



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2026 – 06:43 pm BST

PDB ID : 8OVC / pdb_00008ovc
EMDB ID : EMD-17210
Title : Respiratory supercomplex (III2-IV2) from Mycobacterium smegmatis
Authors : Kovalova, T.; Krol, S.; Sjostrand, D.; Riepl, D.; Gamiz-Hernandez, A.;
Brzezinski, P.; Kaila, V.; Hogbom, M.
Deposited on : 2023-04-25
Resolution : 2.80 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:

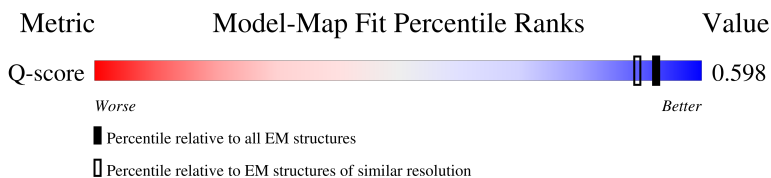
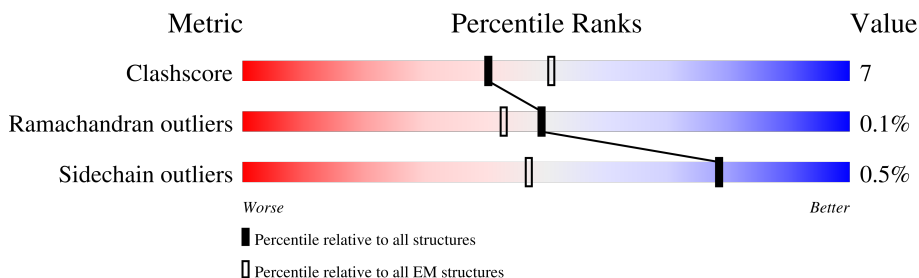
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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.



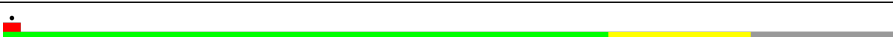
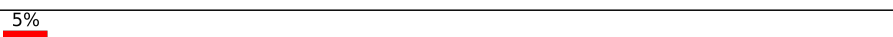
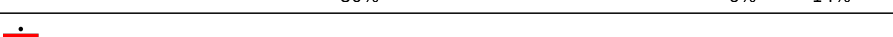
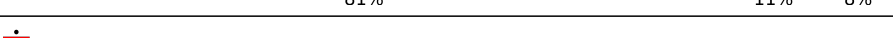
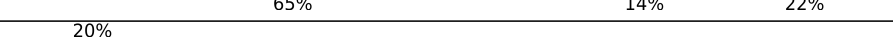
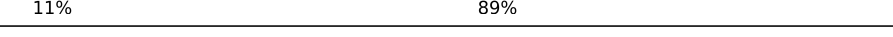
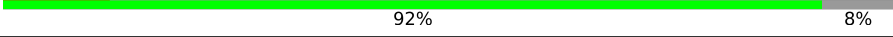
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	C	278	
1	O	278	
2	G	408	
2	M	408	

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Mol	Chain	Length	Quality of chain
3	H	556	
3	N	556	
4	I	100	
4	P	100	
5	J	203	
5	S	203	
6	K	139	
6	T	139	
7	L	575	
7	R	575	
8	Q	341	
8	X	341	
9	U	79	
9	Z	79	
10	V	157	
10	a	157	
11	W	186	
11	b	186	
12	Y	236	
12	c	236	
13	E	10	
13	f	10	
14	F	25	
14	e	25	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEC	C	301	X	-	-	-
15	HEC	C	302	X	-	-	-
15	HEC	O	301	X	-	-	-
15	HEC	O	302	X	-	-	-
16	MQ9	H	607	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 46771 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome bc1 complex cytochrome c subunit.

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

There are 20 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	381	Total	C	N	O	S	0	0
			2973	1922	503	537	11		
2	G	380	Total	C	N	O	S	0	0
			2964	1917	501	535	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	535	Total	C	N	O	S	0	0
			4181	2751	711	701	18		
3	H	533	Total	C	N	O	S	0	0
			4167	2743	707	699	18		

There are 20 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	86	Total	C	N	O	S	0	0
			688	443	125	115	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	86	Total	C	N	O	S	0	0
			688	443	125	115	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		
5	J	186	Total	C	N	O	S	0	0
			1455	976	231	241	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	552	Total	C	N	O	S	0	0
			4373	2938	695	714	26		
7	L	551	Total	C	N	O	S	0	0
			4369	2936	694	713	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	286	Total	C	N	O	S	0	0
			2287	1483	377	419	8		
8	X	301	Total	C	N	O	S	0	0
			2398	1552	399	437	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	66	Total	C	N	O	S	0	0
			499	329	84	85	1		
9	Z	68	Total	C	N	O	S	0	0
			511	336	86	87	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	144	Total	C	N	O	S	0	0
			1032	653	175	202	2		
10	a	143	Total	C	N	O	S	0	0
			1024	647	174	201	2		

- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	146	Total	C	N	O	S	0	0
			1051	652	176	222	1		
11	b	148	Total	C	N	O	S	0	0
			1074	666	179	228	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	26	Total	C	N	O	S	0	0
			173	106	27	39	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

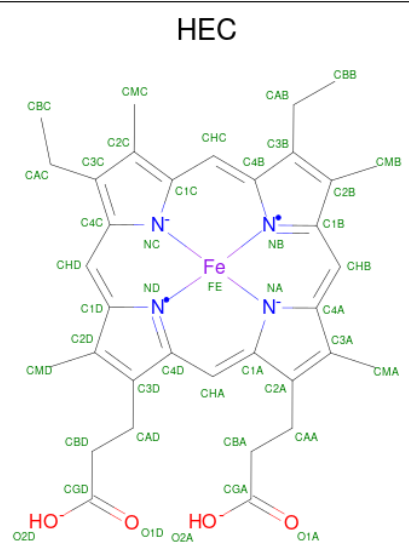
- Molecule 13 is a protein called Co-purified unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	E	7	Total	C	N	O	0	0
			35	21	7	7		
13	f	7	Total	C	N	O	0	0
			35	21	7	7		

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

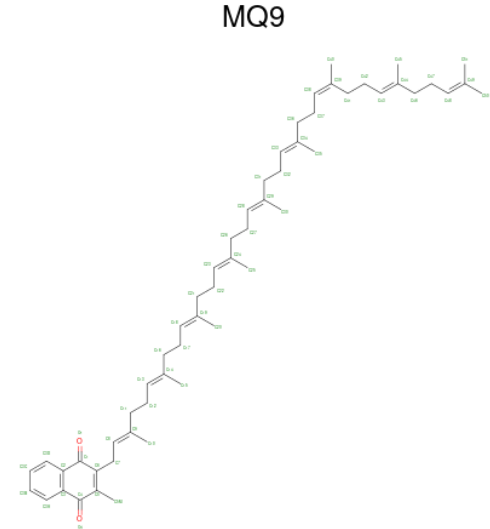
Mol	Chain	Residues	Atoms				AltConf	Trace
14	F	23	Total	C	N	O	0	0
			115	69	23	23		
14	e	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 15 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



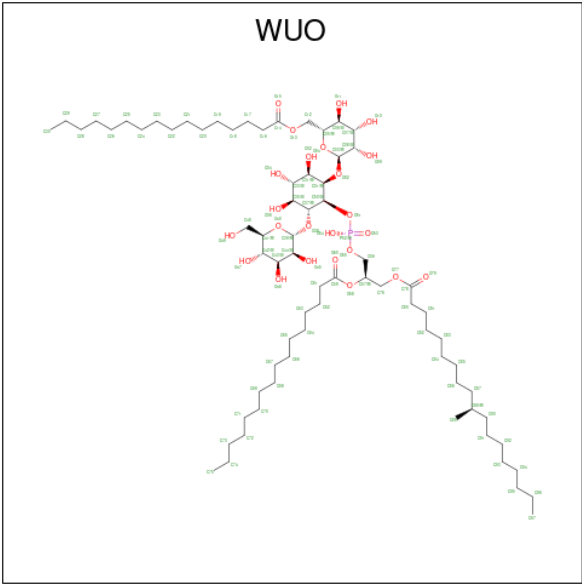
Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 43	C 34	Fe 1	N 4	O 4	0
15	O	1	Total 43	C 34	Fe 1	N 4	O 4	0
15	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
15	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 16 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	O	1	Total	C	O	0
			58	56	2	
16	N	1	Total	C	O	0
			58	56	2	
16	N	1	Total	C	O	0
			58	56	2	
16	N	1	Total	C	O	0
			58	56	2	
16	C	1	Total	C	O	0
			58	56	2	
16	G	1	Total	C	O	0
			43	41	2	
16	H	1	Total	C	O	0
			58	56	2	
16	H	1	Total	C	O	0
			43	41	2	
16	H	1	Total	C	O	0
			58	56	2	
16	H	1	Total	C	O	0
			58	56	2	

- Molecule 17 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (CCD ID: WUO) (formula: C₇₂H₁₃₅O₂₄P).



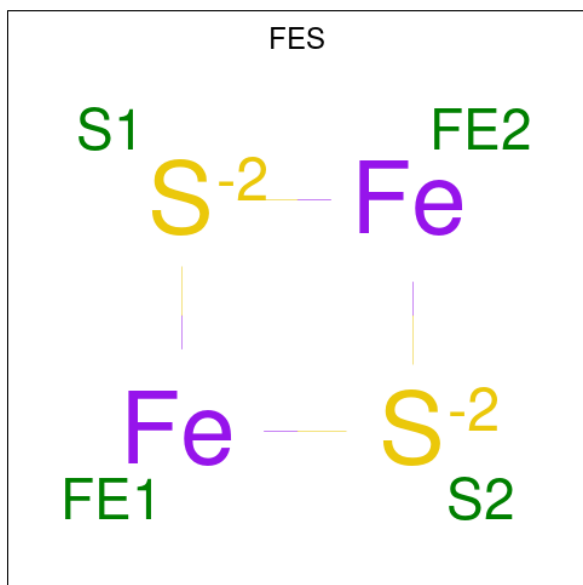
Mol	Chain	Residues	Atoms				AltConf
17	O	1	Total	C	O	P	0
			97	72	24	1	

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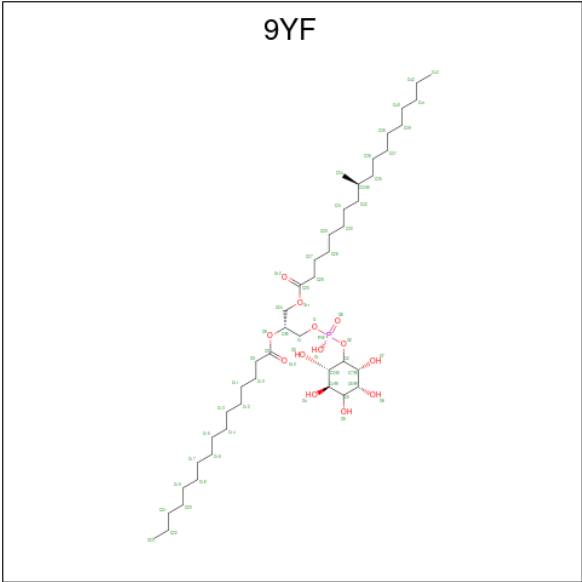
Mol	Chain	Residues	Atoms				AltConf
17	W	1	Total	C	O	P	0
			97	72	24	1	
17	C	1	Total	C	O	P	0
			97	72	24	1	
17	I	1	Total	C	O	P	0
			97	72	24	1	

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



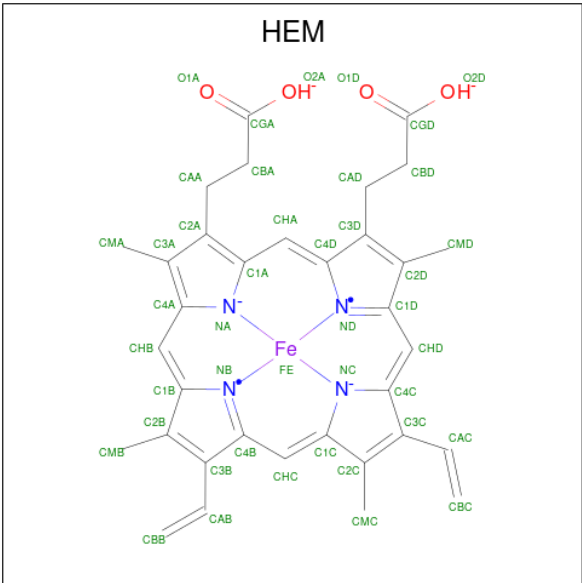
Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	Fe	S	0
			4	2	2	
18	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 19 is (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: $\text{C}_{44}\text{H}_{85}\text{O}_{13}\text{P}$).



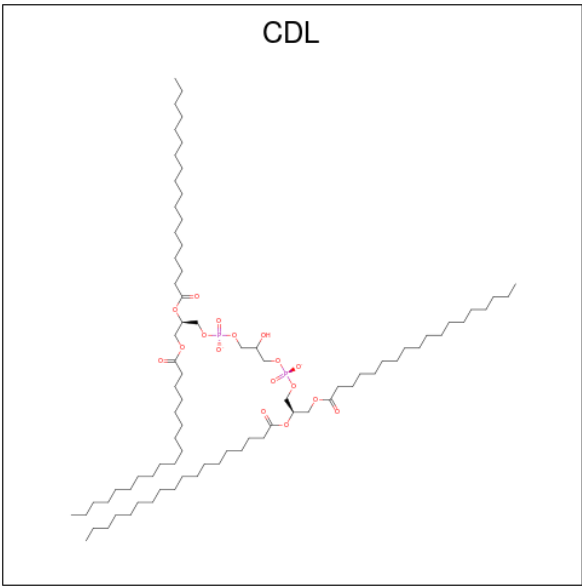
Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			58	44	13	1	
19	W	1	Total	C	O	P	0
			58	44	13	1	
19	G	1	Total	C	O	P	0
			58	44	13	1	
19	b	1	Total	C	O	P	0
			58	44	13	1	

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



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

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



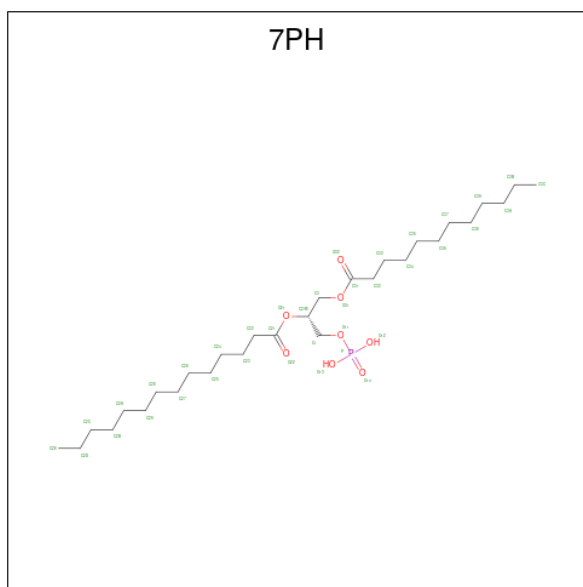
Mol	Chain	Residues	Atoms				AltConf
21	N	1	Total	C	O	P	0
			77	58	17	2	
21	N	1	Total	C	O	P	0
			79	60	17	2	
21	P	1	Total	C	O	P	0
			77	58	17	2	
21	T	1	Total	C	O	P	0
			79	60	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	G	1	Total	C	O	P	0
			79	60	17	2	
21	H	1	Total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

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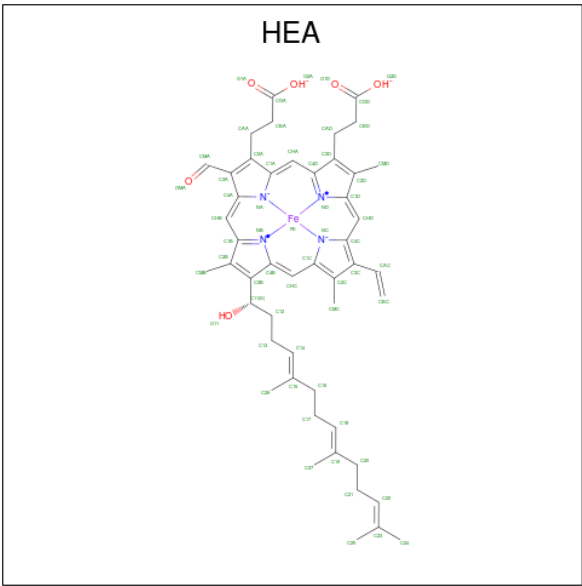
Mol	Chain	Residues	Atoms				AltConf
21	H	1	Total	C	O	P	0
			74	55	17	2	
21	H	1	Total	C	O	P	0
			77	58	17	2	
21	H	1	Total	C	O	P	0
			79	60	17	2	
21	H	1	Total	C	O	P	0
			79	60	17	2	
21	I	1	Total	C	O	P	0
			77	58	17	2	
21	I	1	Total	C	O	P	0
			77	58	17	2	
21	L	1	Total	C	O	P	0
			79	60	17	2	
21	L	1	Total	C	O	P	0
			77	58	17	2	

- Molecule 22 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
22	S	1	Total	C	O	P	0
			38	29	8	1	
22	S	1	Total	C	O	P	0
			38	29	8	1	
22	J	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 23 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 24 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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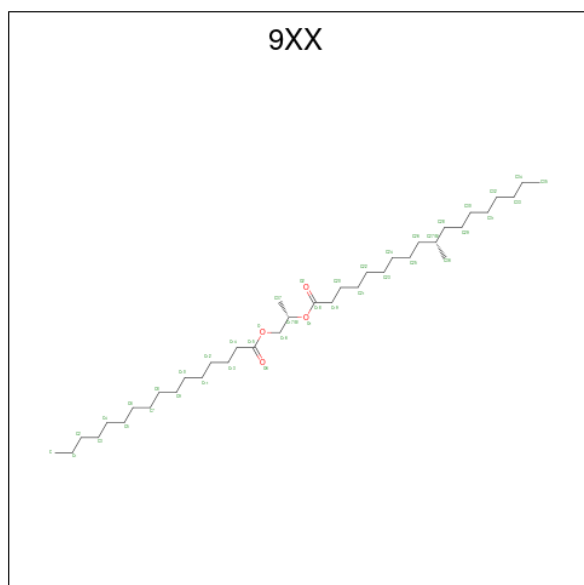
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Mol	Chain	Residues	Atoms		AltConf
25	L	1	Total	Mg	0
			1	1	

- Molecule 26 is CALCIUM ION (CCD ID: CA) (formula: Ca).

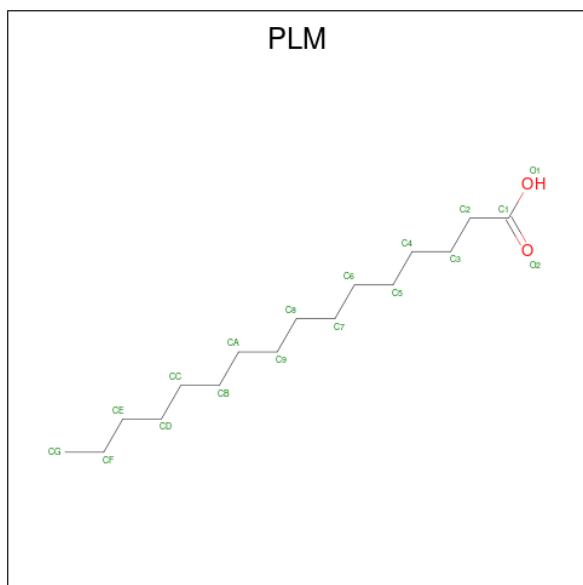
Mol	Chain	Residues	Atoms		AltConf
26	R	1	Total	Ca	0
			1	1	
26	L	1	Total	Ca	0
			1	1	

- Molecule 27 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C₃₈H₇₄O₄).



Mol	Chain	Residues	Atoms			AltConf
27	R	1	Total	C	O	0
			42	38	4	
27	Y	1	Total	C	O	0
			32	28	4	
27	H	1	Total	C	O	0
			32	28	4	
27	b	1	Total	C	O	0
			32	28	4	

- Molecule 28 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
28	W	1	Total	C	O	0
			11	10	1	
28	Y	1	Total	C	O	0
			11	10	1	
28	L	1	Total	C	O	0
			11	10	1	
28	c	1	Total	C	O	0
			11	10	1	

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		AltConf
29	O	25	Total	O	0
			25	25	
29	M	15	Total	O	0
			15	15	
29	N	22	Total	O	0
			22	22	
29	P	3	Total	O	0
			3	3	
29	S	1	Total	O	0
			1	1	
29	T	3	Total	O	0
			3	3	
29	R	14	Total	O	0
			14	14	
29	Q	5	Total	O	0
			5	5	

Continued on next page...

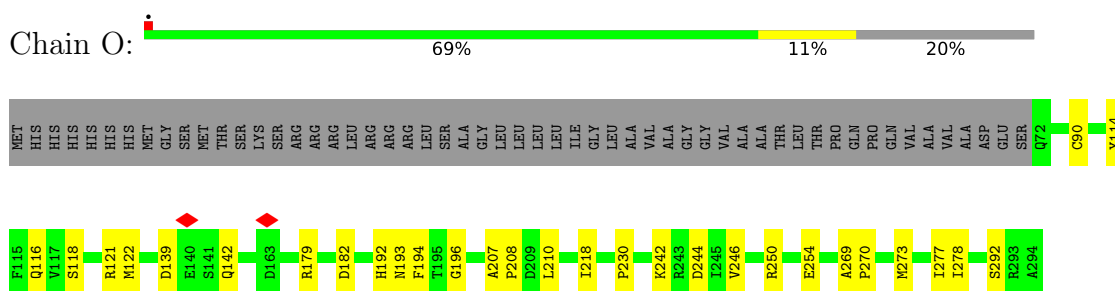
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
29	V	1	Total 1	O 1	0
29	W	5	Total 5	O 5	0
29	Y	2	Total 2	O 2	0
29	C	30	Total 30	O 30	0
29	G	24	Total 24	O 24	0
29	H	39	Total 39	O 39	0
29	I	5	Total 5	O 5	0
29	K	6	Total 6	O 6	0
29	L	25	Total 25	O 25	0
29	X	9	Total 9	O 9	0
29	Z	1	Total 1	O 1	0
29	b	12	Total 12	O 12	0
29	c	2	Total 2	O 2	0

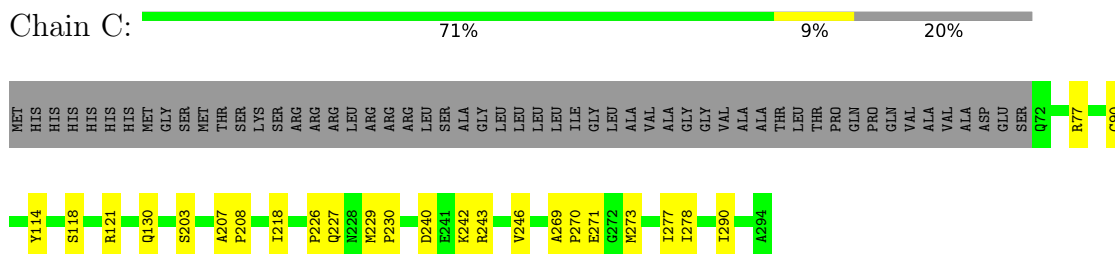
3 Residue-property plots [i](#)

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.

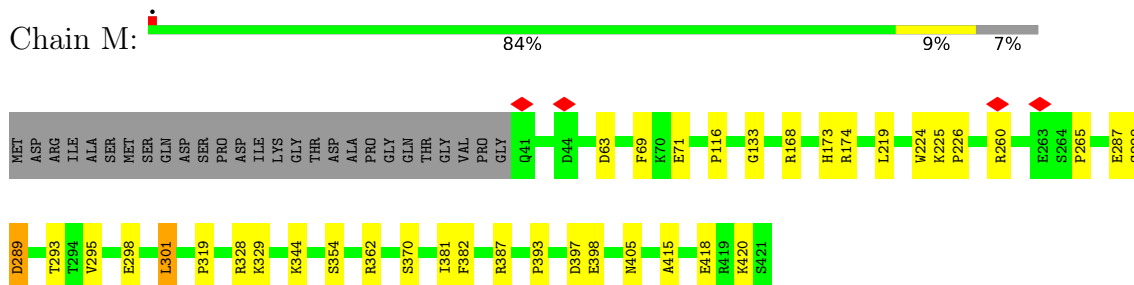
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit



- Molecule 1: Cytochrome bc1 complex cytochrome c subunit

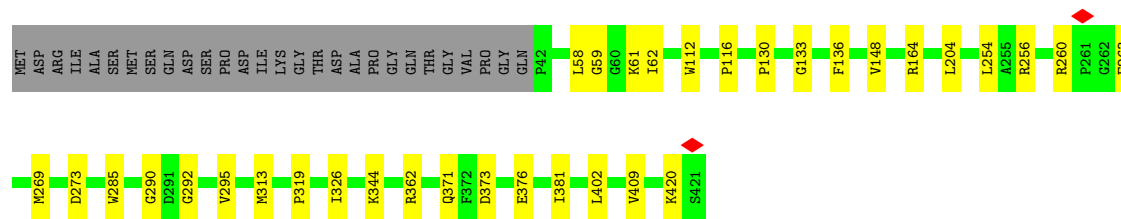


- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

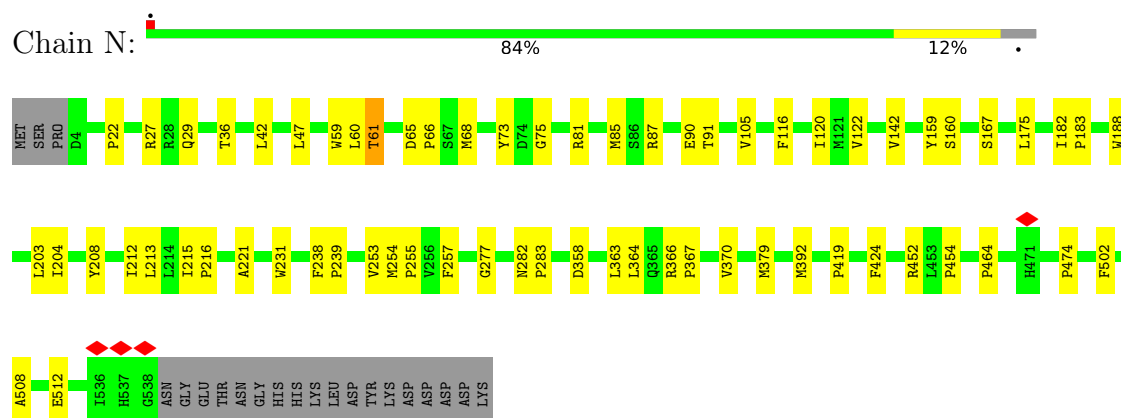


- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

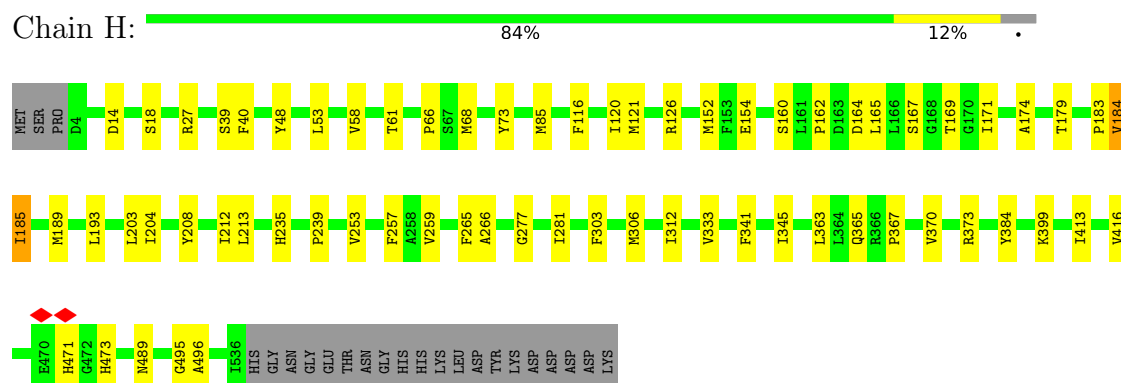




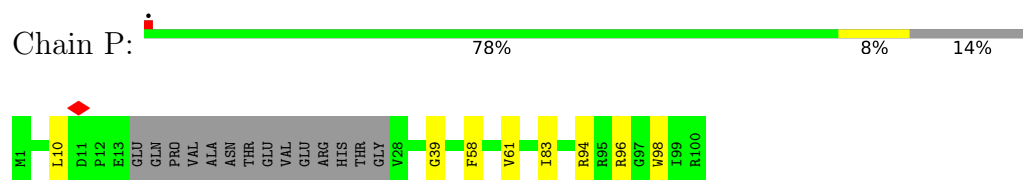
- Molecule 3: Cytochrome bc1 complex cytochrome b subunit



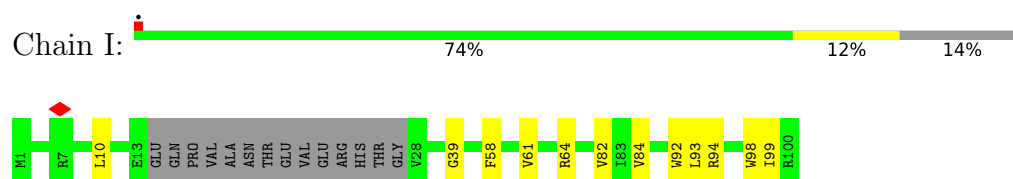
- Molecule 3: Cytochrome bc1 complex cytochrome b subunit



- Molecule 4: Transmembrane protein

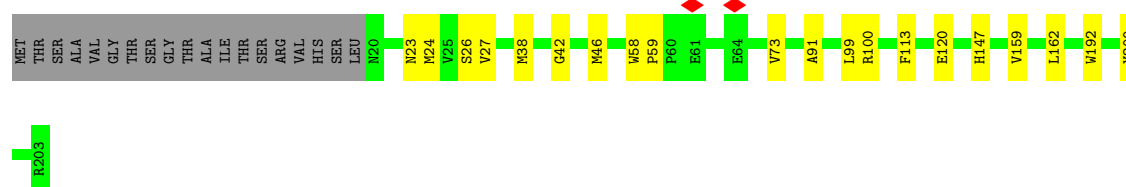


- Molecule 4: Transmembrane protein



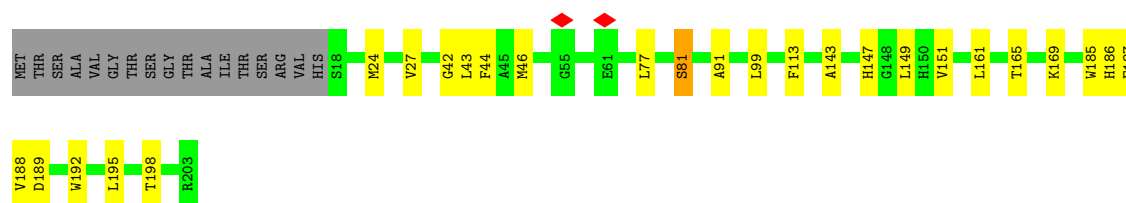
- Molecule 5: Probable cytochrome c oxidase subunit 3

Chain S: 

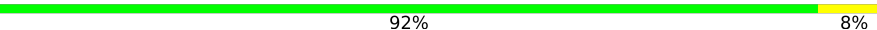


- Molecule 5: Probable cytochrome c oxidase subunit 3

Chain J: 



- Molecule 6: Cytochrome c oxidase polypeptide 4

Chain T: 



- Molecule 6: Cytochrome c oxidase polypeptide 4

Chain K: 

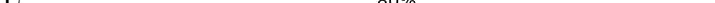


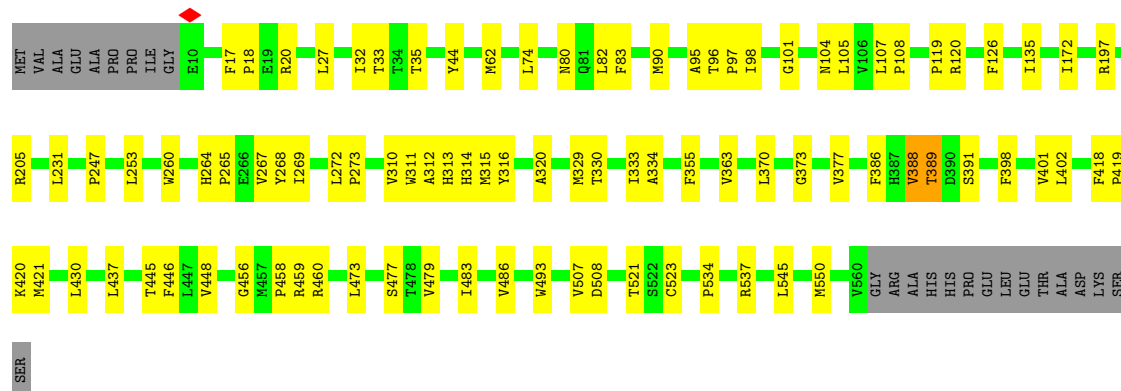
- Molecule 7: Cytochrome c oxidase subunit 1

Chain R: 



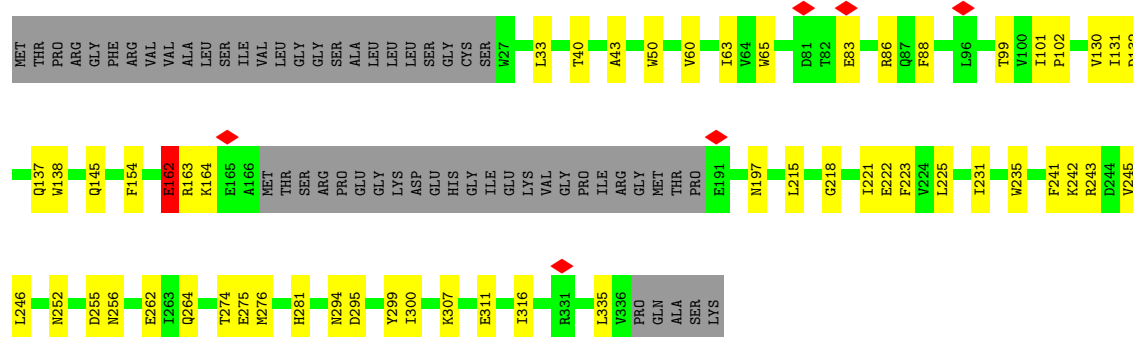
- Molecule 7: Cytochrome c oxidase subunit 1

Chain L:  80% 16% .



