



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 06:08 AM UTC

PDB ID : 9DM1 / pdb_00009dm1
EMDB ID : EMD-46995
Title : Mycobacterial supercomplex malate:quinone oxidoreductase assembly
Authors : Di Trani, J.M.; Rubinstein, J.L.
Deposited on : 2024-09-11
Resolution : 3.20 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:

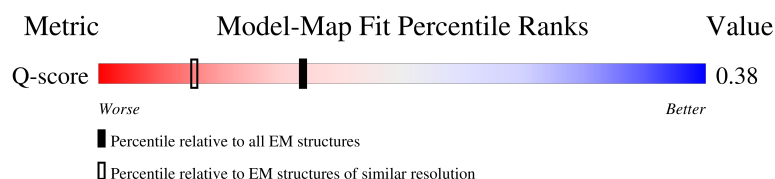
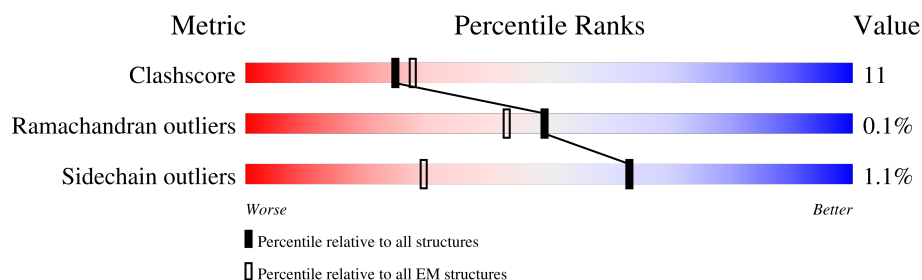
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	L	566	
1	R	566	
2	E	535	
2	F	535	

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Mol	Chain	Length	Quality of chain
3	D	216	92% 97% .
3	G	216	91% 99% .
4	K	312	43% 84% 16%
4	Q	312	44% 80% 19% .
5	S	203	25% 82% 17%
5	X	203	26% 83% 16% .
6	T	139	29% 83% 17% .
6	Z	139	28% 81% 19%
7	U	79	81% 82% 18%
7	a	79	84% 94% 6%
8	V	145	74% 81% 18% .
8	b	145	75% 80% 20%
9	J	100	20% 73% 19% 8%
9	P	100	23% 80% 11% 8%
10	I	223	6% 81% 18% .
10	O	223	6% 79% 21%
11	W	159	39% 83% 16% .
11	c	159	38% 81% 18% .
12	M	382	13% 84% 15%
12	Y	382	12% 84% 16%
13	A	510	85% 94% 5%

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
16	CDL	R	604	-	-	X	-
16	CDL	S	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CDL	T	201	-	-	X	-
16	CDL	X	301	-	-	X	-
16	CDL	X	302	-	-	X	-
16	CDL	Z	202	-	-	X	-
16	CDL	Z	203	-	-	X	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 51339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	552	Total	C	N	O	S	0	0
			4370	2937	695	712	26		
1	L	552	Total	C	N	O	S	0	0
			4370	2937	695	712	26		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	32	ILE	VAL	conflict	UNP A0A0K0XH24
R	47	VAL	ALA	conflict	UNP A0A0K0XH24
R	54	VAL	ILE	conflict	UNP A0A0K0XH24
R	357	THR	SER	conflict	UNP A0A0K0XH24
R	452	LEU	VAL	conflict	UNP A0A0K0XH24
R	467	THR	SER	conflict	UNP A0A0K0XH24
R	476	ILE	VAL	conflict	UNP A0A0K0XH24
R	479	VAL	ILE	conflict	UNP A0A0K0XH24
L	32	ILE	VAL	conflict	UNP A0A0K0XH24
L	47	VAL	ALA	conflict	UNP A0A0K0XH24
L	54	VAL	ILE	conflict	UNP A0A0K0XH24
L	357	THR	SER	conflict	UNP A0A0K0XH24
L	452	LEU	VAL	conflict	UNP A0A0K0XH24
L	467	THR	SER	conflict	UNP A0A0K0XH24
L	476	ILE	VAL	conflict	UNP A0A0K0XH24
L	479	VAL	ILE	conflict	UNP A0A0K0XH24

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

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

- Molecule 3 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	216	Total	C	N	O	S	0	0
			1092	645	217	229	1		
3	G	216	Total	C	N	O	S	0	0
			1092	645	217	229	1		

