 (6%)
21	MQ9	B	610	-	44,44,59	3.95	16 (36%)	54,57,75	3.20	22 (40%)
21	MQ9	O	304	-	59,59,59	3.89	18 (30%)	72,75,75	3.43	32 (44%)
16	9Y0	P	202	-	40,40,48	1.38	4 (10%)	43,45,53	0.99	2 (4%)
15	CDL	M	503	-	94,94,99	1.19	6 (6%)	100,106,111	0.93	5 (5%)
17	PLM	K	203	9	16,16,17	0.47	0	15,15,17	0.44	0
21	MQ9	N	610	-	44,44,59	3.95	16 (36%)	54,57,75	3.20	22 (40%)
15	CDL	R	605	-	75,75,99	1.25	7 (9%)	81,87,111	1.04	4 (4%)
19	9YF	M	501	-	58,58,58	0.87	3 (5%)	69,71,71	0.96	4 (5%)
14	HEA	F	602	2	66,67,67	5.49	24 (36%)	78,103,103	5.14	55 (70%)
15	CDL	P	201	-	87,87,99	1.20	8 (9%)	93,99,111	0.95	5 (5%)
15	CDL	N	604	16	73,73,99	1.32	7 (9%)	79,85,111	1.04	5 (6%)
19	9YF	O	303	-	58,58,58	0.85	4 (6%)	69,71,71	0.94	3 (4%)
14	HEA	R	601	2	66,67,67	5.11	20 (30%)	78,103,103	6.59	56 (71%)
19	9YF	A	503	-	58,58,58	1.16	4 (6%)	69,71,71	1.23	7 (10%)
15	CDL	T	201	-	78,78,99	1.25	7 (8%)	84,90,111	0.92	4 (4%)
22	HEC	C	301	11	50,50,50	1.78	6 (12%)	68,82,82	1.54	8 (11%)
15	CDL	B	603	16	73,73,99	1.32	7 (9%)	79,85,111	1.04	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	MQ9	B	608	-	49,49,59	3.95	16 (32%)	60,63,75	3.30	25 (41%)
15	CDL	A	502	-	94,94,99	1.19	6 (6%)	100,106,111	0.93	5 (5%)
21	MQ9	N	608	-	49,49,59	3.95	16 (32%)	60,63,75	3.31	26 (43%)
18	9XX	W	204	9	41,41,41	1.15	3 (7%)	44,44,44	1.11	3 (6%)
23	FES	A	501	12	0,4,4	-	-	-	-	-
20	HEM	N	602	10	49,49,50	1.20	4 (8%)	66,81,82	1.39	9 (13%)
15	CDL	H	201	-	78,78,99	1.25	7 (8%)	84,90,111	0.92	4 (4%)
18	9XX	Y	302	8	31,31,41	1.27	3 (9%)	34,34,44	1.14	2 (5%)
21	MQ9	B	609	-	59,59,59	3.97	19 (32%)	72,75,75	3.44	35 (48%)
20	HEM	N	603	10	50,50,50	1.49	7 (14%)	66,82,82	1.14	7 (10%)
14	HEA	F	601	2	66,67,67	5.10	20 (30%)	78,103,103	6.59	56 (71%)
21	MQ9	B	607	-	44,44,59	3.94	17 (38%)	54,57,75	3.23	23 (42%)
17	PLM	W	203	9	16,16,17	0.48	0	15,15,17	0.44	0

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
19	9YF	C	303	-	-	33/54/78/78	0/1/1/1
15	CDL	F	606	-	-	51/91/91/110	-
22	HEC	O	302	11	1/1/3/7	4/14/54/54	-
15	CDL	B	611	-	-	44/76/76/110	-
15	CDL	N	606	-	-	41/89/89/110	-
16	9Y0	B	606	15	-	33/52/52/52	-
19	9YF	M	504	-	-	29/54/78/78	0/1/1/1
21	MQ9	N	607	-	-	19/35/55/73	0/2/2/2
18	9XX	K	204	9	-	22/43/43/43	-
16	9Y0	S	301	-	-	23/46/46/52	-
17	PLM	Y	301	8	-	0/7/8/15	-
16	9Y0	G	301	-	-	22/46/46/52	-
15	CDL	F	605	-	-	39/86/86/110	-
15	CDL	N	601	-	-	42/76/76/110	-
16	9Y0	B	612	15	-	34/52/52/52	-
21	MQ9	N	609	-	-	25/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	9YF	W	202	-	-	24/54/78/78	0/1/1/1
15	CDL	R	606	-	-	49/91/91/110	-
15	CDL	B	605	-	-	42/89/89/110	-
20	HEM	B	601	10	-	4/12/52/54	-
19	9YF	K	202	-	-	28/54/78/78	0/1/1/1
16	9Y0	W	201	-	-	29/41/41/52	-
23	FES	M	502	12	-	-	0/1/1/1
16	9Y0	K	201	-	-	27/41/41/52	-
14	HEA	R	602	2	-	16/36/76/76	-
18	9XX	Z	302	8	-	13/33/33/43	-
17	PLM	Z	301	8	-	0/7/8/15	-
22	HEC	O	301	11	-	3/14/54/54	-
15	CDL	N	605	-	-	49/87/87/110	-
21	MQ9	C	304	-	-	31/53/73/73	0/2/2/2
16	9Y0	D	202	-	-	26/44/44/52	-
19	9YF	A	504	-	-	21/54/78/78	0/1/1/1
22	HEC	C	302	11	1/1/3/7	4/14/54/54	-
20	HEM	B	602	10	-	5/14/54/54	-
15	CDL	D	201	-	-	56/98/98/110	-
15	CDL	B	604	-	-	49/87/87/110	-
21	MQ9	B	610	-	-	19/35/55/73	0/2/2/2
21	MQ9	O	304	-	-	31/53/73/73	0/2/2/2
16	9Y0	P	202	-	-	26/44/44/52	-
15	CDL	M	503	-	-	61/105/105/110	-
17	PLM	K	203	9	-	4/13/14/15	-
21	MQ9	N	610	-	-	19/35/55/73	0/2/2/2
15	CDL	R	605	-	-	38/86/86/110	-
19	9YF	M	501	-	-	21/54/78/78	0/1/1/1
14	HEA	F	602	2	-	16/36/76/76	-
15	CDL	P	201	-	-	57/98/98/110	-
15	CDL	N	604	16	-	52/84/84/110	-
19	9YF	O	303	-	-	33/54/78/78	0/1/1/1
14	HEA	R	601	2	-	20/36/76/76	-
19	9YF	A	503	-	-	26/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	T	201	-	-	52/89/89/110	-
22	HEC	C	301	11	-	3/14/54/54	-
15	CDL	B	603	16	-	51/84/84/110	-
21	MQ9	B	608	-	-	21/41/61/73	0/2/2/2
15	CDL	A	502	-	-	61/105/105/110	-
21	MQ9	N	608	-	-	21/41/61/73	0/2/2/2
18	9XX	W	204	9	-	24/43/43/43	-
23	FES	A	501	12	-	-	0/1/1/1
20	HEM	N	602	10	-	4/12/52/54	-
15	CDL	H	201	-	-	52/89/89/110	-
18	9XX	Y	302	8	-	13/33/33/43	-
21	MQ9	B	609	-	-	25/53/73/73	0/2/2/2
20	HEM	N	603	10	-	5/14/54/54	-
14	HEA	F	601	2	-	20/36/76/76	-
21	MQ9	B	607	-	-	19/35/55/73	0/2/2/2
17	PLM	W	203	9	-	4/13/14/15	-

The worst 5 of 506 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	602	HEA	CHA-C1A	16.63	1.70	1.38
14	R	602	HEA	CHA-C1A	16.58	1.70	1.38
14	F	602	HEA	CHD-C1D	16.08	1.71	1.38
14	R	602	HEA	CHD-C1D	16.04	1.71	1.38
14	R	601	HEA	CHD-C1D	16.00	1.71	1.38

The worst 5 of 722 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	601	HEA	C3C-C4C-NC	18.72	121.77	110.25
14	R	601	HEA	C3C-C4C-NC	18.61	121.70	110.25
14	R	601	HEA	CHA-C4D-C3D	-14.29	103.83	124.84
14	F	601	HEA	CHA-C4D-C3D	-14.23	103.92	124.84
14	R	602	HEA	C1A-CHA-C4D	-14.20	95.42	126.06

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	302	HEC	NA
22	O	302	HEC	NA

5 of 1735 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	F	601	HEA	C1A-C2A-CAA-CBA
14	F	601	HEA	C3A-C2A-CAA-CBA
14	F	601	HEA	C2A-C3A-CMA-OMA
14	F	601	HEA	C4A-C3A-CMA-OMA
14	F	601	HEA	C17-C18-C19-C20

There are no ring outliers.

49 monomers are involved in 152 short contacts:

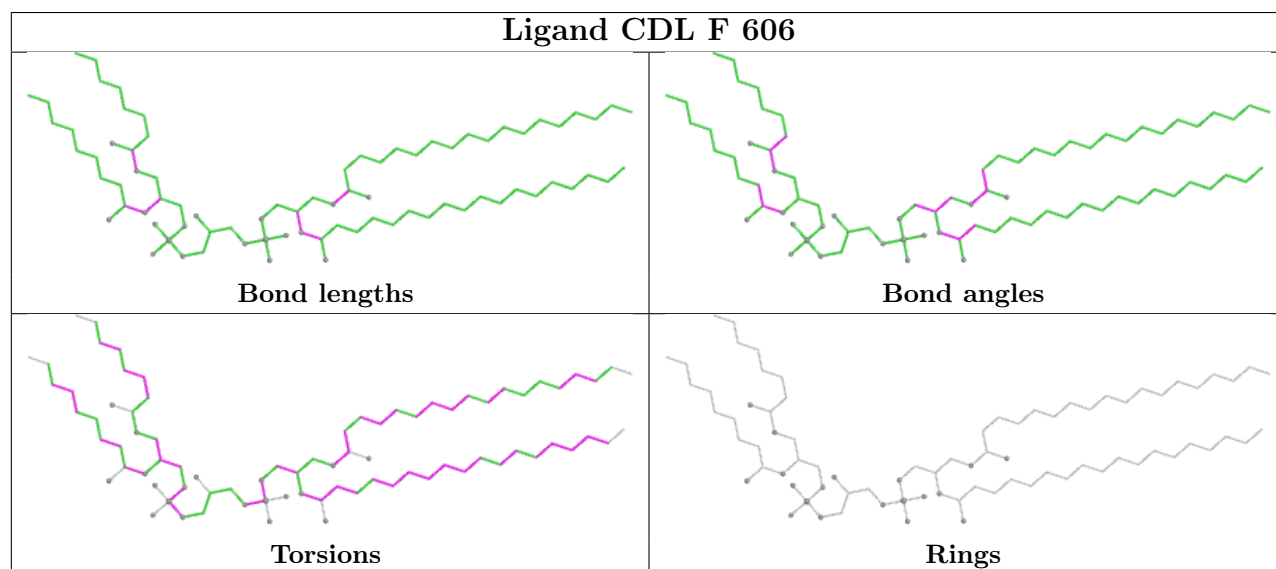
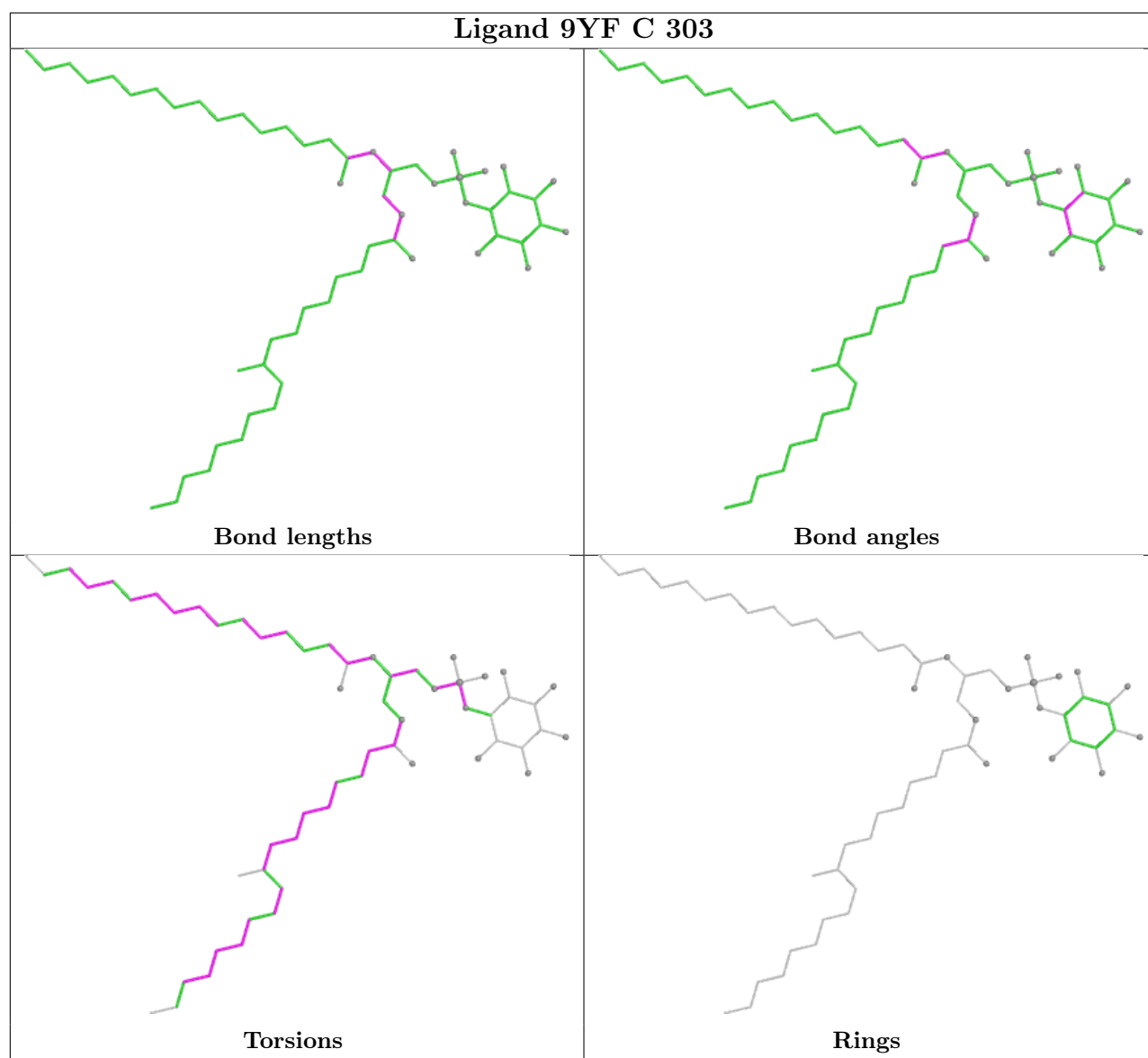
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	303	9YF	1	0
15	F	606	CDL	4	0
22	O	302	HEC	3	0
15	B	611	CDL	2	0
15	N	606	CDL	3	0
19	M	504	9YF	6	0
21	N	607	MQ9	1	0
15	F	605	CDL	2	0
15	N	601	CDL	2	0
21	N	609	MQ9	3	0
19	W	202	9YF	1	0
15	R	606	CDL	6	0
15	B	605	CDL	2	0
20	B	601	HEM	2	0
19	K	202	9YF	1	0
23	M	502	FES	2	0
14	R	602	HEA	5	0
22	O	301	HEC	2	0
15	N	605	CDL	4	0
21	C	304	MQ9	7	0
22	C	302	HEC	3	0
20	B	602	HEM	1	0
15	D	201	CDL	6	0
15	B	604	CDL	4	0
21	B	610	MQ9	1	0
21	O	304	MQ9	7	0
15	M	503	CDL	3	0

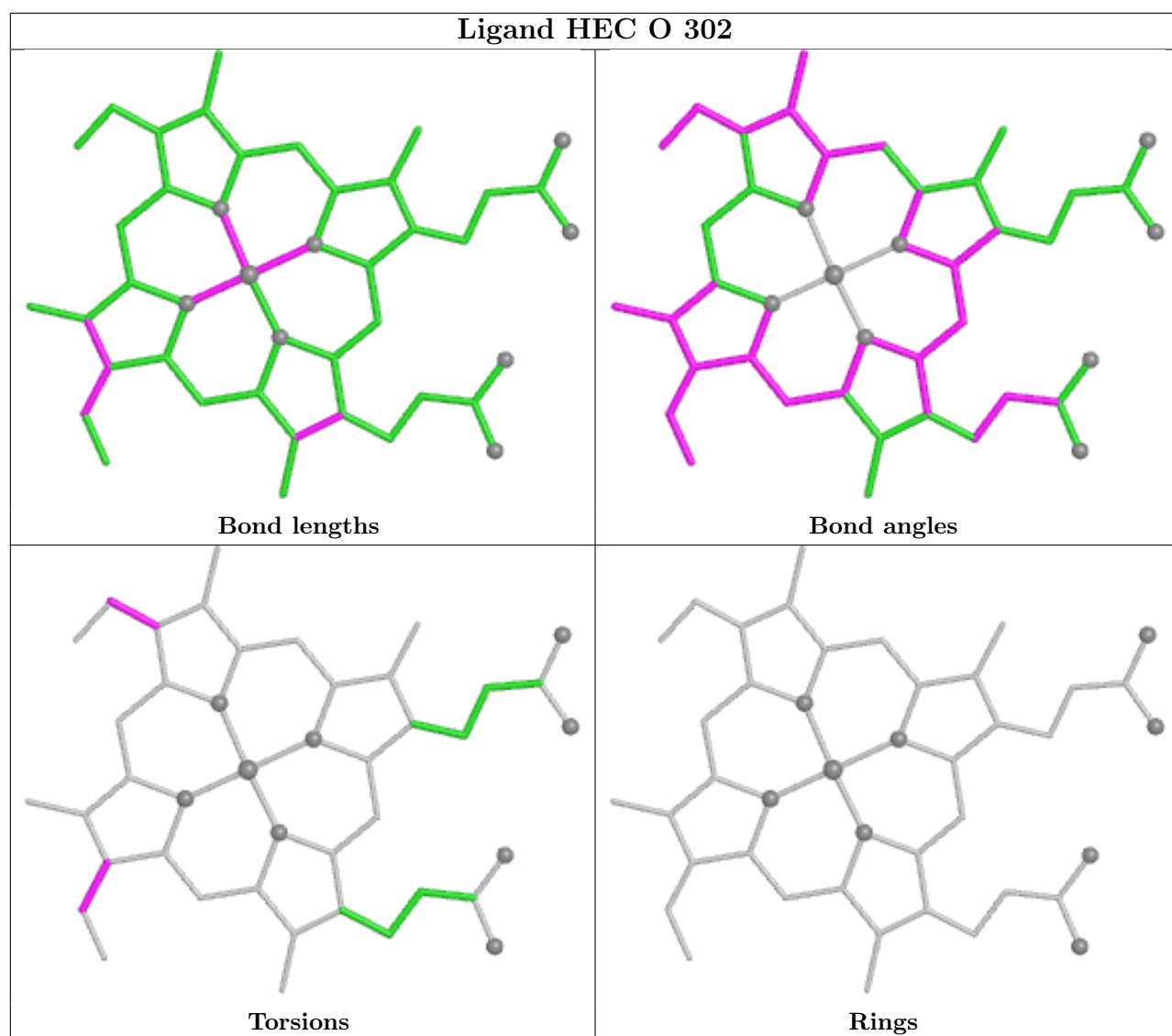
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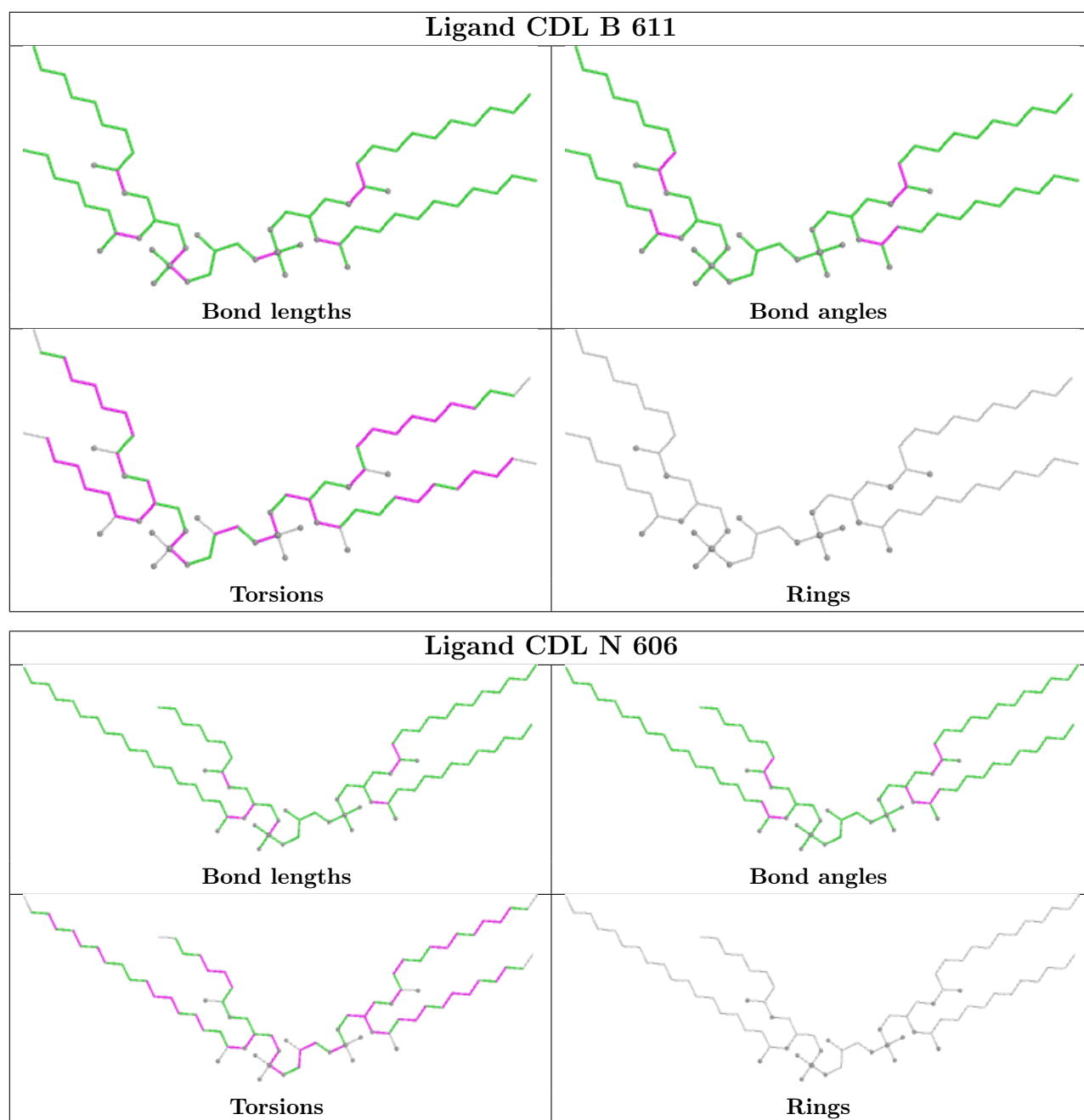
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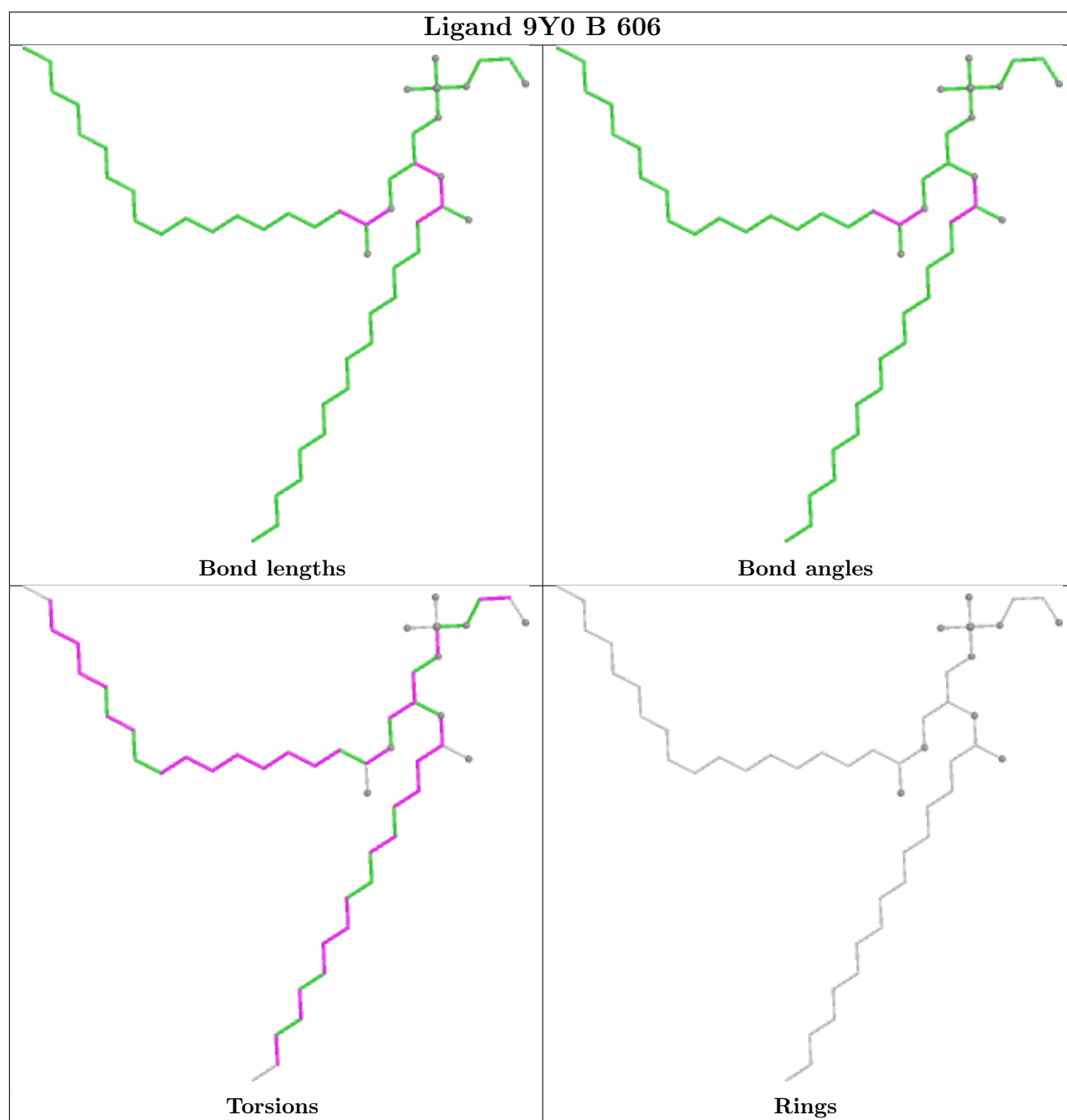
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	203	PLM	1	0
21	N	610	MQ9	1	0
15	R	605	CDL	2	0
14	F	602	HEA	6	0
15	P	201	CDL	5	0
15	N	604	CDL	8	0
19	O	303	9YF	1	0
14	R	601	HEA	6	0
19	A	503	9YF	17	0
15	T	201	CDL	2	0
22	C	301	HEC	2	0
15	B	603	CDL	7	0
21	B	608	MQ9	3	0
15	A	502	CDL	3	0
21	N	608	MQ9	1	0
23	A	501	FES	1	0
20	N	602	HEM	2	0
15	H	201	CDL	2	0
21	B	609	MQ9	2	0
20	N	603	HEM	1	0
14	F	601	HEA	5	0
21	B	607	MQ9	1	0