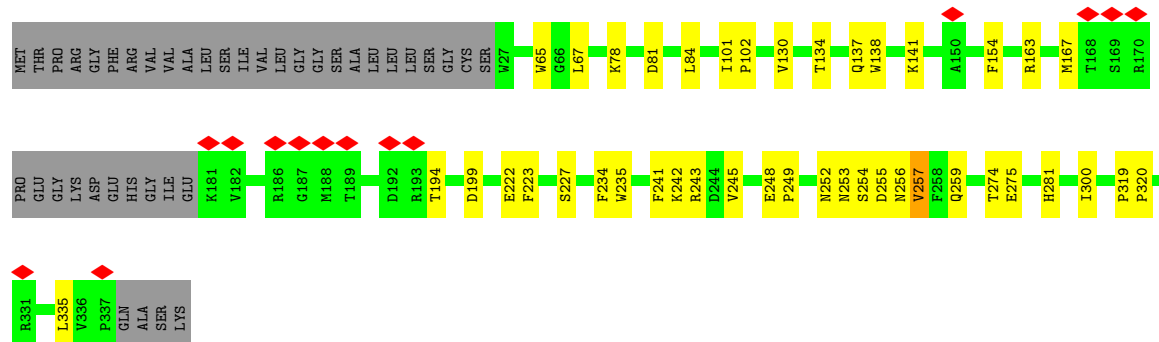
- Molecule 8: cytochrome-c oxidase

Chain Q:  68% 16% 16%

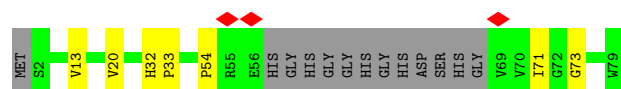
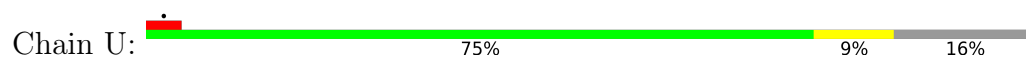


- Molecule 8: cytochrome-c oxidase

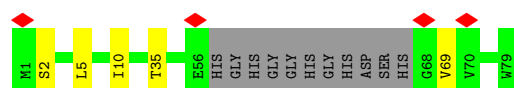
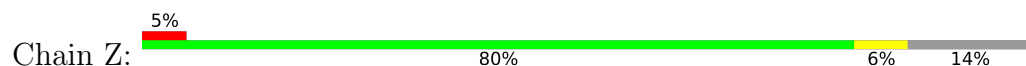
Chain X: 76% 12% 12%



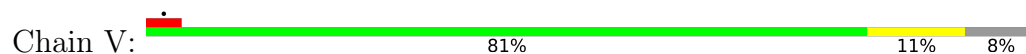
- Molecule 9: Cytochrome c oxidase subunit



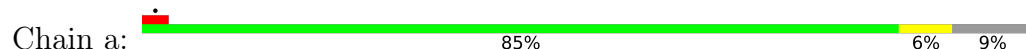
- Molecule 9: Cytochrome c oxidase subunit



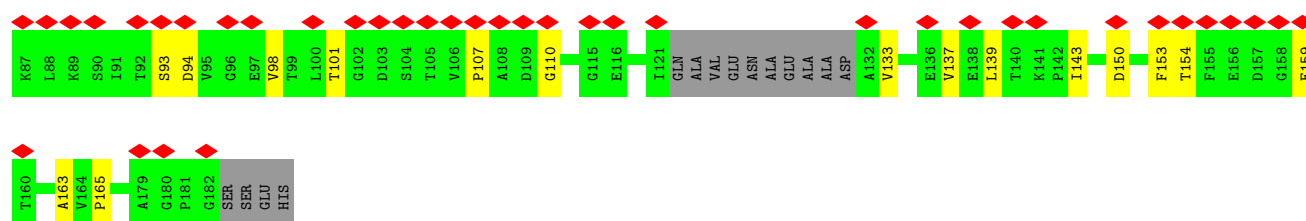
- Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575



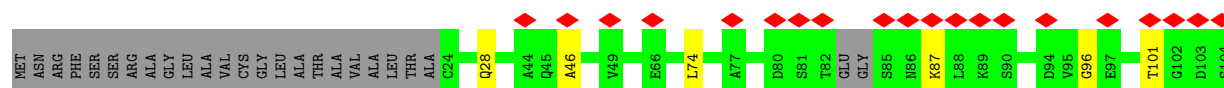
- Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575

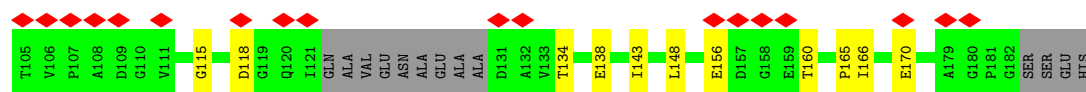


- Molecule 11: LpqE protein

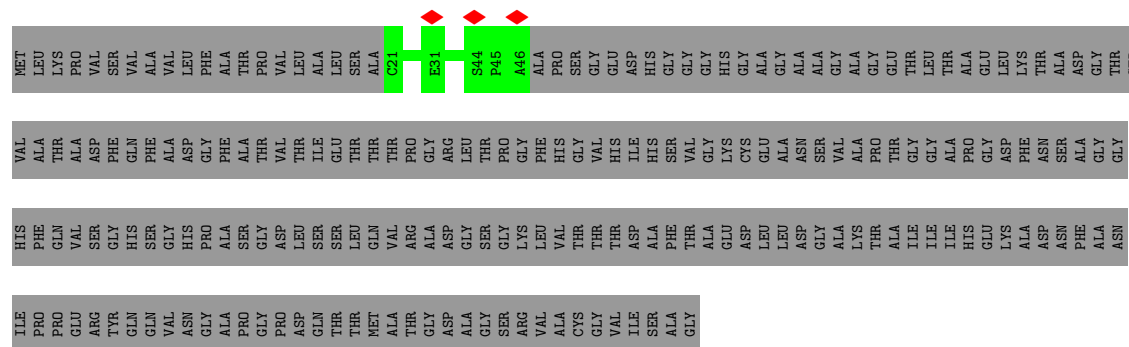


- Molecule 11: LpqE protein

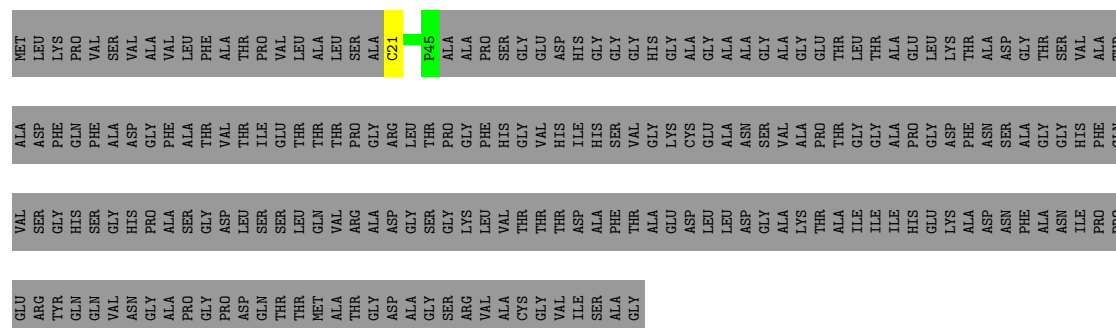




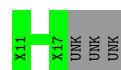
- Molecule 12: Superoxide dismutase [Cu-Zn]



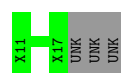
- Molecule 12: Superoxide dismutase [Cu-Zn]



- Molecule 13: Co-purified unknown peptide

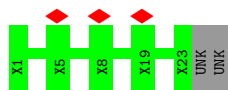


- Molecule 13: Co-purified unknown peptide



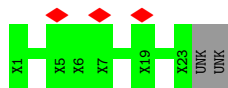
- Molecule 14: Co-purified unknown peptide





- Molecule 14: Co-purified unknown peptide

Chain e: 12% 92% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90918	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 ($e^-/\text{\AA}^2$)	48.2	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.509	Depositor
Minimum map value	-0.830	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.194	Depositor
Map size (Å)	457.056, 457.056, 457.056	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8464, 0.8464, 0.8464	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, CDL, HEM, 7PH, WUO, 9XX, HEC, PLM, 9YF, CA, FES, MG, MQ9, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.51	0/1660	0.78	0/2250
1	O	0.50	0/1660	0.80	0/2250
2	G	0.45	0/3043	0.77	0/4124
2	M	0.49	0/3052	0.80	0/4137
3	H	0.52	0/4299	0.80	1/5862 (0.0%)
3	N	0.49	0/4314	0.77	0/5882
4	I	0.57	0/708	0.85	0/961
4	P	0.44	0/708	0.75	0/961
5	J	0.54	0/1502	0.83	0/2051
5	S	0.46	0/1488	0.77	0/2032
6	K	0.45	0/1112	0.80	0/1524
6	T	0.44	0/1112	0.80	0/1524
7	L	0.50	0/4529	0.79	1/6187 (0.0%)
7	R	0.51	0/4533	0.81	2/6192 (0.0%)
8	Q	0.44	0/2350	0.76	0/3199
8	X	0.49	0/2464	0.78	0/3353
9	U	0.50	0/515	0.80	1/704 (0.1%)
9	Z	0.48	0/527	0.81	0/719
10	V	0.50	0/1050	0.80	0/1434
10	a	0.52	0/1042	0.80	0/1423
11	W	0.48	0/1067	0.77	0/1464
11	b	0.47	0/1090	0.77	0/1494
12	Y	0.58	0/180	0.81	0/251
12	c	0.60	0/175	0.79	0/244
All	All	0.49	0/44180	0.79	5/60222 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	20	VAL	N-CA-C	-5.89	107.07	112.96
7	L	389	THR	CB-CA-C	-5.41	99.50	109.46
3	H	416	VAL	N-CA-C	-5.06	108.90	113.71
7	R	526	PRO	CA-C-N	5.03	127.27	120.38
7	R	526	PRO	C-N-CA	5.03	127.27	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1623	0	1560	18	0
1	O	1623	0	1560	24	0
2	G	2964	0	2974	24	0
2	M	2973	0	2981	26	0
3	H	4167	0	4192	60	0
3	N	4181	0	4201	58	0
4	I	688	0	672	11	0
4	P	688	0	672	9	0
5	J	1455	0	1455	18	0
5	S	1441	0	1439	14	0
6	K	1077	0	1058	17	0
6	T	1077	0	1058	12	0
7	L	4369	0	4346	84	0
7	R	4373	0	4349	94	0
8	Q	2287	0	2232	40	0
8	X	2398	0	2355	32	0
9	U	499	0	504	6	0
9	Z	511	0	519	4	0
10	V	1032	0	1046	15	0
10	a	1024	0	1035	6	0
11	W	1051	0	1008	17	0
11	b	1074	0	1042	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Y	173	0	156	0	0
12	c	168	0	151	2	0
13	E	35	0	9	0	0
13	f	35	0	9	0	0
14	F	115	0	26	0	0
14	e	115	0	26	0	0
15	C	86	0	60	4	0
15	O	86	0	60	6	0
16	C	58	0	80	16	0
16	G	43	0	53	6	0
16	H	217	0	293	39	0
16	N	174	0	240	25	0
16	O	58	0	80	5	0
17	C	97	0	0	0	0
17	I	97	0	0	2	0
17	O	97	0	0	1	0
17	W	97	0	0	1	0
18	G	4	0	0	0	0
18	M	4	0	0	0	0
19	G	58	0	0	2	0
19	M	58	0	0	7	0
19	W	58	0	0	3	0
19	b	58	0	0	3	0
20	H	86	0	60	15	0
20	N	86	0	60	10	0
21	G	79	0	105	2	0
21	H	383	0	492	21	0
21	I	154	0	196	9	0
21	L	156	0	203	3	0
21	N	156	0	203	9	0
21	P	77	0	98	3	0
21	R	154	0	196	6	0
21	T	79	0	105	4	0
22	J	38	0	55	0	0
22	S	76	0	110	3	0
23	L	120	0	108	13	0
23	R	120	0	108	22	0
24	L	1	0	0	0	0
24	Q	2	0	0	0	0
24	R	1	0	0	0	0
24	X	2	0	0	0	0
25	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	R	1	0	0	0	0
26	L	1	0	0	0	0
26	R	1	0	0	0	0
27	H	32	0	0	0	0
27	R	42	0	0	1	0
27	Y	32	0	0	0	0
27	b	32	0	0	0	0
28	L	11	0	16	0	0
28	W	11	0	16	2	0
28	Y	11	0	16	0	0
28	c	11	0	16	1	0
29	C	30	0	0	0	0
29	G	24	0	0	0	0
29	H	39	0	0	0	0
29	I	5	0	0	0	0
29	K	6	0	0	0	0
29	L	25	0	0	0	0
29	M	15	0	0	0	0
29	N	22	0	0	0	0
29	O	25	0	0	1	0
29	P	3	0	0	0	0
29	Q	5	0	0	0	0
29	R	14	0	0	0	0
29	S	1	0	0	0	0
29	T	3	0	0	0	0
29	V	1	0	0	0	0
29	W	5	0	0	0	0
29	X	9	0	0	0	0
29	Y	2	0	0	0	0
29	Z	1	0	0	0	0
29	b	12	0	0	0	0
29	c	2	0	0	0	0
All	All	46771	0	45664	643	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 643 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:264:HIS:NE2	7:L:268:TYR:HE2	1.35	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:264:HIS:NE2	7:L:268:TYR:CE2	2.12	1.16
7:R:406:ILE:HD11	23:R:603:HEA:CBC	1.77	1.12
1:O:192:HIS:CE1	1:O:210:LEU:HD21	1.84	1.10
23:R:602:HEA:HBC1	23:R:602:HEA:HHD	1.34	1.09

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	C	221/278 (80%)	210 (95%)	11 (5%)	0	100	100
1	O	221/278 (80%)	209 (95%)	11 (5%)	1 (0%)	24	55
2	G	378/408 (93%)	358 (95%)	18 (5%)	2 (0%)	24	55
2	M	379/408 (93%)	360 (95%)	18 (5%)	1 (0%)	36	66
3	H	531/556 (96%)	511 (96%)	19 (4%)	1 (0%)	43	72
3	N	533/556 (96%)	504 (95%)	29 (5%)	0	100	100
4	I	82/100 (82%)	80 (98%)	2 (2%)	0	100	100
4	P	82/100 (82%)	79 (96%)	3 (4%)	0	100	100
5	J	184/203 (91%)	178 (97%)	6 (3%)	0	100	100
5	S	182/203 (90%)	180 (99%)	2 (1%)	0	100	100
6	K	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
6	T	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
7	L	549/575 (96%)	527 (96%)	22 (4%)	0	100	100
7	R	550/575 (96%)	514 (94%)	36 (6%)	0	100	100
8	Q	282/341 (83%)	260 (92%)	21 (7%)	1 (0%)	30	60
8	X	297/341 (87%)	277 (93%)	20 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	U	62/79 (78%)	60 (97%)	2 (3%)	0	100	100
9	Z	64/79 (81%)	56 (88%)	8 (12%)	0	100	100
10	V	142/157 (90%)	134 (94%)	8 (6%)	0	100	100
10	a	141/157 (90%)	131 (93%)	10 (7%)	0	100	100
11	W	140/186 (75%)	130 (93%)	10 (7%)	0	100	100
11	b	142/186 (76%)	129 (91%)	13 (9%)	0	100	100
12	Y	24/236 (10%)	20 (83%)	4 (17%)	0	100	100
12	c	23/236 (10%)	20 (87%)	3 (13%)	0	100	100
All	All	5483/6516 (84%)	5190 (95%)	287 (5%)	6 (0%)	49	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	184	VAL
1	O	196	GLY
8	Q	162	GLU
2	G	292	GLY
2	M	116	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	C	163/206 (79%)	163 (100%)	0	100	100
1	O	163/206 (79%)	163 (100%)	0	100	100
2	G	311/333 (93%)	310 (100%)	1 (0%)	86	95
2	M	312/333 (94%)	307 (98%)	5 (2%)	55	83
3	H	428/448 (96%)	425 (99%)	3 (1%)	76	91
3	N	429/448 (96%)	427 (100%)	2 (0%)	81	93
4	I	71/83 (86%)	71 (100%)	0	100	100
4	P	71/83 (86%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	148/161 (92%)	146 (99%)	2 (1%)	59	85
5	S	146/161 (91%)	146 (100%)	0	100	100
6	K	106/106 (100%)	106 (100%)	0	100	100
6	T	106/106 (100%)	106 (100%)	0	100	100
7	L	453/471 (96%)	450 (99%)	3 (1%)	76	91
7	R	453/471 (96%)	451 (100%)	2 (0%)	84	94
8	Q	244/288 (85%)	243 (100%)	1 (0%)	84	94
8	X	257/288 (89%)	254 (99%)	3 (1%)	63	87
9	U	51/59 (86%)	51 (100%)	0	100	100
9	Z	52/59 (88%)	52 (100%)	0	100	100
10	V	106/114 (93%)	106 (100%)	0	100	100
10	a	105/114 (92%)	105 (100%)	0	100	100
11	W	114/146 (78%)	114 (100%)	0	100	100
11	b	119/146 (82%)	119 (100%)	0	100	100
12	Y	20/167 (12%)	20 (100%)	0	100	100
12	c	20/167 (12%)	20 (100%)	0	100	100
All	All	4448/5164 (86%)	4426 (100%)	22 (0%)	78	93

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	81	SER
7	L	388	VAL
7	L	315	MET
7	L	389	THR
3	N	392	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
7	L	314	HIS
7	L	449	GLN
11	W	55	HIS
10	V	138	ASN
8	X	122	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 69 ligands modelled in this entry, 10 are monoatomic - leaving 59 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	$\# Z > 2$
23	HEA	L	602	-	66,67,67	2.23	24 (36%)	78,103,103	2.44	35 (44%)
21	CDL	G	504	-	78,78,99	1.03	6 (7%)	84,90,111	1.03	4 (4%)
17	WUO	C	304	-	99,99,99	1.46	13 (13%)	123,125,125	1.39	17 (13%)
16	MQ9	O	303	-	59,59,59	0.50	0	72,75,75	0.45	0
19	9YF	G	502	-	58,58,58	0.85	4 (6%)	69,71,71	1.05	2 (2%)
21	CDL	H	611	-	78,78,99	1.03	8 (10%)	84,90,111	1.09	5 (5%)
22	7PH	S	401	-	37,37,37	0.30	0	41,42,42	0.34	0
19	9YF	M	502	-	58,58,58	0.85	4 (6%)	69,71,71	1.03	2 (2%)
19	9YF	b	201	-	58,58,58	0.85	4 (6%)	69,71,71	1.04	2 (2%)
16	MQ9	N	601	-	59,59,59	0.42	0	72,75,75	0.63	1 (1%)
23	HEA	L	603	7	66,67,67	3.90	30 (45%)	78,103,103	2.53	34 (43%)
18	FES	M	501	2	0,4,4	-	-	-	-	-
16	MQ9	H	607	-	44,44,59	0.38	0	54,57,75	0.36	0
27	9XX	Y	302	-	31,31,41	1.10	4 (12%)	34,34,44	1.26	2 (5%)
27	9XX	R	608	-	41,41,41	1.08	3 (7%)	44,44,44	1.65	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	FES	G	503	2	0,4,4	-	-	-		
15	HEC	C	302	1	50,50,50	1.33	7 (14%)	68,82,82	1.31	9 (13%)
16	MQ9	H	609	-	59,59,59	0.35	0	72,75,75	0.32	0
20	HEM	N	602	3	50,50,50	1.73	12 (24%)	66,82,82	2.11	19 (28%)
20	HEM	H	610	3	50,50,50	2.06	15 (30%)	66,82,82	1.87	19 (28%)
27	9XX	H	612	-	31,31,41	1.10	4 (12%)	34,34,44	1.37	3 (8%)
16	MQ9	G	501	-	44,44,59	0.37	0	54,57,75	0.36	0
21	CDL	T	201	-	78,78,99	0.29	0	84,90,111	0.34	0
28	PLM	W	403	-	10,10,17	0.42	0	9,9,17	0.45	0
16	MQ9	H	602	-	59,59,59	1.56	7 (11%)	72,75,75	1.29	10 (13%)
21	CDL	H	601	-	73,73,99	0.43	0	79,85,111	0.66	2 (2%)
15	HEC	O	302	1	50,50,50	1.33	6 (12%)	68,82,82	1.31	9 (13%)
15	HEC	O	301	1	50,50,50	1.34	7 (14%)	68,82,82	1.17	3 (4%)
23	HEA	R	602	-	66,67,67	2.23	23 (34%)	78,103,103	2.44	36 (46%)
23	HEA	R	603	7	66,67,67	2.42	24 (36%)	78,103,103	2.55	32 (41%)
16	MQ9	H	608	-	59,59,59	0.35	0	72,75,75	0.31	0
21	CDL	N	603	-	76,76,99	0.29	0	82,88,111	0.34	0
28	PLM	L	608	-	10,10,17	0.41	0	9,9,17	0.46	0
28	PLM	c	301	-	10,10,17	0.40	0	9,9,17	0.45	0
21	CDL	P	301	-	76,76,99	0.29	0	82,88,111	0.34	0
19	9YF	W	402	-	58,58,58	0.85	4 (6%)	69,71,71	1.05	2 (2%)
22	7PH	S	402	-	37,37,37	0.31	0	41,42,42	0.34	0
17	WUO	O	304	-	99,99,99	1.37	5 (5%)	123,125,125	1.25	16 (13%)
21	CDL	I	302	-	76,76,99	0.29	0	82,88,111	0.35	0
21	CDL	L	601	-	78,78,99	1.06	7 (8%)	84,90,111	0.95	2 (2%)
27	9XX	b	202	-	31,31,41	1.11	4 (12%)	34,34,44	1.35	4 (11%)
21	CDL	N	604	-	78,78,99	0.29	0	84,90,111	0.34	0
21	CDL	H	605	-	76,76,99	0.29	0	82,88,111	0.34	0
21	CDL	R	605	-	76,76,99	0.29	0	82,88,111	0.39	0
21	CDL	H	606	-	78,78,99	0.29	0	84,90,111	0.34	0
17	WUO	W	401	-	99,99,99	1.37	5 (5%)	123,125,125	1.24	16 (13%)
16	MQ9	N	605	-	59,59,59	0.35	0	72,75,75	0.31	0
17	WUO	I	303	-	99,99,99	1.37	5 (5%)	123,125,125	1.24	16 (13%)
16	MQ9	N	606	-	59,59,59	0.34	0	72,75,75	0.31	0
20	HEM	H	603	3	50,50,50	1.54	7 (14%)	66,82,82	1.70	15 (22%)
15	HEC	C	301	1	50,50,50	1.34	8 (16%)	68,82,82	1.18	3 (4%)
20	HEM	N	607	3	50,50,50	2.09	18 (36%)	66,82,82	1.67	16 (24%)
21	CDL	L	607	-	76,76,99	0.29	0	82,88,111	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CDL	R	601	-	76,76,99	0.29	0	82,88,111	0.34	0
21	CDL	H	604	-	73,73,99	0.30	0	79,85,111	0.35	0
21	CDL	I	301	-	76,76,99	1.02	7 (9%)	82,88,111	1.10	4 (4%)
22	7PH	J	401	-	37,37,37	0.31	0	41,42,42	0.34	0
28	PLM	Y	301	-	10,10,17	0.45	0	9,9,17	0.52	0
16	MQ9	C	303	-	59,59,59	0.48	0	72,75,75	0.55	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
23	HEA	L	602	-	-	9/36/76/76	-
21	CDL	G	504	-	-	54/89/89/110	-
17	WUO	C	304	-	-	40/84/148/148	0/3/3/3
16	MQ9	O	303	-	-	23/53/73/73	0/2/2/2
19	9YF	G	502	-	-	27/54/78/78	0/1/1/1
21	CDL	H	611	-	-	43/89/89/110	-
22	7PH	S	401	-	-	18/39/39/39	-
19	9YF	M	502	-	-	29/54/78/78	0/1/1/1
19	9YF	b	201	-	-	25/54/78/78	0/1/1/1
16	MQ9	N	601	-	-	30/53/73/73	0/2/2/2
23	HEA	L	603	7	-	12/36/76/76	-
18	FES	M	501	2	-	-	0/1/1/1
16	MQ9	H	607	-	-	20/35/55/73	0/2/2/2
27	9XX	Y	302	-	-	14/33/33/43	-
27	9XX	R	608	-	-	23/43/43/43	-
18	FES	G	503	2	-	-	0/1/1/1
15	HEC	C	302	1	1/1/3/7	6/14/54/54	-
16	MQ9	H	609	-	-	28/53/73/73	0/2/2/2
20	HEM	N	602	3	-	7/14/54/54	-
20	HEM	H	610	3	-	5/14/54/54	-
27	9XX	H	612	-	-	20/33/33/43	-
16	MQ9	G	501	-	-	20/35/55/73	0/2/2/2
21	CDL	T	201	-	-	42/89/89/110	-
28	PLM	W	403	-	-	3/7/8/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MQ9	H	602	-	-	12/53/73/73	0/2/2/2
21	CDL	H	601	-	-	35/84/84/110	-
15	HEC	O	302	1	1/1/3/7	6/14/54/54	-
15	HEC	O	301	1	1/1/3/7	4/14/54/54	-
23	HEA	R	602	-	-	9/36/76/76	-
23	HEA	R	603	7	-	16/36/76/76	-
16	MQ9	H	608	-	-	32/53/73/73	0/2/2/2
21	CDL	N	603	-	-	50/87/87/110	-
28	PLM	L	608	-	-	4/7/8/15	-
28	PLM	c	301	-	-	0/7/8/15	-
21	CDL	P	301	-	-	46/87/87/110	-
19	9YF	W	402	-	-	29/54/78/78	0/1/1/1
22	7PH	S	402	-	-	14/39/39/39	-
17	WUO	O	304	-	-	45/84/148/148	0/3/3/3
21	CDL	I	302	-	-	39/87/87/110	-
21	CDL	L	601	-	-	43/89/89/110	-
27	9XX	b	202	-	-	16/33/33/43	-
21	CDL	N	604	-	-	57/89/89/110	-
21	CDL	H	605	-	-	43/87/87/110	-
21	CDL	R	605	-	-	49/87/87/110	-
21	CDL	H	606	-	-	55/89/89/110	-
17	WUO	W	401	-	-	46/84/148/148	0/3/3/3
16	MQ9	N	605	-	-	21/53/73/73	0/2/2/2
17	WUO	I	303	-	-	44/84/148/148	0/3/3/3
16	MQ9	N	606	-	-	22/53/73/73	0/2/2/2
20	HEM	H	603	3	-	7/14/54/54	-
15	HEC	C	301	1	1/1/3/7	4/14/54/54	-
20	HEM	N	607	3	-	6/14/54/54	-
21	CDL	L	607	-	-	43/87/87/110	-
21	CDL	R	601	-	-	37/87/87/110	-
21	CDL	H	604	-	-	41/84/84/110	-
21	CDL	I	301	-	-	44/87/87/110	-
22	7PH	J	401	-	-	20/39/39/39	-
28	PLM	Y	301	-	-	1/7/8/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MQ9	C	303	-	-	23/53/73/73	0/2/2/2

The worst 5 of 275 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	603	HEA	C3B-C2B	8.15	1.53	1.34
23	L	603	HEA	C3A-C2A	7.79	1.53	1.36
23	L	603	HEA	FE-NB	7.51	2.18	1.94
23	L	603	HEA	CHD-C1D	7.45	1.53	1.38
23	L	603	HEA	C3D-C2D	7.44	1.52	1.36

The worst 5 of 348 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	602	HEA	C3B-C4B-NB	6.64	117.71	109.84
17	C	304	WUO	O58-C59-C61	6.64	125.81	111.50
23	L	602	HEA	C3B-C4B-NB	6.61	117.67	109.84
23	R	603	HEA	C2B-C1B-NB	6.61	117.80	109.88
23	R	603	HEA	C3D-C4D-ND	6.08	116.24	110.36

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	O	301	HEC	NA
15	O	302	HEC	NA
15	C	301	HEC	NA
15	C	302	HEC	NA

5 of 1461 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	O	303	MQ9	C14-C16-C17-C18
16	O	303	MQ9	C17-C18-C19-C21
16	O	303	MQ9	C18-C19-C21-C22
16	O	303	MQ9	C20-C19-C21-C22
16	O	303	MQ9	C32-C33-C34-C35

There are no ring outliers.

50 monomers are involved in 235 short contacts:

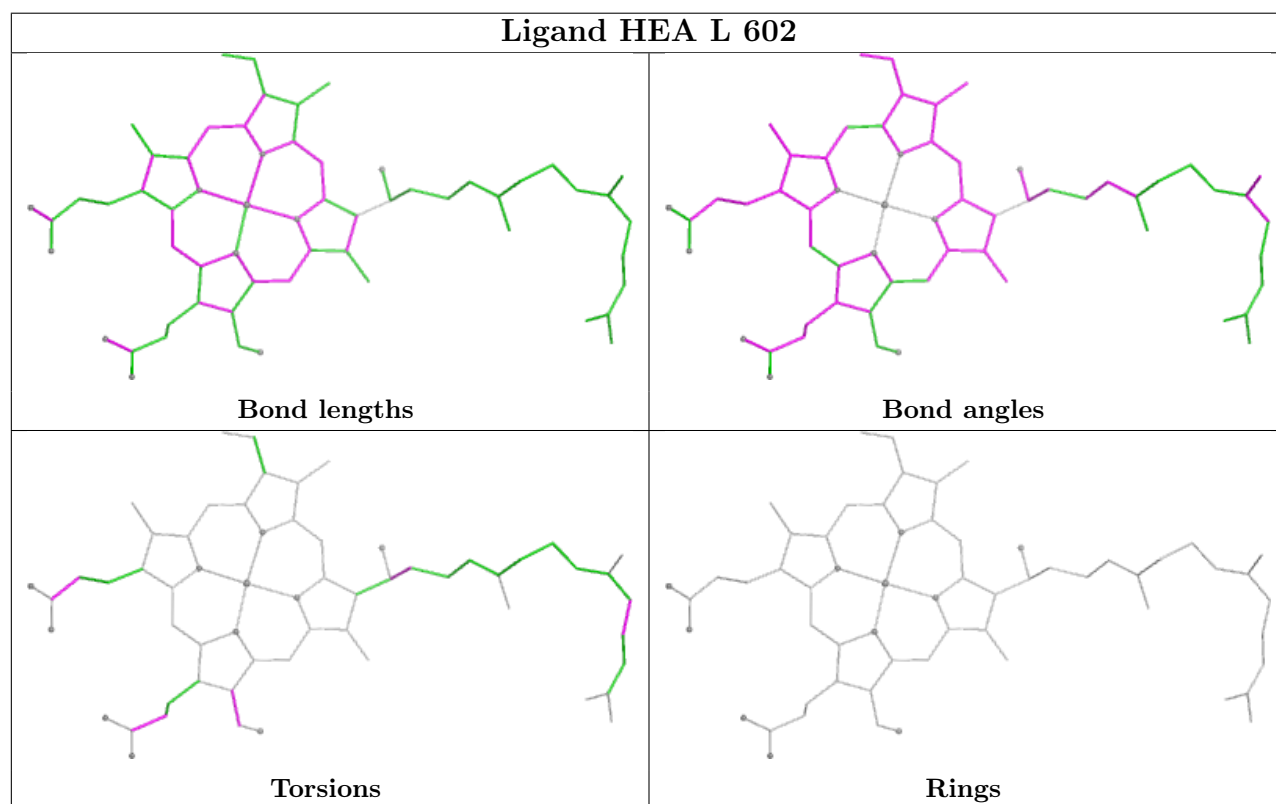
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	602	HEA	7	0
21	G	504	CDL	2	0
16	O	303	MQ9	5	0
19	G	502	9YF	2	0
21	H	611	CDL	4	0
22	S	401	7PH	1	0
19	M	502	9YF	7	0
19	b	201	9YF	3	0
16	N	601	MQ9	9	0
23	L	603	HEA	6	0
16	H	607	MQ9	22	0
27	R	608	9XX	1	0
15	C	302	HEC	3	0
16	H	609	MQ9	7	0
20	N	602	HEM	6	0
20	H	610	HEM	5	0
16	G	501	MQ9	6	0
21	T	201	CDL	4	0
28	W	403	PLM	2	0
16	H	602	MQ9	3	0
21	H	601	CDL	4	0
15	O	302	HEC	2	0
15	O	301	HEC	4	0
23	R	602	HEA	7	0
23	R	603	HEA	15	0
16	H	608	MQ9	17	0
21	N	603	CDL	4	0
28	c	301	PLM	1	0
21	P	301	CDL	3	0
19	W	402	9YF	3	0
22	S	402	7PH	2	0
17	O	304	WUO	1	0
21	I	302	CDL	5	0
21	L	601	CDL	1	0
21	N	604	CDL	7	0
21	H	605	CDL	3	0
21	R	605	CDL	5	0
21	H	606	CDL	4	0
17	W	401	WUO	1	0
16	N	605	MQ9	10	0
17	I	303	WUO	2	0
16	N	606	MQ9	9	0
20	H	603	HEM	10	0

