



wwPDB EM Validation Summary Report ⓘ

Aug 23, 2026 – 11:57 am BST

PDB ID : 8OVD / pdb_00008ovd
EMDB ID : EMD-17211
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 : 2.30 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:

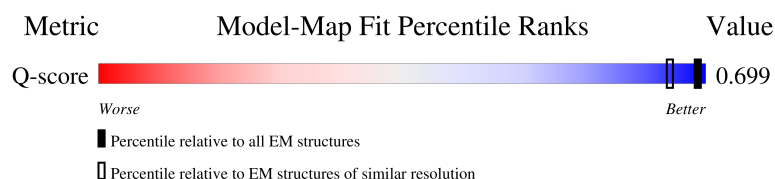
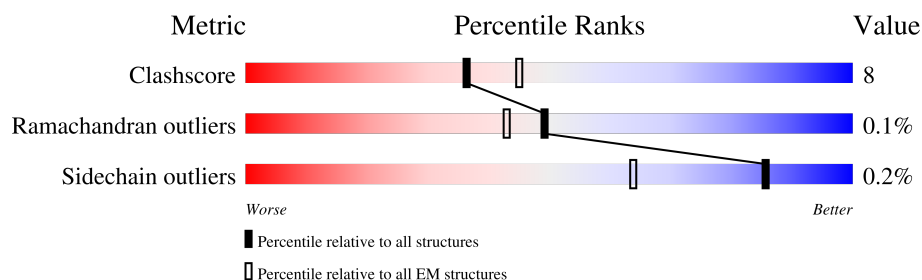
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.30 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	4254 (1.80 - 2.80)

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	

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
13	HEC	C	301	X	-	-	-
13	HEC	C	302	X	-	-	-
13	HEC	O	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	HEC	O	302	X	-	-	-
21	CDL	H	903	-	-	X	-
21	CDL	N	602	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 47246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 20 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 20 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Transmembrane protein.

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

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

- 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	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	299	Total	C	N	O	S	0	0
			2382	1541	396	435	10		
8	X	300	Total	C	N	O	S	0	0
			2391	1547	398	436	10		

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

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

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

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

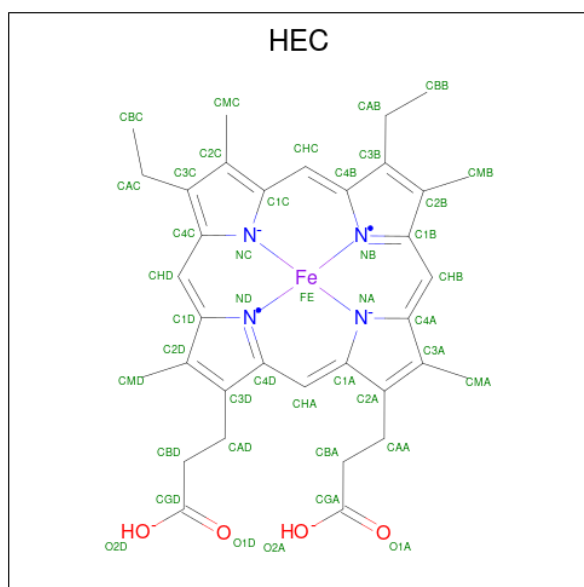
- Molecule 11 is a protein called LpqE protein.

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

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

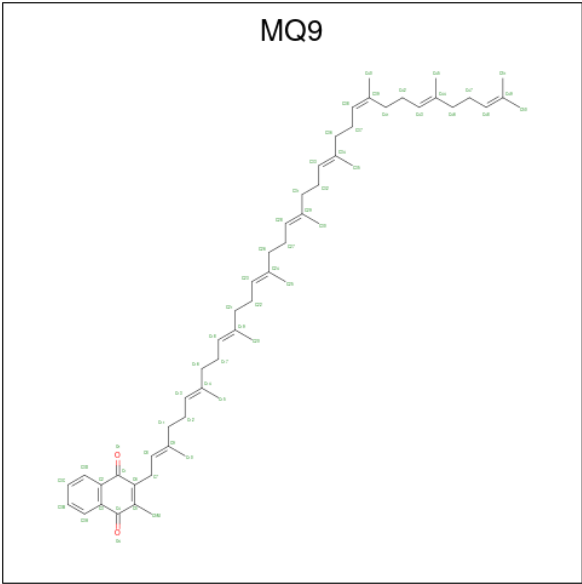
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	25	Total	C	N	O	S	0	0
			168	103	26	38	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 14 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



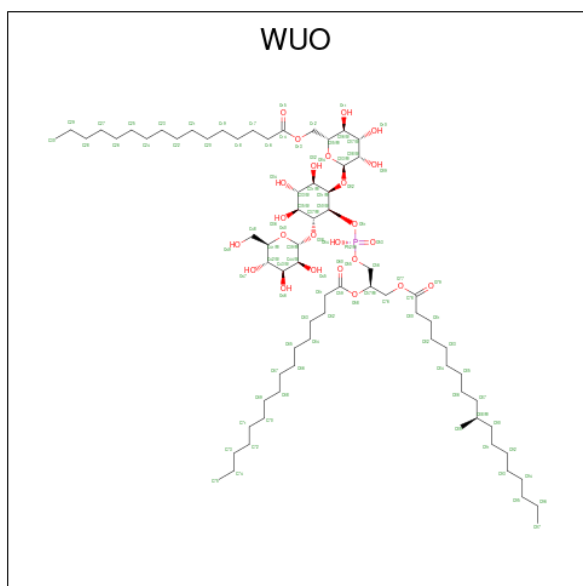
Mol	Chain	Residues	Atoms			AltConf
14	O	1	Total	C	O	0
			58	56	2	
14	M	1	Total	C	O	0
			58	56	2	
14	N	1	Total	C	O	0
			43	41	2	
14	N	1	Total	C	O	0
			58	56	2	
14	N	1	Total	C	O	0
			58	56	2	
14	T	1	Total	C	O	0
			58	56	2	
14	C	1	Total	C	O	0
			58	56	2	
14	G	1	Total	C	O	0
			58	56	2	

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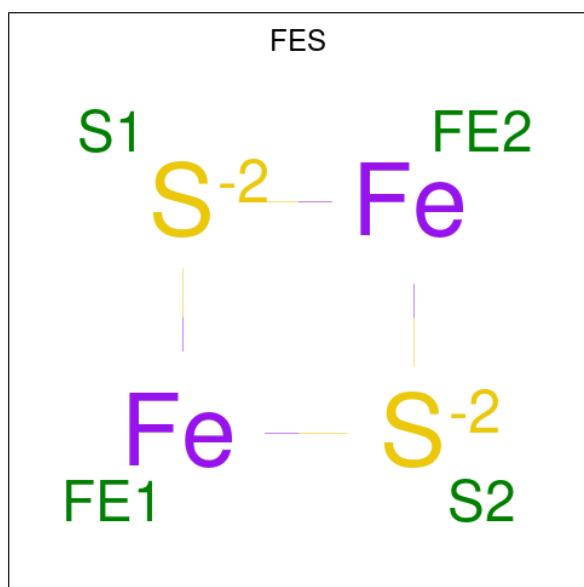
Mol	Chain	Residues	Atoms			AltConf
14	H	1	Total	C	O	0
			43	41	2	
14	H	1	Total	C	O	0
			58	56	2	
14	H	1	Total	C	O	0
			58	56	2	
14	K	1	Total	C	O	0
			58	56	2	

- Molecule 15 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (CCD ID: WUO) (formula: $C_{72}H_{135}O_{24}P$).



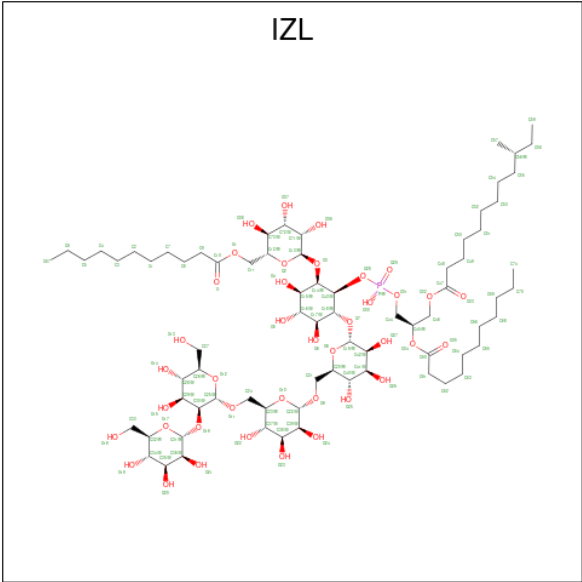
Mol	Chain	Residues	Atoms				AltConf
15	O	1	Total	C	O	P	0
			97	72	24	1	
15	P	1	Total	C	O	P	0
			97	72	24	1	
15	C	1	Total	C	O	P	0
			97	72	24	1	
15	I	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



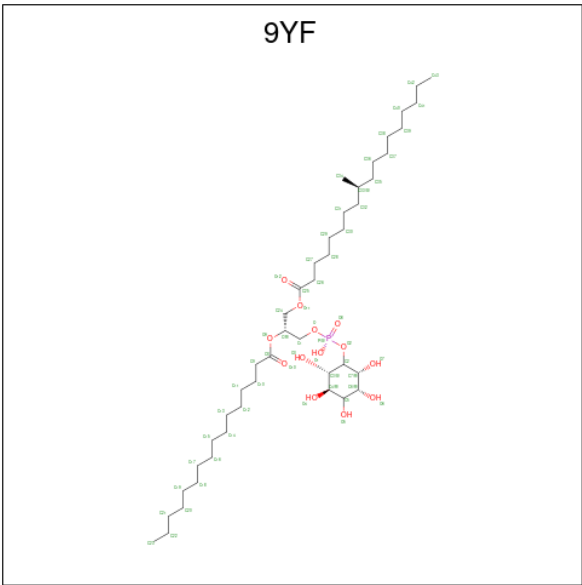
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	Fe	S	0
			4	2	2	
16	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is [(2 {R})-3-[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (CCD ID: IZL) (formula: C₇₄H₁₃₃O₃₉P).



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

- Molecule 18 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).



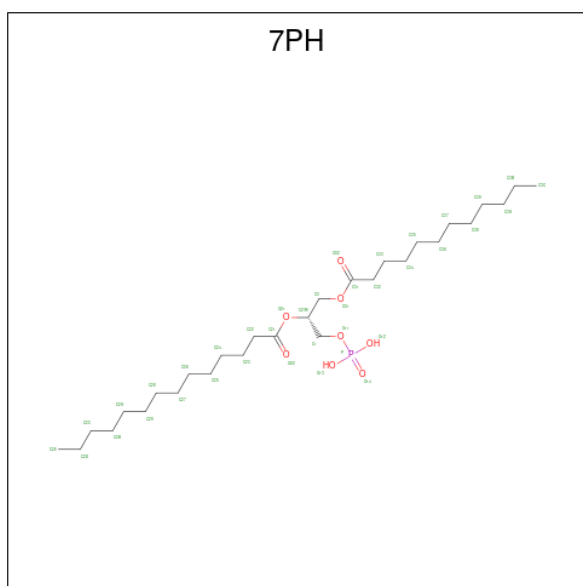
Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			58	44	13	1	

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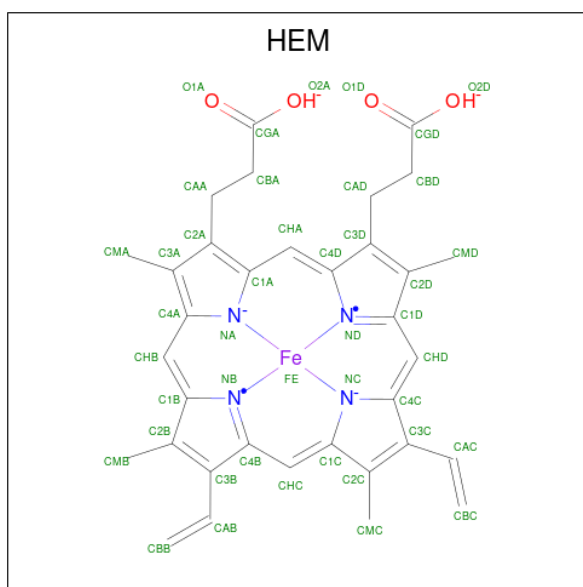
Mol	Chain	Residues	Atoms				AltConf
18	W	1	Total	C	O	P	0
			58	44	13	1	
18	G	1	Total	C	O	P	0
			58	44	13	1	
18	b	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 19 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



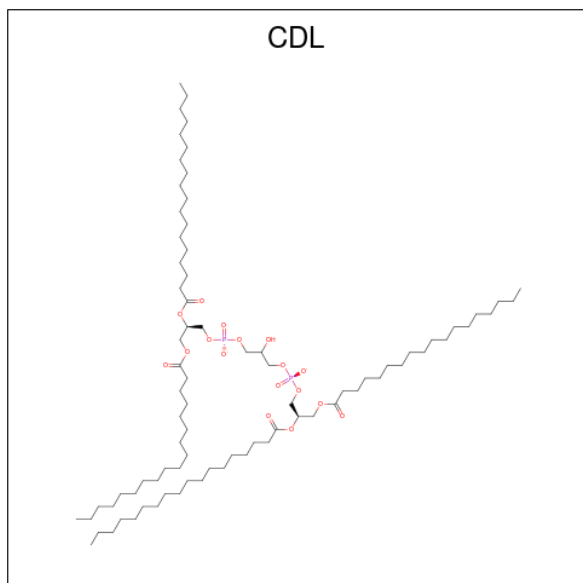
Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			38	29	8	1	
19	N	1	Total	C	O	P	0
			38	29	8	1	
19	S	1	Total	C	O	P	0
			38	29	8	1	
19	G	1	Total	C	O	P	0
			38	29	8	1	
19	H	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



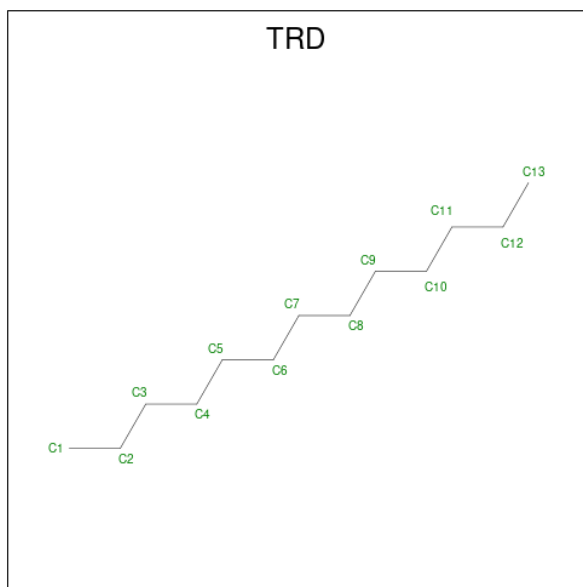
Mol	Chain	Residues	Atoms					AltConf
20	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	H	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	H	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



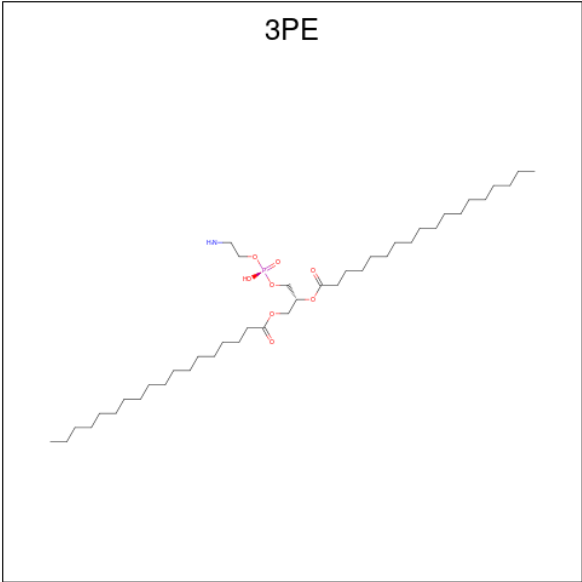
Mol	Chain	Residues	Atoms				AltConf
21	N	1	Total	C	O	P	0
			74	55	17	2	
21	N	1	Total	C	O	P	0
			77	58	17	2	
21	N	1	Total	C	O	P	0
			79	60	17	2	
21	P	1	Total	C	O	P	0
			77	58	17	2	
21	T	1	Total	C	O	P	0
			79	60	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	C	1	Total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

- Molecule 22 is TRIDECANE (CCD ID: TRD) (formula: C₁₃H₂₈).



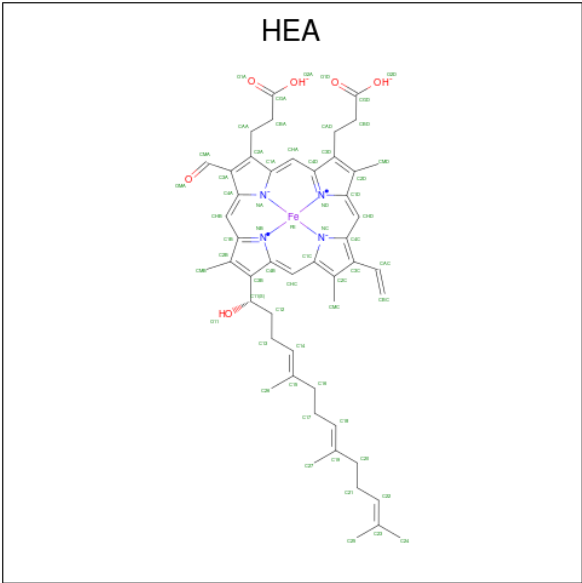
Mol	Chain	Residues	Atoms	AltConf
22	S	1	Total C 13 13	0
22	T	1	Total C 13 13	0
22	R	1	Total C 13 13	0
22	R	1	Total C 13 13	0
22	Q	1	Total C 13 13	0
22	J	1	Total C 13 13	0
22	K	1	Total C 13 13	0
22	L	1	Total C 13 13	0
22	L	1	Total C 13 13	0
22	X	1	Total C 13 13	0

- Molecule 23 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



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

- Molecule 24 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

- Molecule 25 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

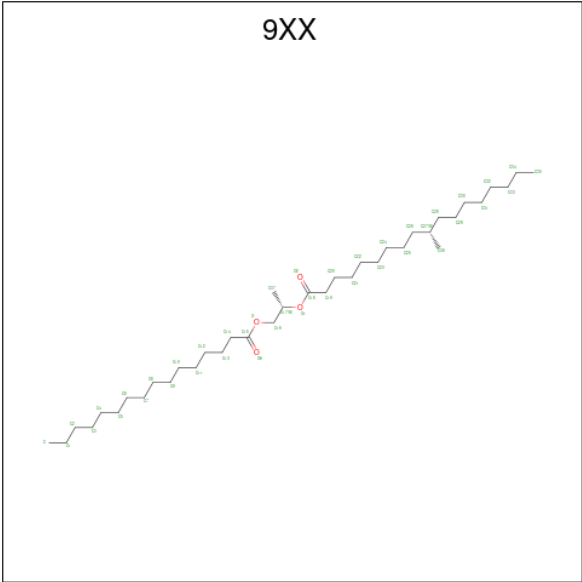
- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

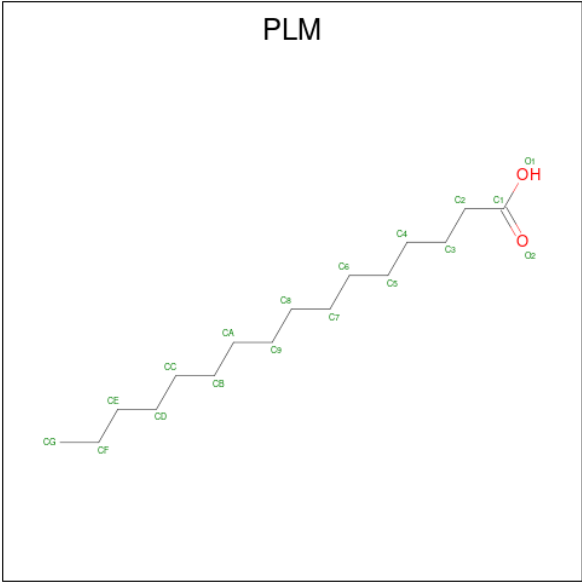
Mol	Chain	Residues	Atoms		AltConf
27	R	1	Total	Ca	0
			1	1	
27	L	1	Total	Ca	0
			1	1	

- Molecule 28 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C₃₈H₇₄O₄).



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

- Molecule 29 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
29	W	1	Total	C	O	0
			11	10	1	
29	Y	1	Total	C	O	0
			11	10	1	
29	b	1	Total	C	O	0
			11	10	1	
29	c	1	Total	C	O	0
			11	10	1	

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	O	43	Total	O	0
			43	43	
30	M	51	Total	O	0
			51	51	
30	N	67	Total	O	0
			67	67	
30	P	2	Total	O	0
			2	2	
30	S	6	Total	O	0
			6	6	
30	T	11	Total	O	0
			11	11	
30	R	68	Total	O	0
			68	68	
30	Q	30	Total	O	0
			30	30	
30	W	4	Total	O	0
			4	4	
30	C	56	Total	O	0
			56	56	
30	G	60	Total	O	0
			60	60	
30	H	64	Total	O	0
			64	64	
30	I	3	Total	O	0
			3	3	
30	J	8	Total	O	0
			8	8	
30	K	14	Total	O	0
			14	14	
30	L	78	Total	O	0
			78	78	

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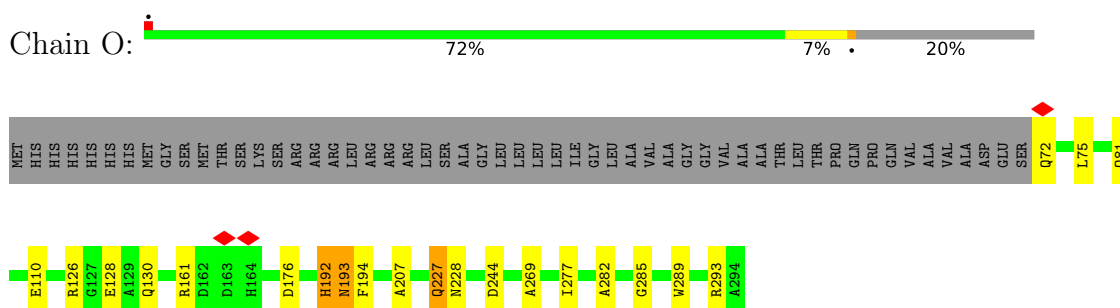
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Mol	Chain	Residues	Atoms		AltConf
30	X	35	Total 35	O 35	0
30	Z	2	Total 2	O 2	0
30	a	1	Total 1	O 1	0
30	b	10	Total 10	O 10	0
30	c	1	Total 1	O 1	0

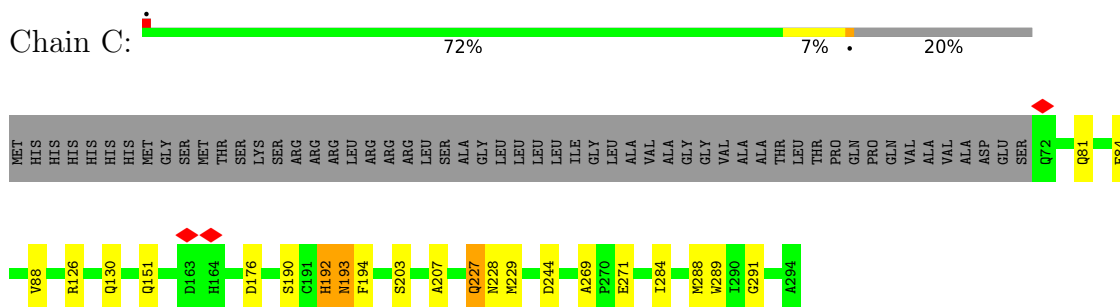
3 Residue-property plots [i](#)

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.

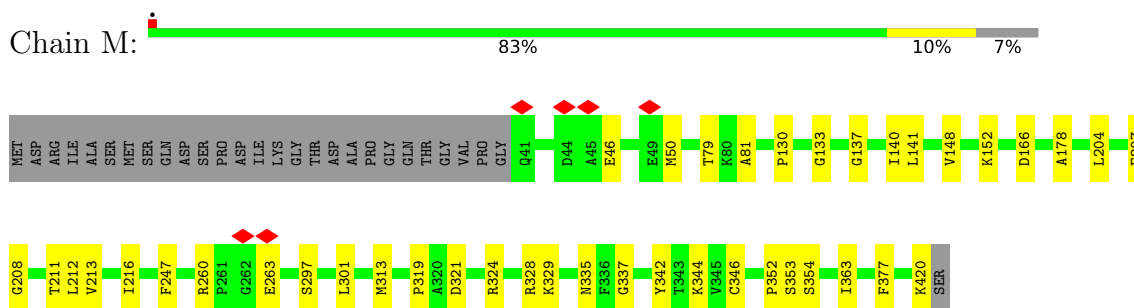
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit



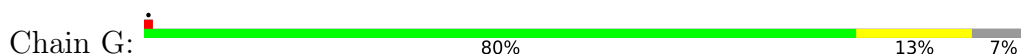
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit

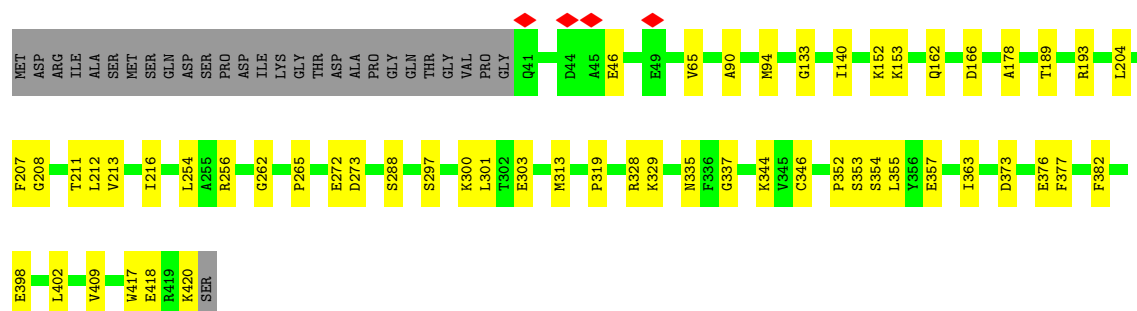


- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

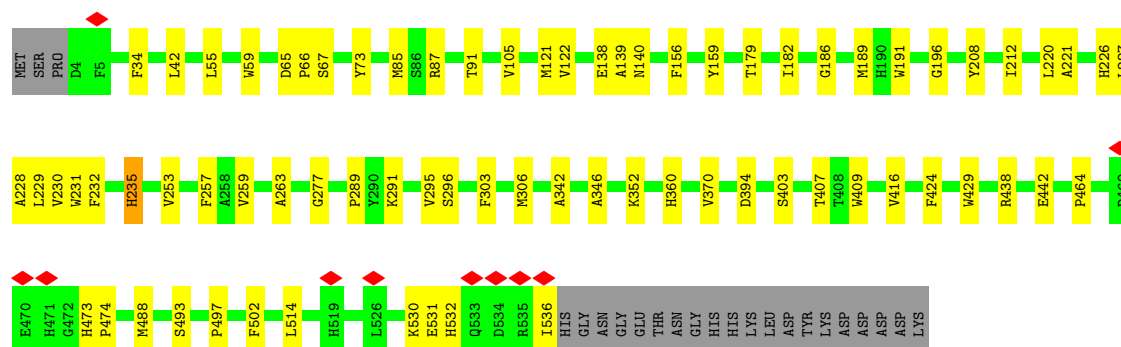
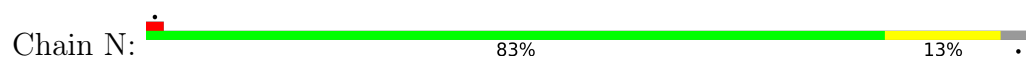


- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

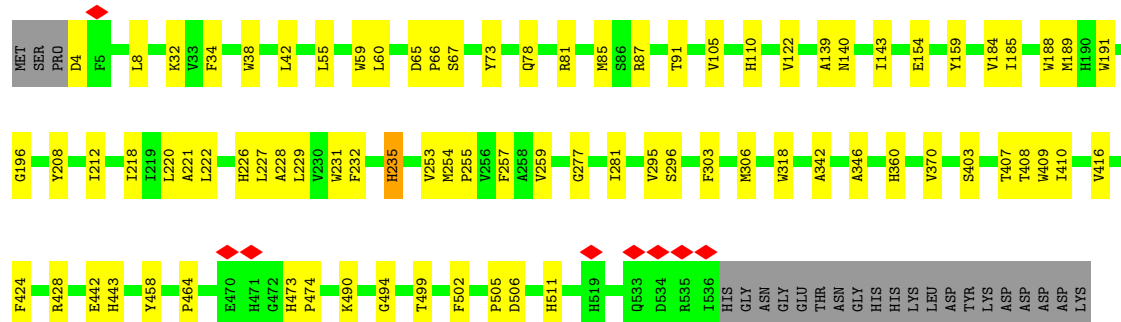
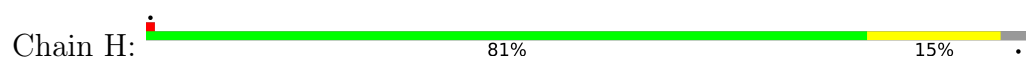




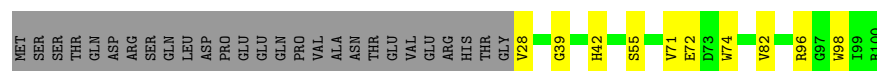
- Molecule 3: Cytochrome bc1 complex cytochrome b subunit



- Molecule 3: Cytochrome bc1 complex cytochrome b subunit

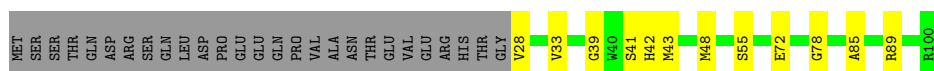


- Molecule 4: Transmembrane protein

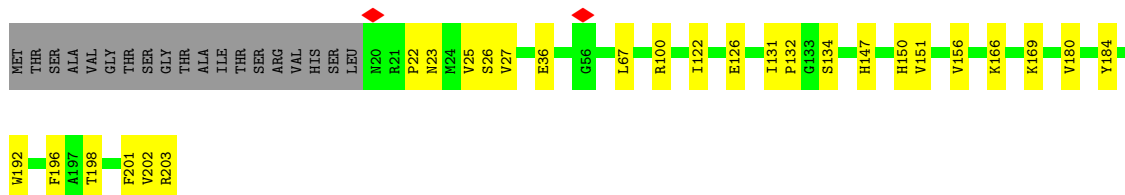
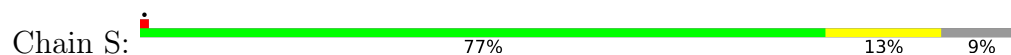


- Molecule 4: Transmembrane protein

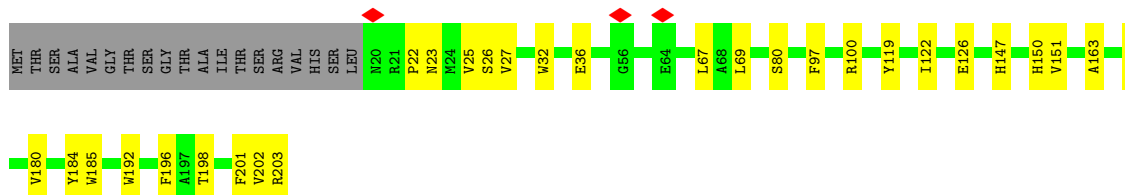
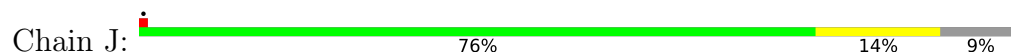




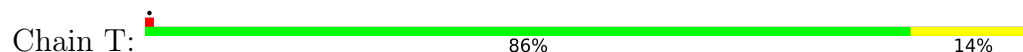
- Molecule 5: Probable cytochrome c oxidase subunit 3



- Molecule 5: Probable cytochrome c oxidase subunit 3



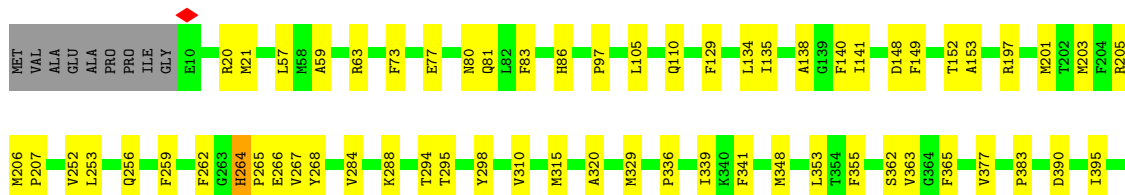
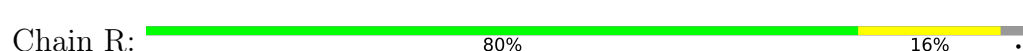
- Molecule 6: Cytochrome c oxidase polypeptide 4

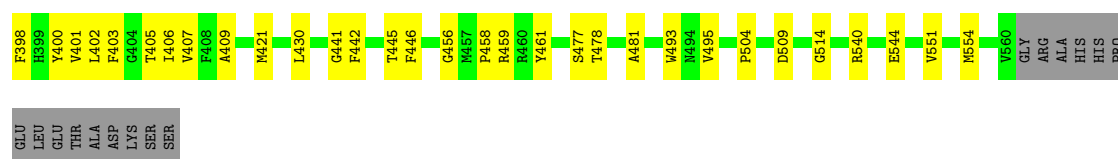


- Molecule 6: Cytochrome c oxidase polypeptide 4



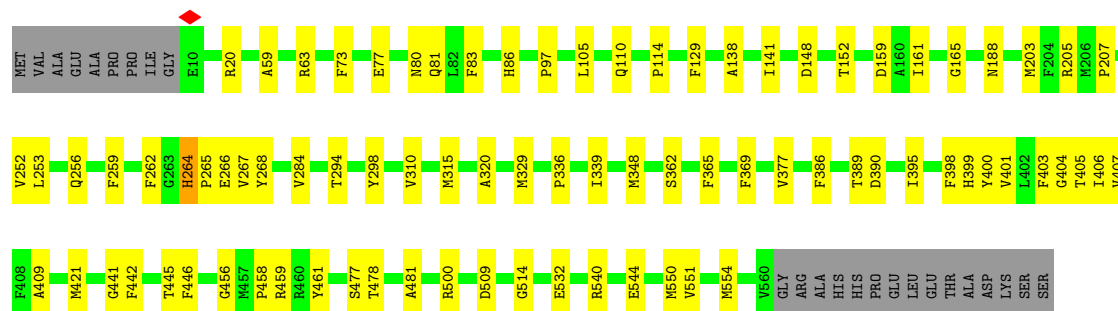
- Molecule 7: Cytochrome c oxidase subunit 1





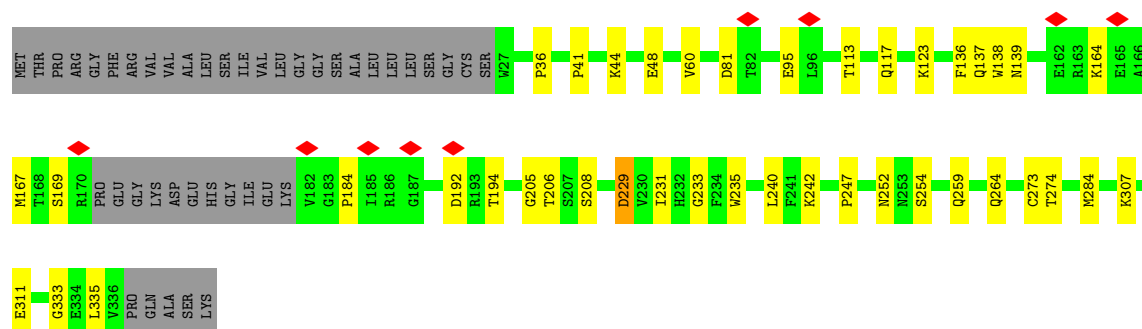
• Molecule 7: Cytochrome c oxidase subunit 1

Chain L: 81% 14% .