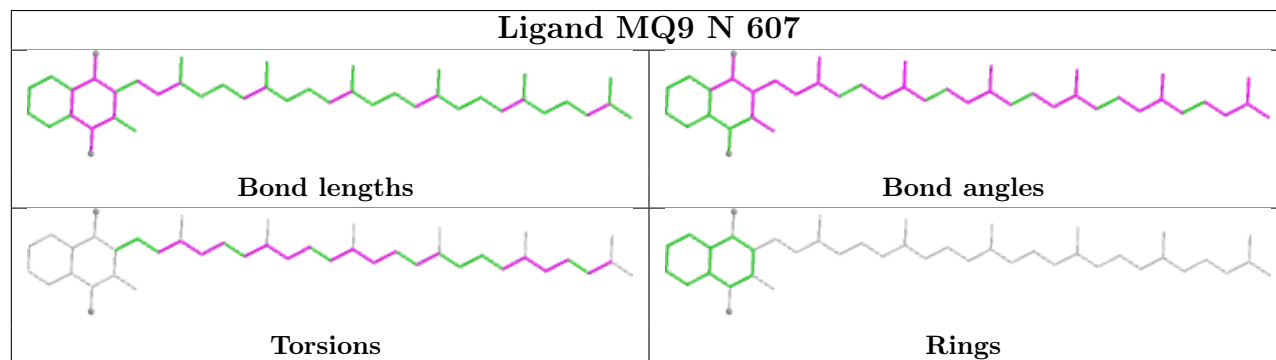
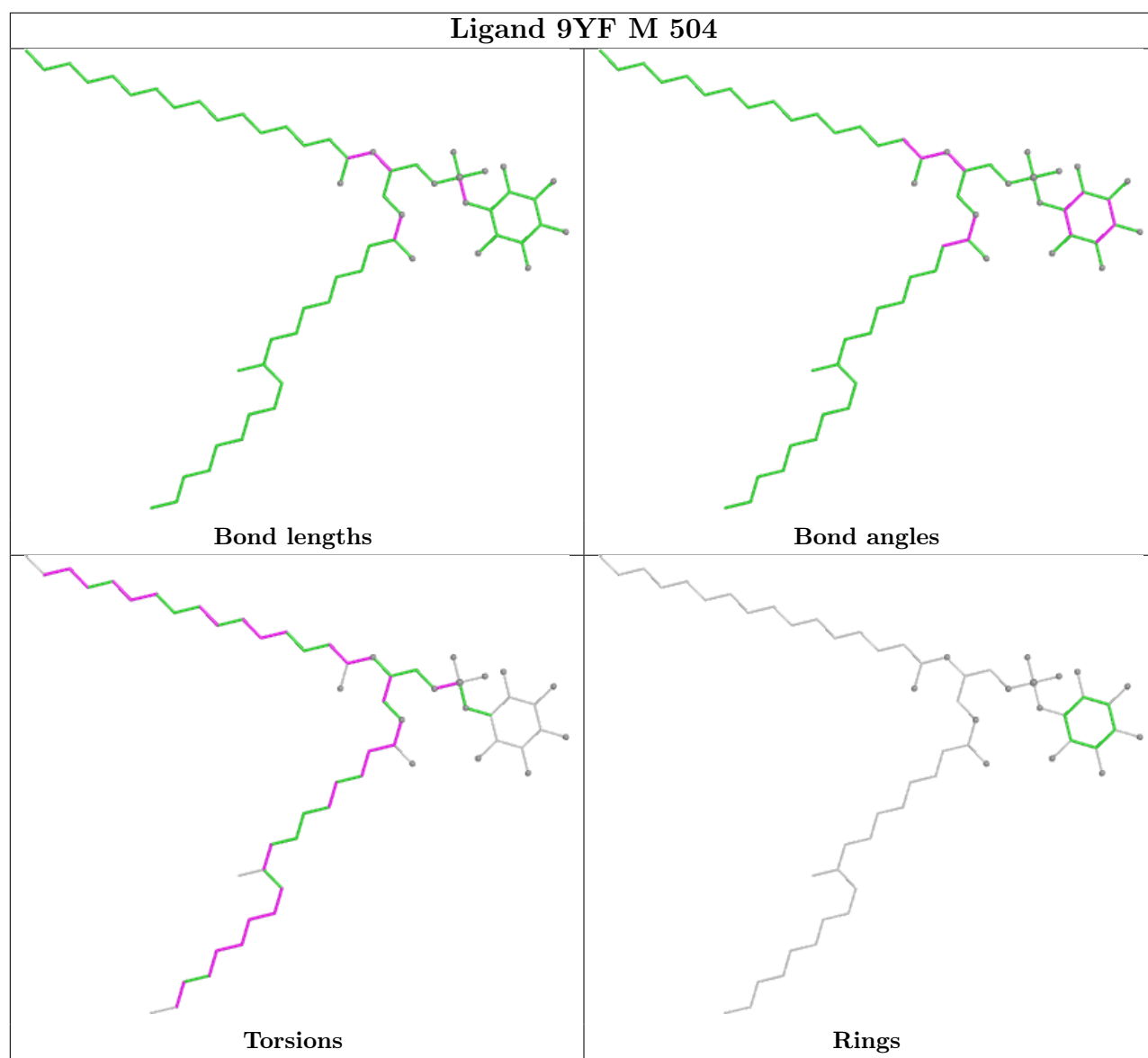
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

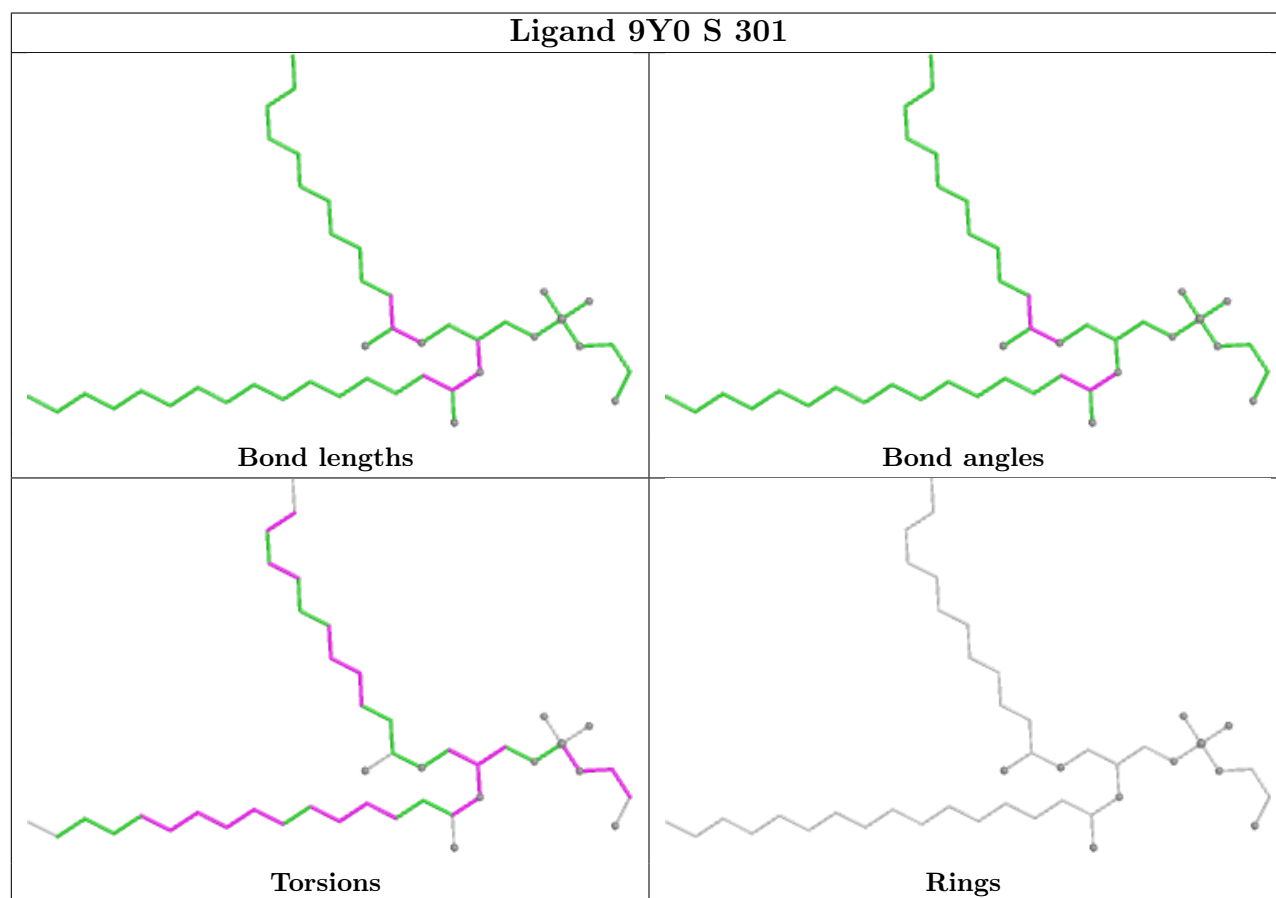
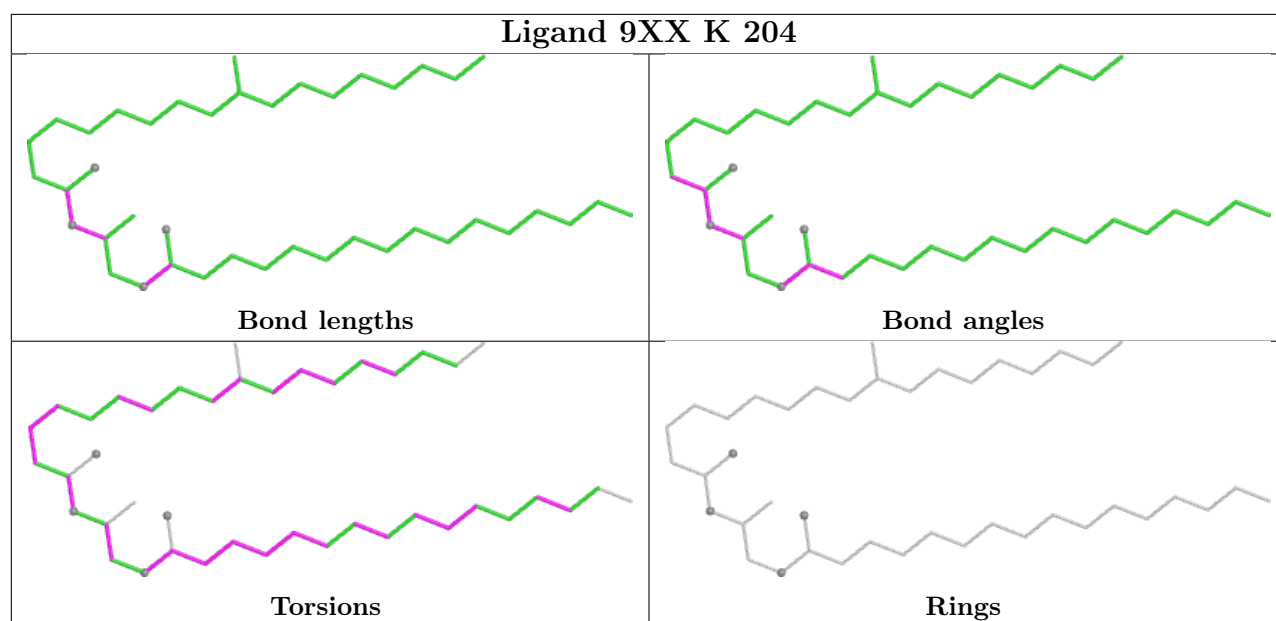


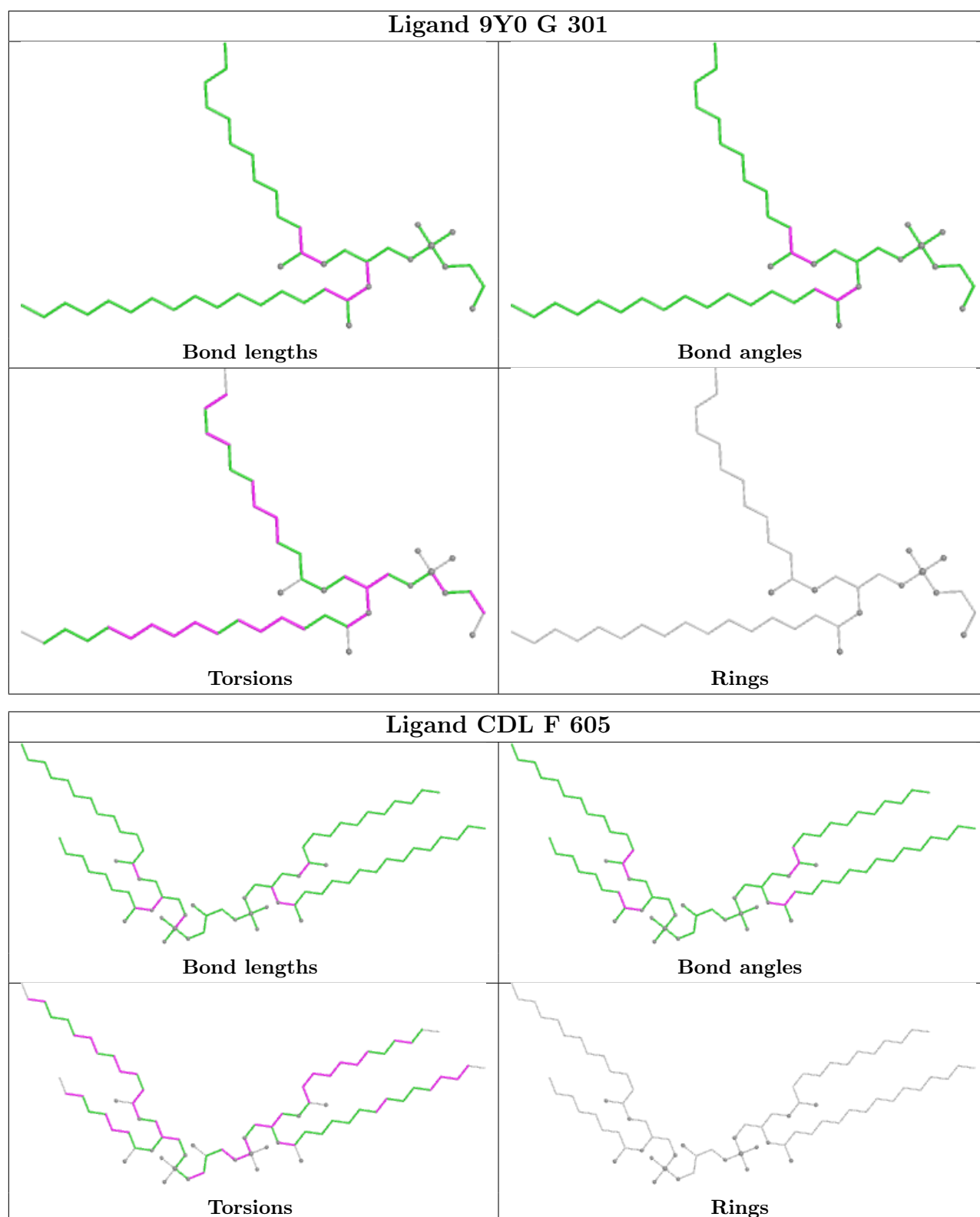


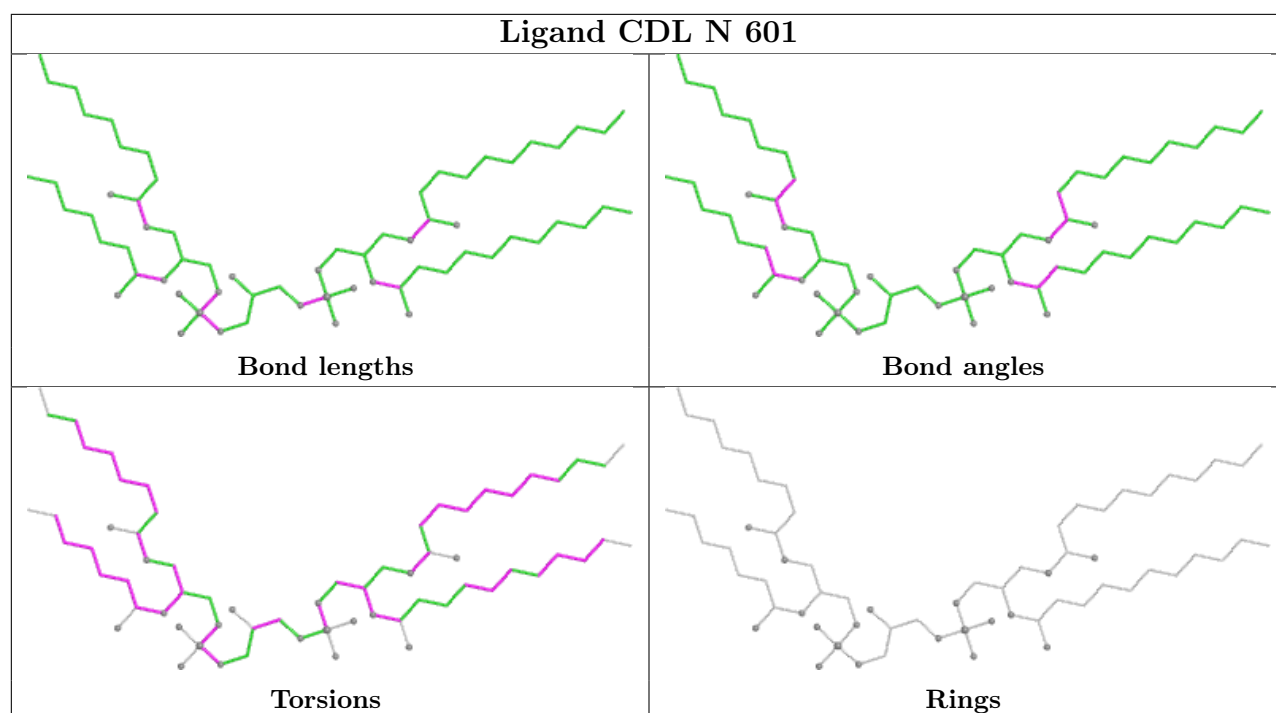


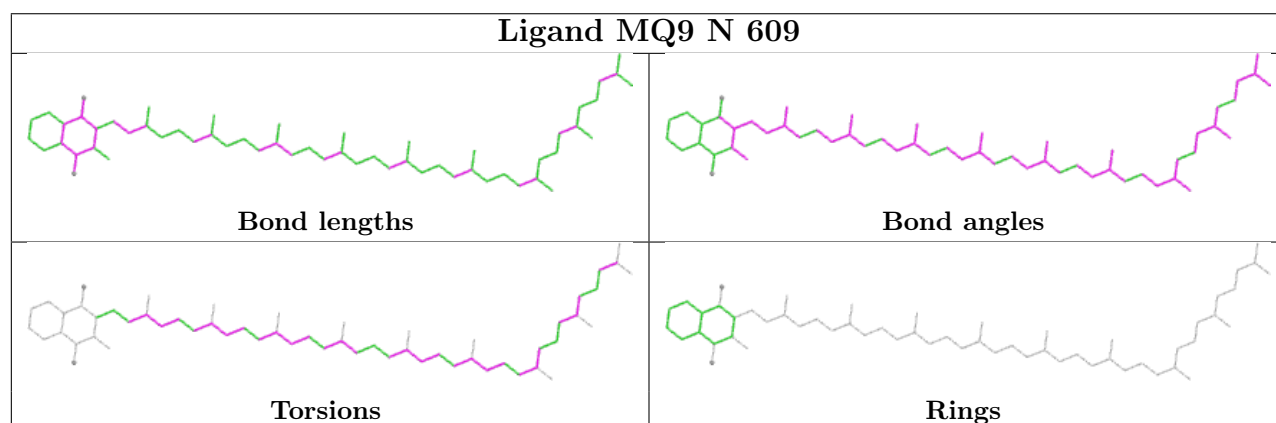
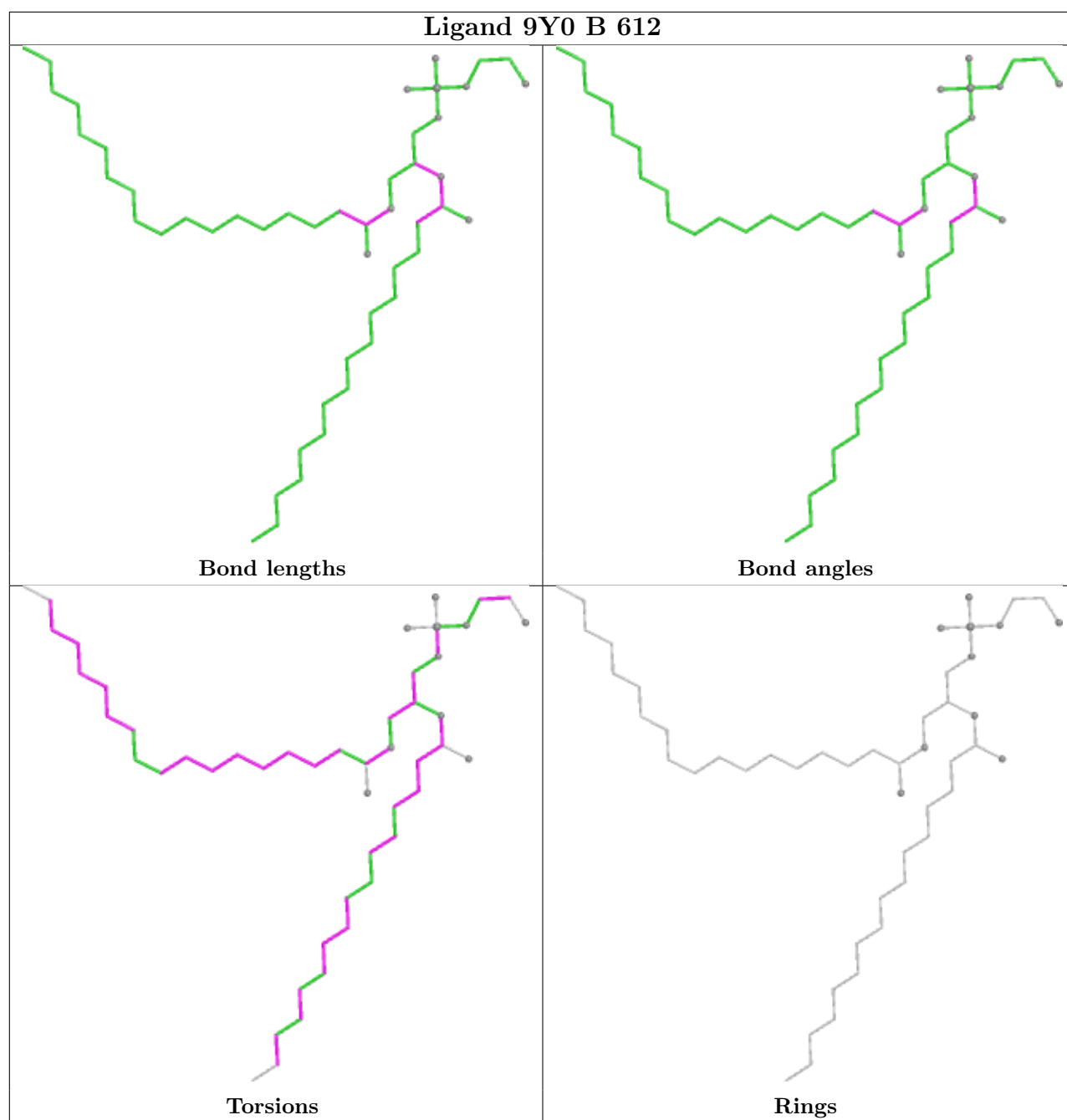