- Molecule 4 is a protein called Cytochrome aa3 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	312	Total	C	N	O	S	0	0
			2465	1592	412	451	10		
4	K	312	Total	C	N	O	S	0	0
			2465	1592	412	451	10		

- Molecule 5 is a protein called Cytochrome aa3 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	203	Total	C	N	O	S	0	0
			1560	1039	253	260	8		
5	X	203	Total	C	N	O	S	0	0
			1560	1039	253	260	8		

- 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	Z	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	79	Total	C	N	O	S	0	0
			591	381	107	101	2		
7	a	79	Total	C	N	O	S	0	0
			591	381	107	101	2		

- Molecule 8 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	145	Total	C	N	O	S	0	0
			1041	658	176	205	2		
8	b	145	Total	C	N	O	S	0	0
			1041	658	176	205	2		

- Molecule 9 is a protein called Conserved transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	92	Total	C	N	O	S	0	0
			736	471	136	124	5		
9	J	92	Total	C	N	O	S	0	0
			736	471	136	124	5		

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

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

- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	158	Total	C	N	O	S	0	0
			1149	708	192	248	1		
11	W	158	Total	C	N	O	S	0	0
			1149	708	192	248	1		

- Molecule 12 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

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

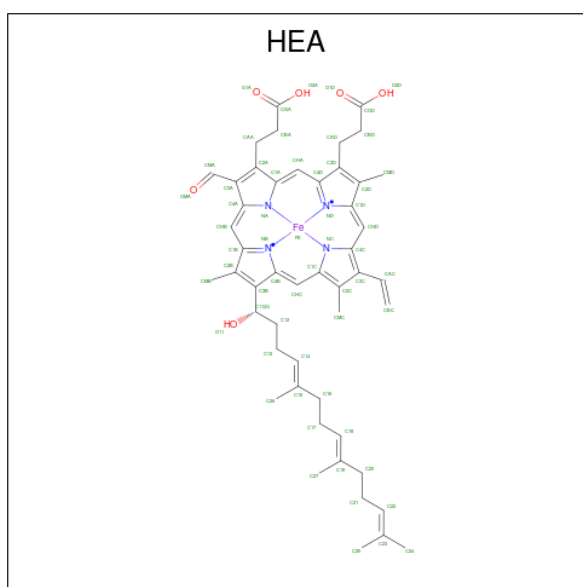
- Molecule 13 is a protein called Probable malate:quinone oxidoreductase.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	A	485	Total	C	N	O	0	0
			2377	1407	485	485		

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

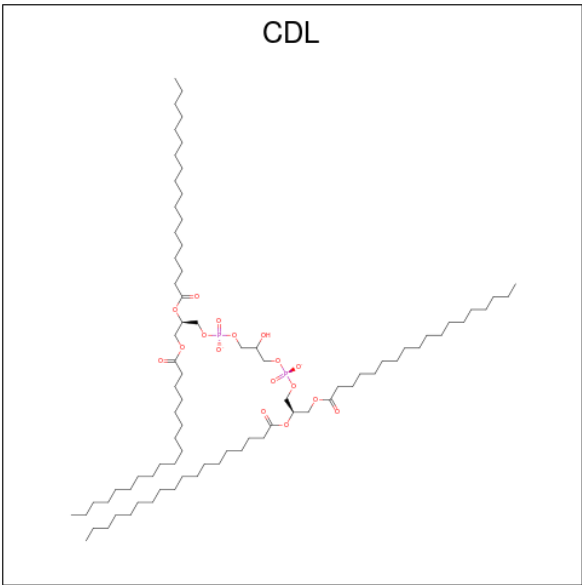
Mol	Chain	Residues	Atoms		AltConf
14	R	1	Total 1	Cu 1	0
14	L	1	Total 1	Cu 1	0
14	Q	2	Total 2	Cu 2	0
14	K	2	Total 2	Cu 2	0