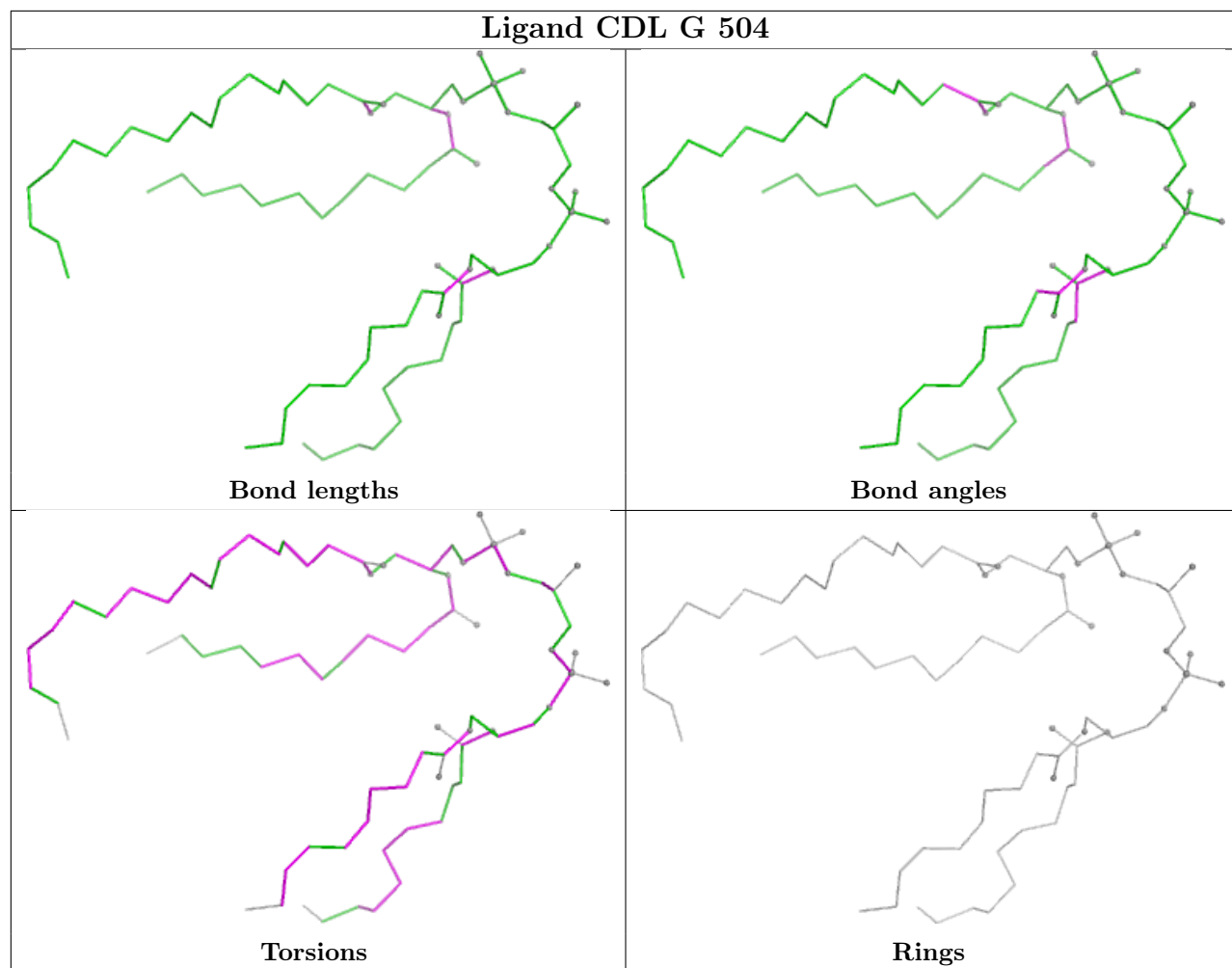
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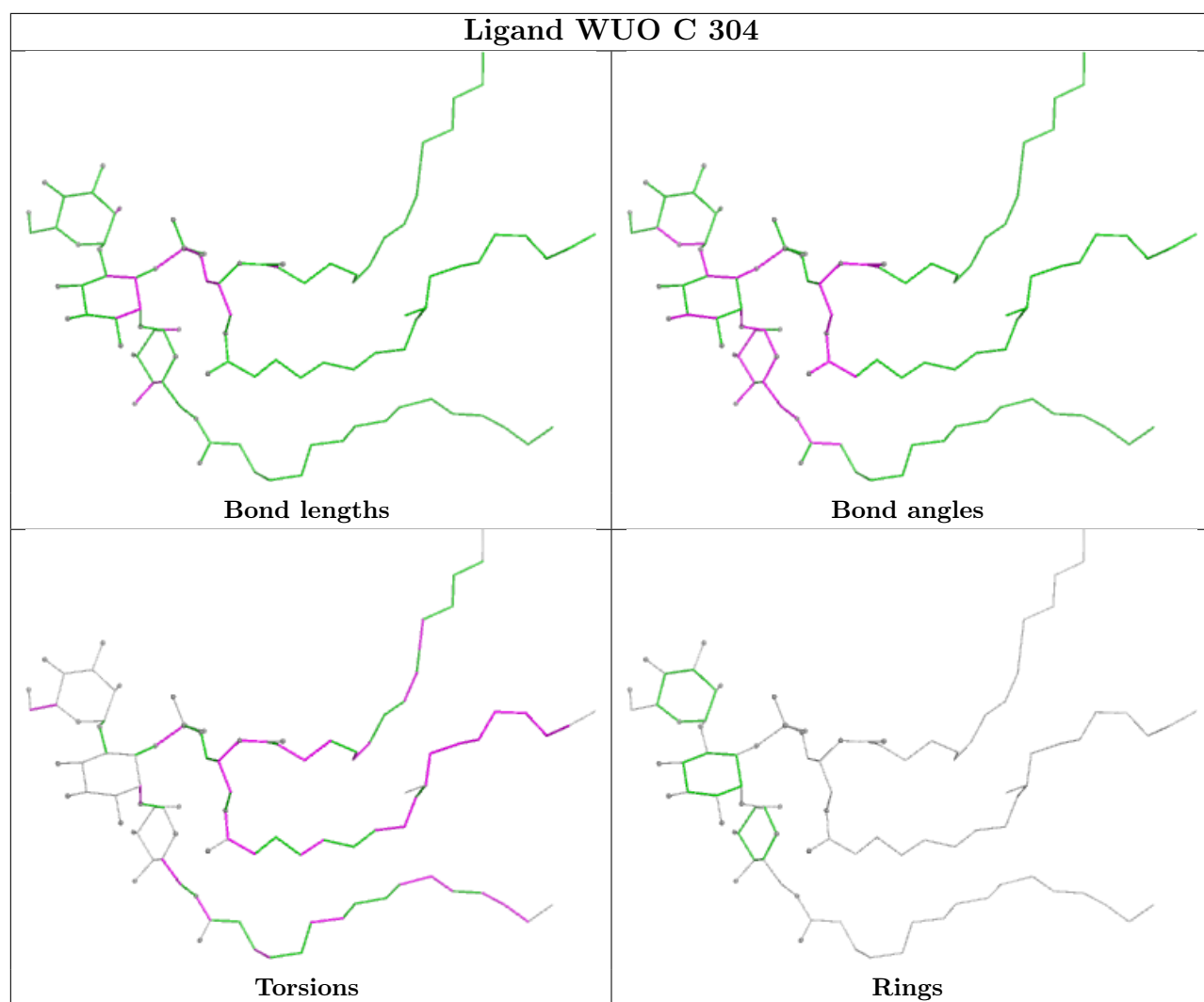
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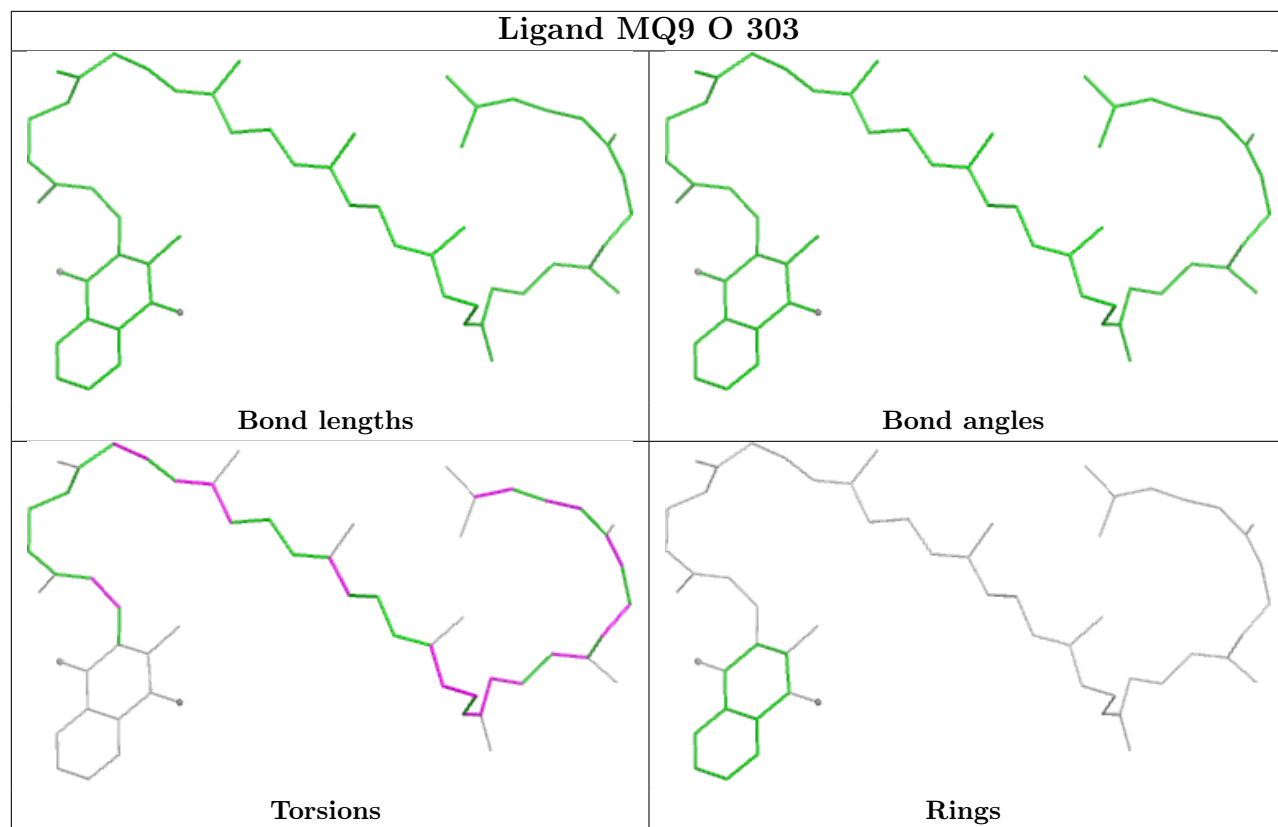
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	301	HEC	1	0
20	N	607	HEM	4	0
21	L	607	CDL	2	0
21	R	601	CDL	1	0
21	H	604	CDL	9	0
21	I	301	CDL	4	0
16	C	303	MQ9	16	0

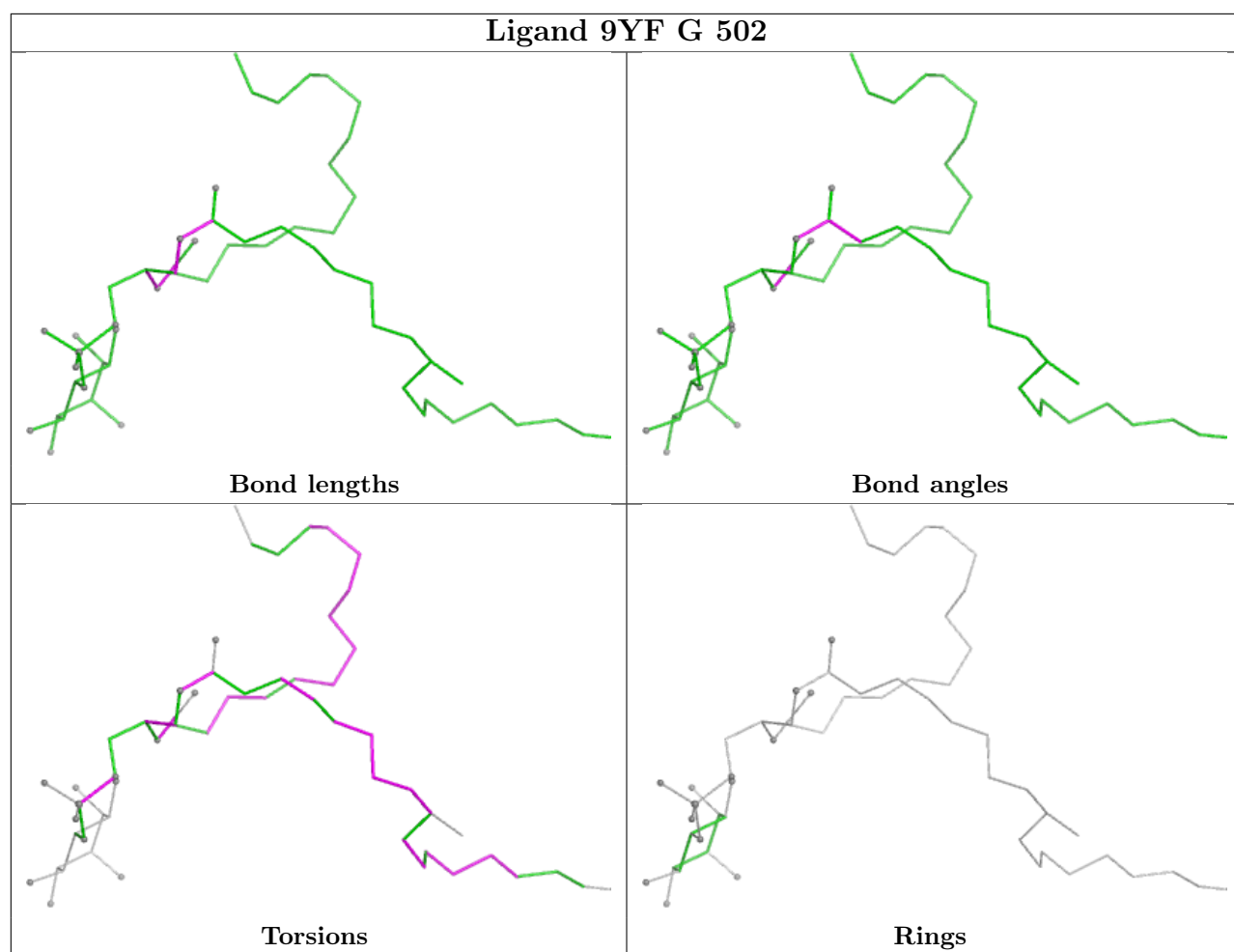
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

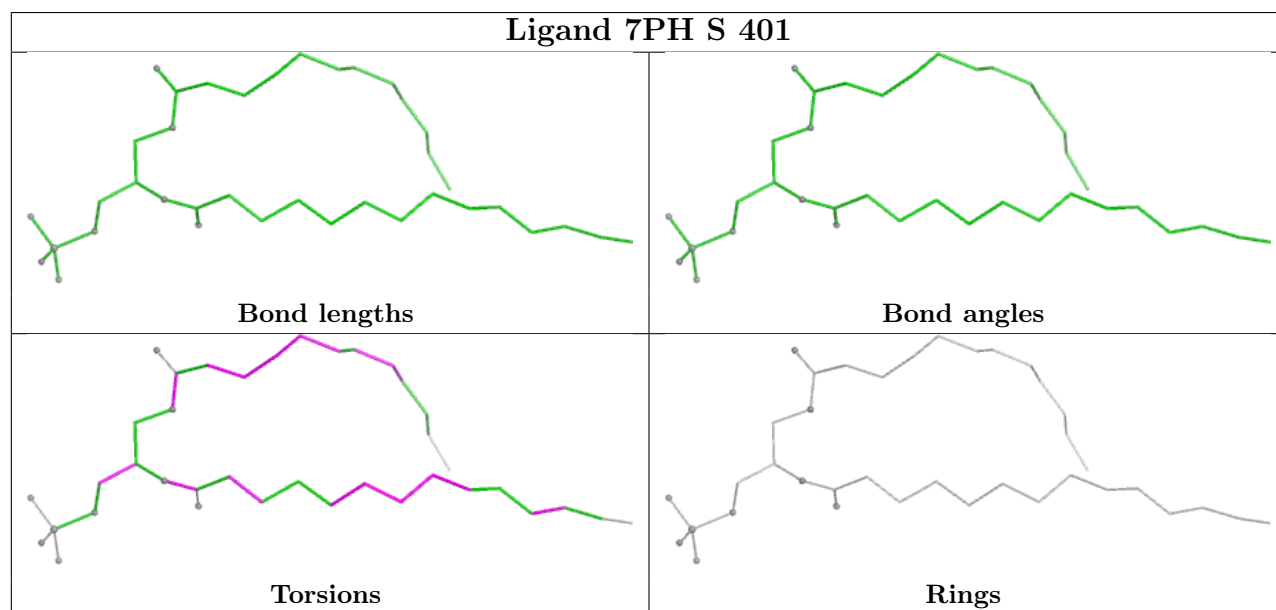
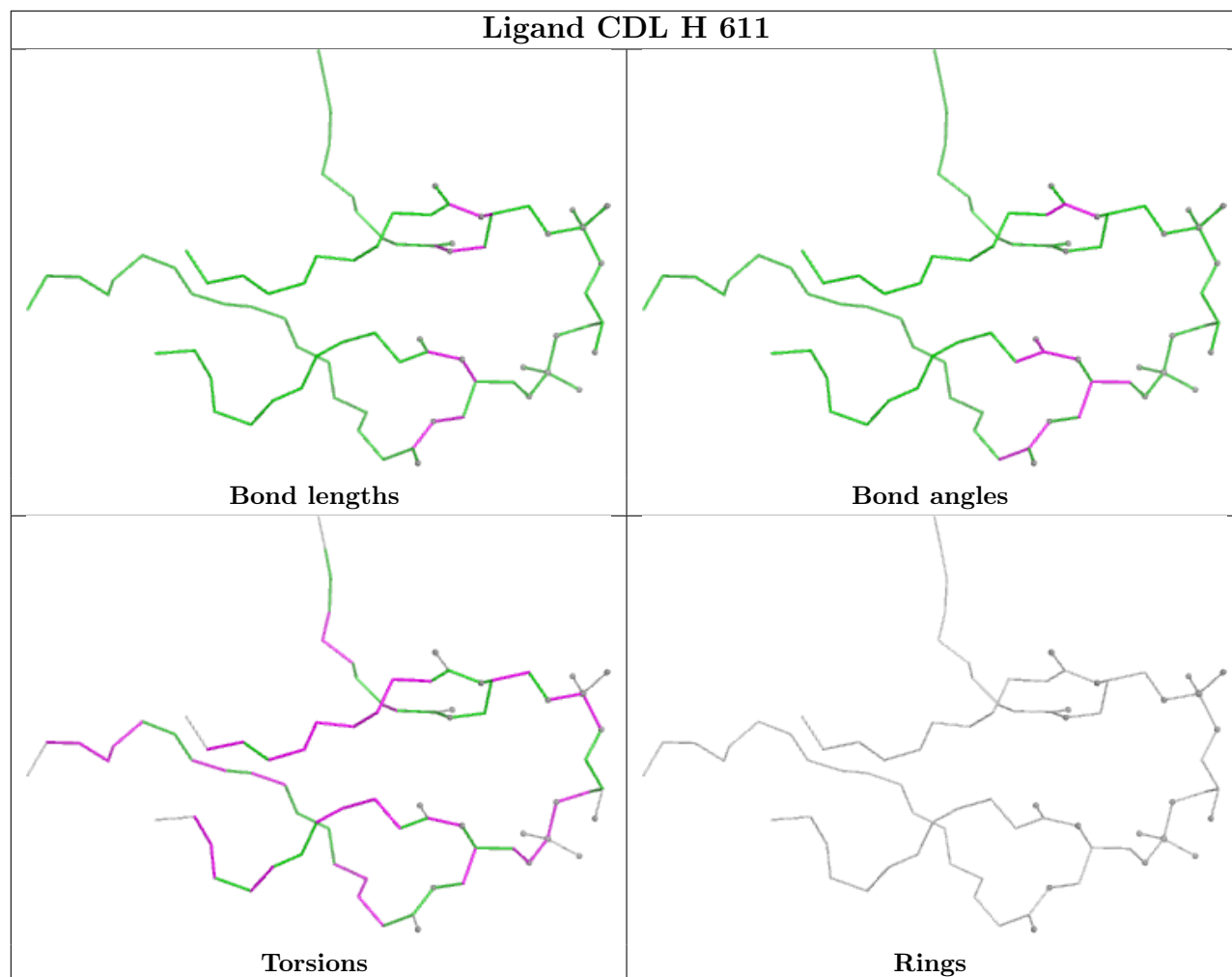


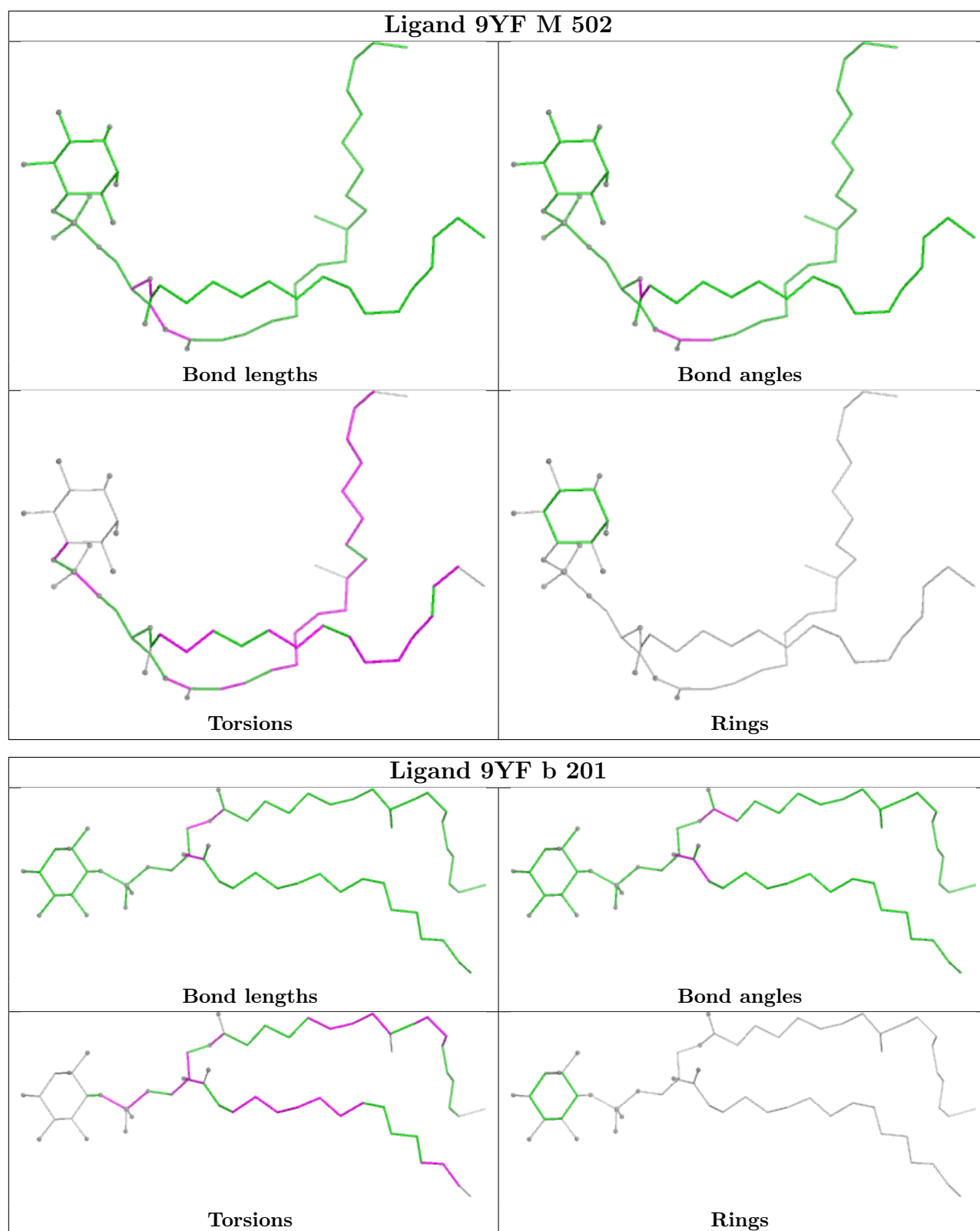


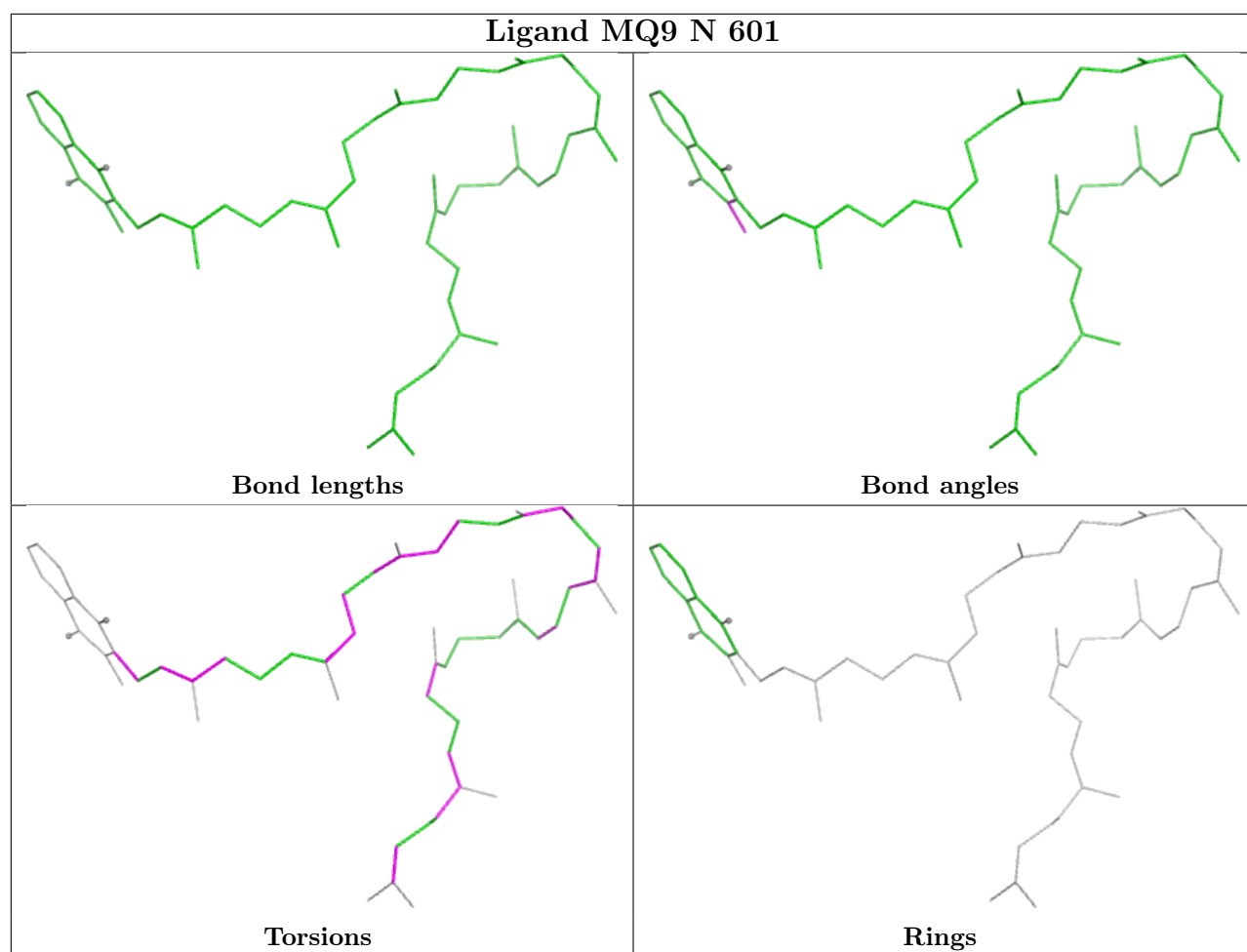


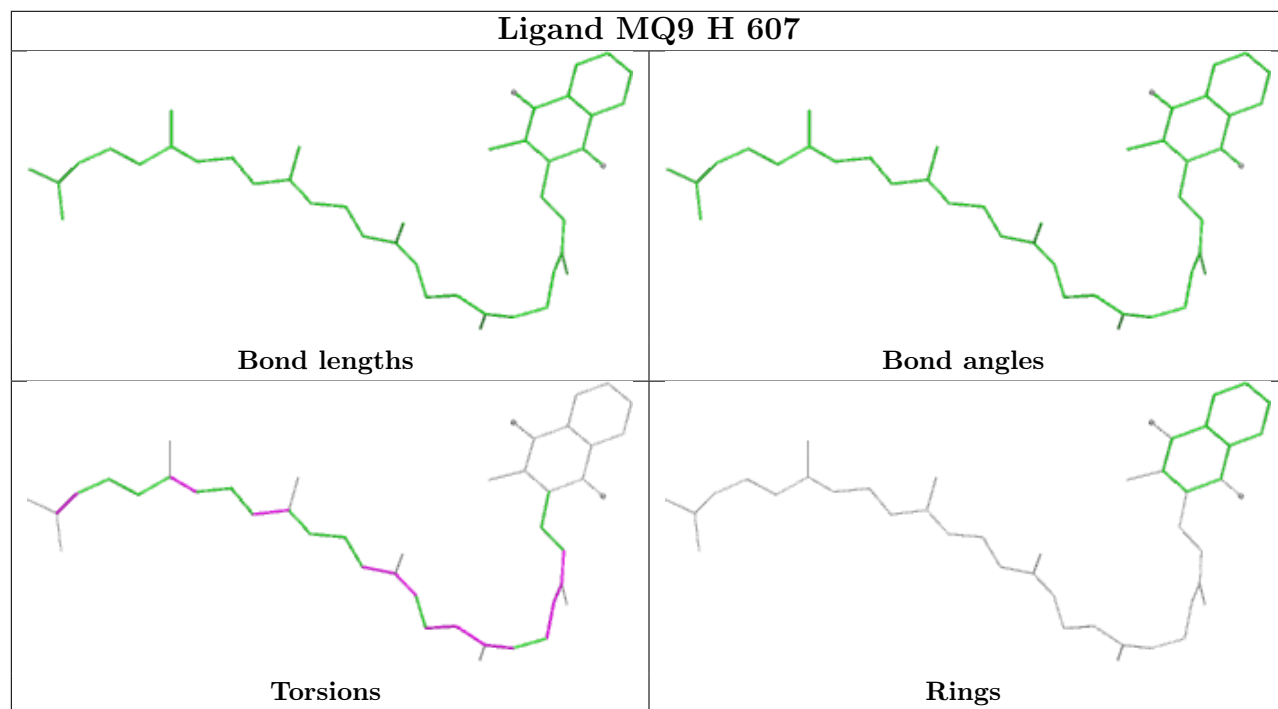
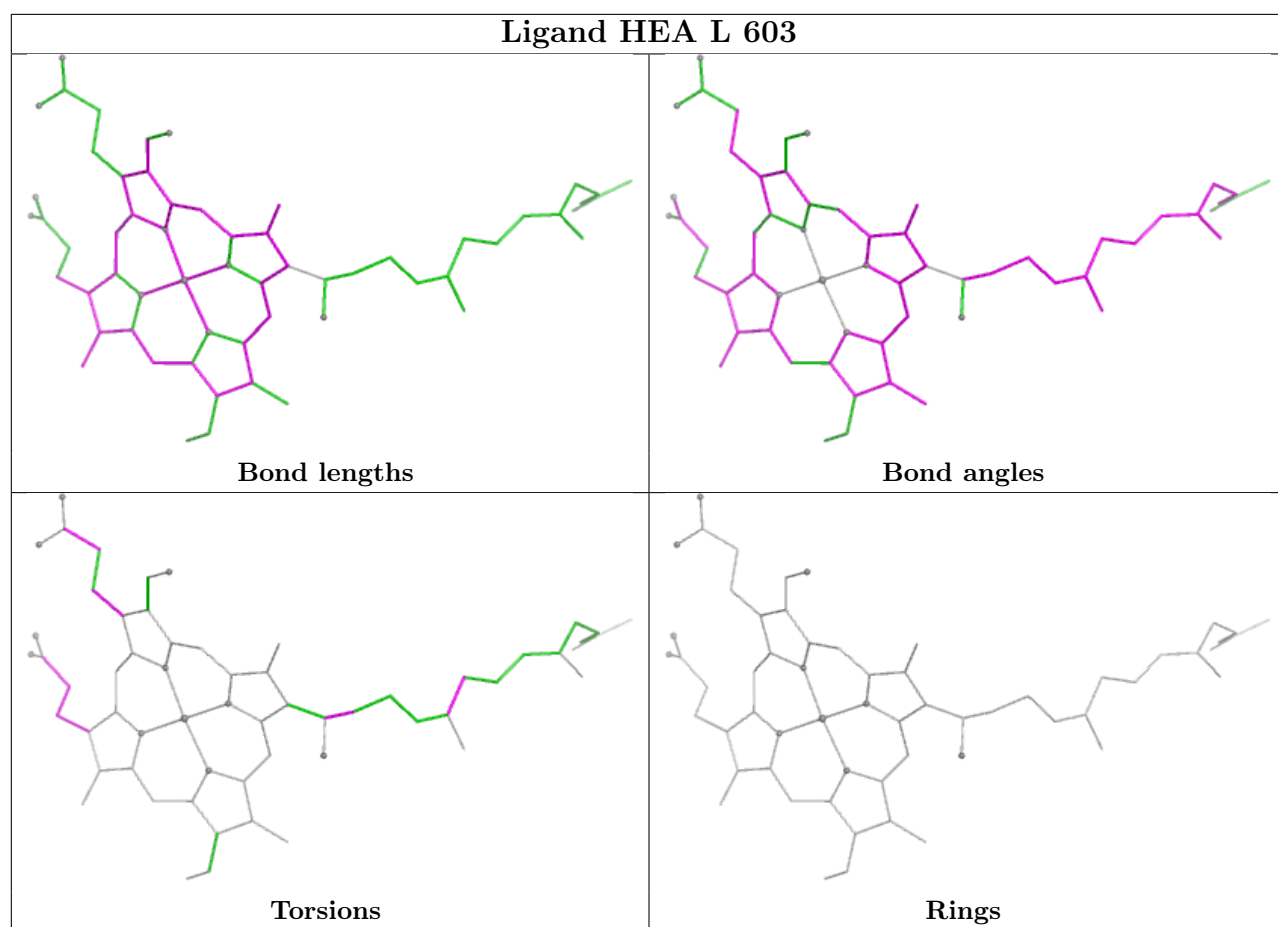