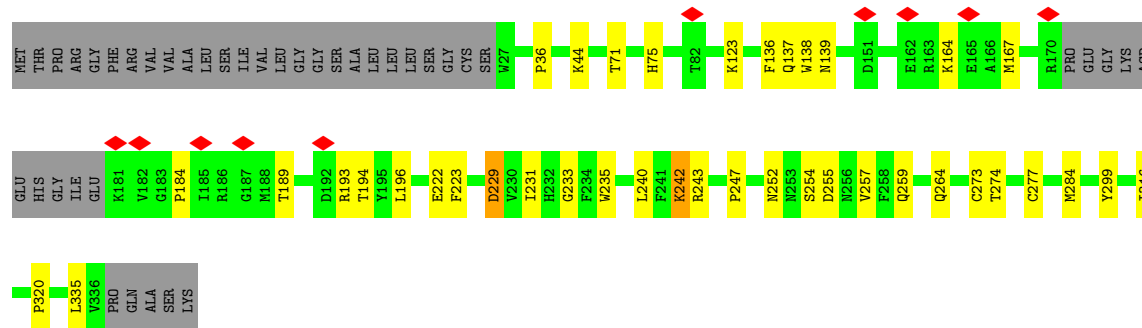
• Molecule 8: cytochrome-c oxidase

Chain Q: 76% 12% 12%

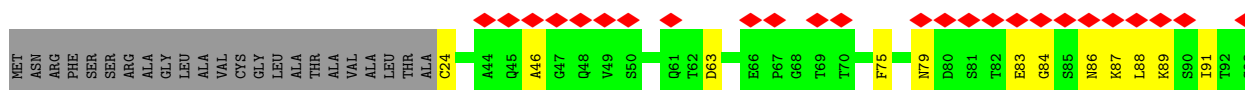
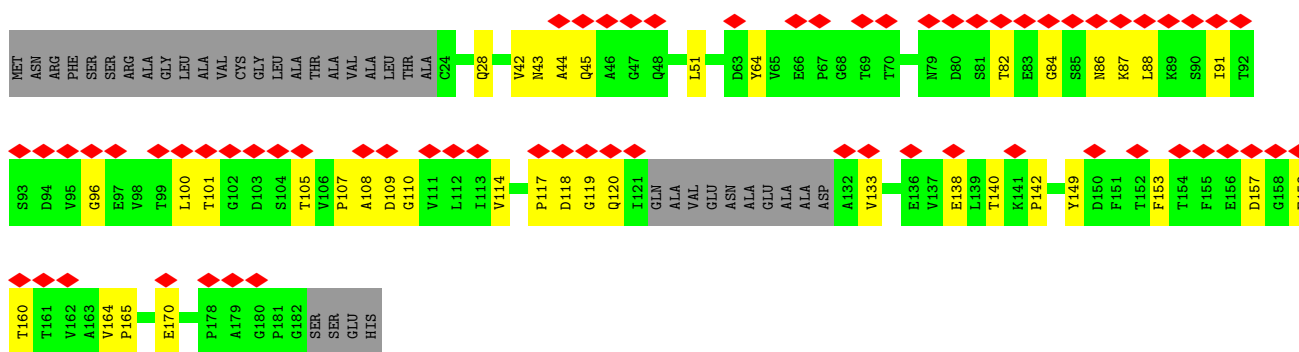
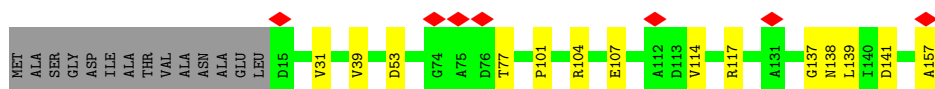
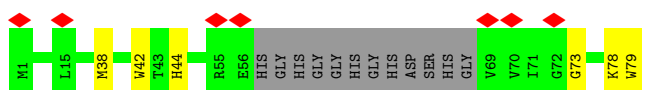


• Molecule 8: cytochrome-c oxidase

Chain X: 76% 11% 12%



• Molecule 9: Cytochrome c oxidase subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.515	Depositor
Minimum map value	-1.210	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	447.12, 447.12, 447.12	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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: HEC, HEM, CU, 3PE, 7PH, WUO, FES, MG, IZL, PLM, CDL, MQ9, CA, 9YF, HEA, TRD, 9XX

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	0.45	1/1660 (0.1%)	0.61	3/2250 (0.1%)
1	O	0.46	2/1660 (0.1%)	0.61	3/2250 (0.1%)
2	G	0.39	2/3046 (0.1%)	0.48	0/4129
2	M	0.34	0/3046	0.44	0/4129
3	H	0.37	0/4299	0.49	0/5862
3	N	0.37	0/4299	0.51	0/5862
4	I	0.29	0/606	0.38	0/825
4	P	0.28	0/606	0.37	0/825
5	J	0.30	0/1488	0.43	0/2032
5	S	0.30	0/1488	0.42	0/2032
6	K	0.29	0/1112	0.40	0/1524
6	T	0.29	0/1112	0.43	0/1524
7	L	0.45	3/4529 (0.1%)	0.64	7/6187 (0.1%)
7	R	0.45	3/4529 (0.1%)	0.63	7/6187 (0.1%)
8	Q	0.36	0/2447	0.46	0/3330
8	X	0.37	0/2456	0.48	0/3341
9	U	0.24	0/515	0.34	0/704
9	Z	0.25	0/523	0.37	0/714
10	V	0.26	0/1042	0.40	0/1423
10	a	0.27	0/1042	0.45	0/1423
11	W	0.24	0/1100	0.45	0/1508
11	b	0.22	0/1100	0.47	0/1508
12	Y	0.34	0/175	0.47	0/244
12	c	0.30	0/175	0.44	0/244
All	All	0.37	11/44055 (0.0%)	0.51	20/60057 (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
7	L	0	1
7	R	0	1
All	All	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	268	TYR	C-N	8.88	1.44	1.34
7	L	268	TYR	C-N	8.54	1.44	1.34
2	G	46	GLU	C-N	-8.36	1.23	1.33
7	R	267	VAL	CA-CB	-6.63	1.45	1.54
7	L	267	VAL	CA-CB	-6.63	1.45	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	262	PHE	CA-C-N	11.21	132.33	120.00
7	L	262	PHE	C-N-CA	11.21	132.33	120.00
7	R	262	PHE	CA-C-N	10.66	131.73	120.00
7	R	262	PHE	C-N-CA	10.66	131.73	120.00
1	C	192	HIS	CA-C-O	-7.93	109.68	119.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	L	264	HIS	Sidechain
7	R	264	HIS	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1623	0	1560	26	0
1	O	1623	0	1560	21	0
2	G	2967	0	2976	51	0
2	M	2967	0	2976	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	4167	0	4192	85	0
3	N	4167	0	4192	72	0
4	I	586	0	578	11	0
4	P	586	0	578	10	0
5	J	1441	0	1439	22	0
5	S	1441	0	1439	24	0
6	K	1077	0	1058	11	0
6	T	1077	0	1058	17	0
7	L	4369	0	4345	63	0
7	R	4369	0	4345	69	0
8	Q	2382	0	2335	33	0
8	X	2391	0	2348	39	0
9	U	499	0	504	9	0
9	Z	507	0	516	6	0
10	V	1024	0	1035	13	0
10	a	1024	0	1035	17	0
11	W	1083	0	1055	27	0
11	b	1083	0	1055	26	0
12	Y	168	0	151	3	0
12	c	168	0	151	2	0
13	C	86	0	60	3	0
13	O	86	0	60	2	0
14	C	58	0	80	1	0
14	G	58	0	77	17	0
14	H	159	0	211	17	0
14	K	58	0	80	9	0
14	M	58	0	77	16	0
14	N	159	0	211	24	0
14	O	58	0	80	3	0
14	T	58	0	80	12	0
15	C	97	0	0	4	0
15	I	97	0	0	2	0
15	O	97	0	0	7	0
15	P	97	0	0	4	0
16	G	4	0	0	0	0
16	M	4	0	0	0	0
17	G	114	0	0	2	0
17	M	114	0	0	0	0
18	G	58	0	0	4	0
18	M	58	0	0	3	0
18	W	58	0	0	1	0
18	b	58	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	G	38	0	55	5	0
19	H	38	0	55	10	0
19	M	38	0	55	5	0
19	N	38	0	55	9	0
19	S	38	0	55	2	0
20	H	86	0	60	4	0
20	N	86	0	60	0	0
21	C	79	0	105	10	0
21	H	230	0	295	37	0
21	I	154	0	196	9	0
21	J	79	0	105	7	0
21	L	79	0	105	8	0
21	N	230	0	295	32	0
21	P	77	0	98	6	0
21	R	154	0	196	6	0
21	T	79	0	105	8	0
22	J	13	0	28	4	0
22	K	13	0	28	0	0
22	L	26	0	56	1	0
22	Q	13	0	28	1	0
22	R	26	0	56	1	0
22	S	13	0	28	4	0
22	T	13	0	28	0	0
22	X	13	0	28	1	0
23	J	32	0	38	1	0
23	S	32	0	38	4	0
24	L	120	0	108	5	0
24	R	120	0	108	12	0
25	L	1	0	0	0	0
25	Q	2	0	0	0	0
25	R	1	0	0	0	0
25	X	2	0	0	0	0
26	L	1	0	0	0	0
26	R	1	0	0	0	0
27	L	1	0	0	0	0
27	R	1	0	0	0	0
28	W	42	0	0	0	0
28	Y	32	0	0	0	0
28	b	32	0	0	0	0
28	c	32	0	0	0	0
29	W	11	0	16	1	0
29	Y	11	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	b	11	0	16	0	0
29	c	11	0	16	1	0
30	C	56	0	0	2	0
30	G	60	0	0	0	0
30	H	64	0	0	0	0
30	I	3	0	0	0	0
30	J	8	0	0	0	0
30	K	14	0	0	0	0
30	L	78	0	0	1	0
30	M	51	0	0	0	0
30	N	67	0	0	0	0
30	O	43	0	0	3	0
30	P	2	0	0	0	0
30	Q	30	0	0	0	0
30	R	68	0	0	0	0
30	S	6	0	0	0	0
30	T	11	0	0	1	0
30	W	4	0	0	0	0
30	X	35	0	0	1	0
30	Z	2	0	0	0	0
30	a	1	0	0	0	0
30	b	10	0	0	0	0
30	c	1	0	0	0	0
All	All	47246	0	46028	713	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 8.

The worst 5 of 713 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)
14:M:505:MQ9:H23	3:H:55:LEU:HD23	1.31	1.12
6:K:100:SER:HB3	14:K:1301:MQ9:H252	1.33	1.09
3:N:55:LEU:HD23	14:G:901:MQ9:H23	1.29	1.08
15:O:304:WUO:C95	14:T:1301:MQ9:H202	1.85	1.06
5:J:198:THR:HG22	22:J:502:TRD:H101	1.38	1.05

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%)	211 (96%)	9 (4%)	1 (0%)	24	31
1	O	221/278 (80%)	208 (94%)	12 (5%)	1 (0%)	24	31
2	G	378/408 (93%)	364 (96%)	14 (4%)	0	100	100
2	M	378/408 (93%)	364 (96%)	14 (4%)	0	100	100
3	H	531/556 (96%)	518 (98%)	12 (2%)	1 (0%)	43	55
3	N	531/556 (96%)	518 (98%)	12 (2%)	1 (0%)	43	55
4	I	71/100 (71%)	68 (96%)	3 (4%)	0	100	100
4	P	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
5	J	182/203 (90%)	179 (98%)	3 (2%)	0	100	100
5	S	182/203 (90%)	180 (99%)	2 (1%)	0	100	100
6	K	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
6	T	137/139 (99%)	134 (98%)	3 (2%)	0	100	100
7	L	549/575 (96%)	543 (99%)	6 (1%)	0	100	100
7	R	549/575 (96%)	542 (99%)	7 (1%)	0	100	100
8	Q	295/341 (86%)	287 (97%)	8 (3%)	0	100	100
8	X	296/341 (87%)	286 (97%)	10 (3%)	0	100	100
9	U	62/79 (78%)	61 (98%)	1 (2%)	0	100	100
9	Z	63/79 (80%)	62 (98%)	1 (2%)	0	100	100
10	V	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
10	a	141/157 (90%)	134 (95%)	7 (5%)	0	100	100
11	W	145/186 (78%)	129 (89%)	16 (11%)	0	100	100
11	b	145/186 (78%)	129 (89%)	16 (11%)	0	100	100
12	Y	23/236 (10%)	20 (87%)	3 (13%)	0	100	100
12	c	23/236 (10%)	20 (87%)	3 (13%)	0	100	100
All	All	5472/6516 (84%)	5301 (97%)	167 (3%)	4 (0%)	49	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	235	HIS
1	O	227	GLN
1	C	227	GLN
3	H	235	HIS

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%)	162 (99%)	1 (1%)	78	89
1	O	163/206 (79%)	162 (99%)	1 (1%)	78	89
2	G	311/333 (93%)	310 (100%)	1 (0%)	86	93
2	M	311/333 (93%)	310 (100%)	1 (0%)	86	93
3	H	428/448 (96%)	428 (100%)	0	100	100
3	N	428/448 (96%)	428 (100%)	0	100	100
4	I	58/83 (70%)	58 (100%)	0	100	100
4	P	58/83 (70%)	58 (100%)	0	100	100
5	J	146/161 (91%)	146 (100%)	0	100	100
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%)	452 (100%)	1 (0%)	87	94
7	R	453/471 (96%)	452 (100%)	1 (0%)	87	94
8	Q	255/288 (88%)	254 (100%)	1 (0%)	84	92
8	X	256/288 (89%)	254 (99%)	2 (1%)	73	86
9	U	51/59 (86%)	51 (100%)	0	100	100
9	Z	52/59 (88%)	52 (100%)	0	100	100
10	V	105/114 (92%)	105 (100%)	0	100	100
10	a	105/114 (92%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	W	121/146 (83%)	121 (100%)	0	100	100
11	b	121/146 (83%)	121 (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	4436/5164 (86%)	4427 (100%)	9 (0%)	85	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	X	229	ASP
8	X	242	LYS
8	Q	229	ASP
1	C	193	ASN
2	G	420	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	20	ASN
8	X	226	ASN
5	J	174	GLN
7	L	249	ASN
8	X	302	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 86 ligands modelled in this entry, 10 are monoatomic - leaving 76 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$
14	MQ9	M	505	14	59,59,59	0.34	0	72,75,75	0.30	0
22	TRD	S	502	-	12,12,12	0.21	0	11,11,11	0.25	0
24	HEA	L	603	7	66,67,67	2.81	28 (42%)	78,103,103	2.14	28 (35%)
15	WUO	O	304	-	99,99,99	1.37	5 (5%)	123,125,125	1.24	16 (13%)
18	9YF	G	904	-	58,58,58	1.39	5 (8%)	69,71,71	1.07	3 (4%)
23	3PE	J	503	-	31,31,50	0.33	0	34,36,55	0.38	0
13	HEC	C	302	1	50,50,50	1.43	4 (8%)	68,82,82	1.41	11 (16%)
14	MQ9	O	303	-	59,59,59	0.36	0	72,75,75	0.32	0
14	MQ9	H	906	-	44,44,59	0.38	0	54,57,75	0.36	0
16	FES	M	501	2	0,4,4	-	-	-	-	-
22	TRD	K	1302	-	12,12,12	0.36	0	11,11,11	0.36	0
15	WUO	I	303	-	99,99,99	1.81	22 (22%)	123,125,125	1.37	16 (13%)
29	PLM	W	203	11	10,10,17	0.93	0	9,9,17	0.59	0
22	TRD	L	608	-	12,12,12	0.22	0	11,11,11	0.47	0
21	CDL	H	903	-	73,73,99	0.30	0	79,85,111	0.36	0
21	CDL	C	305	-	78,78,99	0.29	0	84,90,111	0.34	0
14	MQ9	N	608	-	59,59,59	0.34	0	72,75,75	0.31	0
15	WUO	P	302	-	99,99,99	1.38	5 (5%)	123,125,125	1.24	15 (12%)
19	7PH	S	501	-	37,37,37	0.30	0	41,42,42	0.35	0
15	WUO	C	304	-	99,99,99	1.36	5 (5%)	123,125,125	1.25	17 (13%)
20	HEM	H	908	3	50,50,50	2.63	19 (38%)	66,82,82	2.25	20 (30%)
22	TRD	Q	403	-	12,12,12	0.09	0	11,11,11	0.05	0
13	HEC	C	301	1	50,50,50	1.38	6 (12%)	68,82,82	1.17	6 (8%)
29	PLM	c	301	12	10,10,17	0.80	0	9,9,17	0.65	0
19	7PH	H	901	-	37,37,37	0.30	0	41,42,42	0.34	0
21	CDL	J	501	-	78,78,99	0.99	7 (8%)	84,90,111	1.13	5 (5%)
14	MQ9	C	303	-	59,59,59	0.36	0	72,75,75	0.32	0
28	9XX	Y	302	-	31,31,41	1.10	4 (12%)	34,34,44	1.33	2 (5%)
29	PLM	Y	301	12	10,10,17	0.70	0	9,9,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	MQ9	K	1301	-	59,59,59	0.62	0	72,75,75	0.79	1 (1%)
20	HEM	N	607	3	50,50,50	2.63	19 (38%)	66,82,82	2.25	21 (31%)
21	CDL	H	905	-	78,78,99	0.29	0	84,90,111	0.34	0
13	HEC	O	301	1	50,50,50	1.38	6 (12%)	68,82,82	1.17	6 (8%)
21	CDL	T	1302	-	78,78,99	0.29	0	84,90,111	0.34	0
14	MQ9	N	606	14	59,59,59	0.34	0	72,75,75	0.31	0
28	9XX	c	302	-	31,31,41	1.11	4 (12%)	34,34,44	1.34	2 (5%)
22	TRD	X	403	-	12,12,12	0.09	0	11,11,11	0.05	0
19	7PH	N	609	-	37,37,37	0.30	0	41,42,42	0.34	0
21	CDL	R	605	-	76,76,99	0.29	0	82,88,111	0.34	0
21	CDL	N	603	-	76,76,99	0.29	0	82,88,111	0.34	0
16	FES	G	902	2	0,4,4	-	-	-	-	-
14	MQ9	G	901	14	59,59,59	0.35	0	72,75,75	0.31	0
17	IZL	G	903	-	119,119,119	1.79	22 (18%)	161,163,163	1.18	15 (9%)
18	9YF	W	201	-	58,58,58	1.40	5 (8%)	69,71,71	1.07	3 (4%)
18	9YF	M	503	-	58,58,58	1.40	5 (8%)	69,71,71	1.06	2 (2%)
14	MQ9	H	909	-	59,59,59	0.35	0	72,75,75	0.31	0
19	7PH	M	504	-	37,37,37	0.30	0	41,42,42	0.33	0
19	7PH	G	905	-	37,37,37	0.30	0	41,42,42	0.34	0
22	TRD	R	609	-	12,12,12	0.21	0	11,11,11	0.47	0
29	PLM	b	202	11	10,10,17	0.78	0	9,9,17	0.56	0
23	3PE	S	503	-	31,31,50	0.33	0	34,36,55	0.38	0
21	CDL	I	301	-	76,76,99	0.29	0	82,88,111	0.35	0
24	HEA	R	603	7	66,67,67	2.86	28 (42%)	78,103,103	2.40	33 (42%)
17	IZL	M	502	-	119,119,119	1.75	31 (26%)	161,163,163	1.31	17 (10%)
18	9YF	b	201	-	58,58,58	1.40	5 (8%)	69,71,71	1.07	3 (4%)
24	HEA	L	602	7	66,67,67	2.37	23 (34%)	78,103,103	2.46	29 (37%)
21	CDL	N	602	-	73,73,99	0.30	0	79,85,111	0.36	0
20	HEM	N	601	3	50,50,50	2.48	19 (38%)	66,82,82	2.33	16 (24%)
28	9XX	W	202	-	41,41,41	0.97	4 (9%)	44,44,44	1.39	4 (9%)
22	TRD	L	607	-	12,12,12	0.09	0	11,11,11	0.06	0
14	MQ9	H	907	14	59,59,59	0.35	0	72,75,75	0.32	0
21	CDL	P	301	-	76,76,99	0.29	0	82,88,111	0.35	0
21	CDL	L	601	-	78,78,99	0.29	0	84,90,111	0.34	0
21	CDL	N	604	-	78,78,99	0.29	0	84,90,111	0.34	0
22	TRD	T	1303	-	12,12,12	0.35	0	11,11,11	0.36	0
20	HEM	H	902	3	50,50,50	2.45	16 (32%)	66,82,82	3.14	32 (48%)
13	HEC	O	302	1	50,50,50	1.44	4 (8%)	68,82,82	1.42	12 (17%)
28	9XX	b	203	-	31,31,41	1.07	4 (12%)	34,34,44	1.33	3 (8%)

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	0.35	0
22	TRD	R	608	-	12,12,12	0.09	0	11,11,11	0.06	0
22	TRD	J	502	-	12,12,12	0.21	0	11,11,11	0.25	0
14	MQ9	N	605	-	44,44,59	0.38	0	54,57,75	0.37	0
21	CDL	H	904	-	76,76,99	0.29	0	82,88,111	0.34	0
14	MQ9	T	1301	-	59,59,59	0.66	0	72,75,75	0.65	0
21	CDL	I	302	-	76,76,99	0.30	0	82,88,111	0.40	0
24	HEA	R	602	7	66,67,67	2.36	24 (36%)	78,103,103	2.40	27 (34%)

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
14	MQ9	M	505	14	-	26/53/73/73	0/2/2/2
22	TRD	S	502	-	-	5/10/10/10	-
24	HEA	L	603	7	-	6/36/76/76	-
15	WUO	O	304	-	-	39/84/148/148	0/3/3/3
18	9YF	G	904	-	-	30/54/78/78	0/1/1/1
23	3PE	J	503	-	-	16/35/35/54	-
13	HEC	C	302	1	1/1/3/7	4/14/54/54	-
14	MQ9	O	303	-	-	6/53/73/73	0/2/2/2
14	MQ9	H	906	-	-	14/35/55/73	0/2/2/2
22	TRD	K	1302	-	-	6/10/10/10	-
29	PLM	W	203	11	-	4/7/8/15	-
15	WUO	I	303	-	-	35/84/148/148	0/3/3/3
16	FES	M	501	2	-	-	0/1/1/1
22	TRD	L	608	-	-	1/10/10/10	-
21	CDL	H	903	-	-	44/84/84/110	-
21	CDL	C	305	-	-	46/89/89/110	-
14	MQ9	N	608	-	-	31/53/73/73	0/2/2/2
15	WUO	P	302	-	-	37/84/148/148	0/3/3/3
19	7PH	S	501	-	-	15/39/39/39	-
15	WUO	C	304	-	-	39/84/148/148	0/3/3/3
20	HEM	H	908	3	-	2/14/54/54	-
22	TRD	Q	403	-	-	6/10/10/10	-
13	HEC	C	301	1	1/1/3/7	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PLM	c	301	12	-	3/7/8/15	-
19	7PH	H	901	-	-	22/39/39/39	-
21	CDL	J	501	-	-	50/89/89/110	-
14	MQ9	C	303	-	-	6/53/73/73	0/2/2/2
28	9XX	Y	302	-	-	17/33/33/43	-
29	PLM	Y	301	12	-	2/7/8/15	-
14	MQ9	K	1301	-	-	19/53/73/73	0/2/2/2
20	HEM	N	607	3	-	2/14/54/54	-
21	CDL	H	905	-	-	42/89/89/110	-
13	HEC	O	301	1	1/1/3/7	5/14/54/54	-
21	CDL	T	1302	-	-	53/89/89/110	-
14	MQ9	N	606	14	-	28/53/73/73	0/2/2/2
28	9XX	c	302	-	-	19/33/33/43	-
22	TRD	X	403	-	-	6/10/10/10	-
19	7PH	N	609	-	-	22/39/39/39	-
21	CDL	R	605	-	-	49/87/87/110	-
21	CDL	N	603	-	-	36/87/87/110	-
18	9YF	W	201	-	-	32/54/78/78	0/1/1/1
14	MQ9	G	901	14	-	26/53/73/73	0/2/2/2
17	IZL	G	903	-	-	33/84/208/208	0/6/6/6
19	7PH	M	504	-	-	21/39/39/39	-
18	9YF	M	503	-	-	30/54/78/78	0/1/1/1
14	MQ9	H	909	-	-	31/53/73/73	0/2/2/2
19	7PH	G	905	-	-	21/39/39/39	-
22	TRD	R	609	-	-	1/10/10/10	-
29	PLM	b	202	11	-	3/7/8/15	-
16	FES	G	902	2	-	-	0/1/1/1
23	3PE	S	503	-	-	16/35/35/54	-
21	CDL	I	301	-	-	58/87/87/110	-
24	HEA	R	603	7	-	15/36/76/76	-
17	IZL	M	502	-	-	38/84/208/208	0/6/6/6
18	9YF	b	201	-	-	32/54/78/78	0/1/1/1
24	HEA	L	602	7	-	9/36/76/76	-
21	CDL	N	602	-	-	44/84/84/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	HEM	N	601	3	-	5/14/54/54	-
28	9XX	W	202	-	-	28/43/43/43	-
22	TRD	L	607	-	-	5/10/10/10	-
14	MQ9	H	907	14	-	28/53/73/73	0/2/2/2
21	CDL	P	301	-	-	46/87/87/110	-
21	CDL	L	601	-	-	52/89/89/110	-
21	CDL	N	604	-	-	52/89/89/110	-
22	TRD	T	1303	-	-	6/10/10/10	-
20	HEM	H	902	3	-	4/14/54/54	-
13	HEC	O	302	1	1/1/3/7	4/14/54/54	-
28	9XX	b	203	-	-	21/33/33/43	-
21	CDL	R	601	-	-	38/87/87/110	-
22	TRD	R	608	-	-	5/10/10/10	-
22	TRD	J	502	-	-	5/10/10/10	-
14	MQ9	N	605	-	-	14/35/55/73	0/2/2/2
21	CDL	H	904	-	-	40/87/87/110	-
14	MQ9	T	1301	-	-	19/53/73/73	0/2/2/2
21	CDL	I	302	-	-	49/87/87/110	-
24	HEA	R	602	7	-	8/36/76/76	-

The worst 5 of 329 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	603	HEA	FE-NC	7.31	2.19	1.95
24	L	603	HEA	FE-ND	7.30	2.17	1.94
20	H	902	HEM	FE-NB	7.19	2.17	1.94
24	R	603	HEA	FE-ND	7.18	2.17	1.94
17	G	903	IZL	P-O28	7.09	1.79	1.60

The worst 5 of 365 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	902	HEM	CBC-CAC-C3C	10.41	179.40	127.62
20	H	902	HEM	C4C-C3C-C2C	7.82	113.17	106.75
20	N	601	HEM	C4C-NC-C1C	7.81	112.99	105.35
20	H	902	HEM	O2A-CGA-O1A	-6.51	107.08	123.30
20	N	601	HEM	O2A-CGA-O1A	-6.49	107.12	123.30

All (4) chirality outliers are listed below:

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

5 of 1637 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	M	505	MQ9	C12-C11-C9-C10
14	M	505	MQ9	C12-C13-C14-C15
14	M	505	MQ9	C13-C14-C16-C17
14	M	505	MQ9	C15-C14-C16-C17
14	M	505	MQ9	C18-C19-C21-C22

There are no ring outliers.

58 monomers are involved in 288 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	505	MQ9	16	0
22	S	502	TRD	4	0
24	L	603	HEA	2	0
15	O	304	WUO	7	0
18	G	904	9YF	4	0
23	J	503	3PE	1	0
13	C	302	HEC	3	0
14	O	303	MQ9	3	0
14	H	906	MQ9	1	0
15	I	303	WUO	2	0
29	W	203	PLM	1	0
22	L	608	TRD	1	0
21	H	903	CDL	27	0
21	C	305	CDL	10	0
14	N	608	MQ9	8	0
15	P	302	WUO	4	0
19	S	501	7PH	2	0
15	C	304	WUO	4	0
22	Q	403	TRD	1	0
29	c	301	PLM	1	0
19	H	901	7PH	10	0
21	J	501	CDL	7	0
14	C	303	MQ9	1	0

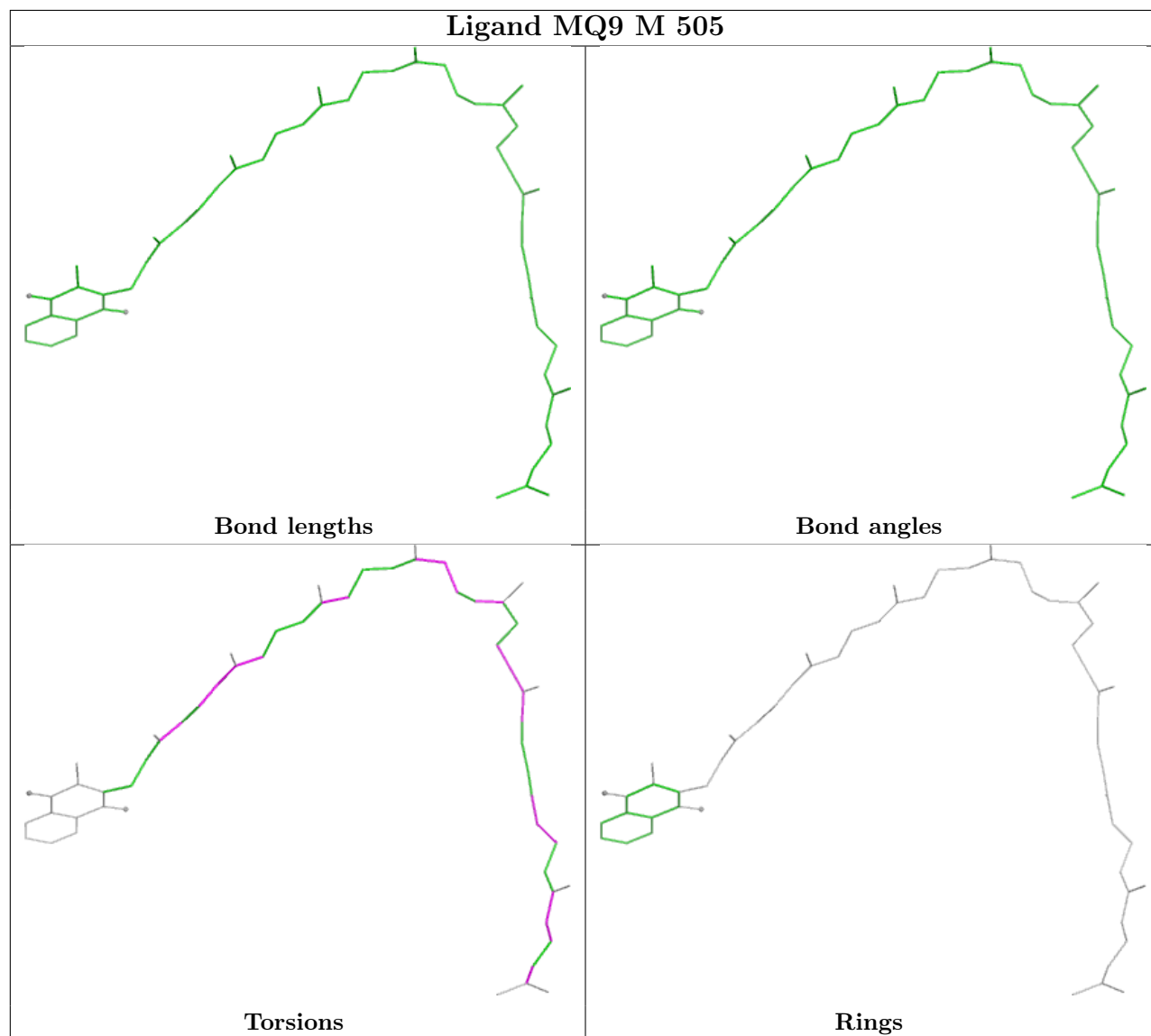
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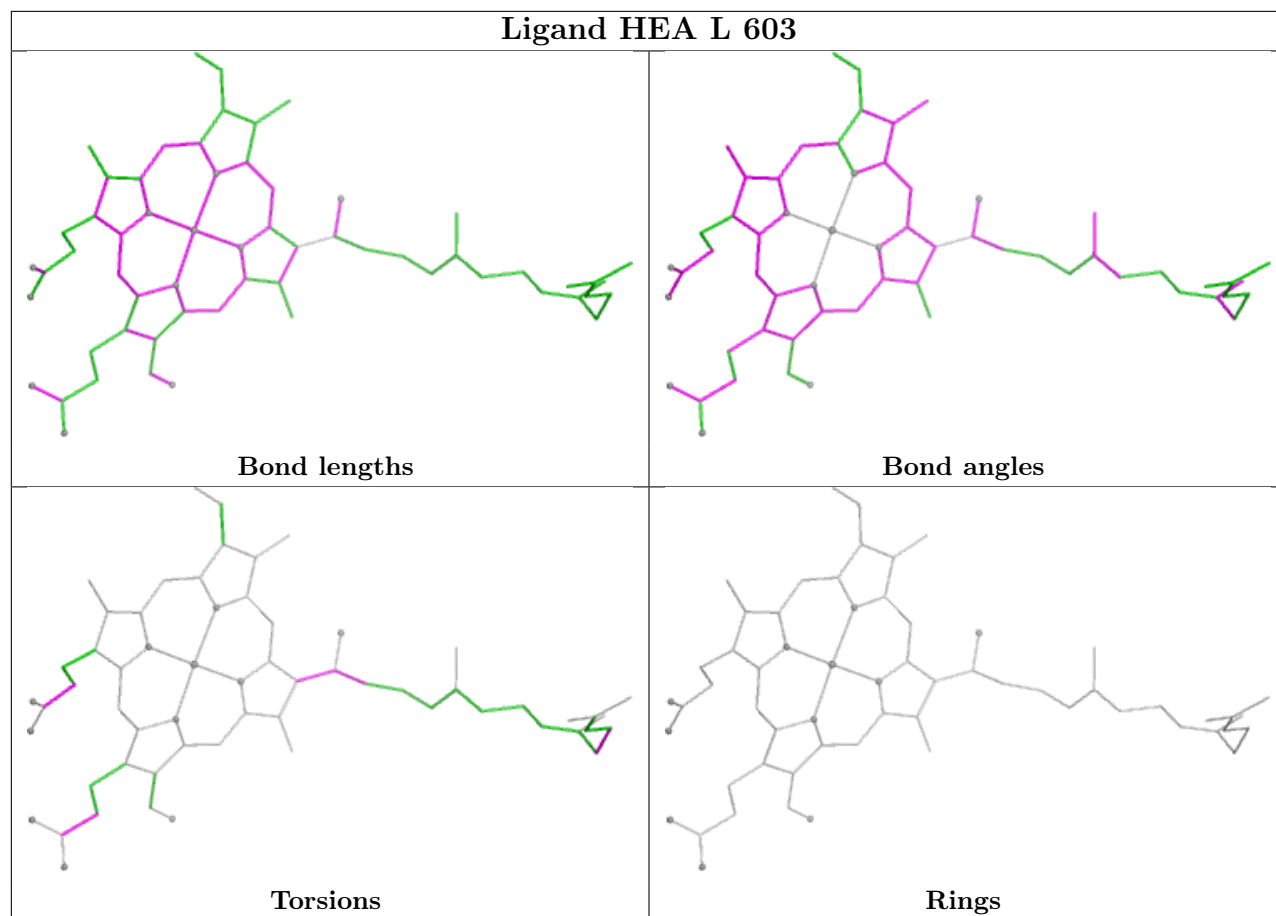
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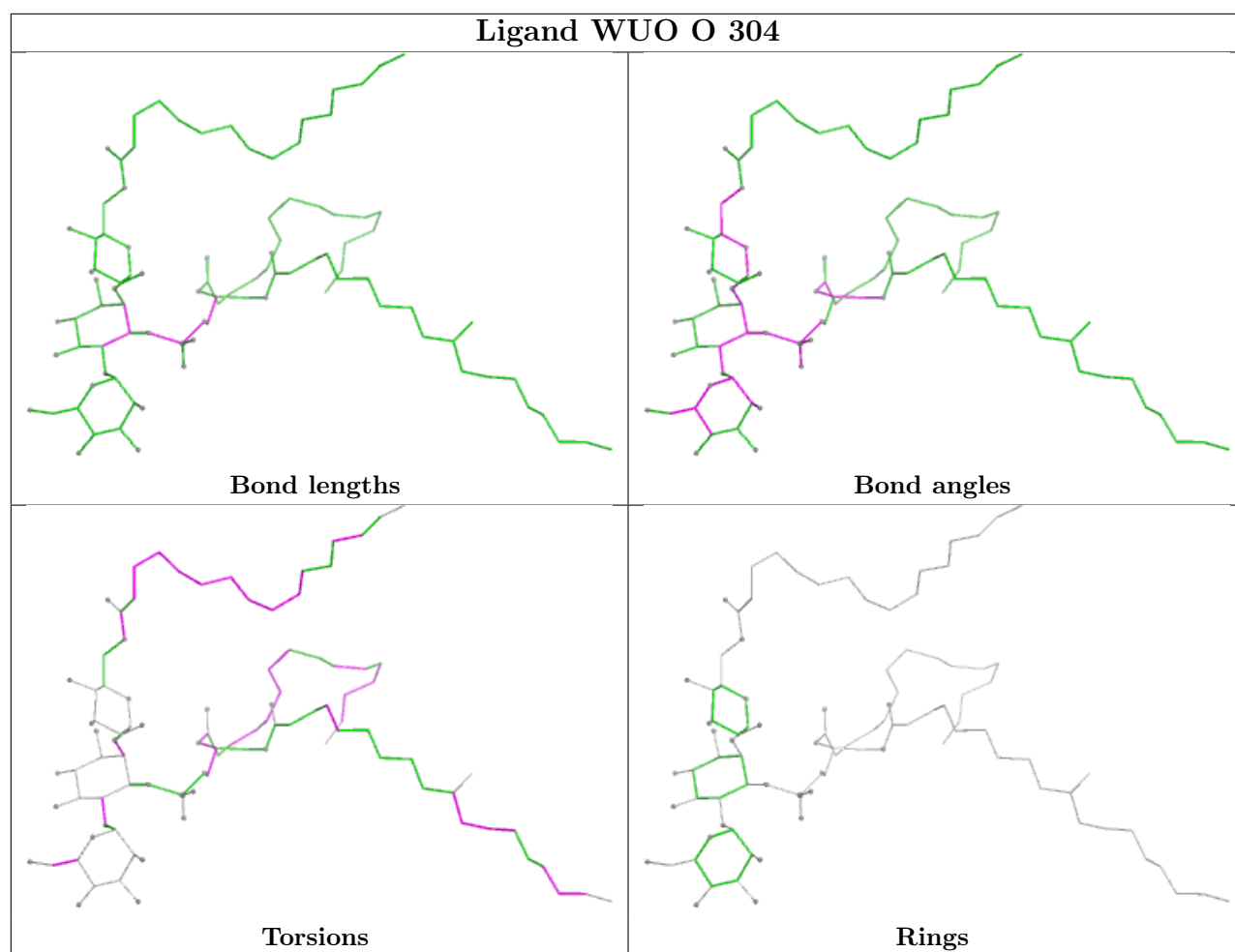
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	K	1301	MQ9	9	0
21	H	905	CDL	8	0
21	T	1302	CDL	8	0
14	N	606	MQ9	15	0
22	X	403	TRD	1	0
19	N	609	7PH	9	0
21	R	605	CDL	4	0
21	N	603	CDL	2	0
14	G	901	MQ9	17	0
17	G	903	IZL	2	0
18	W	201	9YF	1	0
18	M	503	9YF	3	0
14	H	909	MQ9	7	0
19	M	504	7PH	5	0
19	G	905	7PH	5	0
22	R	609	TRD	1	0
23	S	503	3PE	4	0
21	I	301	CDL	5	0
24	R	603	HEA	10	0
18	b	201	9YF	4	0
24	L	602	HEA	3	0
21	N	602	CDL	26	0
14	H	907	MQ9	9	0
21	P	301	CDL	6	0
21	L	601	CDL	8	0
21	N	604	CDL	4	0
20	H	902	HEM	4	0
13	O	302	HEC	2	0
21	R	601	CDL	2	0
22	J	502	TRD	4	0
14	N	605	MQ9	1	0
21	H	904	CDL	3	0
14	T	1301	MQ9	12	0
21	I	302	CDL	5	0
24	R	602	HEA	2	0