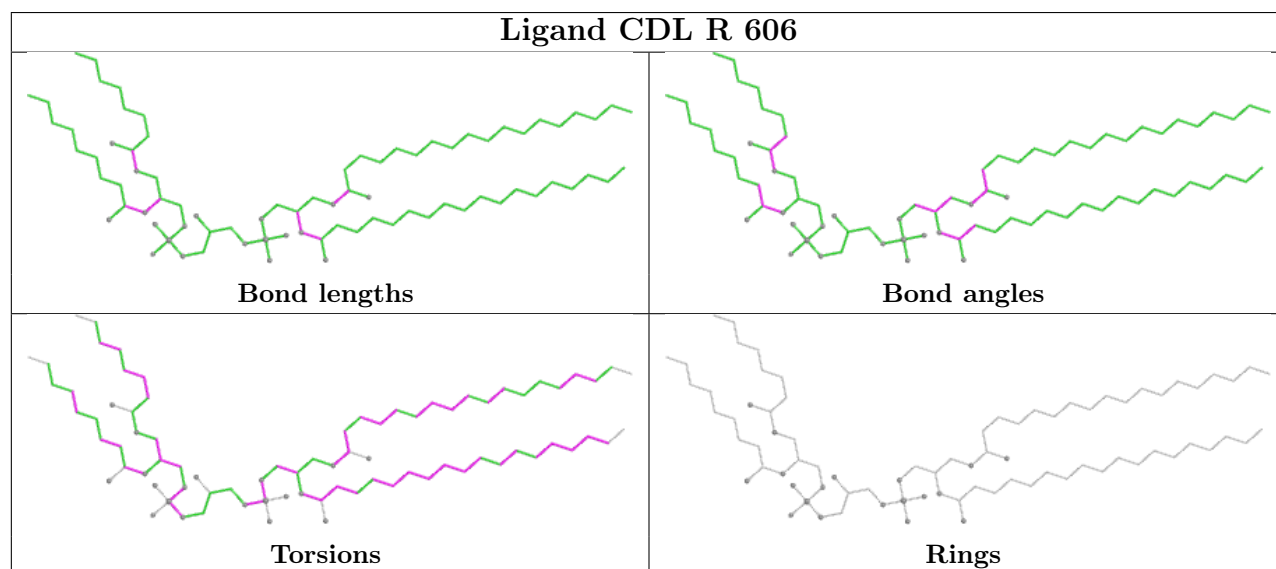
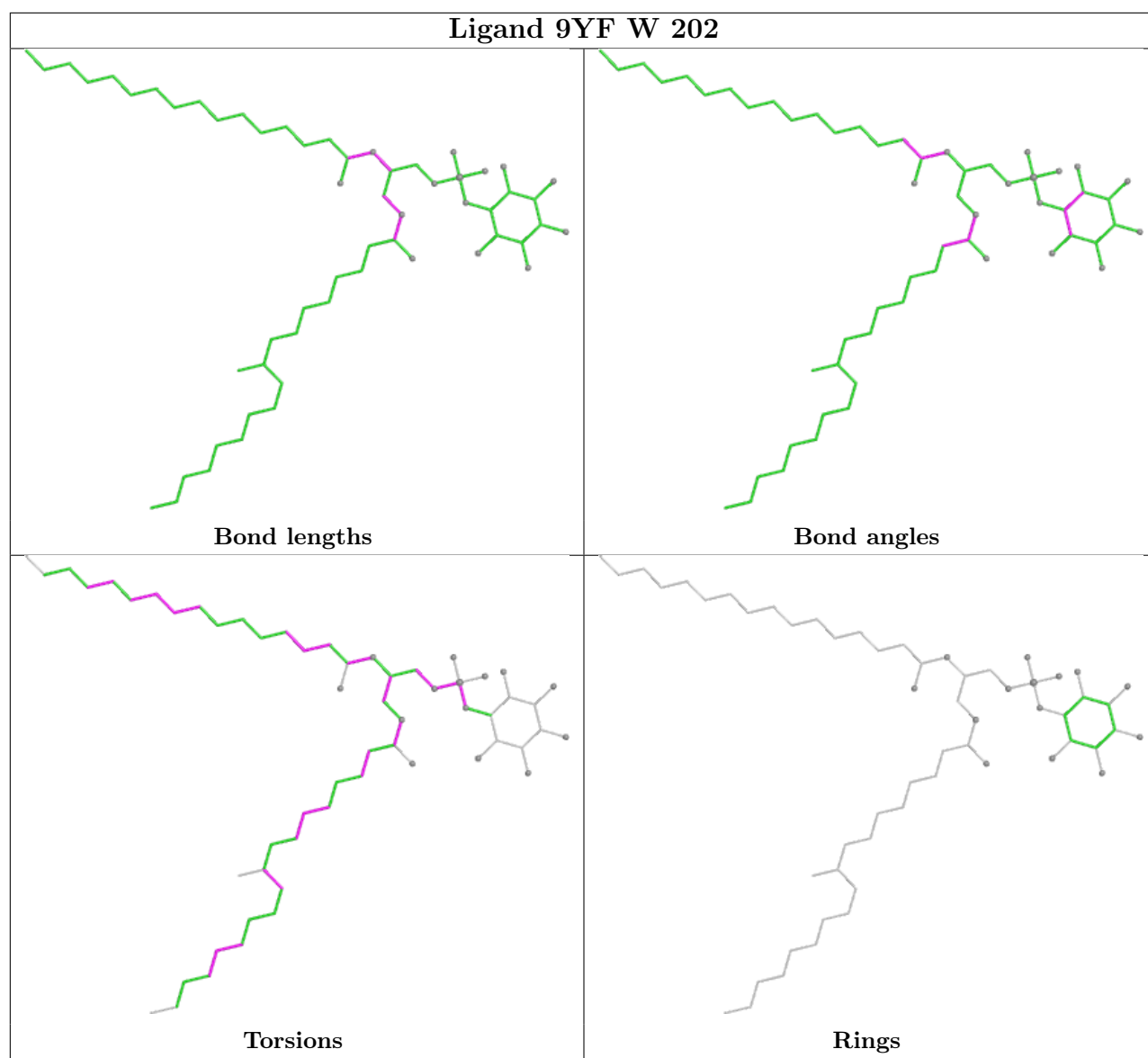


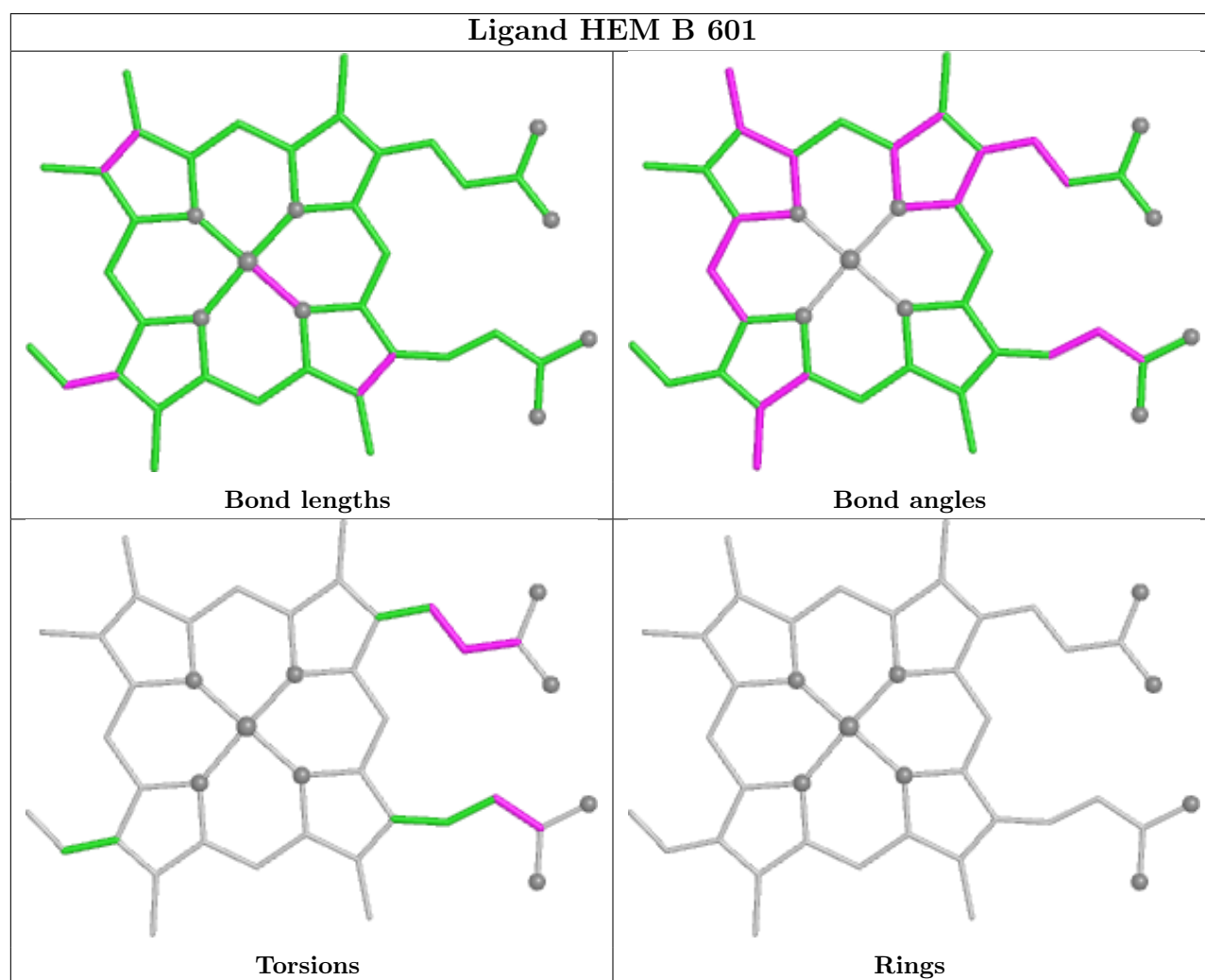
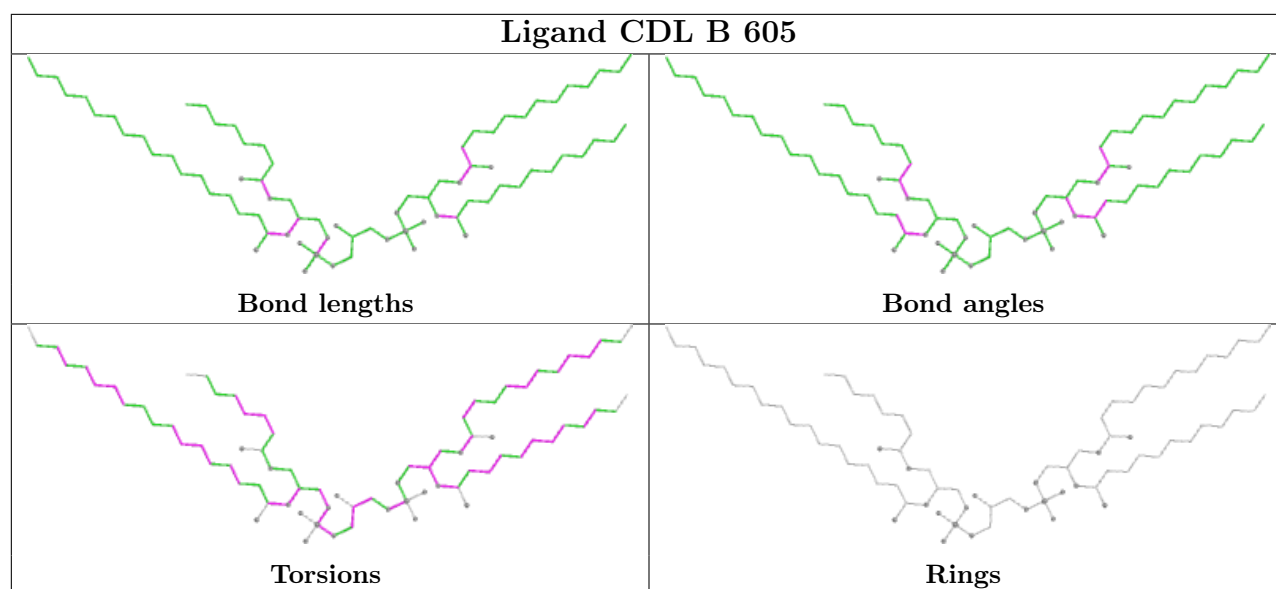


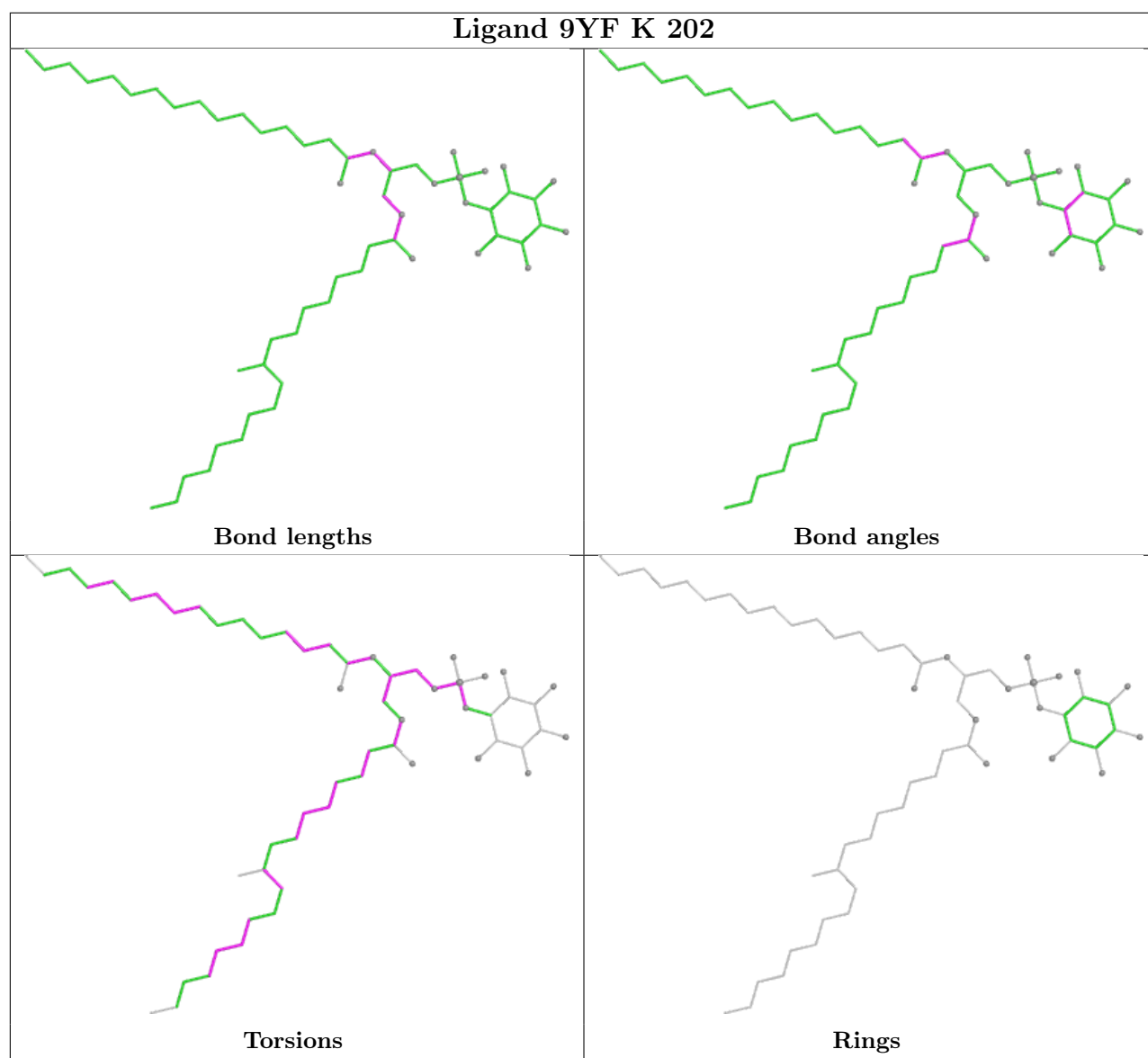


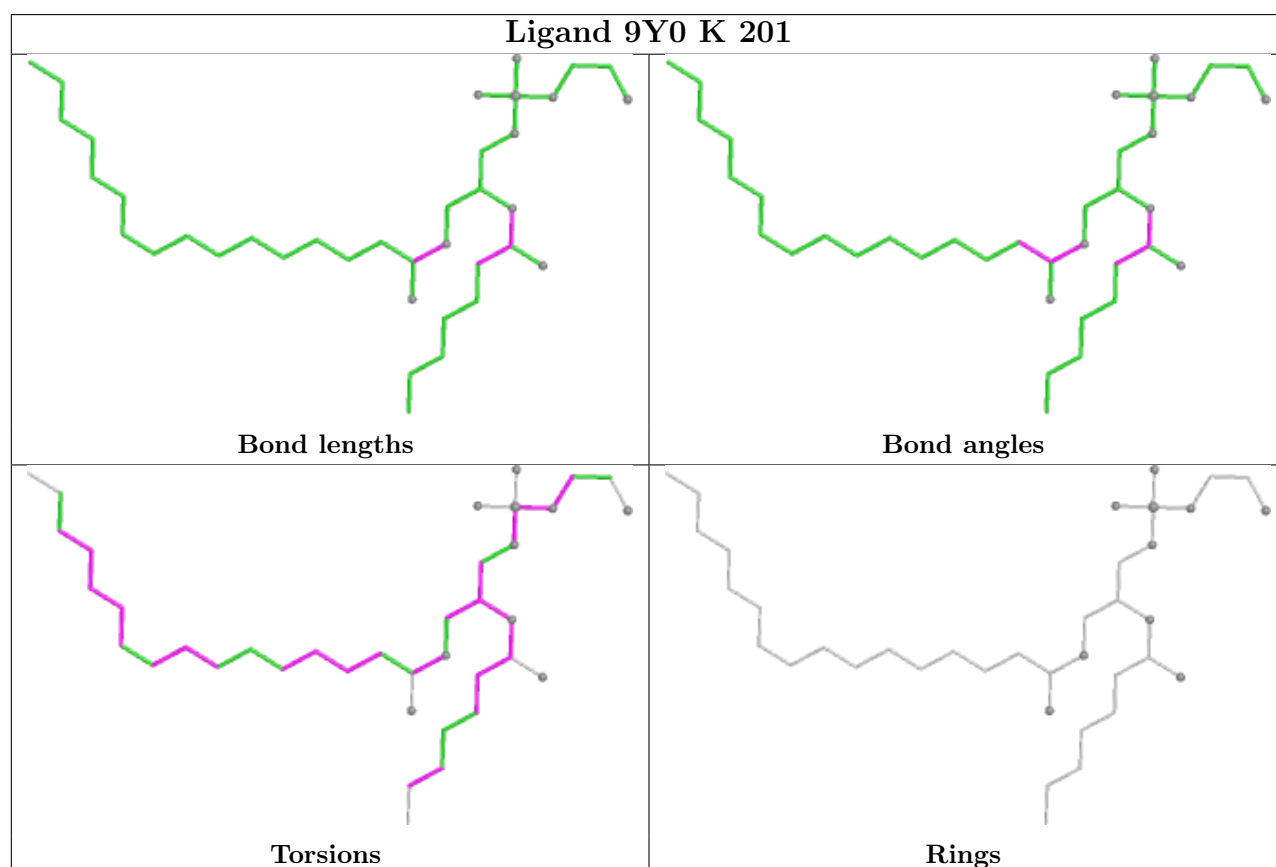
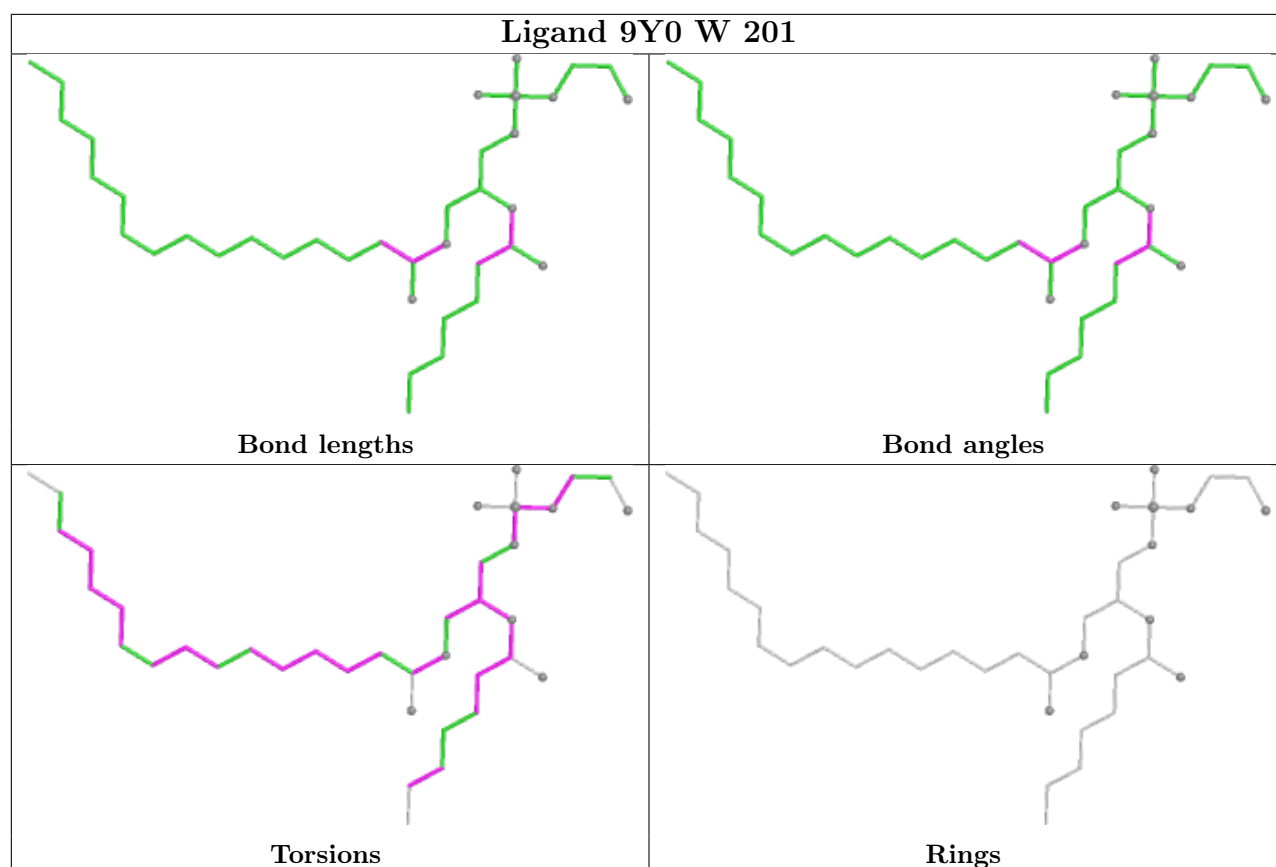