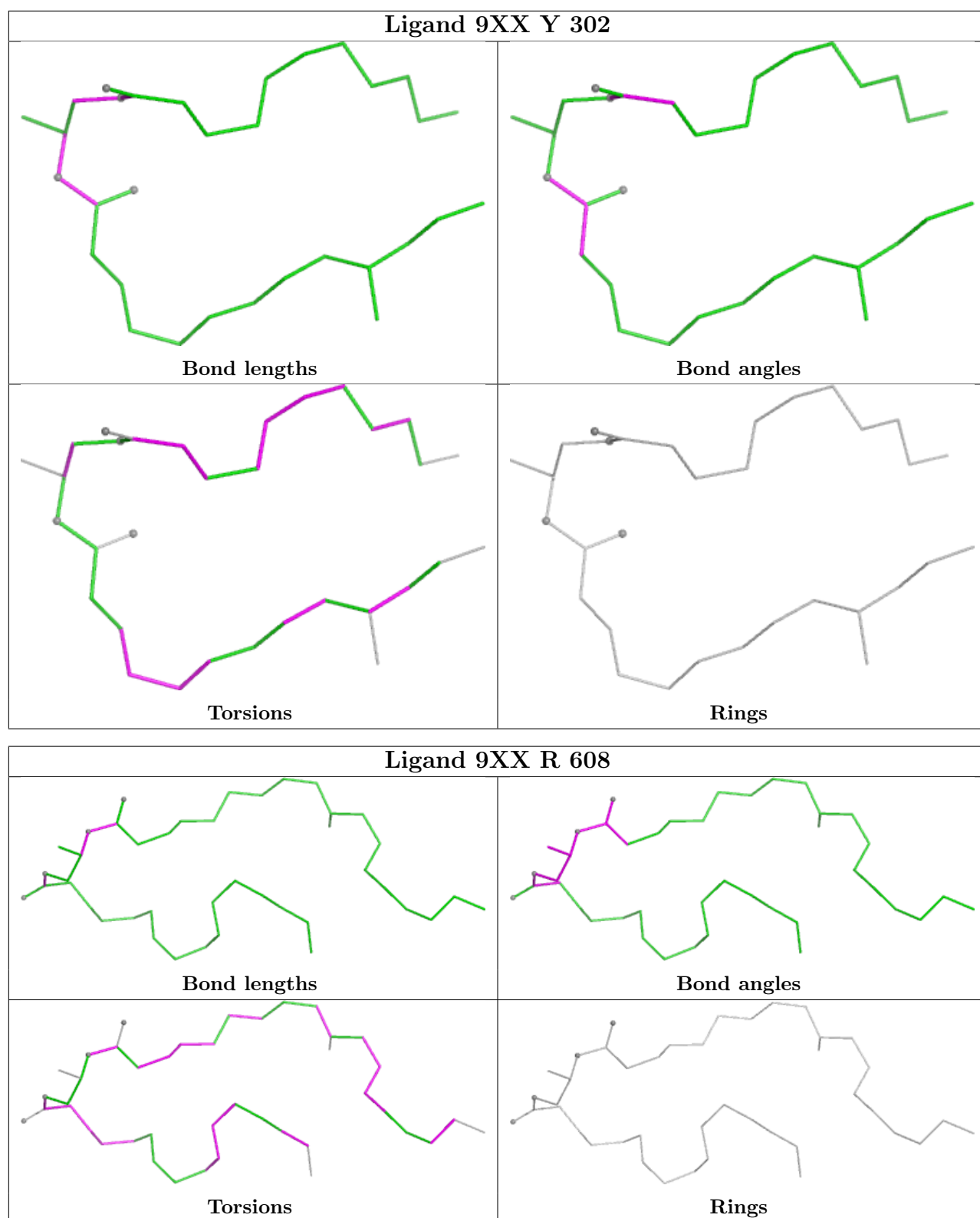


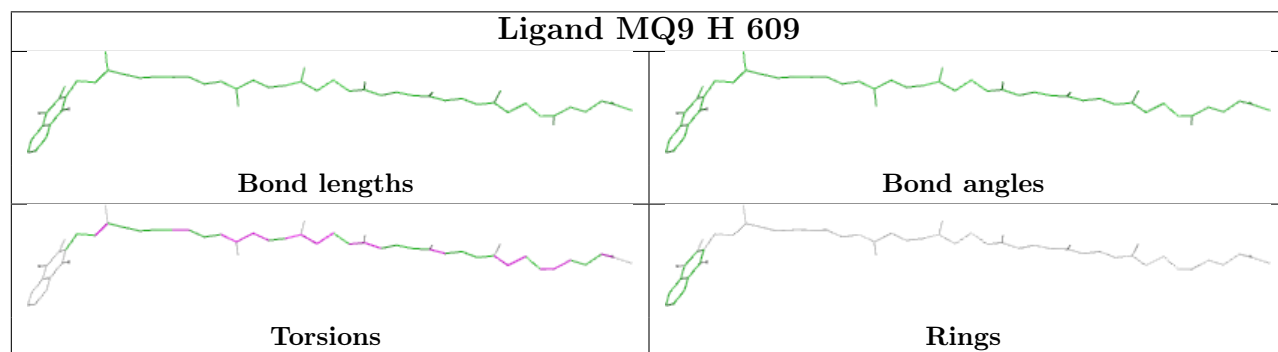
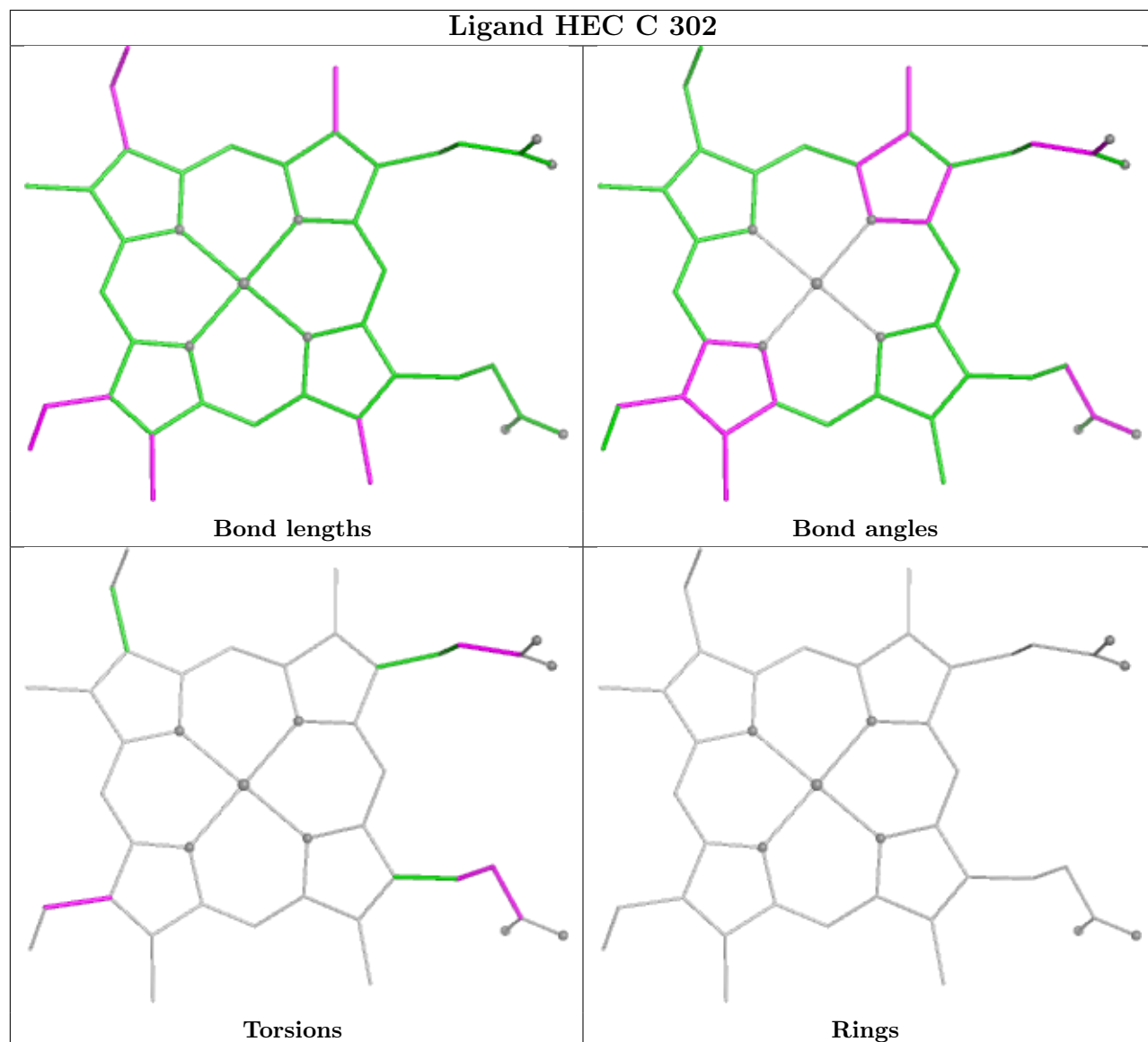


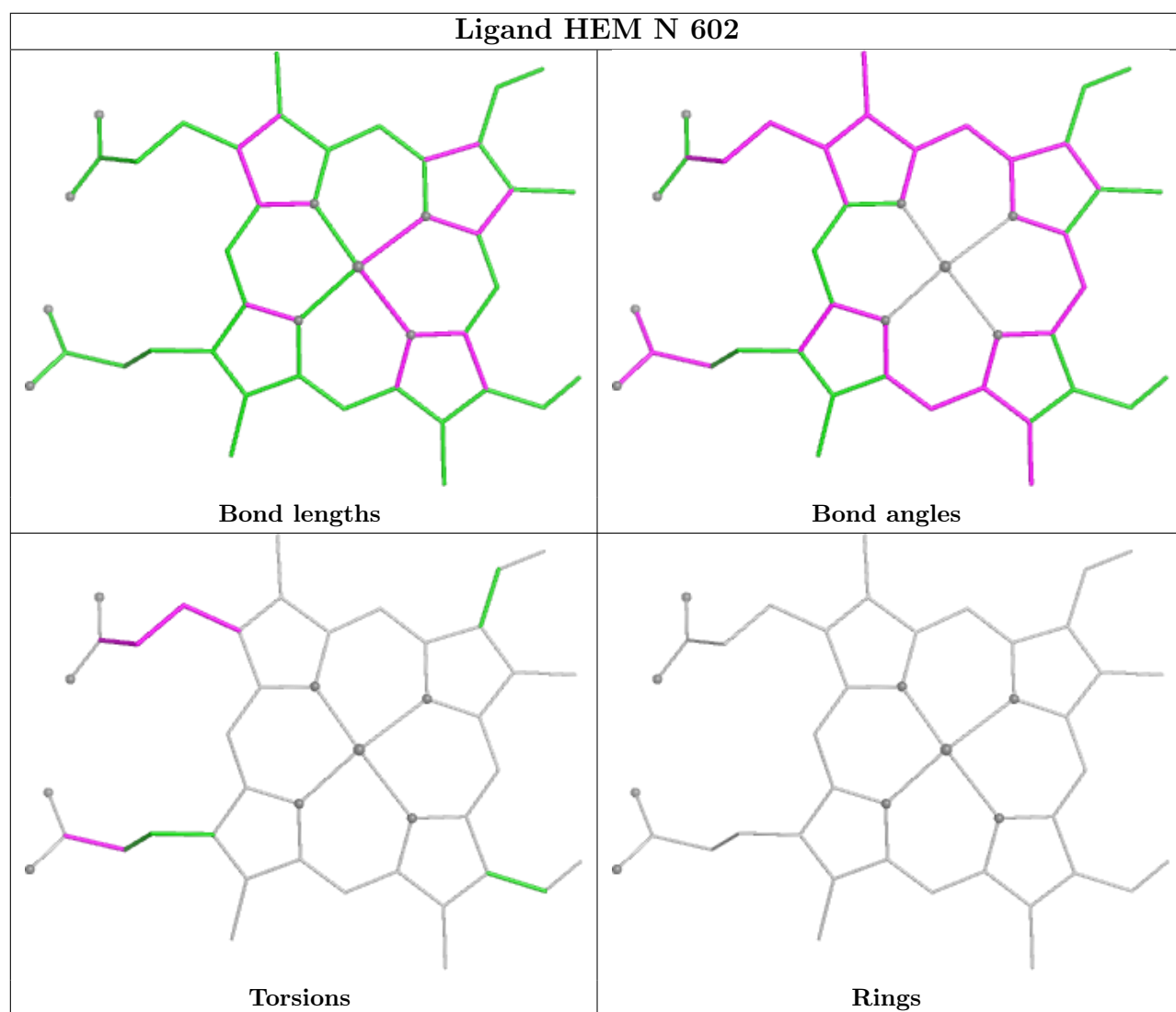


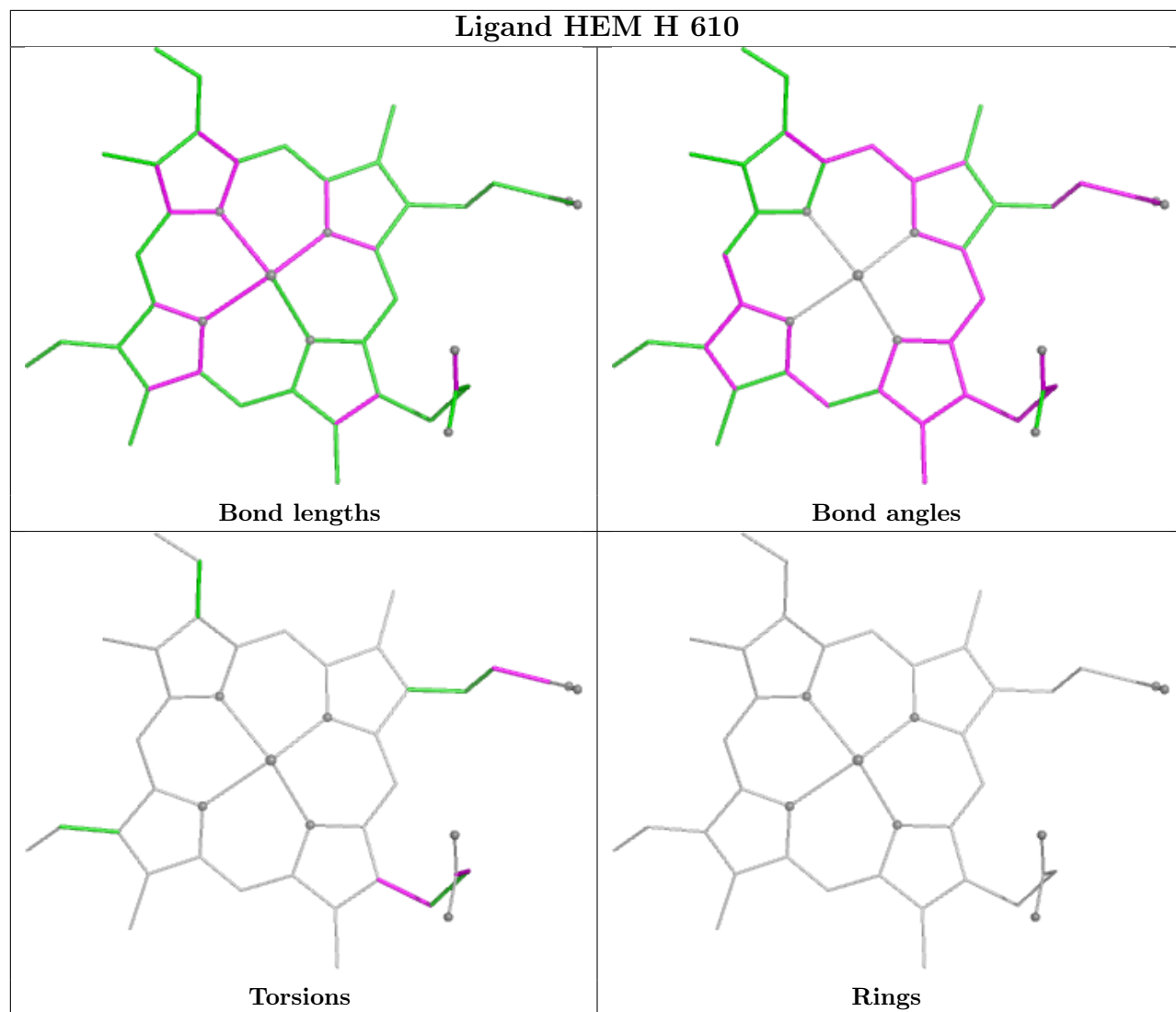


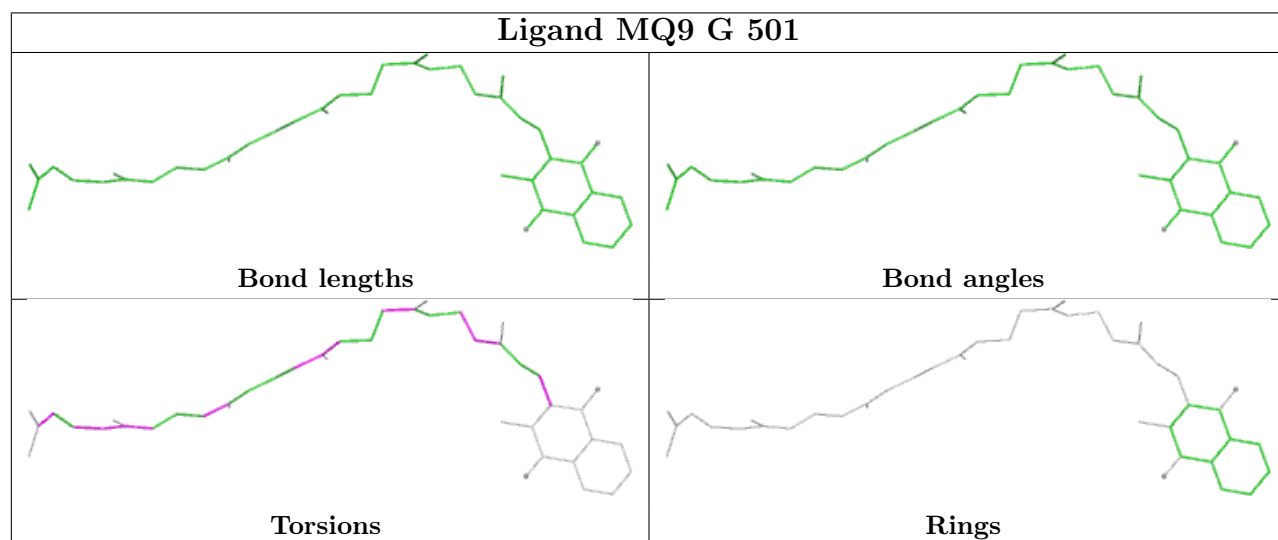
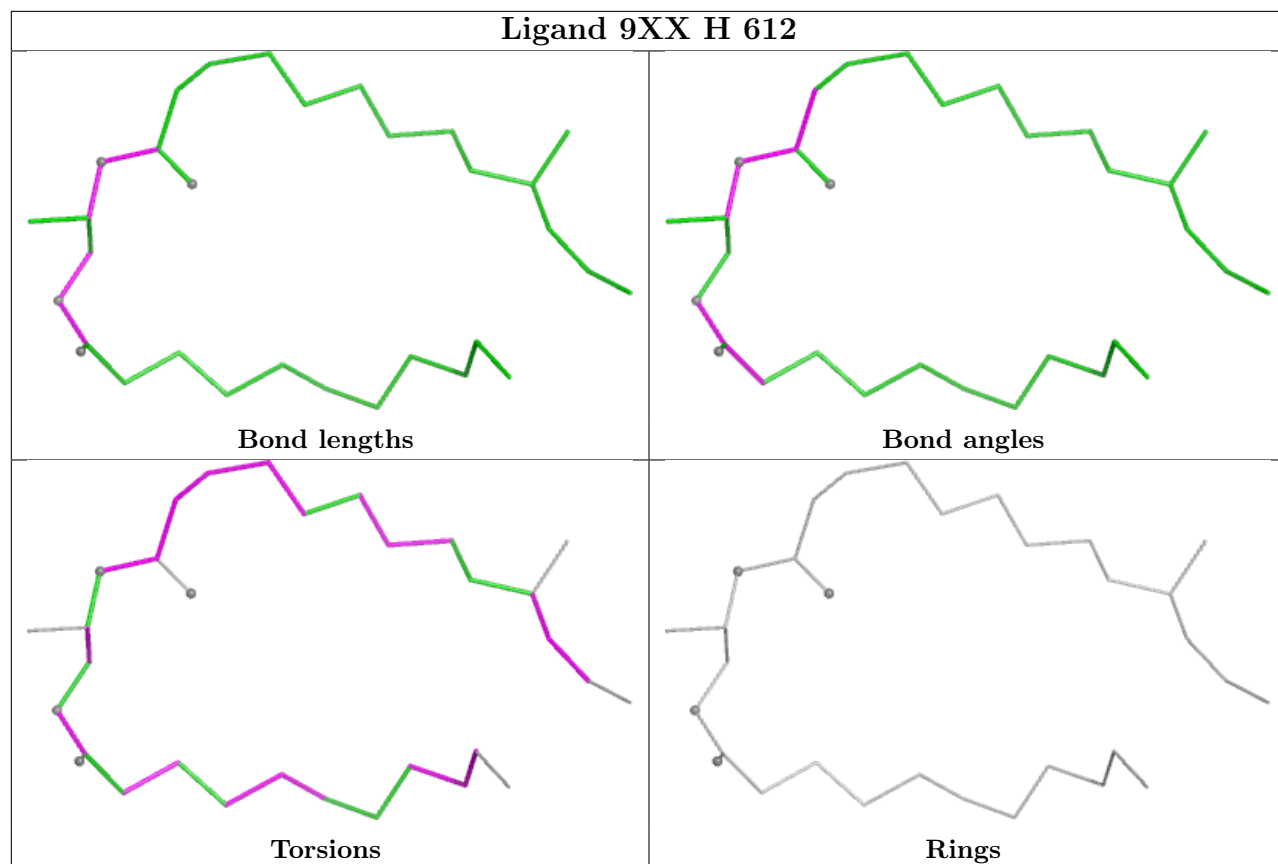


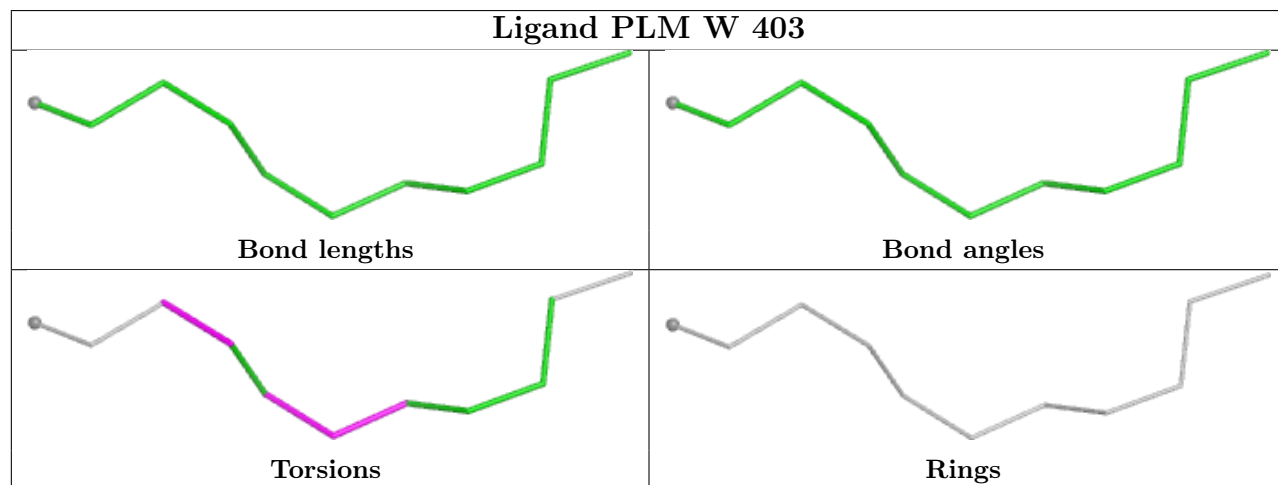
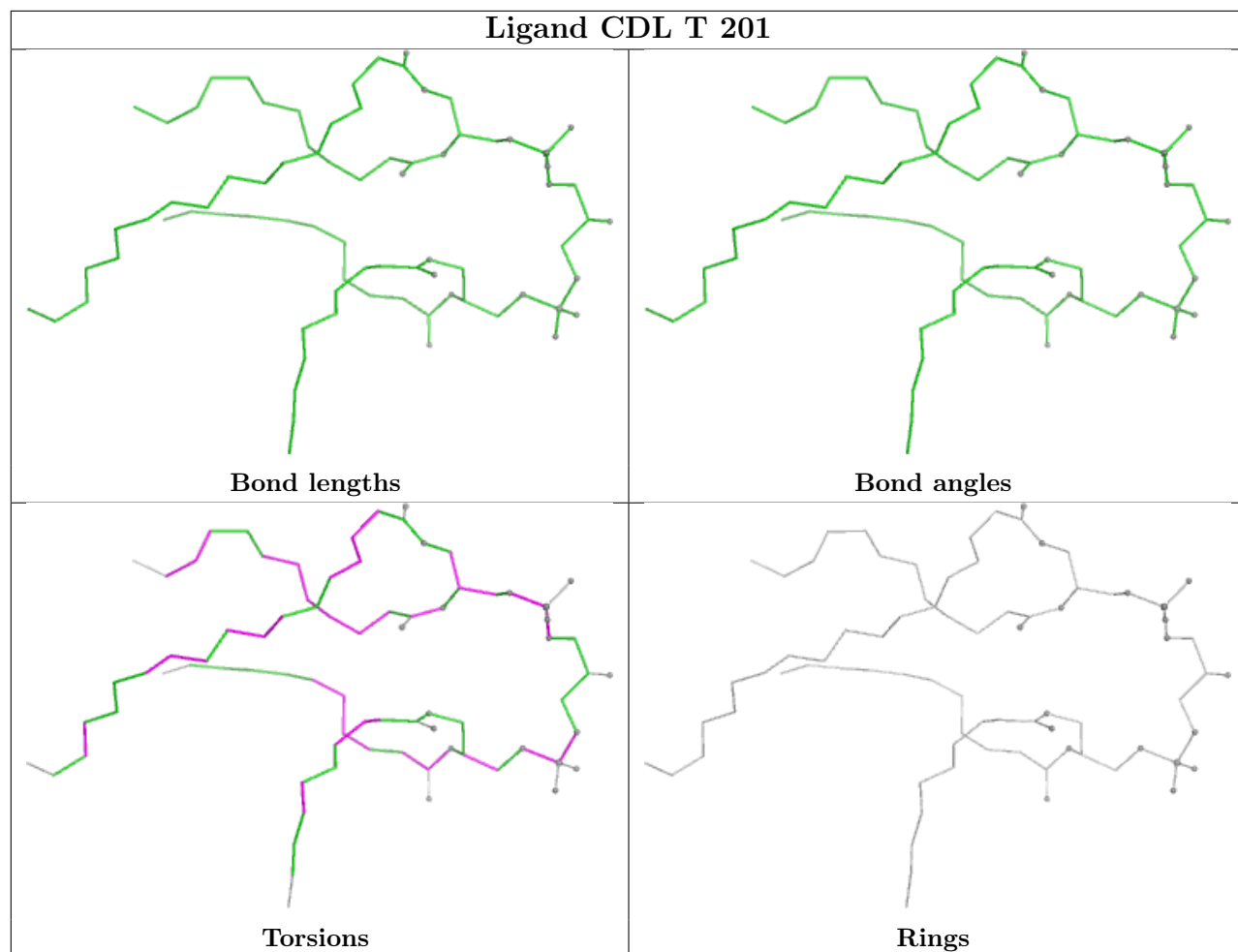