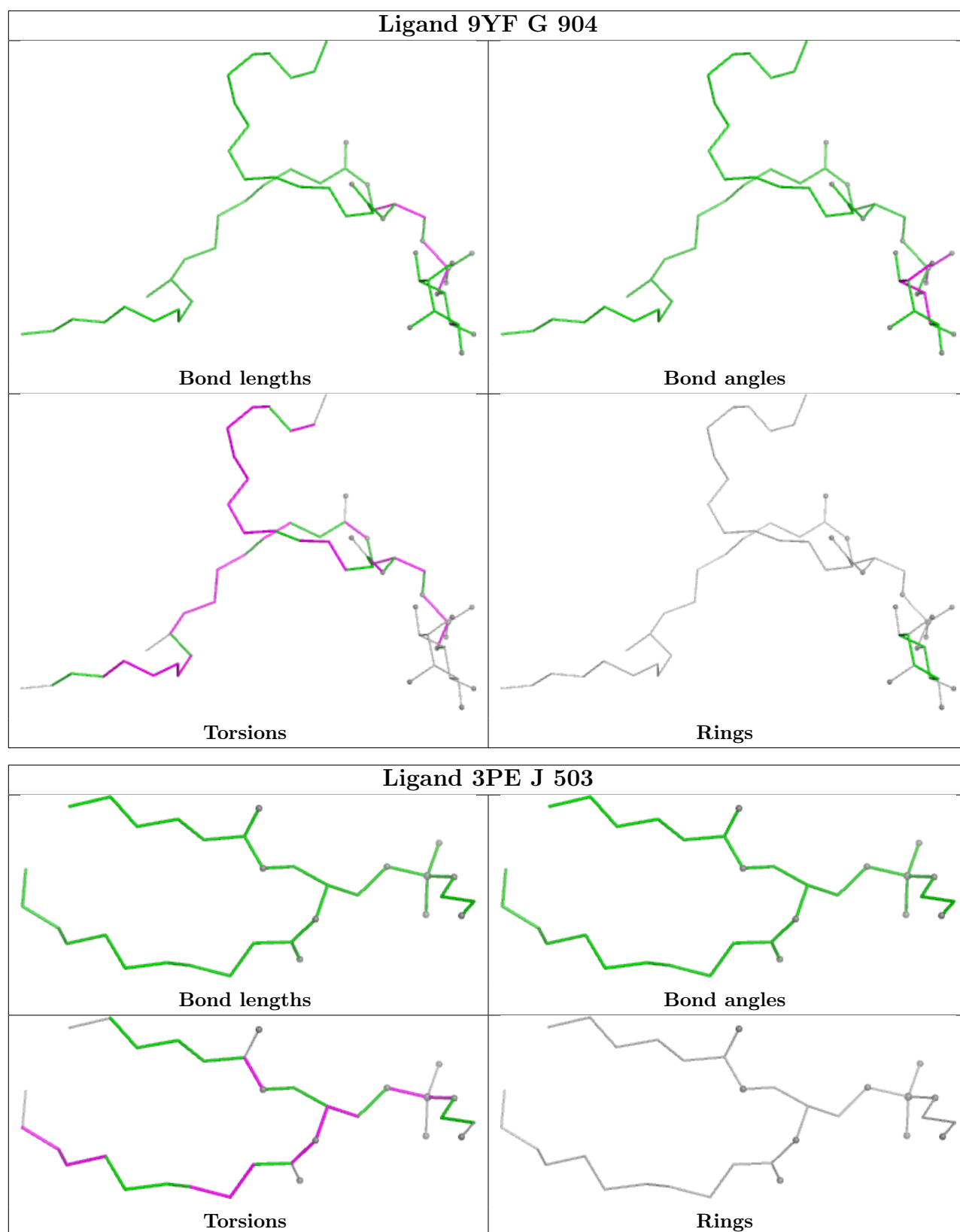
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

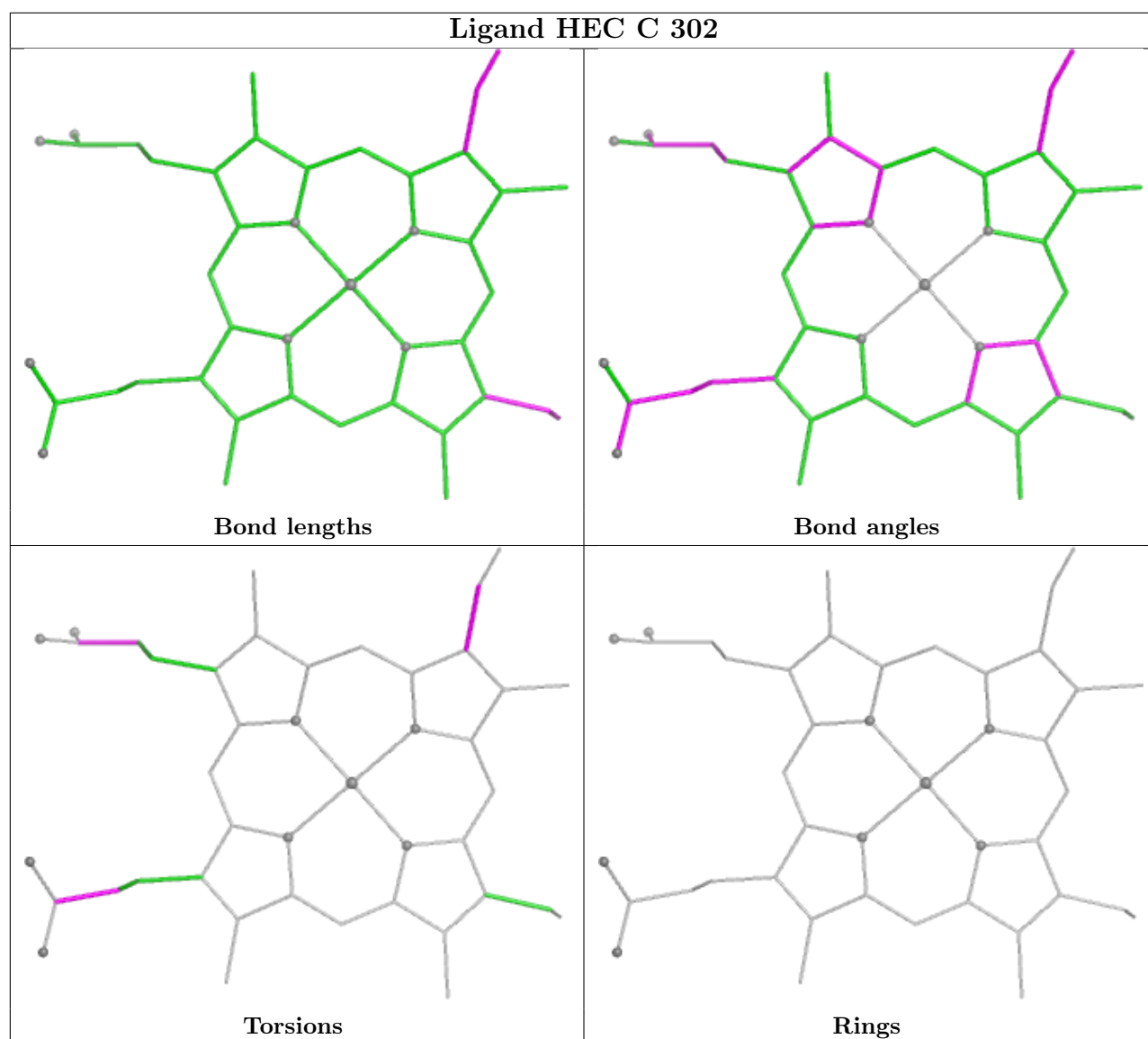
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

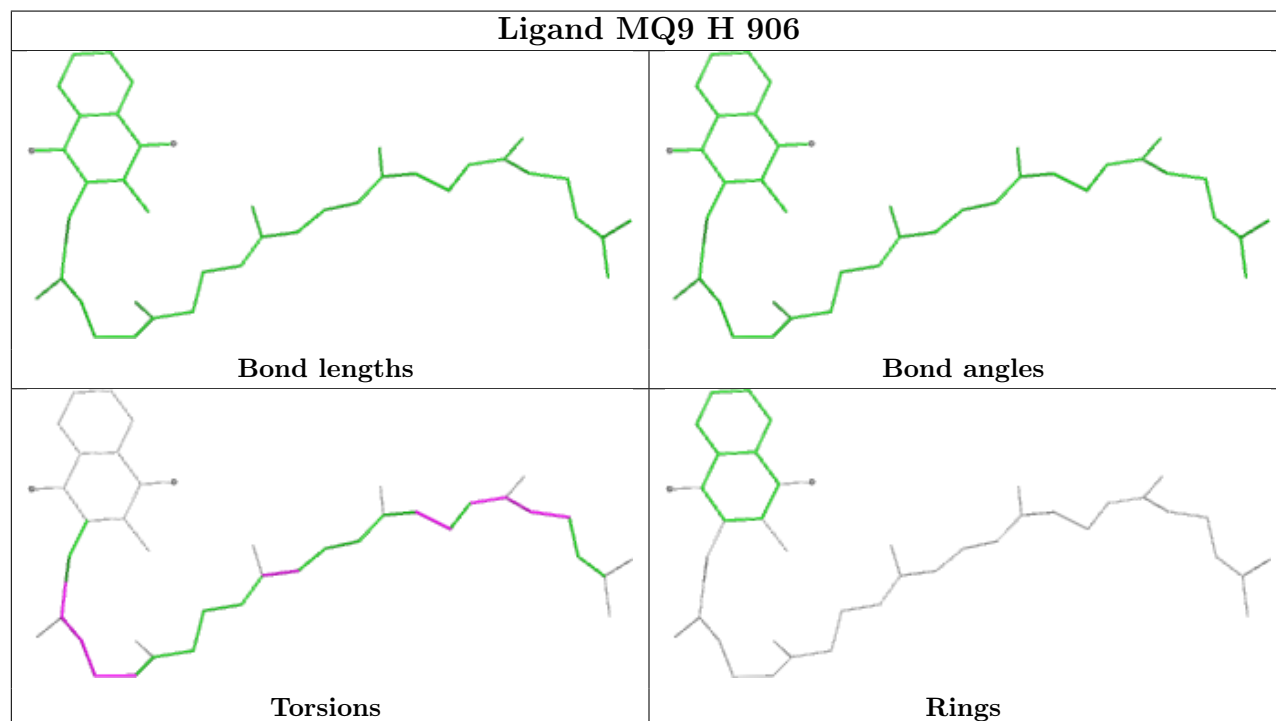
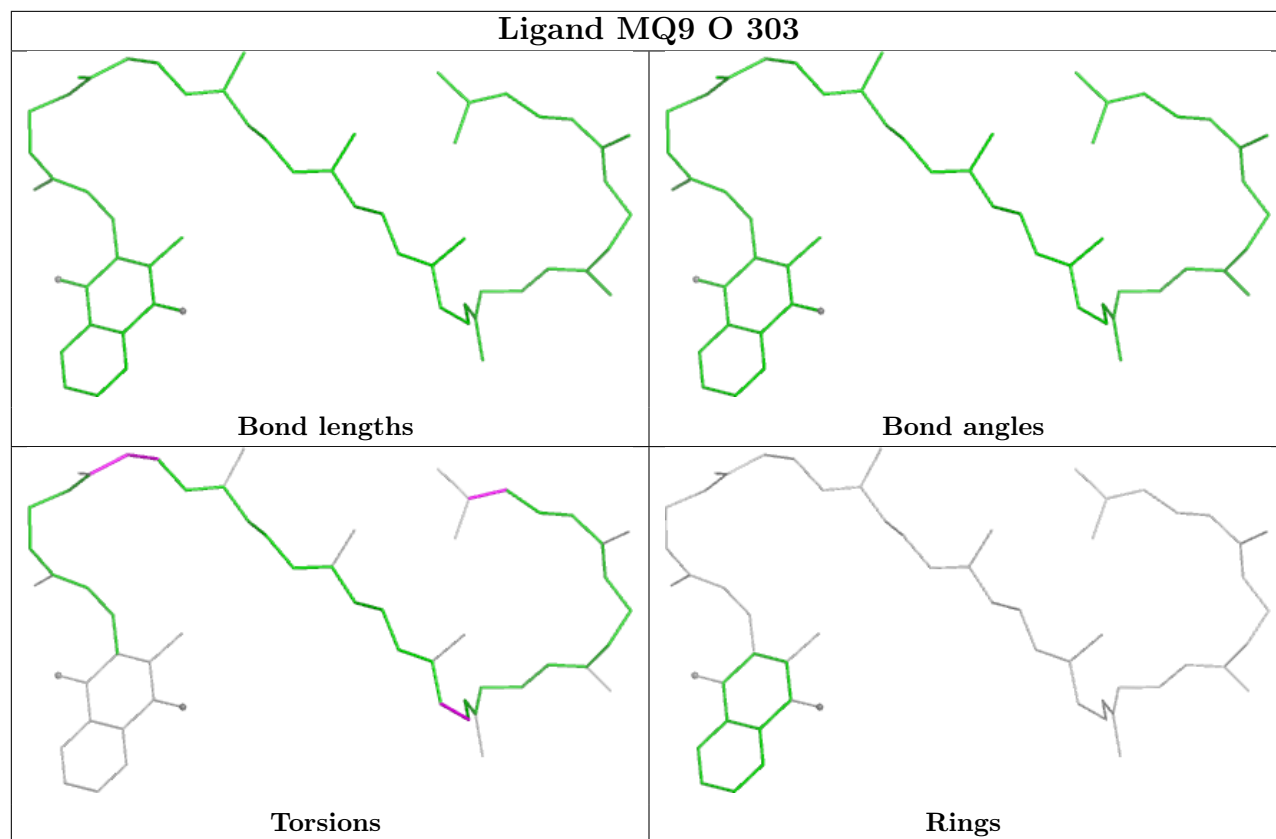


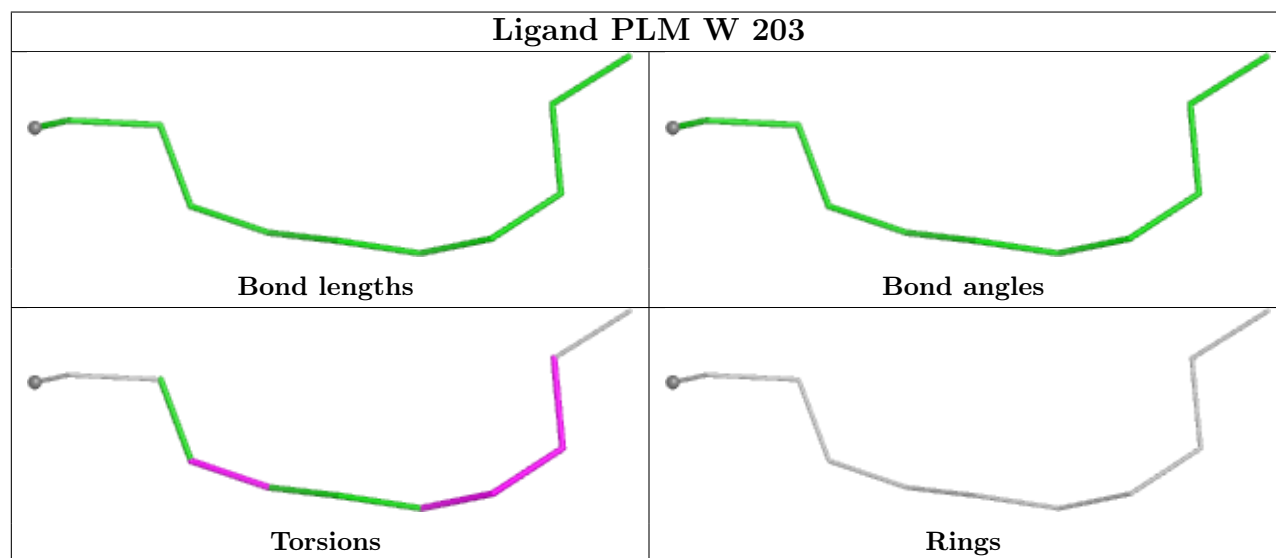
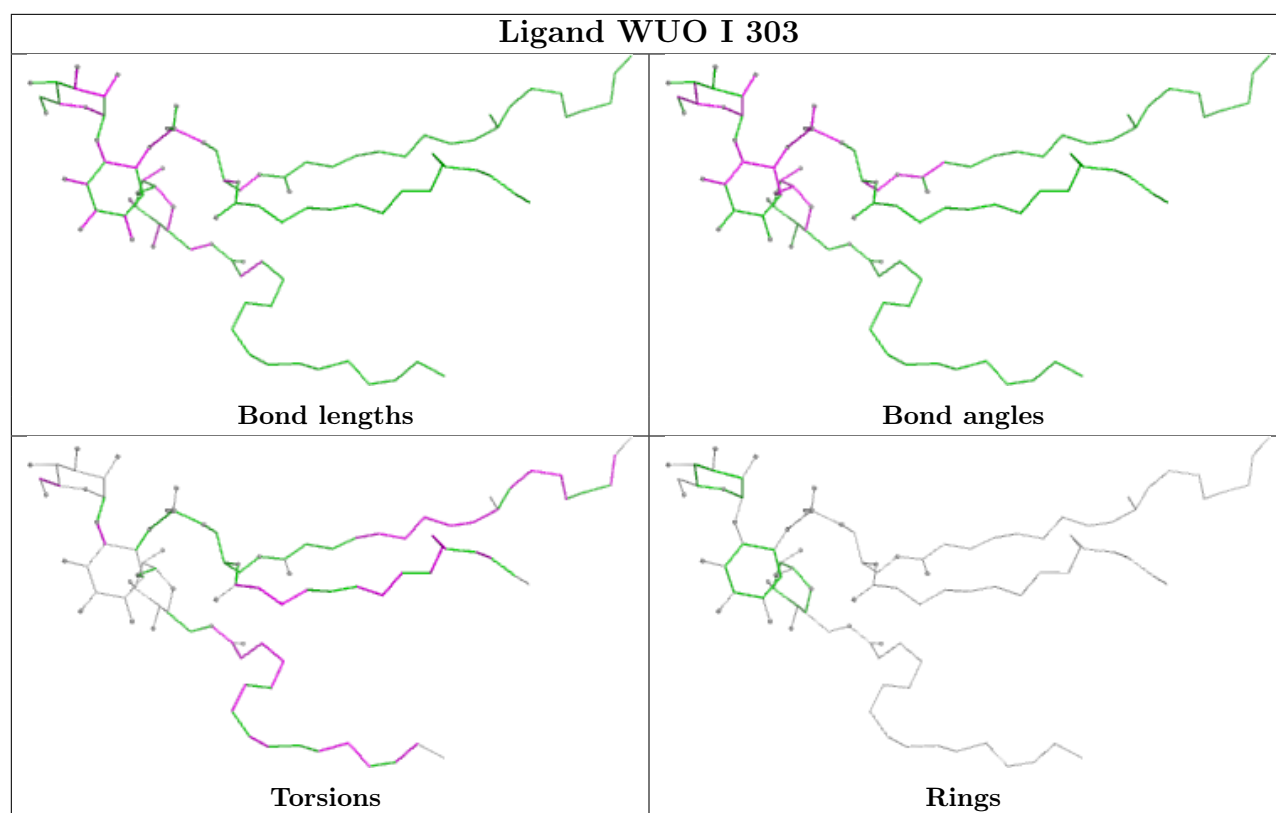


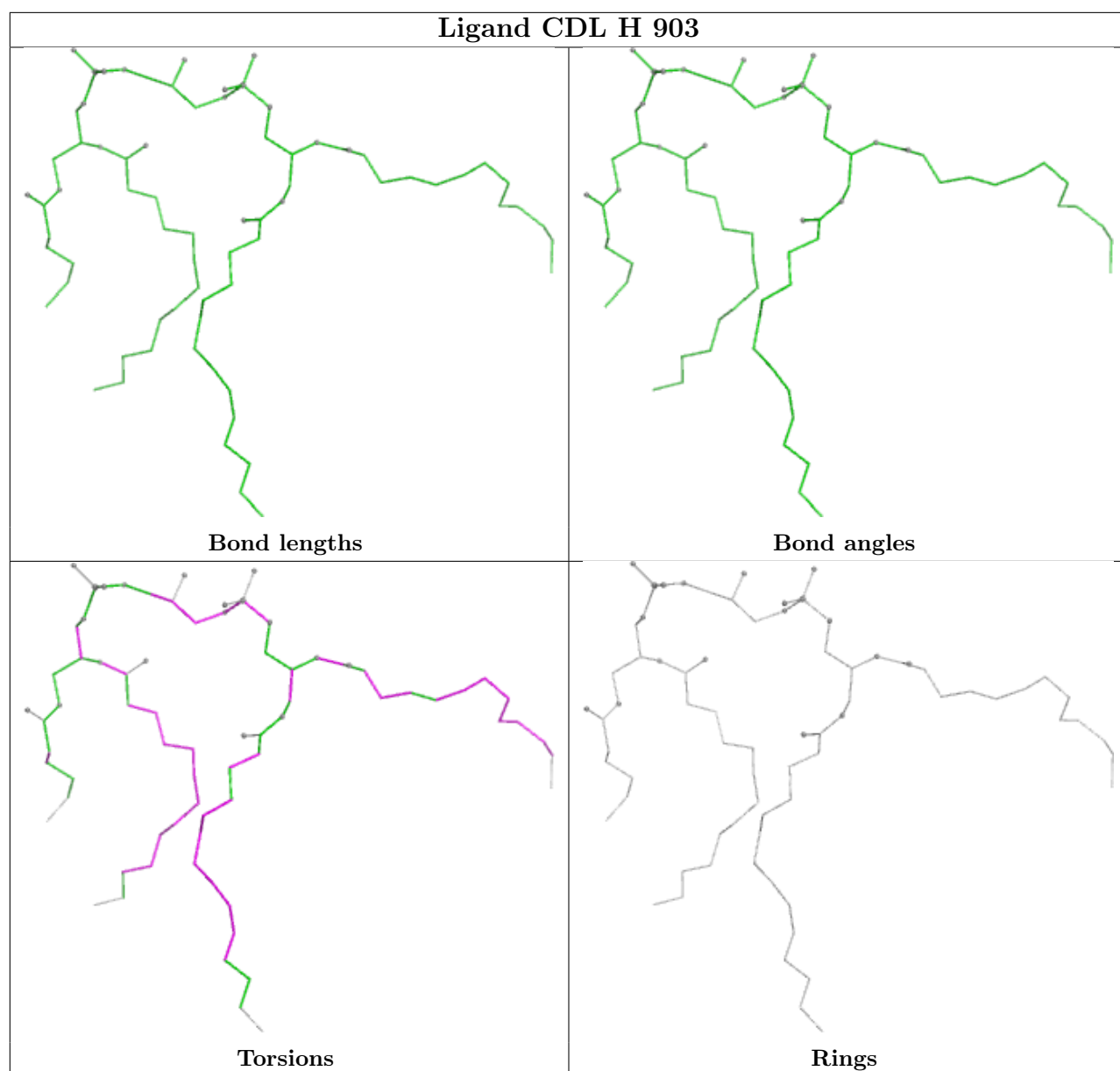


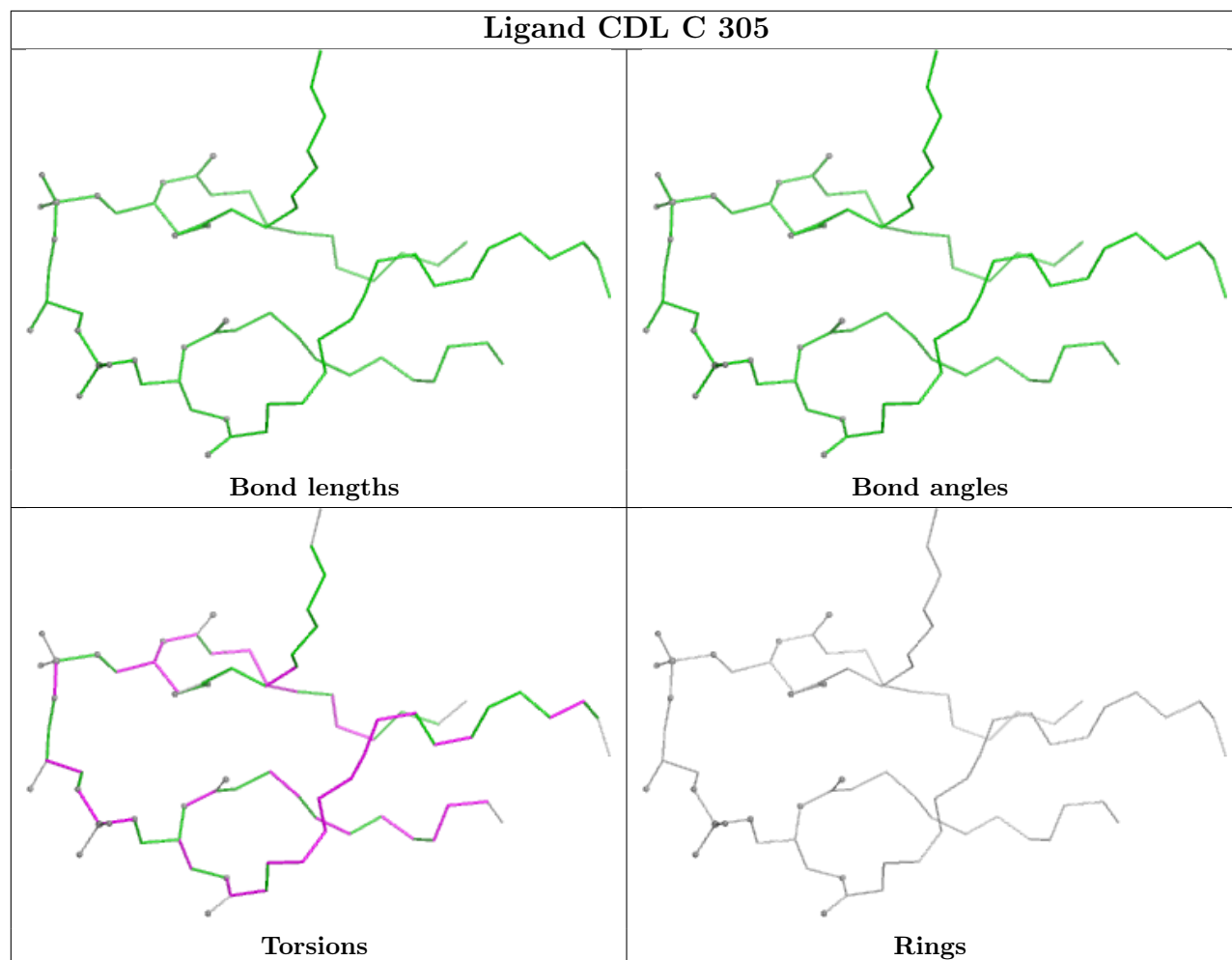
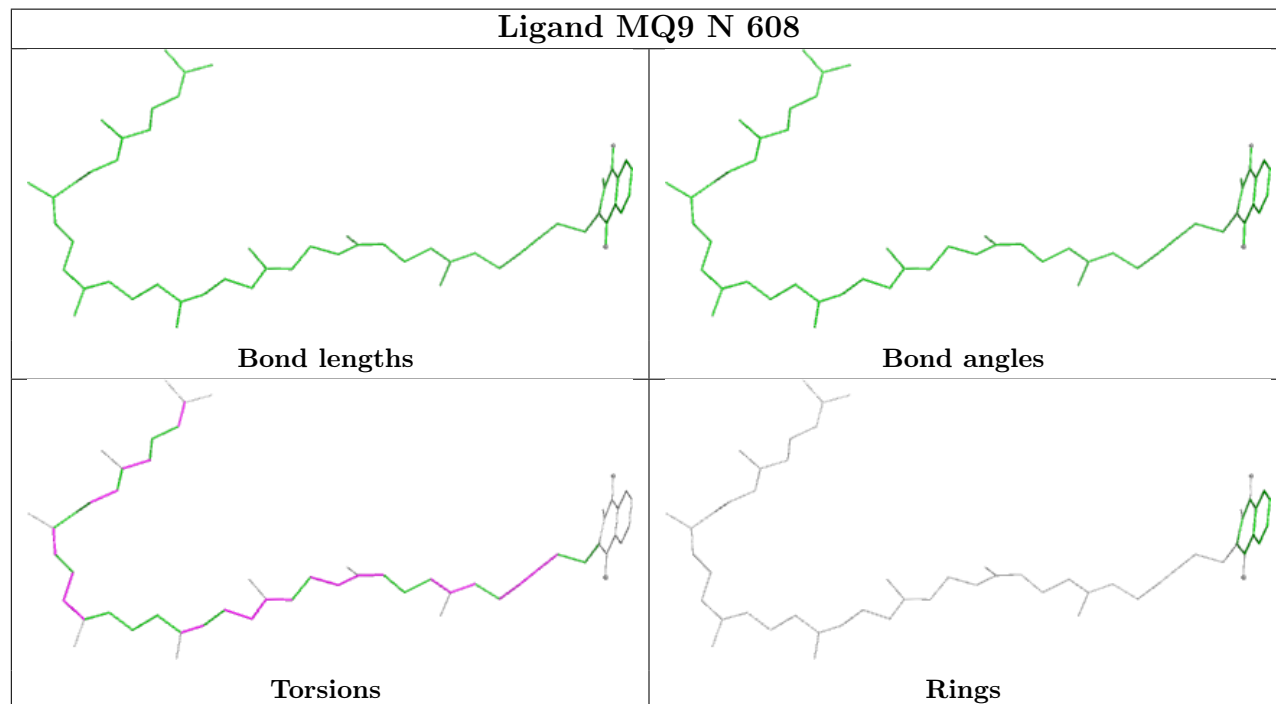


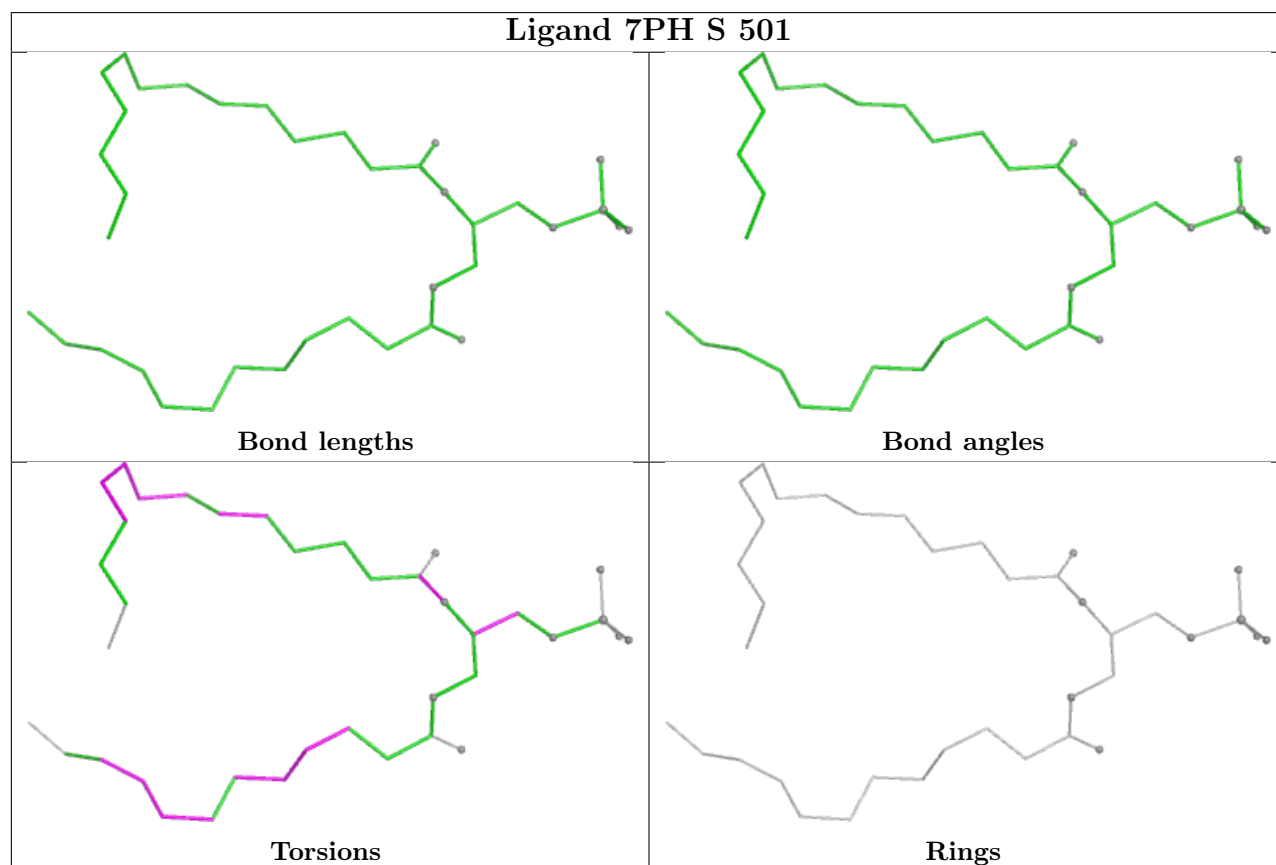
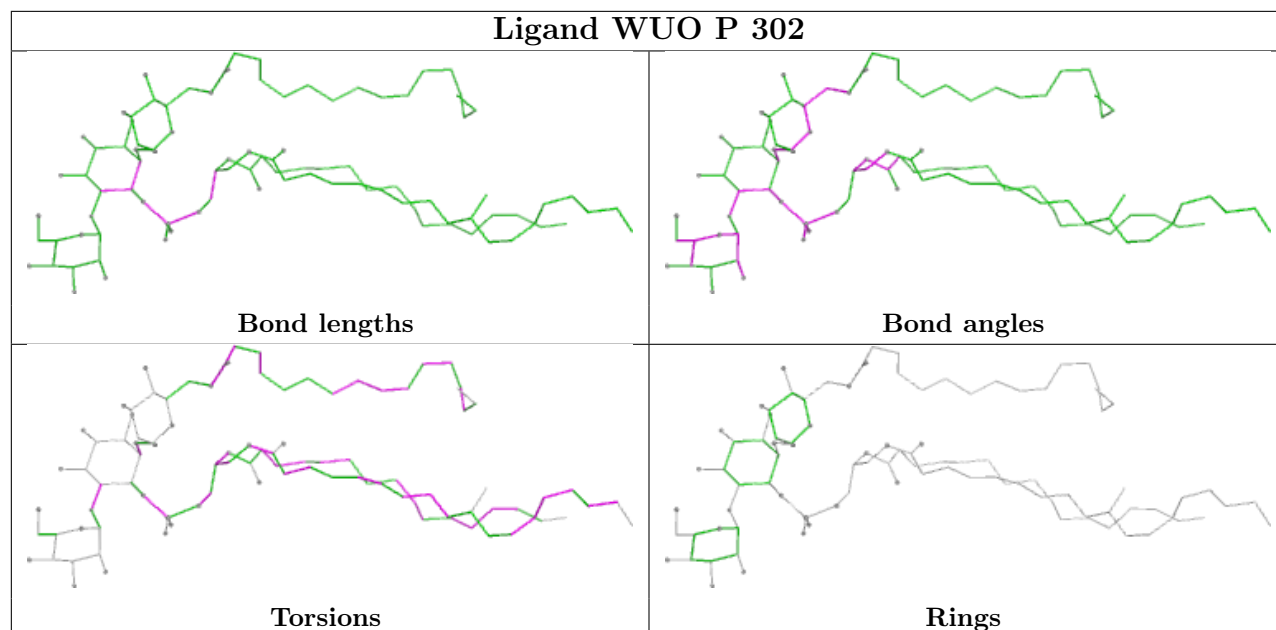