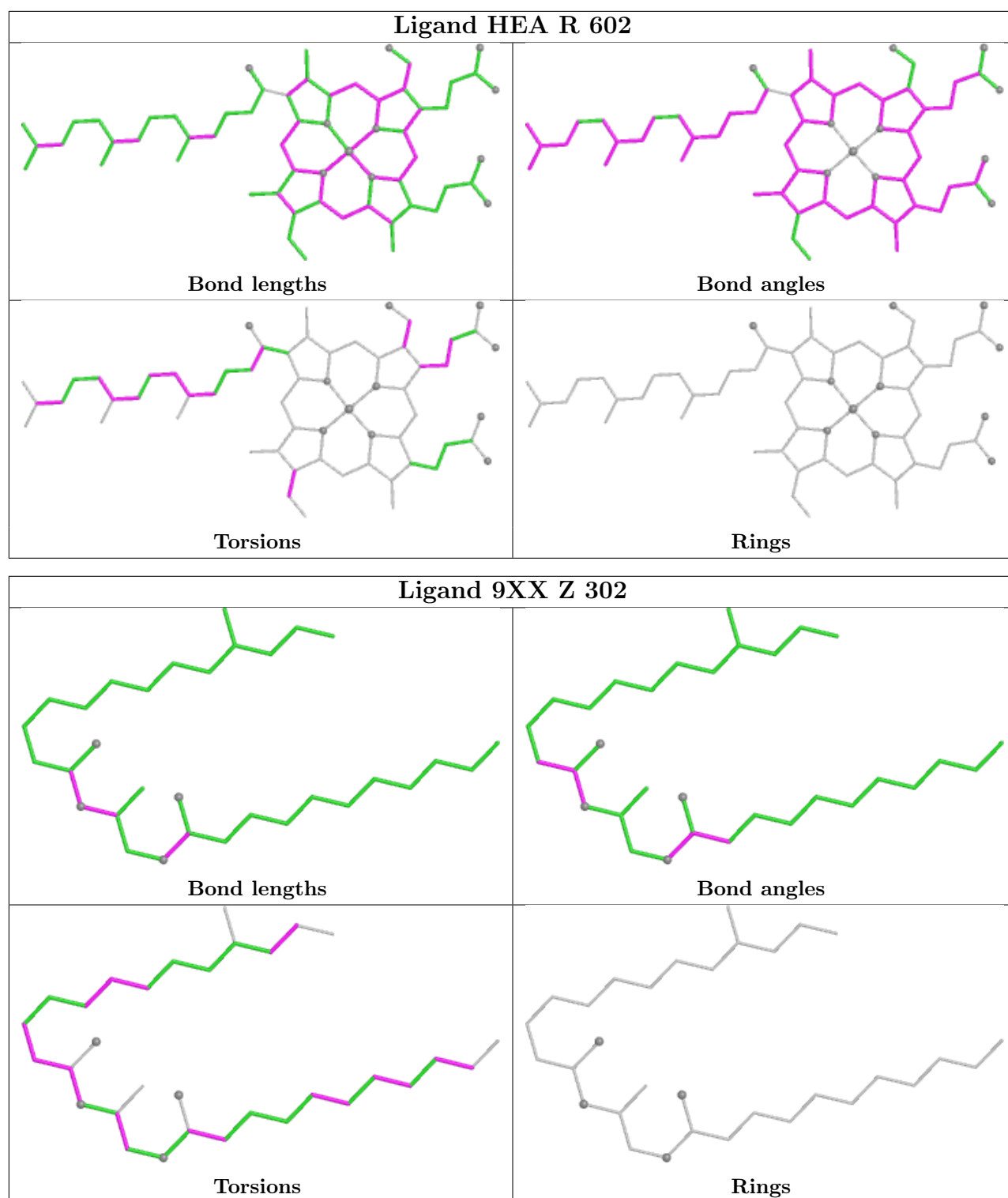


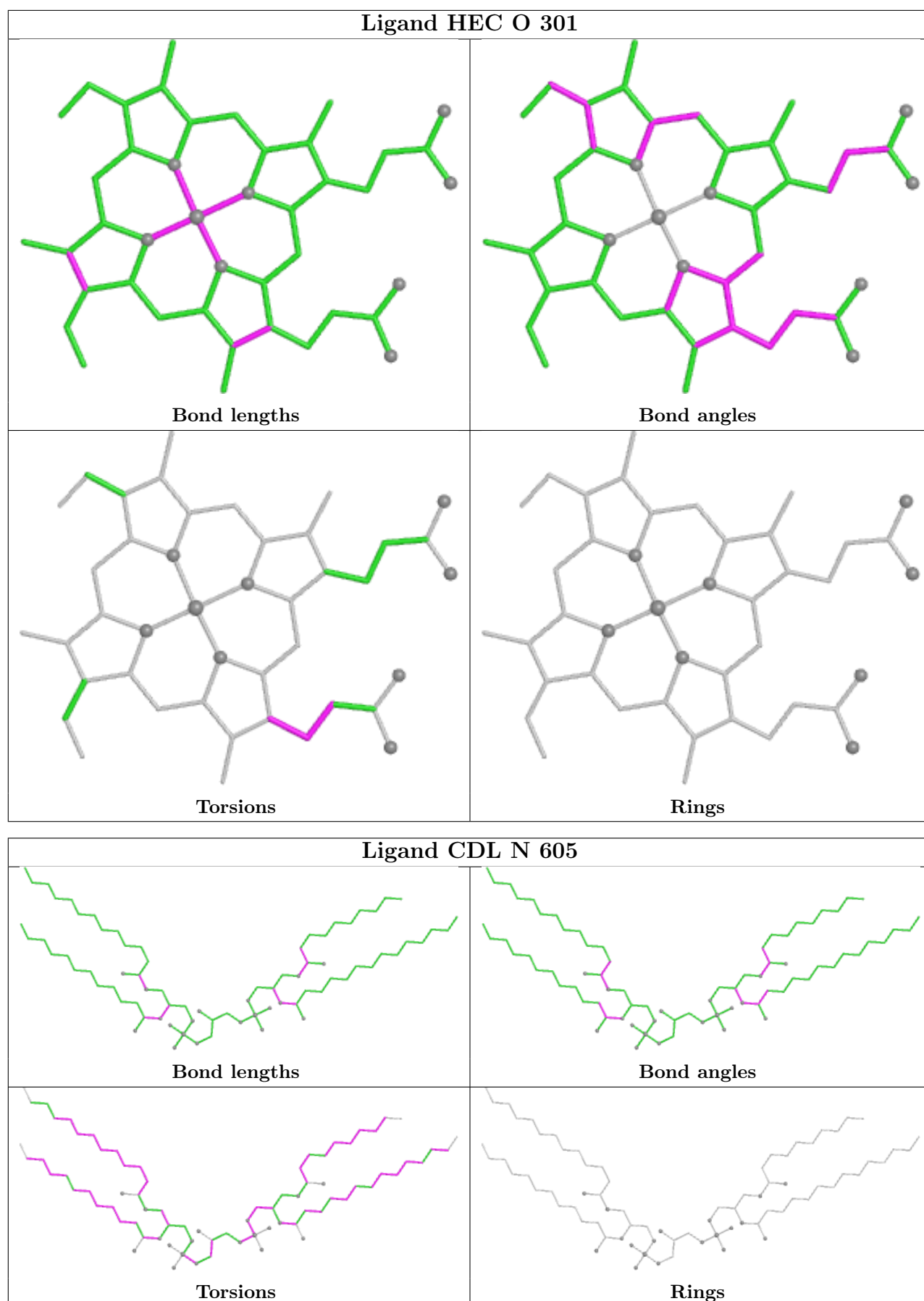


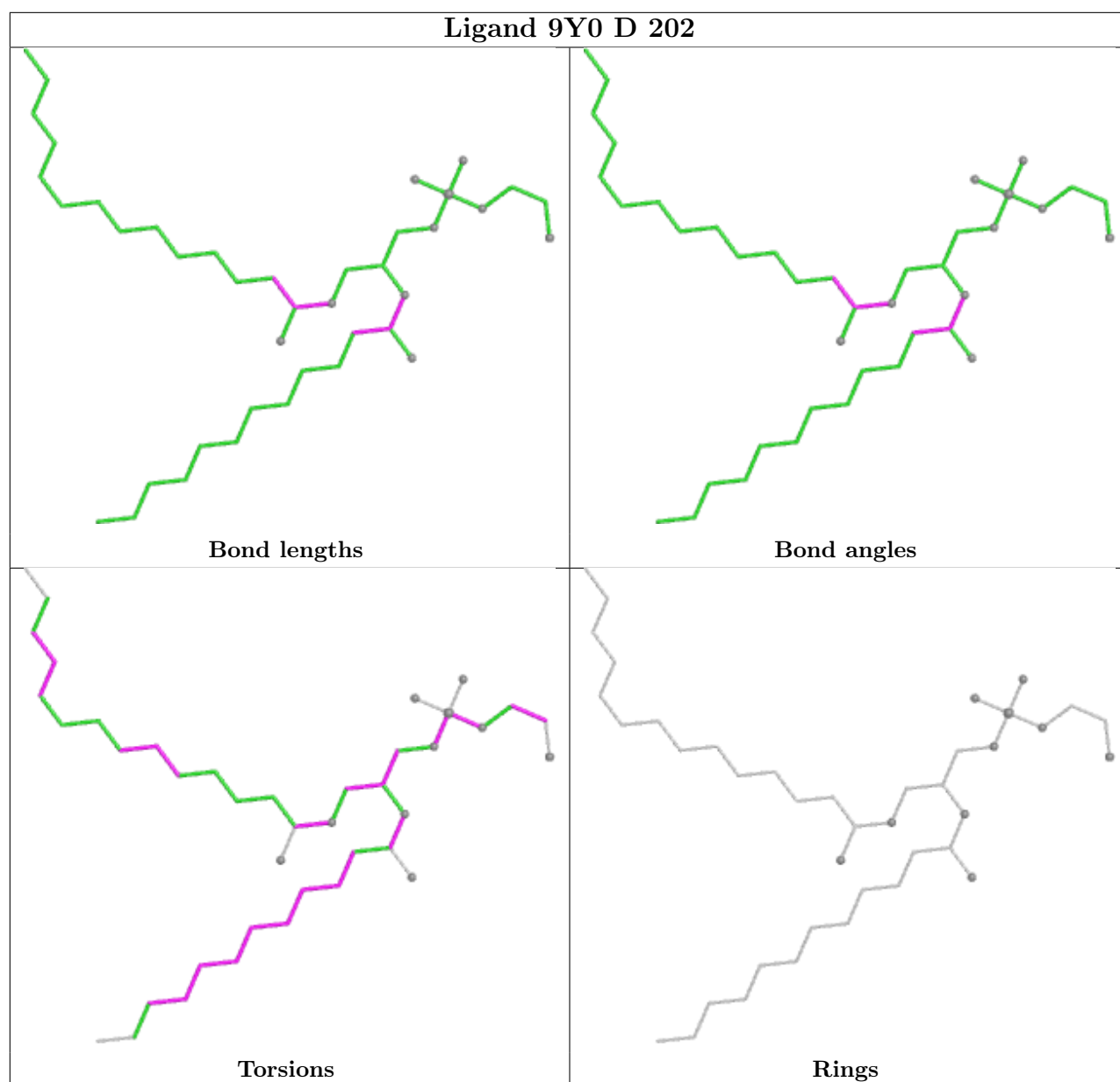
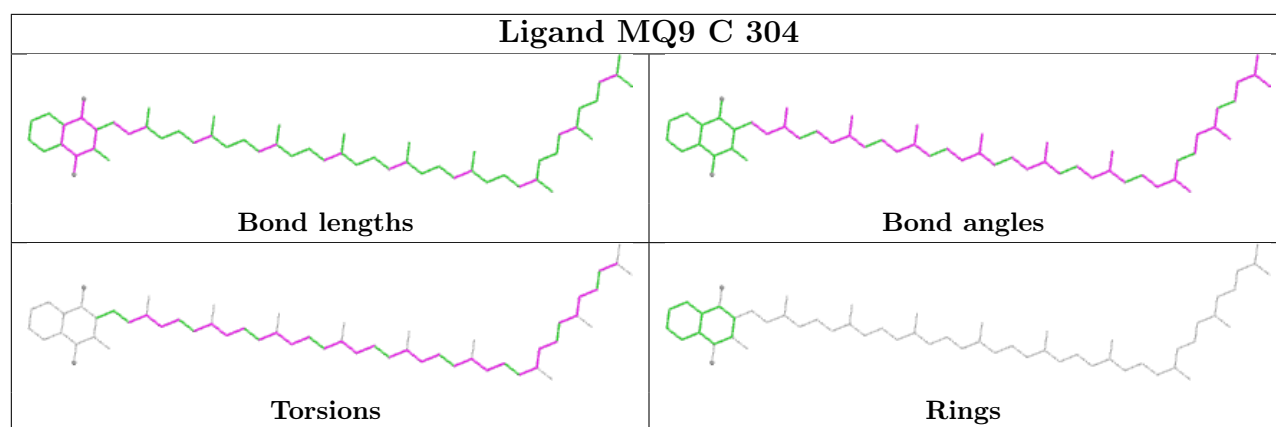


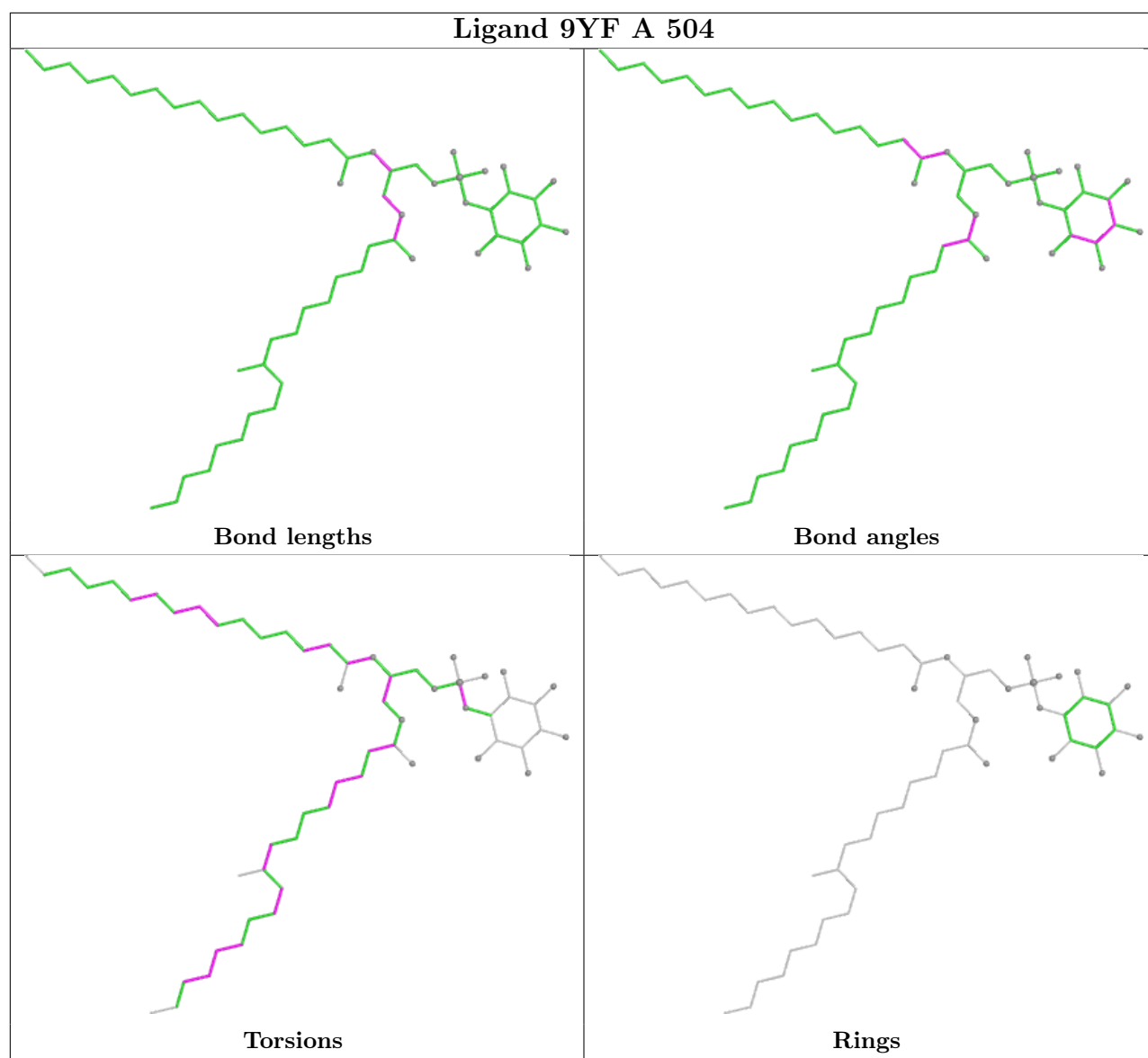


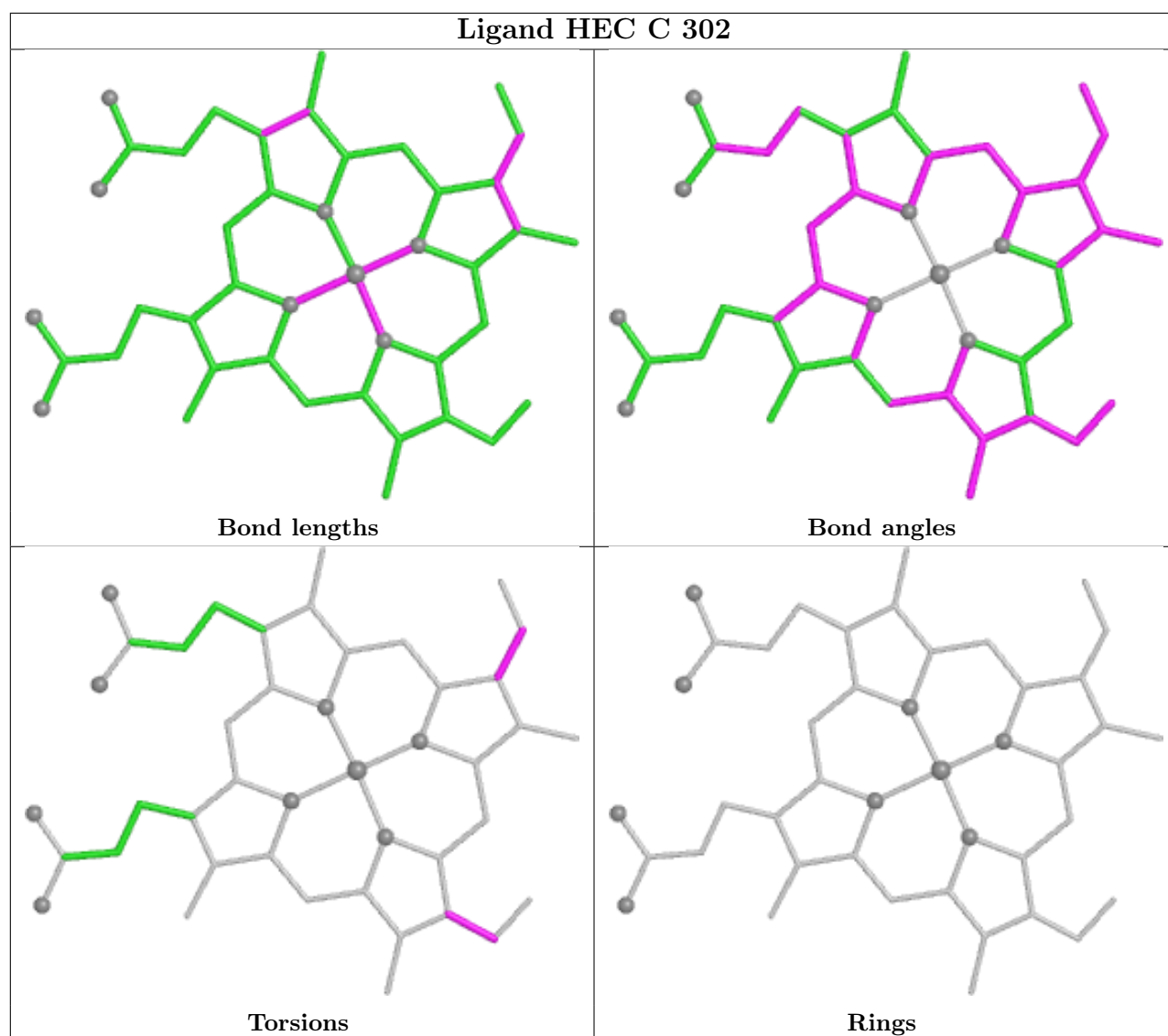


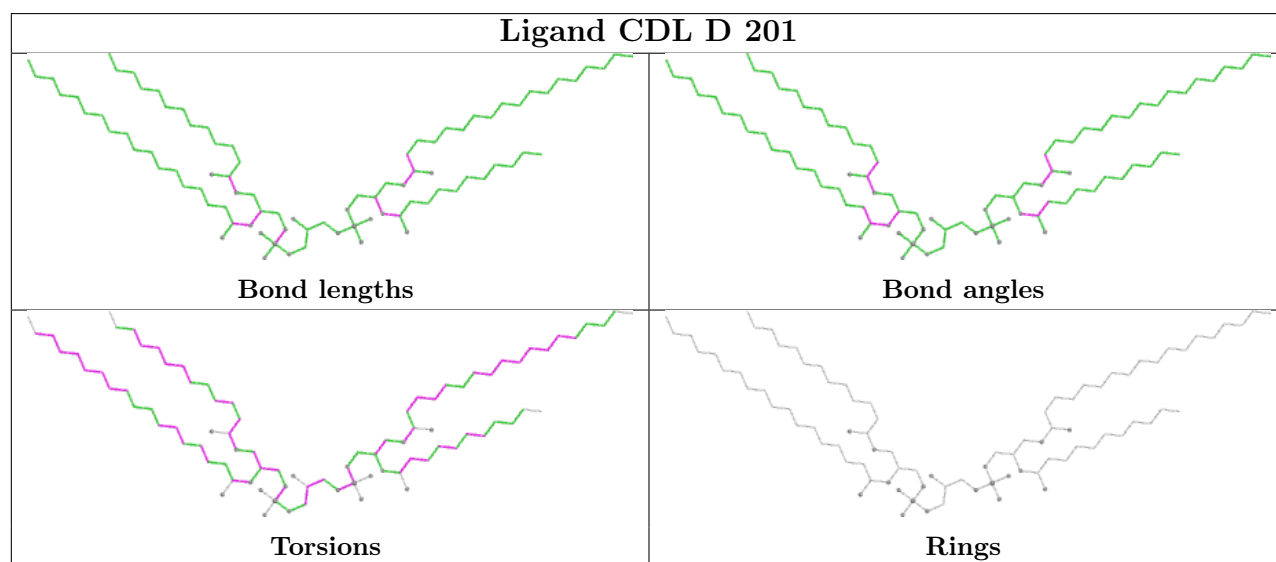
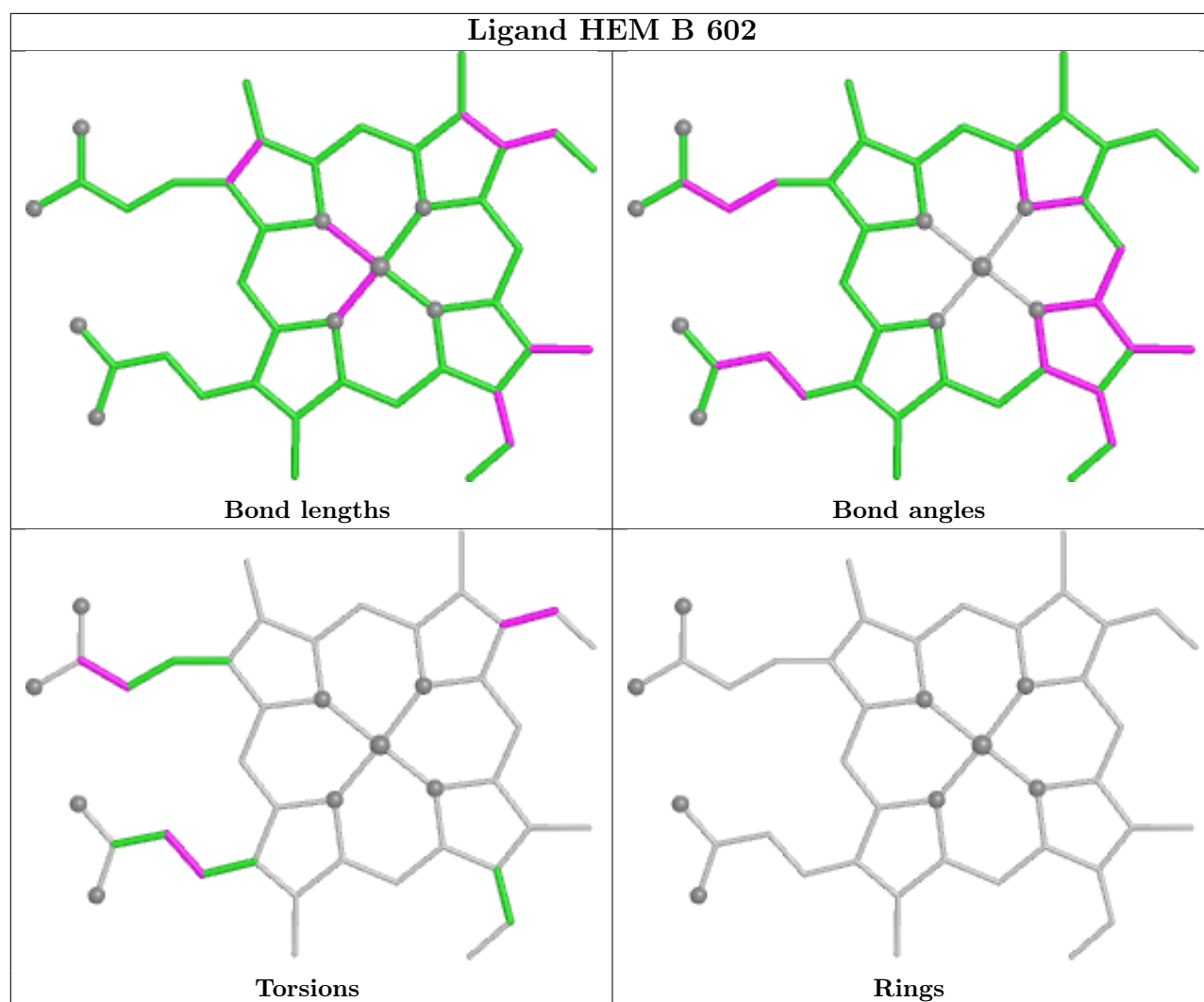


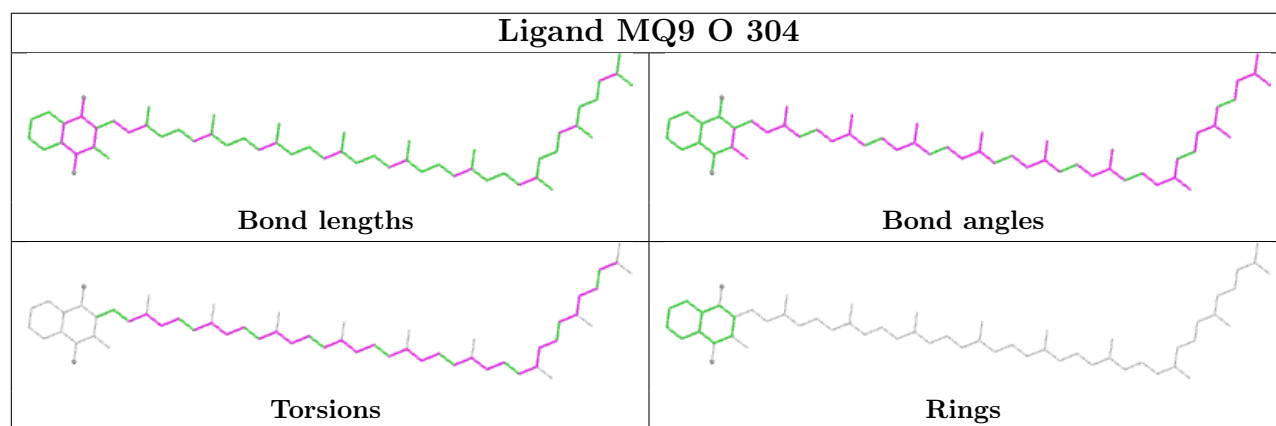
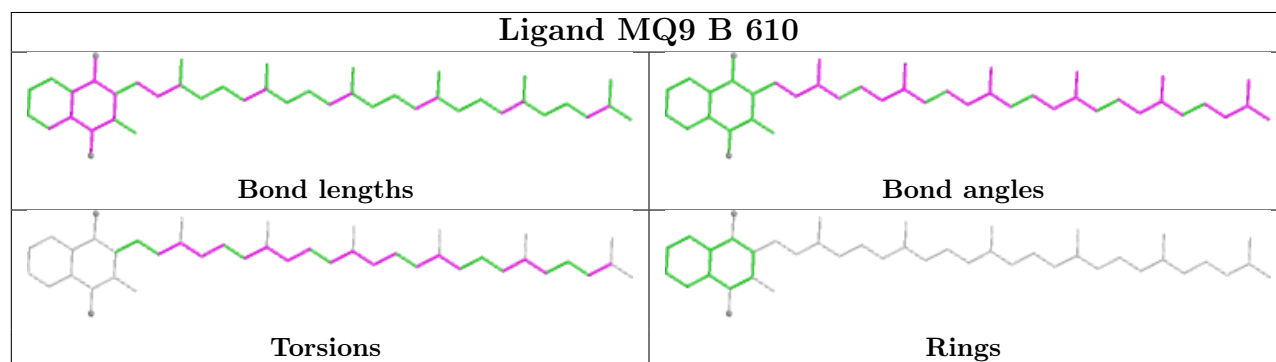
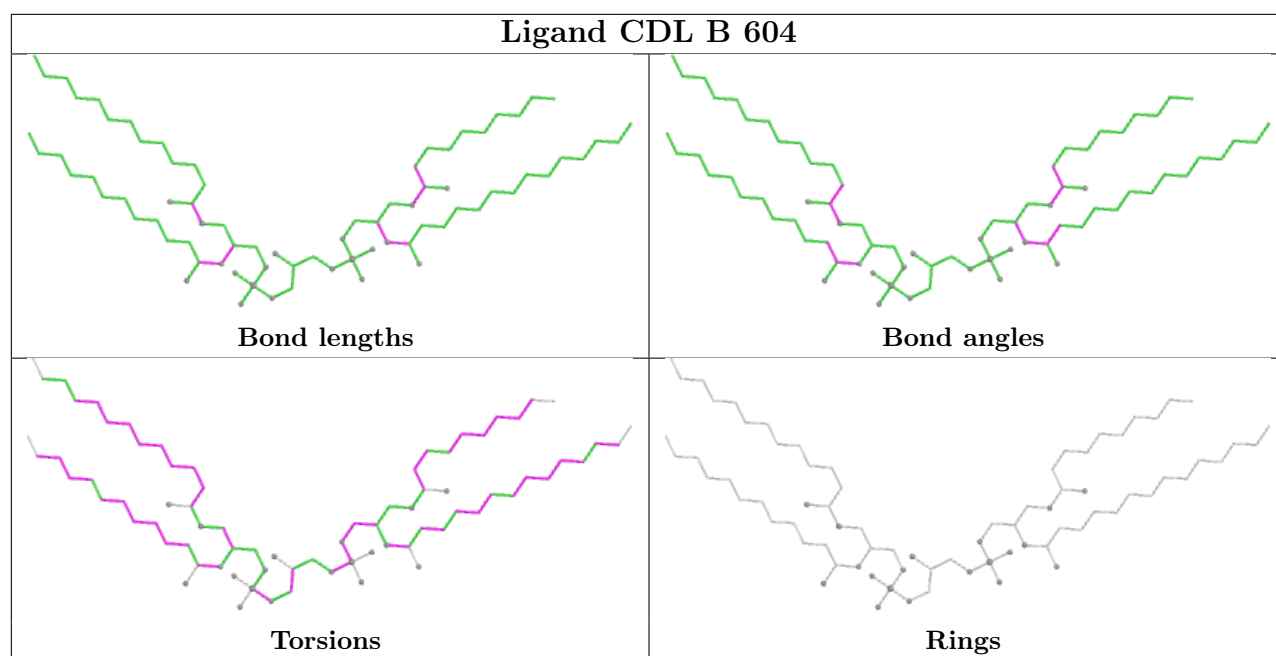