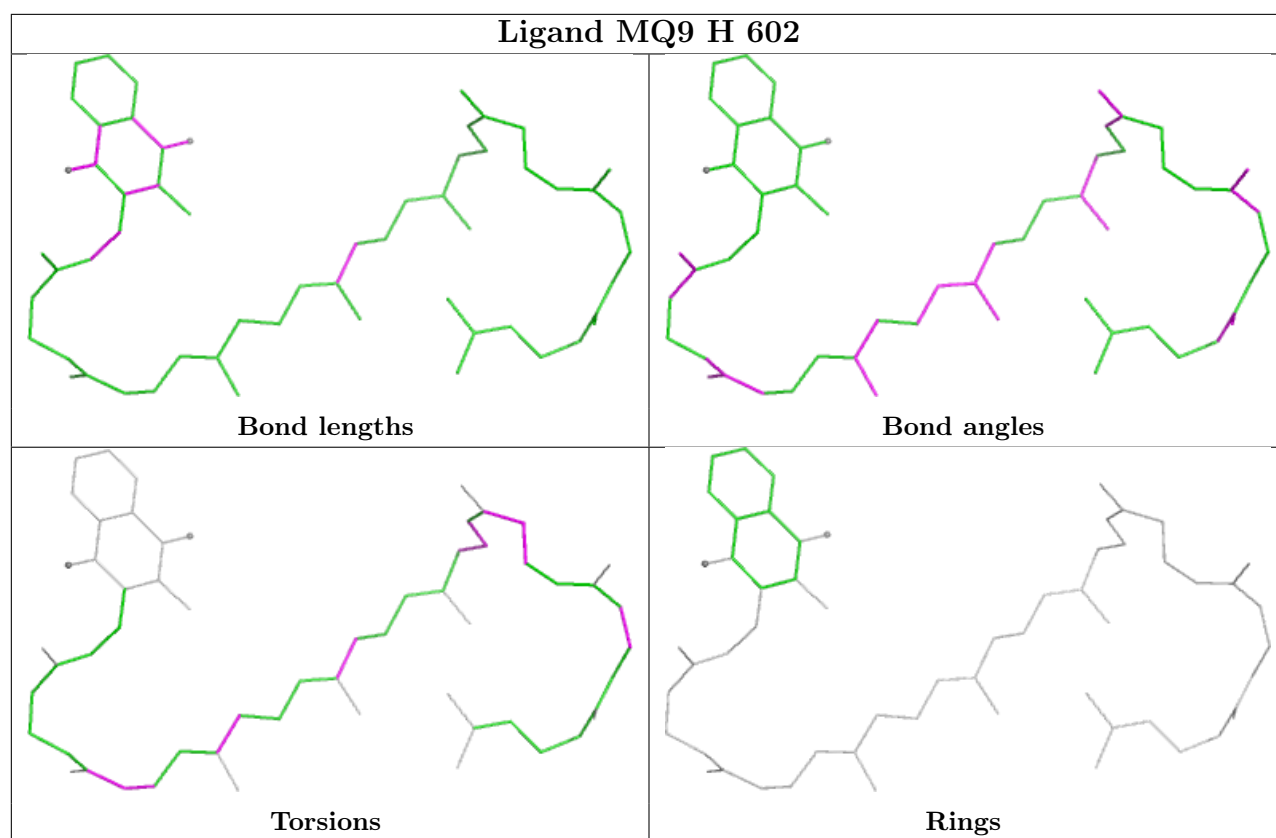


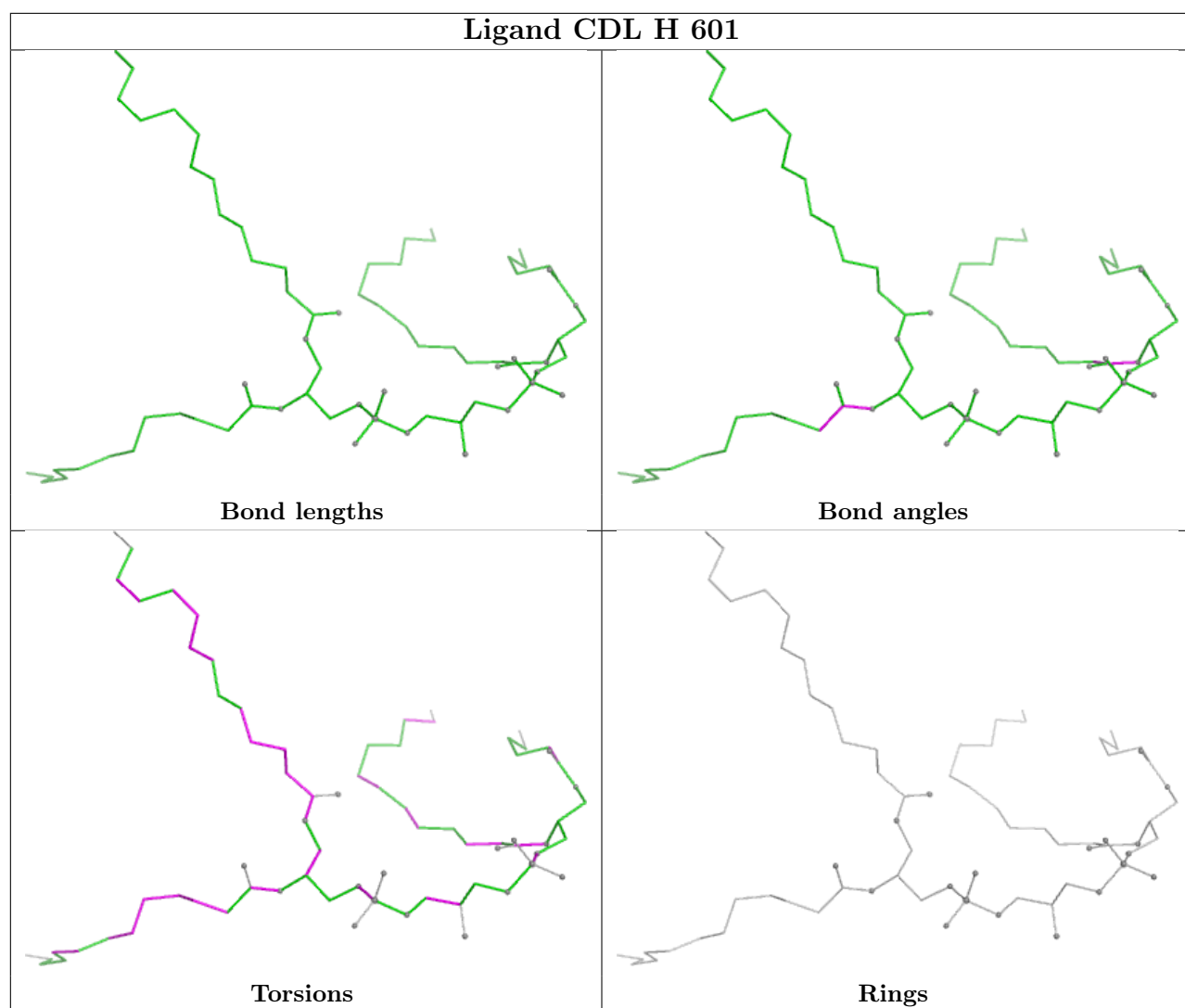


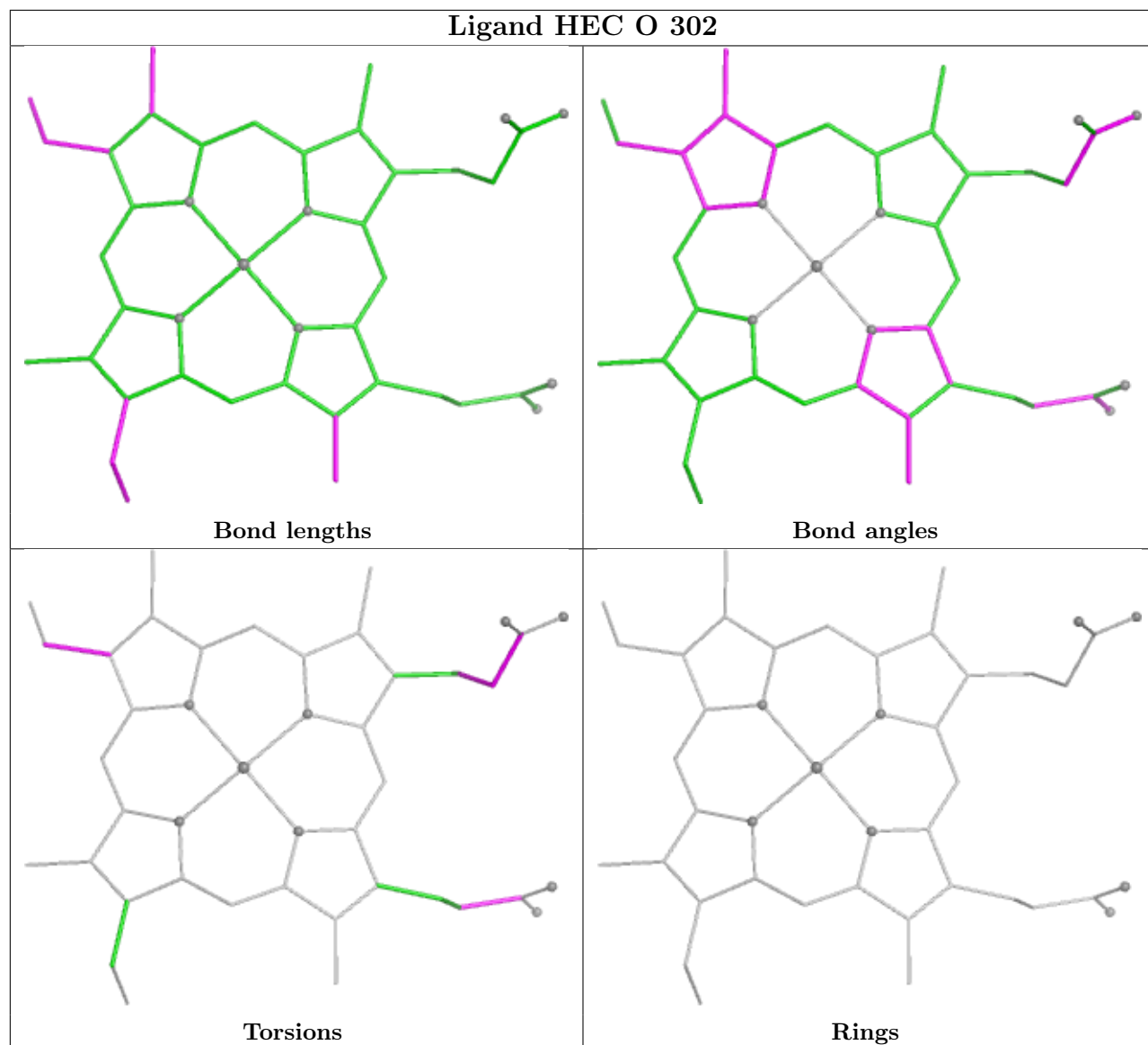


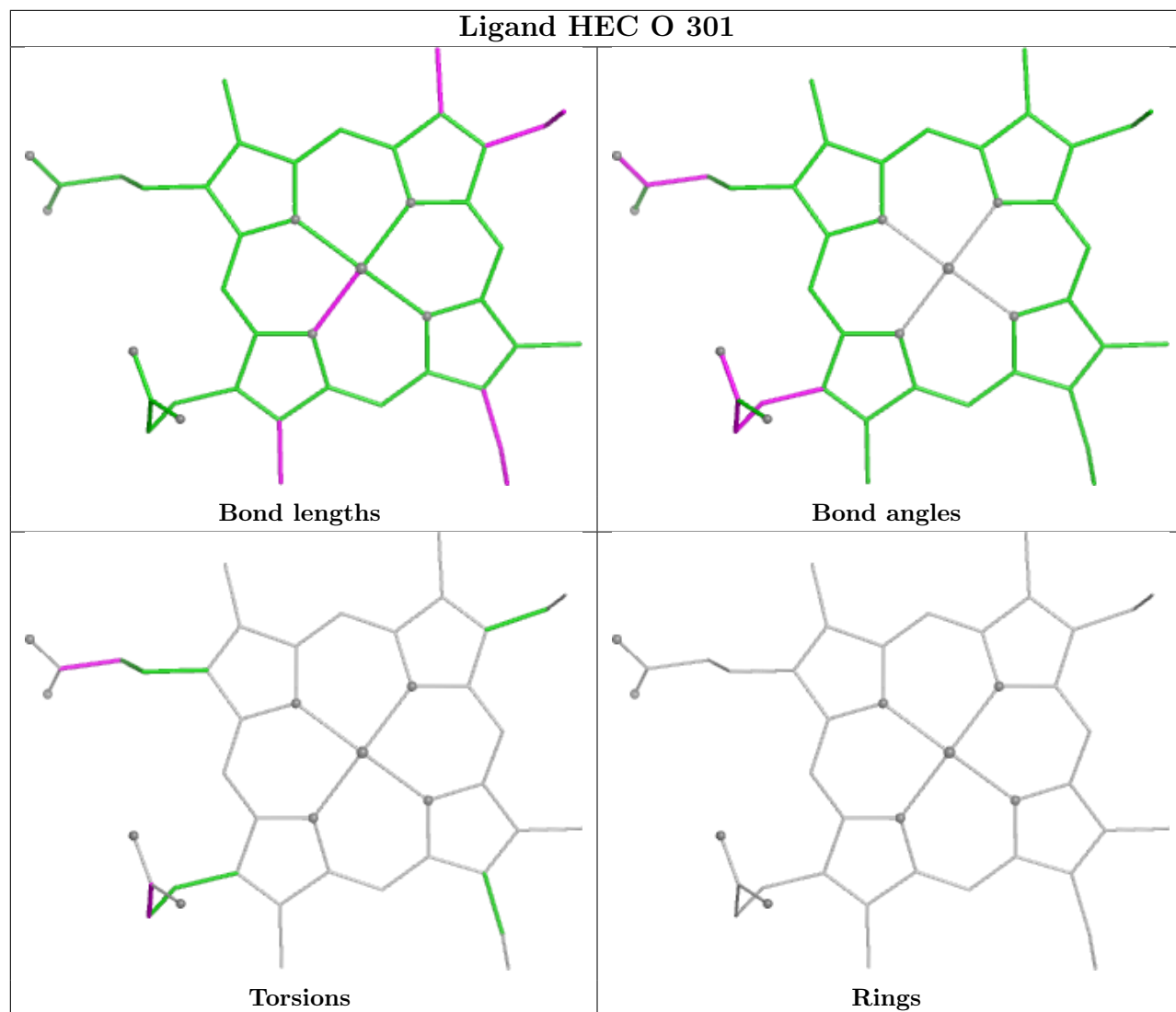


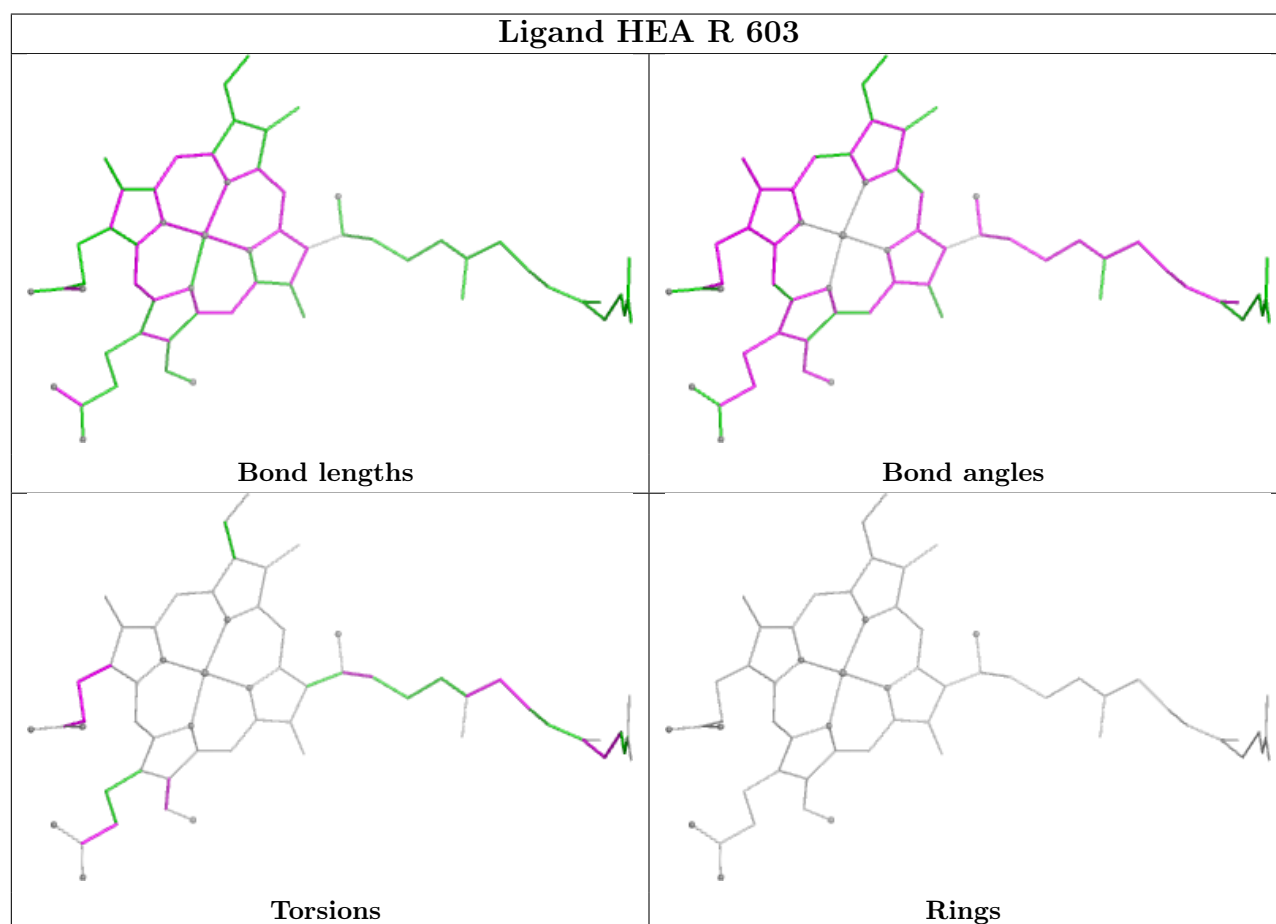
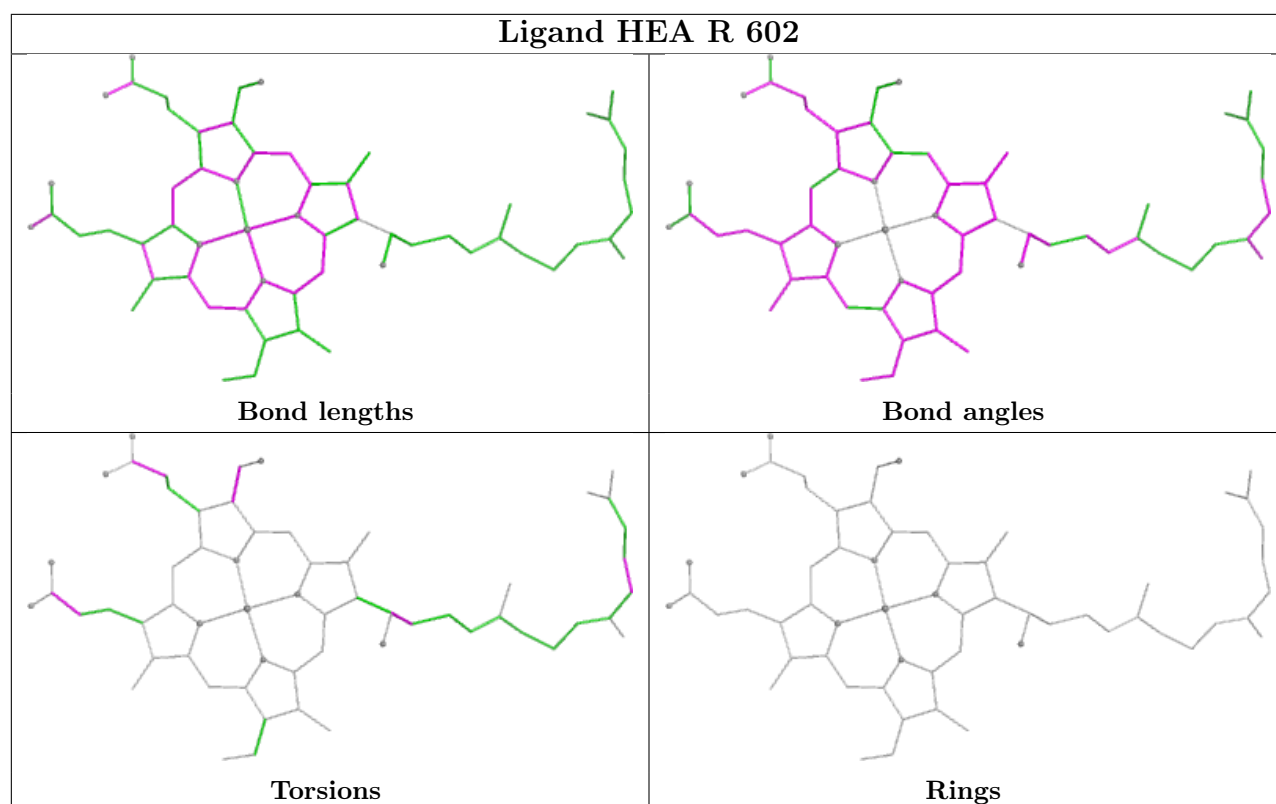


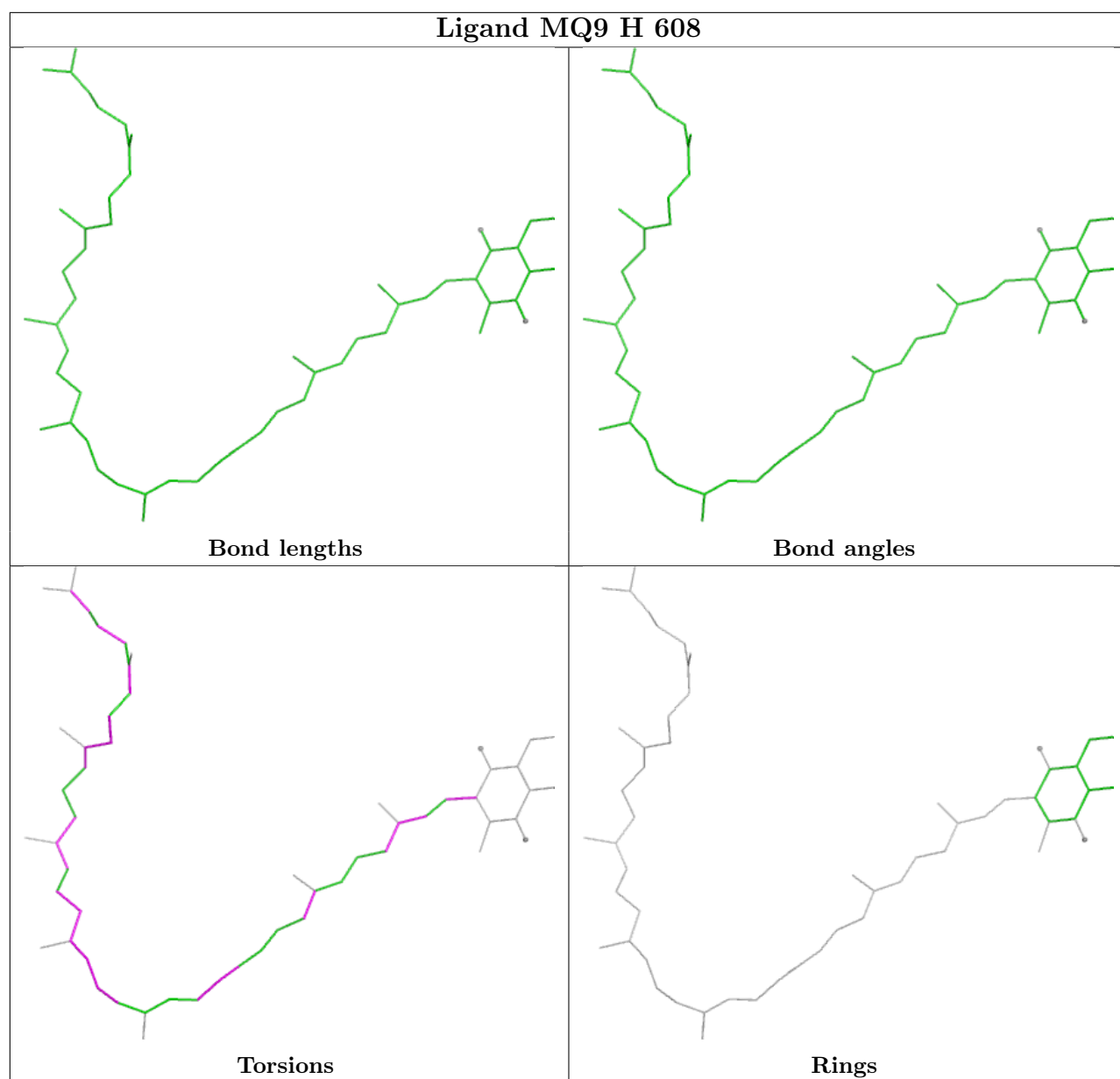


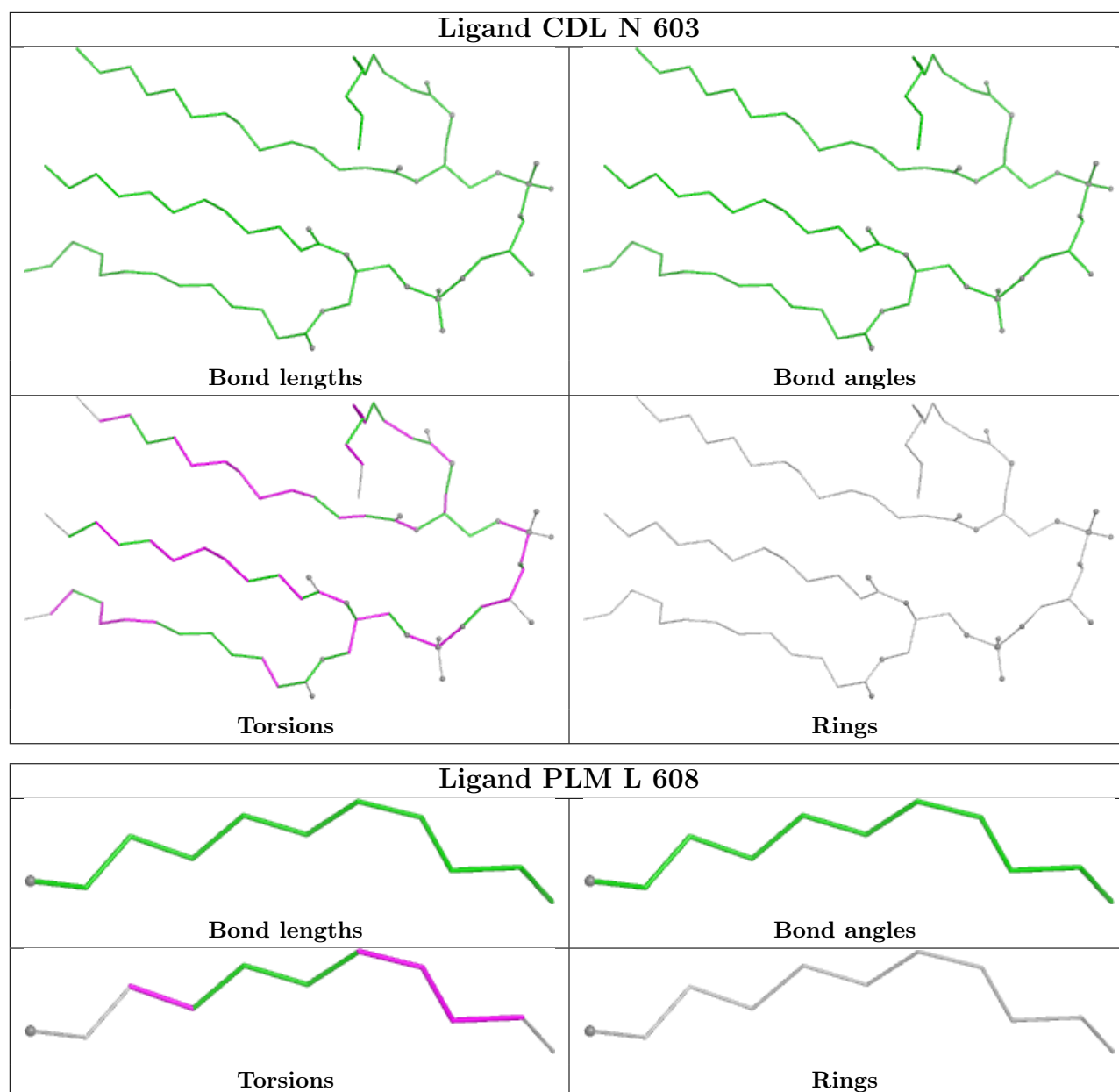


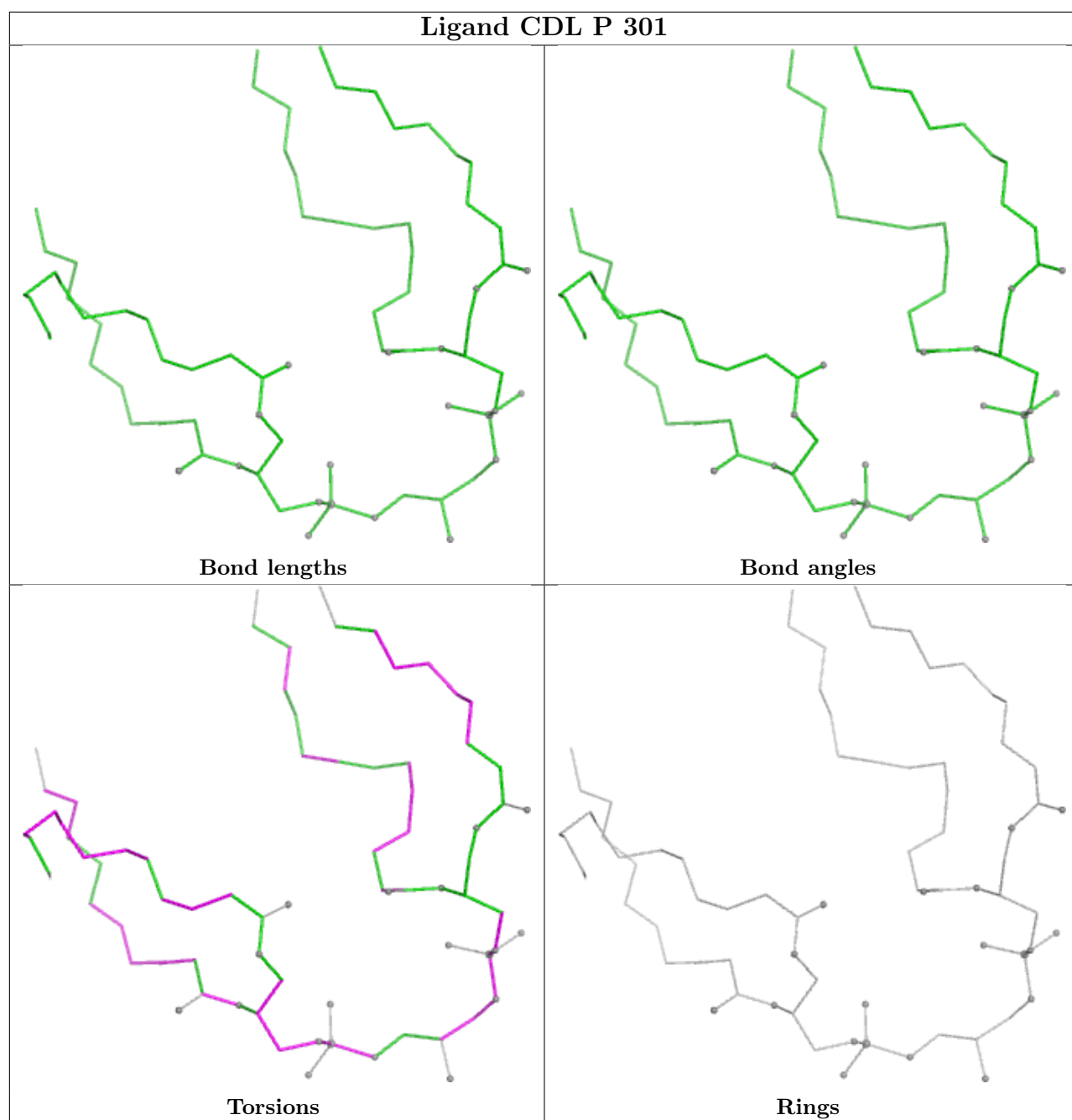


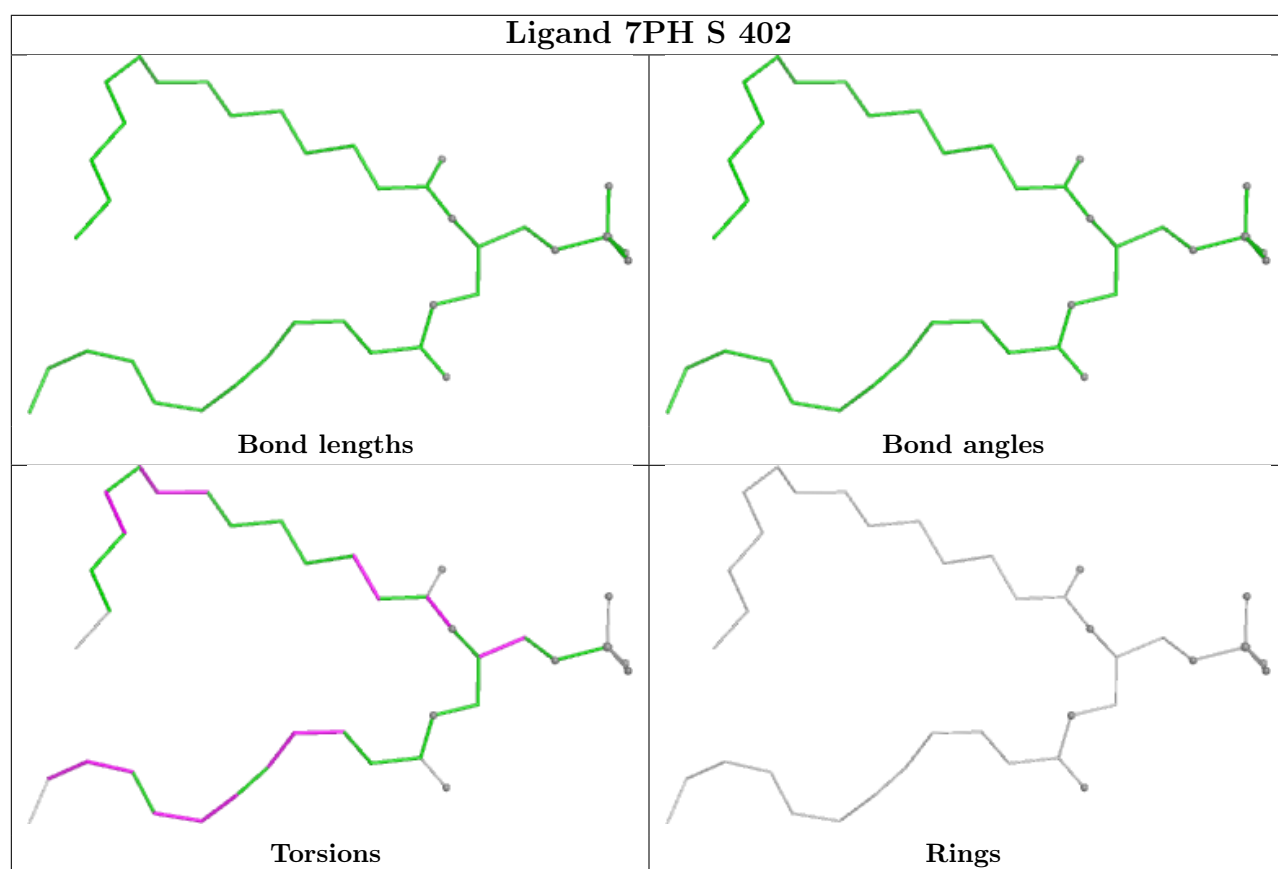
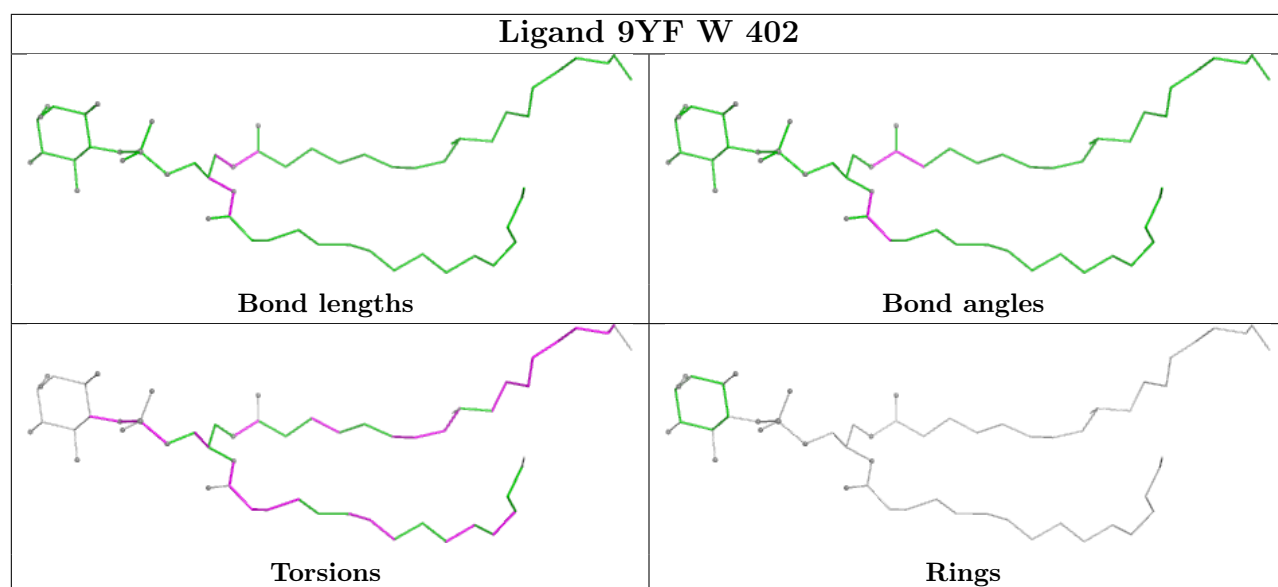


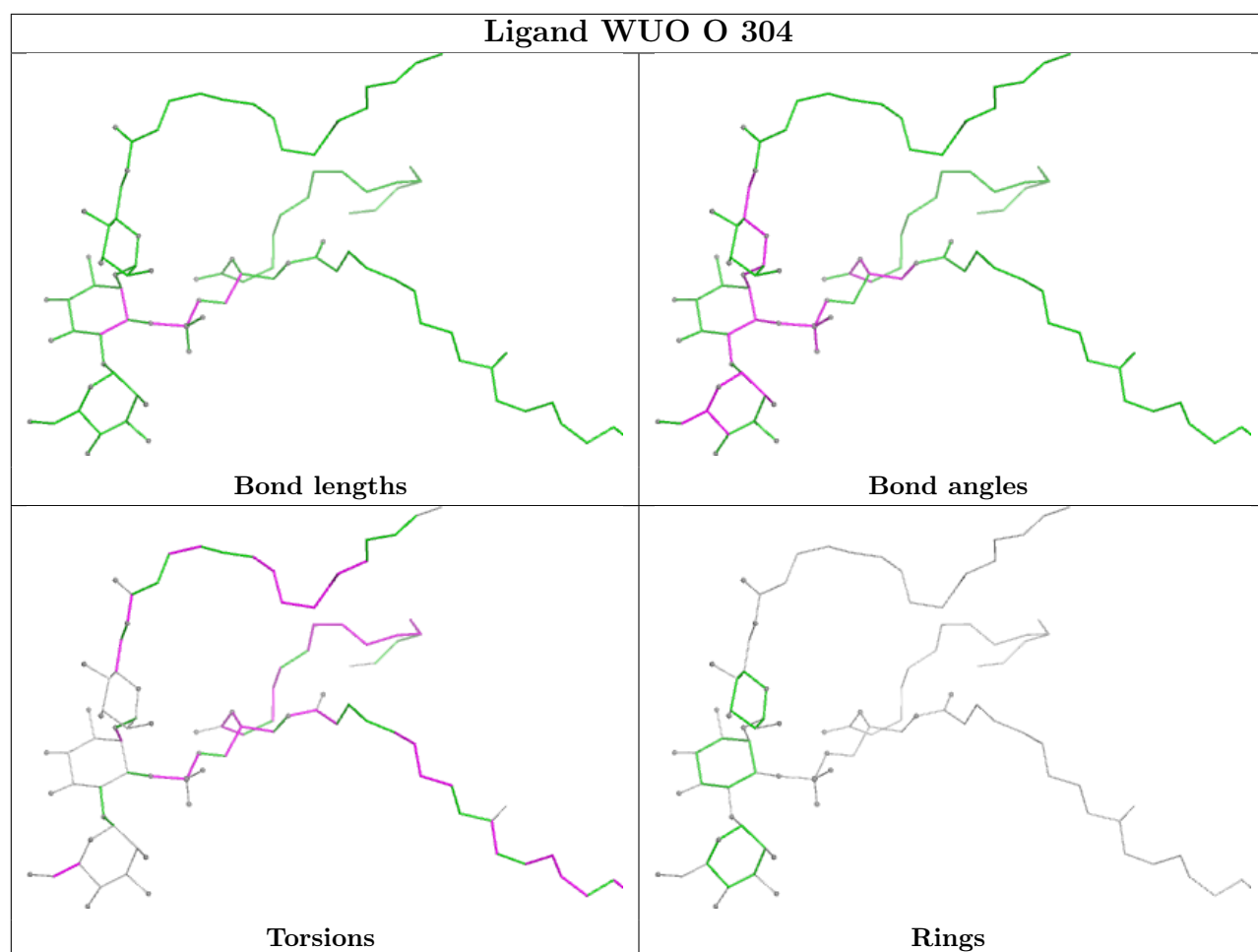


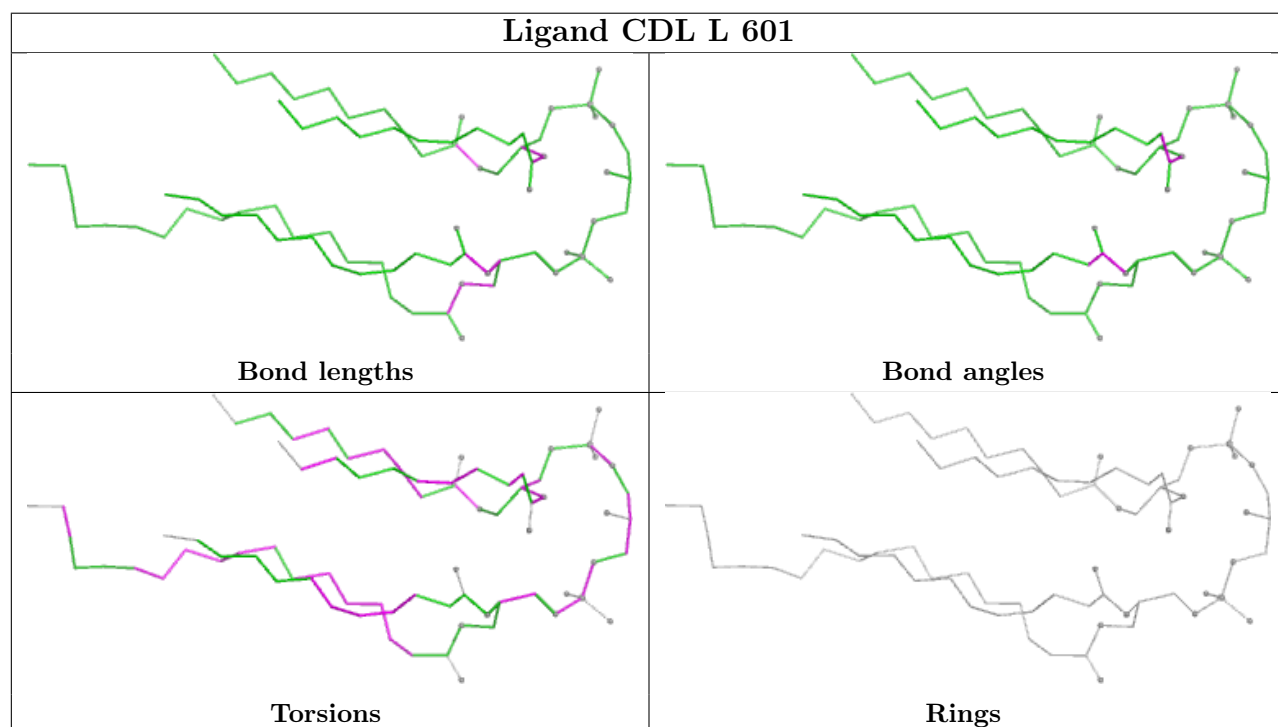
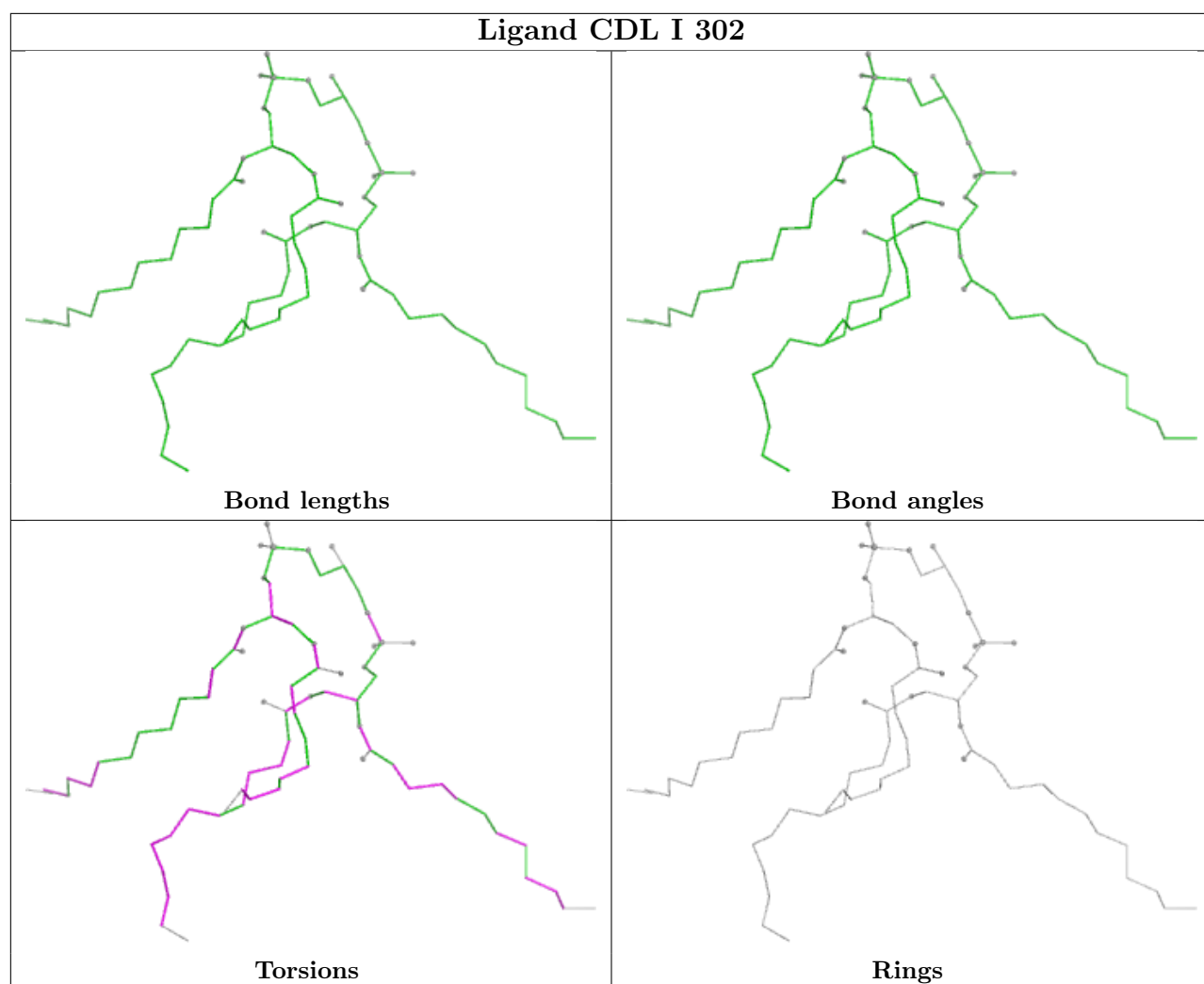