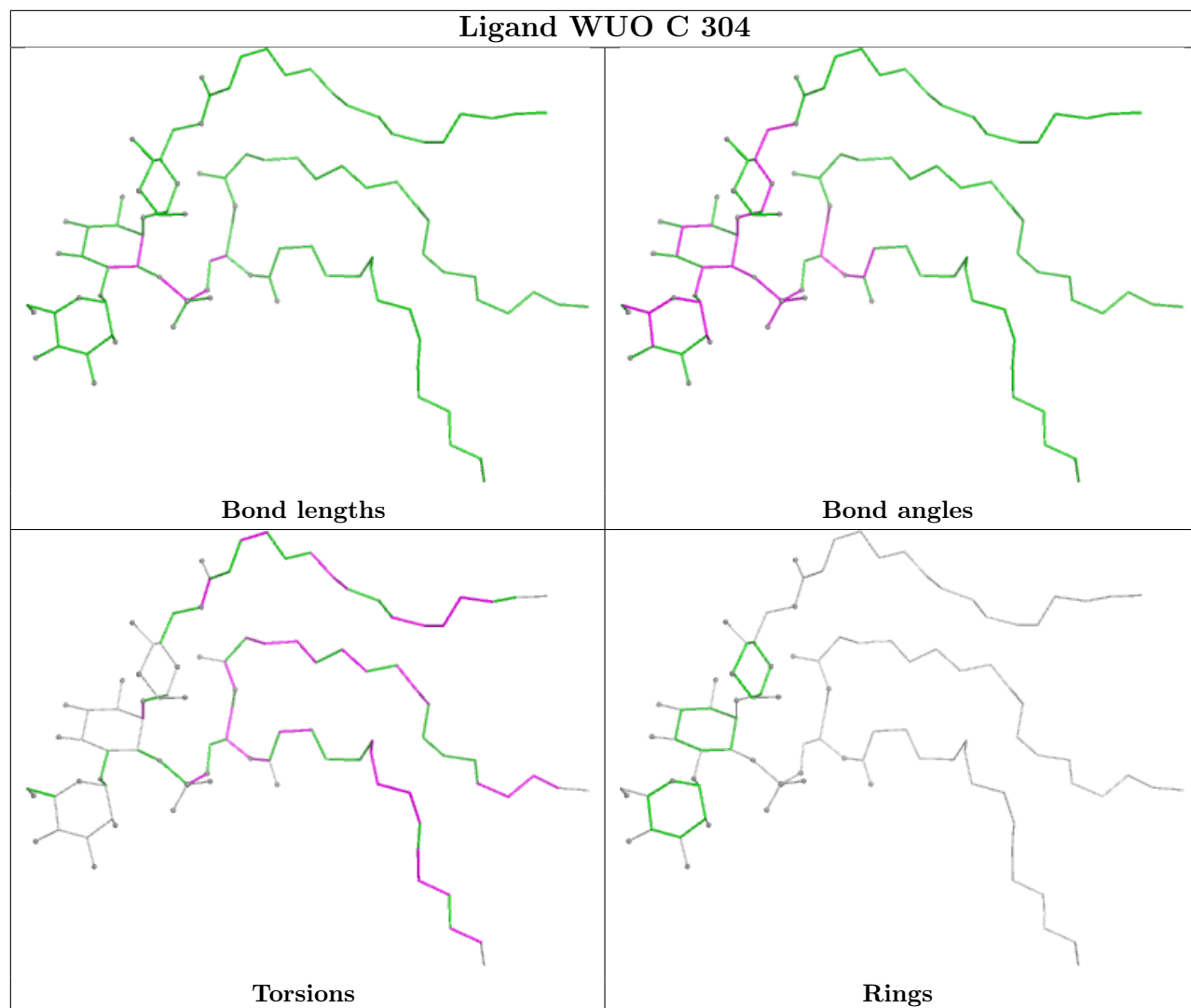


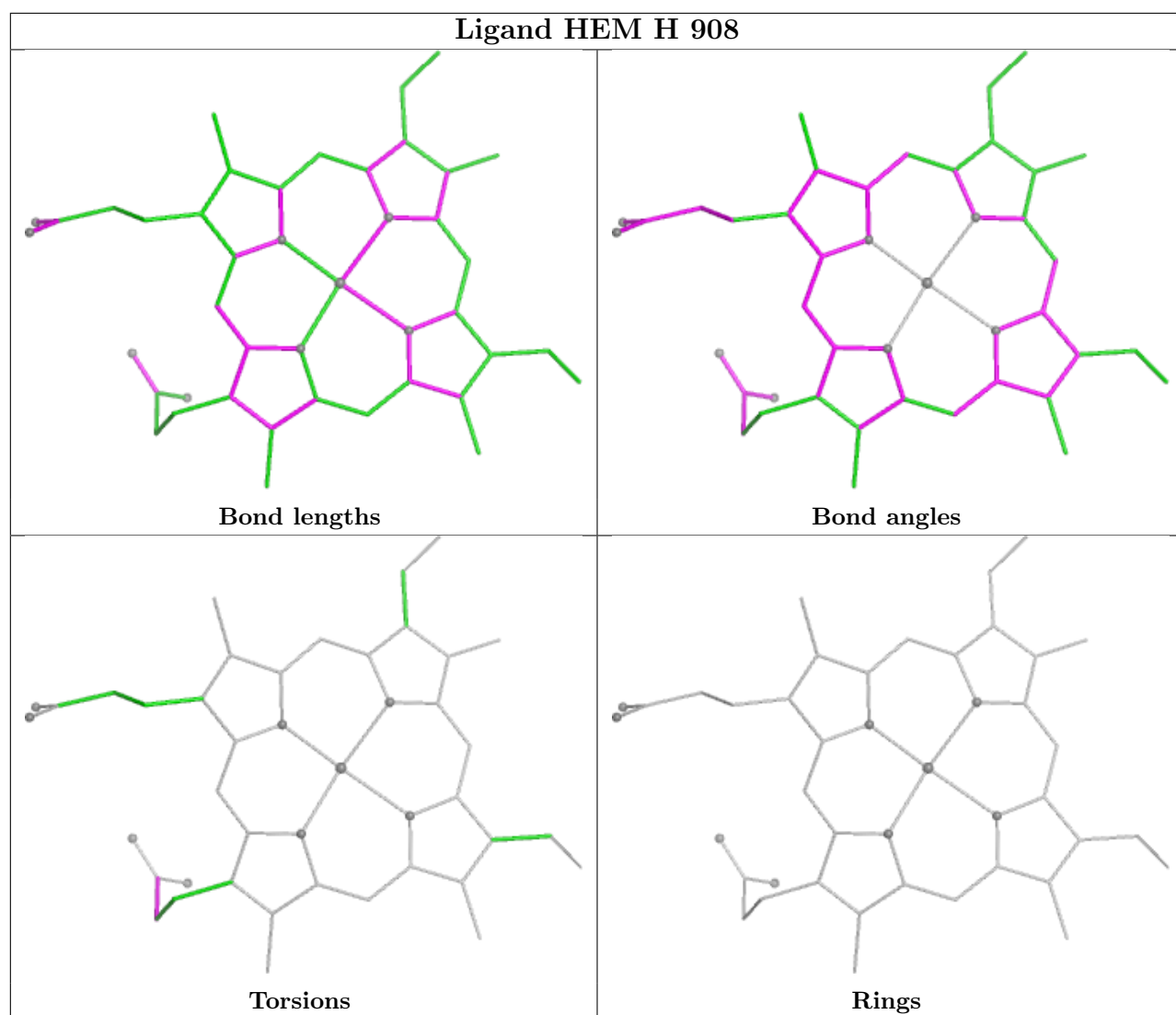


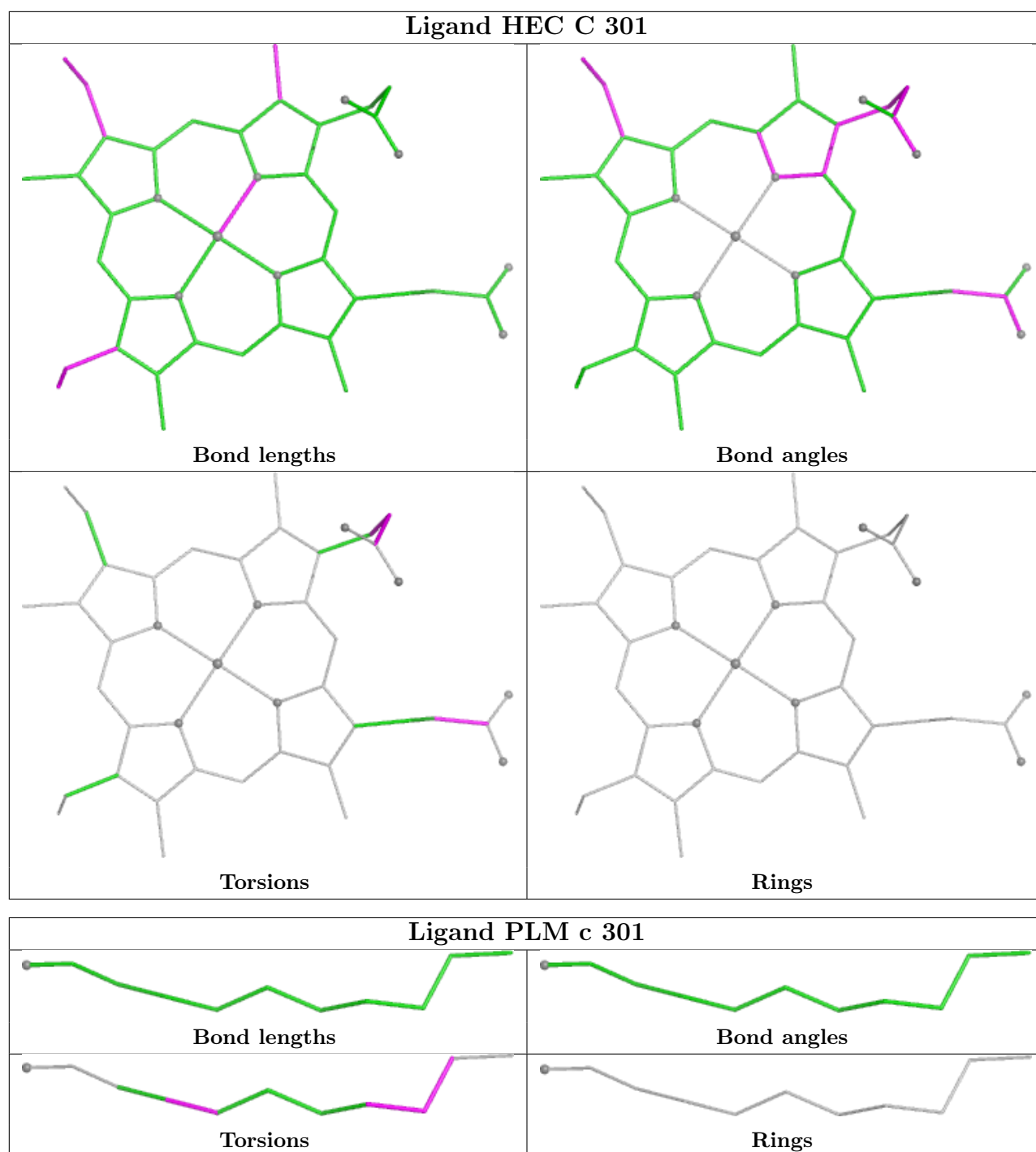


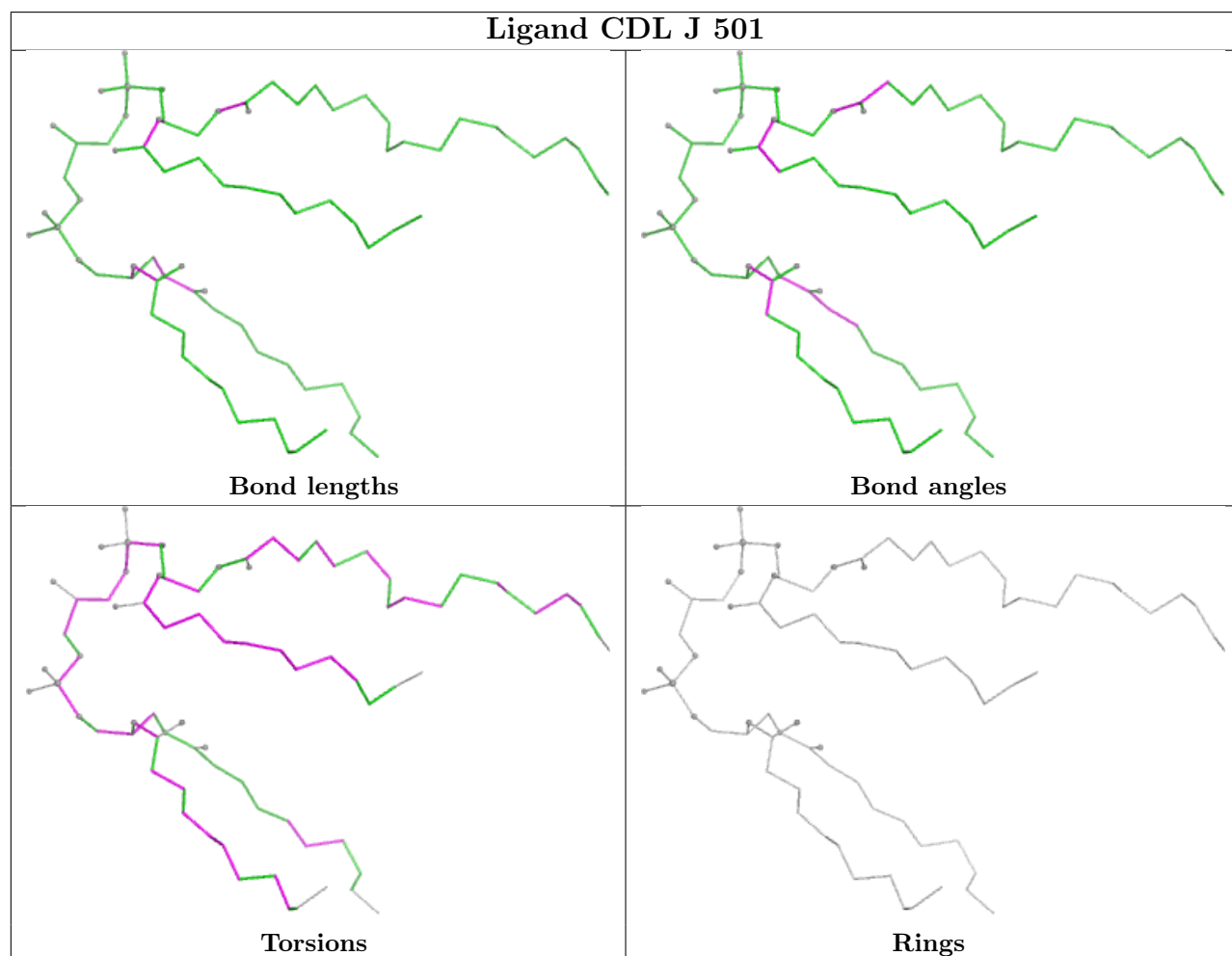
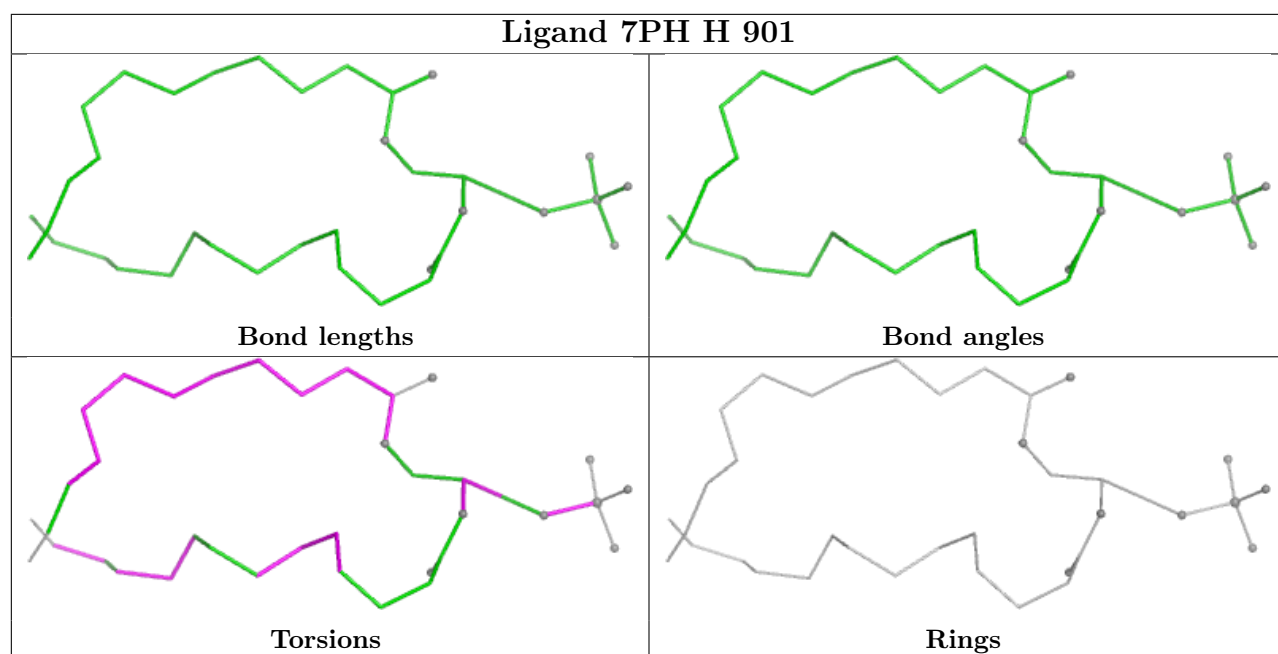
Ligand CDL C 305**Ligand MQ9 N 608**

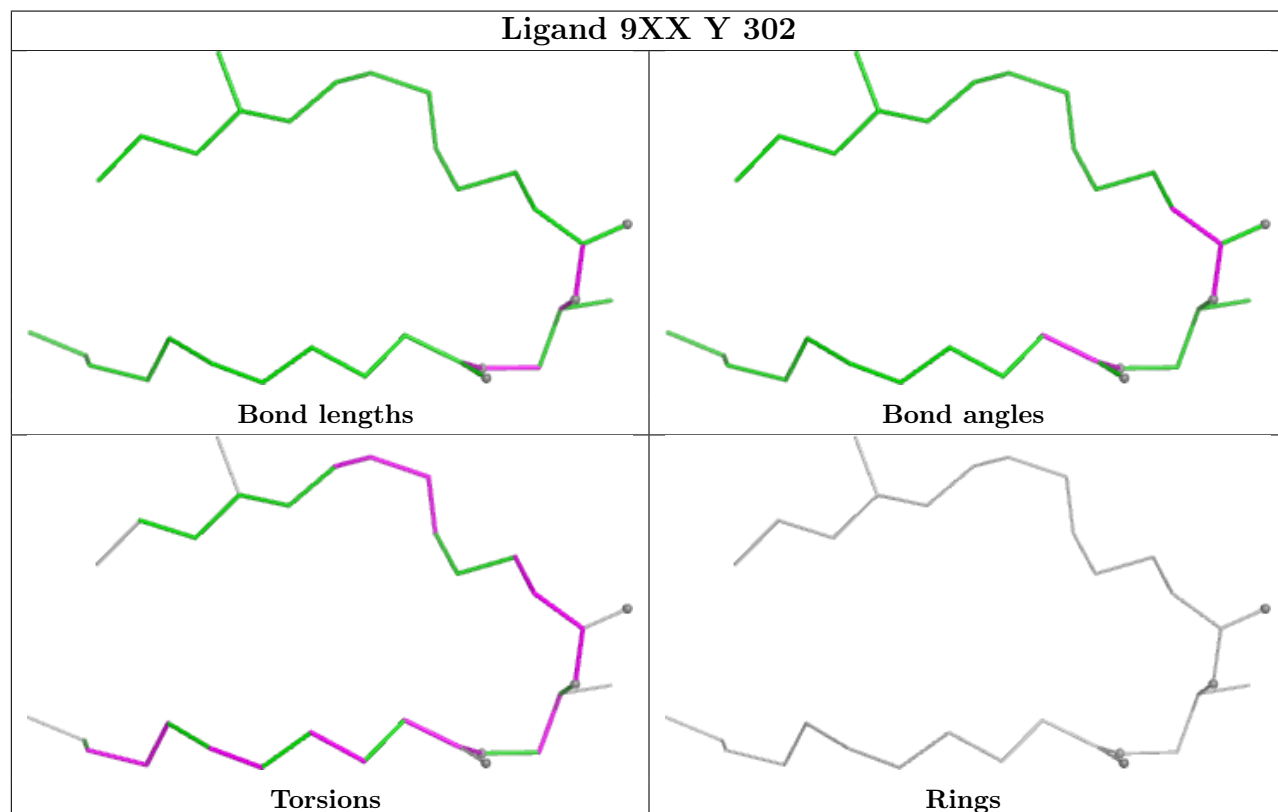
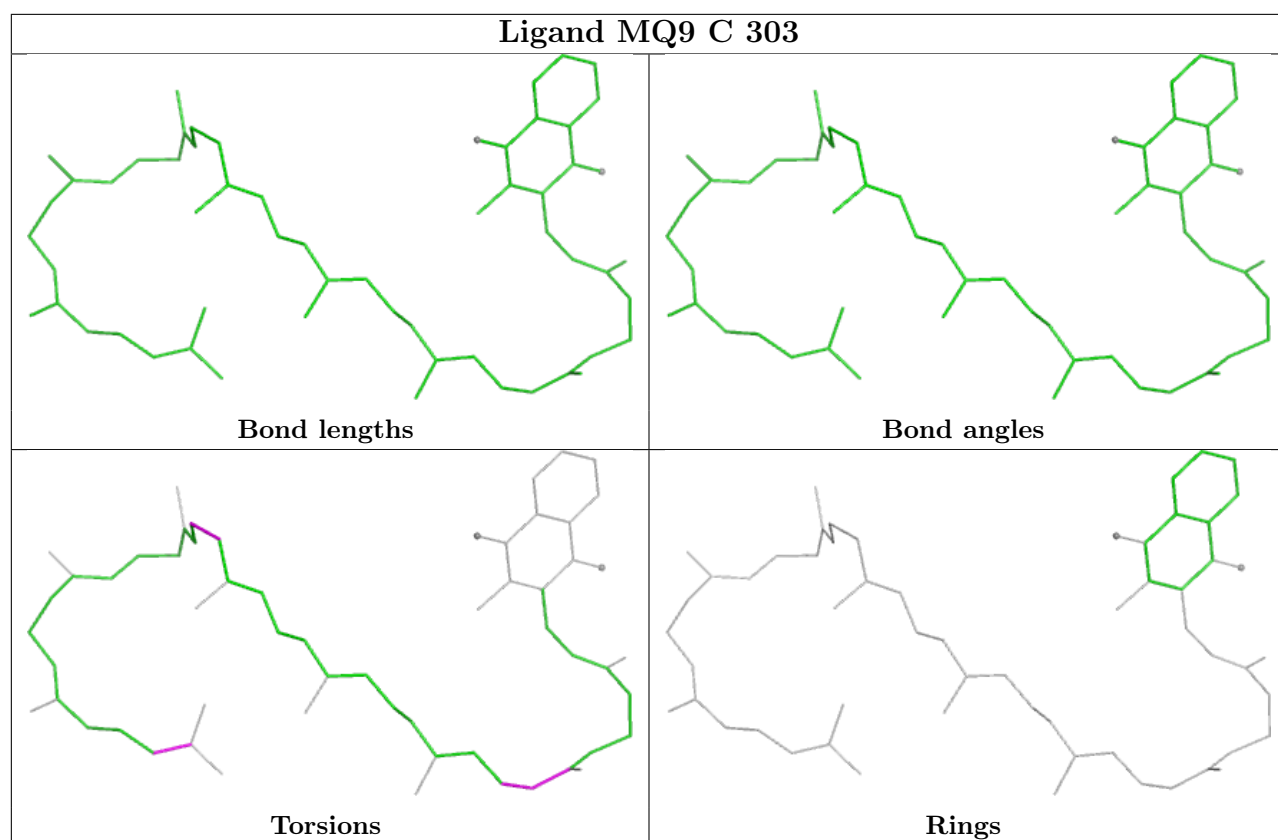


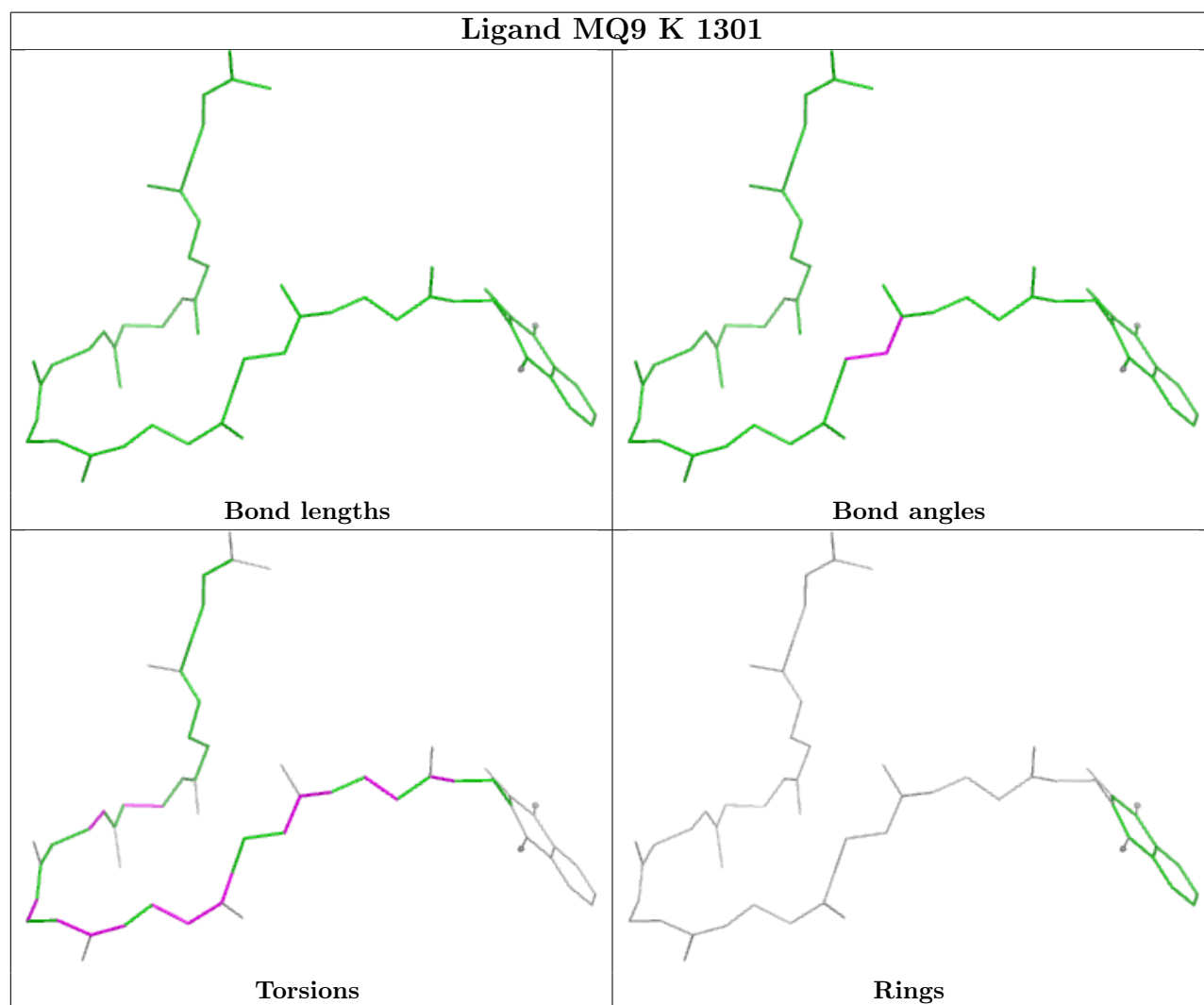
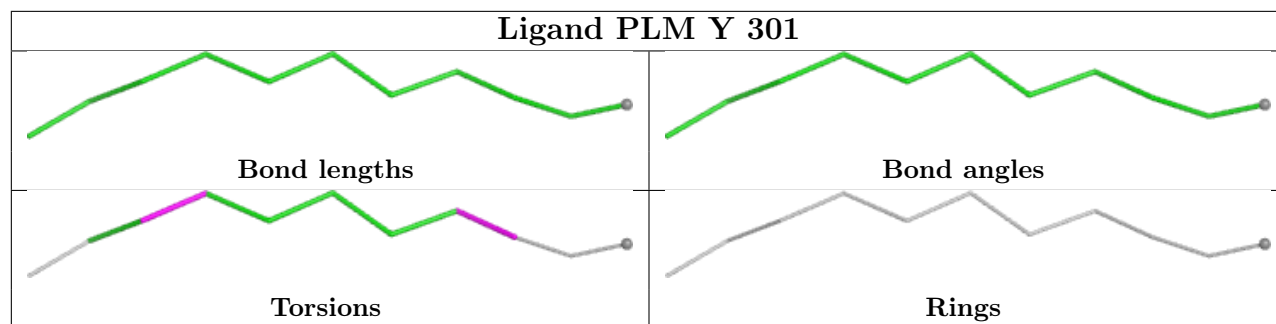