- Molecule 15 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



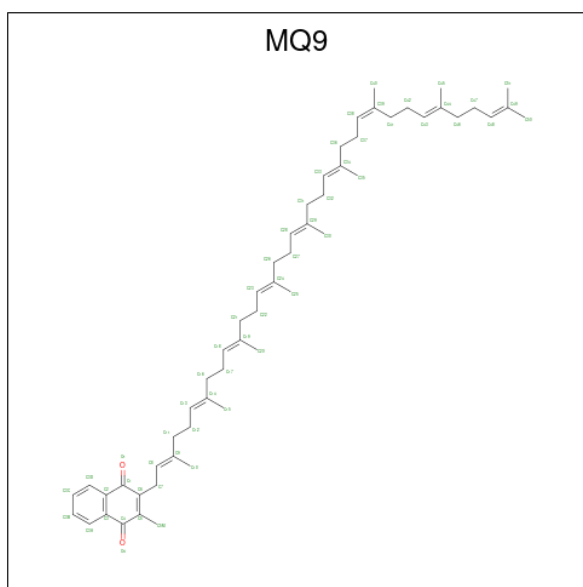
Mol	Chain	Residues	Atoms				AltConf
16	R	1	Total	C	O	P	0
			76	57	17	2	
16	E	1	Total	C	O	P	0
			76	57	17	2	
16	E	1	Total	C	O	P	0
			76	57	17	2	
16	F	1	Total	C	O	P	0
			76	57	17	2	
16	F	1	Total	C	O	P	0
			76	57	17	2	
16	L	1	Total	C	O	P	0
			76	57	17	2	
16	S	1	Total	C	O	P	0
			76	57	17	2	
16	T	1	Total	C	O	P	0
			76	57	17	2	
16	T	1	Total	C	O	P	0
			76	57	17	2	
16	T	1	Total	C	O	P	0
			76	57	17	2	
16	P	1	Total	C	O	P	0
			76	57	17	2	
16	X	1	Total	C	O	P	0
			76	57	17	2	
16	X	1	Total	C	O	P	0
			76	57	17	2	
16	Z	1	Total	C	O	P	0
			76	57	17	2	

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Mol	Chain	Residues	Atoms				AltConf
16	Z	1	Total 76	C 57	O 17	P 2	0
16	J	1	Total 76	C 57	O 17	P 2	0

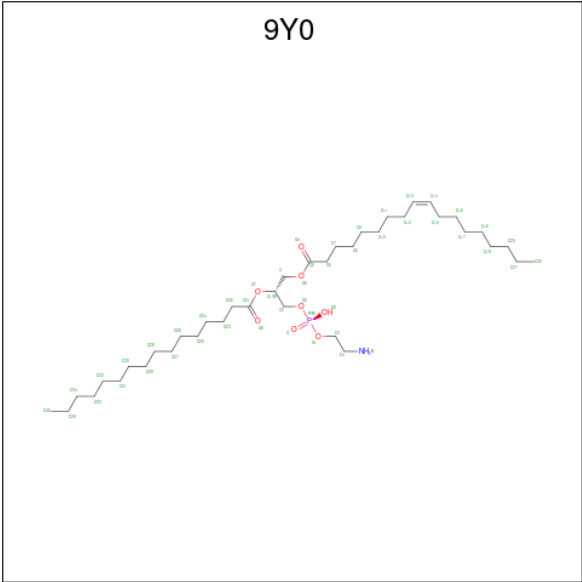
- # HEM

- Molecule 18 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



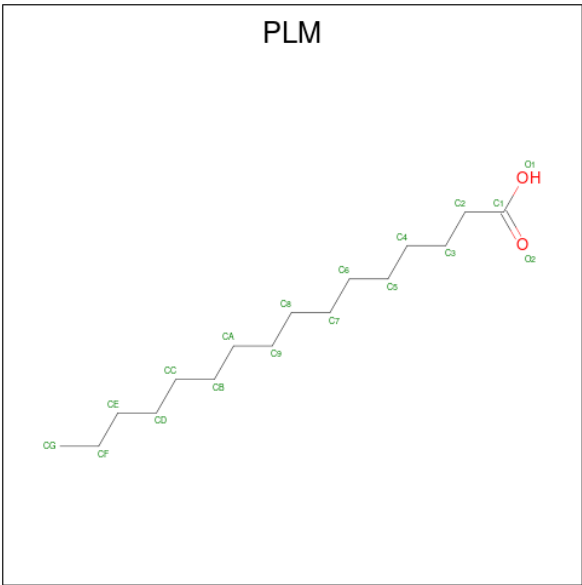
Mol	Chain	Residues	Atoms			AltConf
18	E	1	Total	C	O	0
			58	56	2	
18	E	1	Total	C	O	0
			58	56	2	
18	F	1	Total	C	O	0
			58	56	2	
18	F	1	Total	C	O	0
			58	56	2	
18	F	1	Total	C	O	0
			58	56	2	
18	F	1	Total	C	O	0
			58	56	2	
18	Z	1	Total	C	O	0
			58	56	2	
18	I	1	Total	C	O	0
			58	56	2	

- Molecule 19 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: C₃₉H₇₆NO₈P).