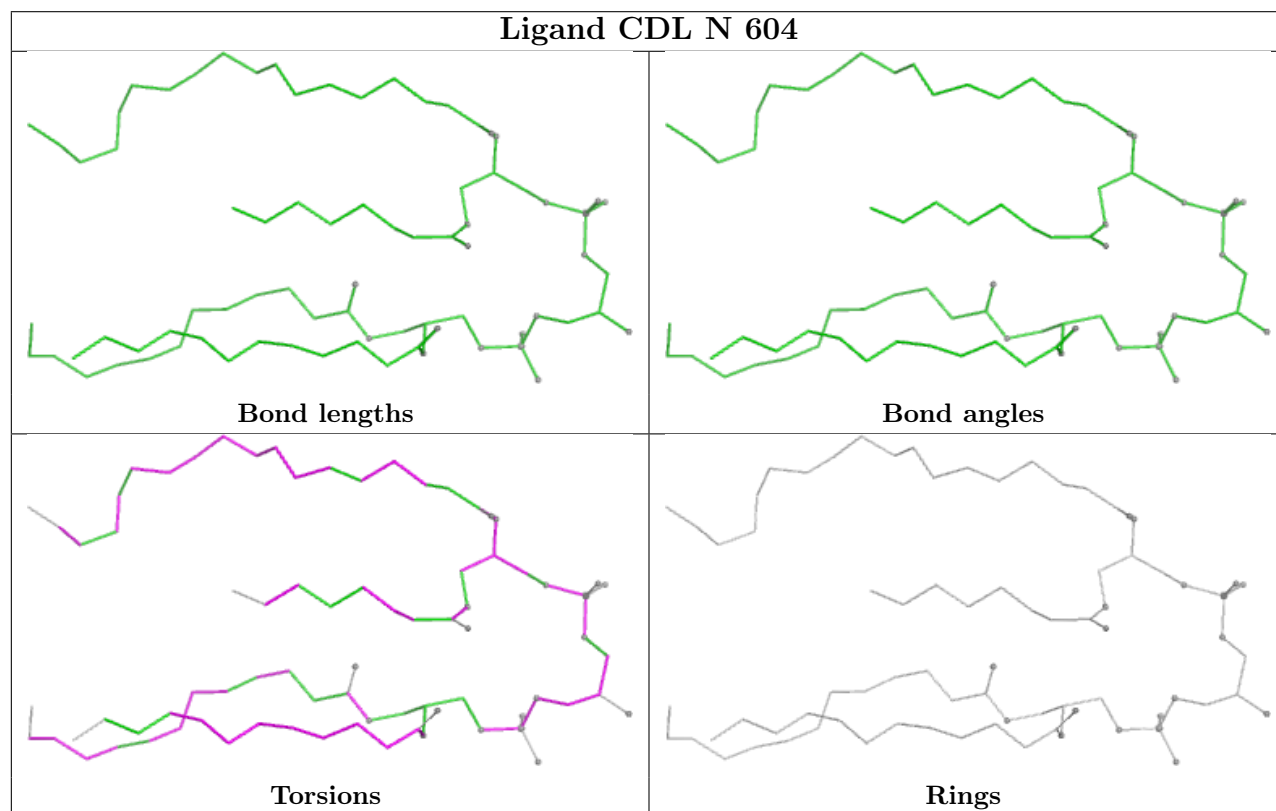
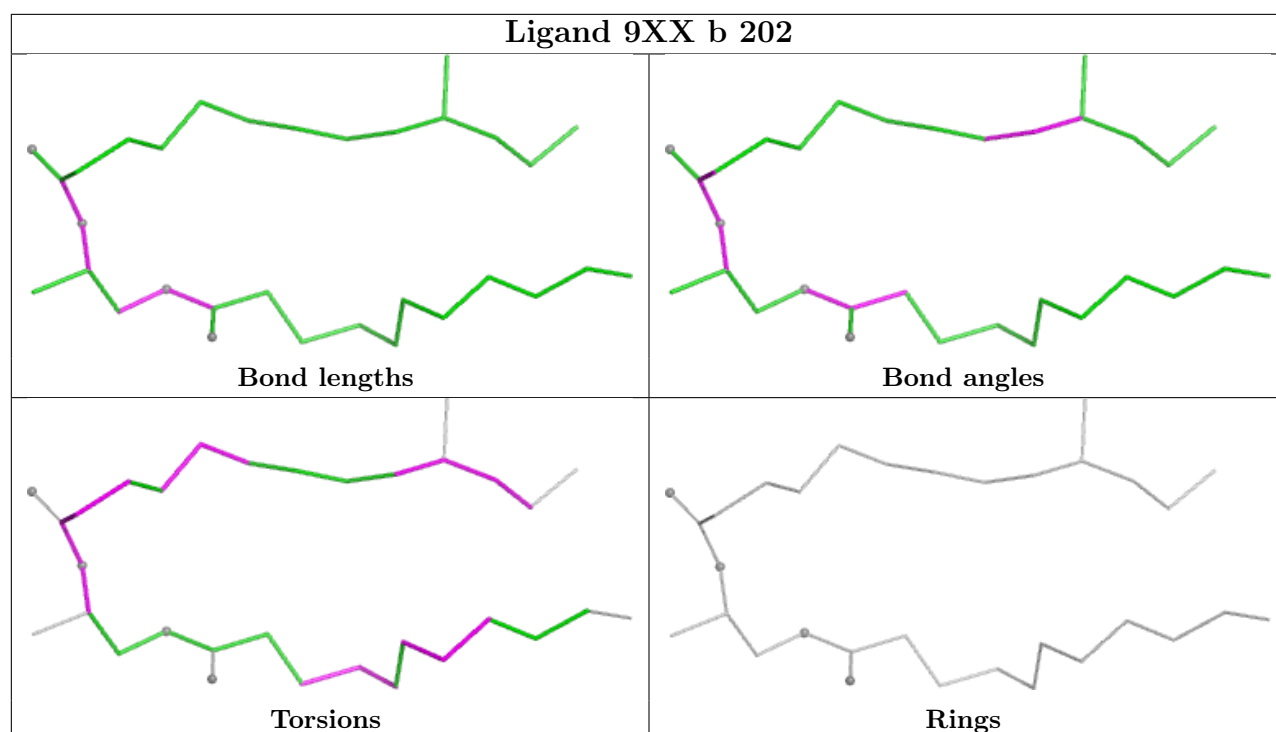


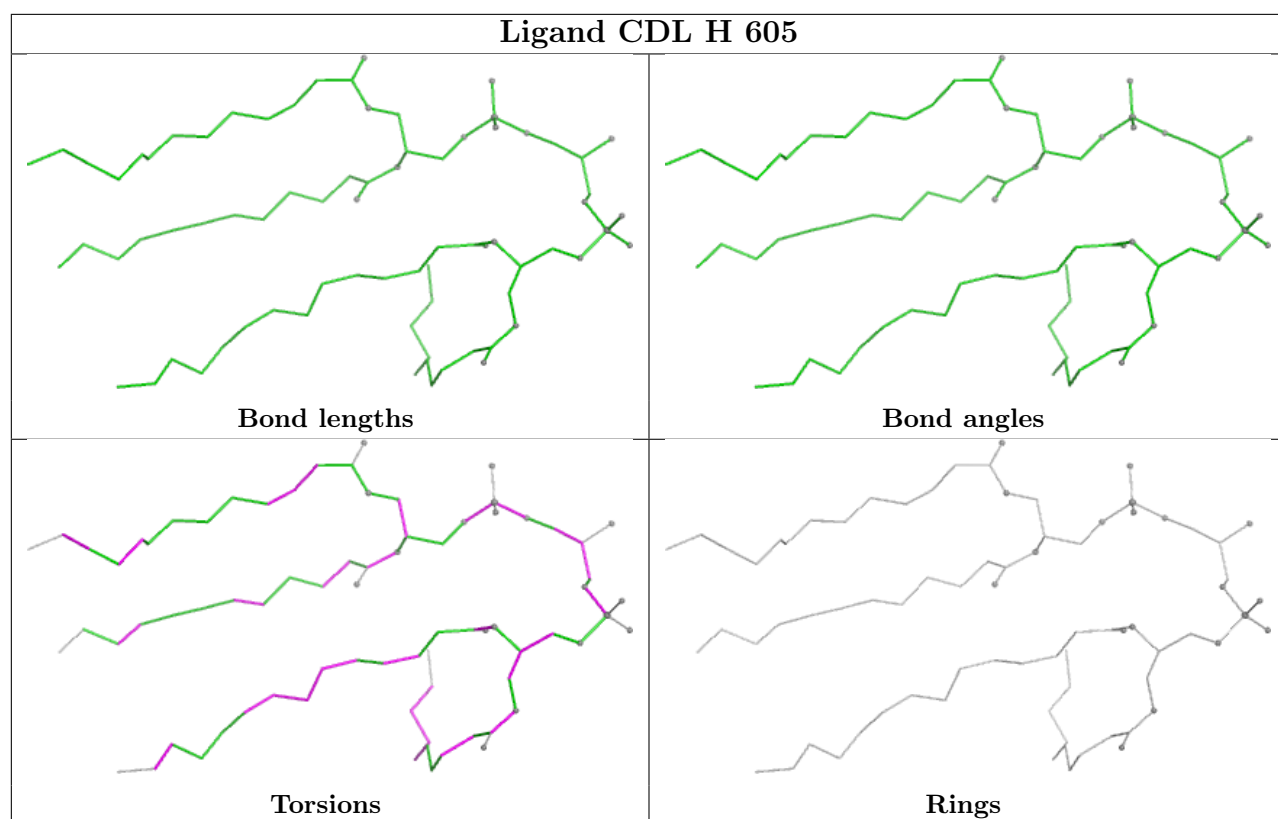


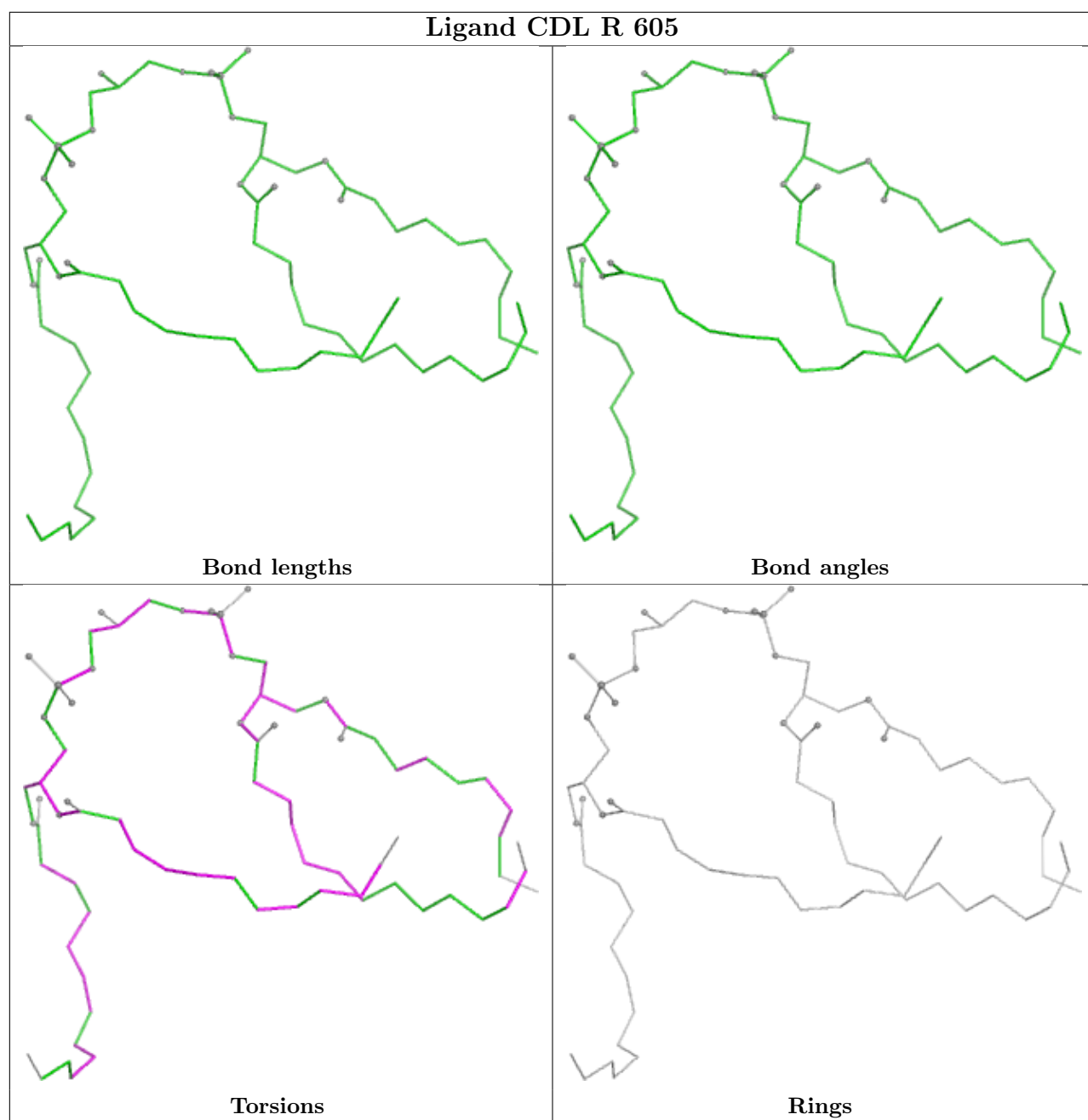


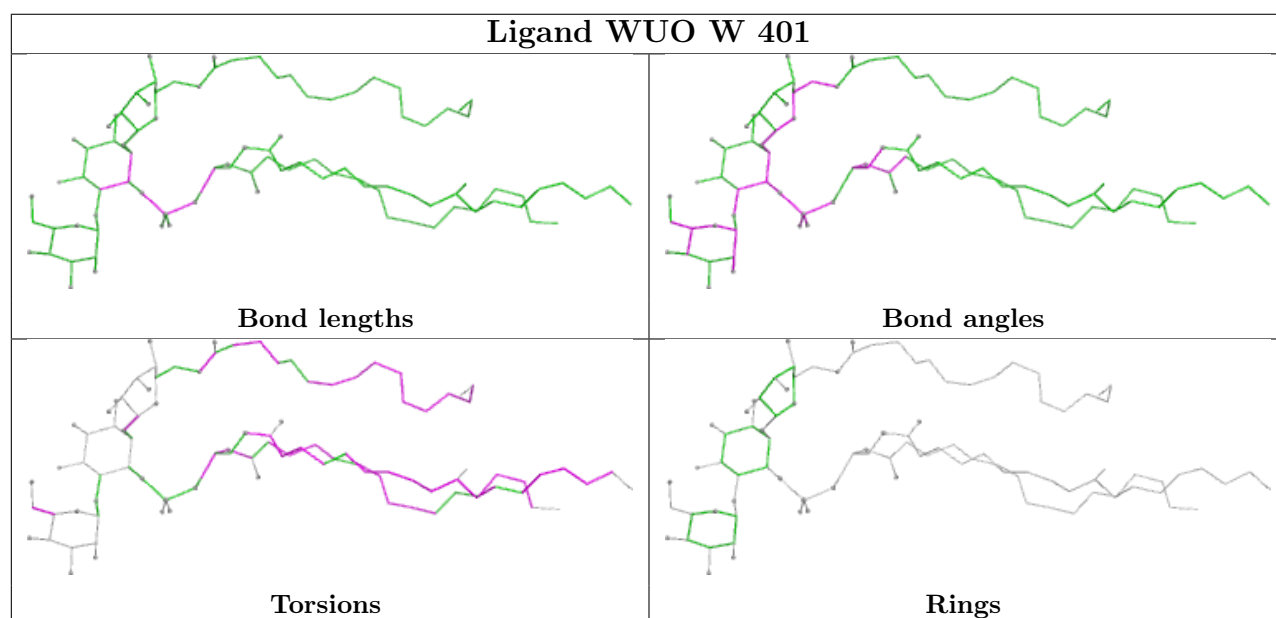
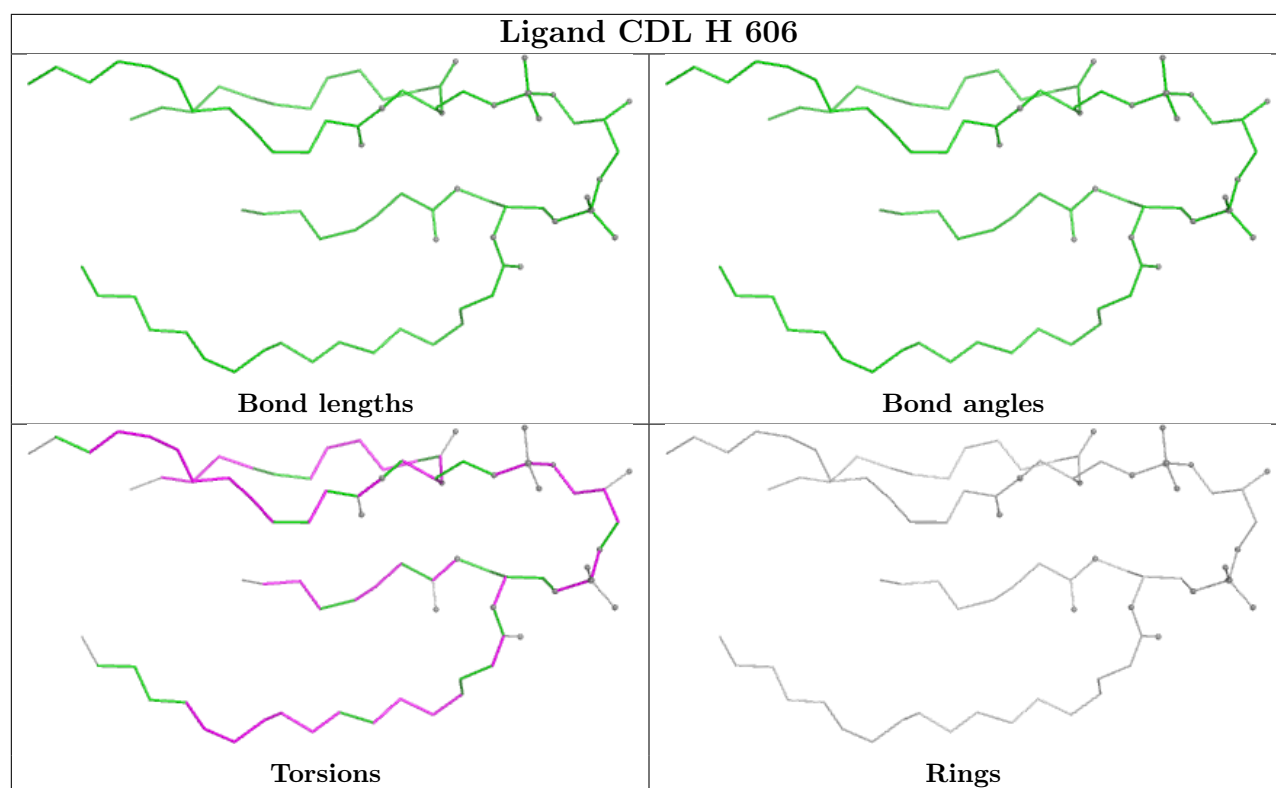


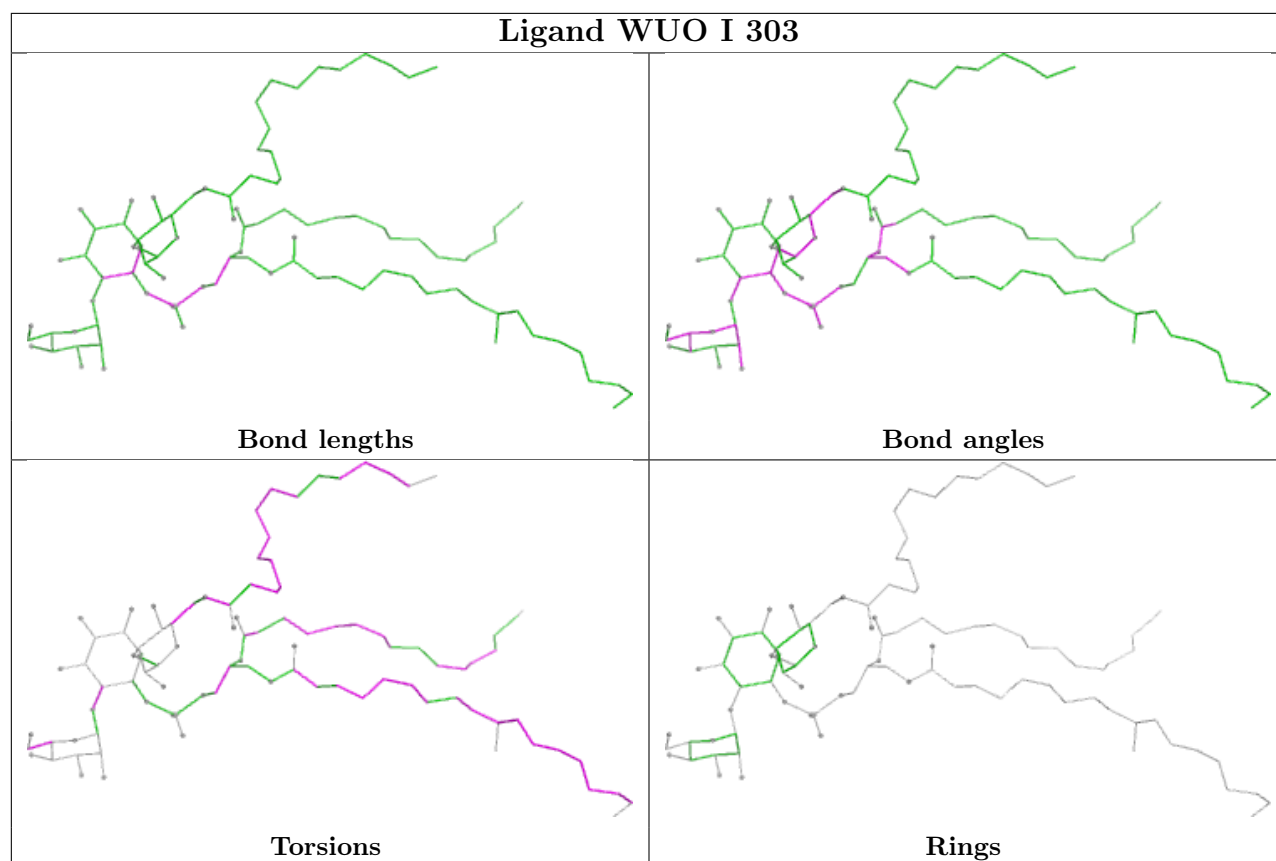
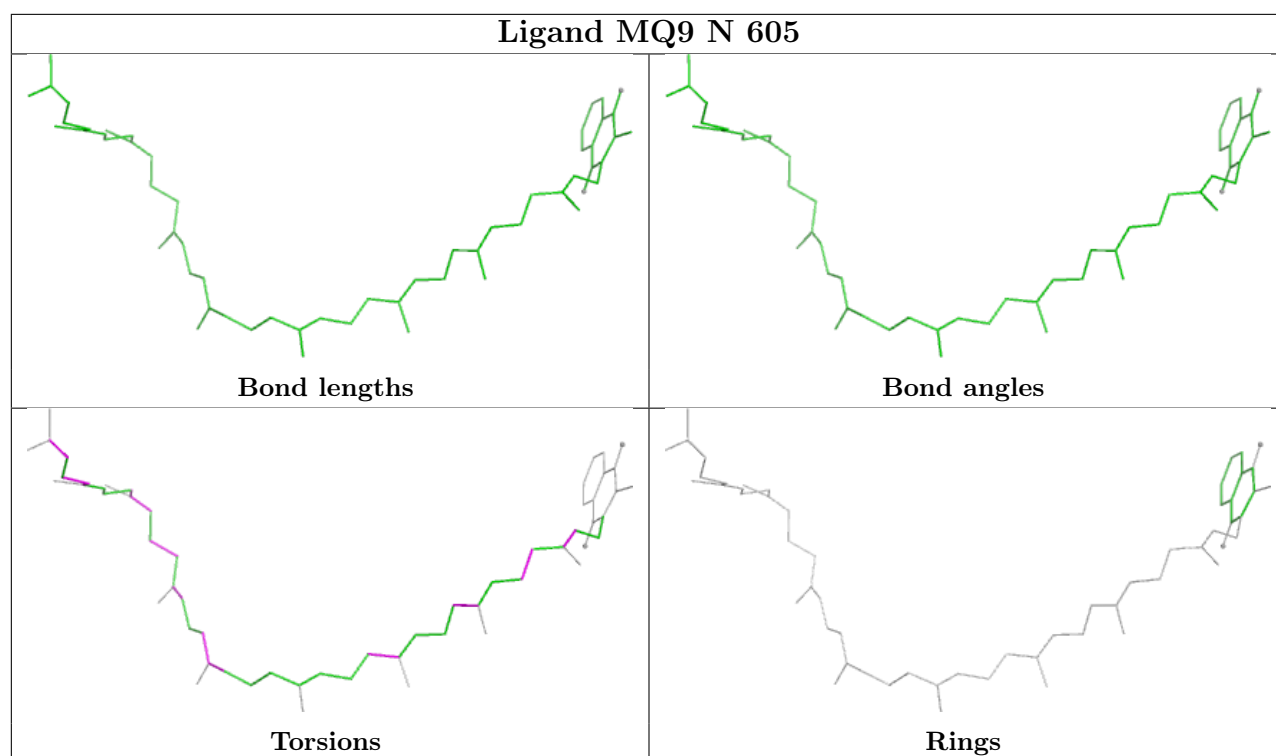