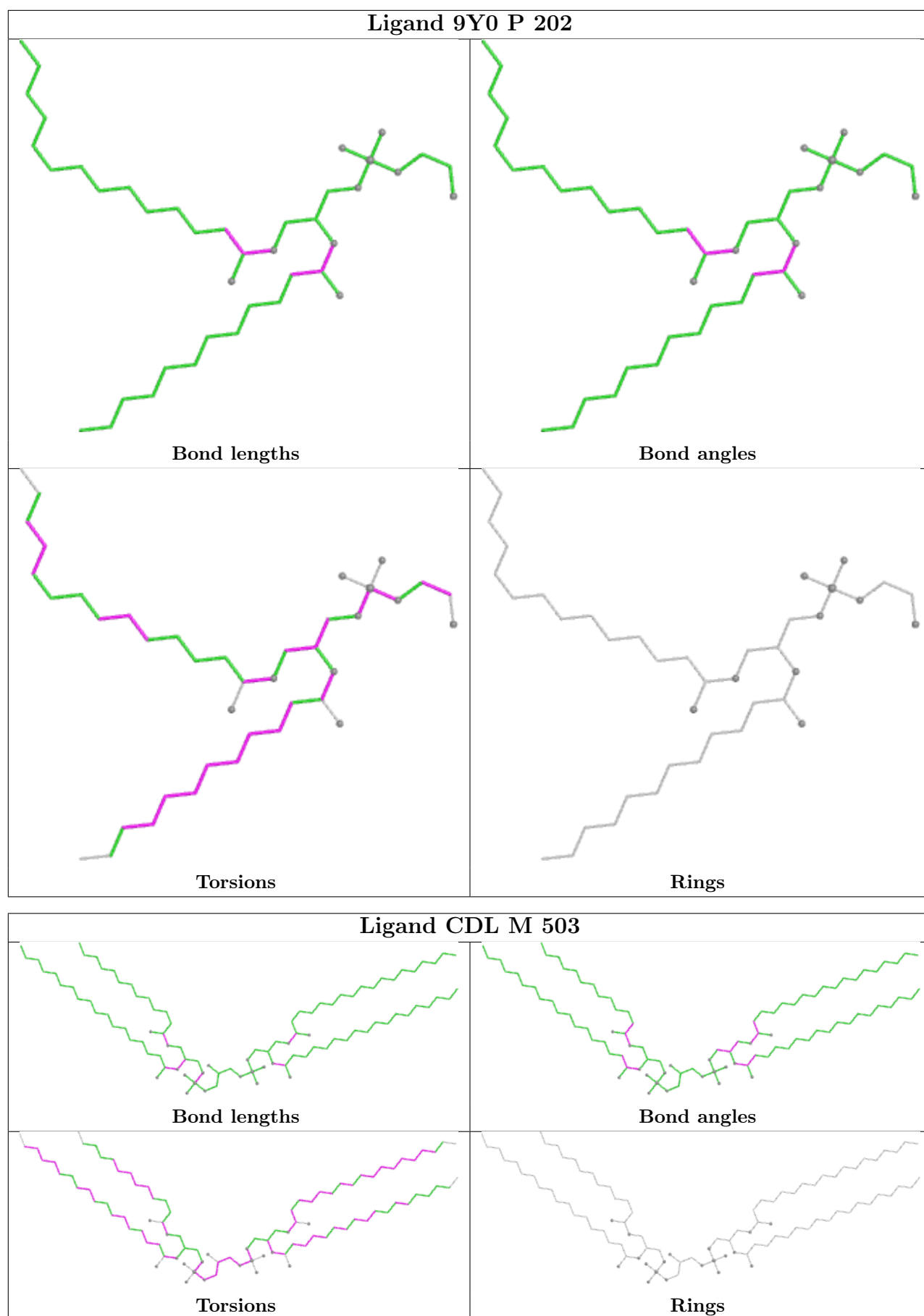


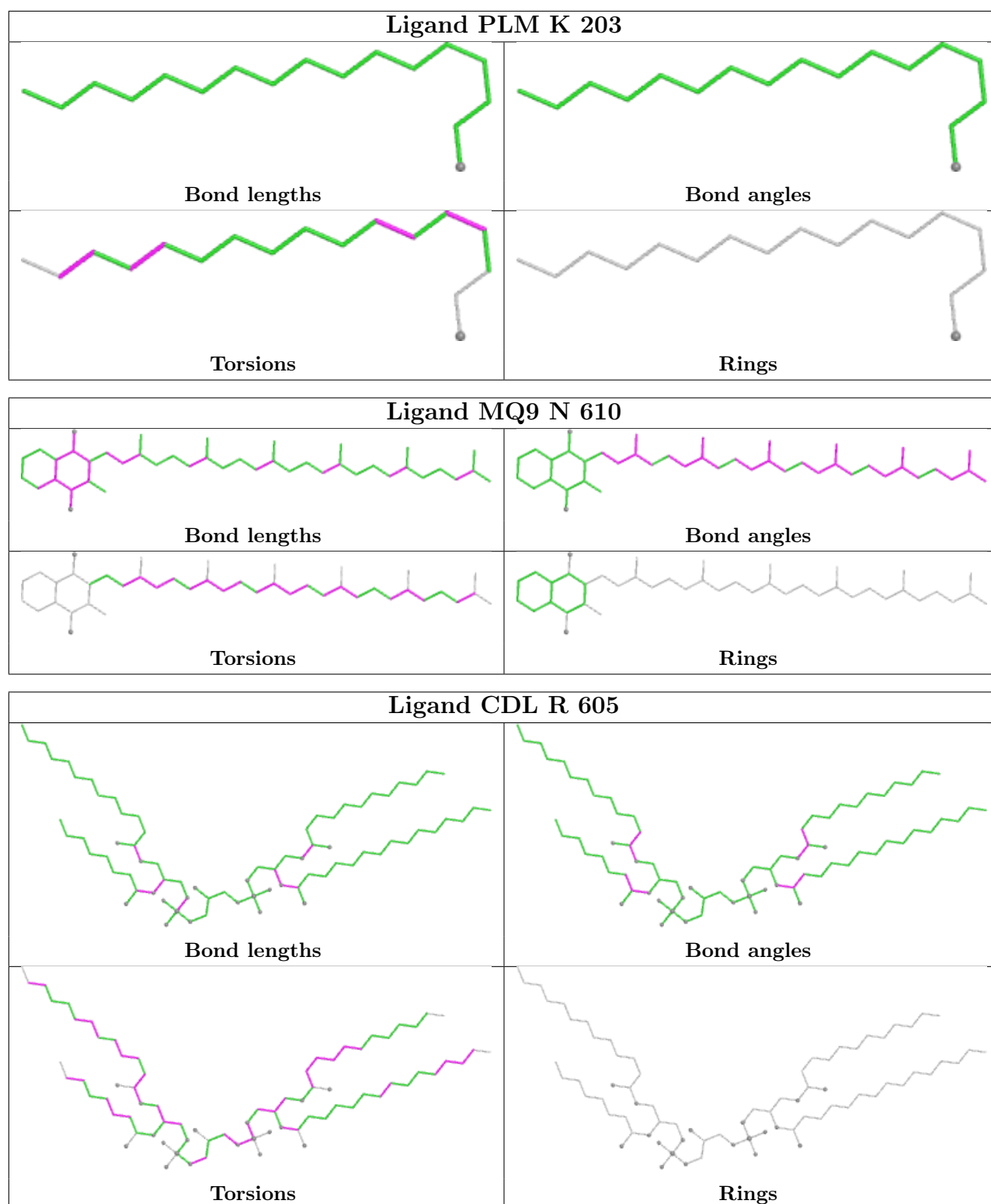


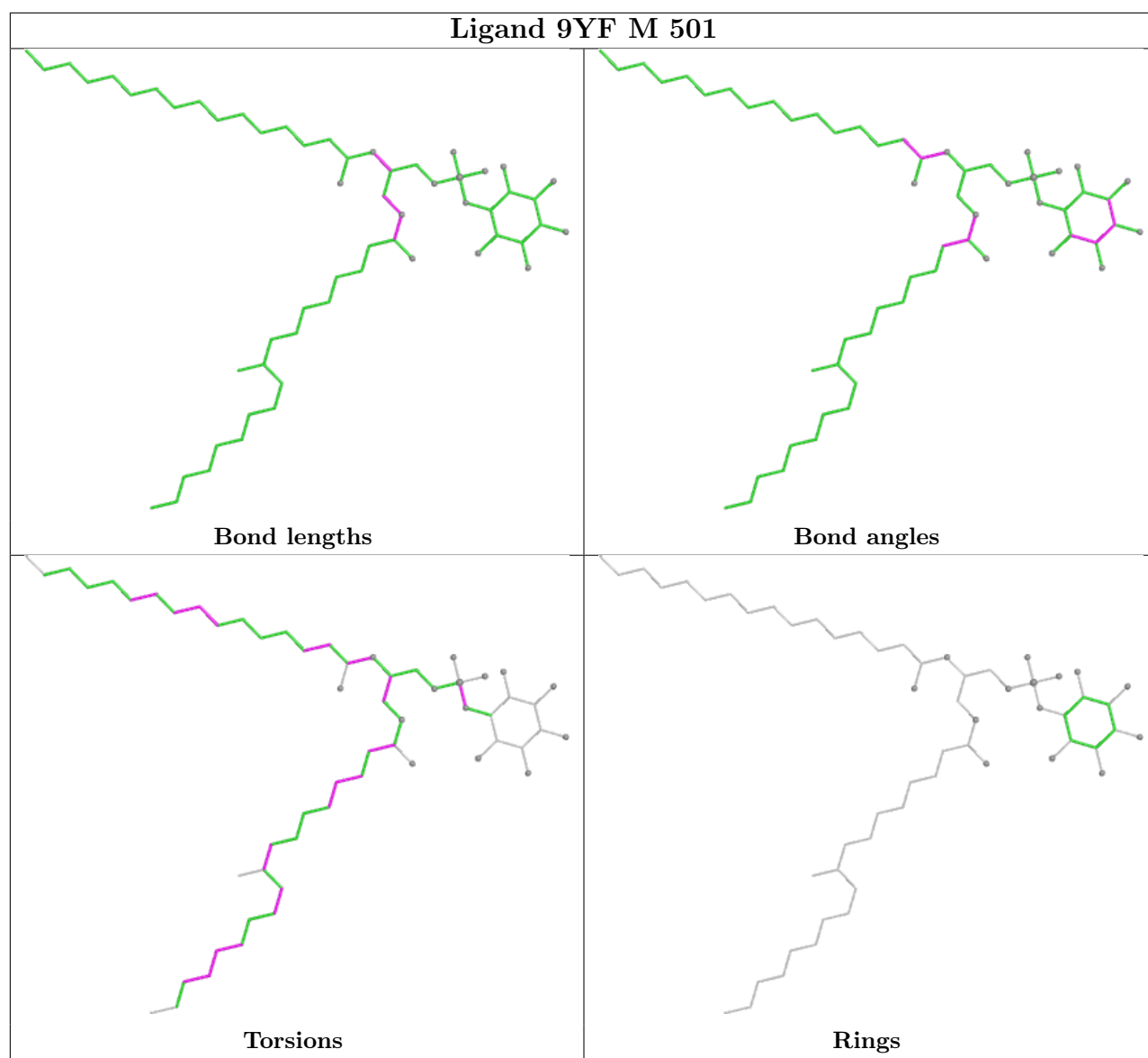


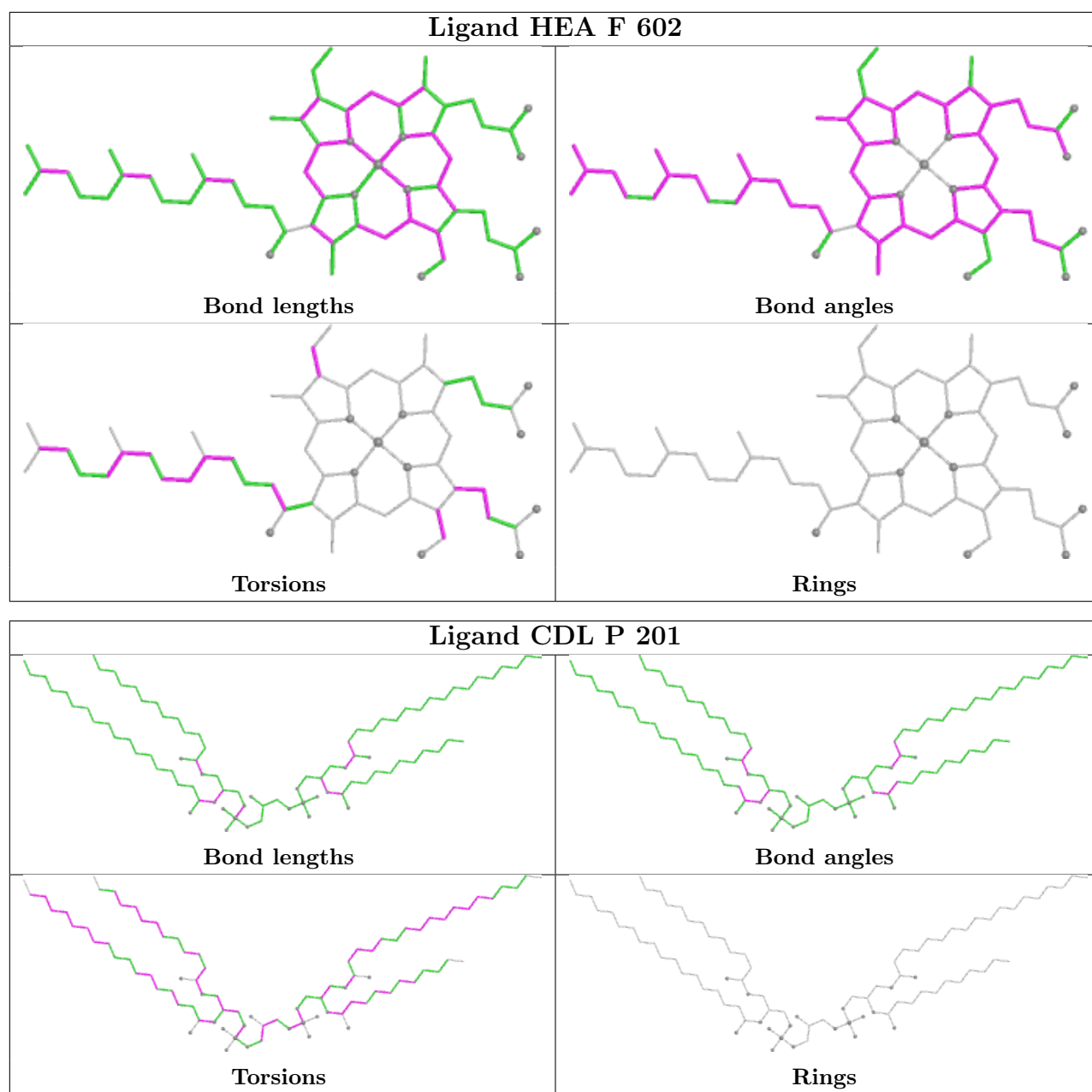


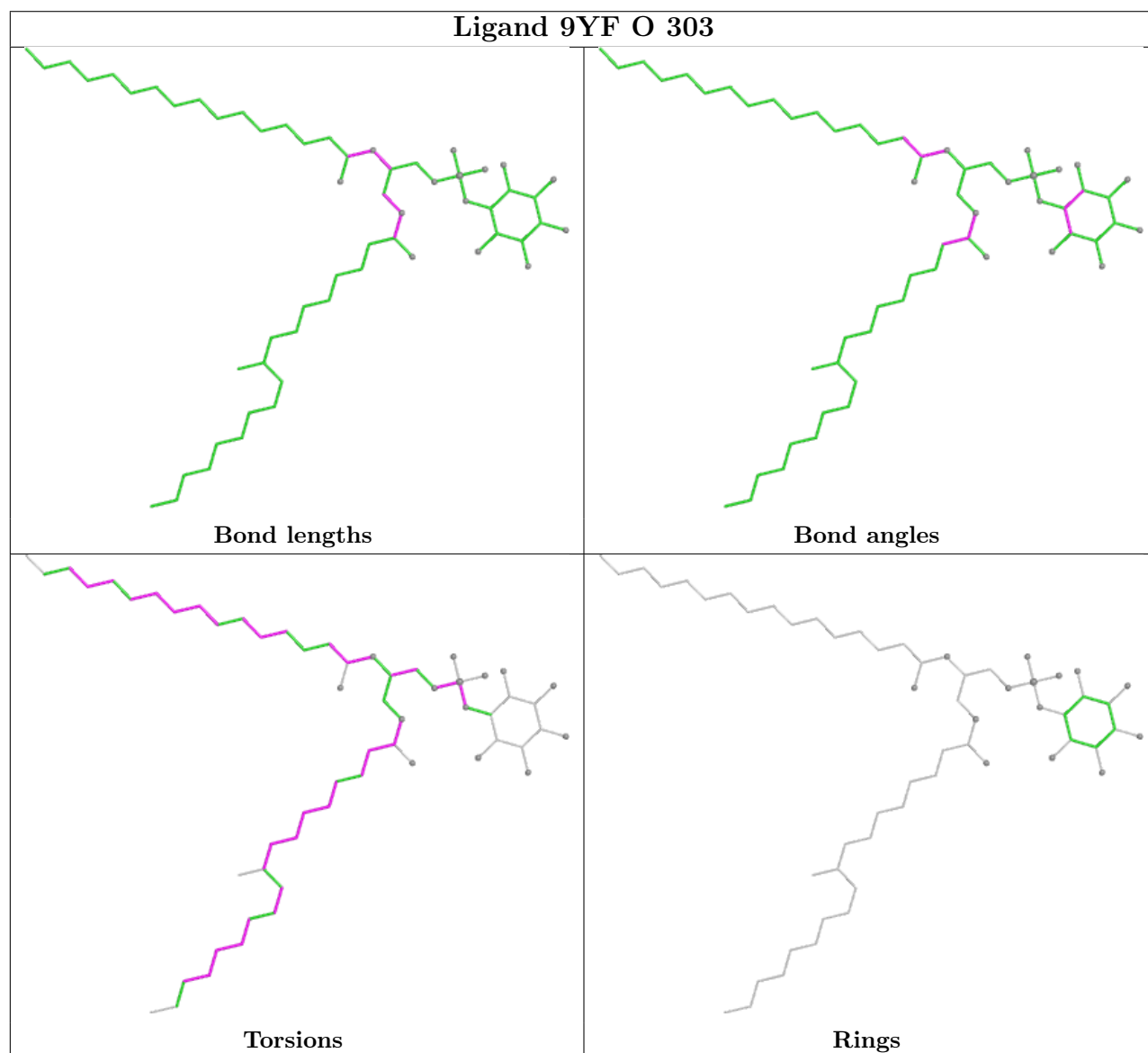
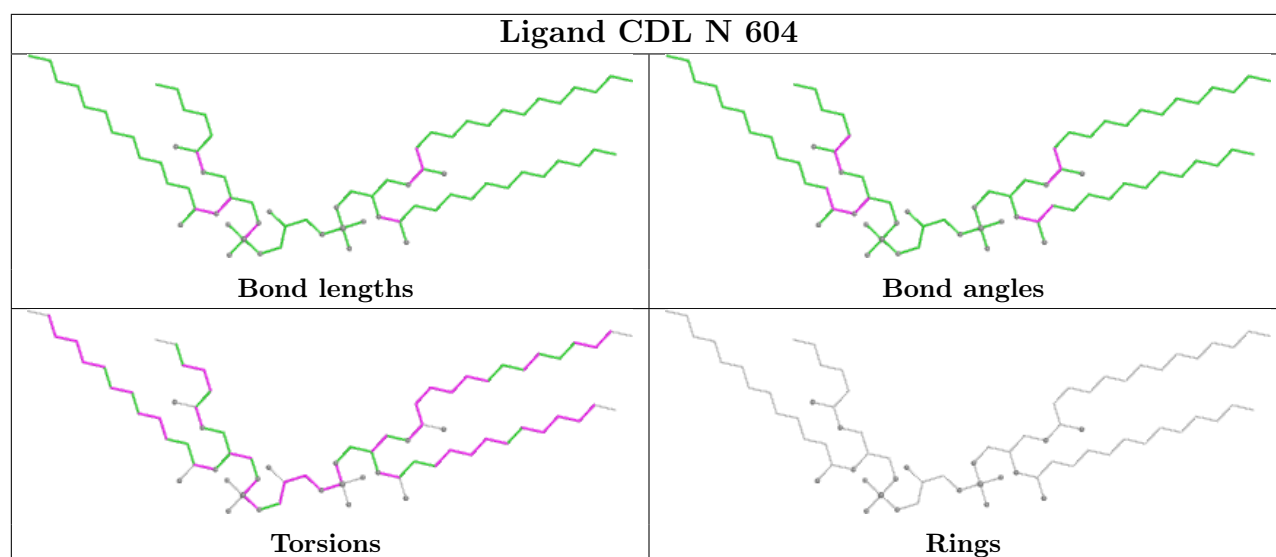