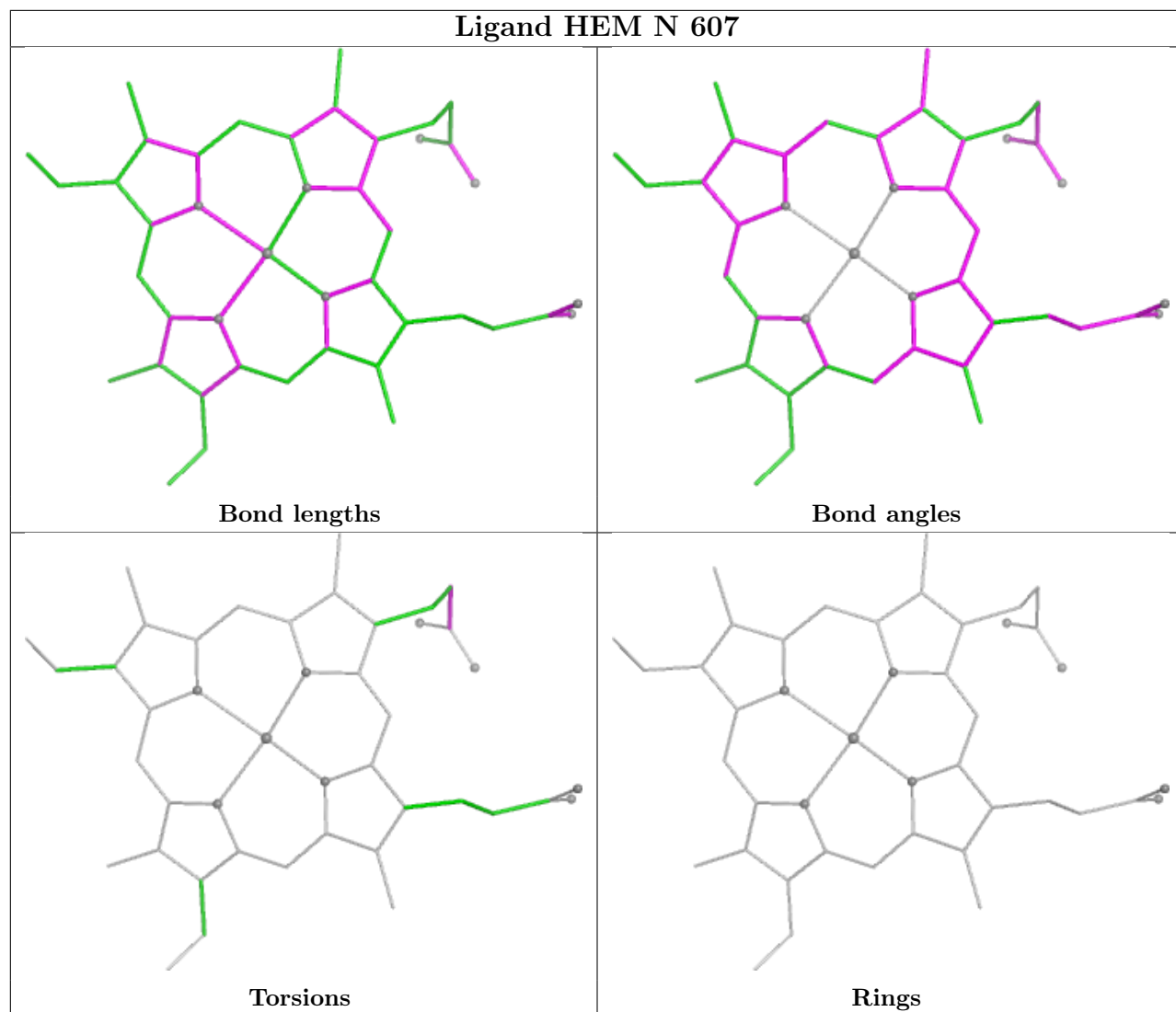


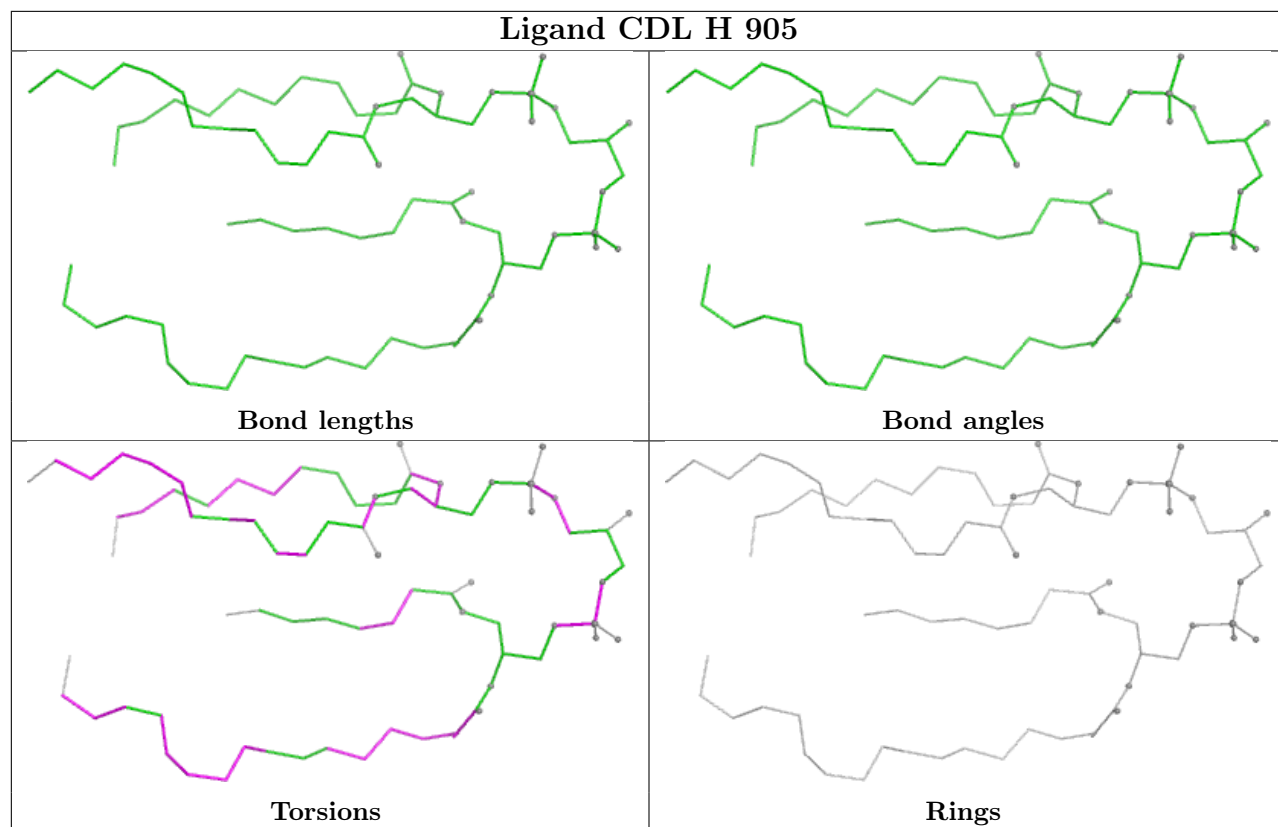


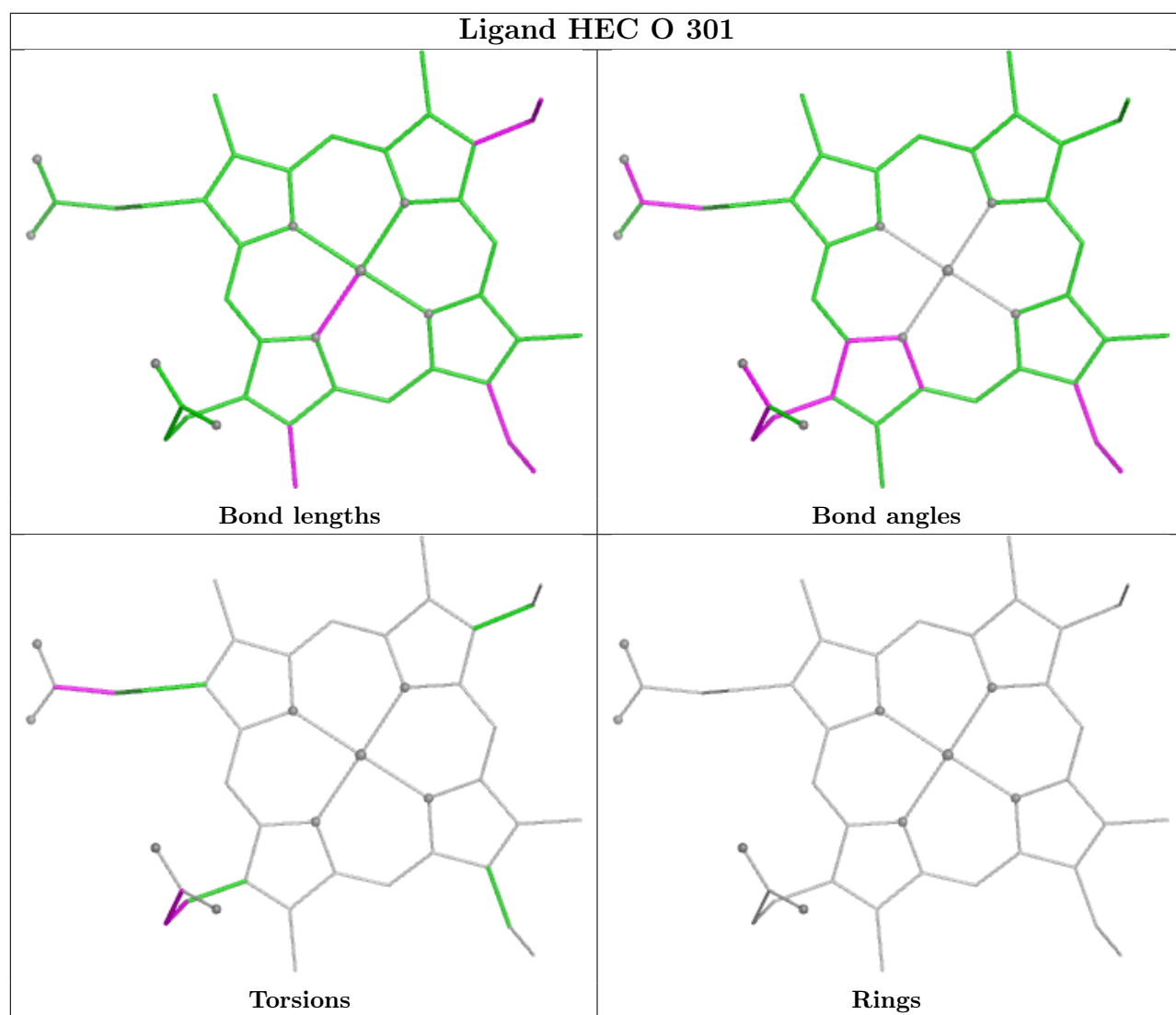


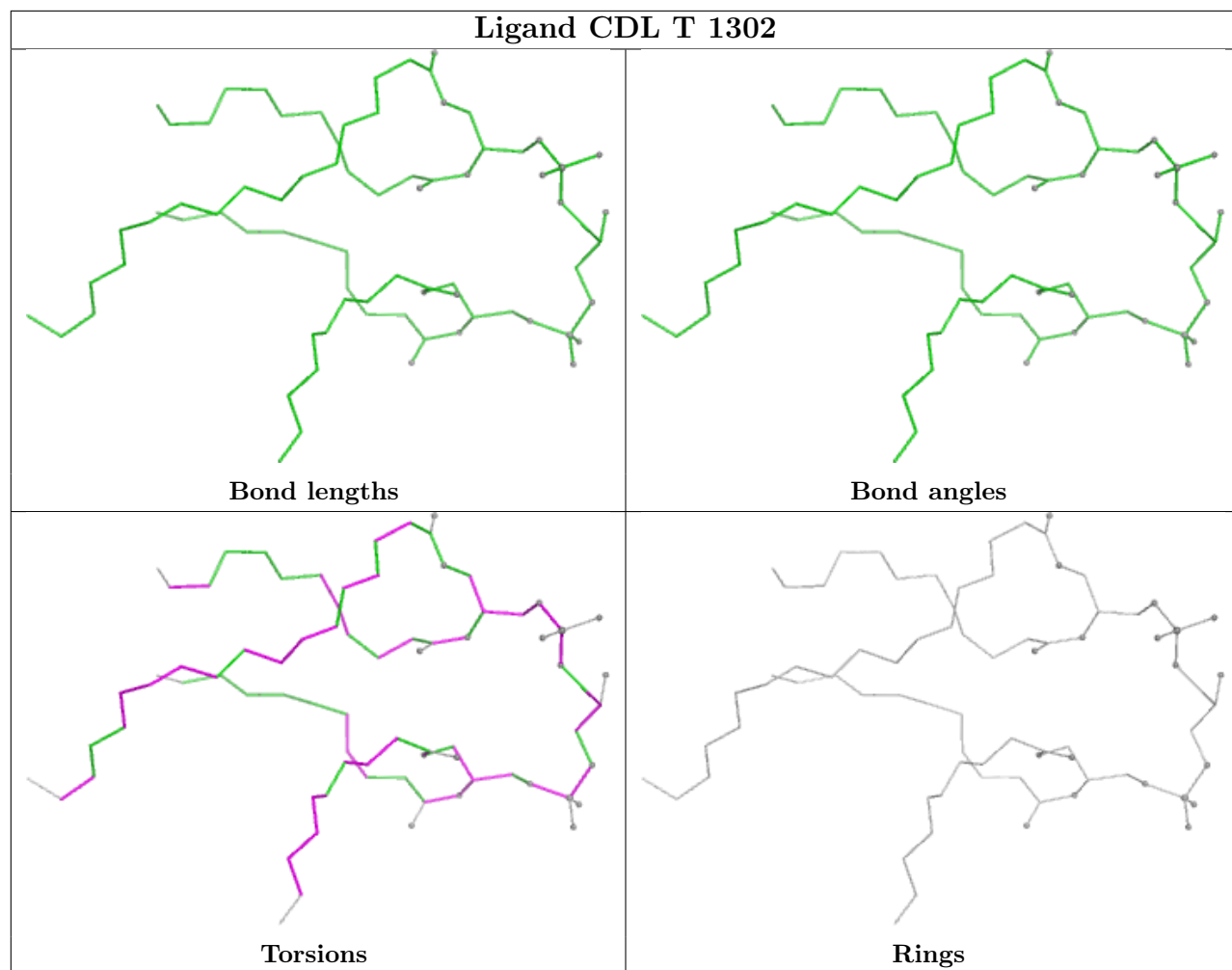


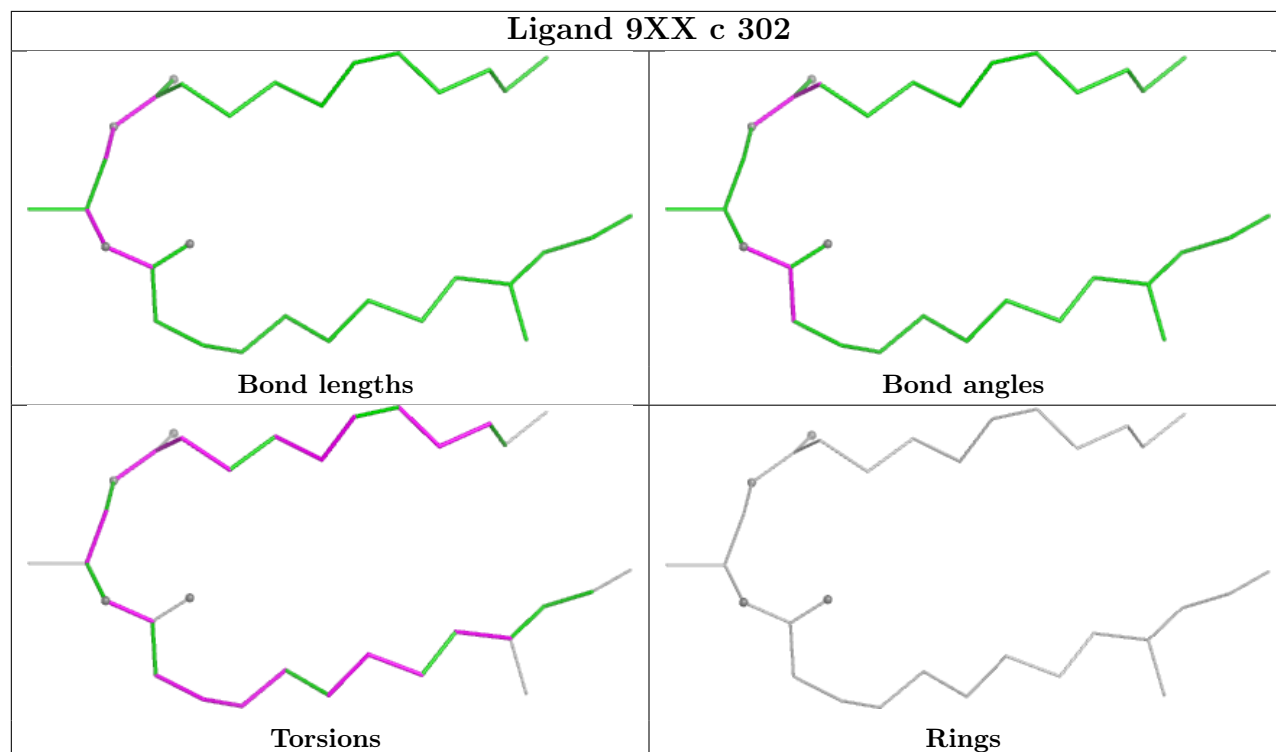
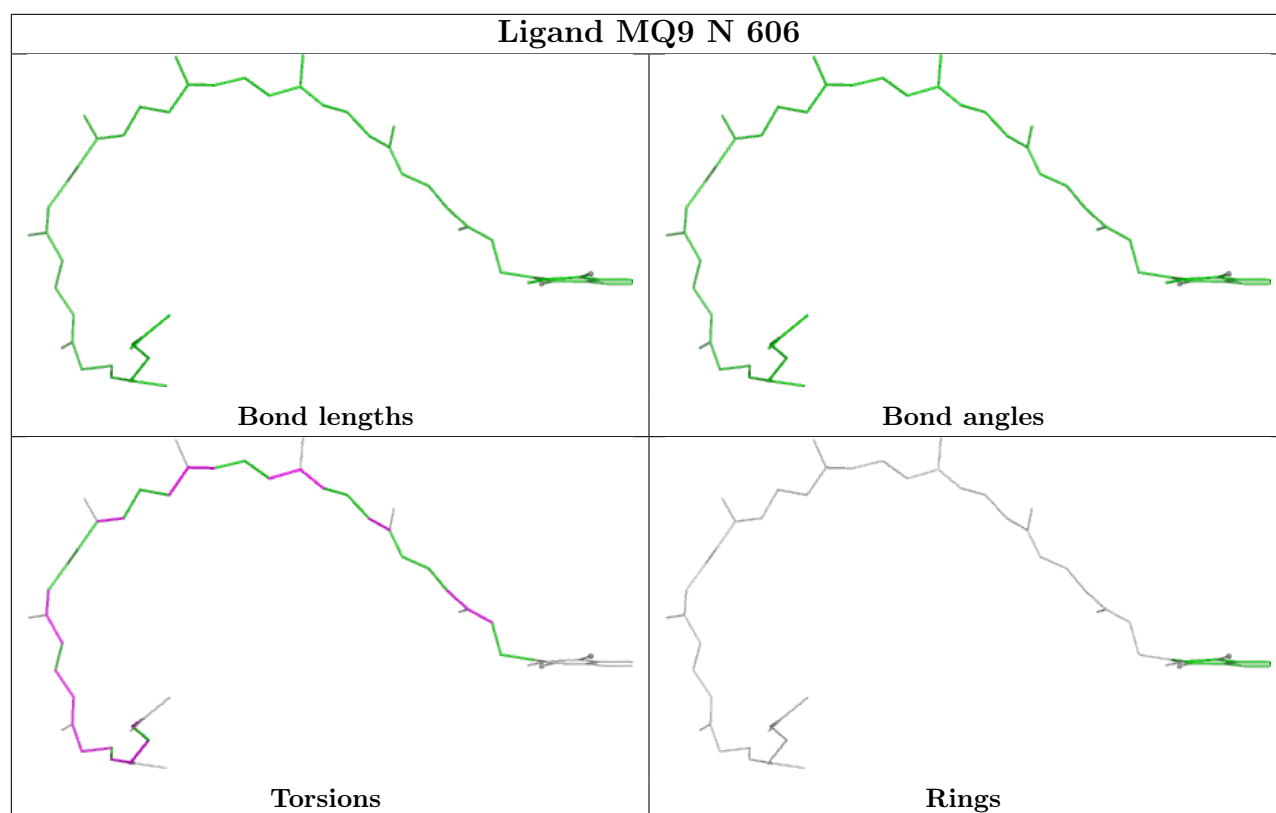


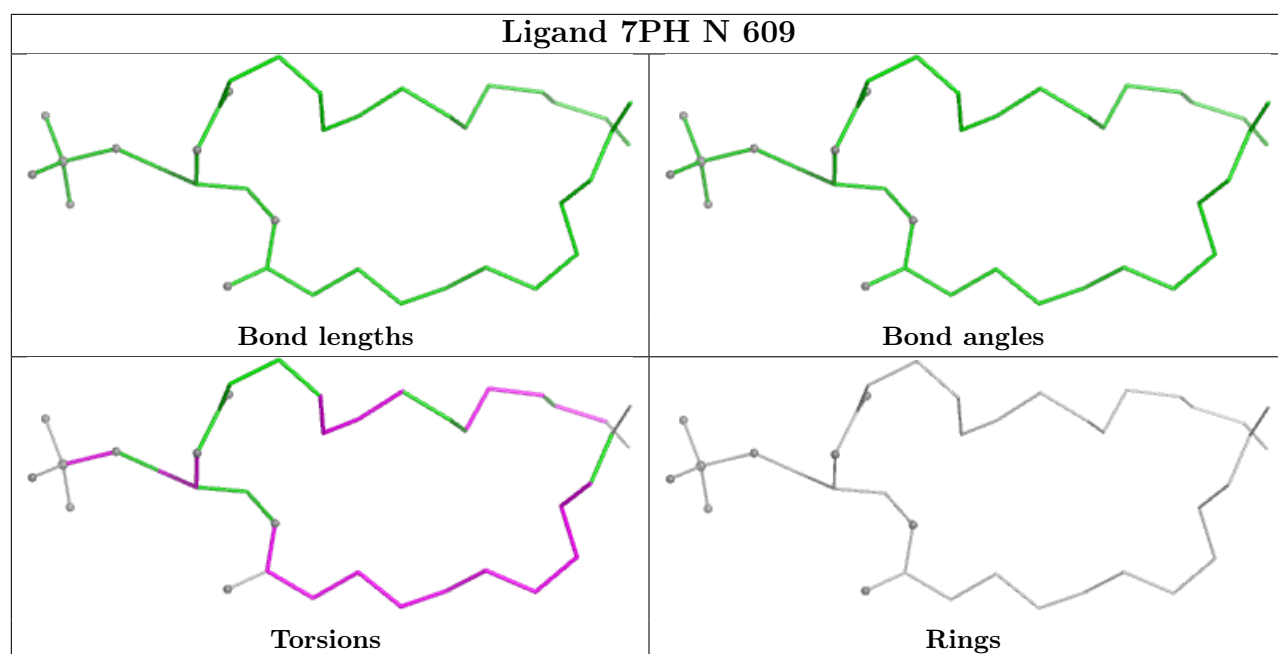


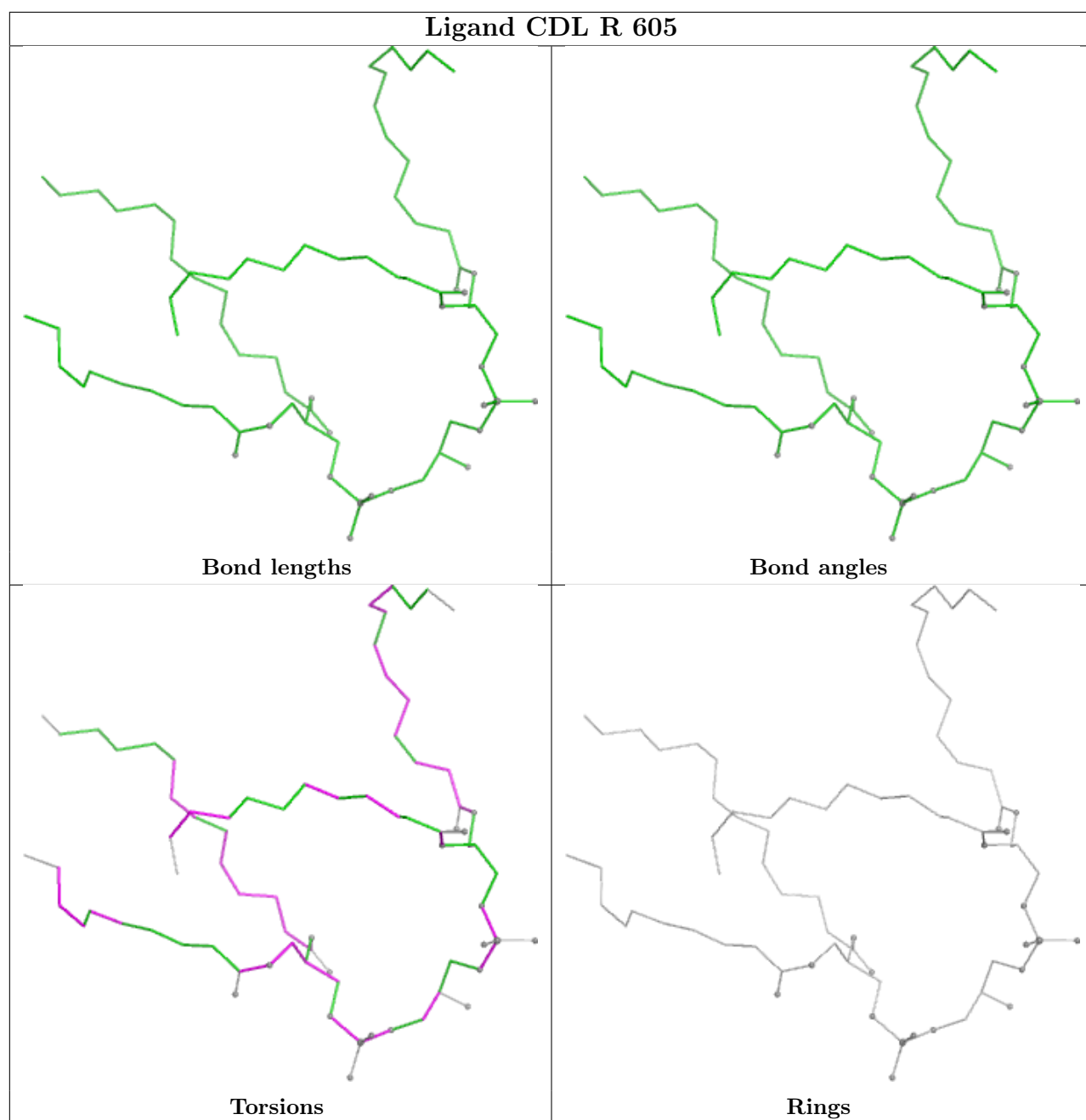


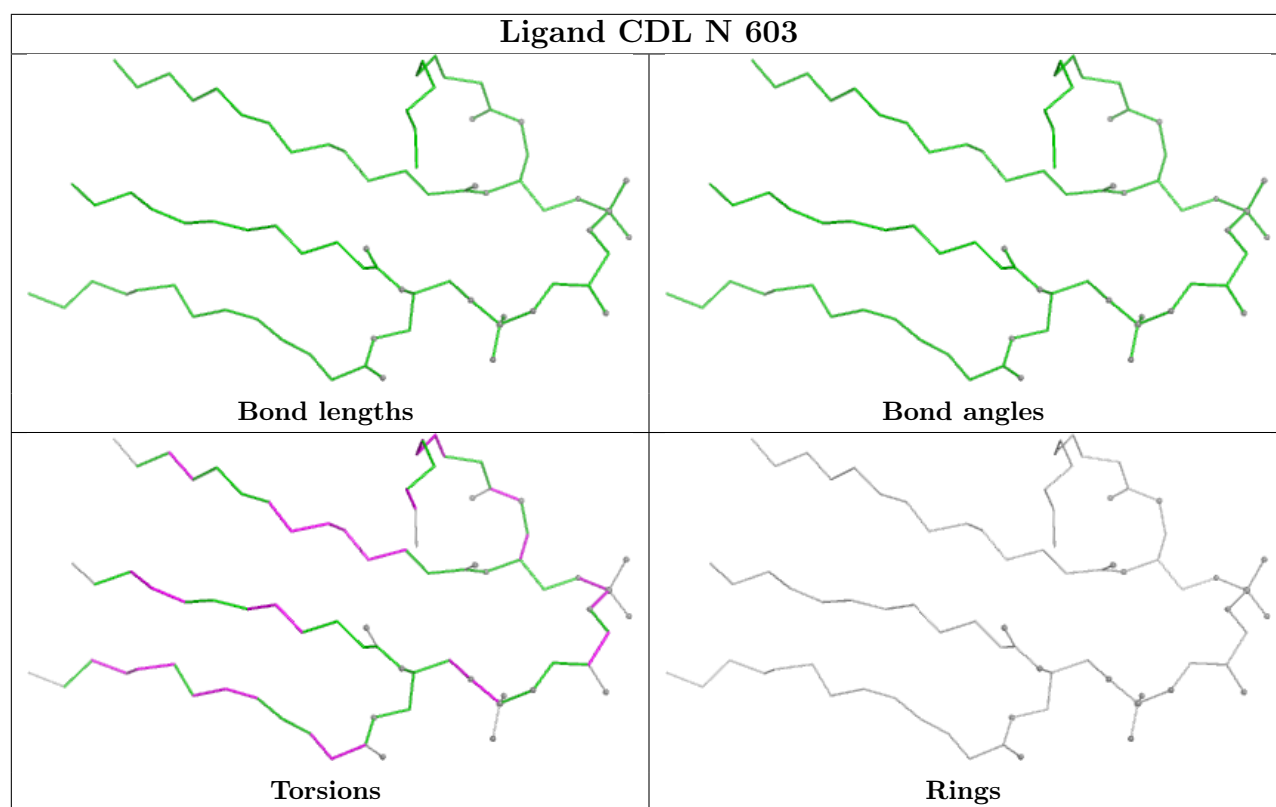


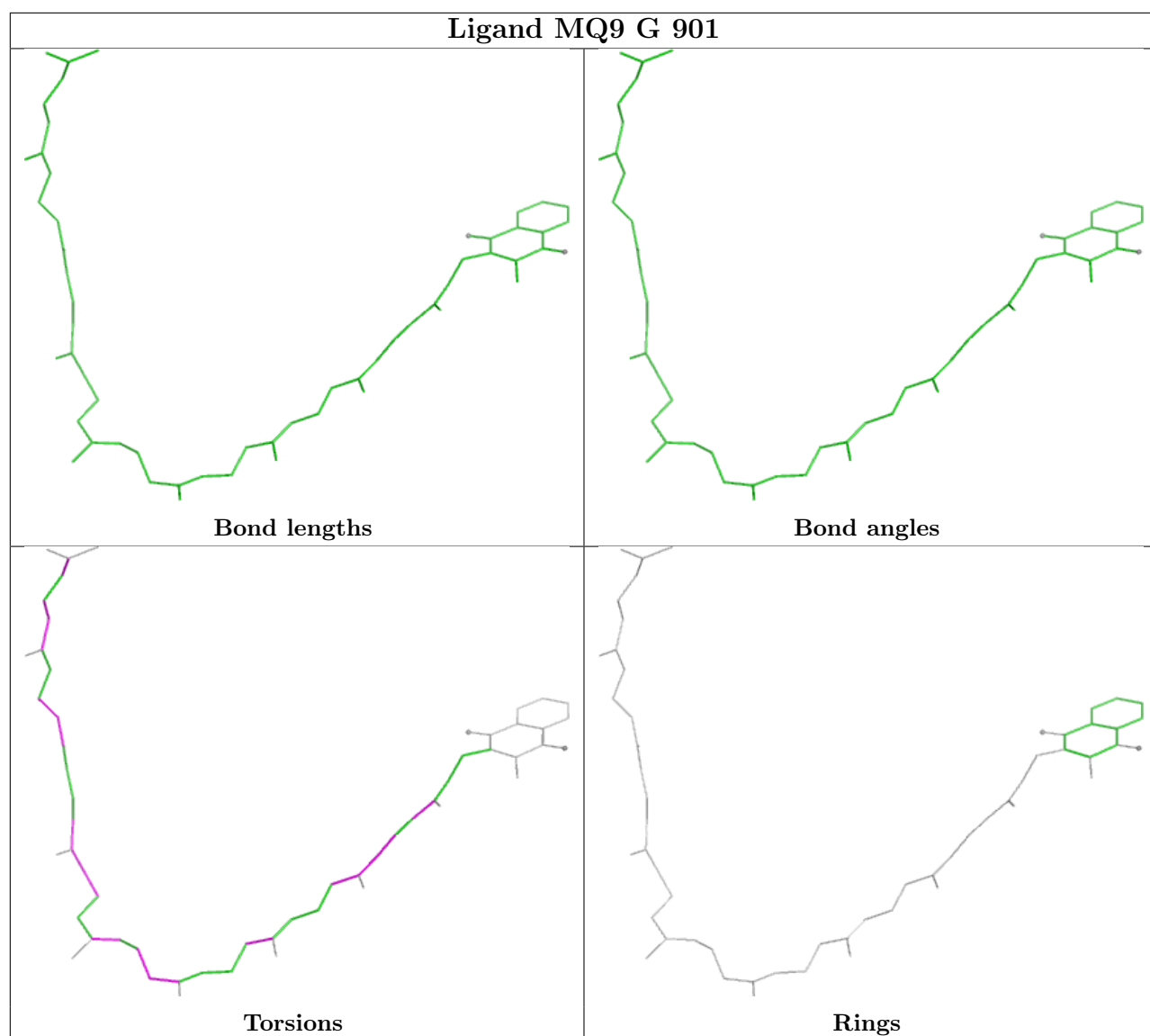


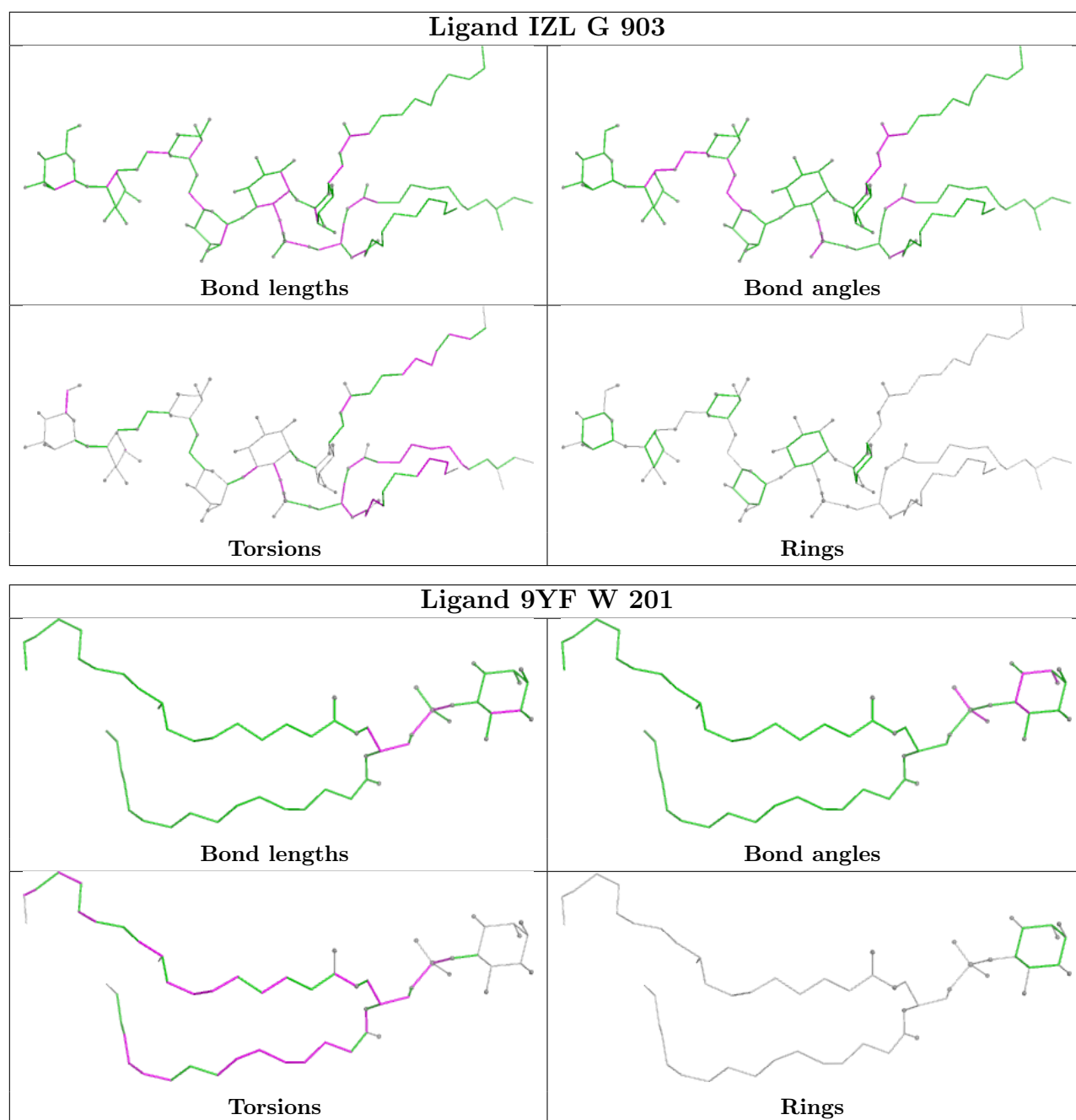


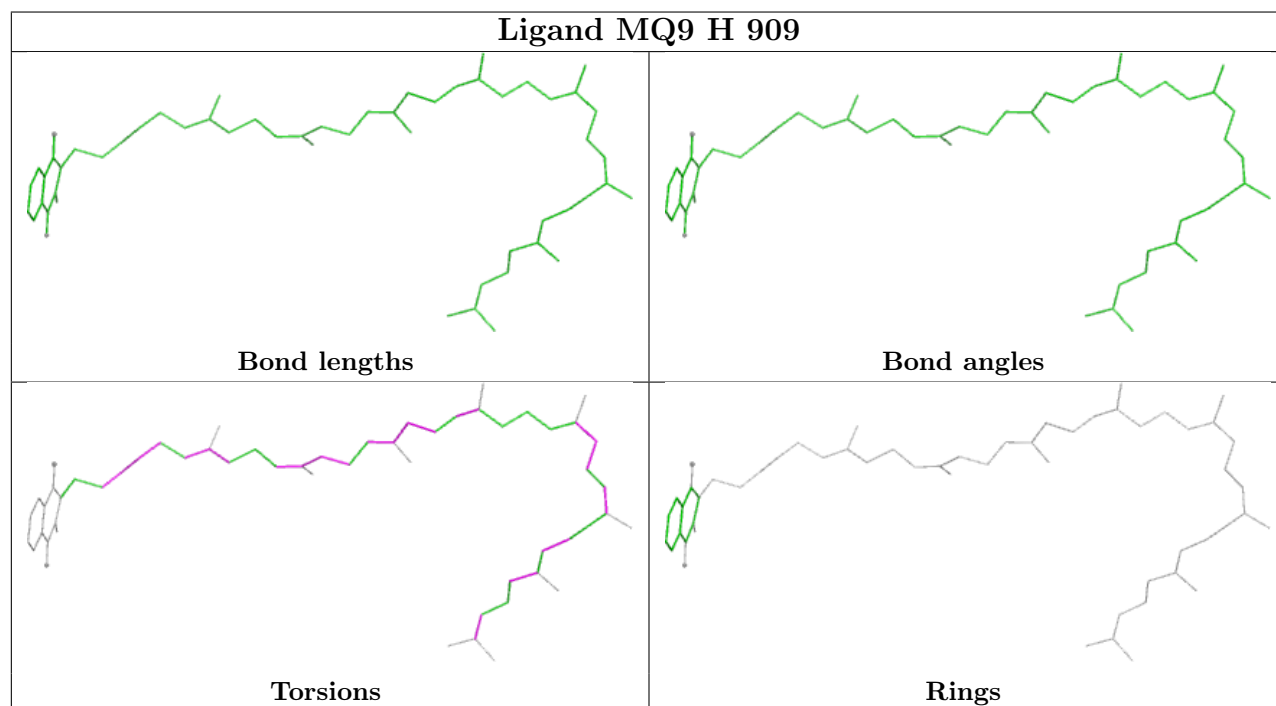
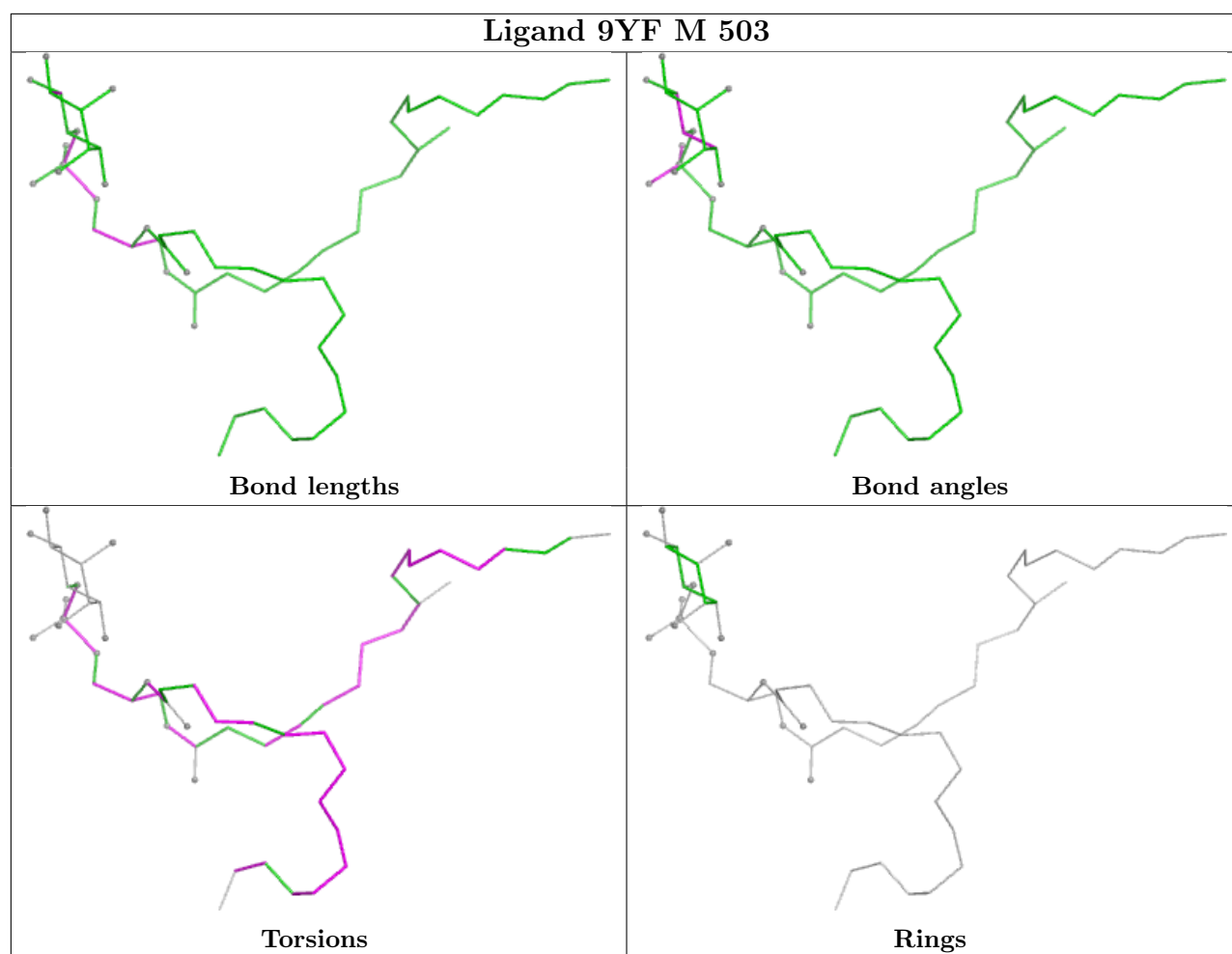