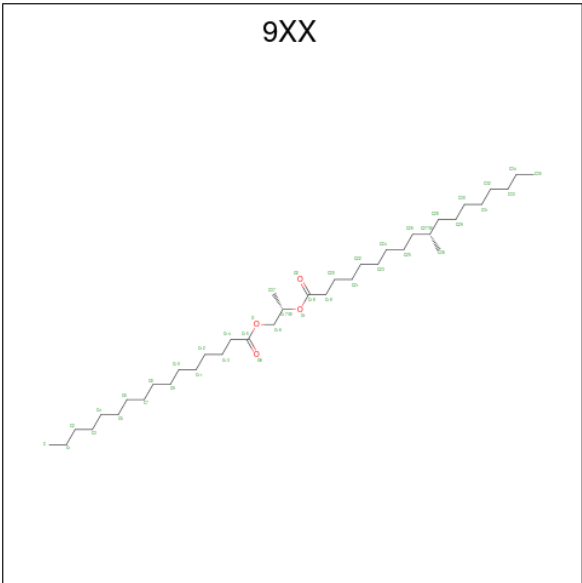
Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	S	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	P	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	X	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	J	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	J	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 20 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



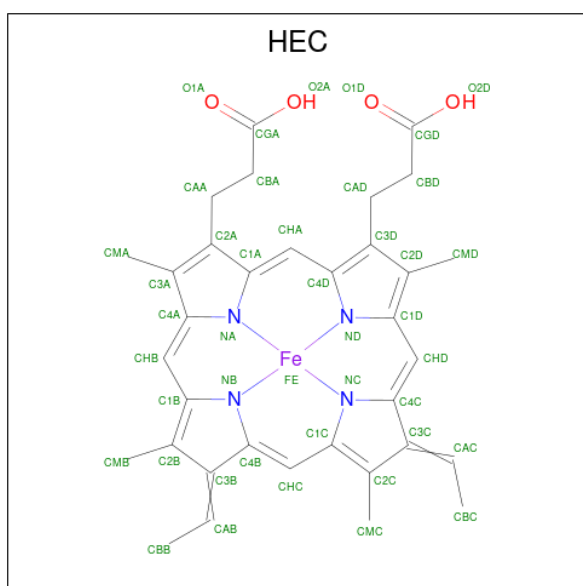
Mol	Chain	Residues	Atoms			AltConf
20	D	1	Total	C	O	0
			11	10	1	
20	G	1	Total	C	O	0
			11	10	1	
20	c	1	Total	C	O	0
			17	16	1	
20	W	1	Total	C	O	0
			17	16	1	

- Molecule 21 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C₃₈H₇₄O₄).



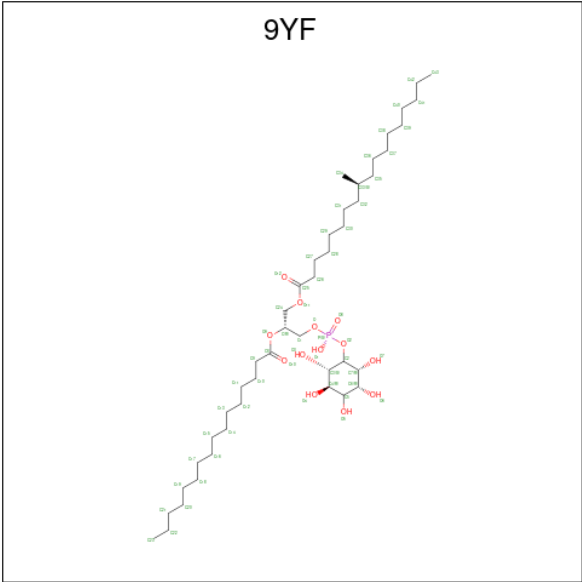
Mol	Chain	Residues	Atoms			AltConf
21	D	1	Total	C	O	0
			32	28	4	
21	G	1	Total	C	O	0
			32	28	4	
21	c	1	Total	C	O	0
			42	38	4	
21	W	1	Total	C	O	0
			42	38	4	