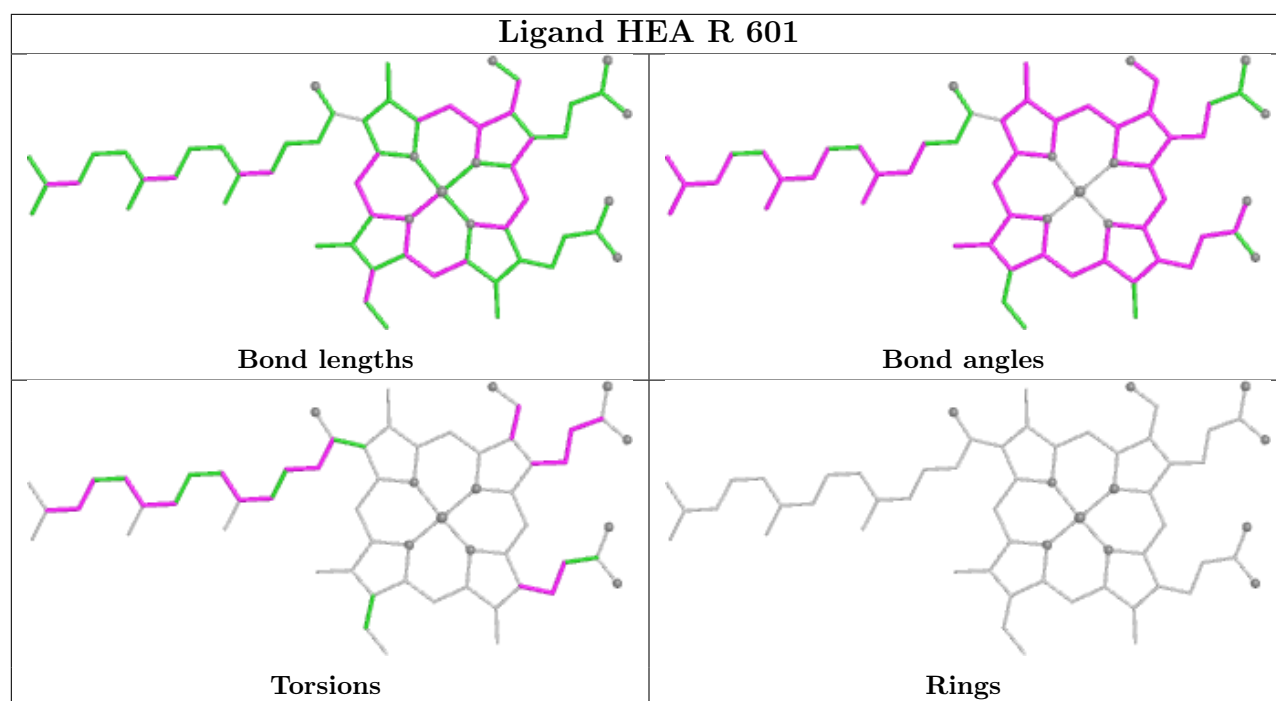


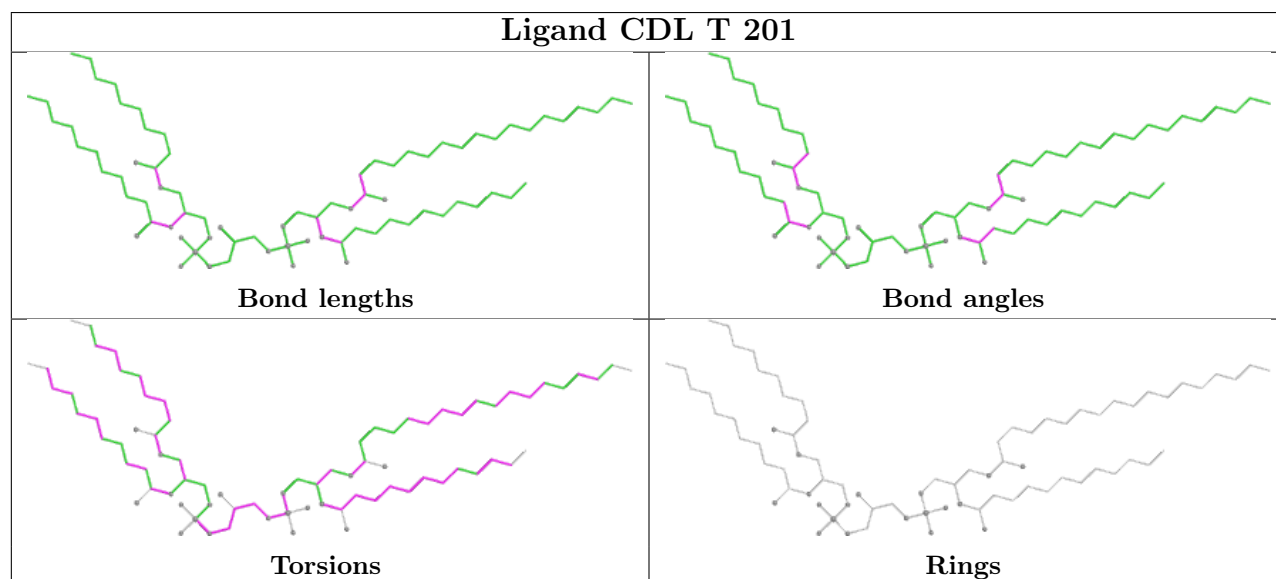
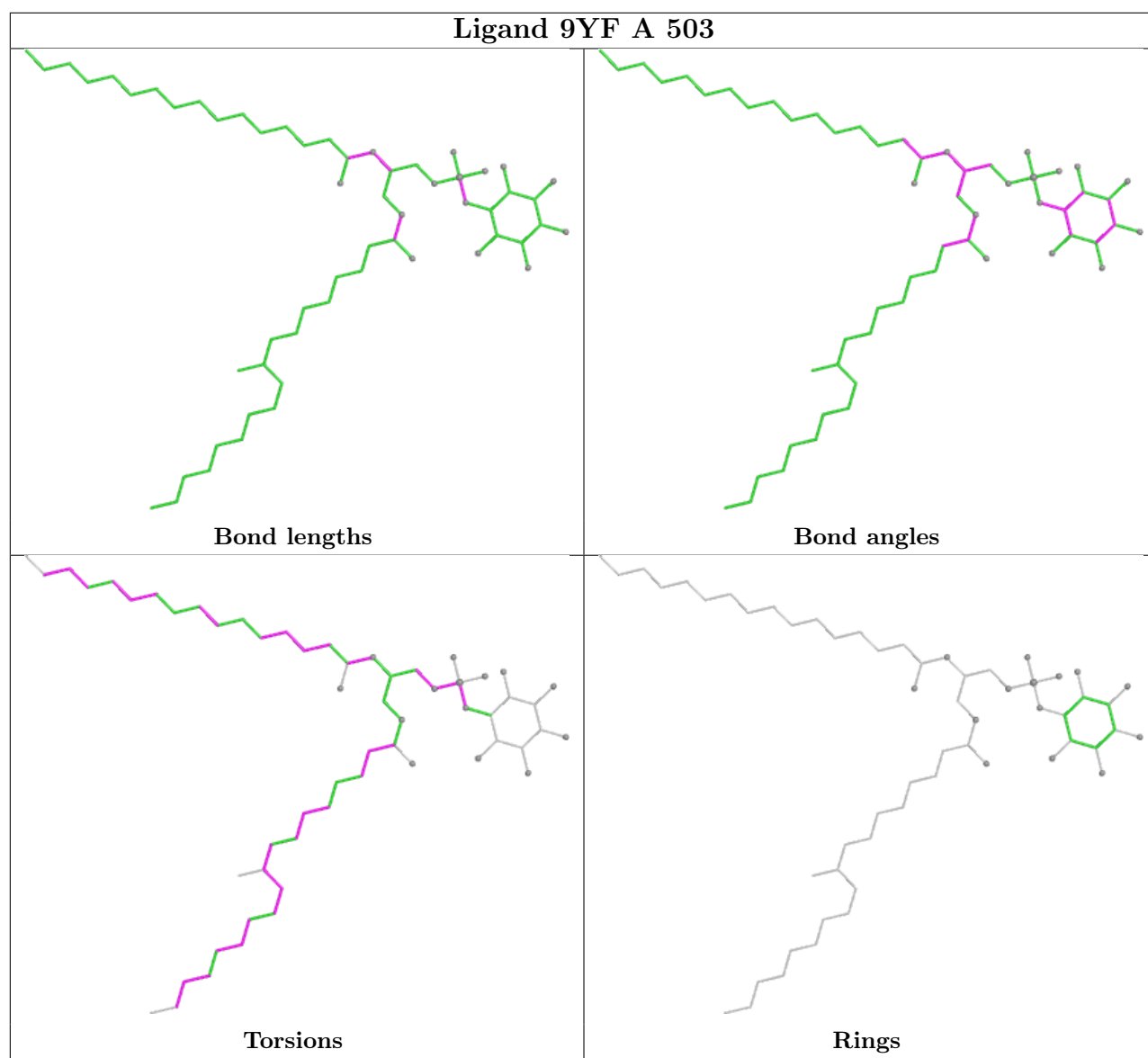


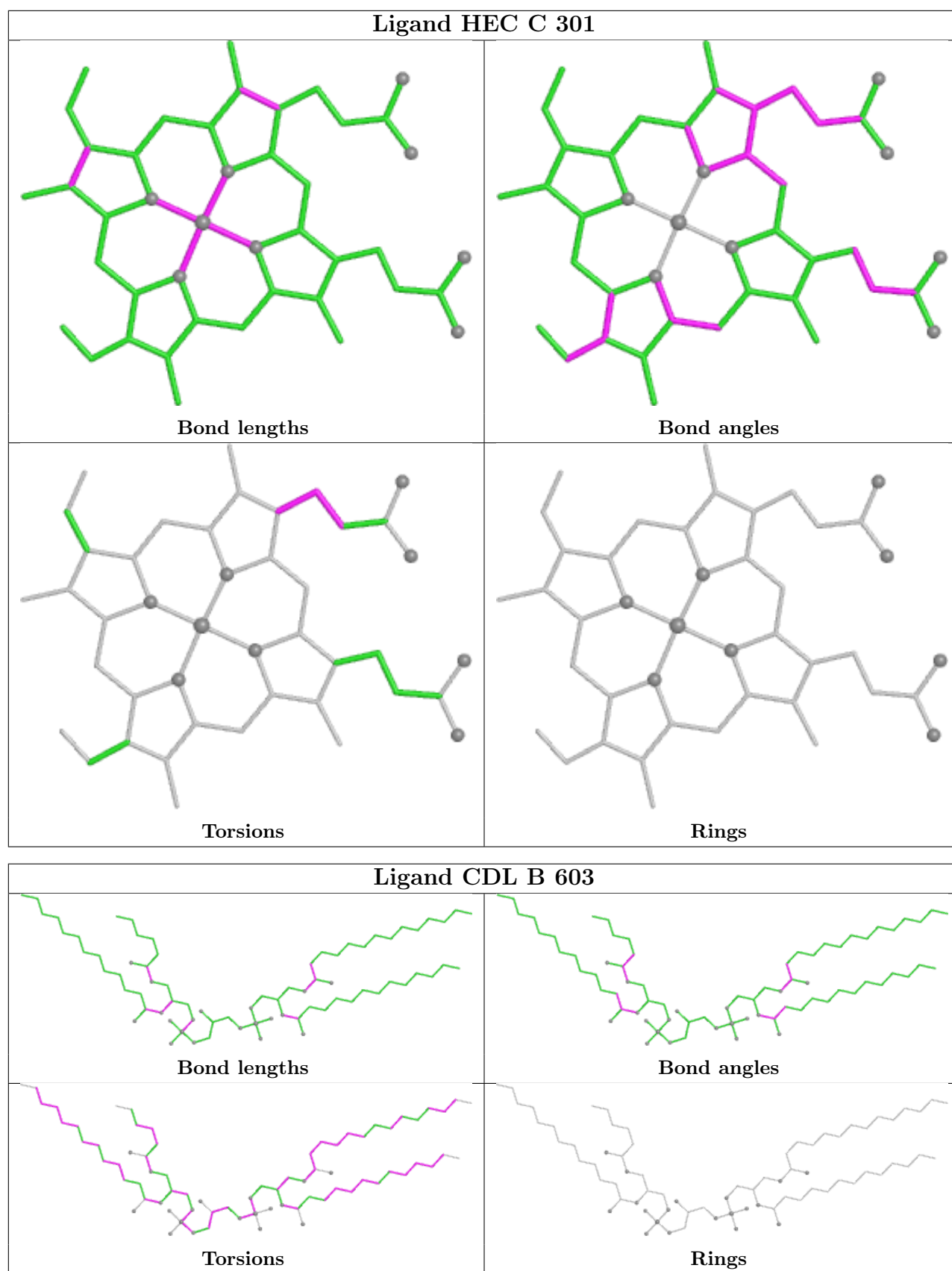


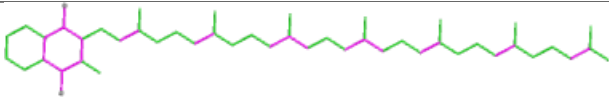
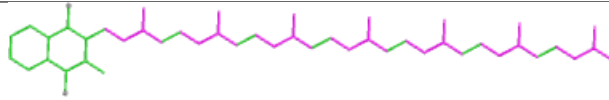
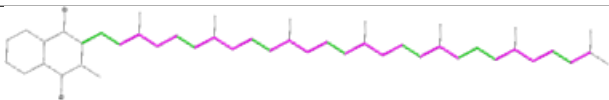
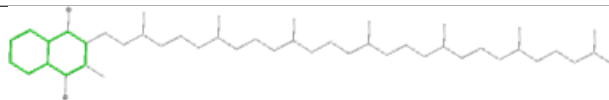


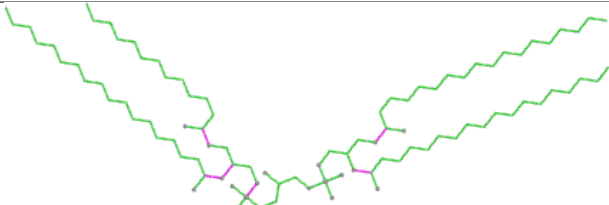
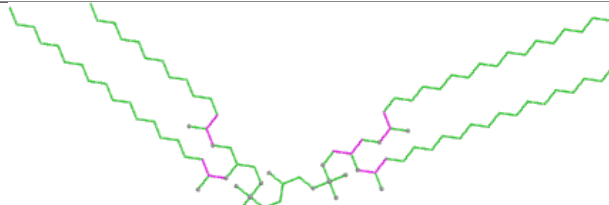
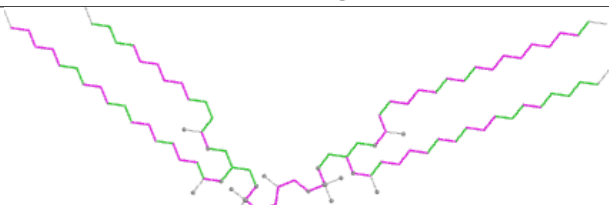
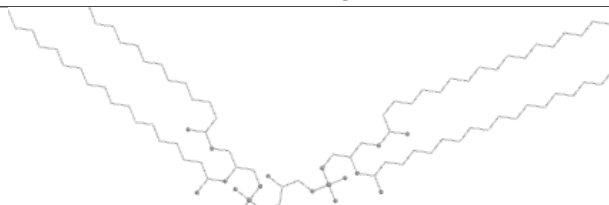


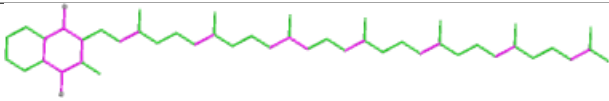
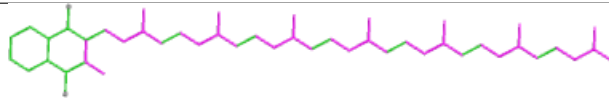
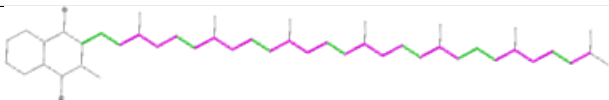
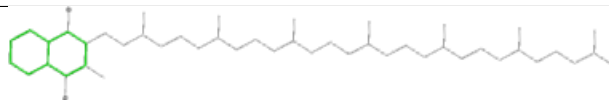


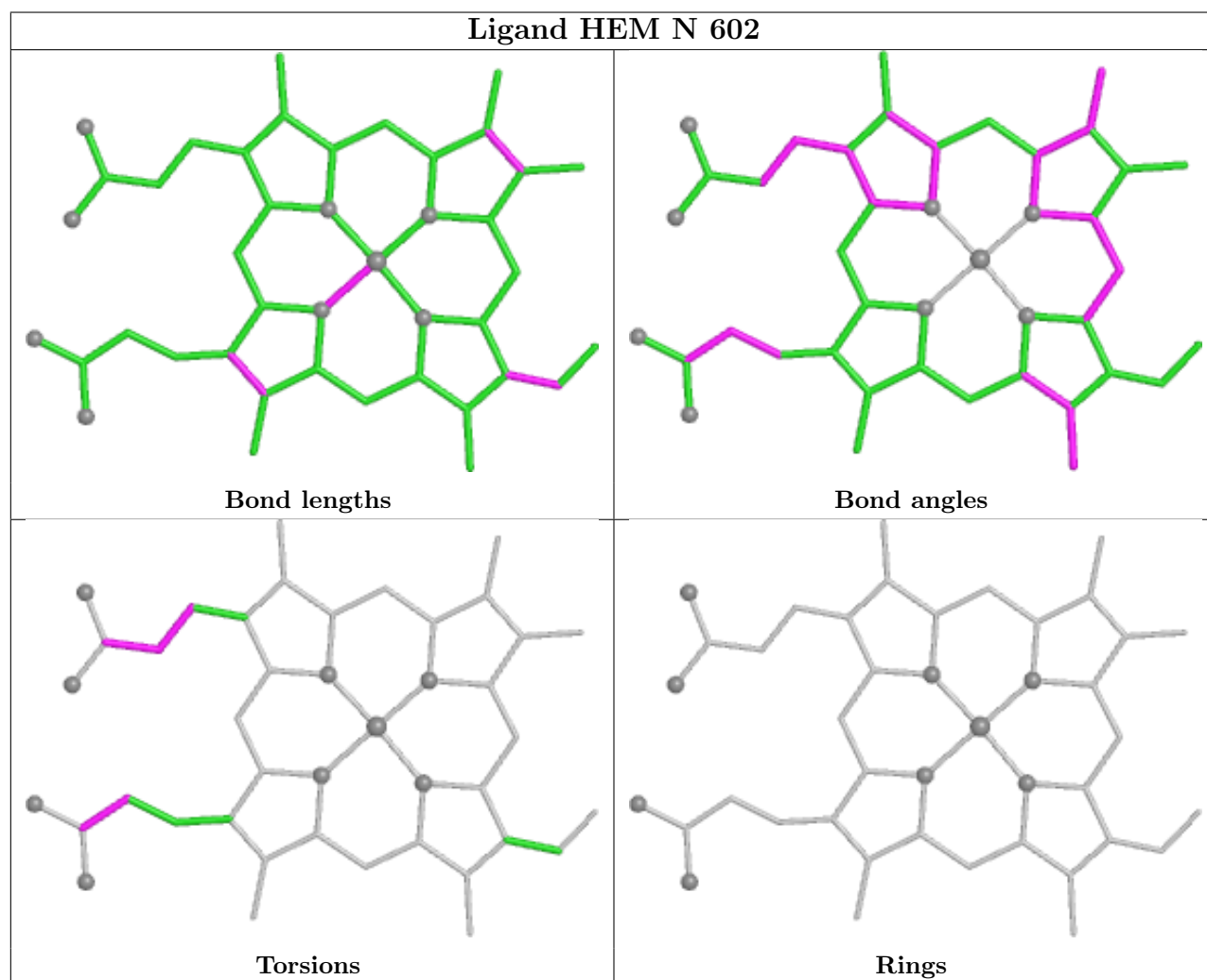
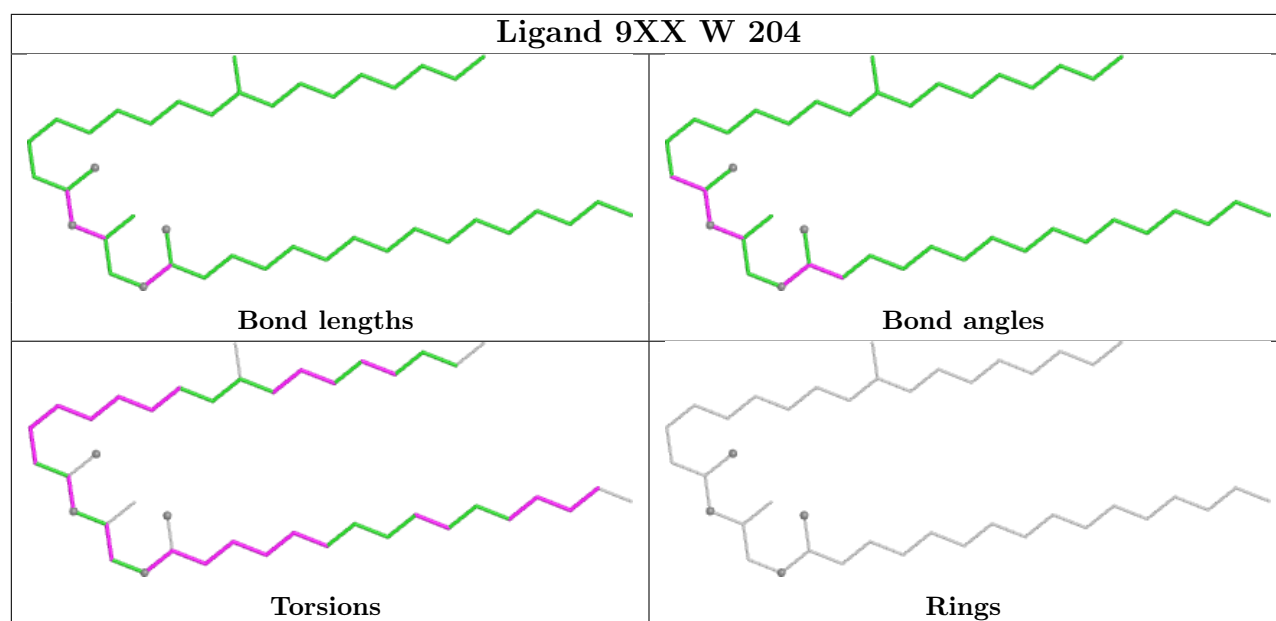


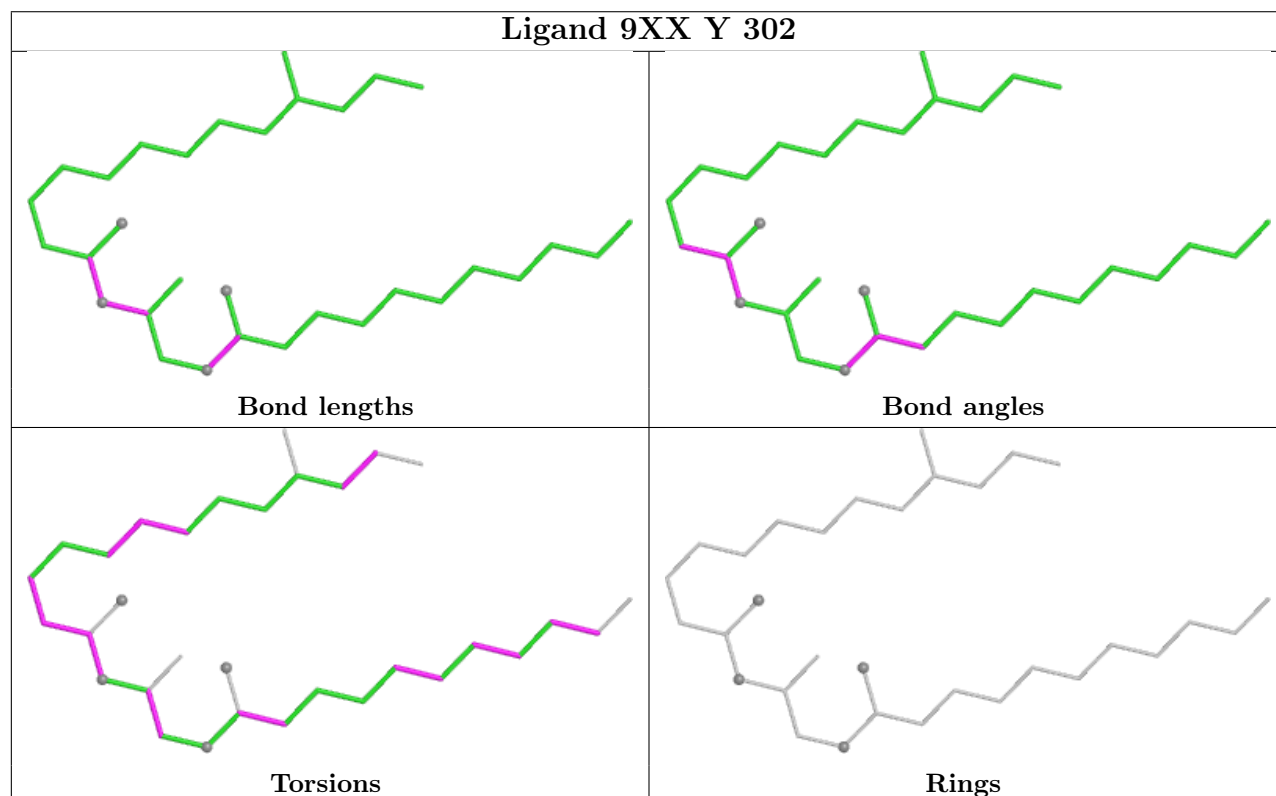
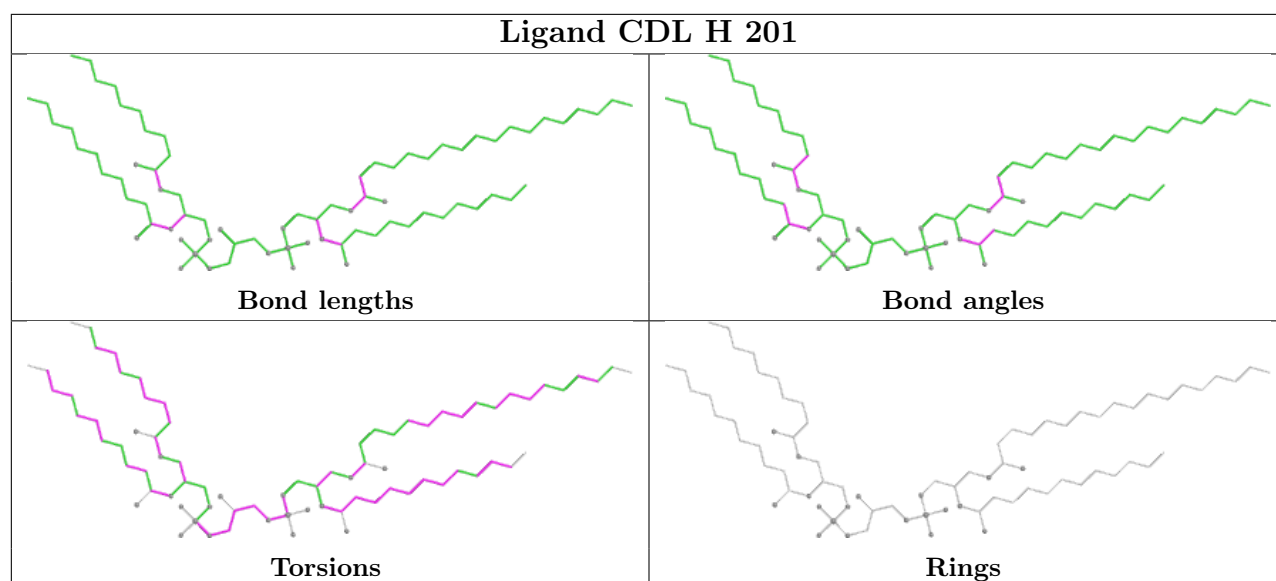