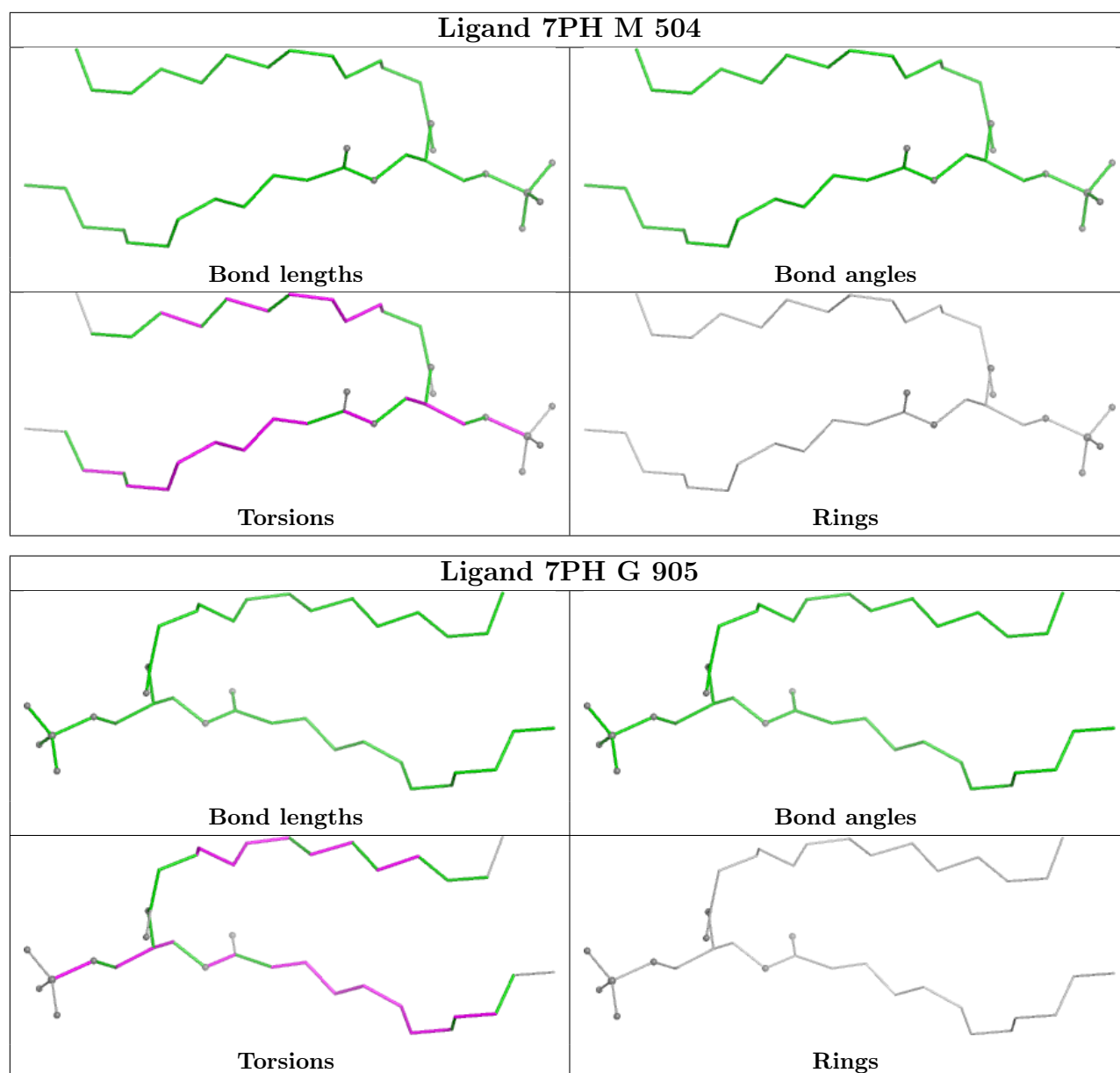


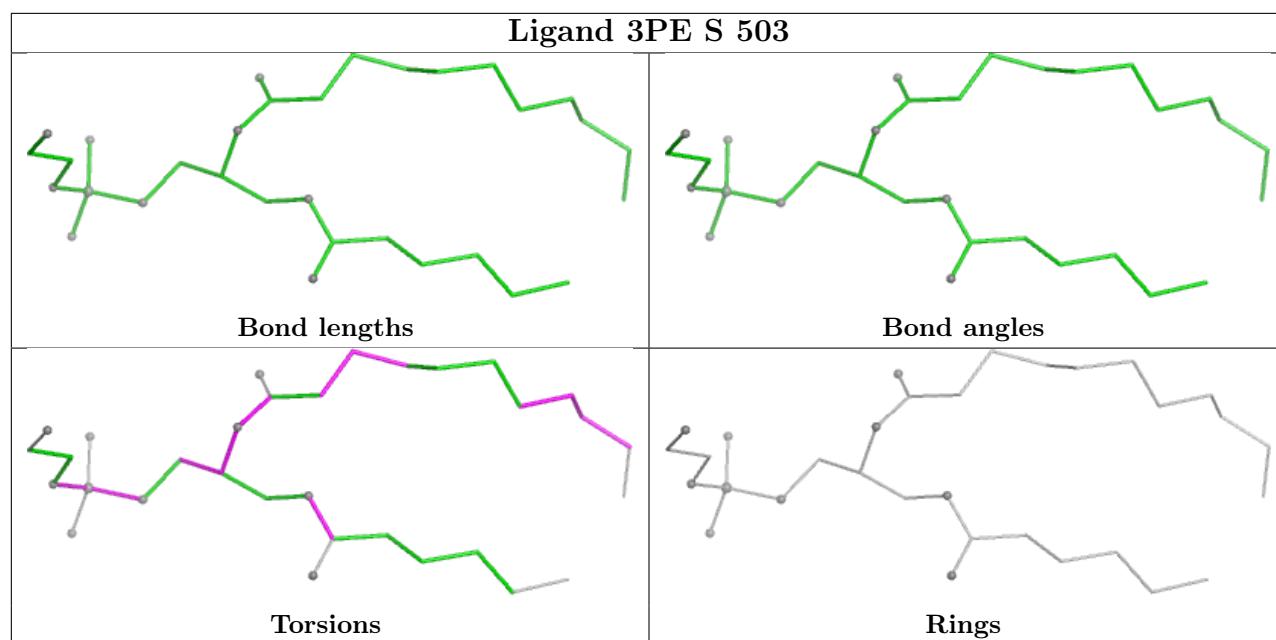
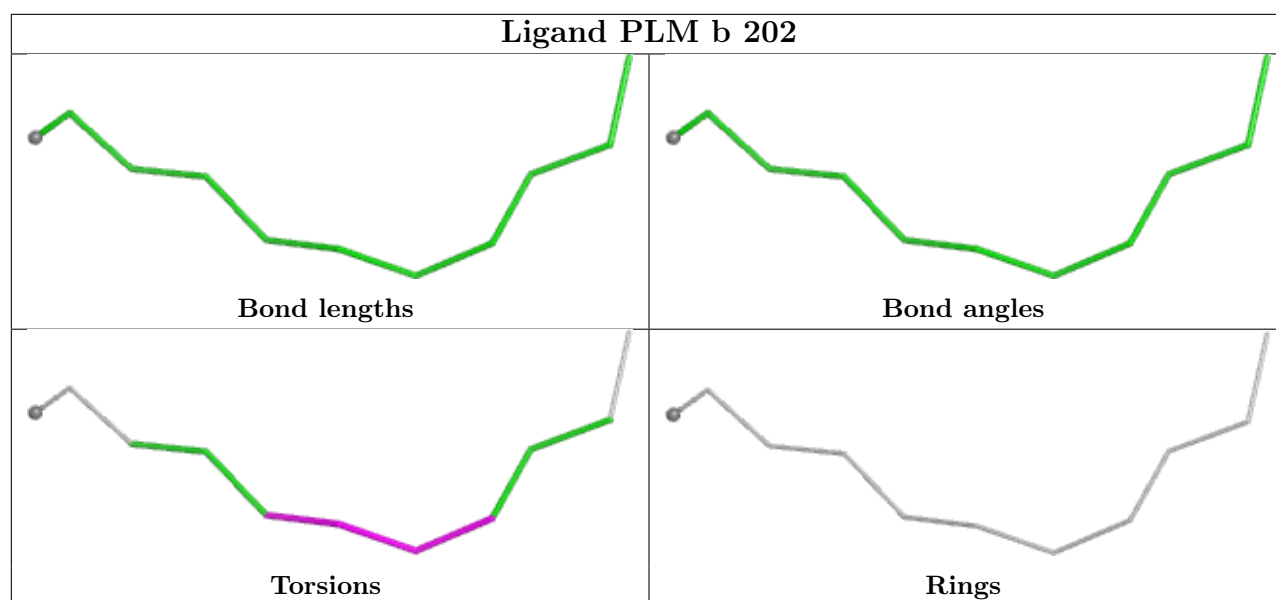


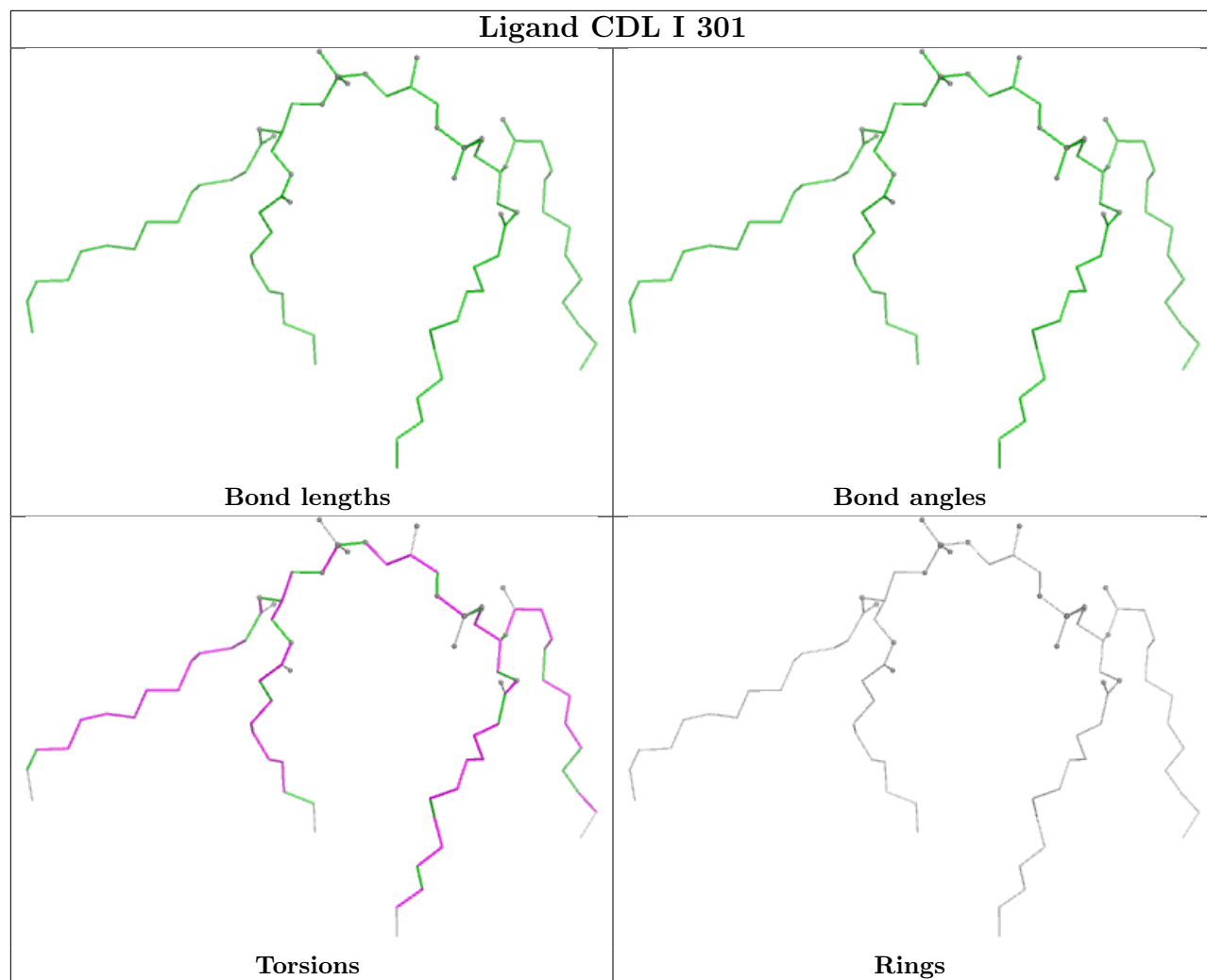


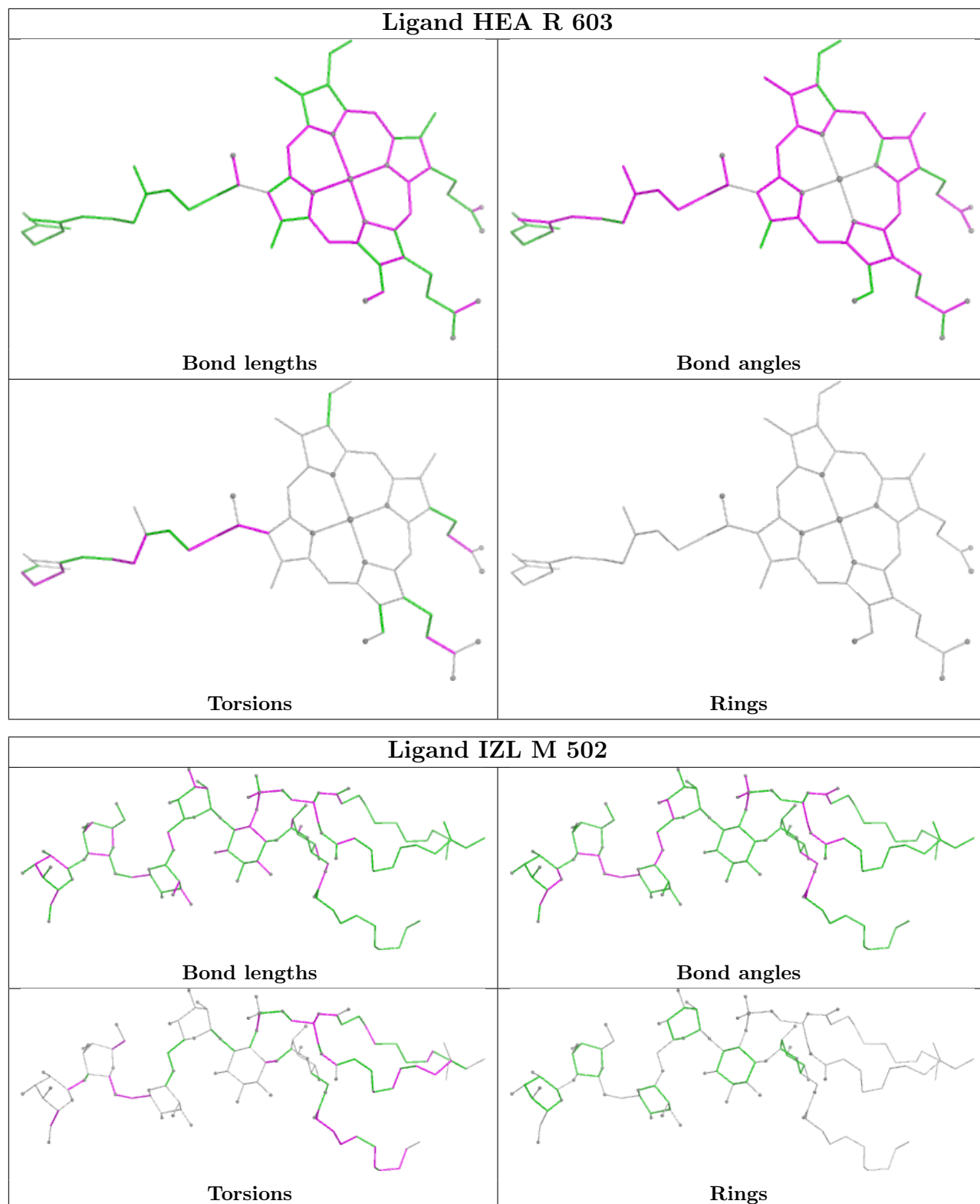


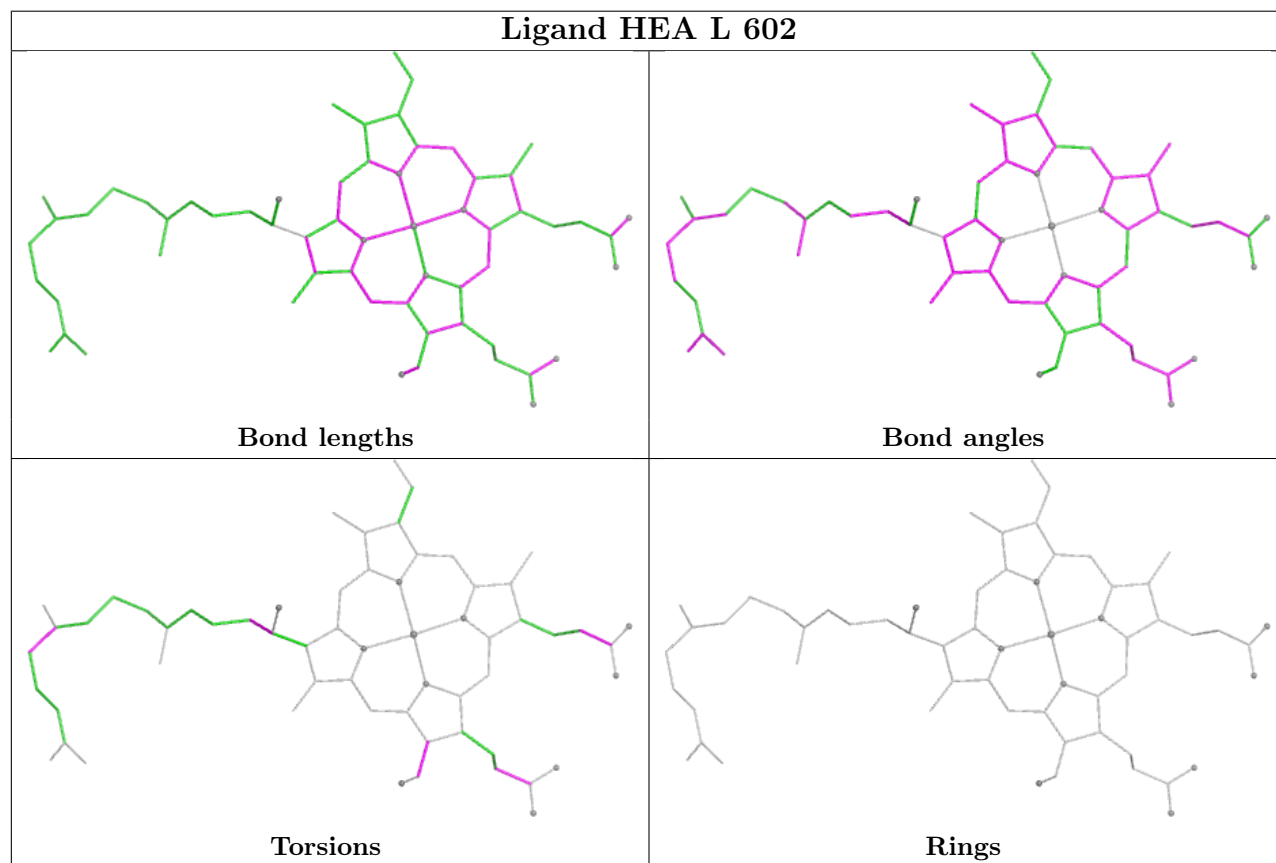
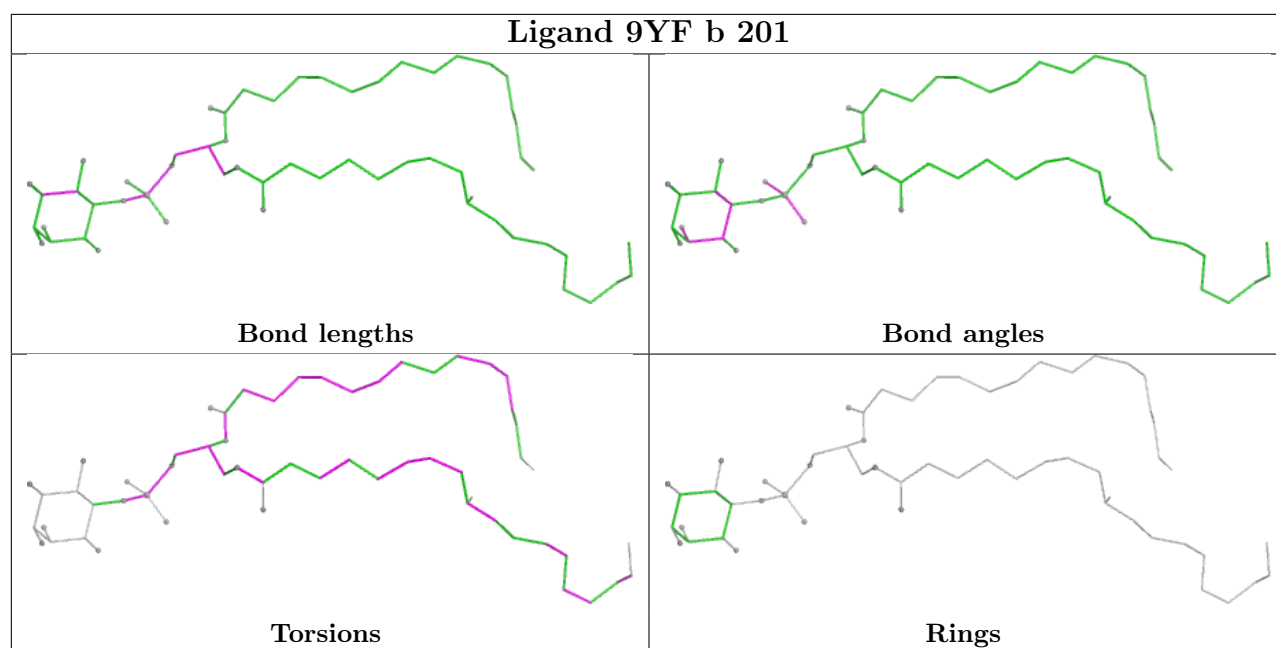


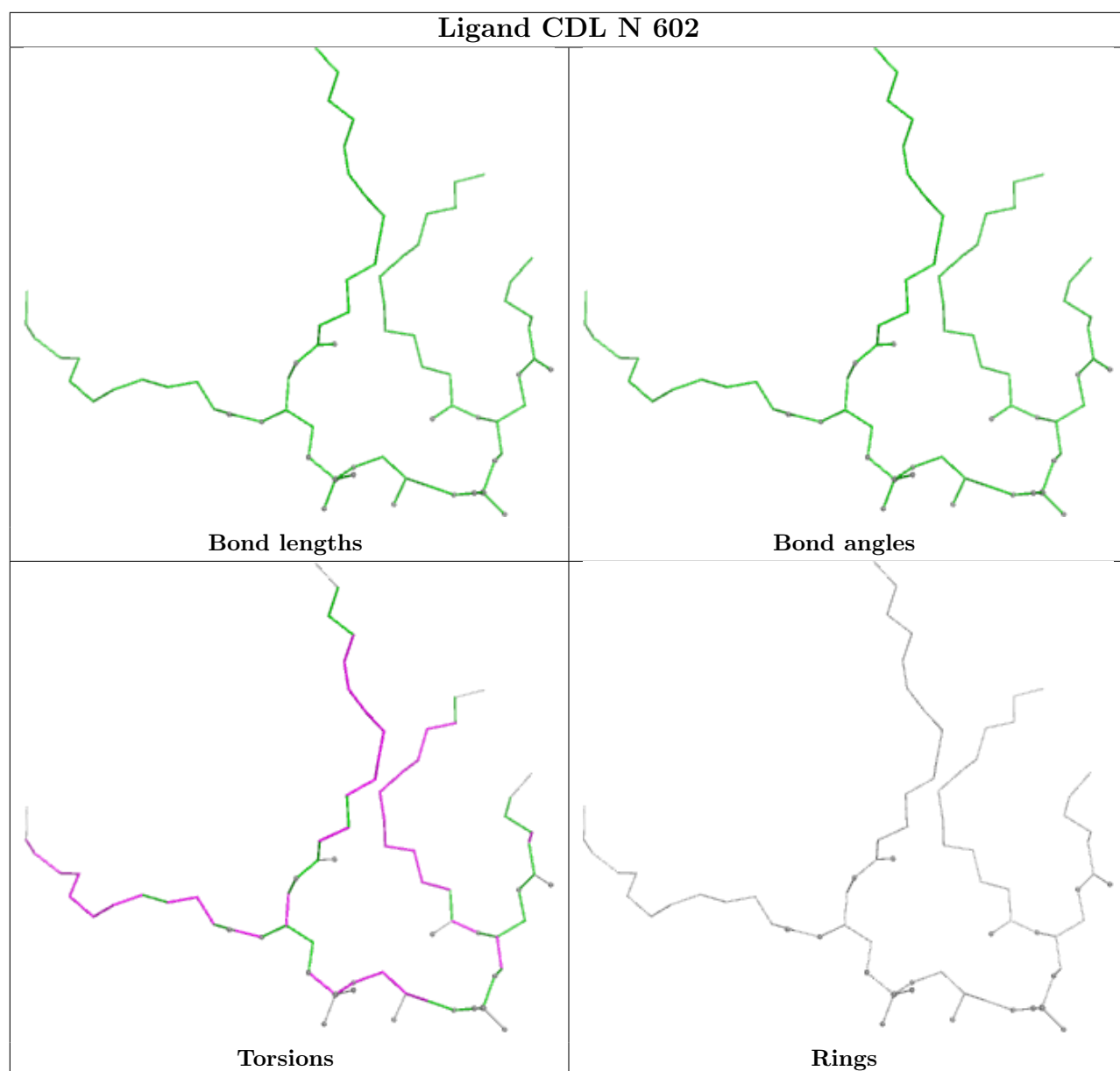


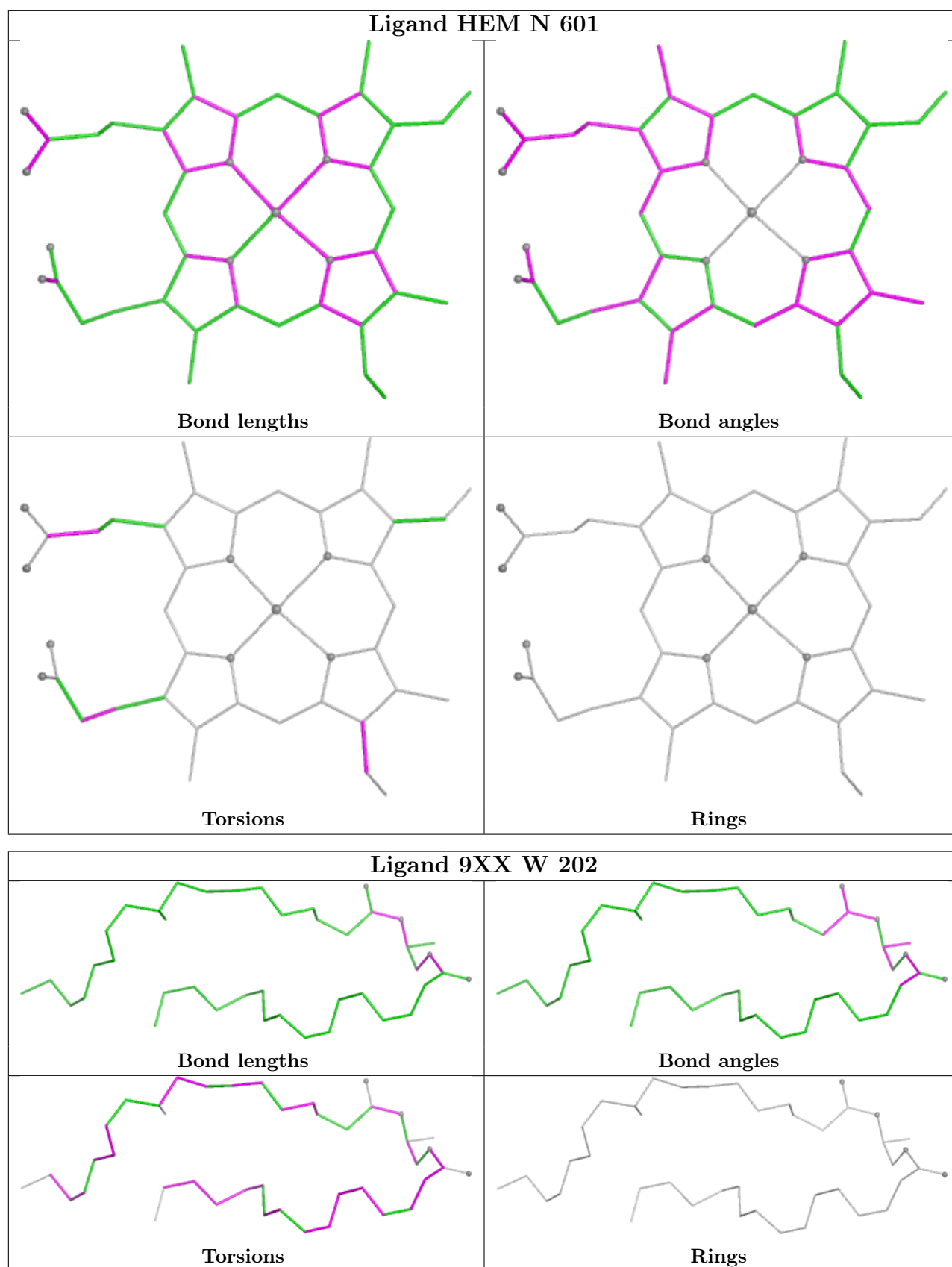


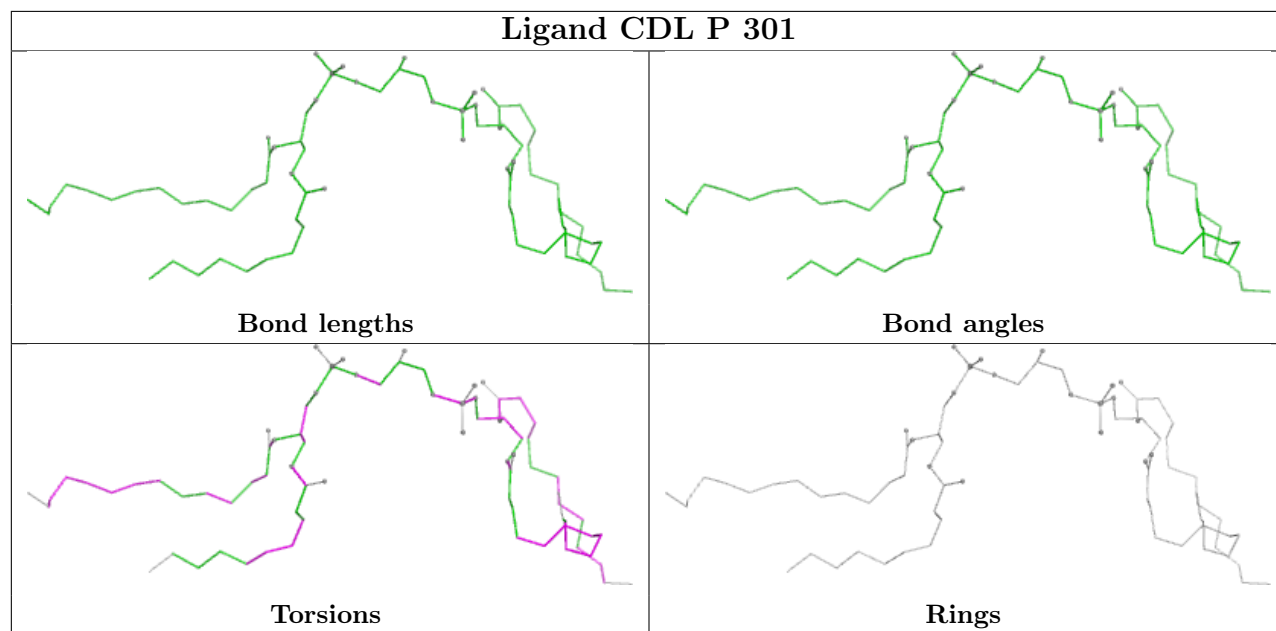
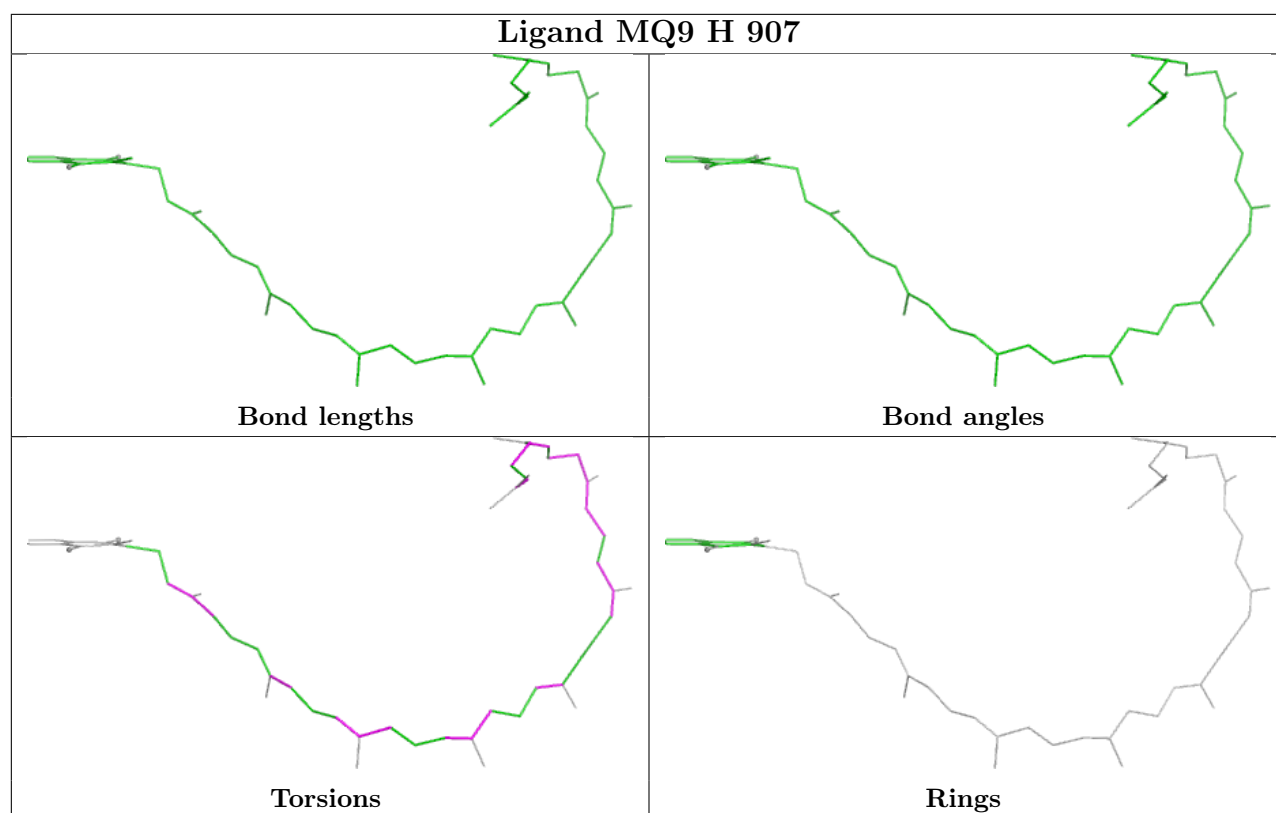


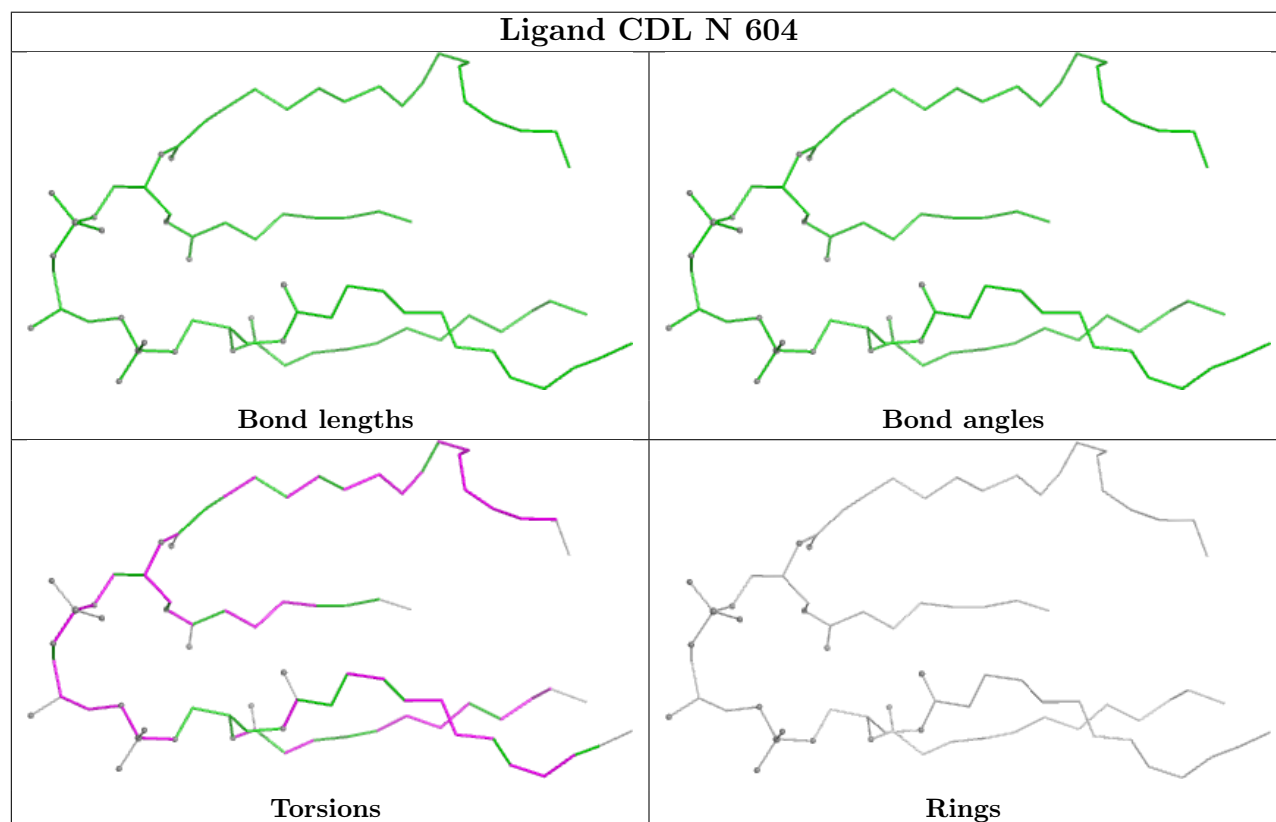
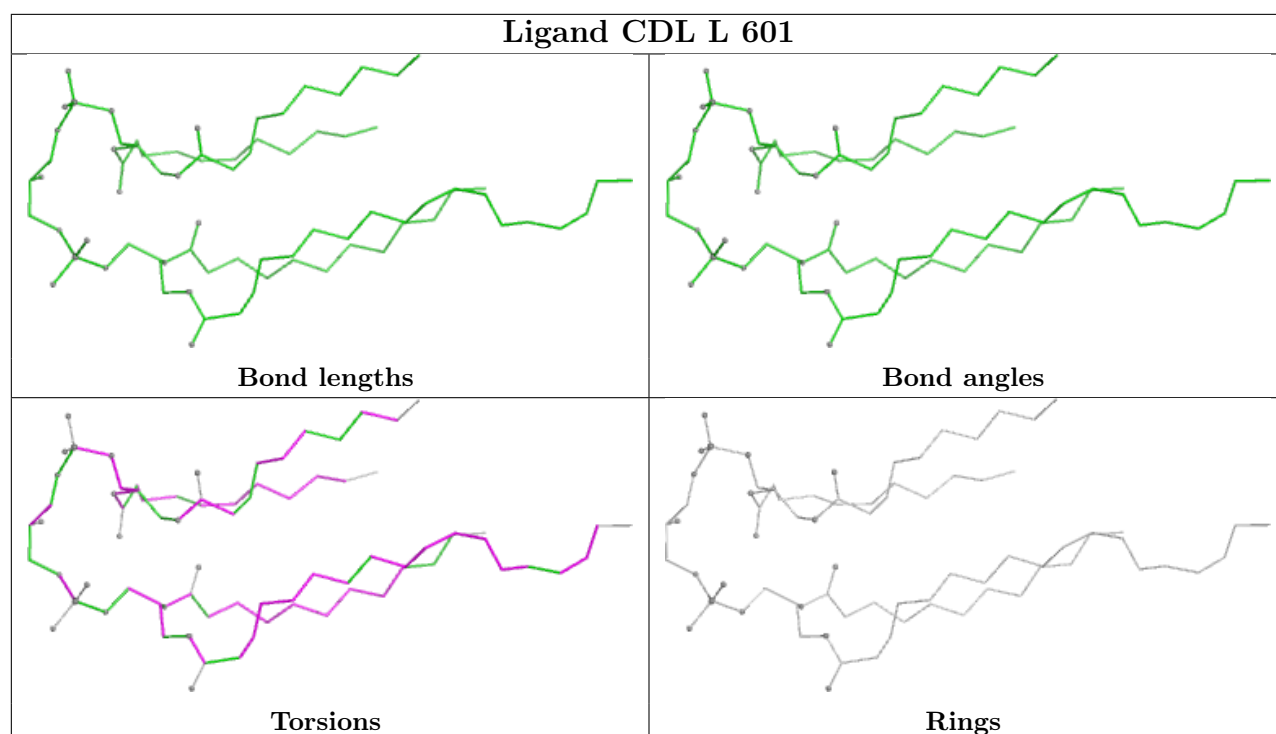