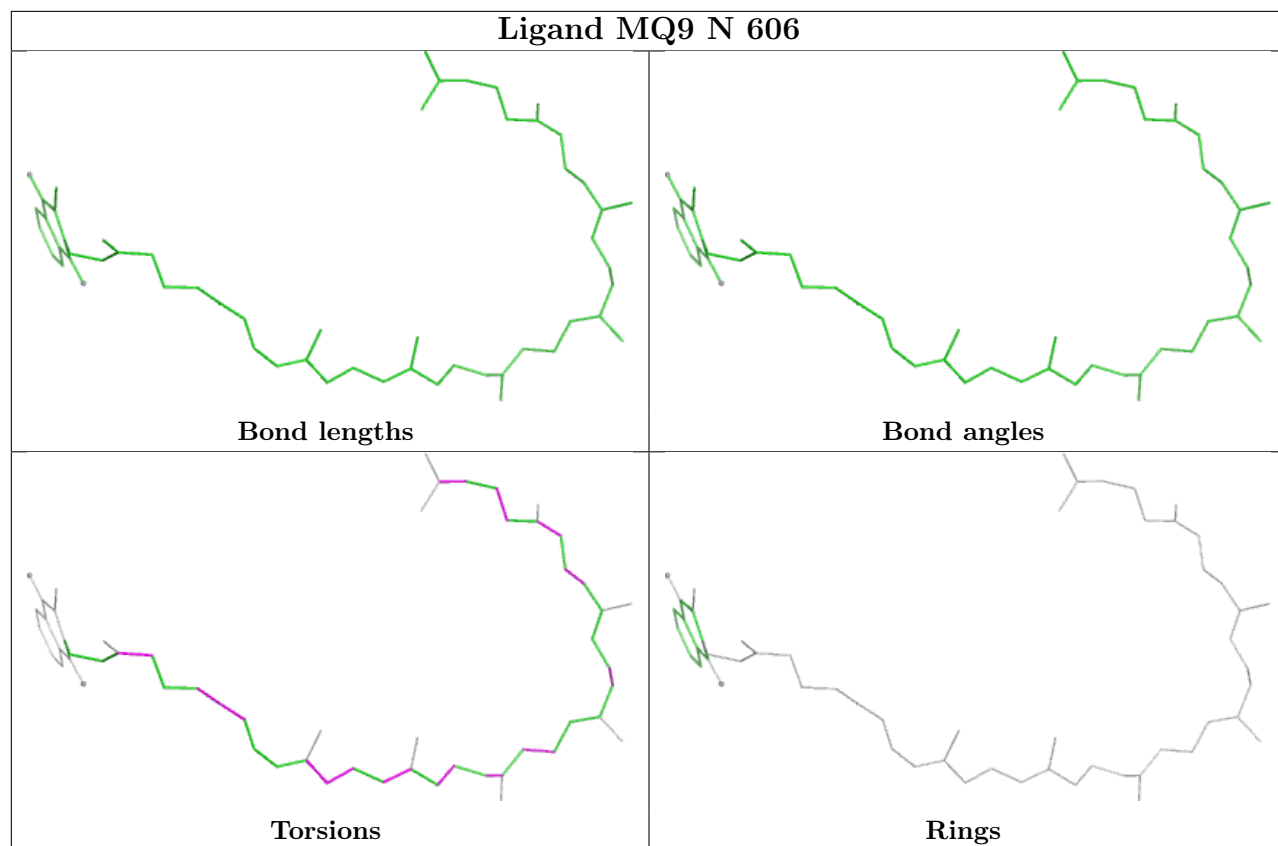


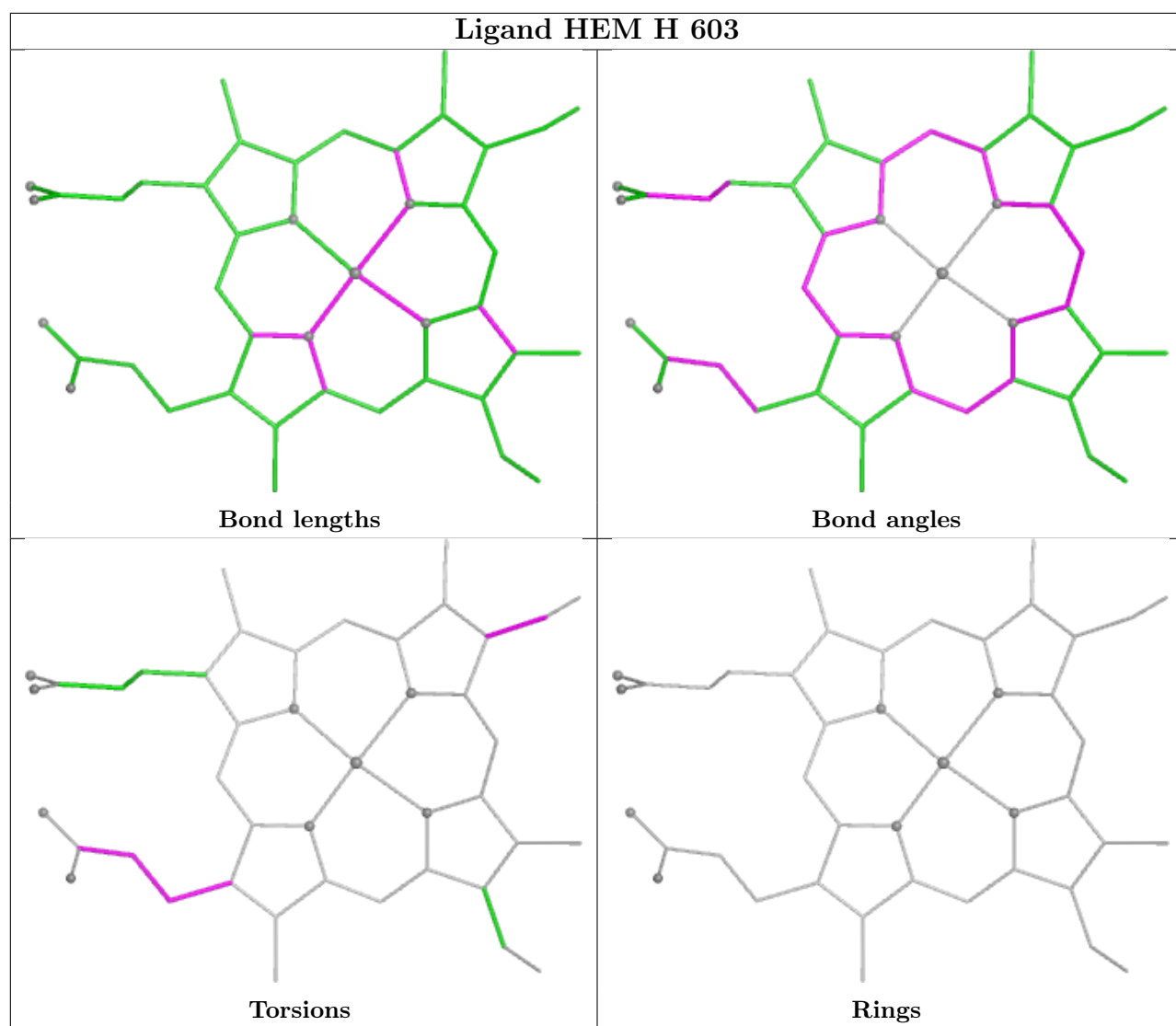


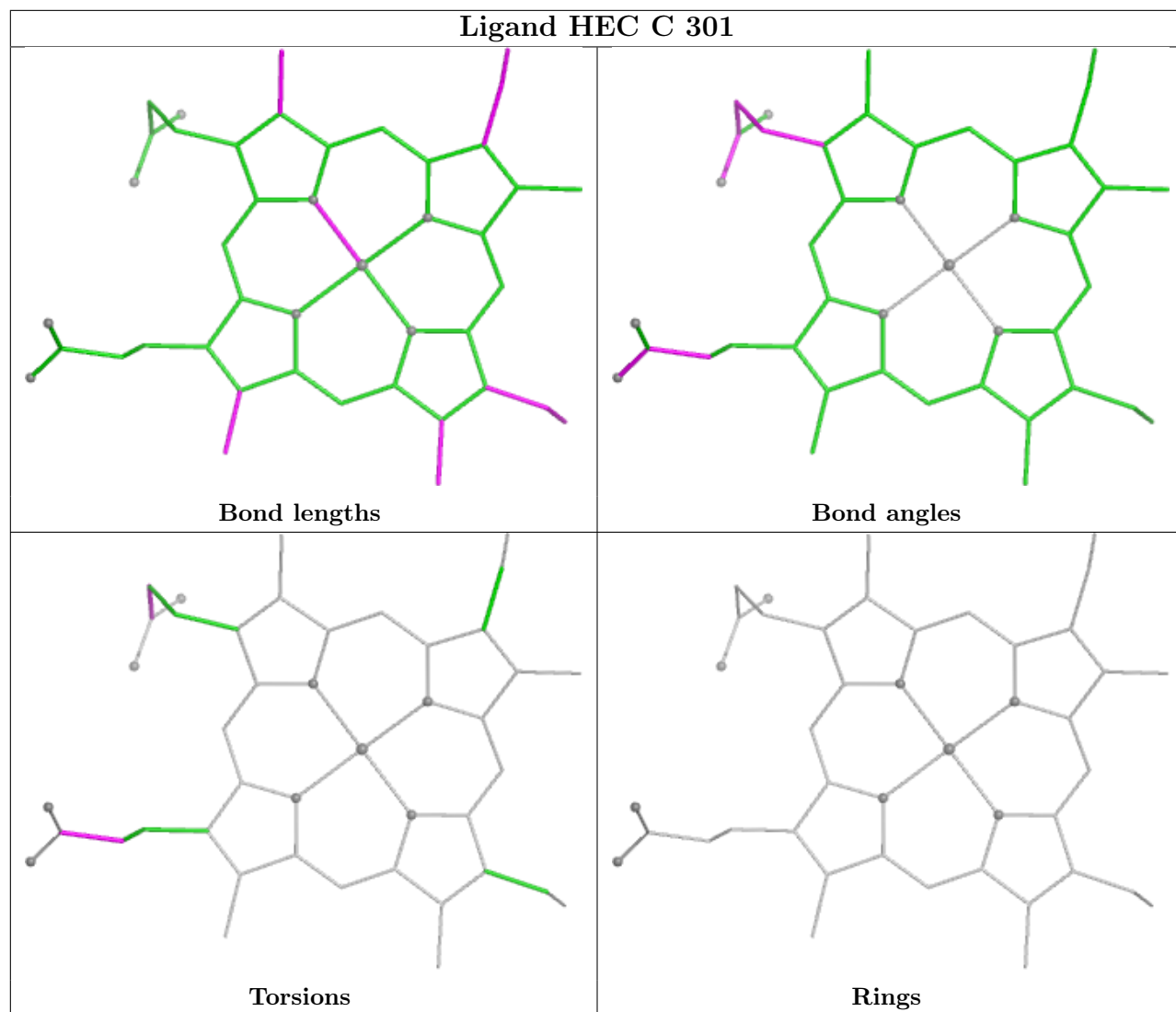


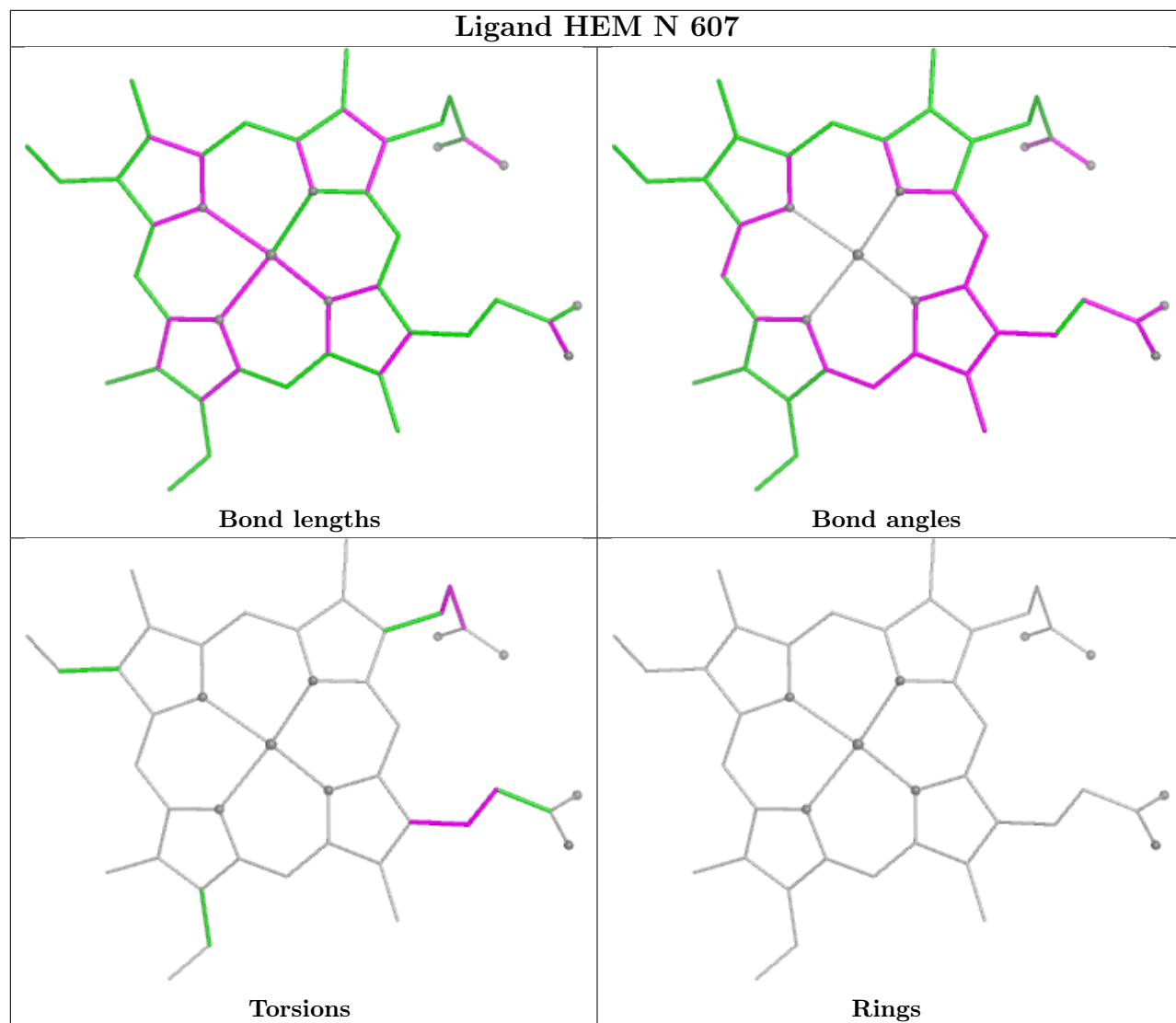


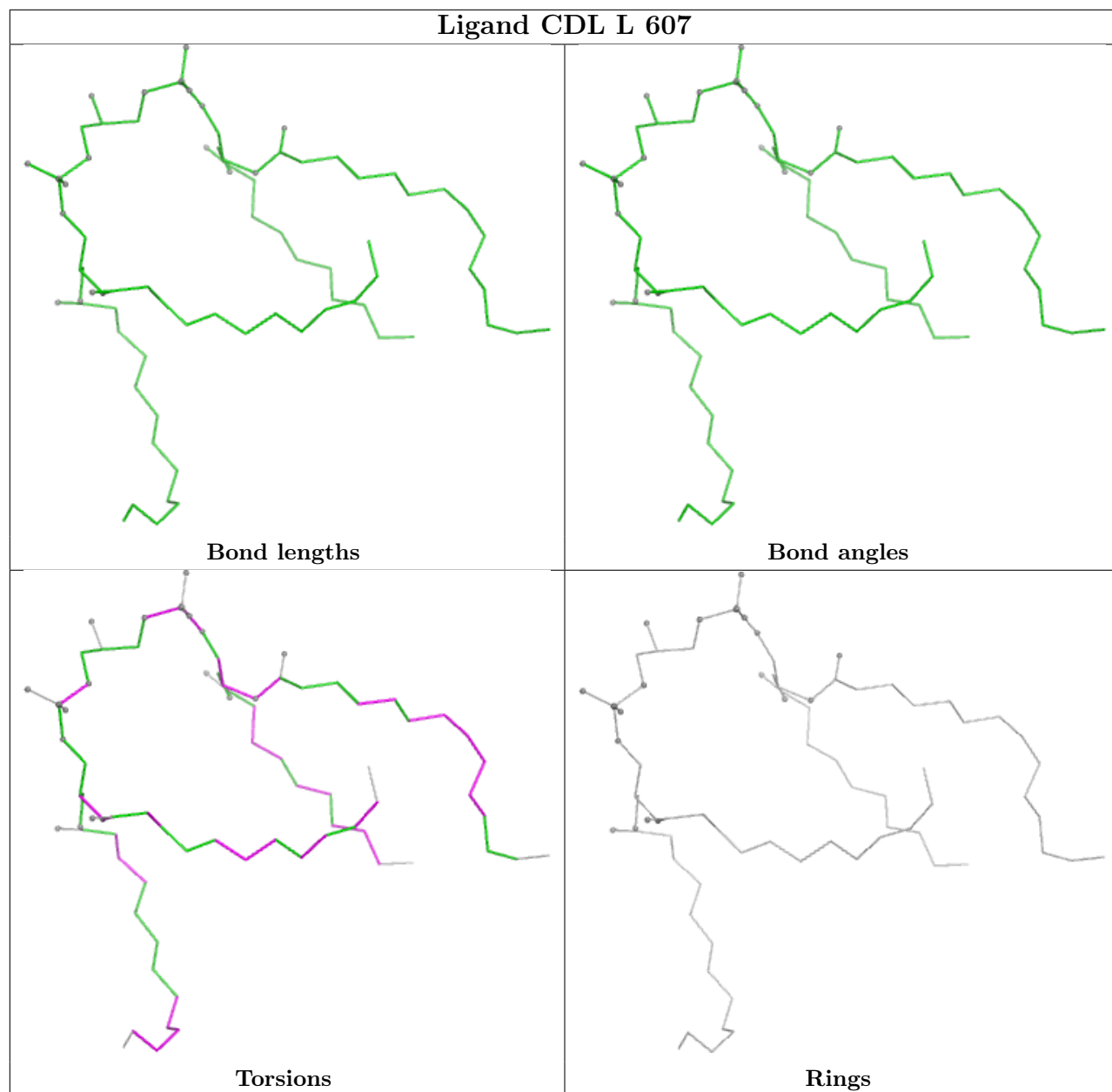


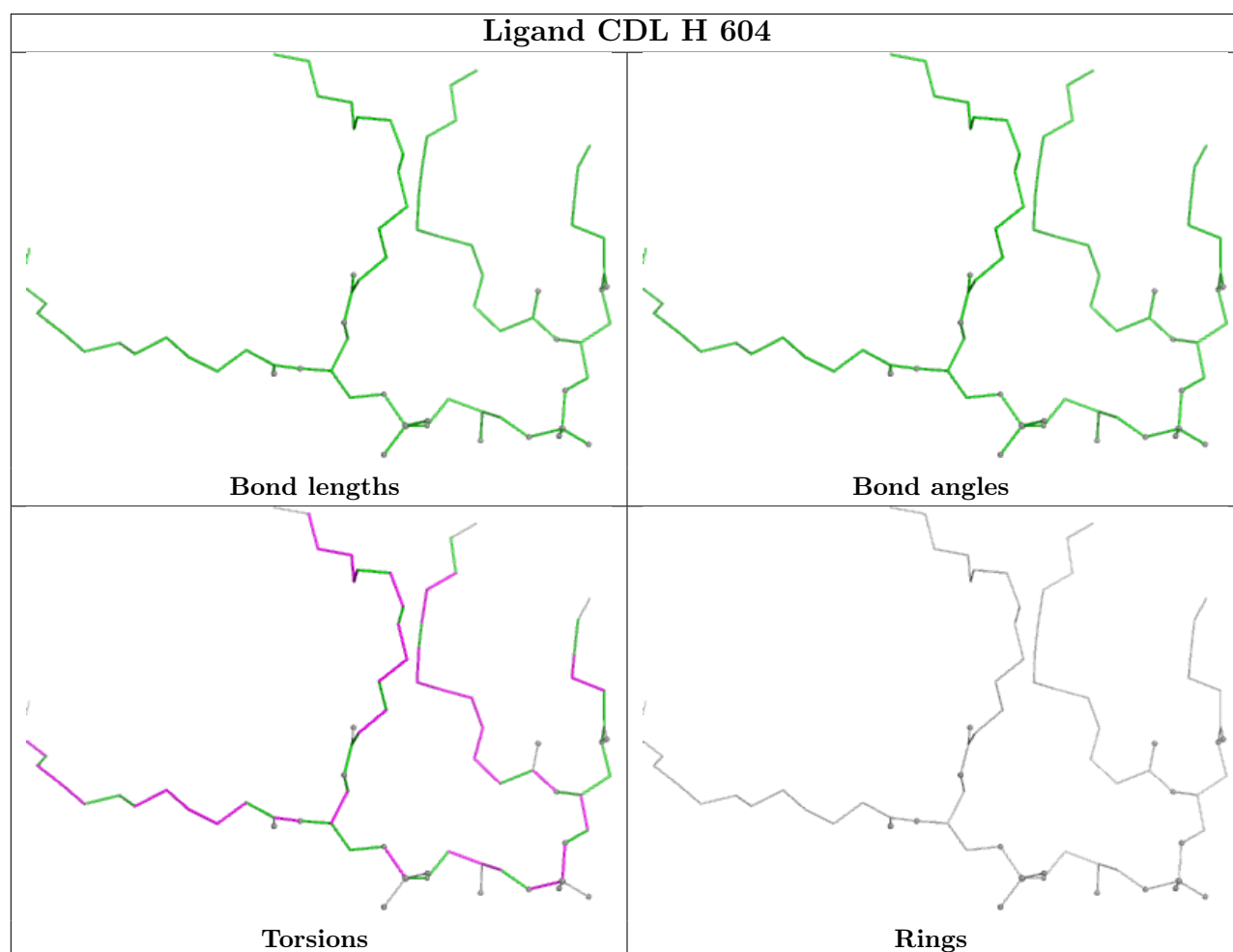
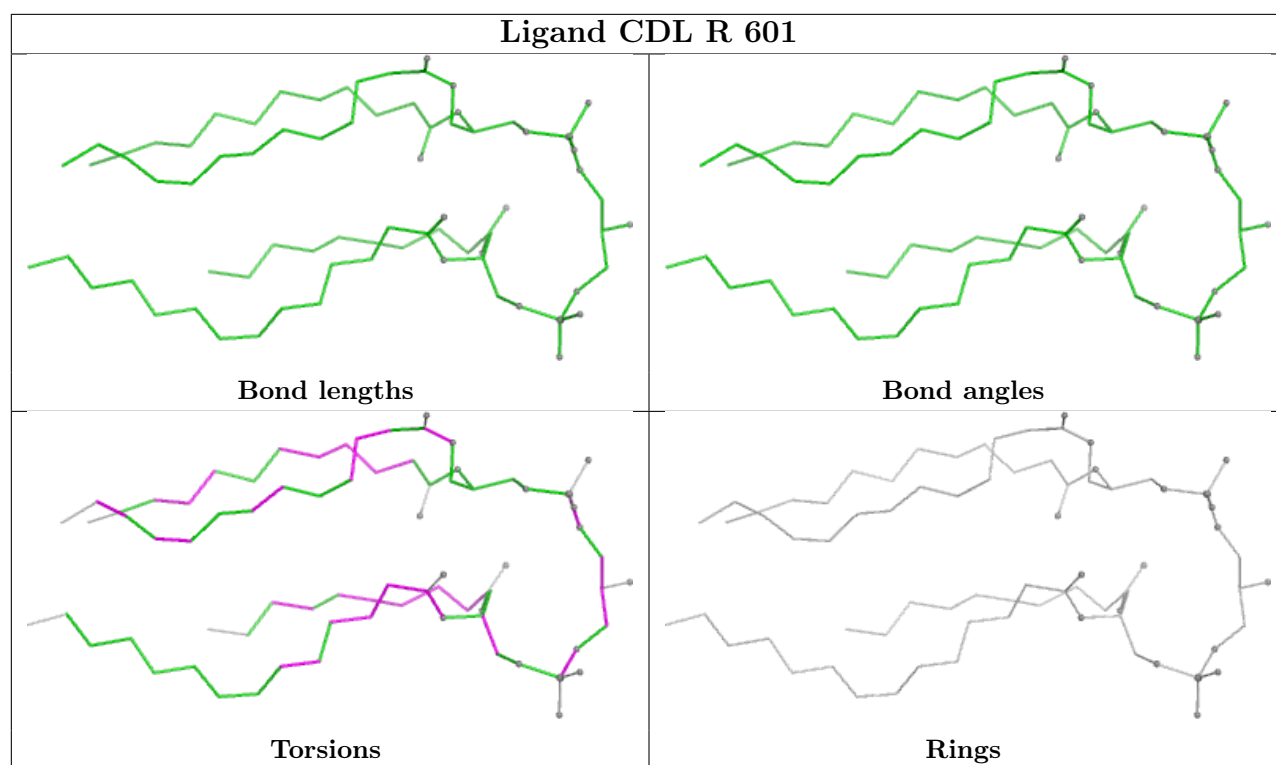


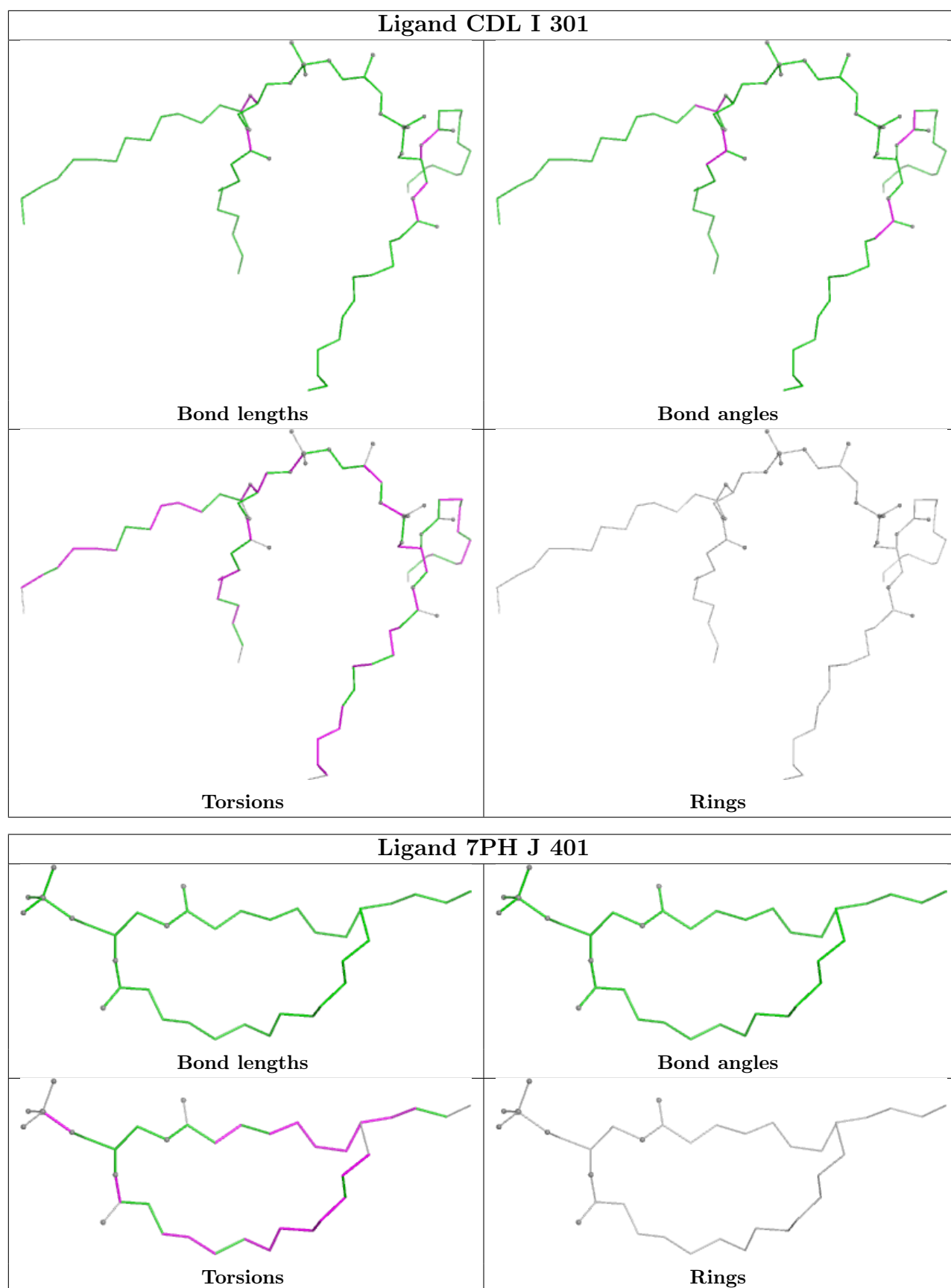


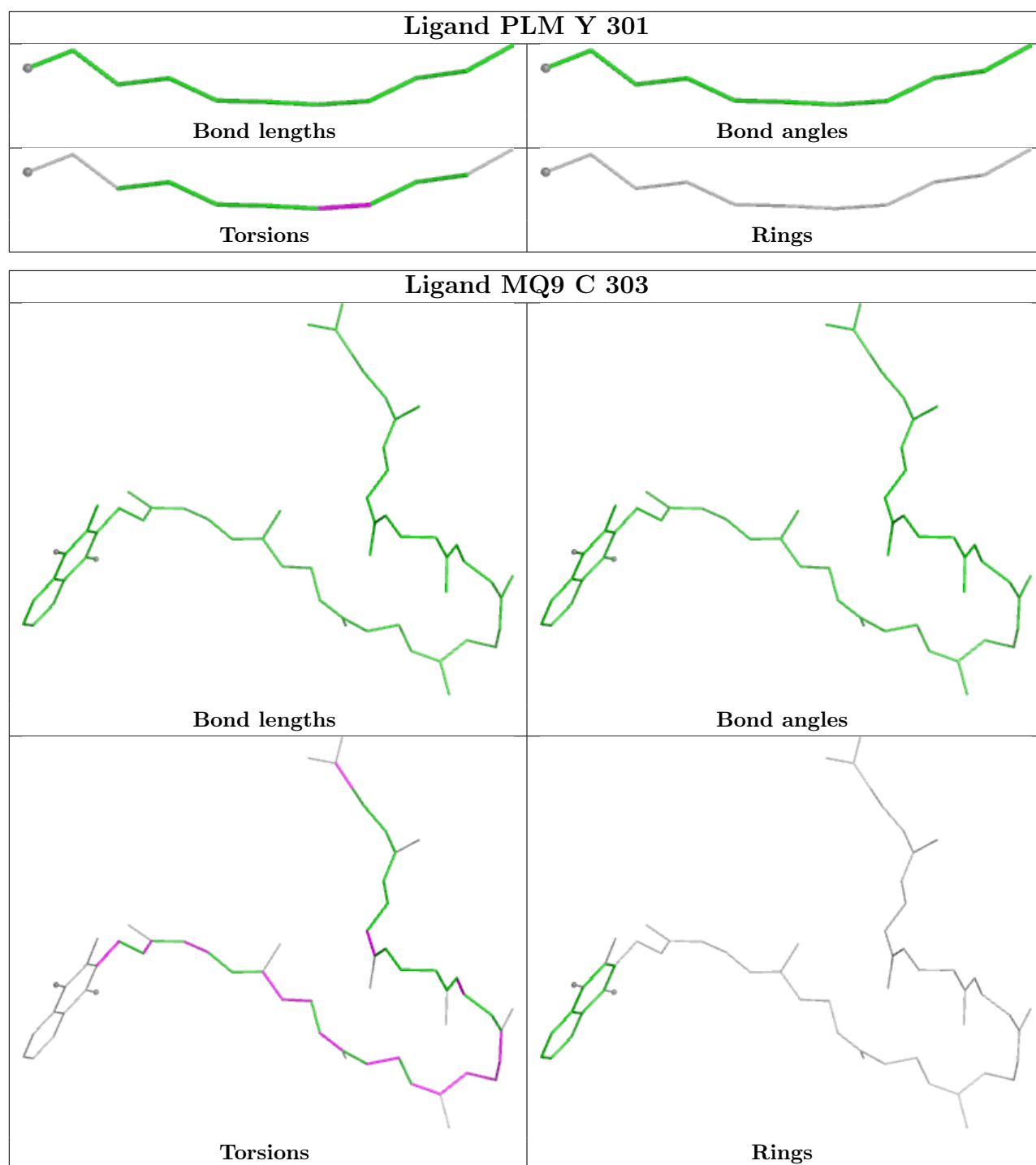












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

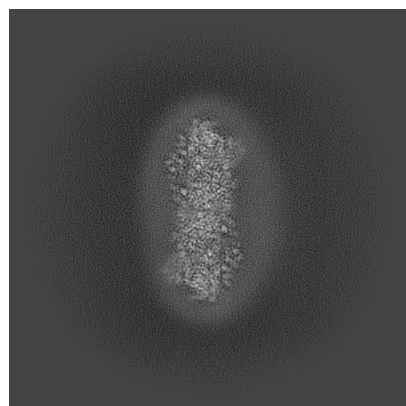
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17210. These allow visual inspection of the internal detail of the map and identification of artifacts.

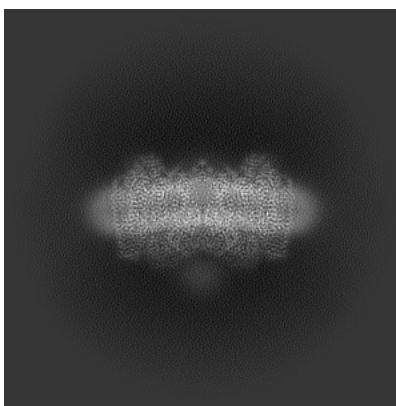
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

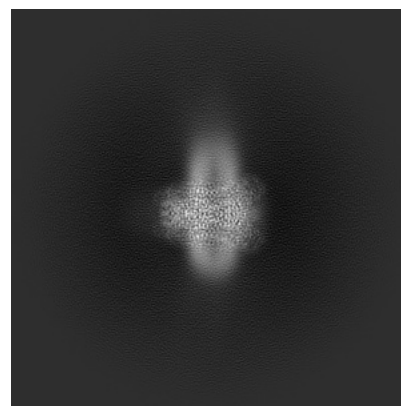
6.1.1 Primary map



X

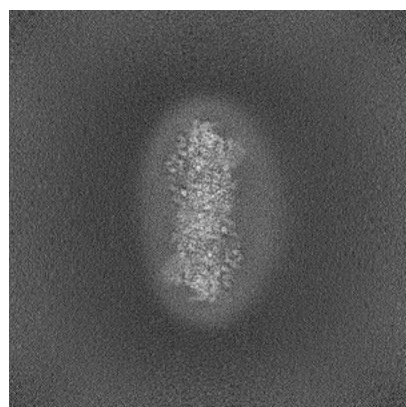


Y

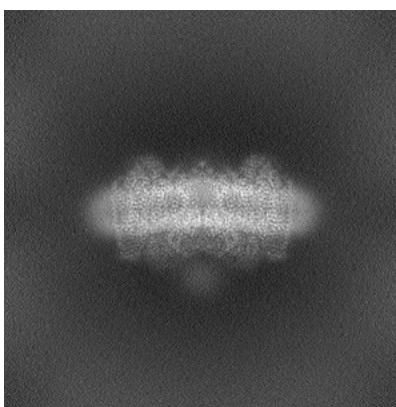


Z

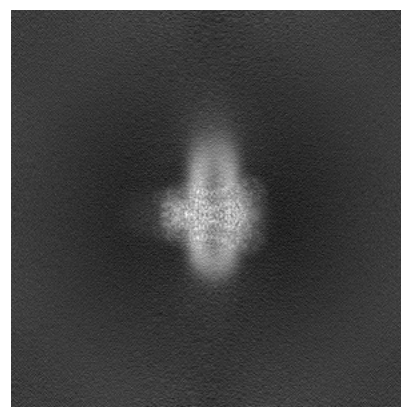
6.1.2 Raw map



X



Y

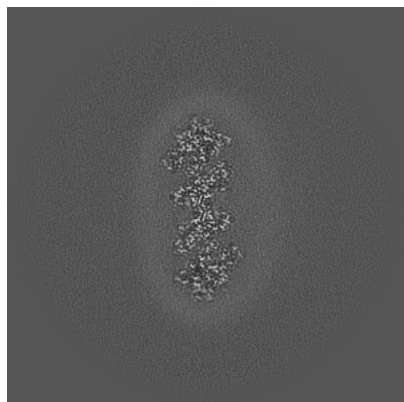


Z

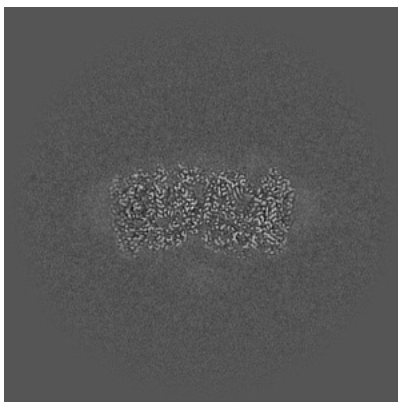
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

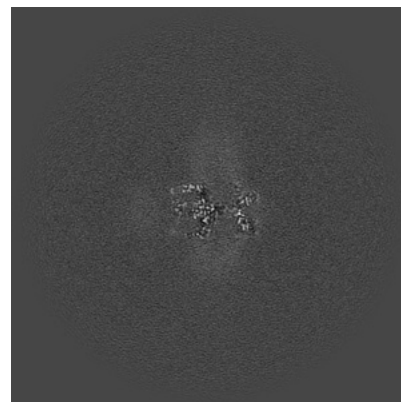
6.2.1 Primary map



X Index: 270

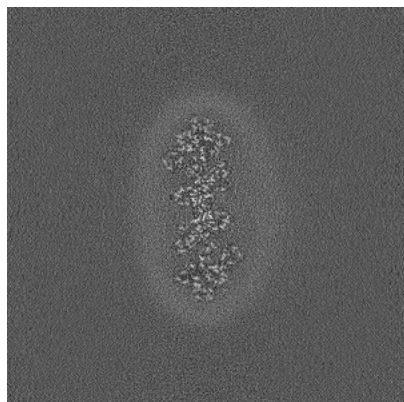


Y Index: 270

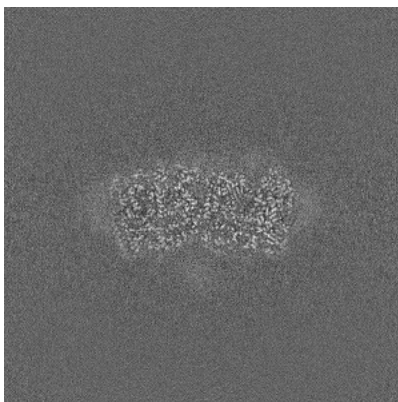


Z Index: 270

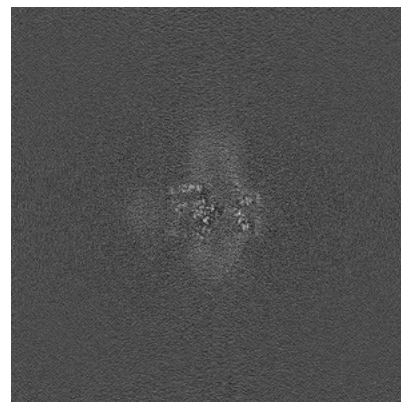
6.2.2 Raw map



X Index: 270



Y Index: 270

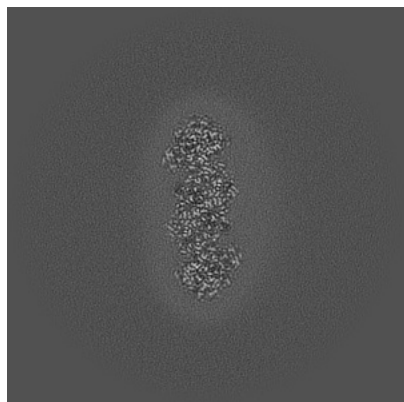


Z Index: 270

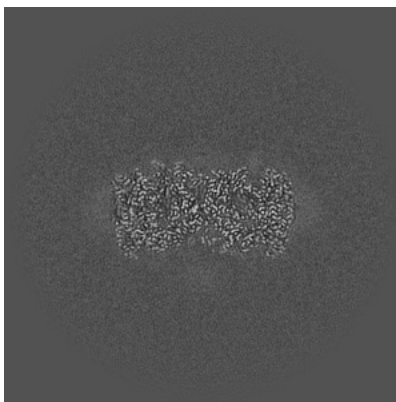
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

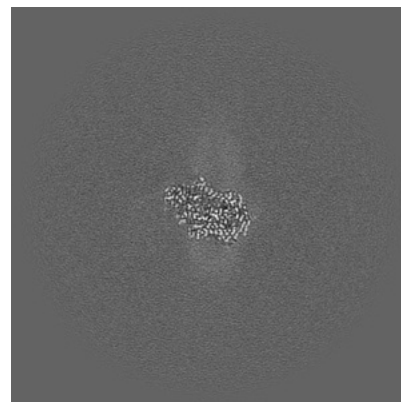
6.3.1 Primary map



X Index: 255

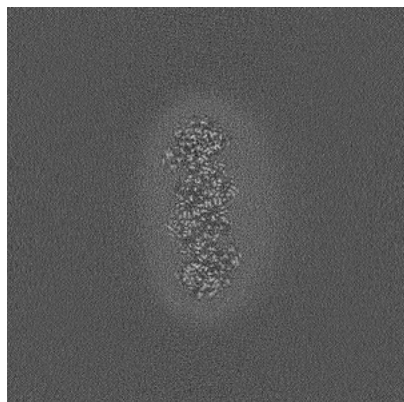


Y Index: 267

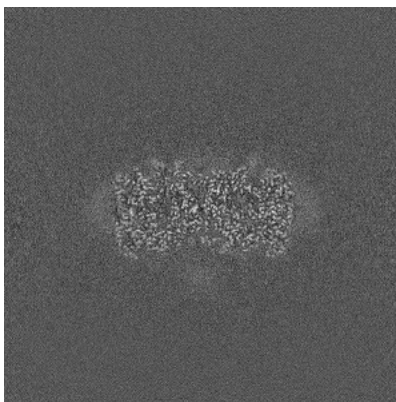


Z Index: 293

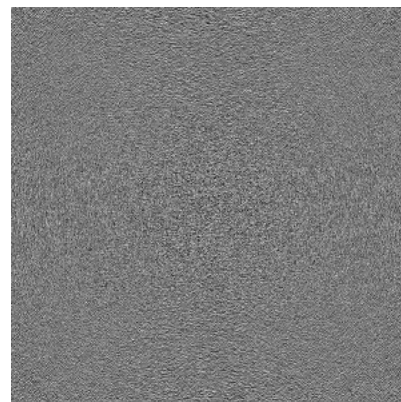
6.3.2 Raw map



X Index: 255



Y Index: 267

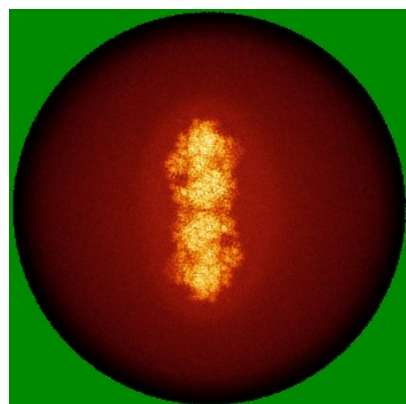


Z Index: 0

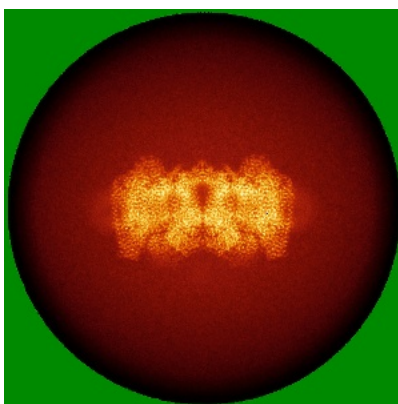
The images above show the largest variance slices of the map in three orthogonal directions.