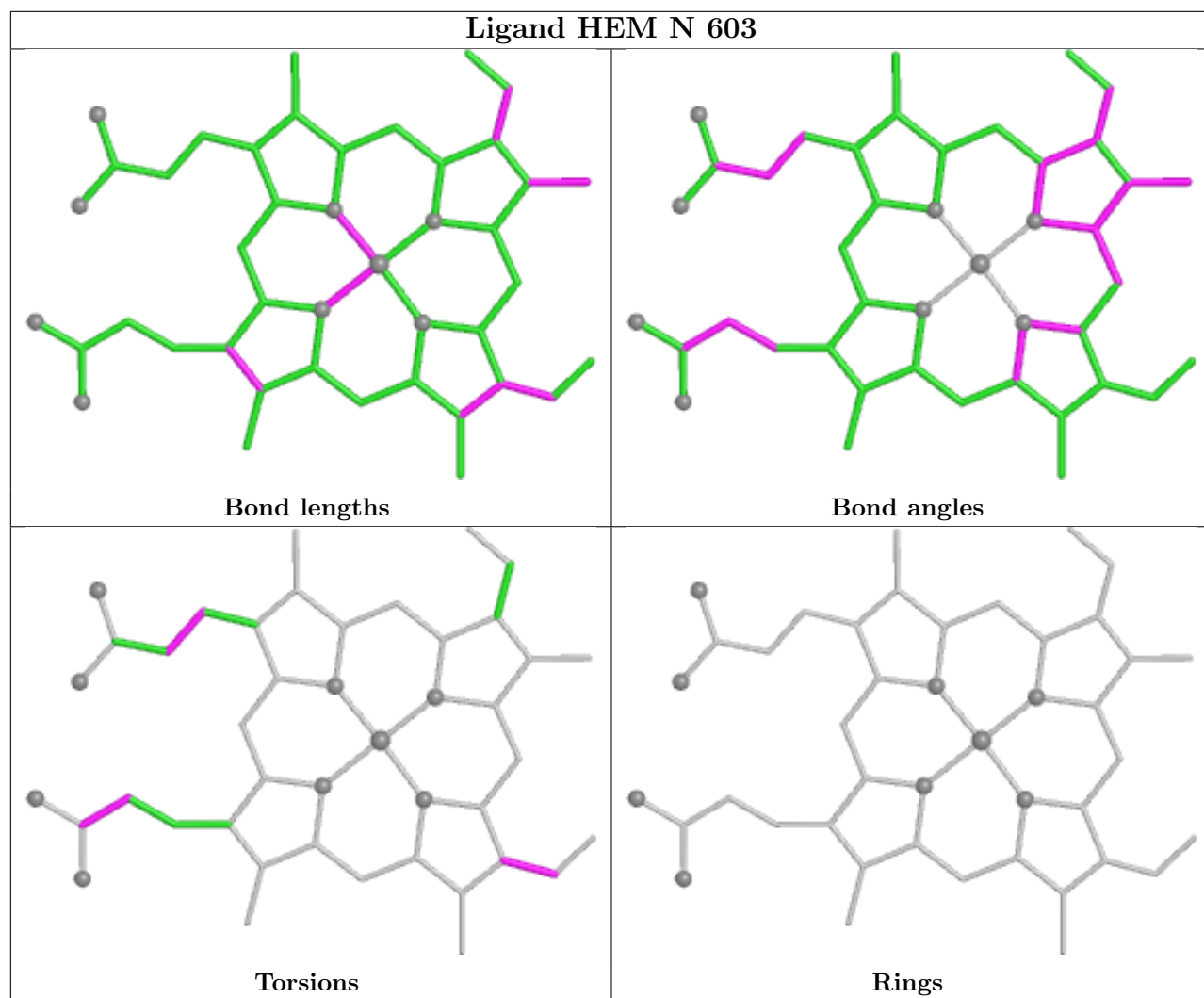
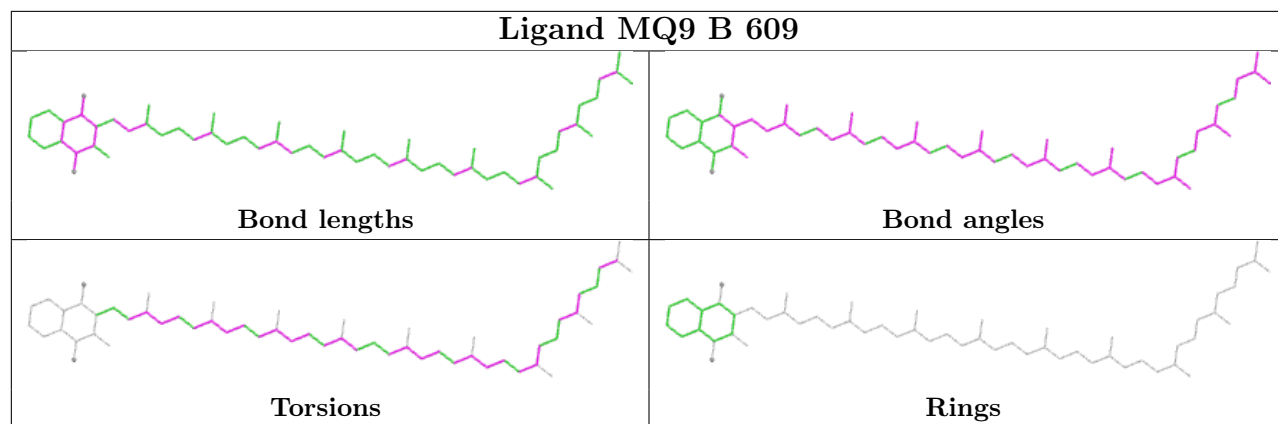
Ligand MQ9 B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

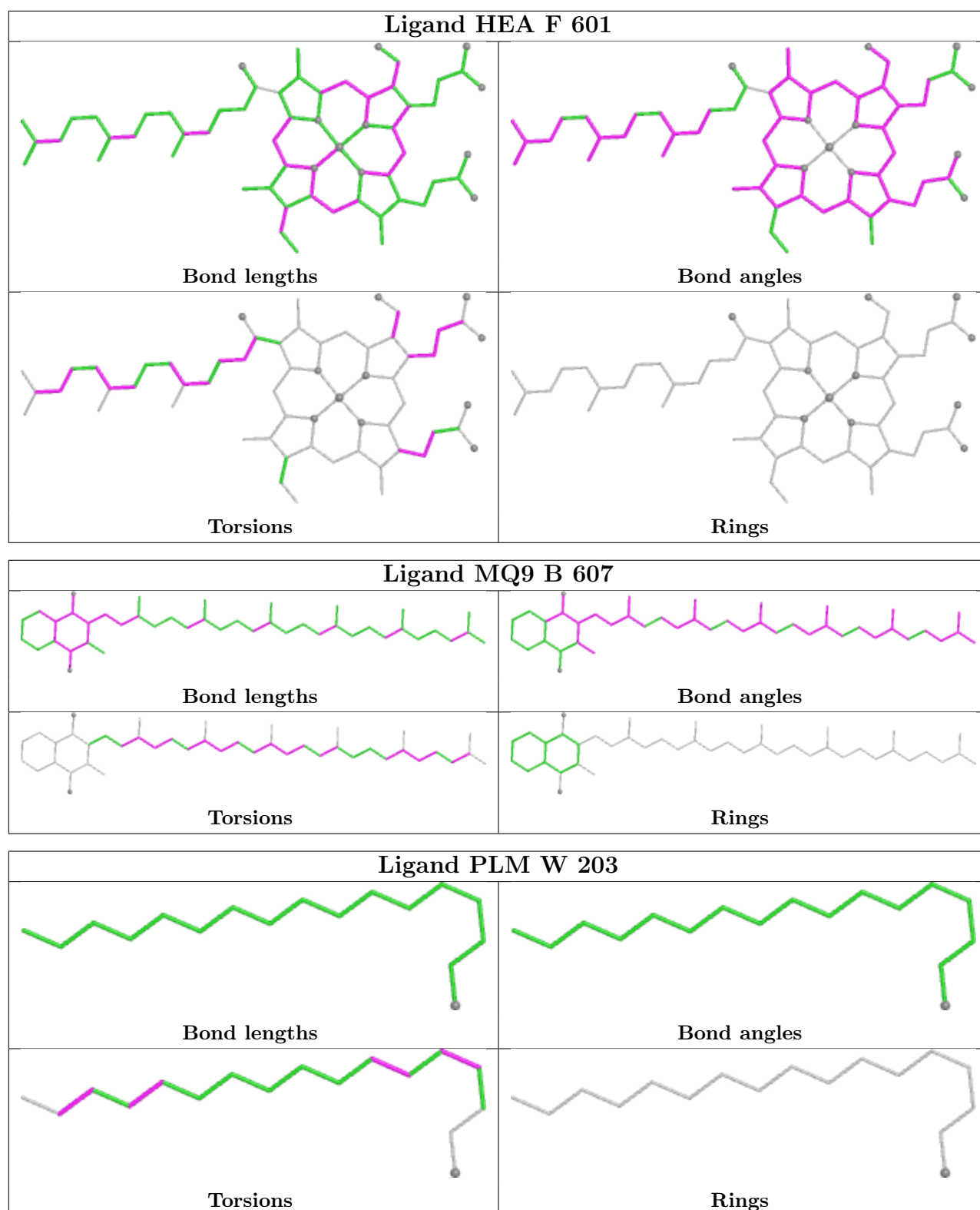
Ligand CDL A 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 N 608	
 Bond lengths	 Bond angles
 Torsions	 Rings









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.

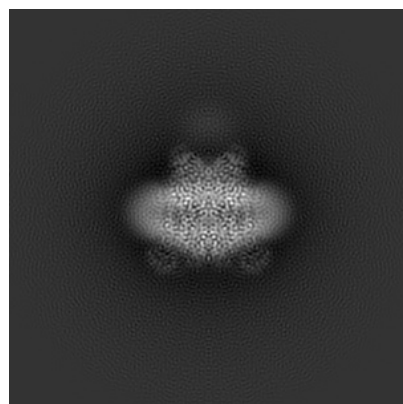
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9610. These allow visual inspection of the internal detail of the map and identification of artifacts.

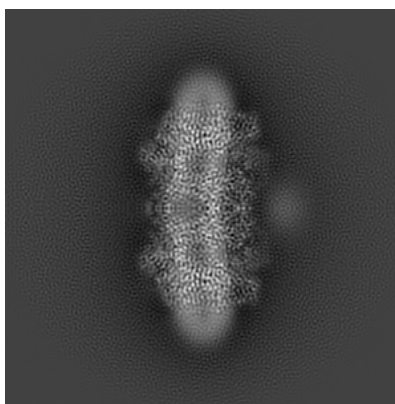
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

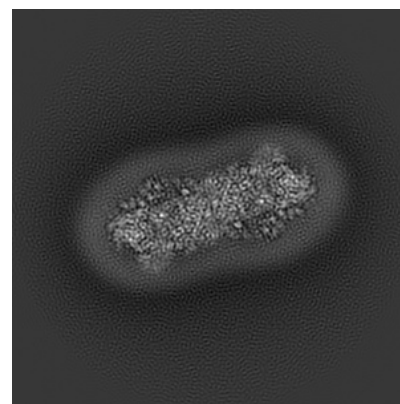
6.1.1 Primary map



X

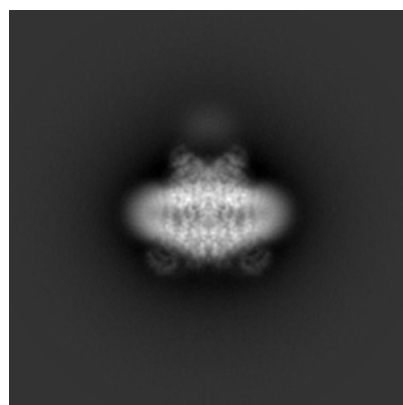


Y

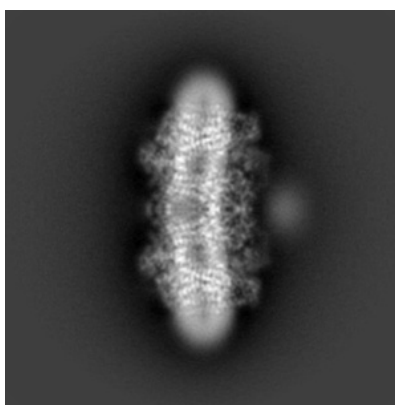


Z

6.1.2 Raw map



X



Y

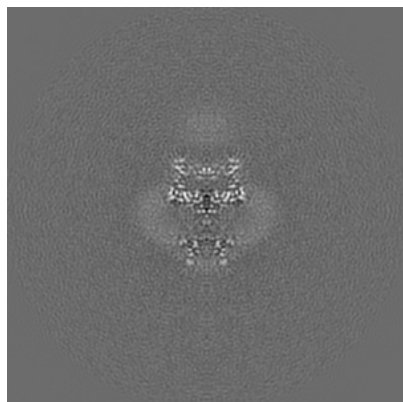


Z

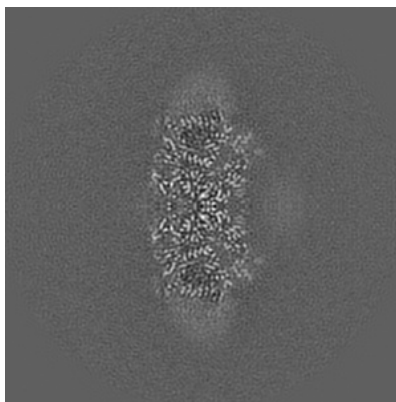
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

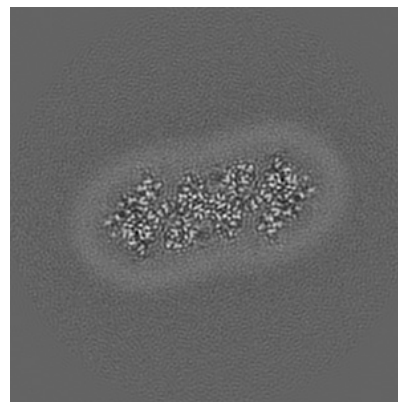
6.2.1 Primary map



X Index: 146

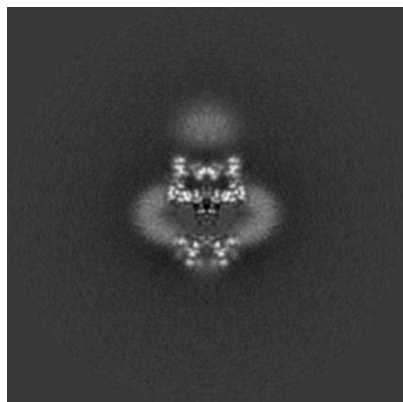


Y Index: 146

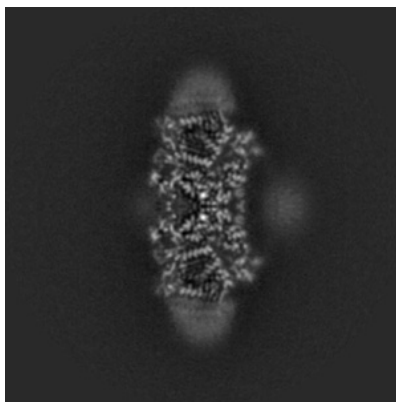


Z Index: 146

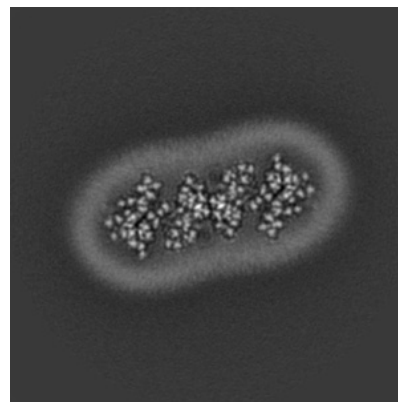
6.2.2 Raw map



X Index: 146



Y Index: 146

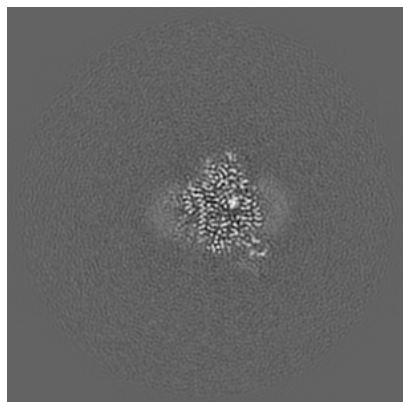


Z Index: 146

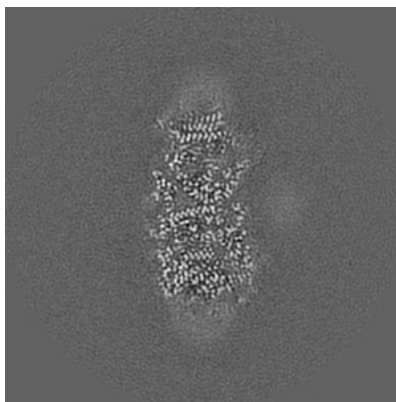
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

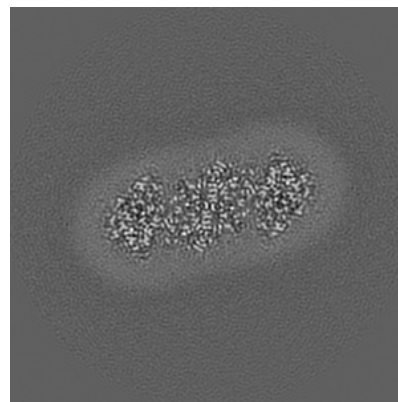
6.3.1 Primary map



X Index: 197

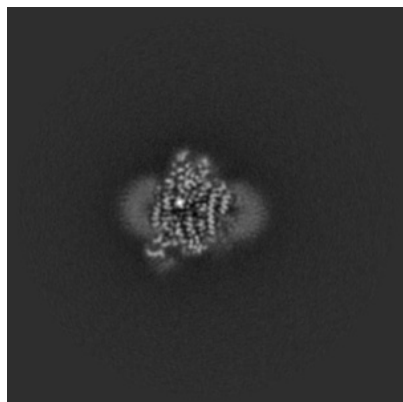


Y Index: 142

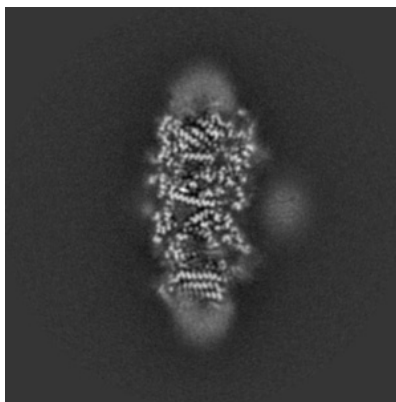


Z Index: 153

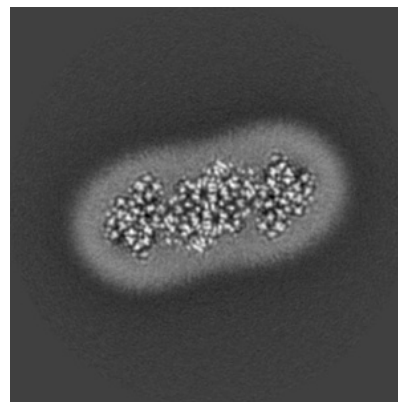
6.3.2 Raw map



X Index: 95



Y Index: 150

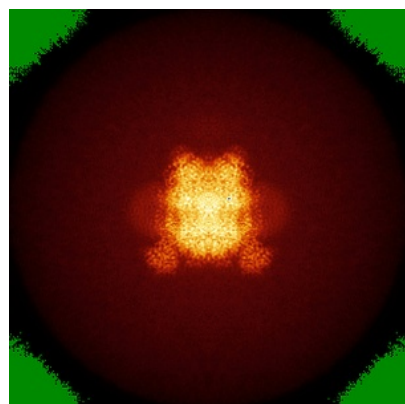


Z Index: 153

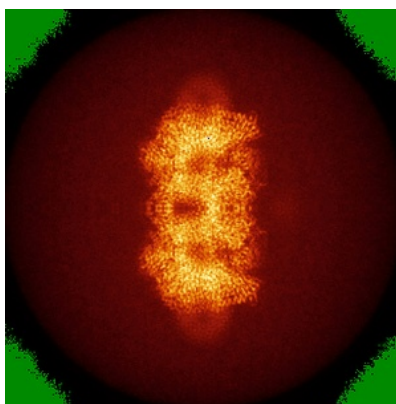
The images above show the largest variance slices of the map in three orthogonal directions.

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

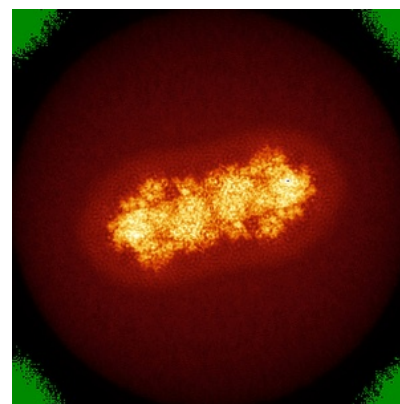
6.4.1 Primary map



X

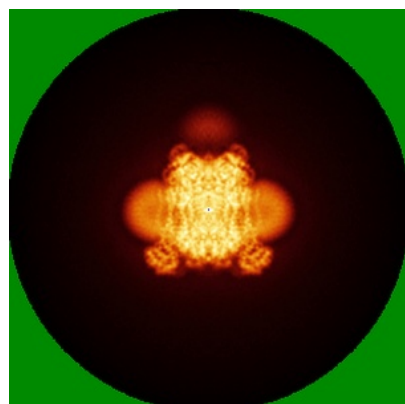


Y

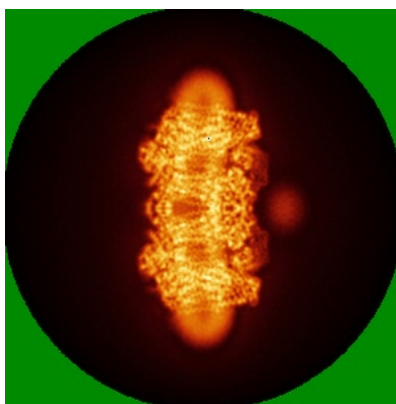


Z

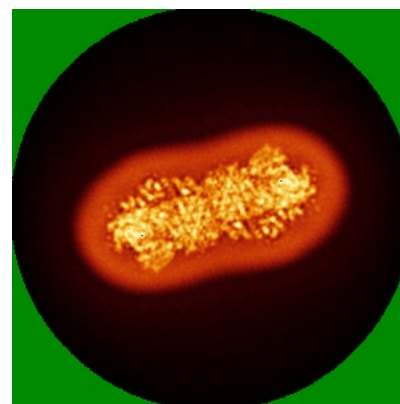
6.4.2 Raw map



X



Y

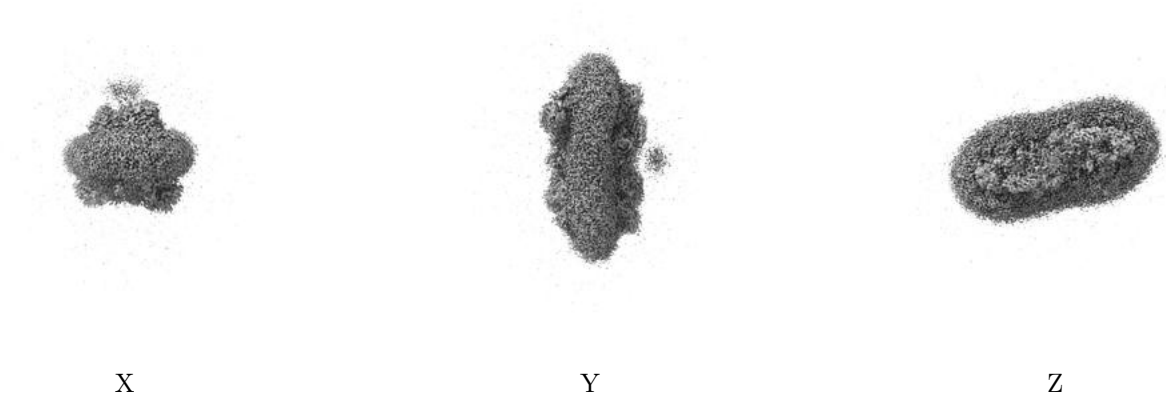


Z

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

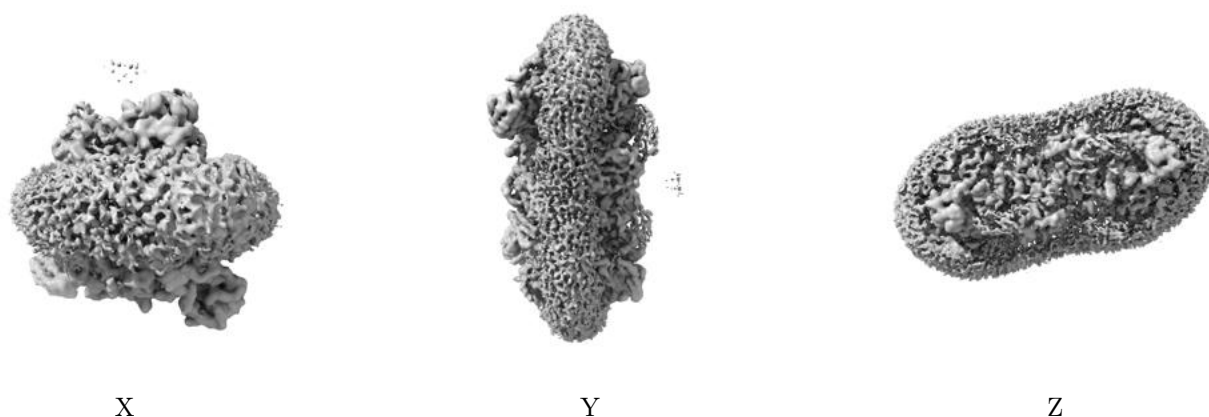
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0452. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

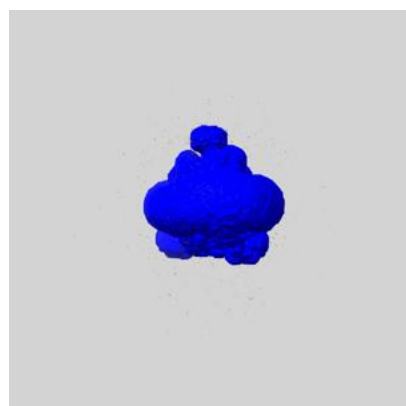
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