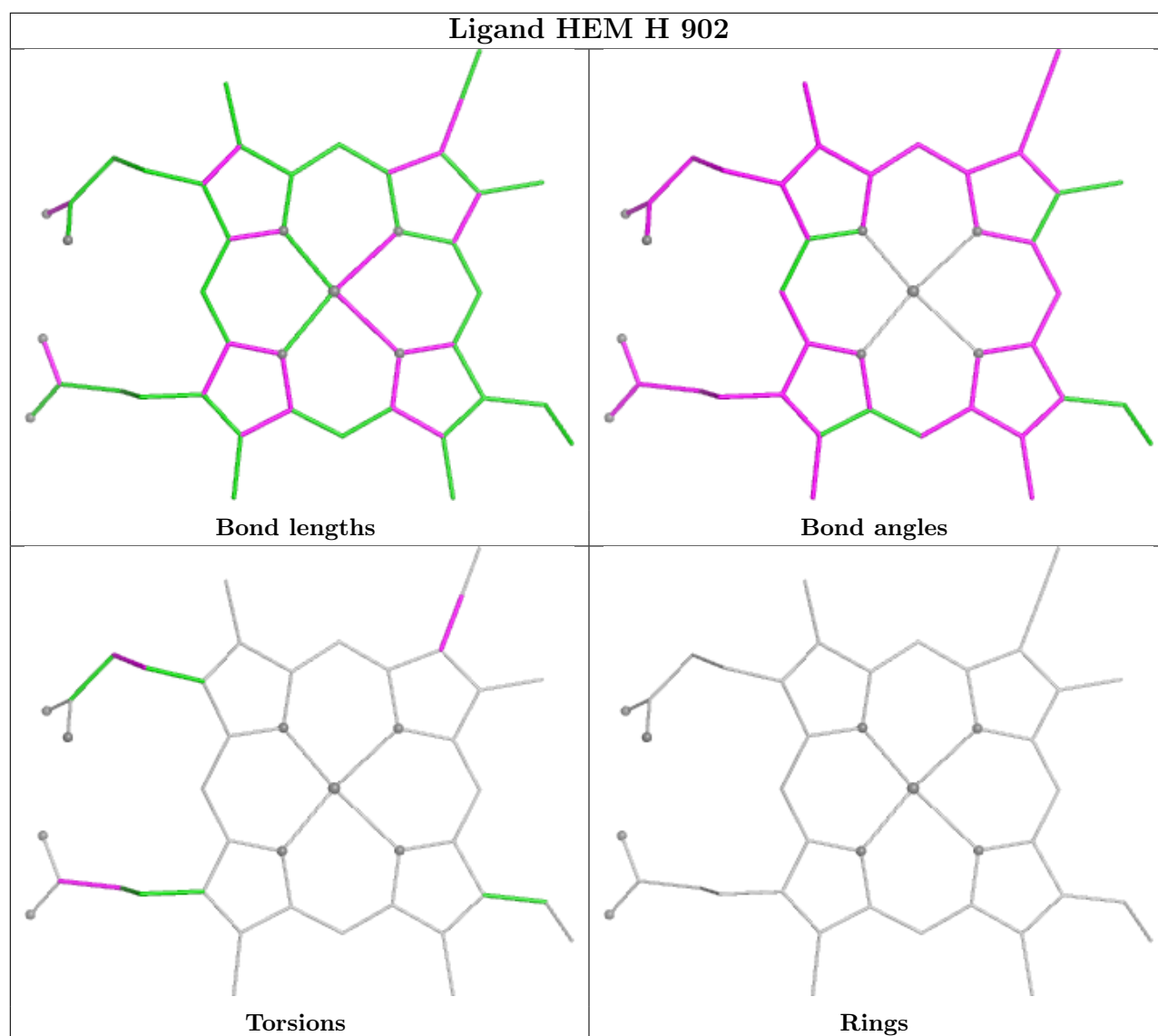


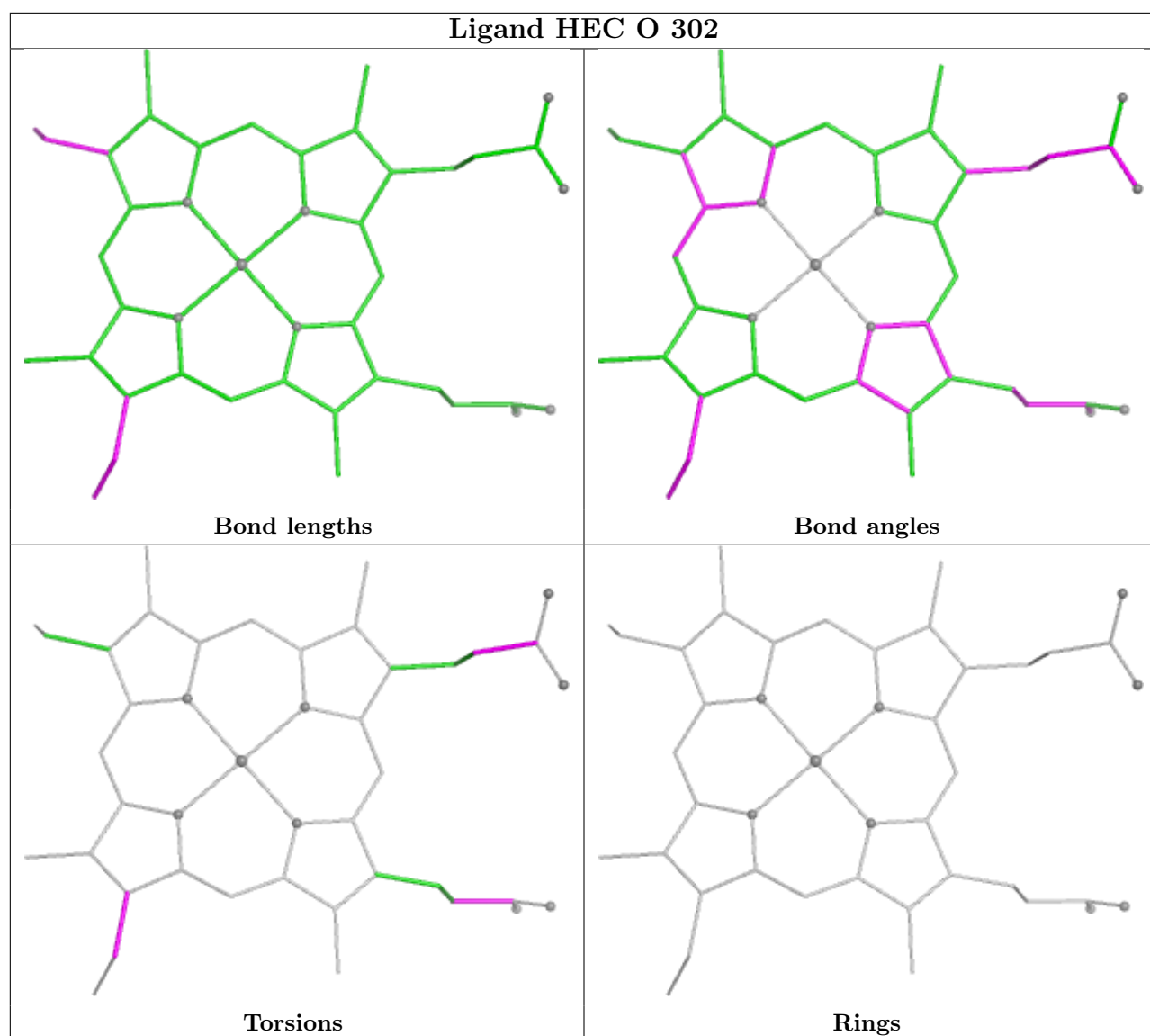


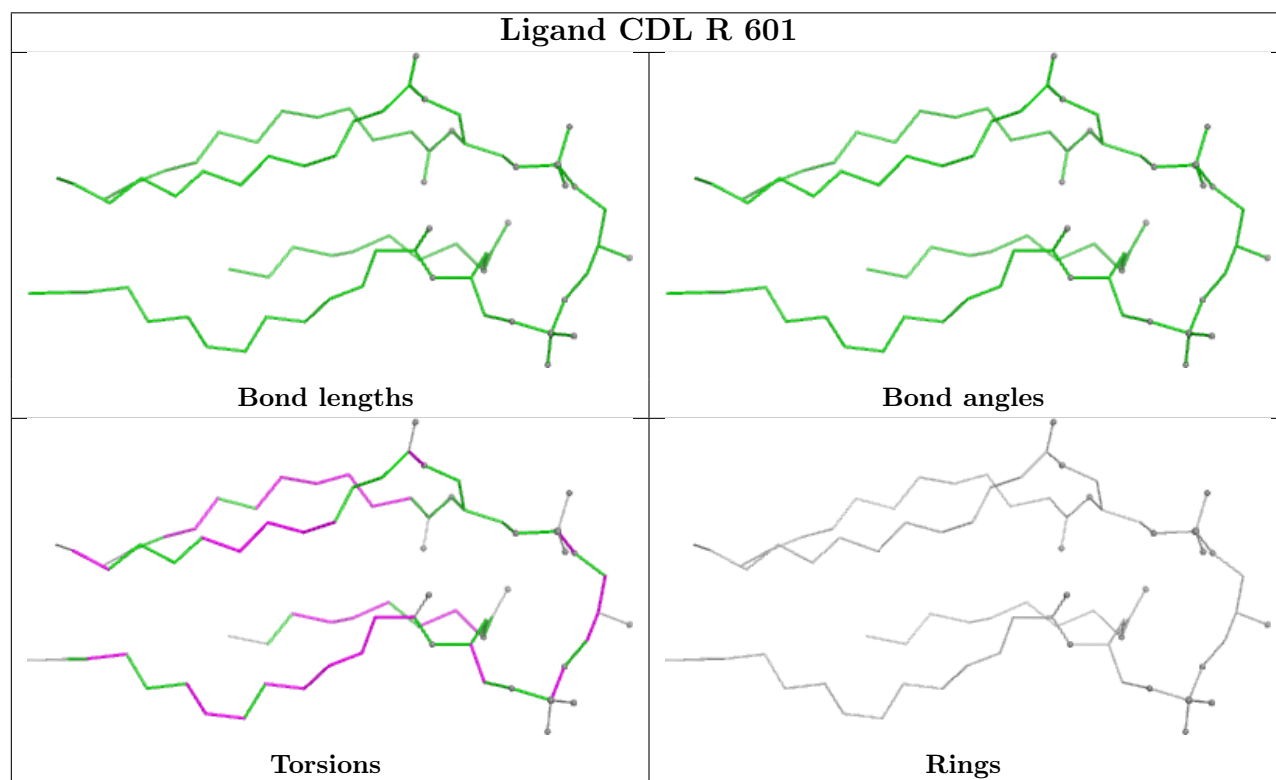
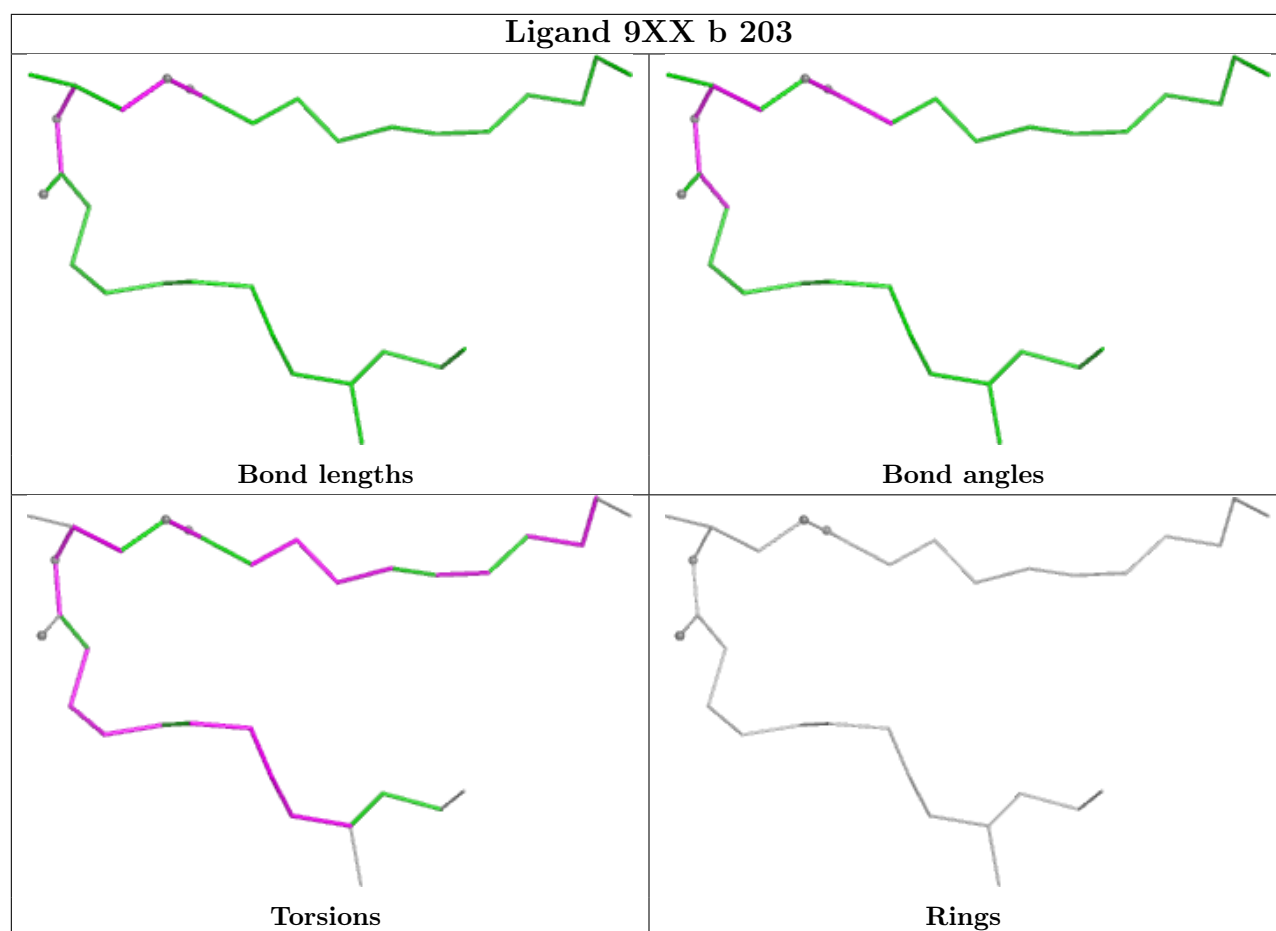


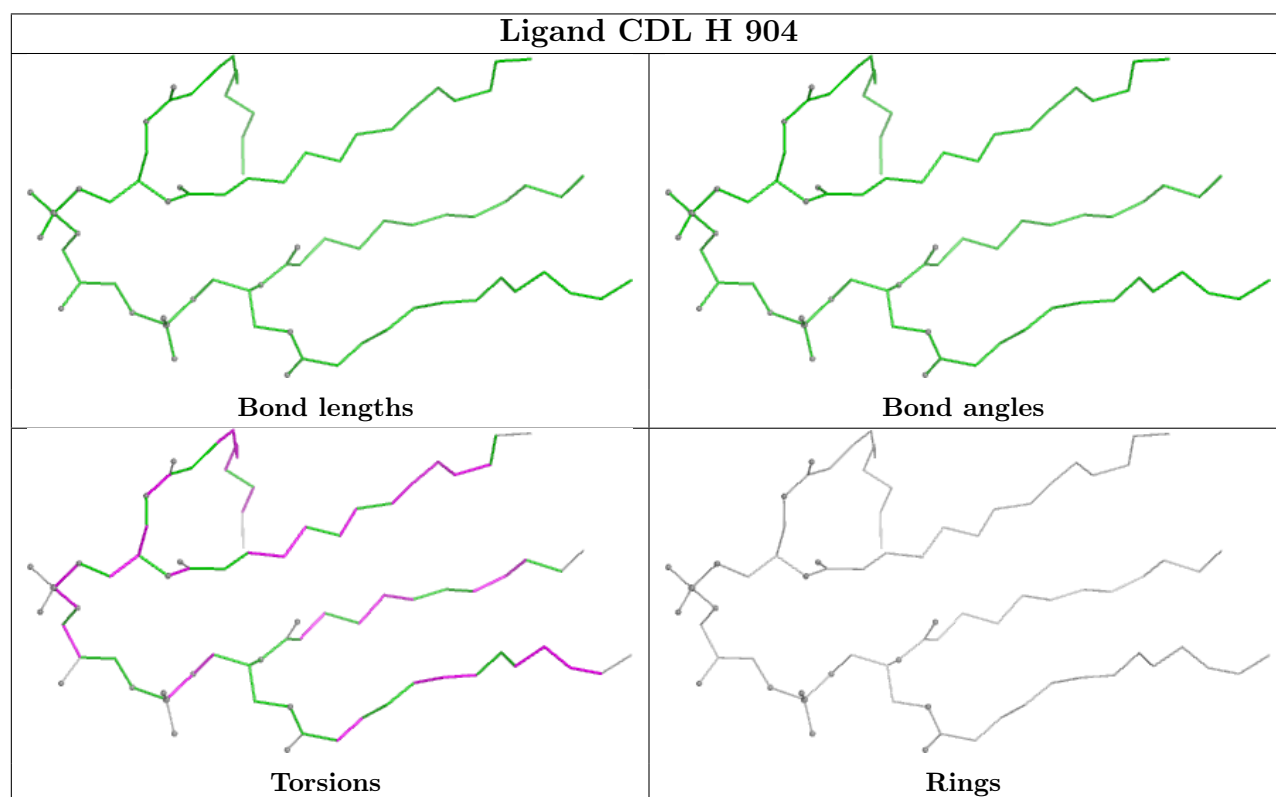
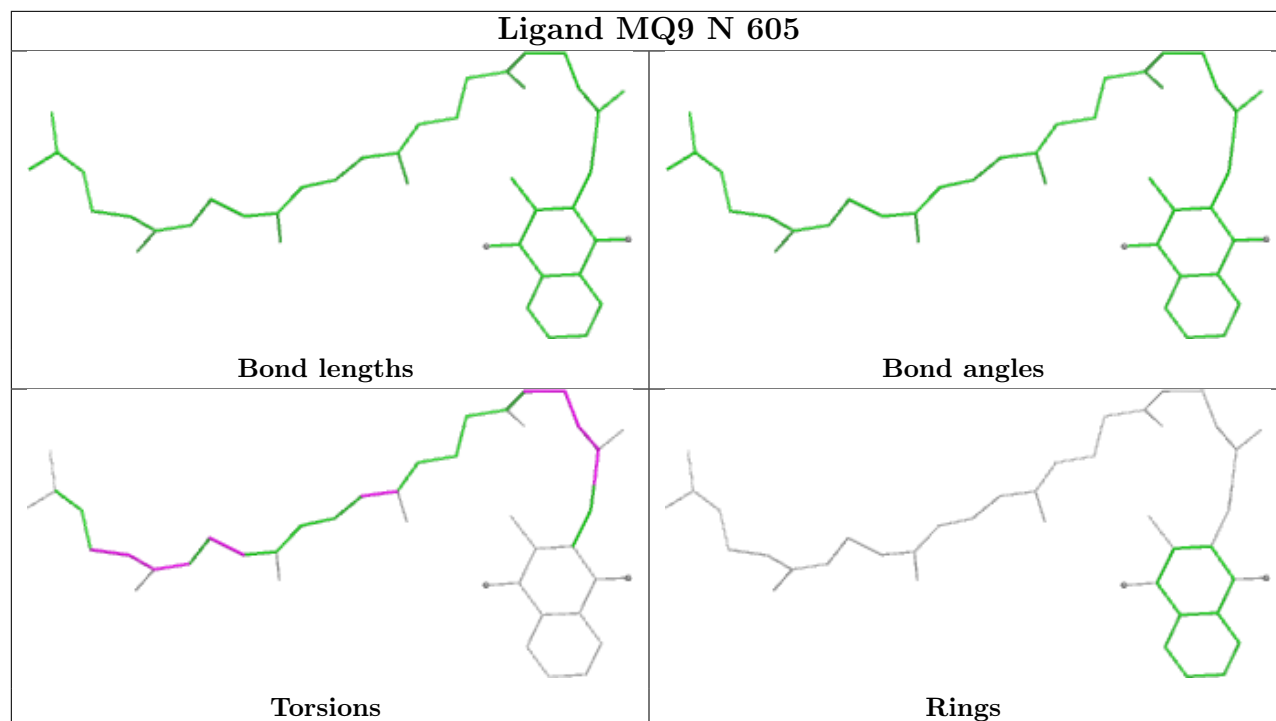


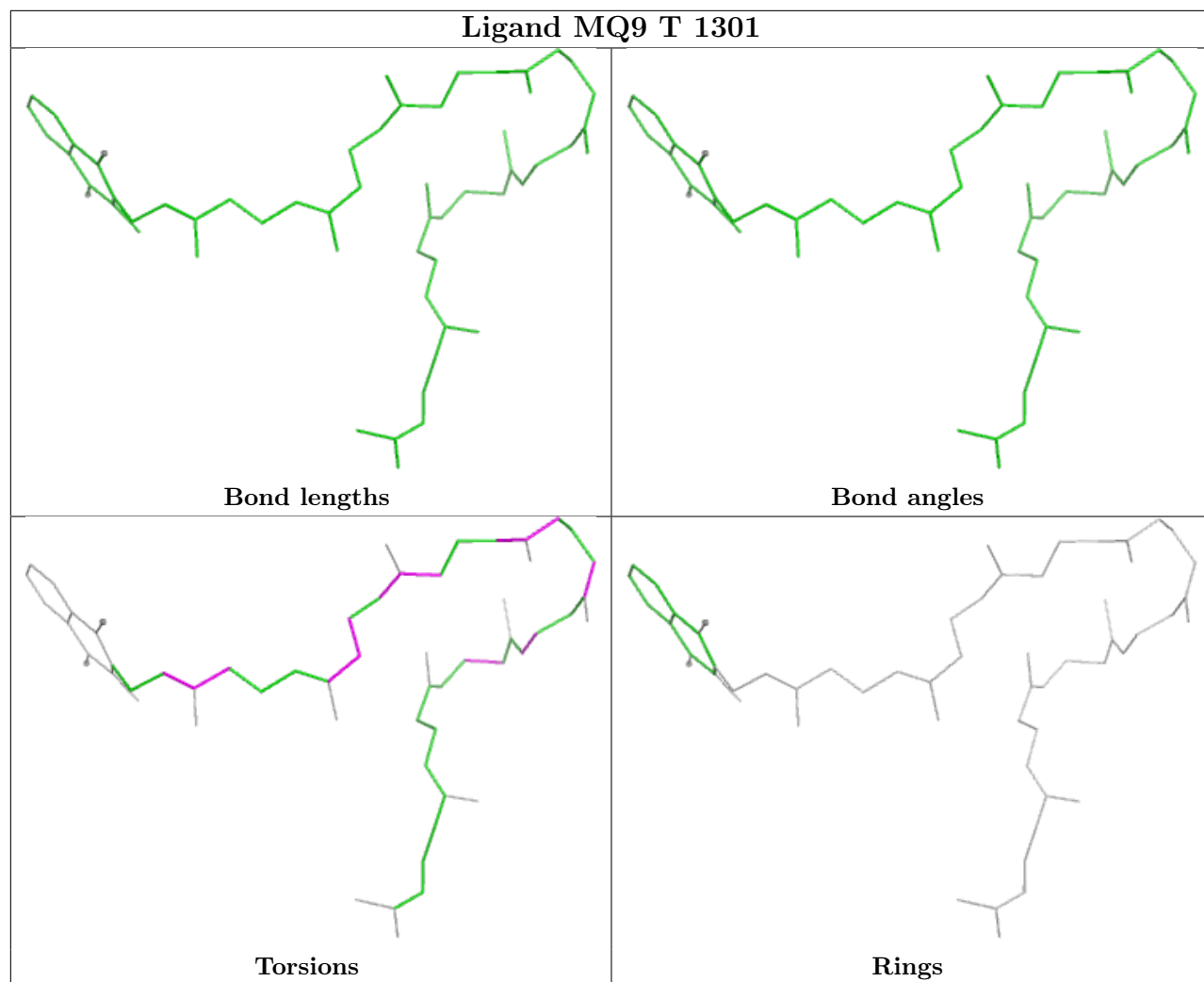


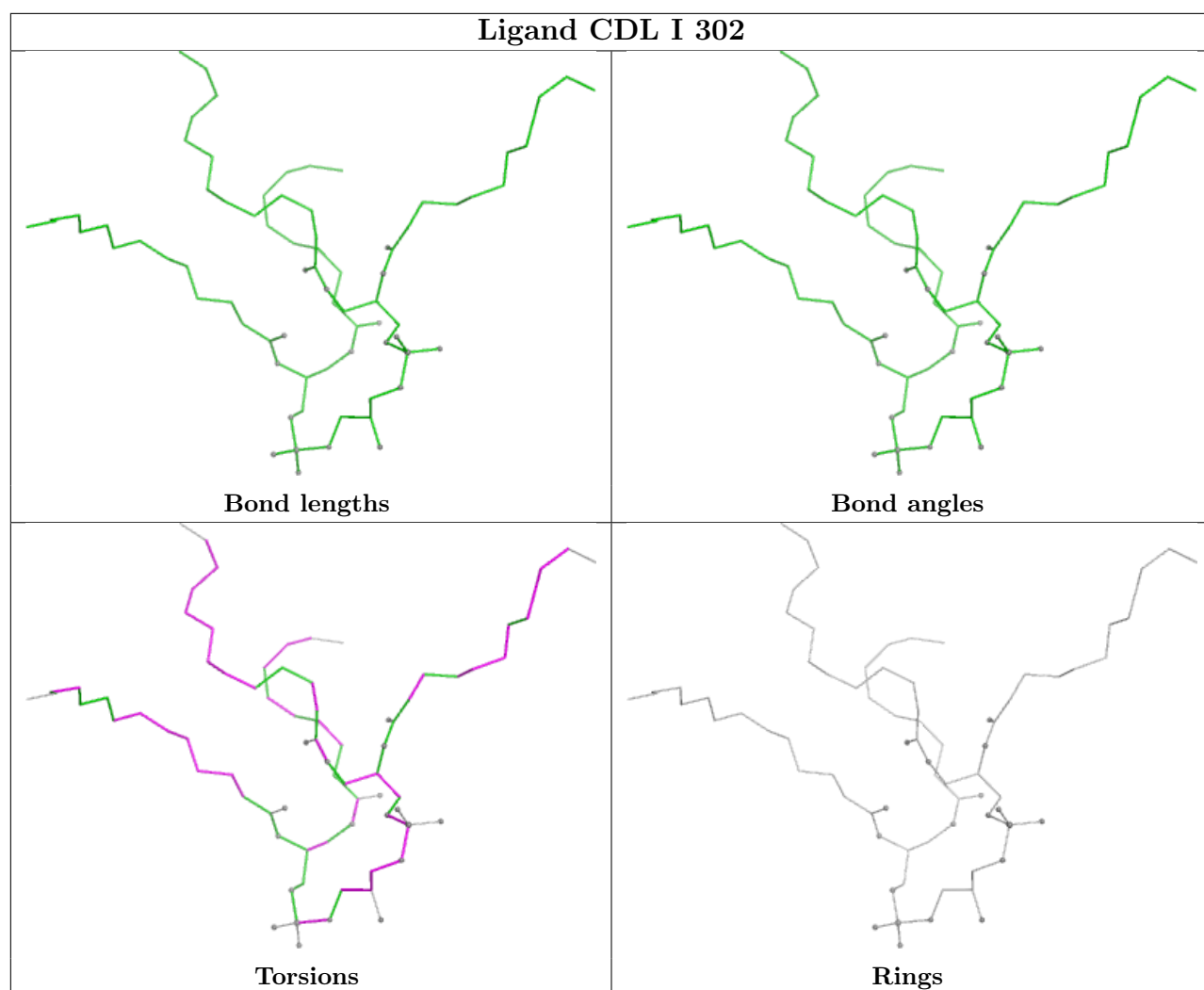


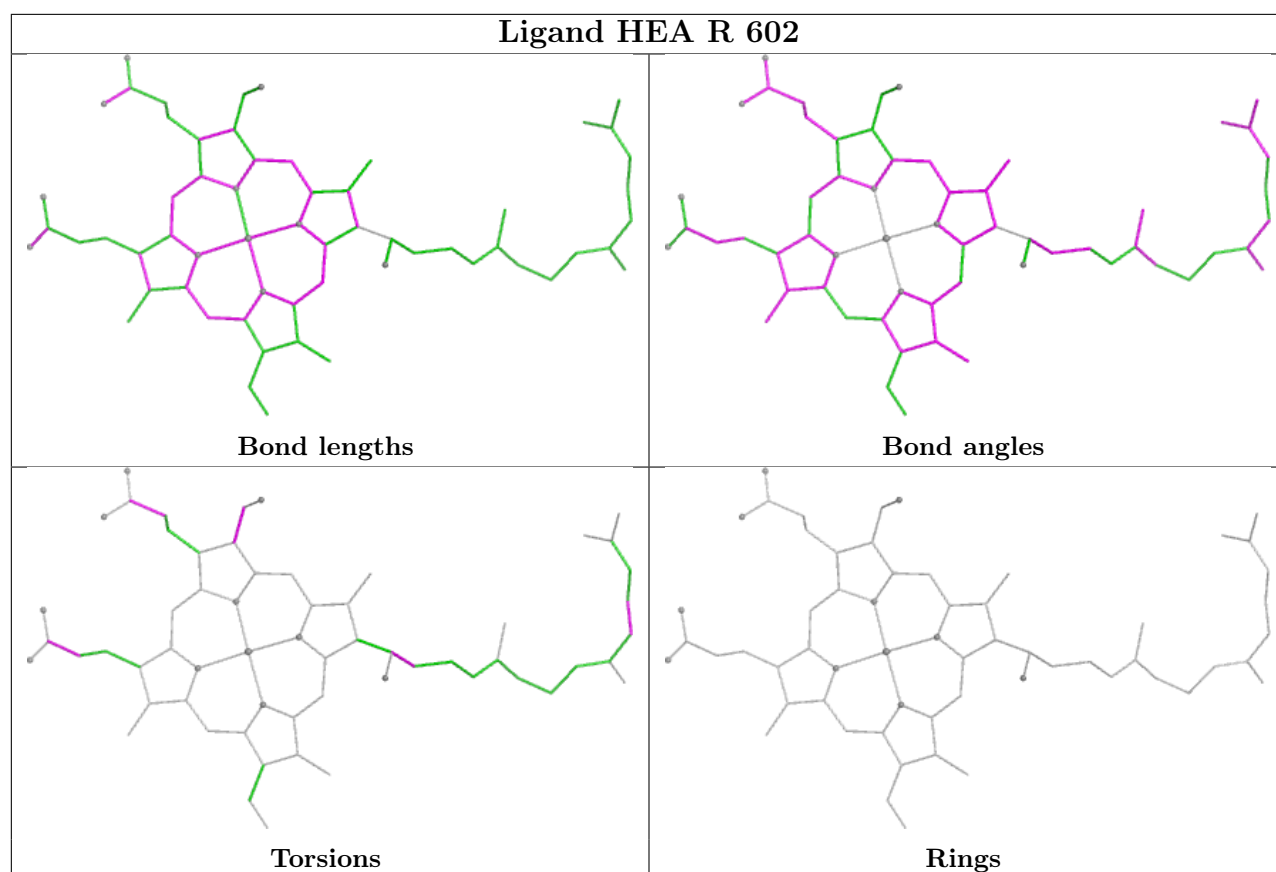












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

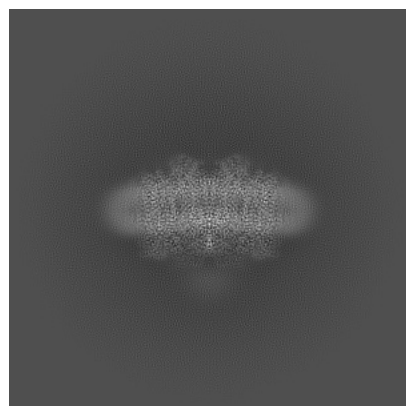
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17211. These allow visual inspection of the internal detail of the map and identification of artifacts.