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

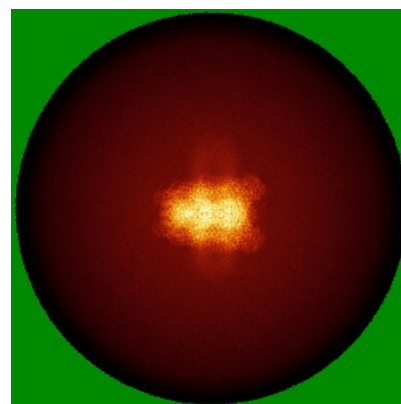
6.4.1 Primary map



X

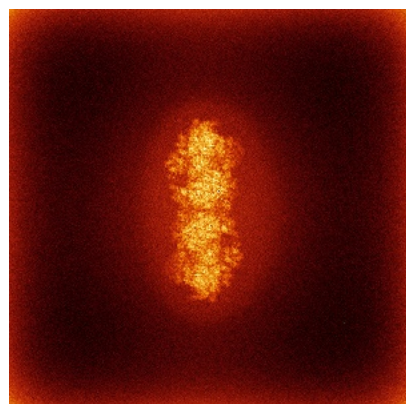


Y

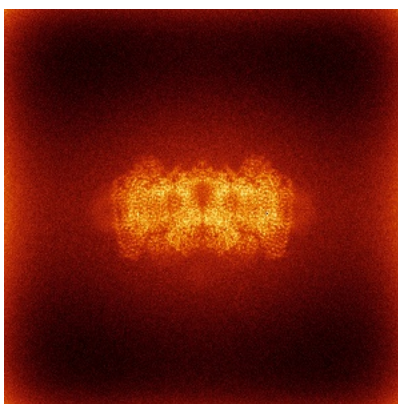


Z

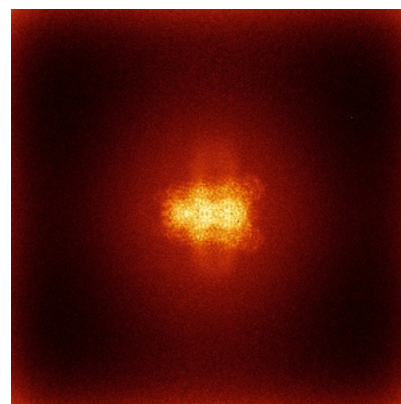
6.4.2 Raw map



X



Y

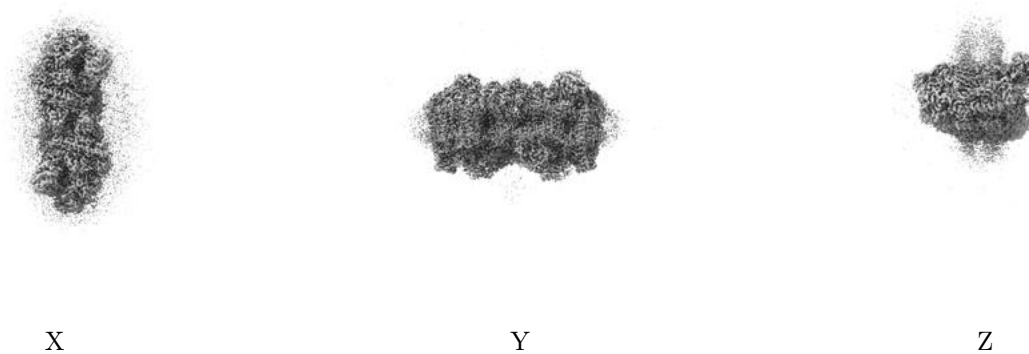


Z

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

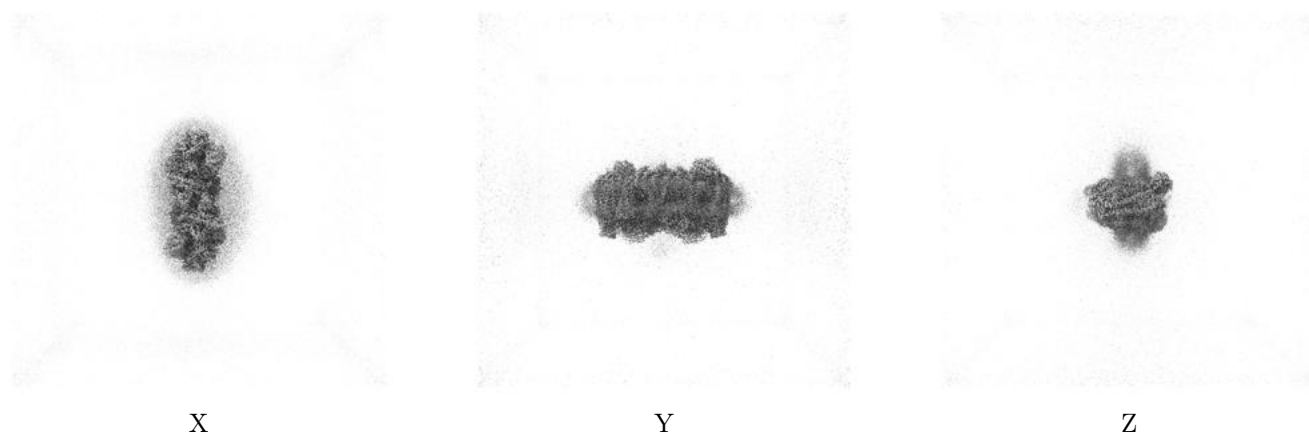
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.194. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

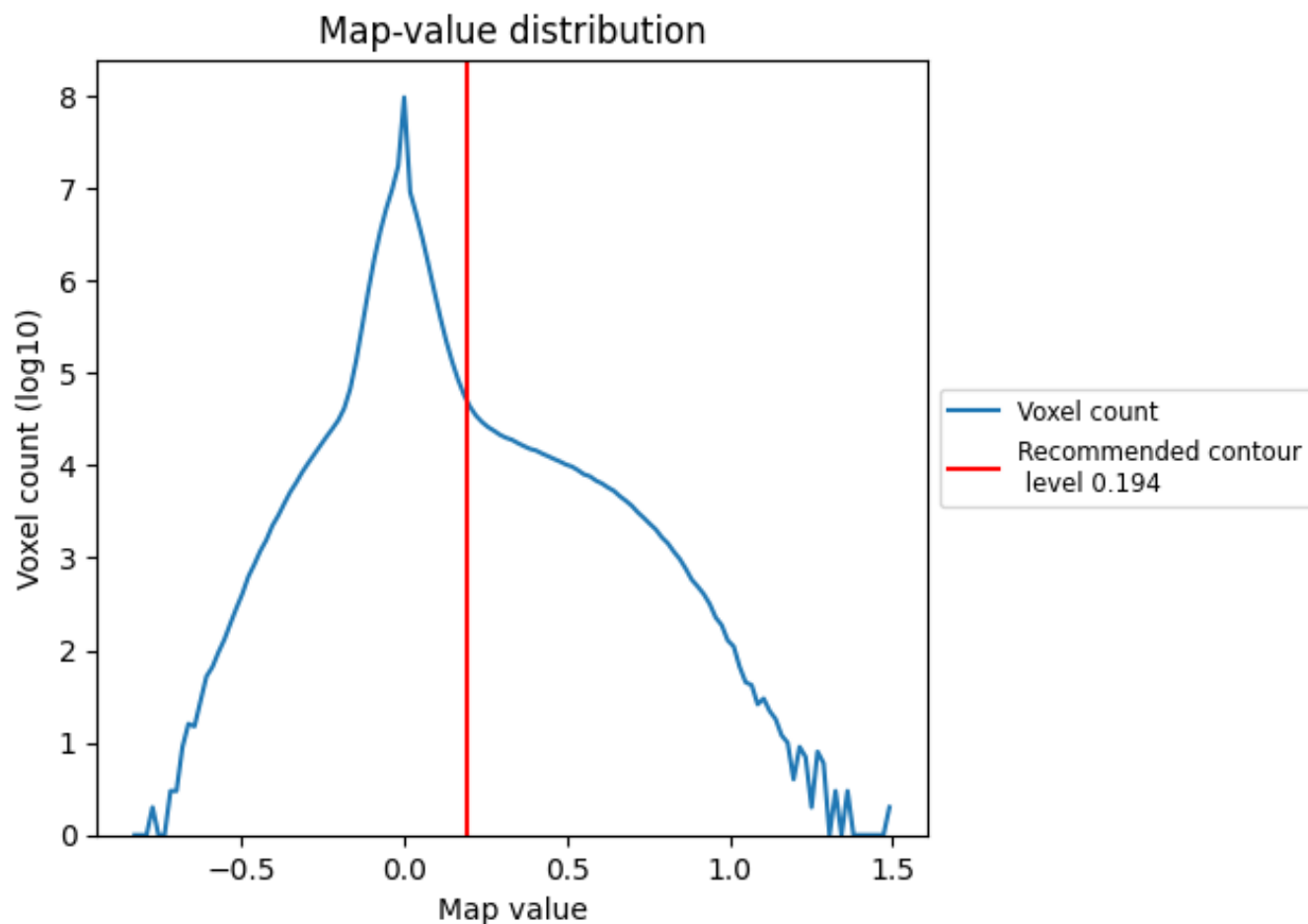
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

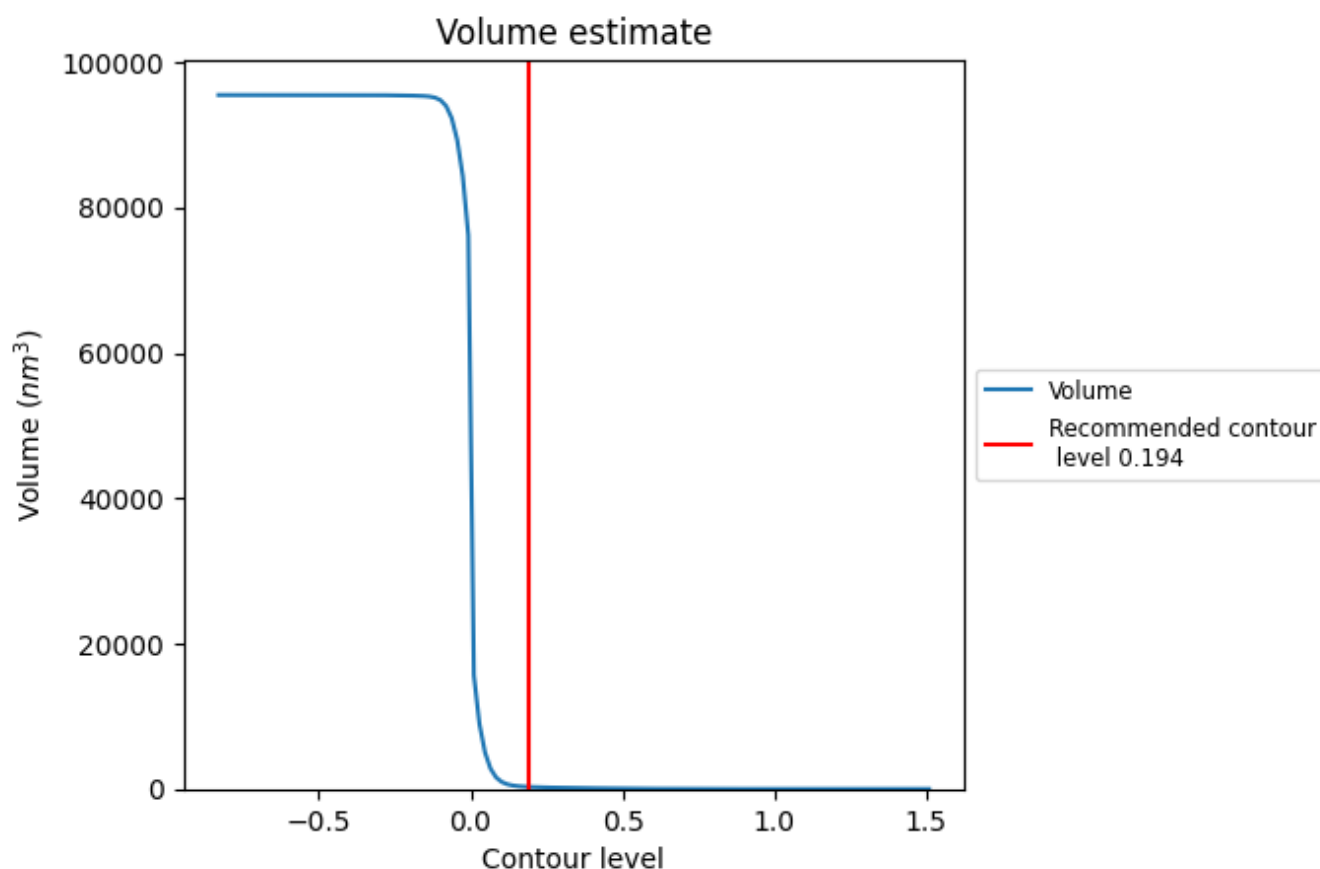
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

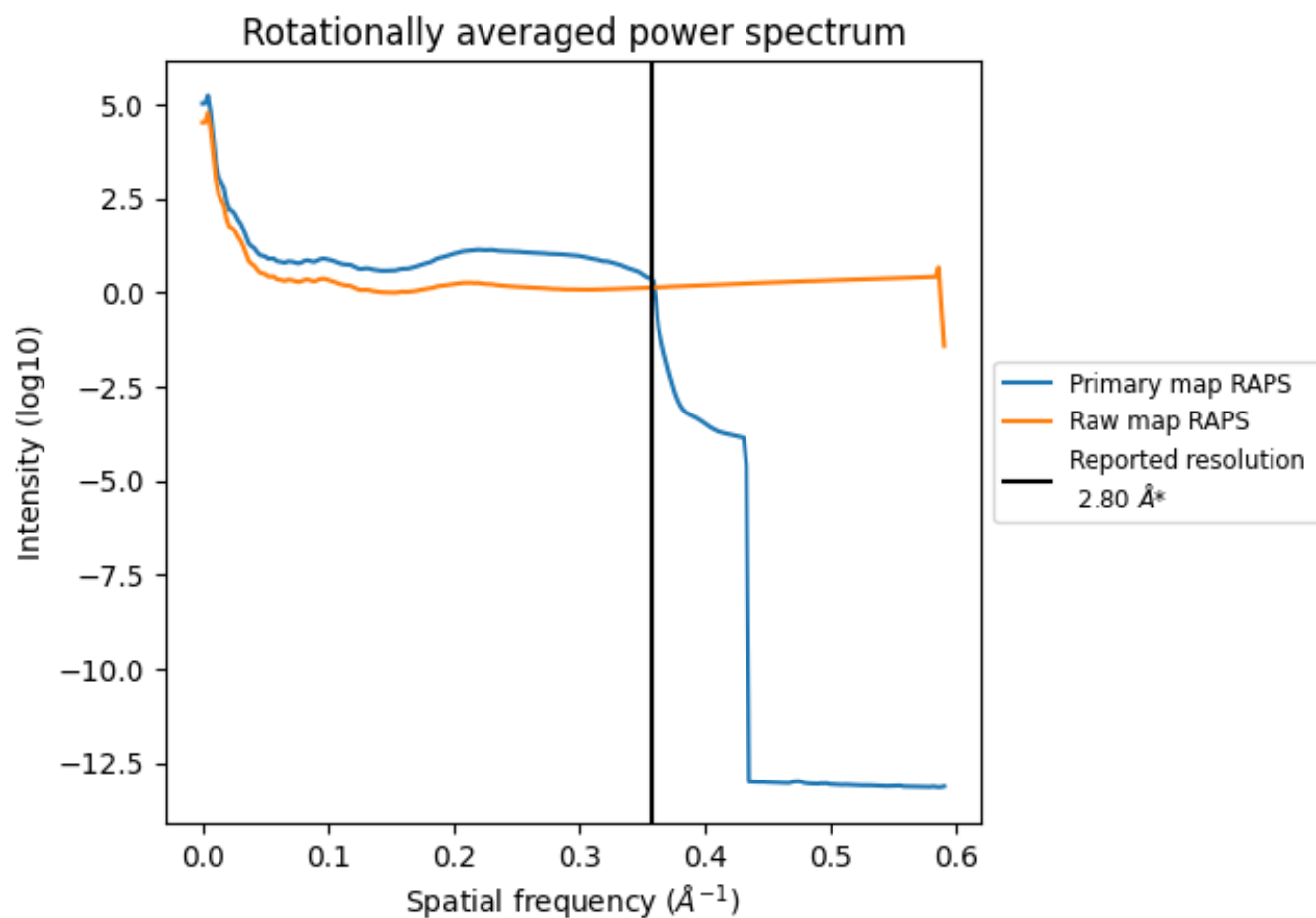
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 274 nm³; this corresponds to an approximate mass of 247 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 ⓘ

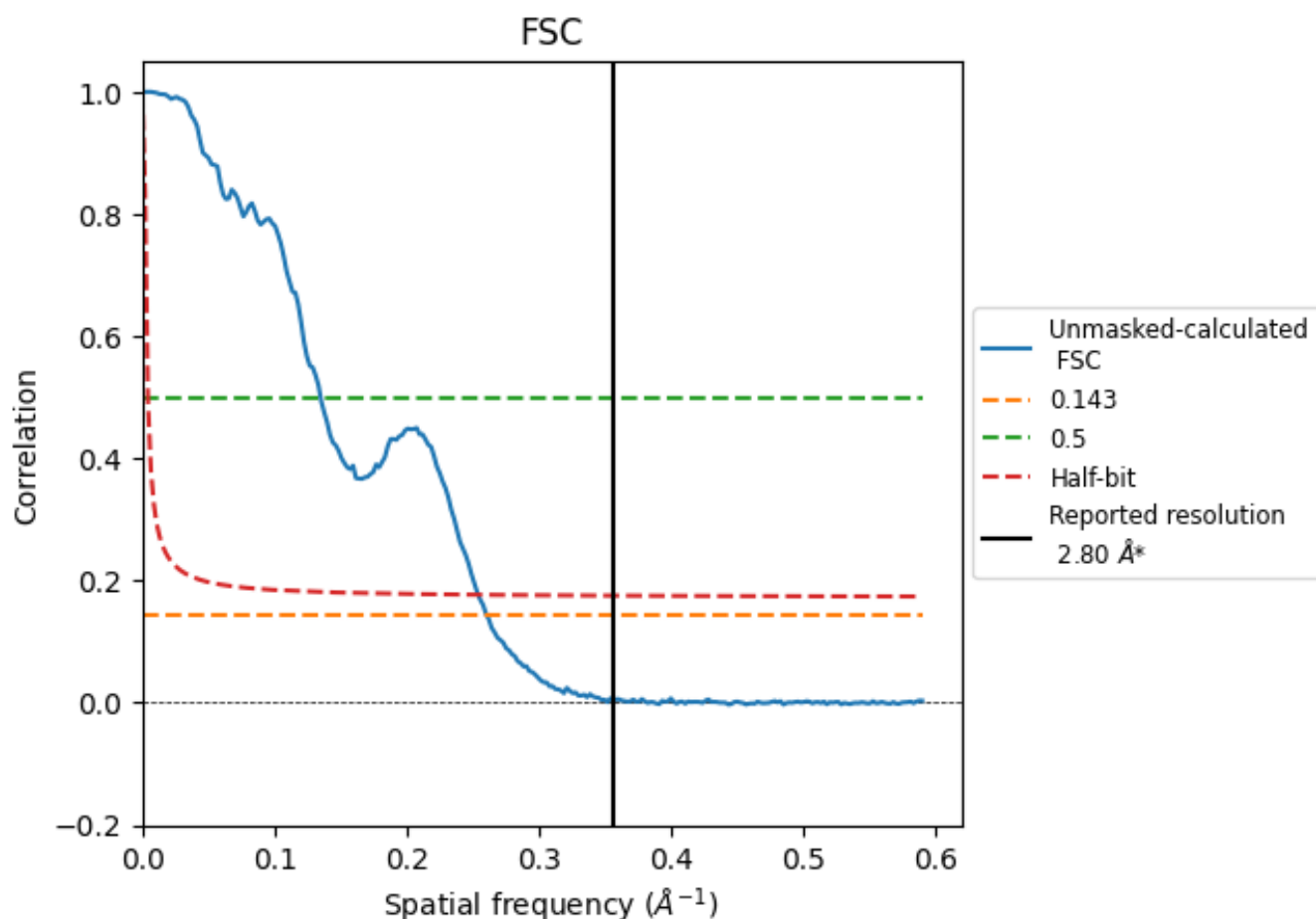


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

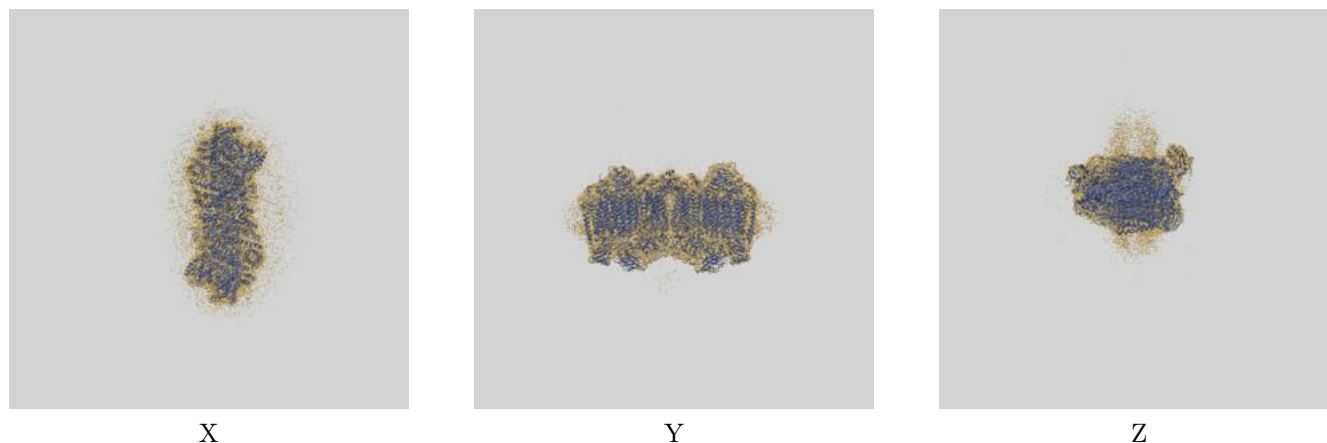
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	7.41	3.93

*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 3.83 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

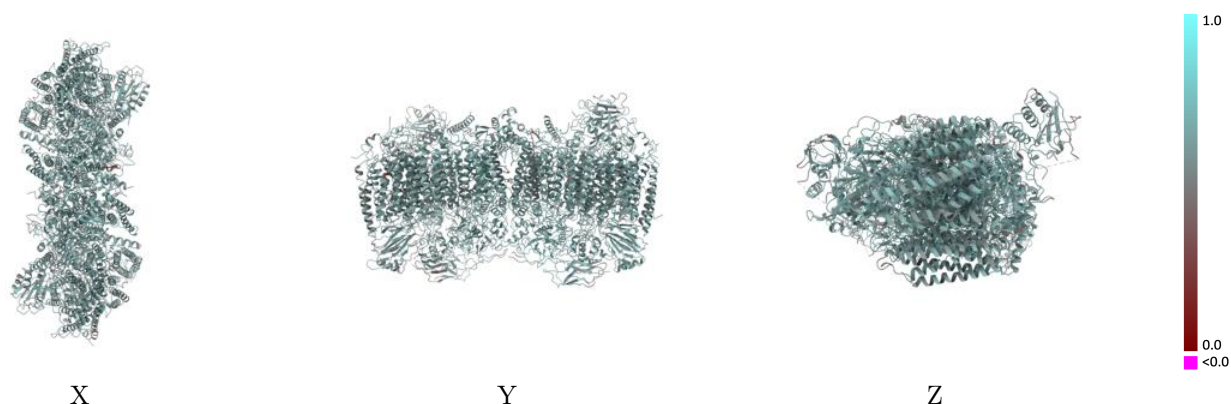
This section contains information regarding the fit between EMDB map EMD-17210 and PDB model 8OVC. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



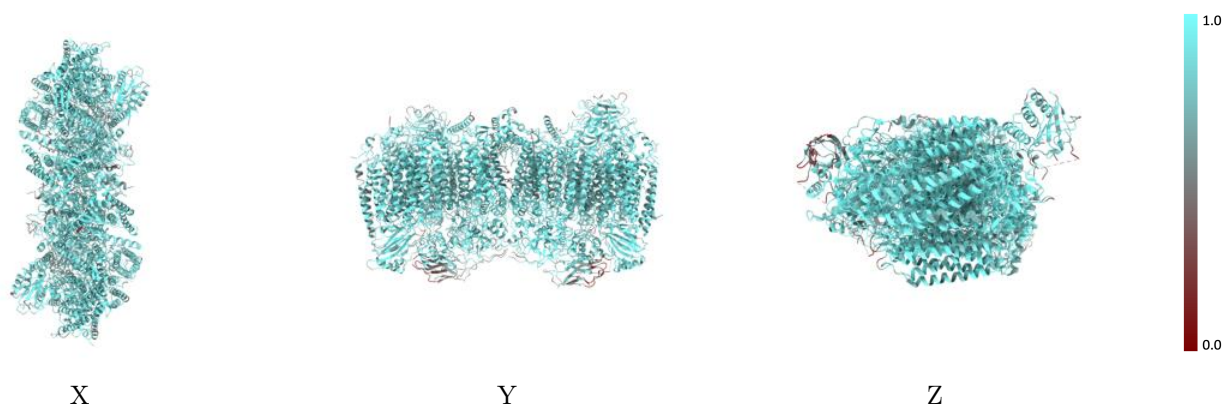
The images above show the 3D surface view of the map at the recommended contour level 0.194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



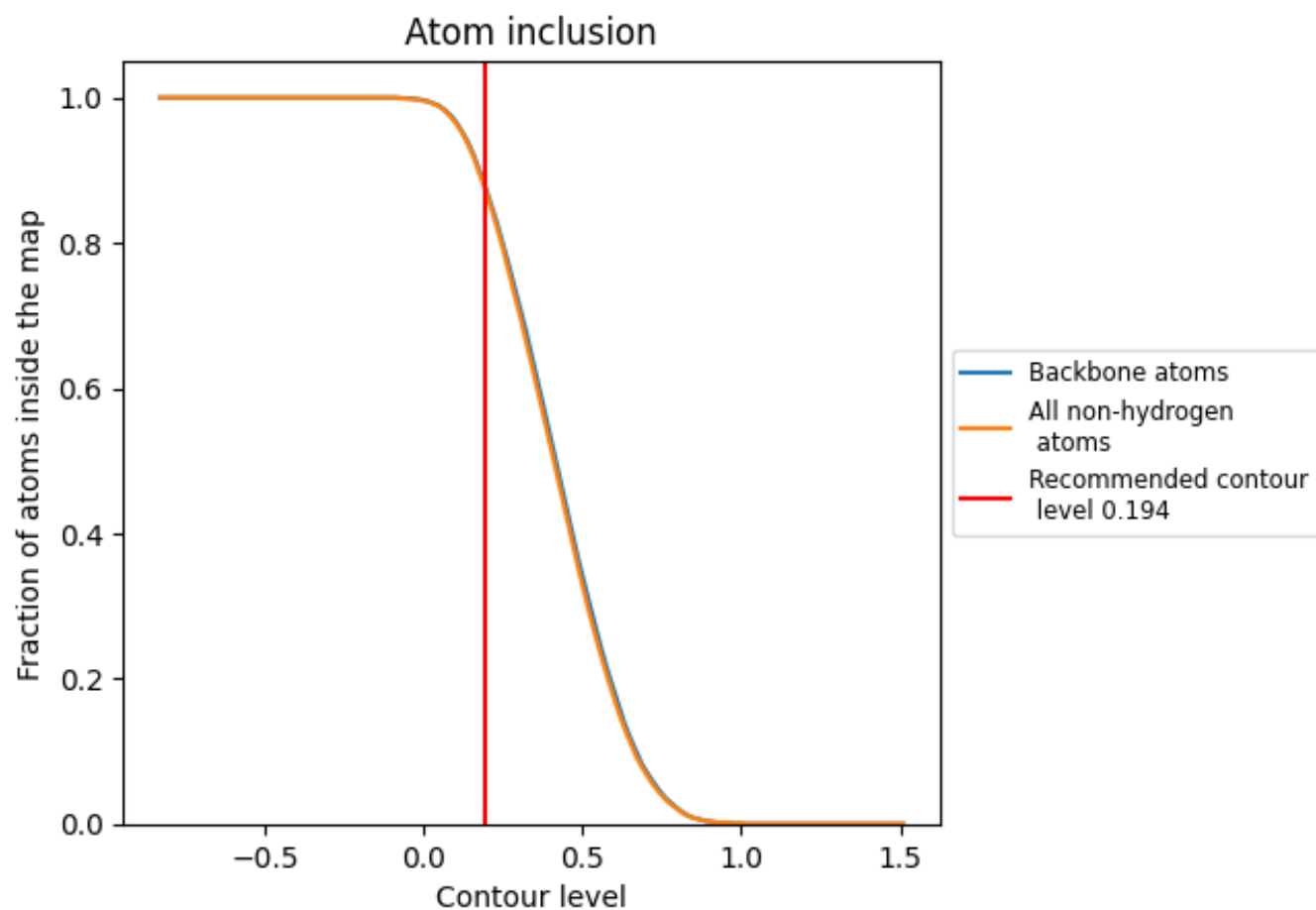
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.194).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5980
C	 0.9220	 0.6240
E	 0.7430	 0.5400
F	 0.6870	 0.4700
G	 0.9030	 0.6170
H	 0.9180	 0.6210
I	 0.8380	 0.5910
J	 0.8960	 0.5980
K	 0.9010	 0.5940
L	 0.9340	 0.6130
M	 0.9030	 0.6120
N	 0.9170	 0.6200
O	 0.9050	 0.6100
P	 0.8560	 0.5920
Q	 0.8200	 0.5570
R	 0.9160	 0.6010
S	 0.8800	 0.5940
T	 0.8790	 0.5820
U	 0.7920	 0.5560
V	 0.7780	 0.5480
W	 0.5380	 0.5340
X	 0.8420	 0.5850
Y	 0.7350	 0.5530
Z	 0.7890	 0.5610
a	 0.8360	 0.5730
b	 0.6010	 0.5630
c	 0.8430	 0.5760
e	 0.7390	 0.4720
f	 0.8290	 0.5120