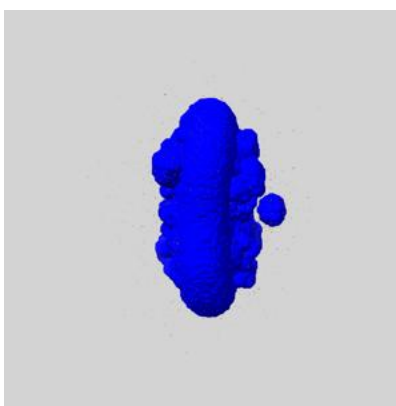
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

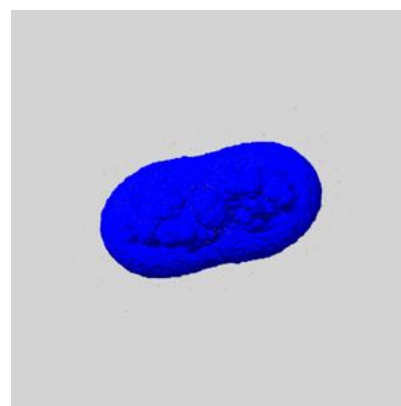
6.6.1 emd_9610_msk_1.map [i](#)



X



Y

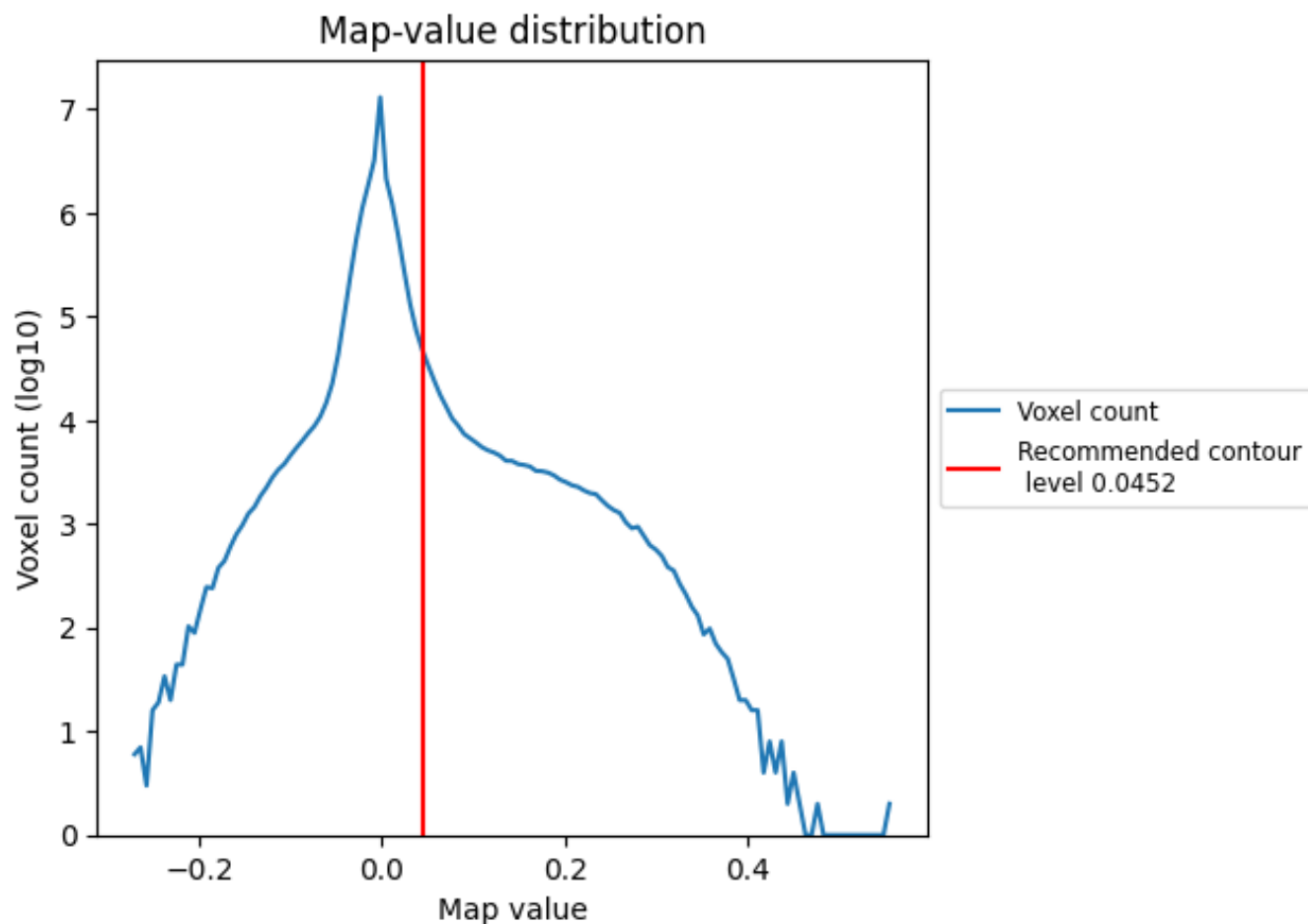


Z

7 Map analysis [i](#)

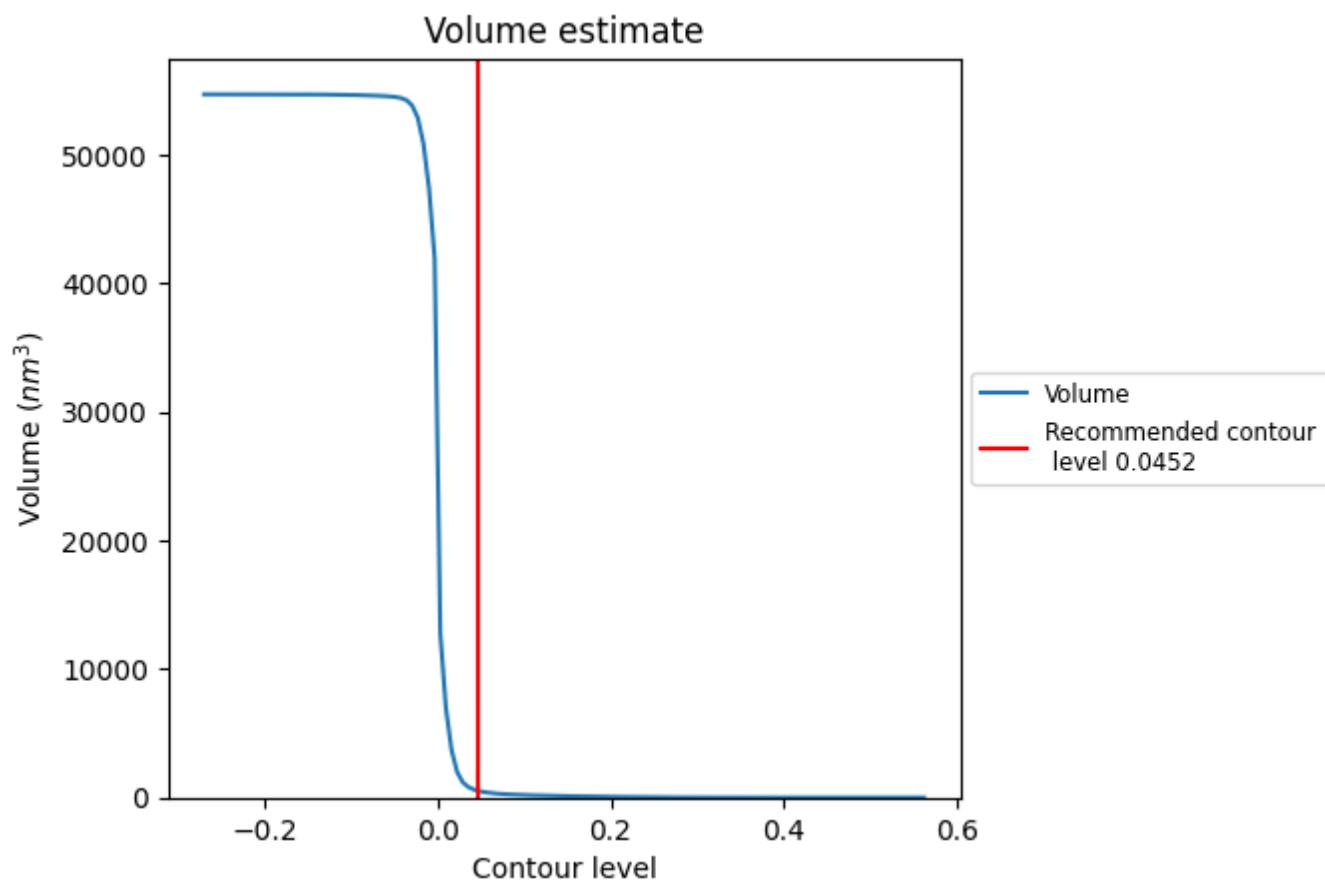
This section contains the results of statistical analysis of the map.

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.

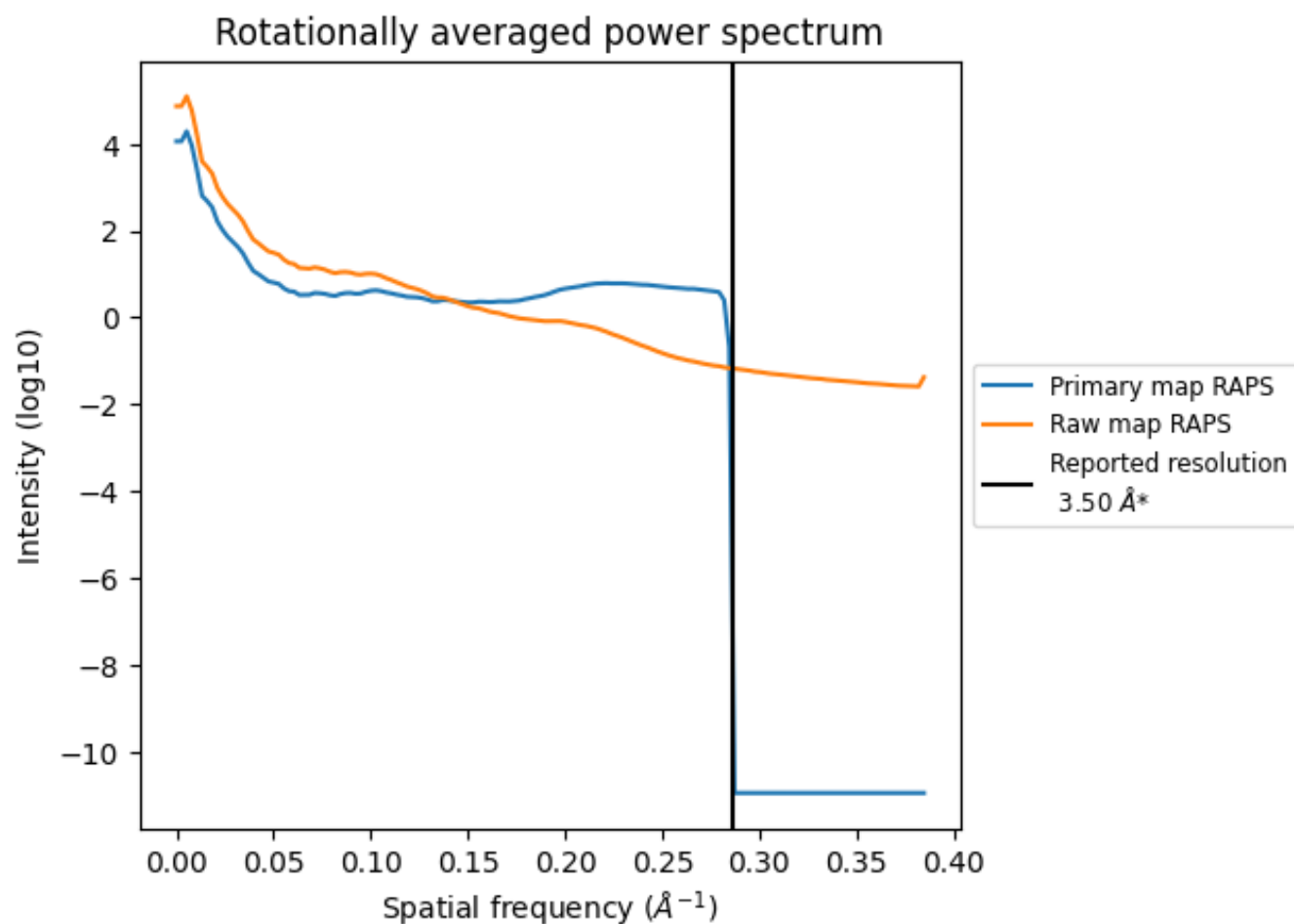
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 554 nm³; this corresponds to an approximate mass of 500 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 ⓘ

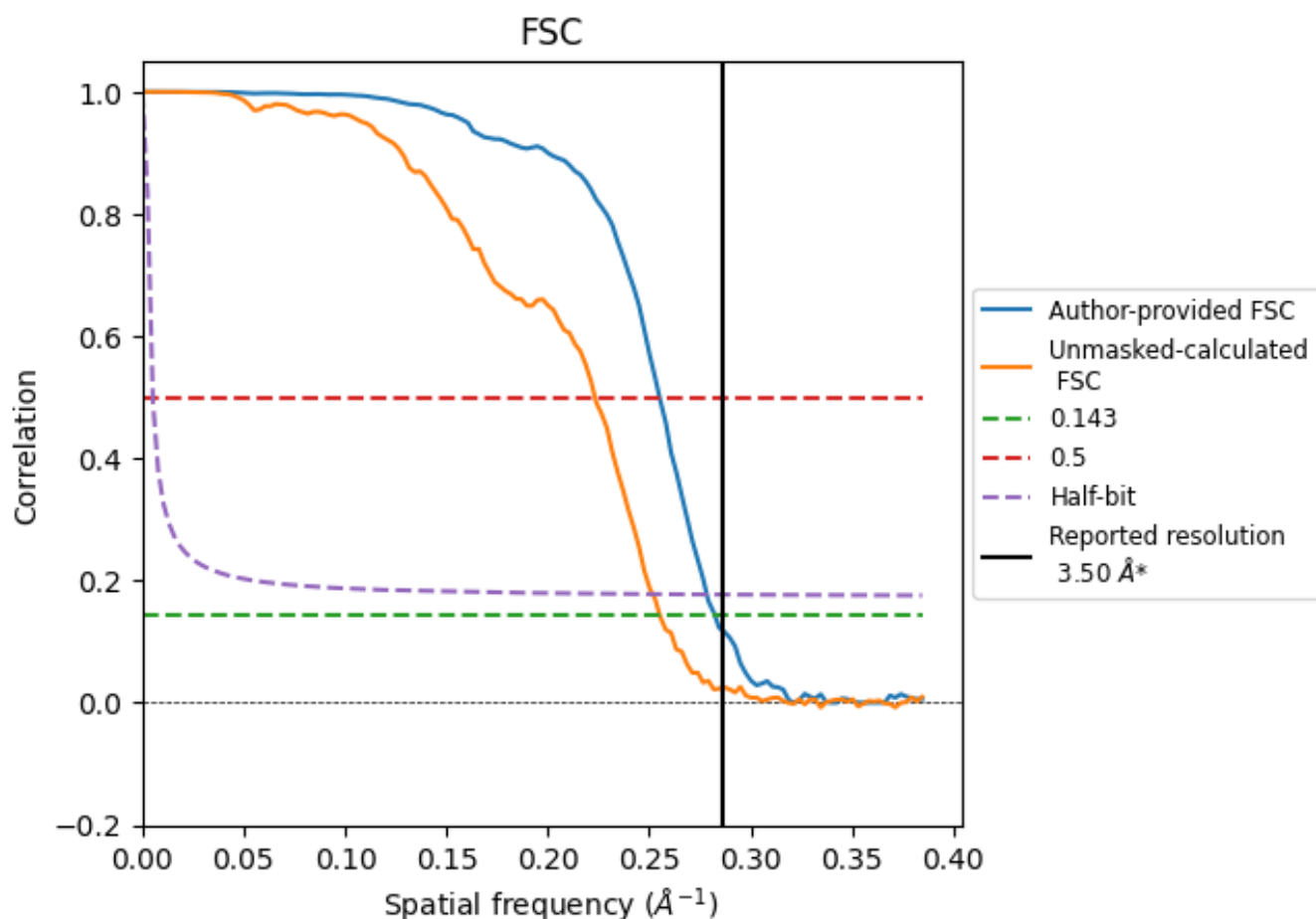


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

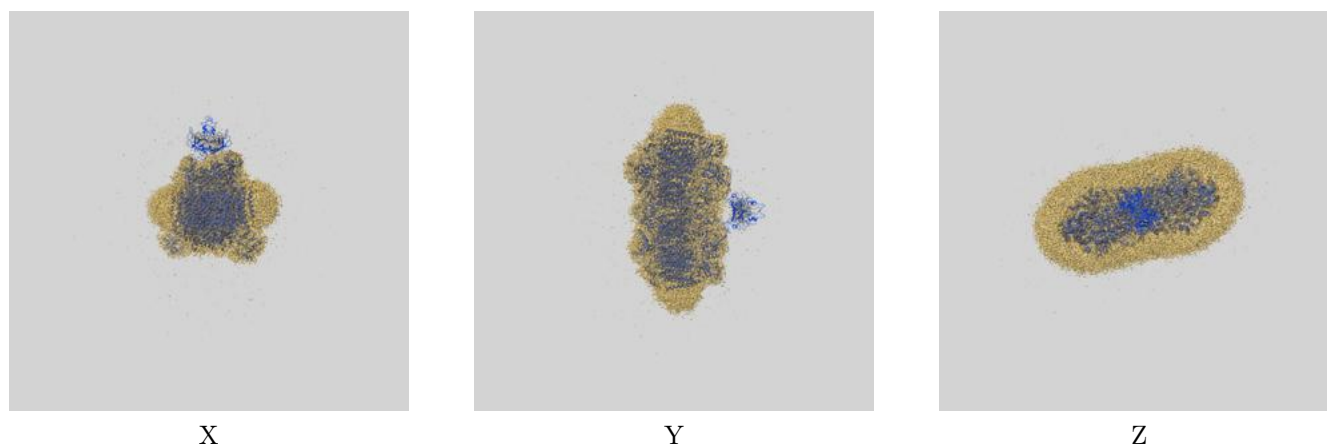
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.54	3.92	3.59
Unmasked-calculated*	3.92	4.48	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

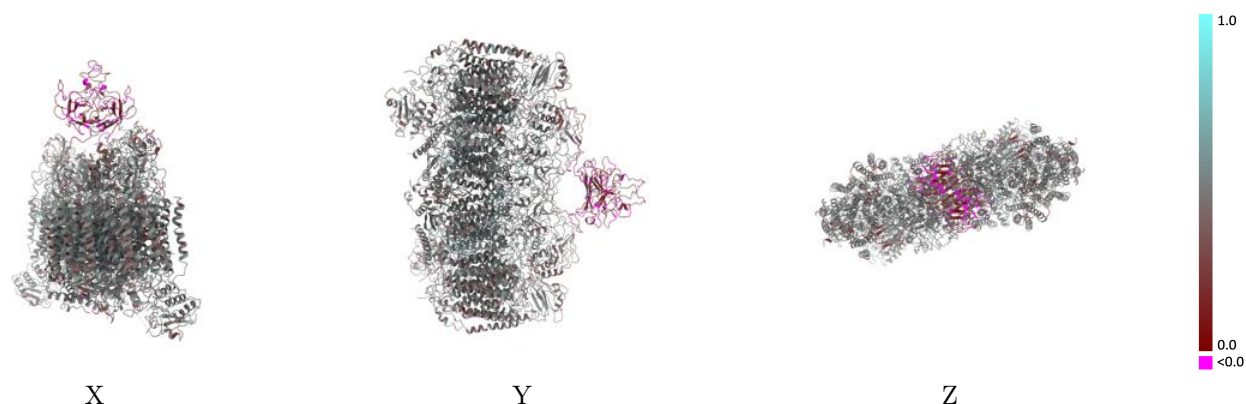
This section contains information regarding the fit between EMDB map EMD-9610 and PDB model 6ADQ. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



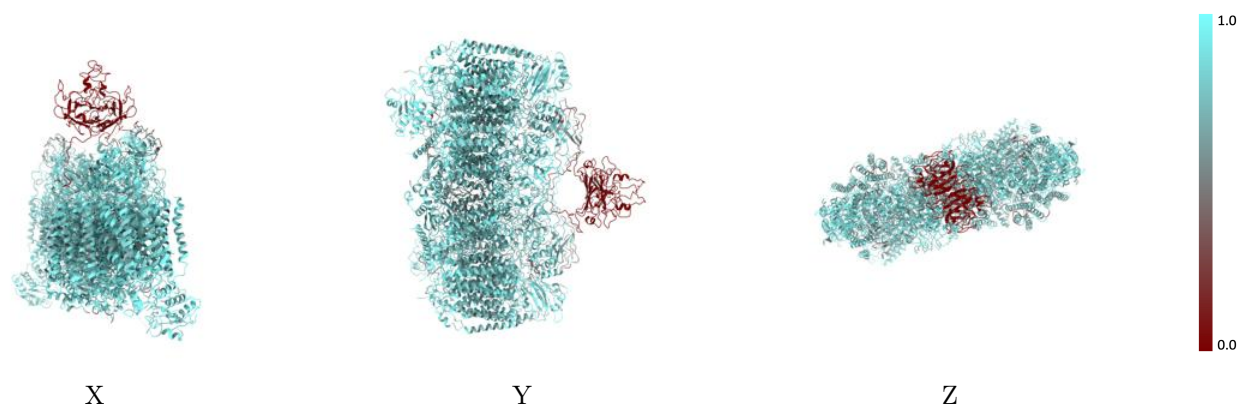
The images above show the 3D surface view of the map at the recommended contour level 0.0452 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



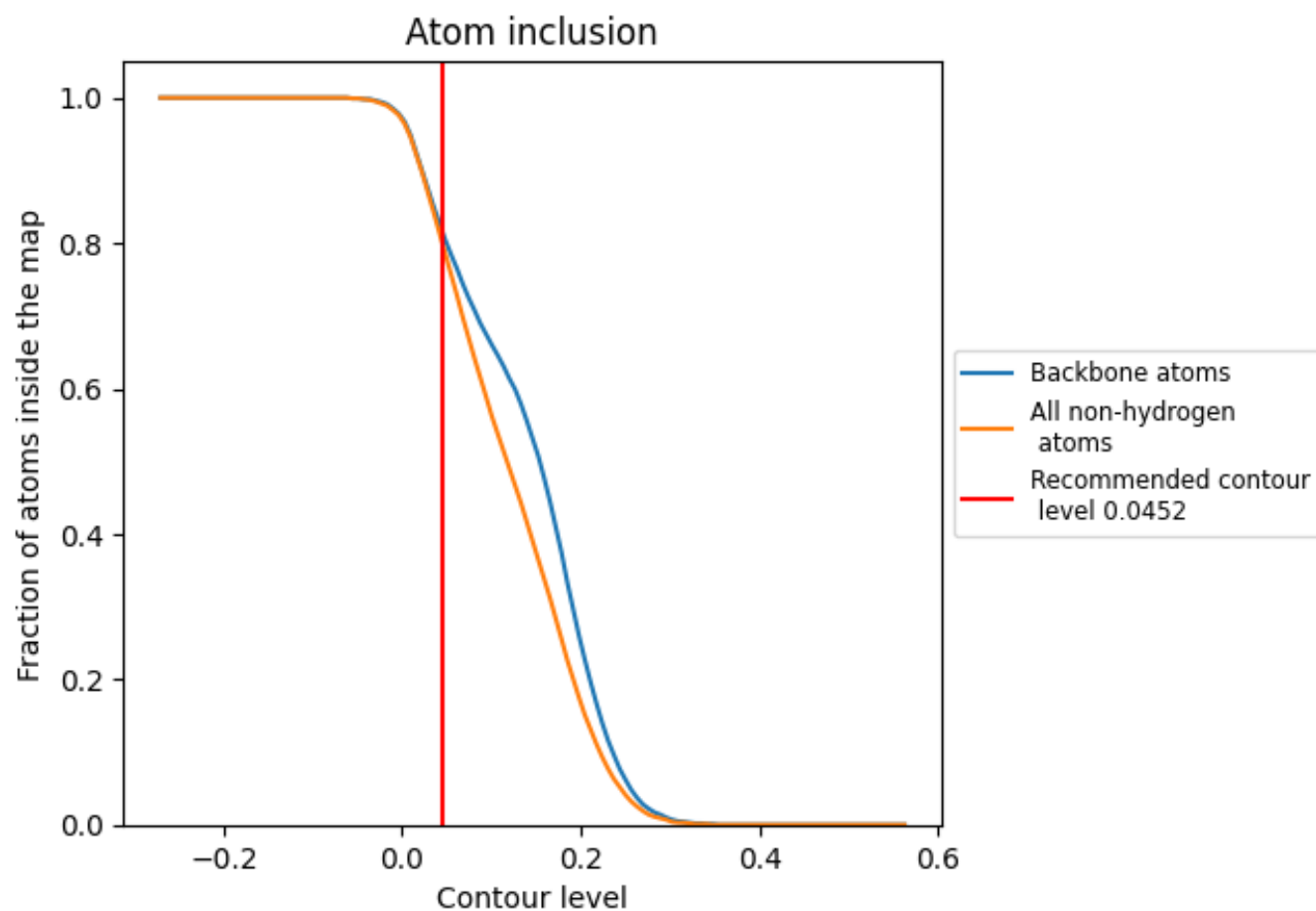
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0452).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.0452) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.4580
A	 0.8490	 0.4820
B	 0.8400	 0.4890
C	 0.8610	 0.4760
D	 0.7920	 0.4690
E	 0.8090	 0.4410
F	 0.8570	 0.4800
G	 0.8020	 0.4460
H	 0.8280	 0.4710
I	 0.8820	 0.4670
J	 0.8600	 0.4500
K	 0.6380	 0.4380
M	 0.8490	 0.4820
N	 0.8450	 0.4910
O	 0.8610	 0.4770
P	 0.7920	 0.4690
Q	 0.8090	 0.4380
R	 0.8570	 0.4810
S	 0.8020	 0.4460
T	 0.8280	 0.4700
U	 0.8760	 0.4620
V	 0.8640	 0.4540
W	 0.6420	 0.4380
Y	 0.1850	 0.1980
Z	 0.1850	 0.2010