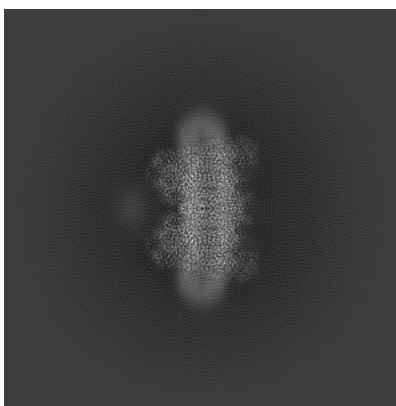
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

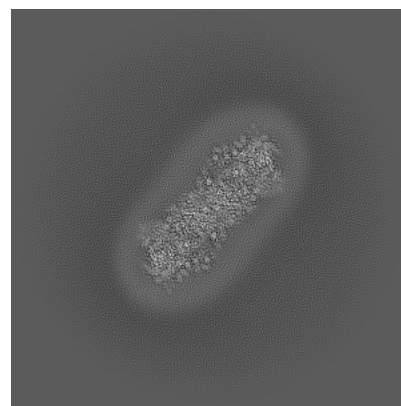
6.1.1 Primary map



X

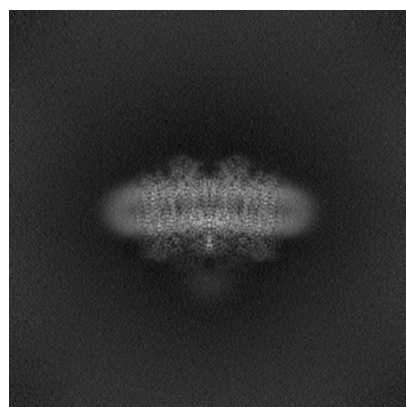


Y

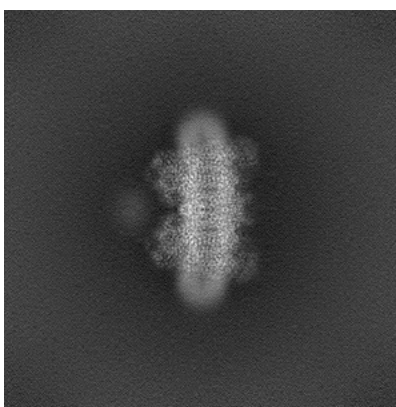


Z

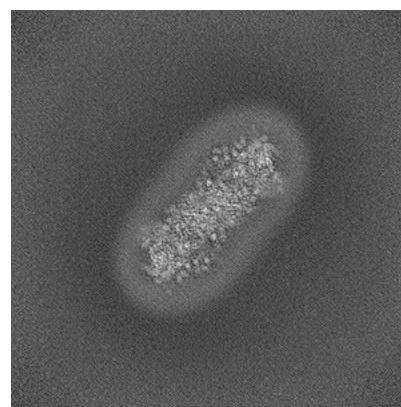
6.1.2 Raw map



X



Y

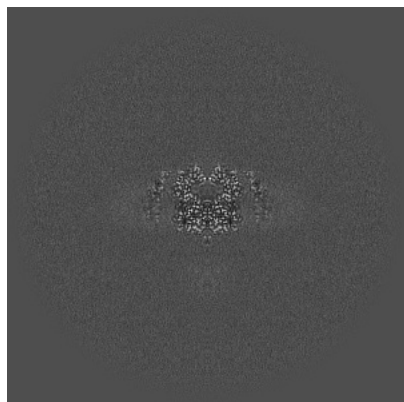


Z

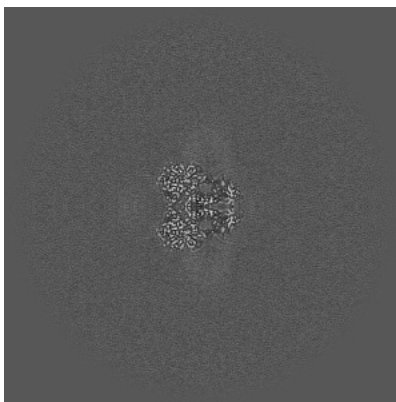
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

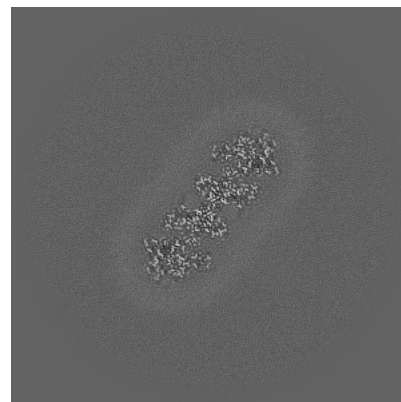
6.2.1 Primary map



X Index: 270

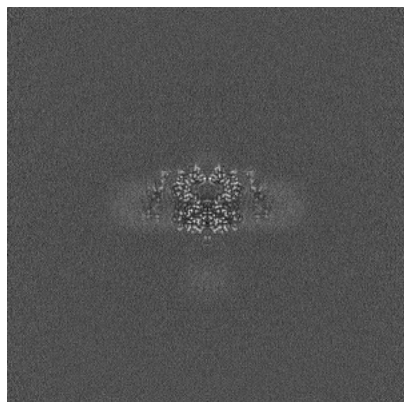


Y Index: 270

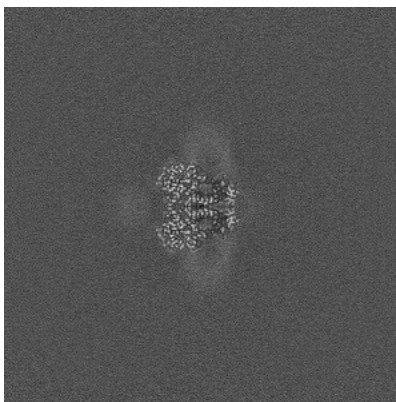


Z Index: 270

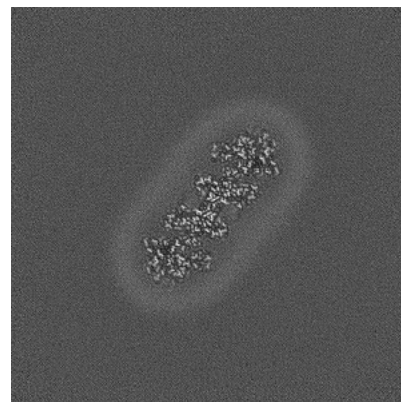
6.2.2 Raw map



X Index: 270



Y Index: 270

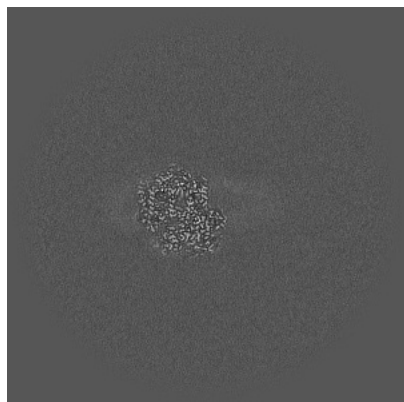


Z Index: 270

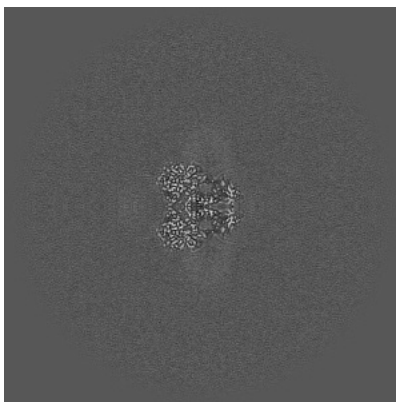
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

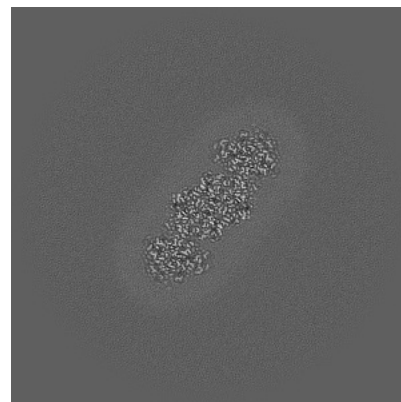
6.3.1 Primary map



X Index: 236

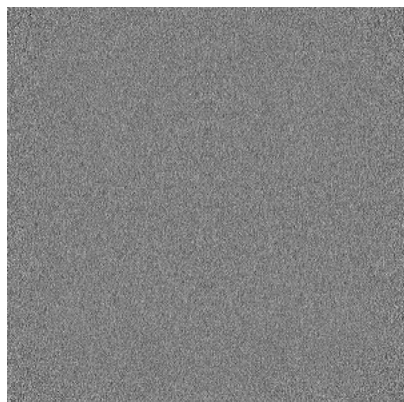


Y Index: 270

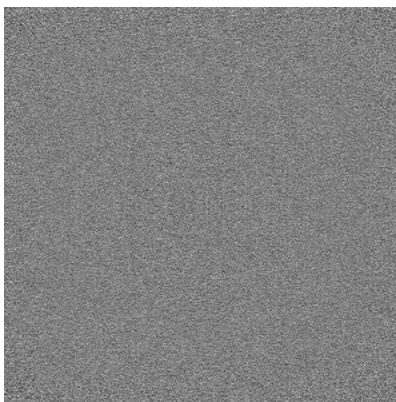


Z Index: 254

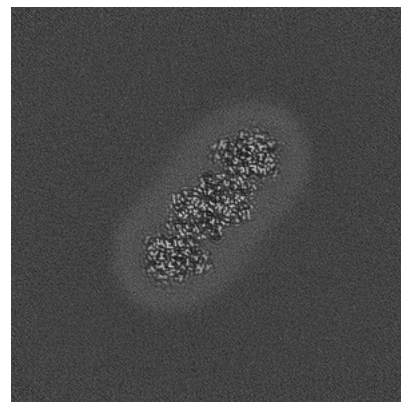
6.3.2 Raw map



X Index: 0



Y Index: 0

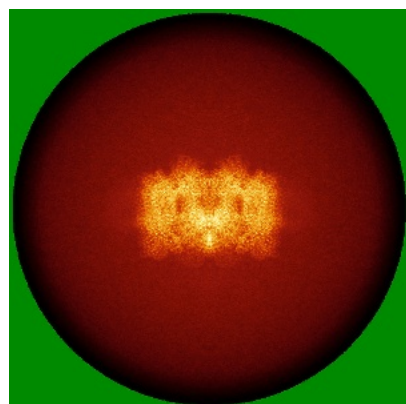


Z Index: 255

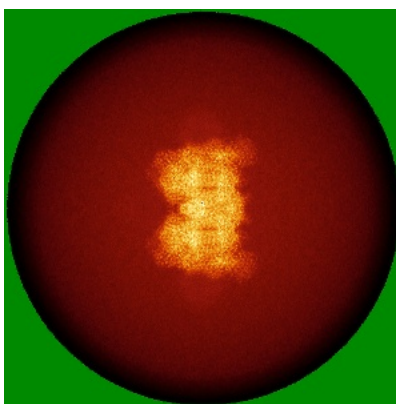
The images above show the largest variance slices of the map in three orthogonal directions.

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

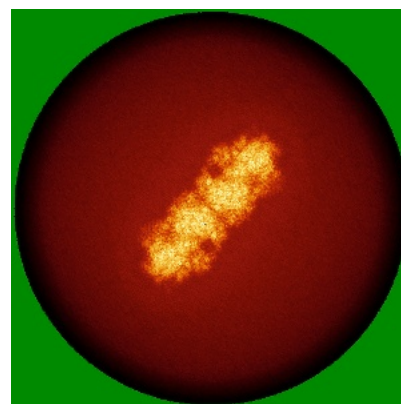
6.4.1 Primary map



X

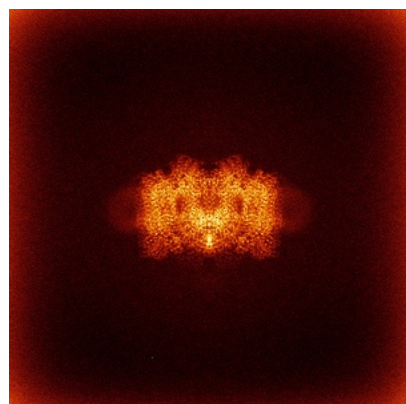


Y

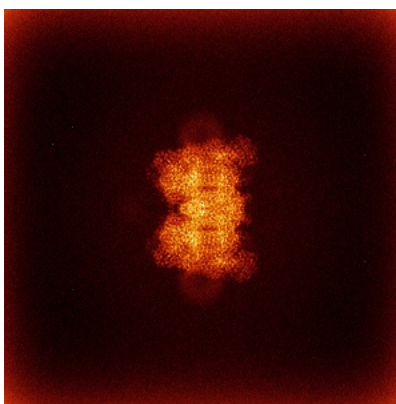


Z

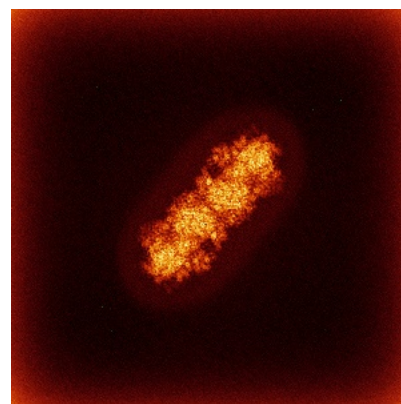
6.4.2 Raw map



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.

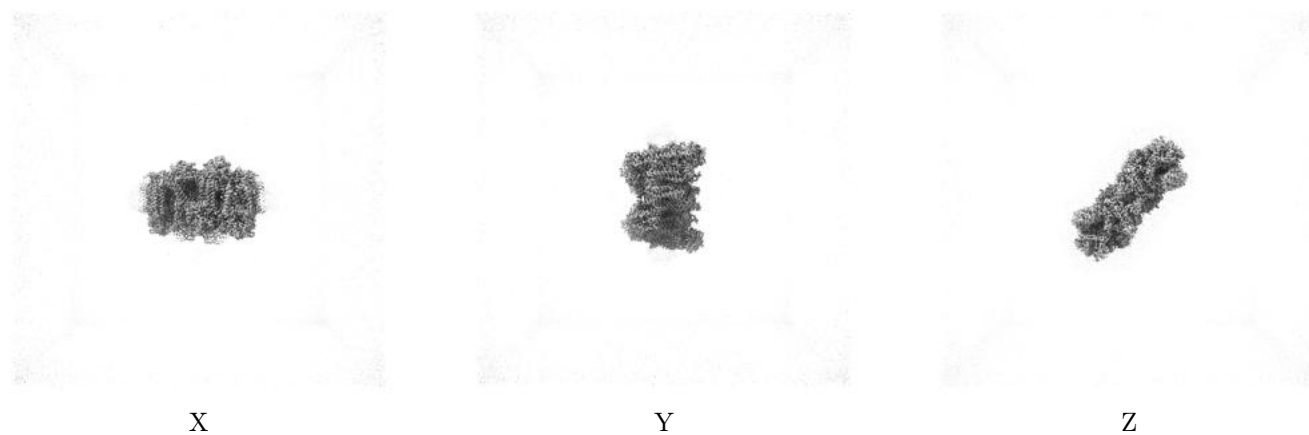
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. 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.

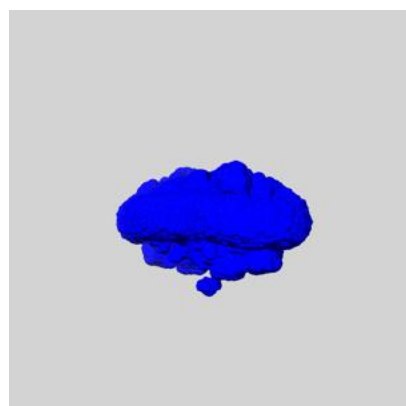
6.6 Mask visualisation [i](#)

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

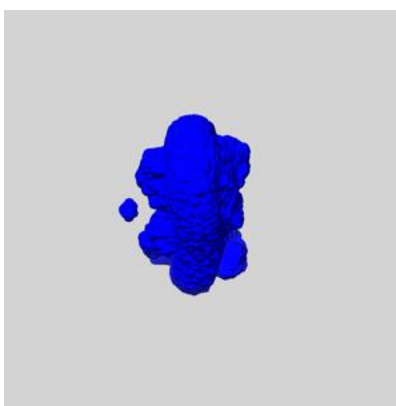
A mask typically either:

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

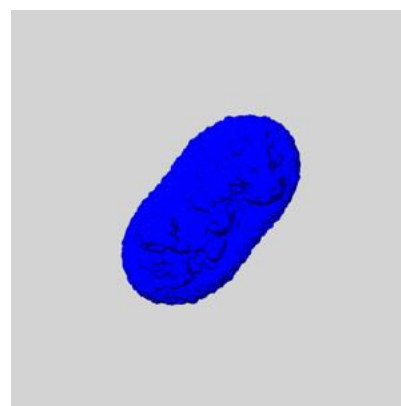
6.6.1 emd_17211_msk_1.map [i](#)



X



Y

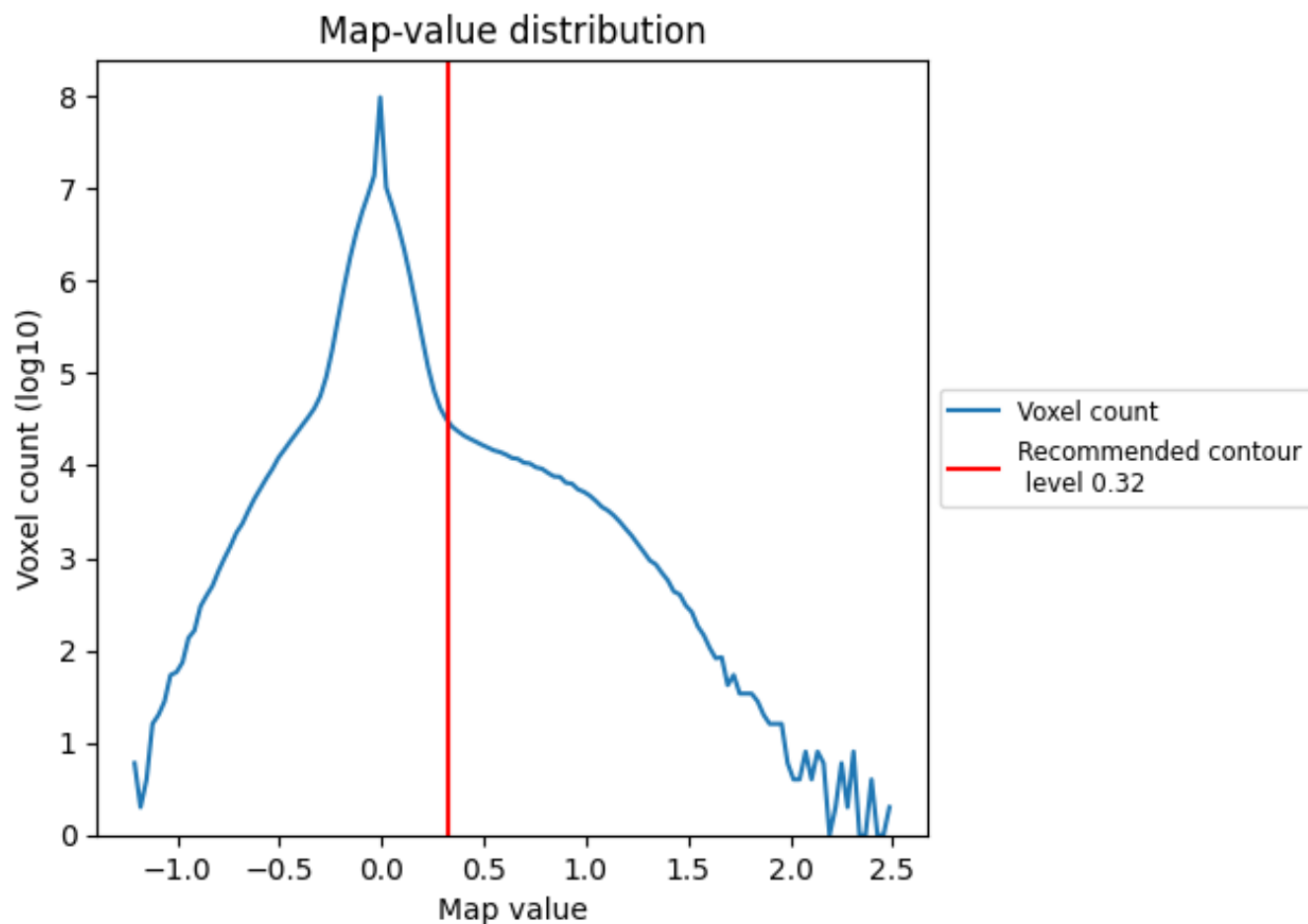


Z

7 Map analysis [i](#)

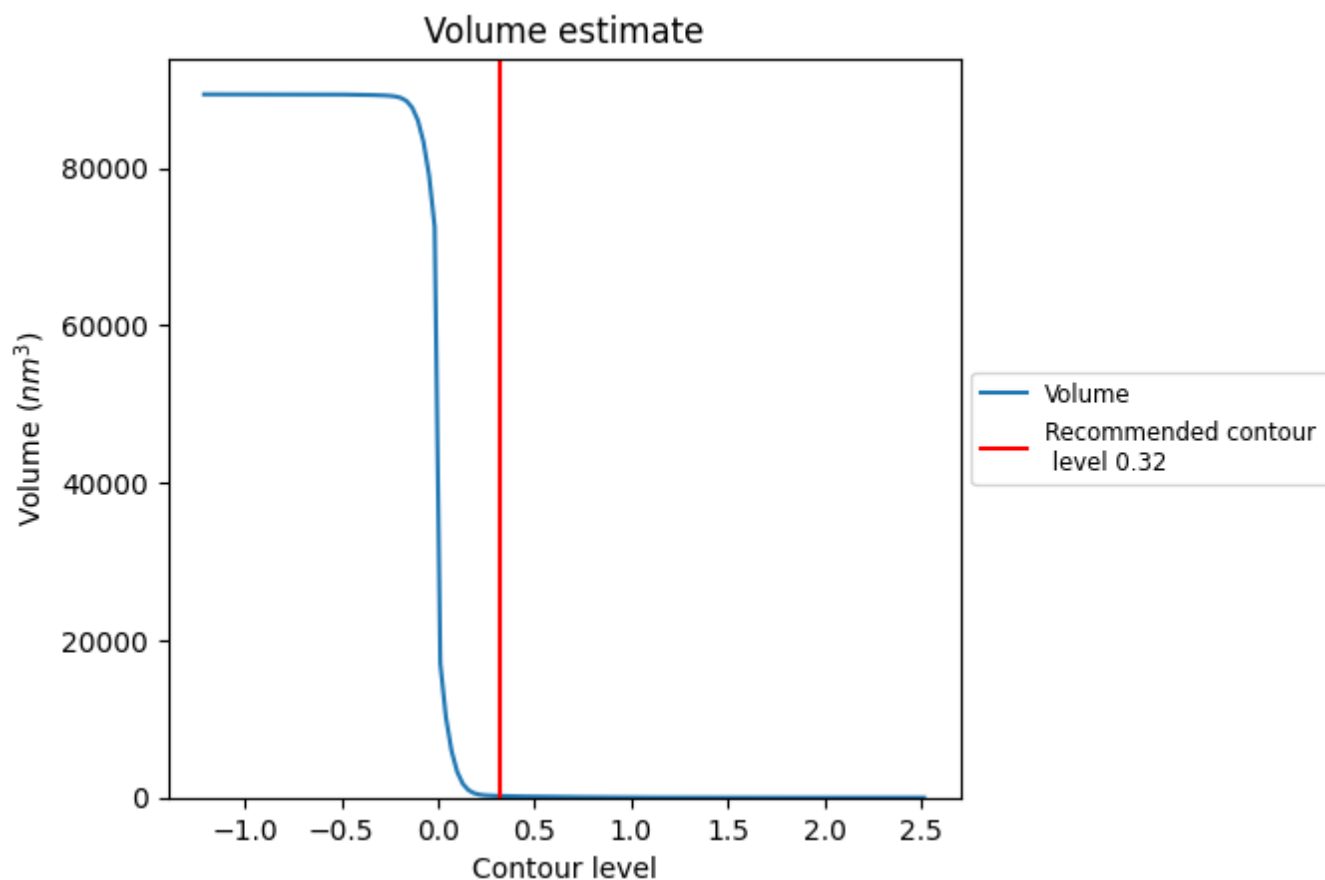
This section contains the results of statistical analysis of the map.

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.

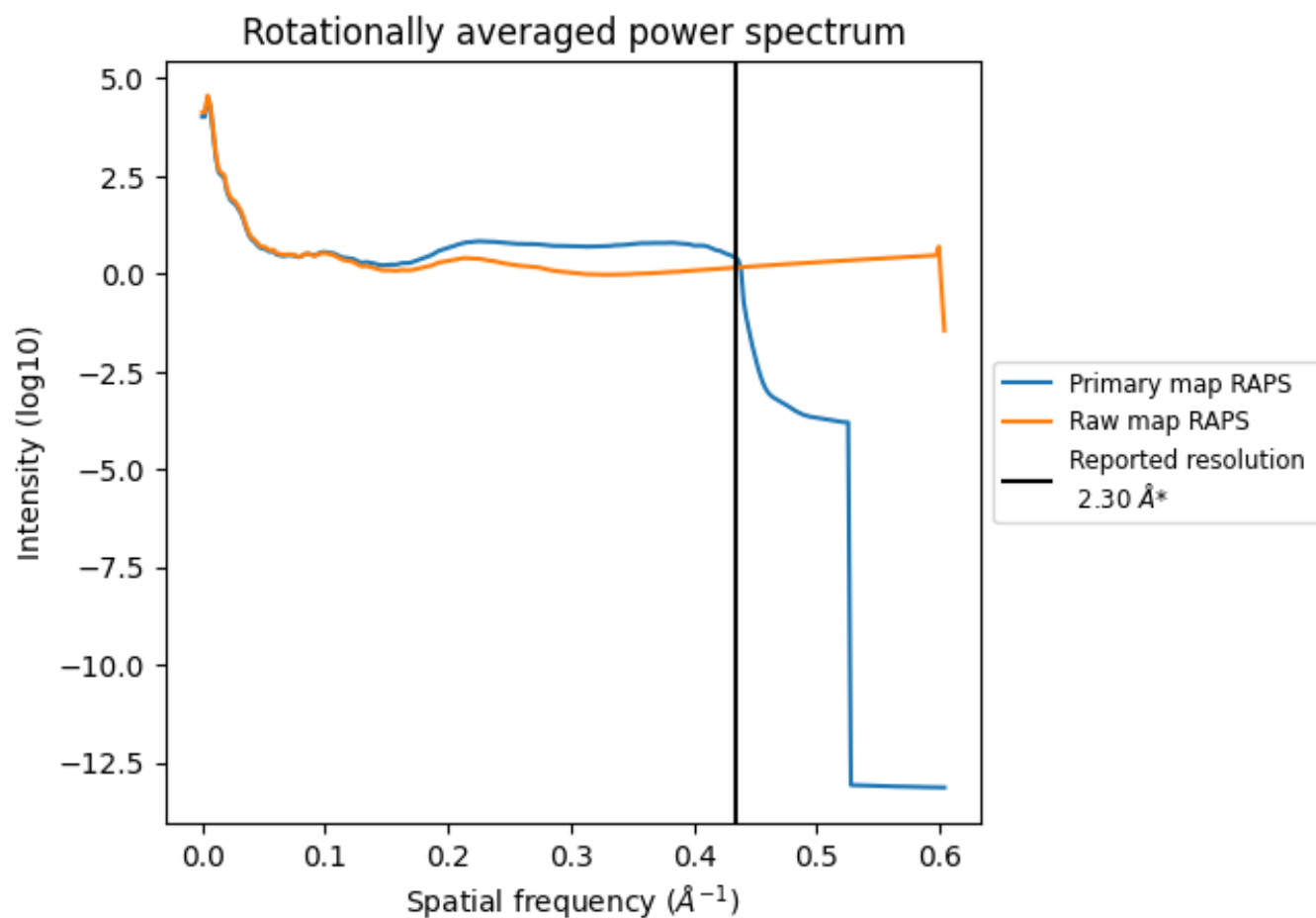
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm^3 ; this corresponds to an approximate mass of 182 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 ⓘ

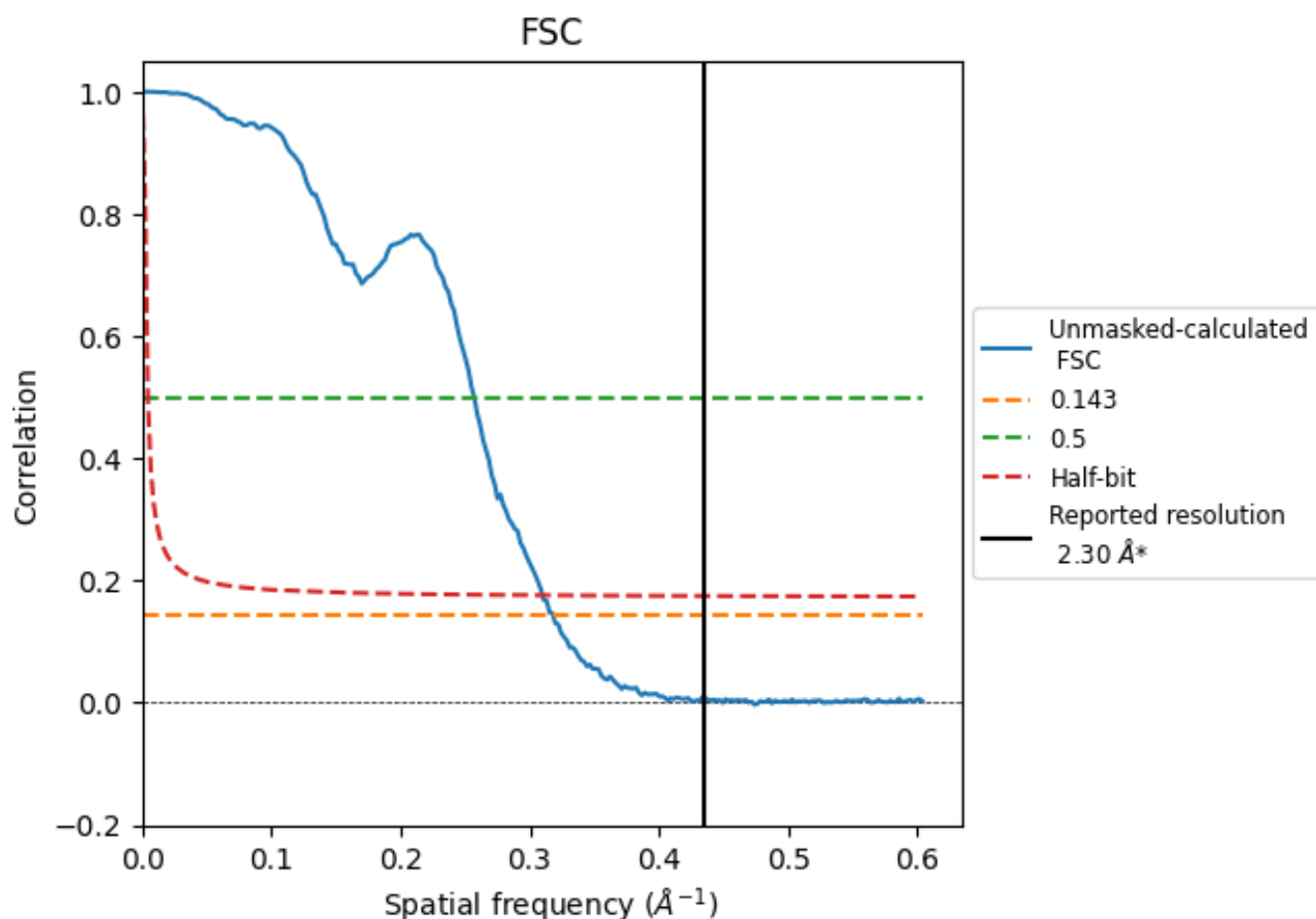


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

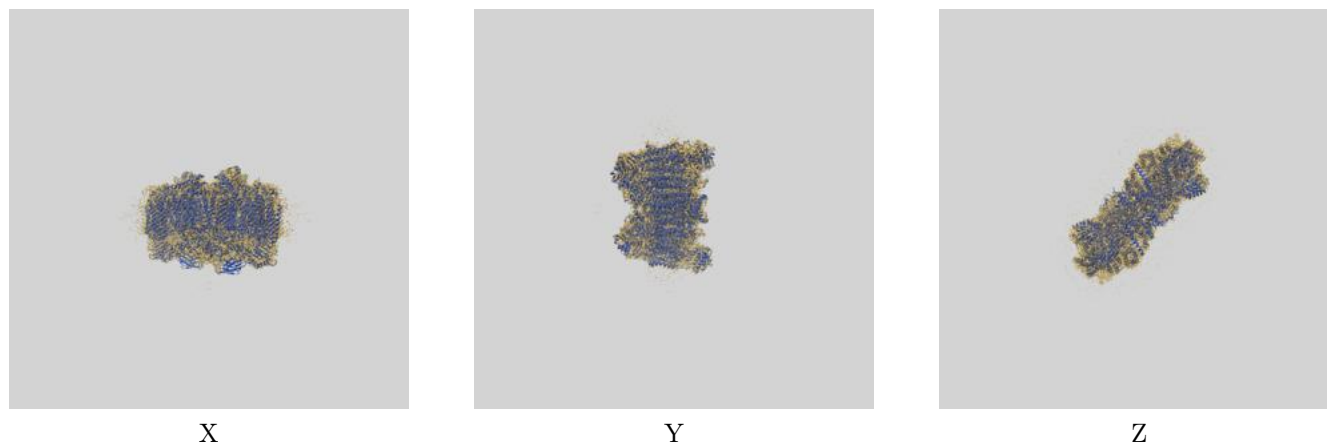
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.89	3.23

*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 3.14 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

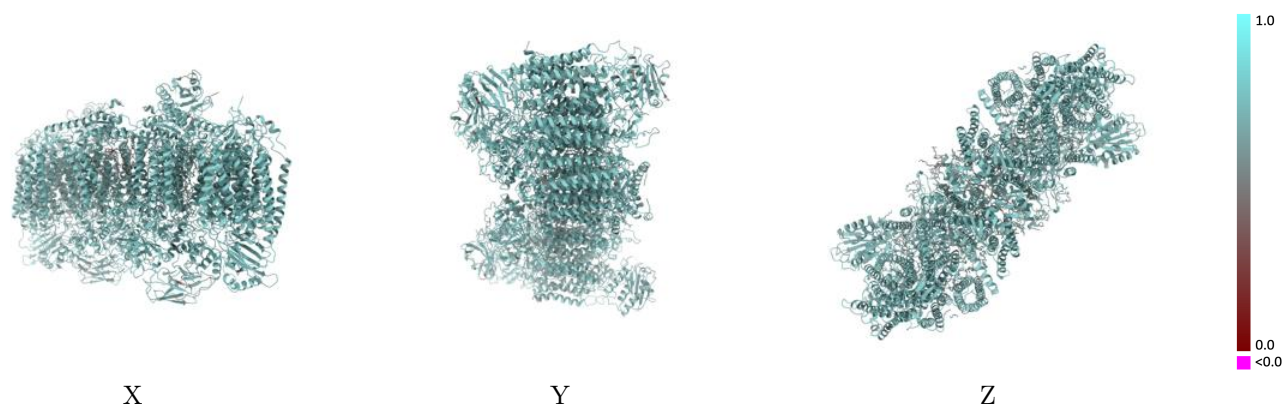
This section contains information regarding the fit between EMDB map EMD-17211 and PDB model 8OVD. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



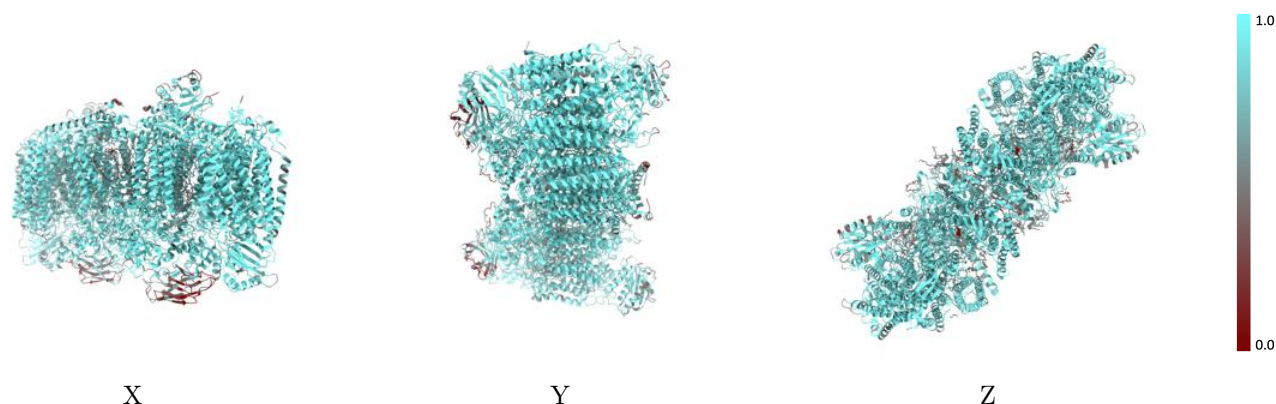
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



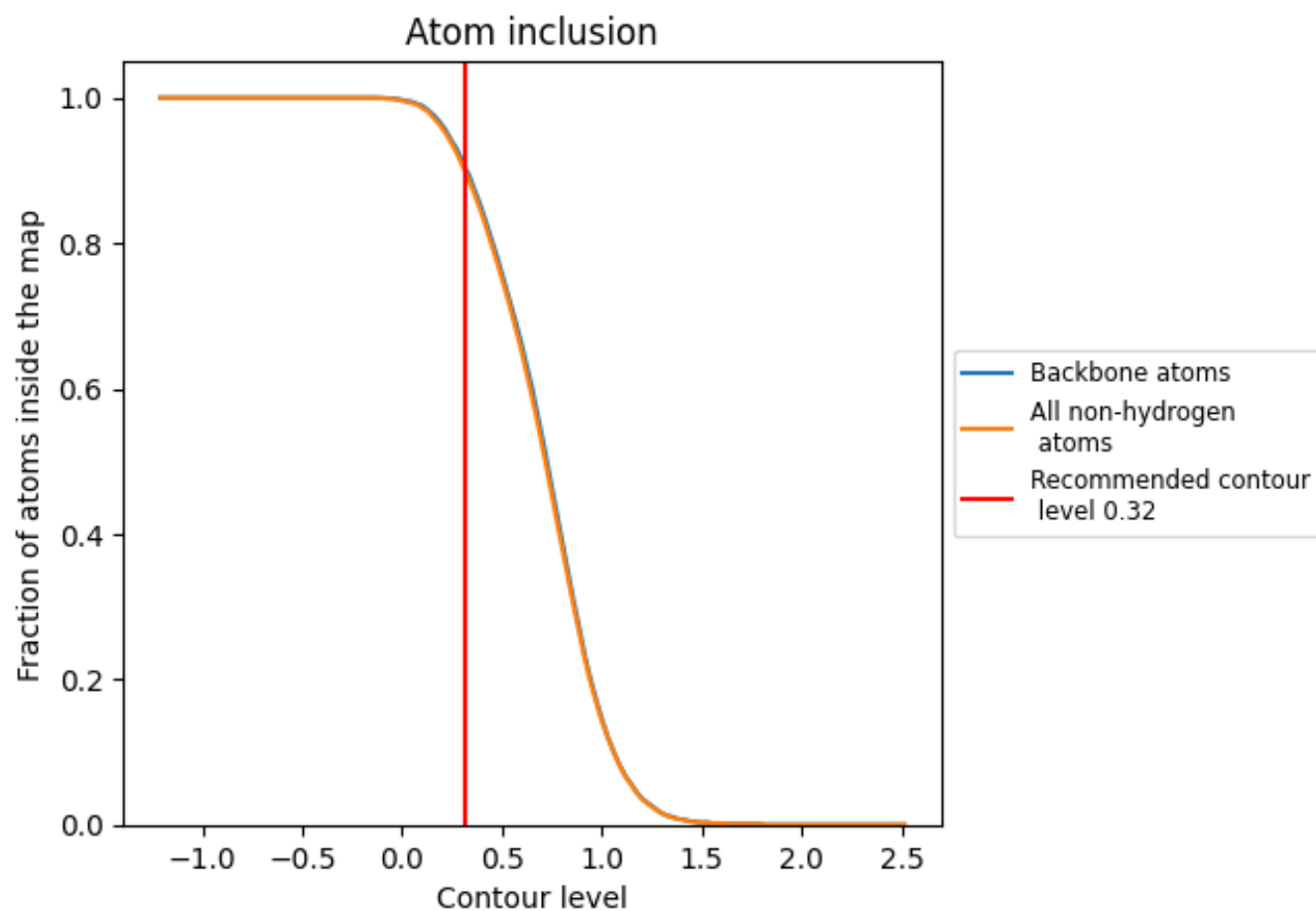
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.6990
C	 0.9310	 0.7130
G	 0.9050	 0.6920
H	 0.9230	 0.7080
I	 0.8360	 0.6890
J	 0.9110	 0.6960
K	 0.9470	 0.7120
L	 0.9800	 0.7200
M	 0.9090	 0.6990
N	 0.9240	 0.7060
O	 0.9430	 0.7140
P	 0.8570	 0.6910
Q	 0.8700	 0.6910
R	 0.9760	 0.7190
S	 0.9320	 0.6990
T	 0.9290	 0.7000
U	 0.8090	 0.6680
V	 0.8310	 0.6700
W	 0.5000	 0.6370
X	 0.8670	 0.6900
Y	 0.7760	 0.6620
Z	 0.7840	 0.6570
a	 0.8150	 0.6630
b	 0.5080	 0.6300
c	 0.7710	 0.6560