- Molecule 22 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



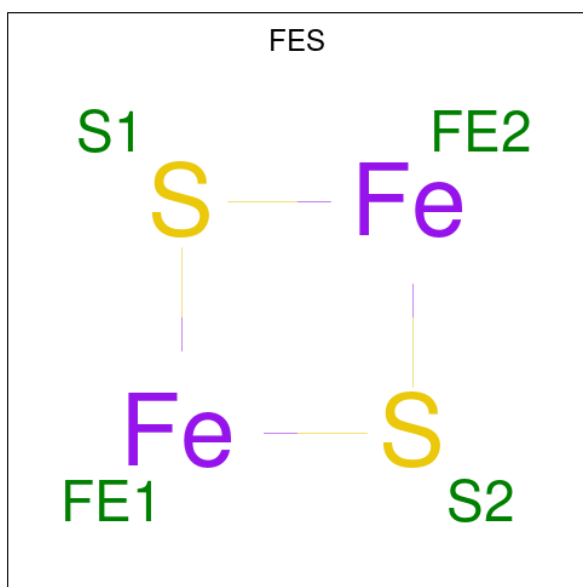
Mol	Chain	Residues	Atoms					AltConf
22	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 23 is (2R)-2-(hexadecanoyloxy)-3-[[[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
23	O	1	Total	C	O	P	0
			58	44	13	1	
23	c	1	Total	C	O	P	0
			58	44	13	1	
23	I	1	Total	C	O	P	0
			58	44	13	1	
23	Y	1	Total	C	O	P	0
			58	44	13	1	
23	Y	1	Total	C	O	P	0
			58	44	13	1	
23	W	1	Total	C	O	P	0
			58	44	13	1	
23	M	1	Total	C	O	P	0
			58	44	13	1	
23	M	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

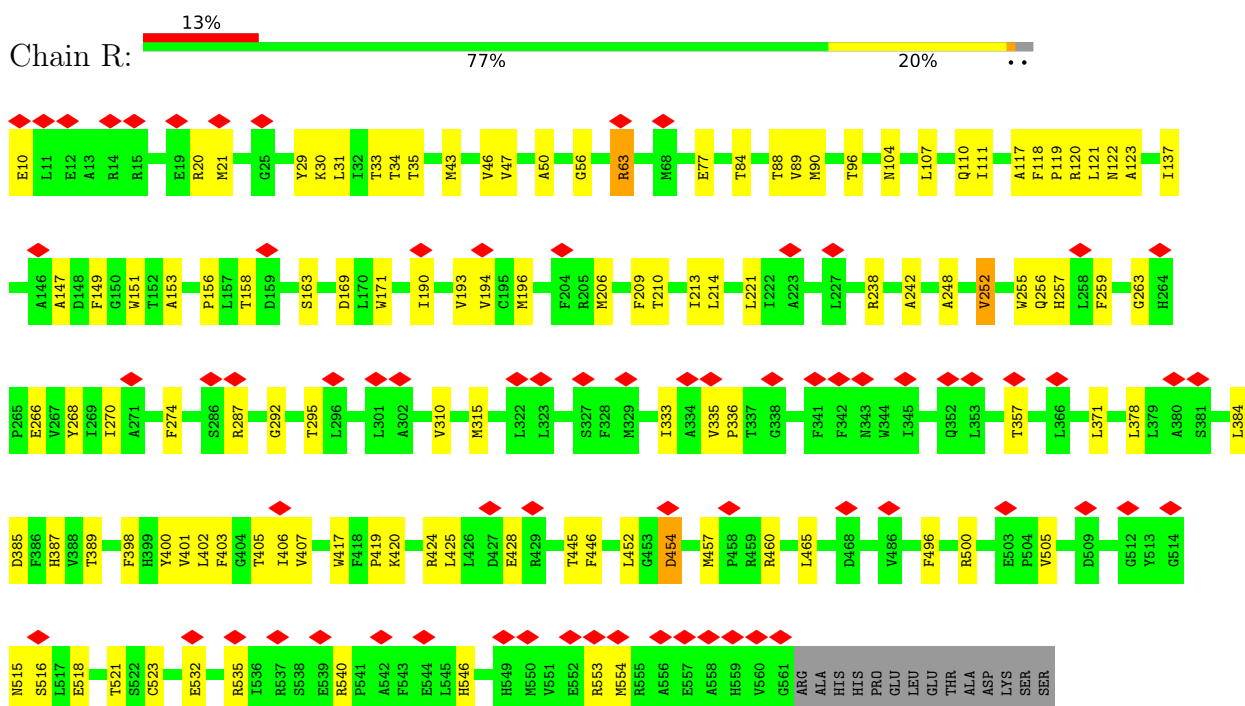


Mol	Chain	Residues	Atoms			AltConf
24	Y	1	Total	Fe	S	0
			4	2	2	
24	M	1	Total	Fe	S	0
			4	2	2	

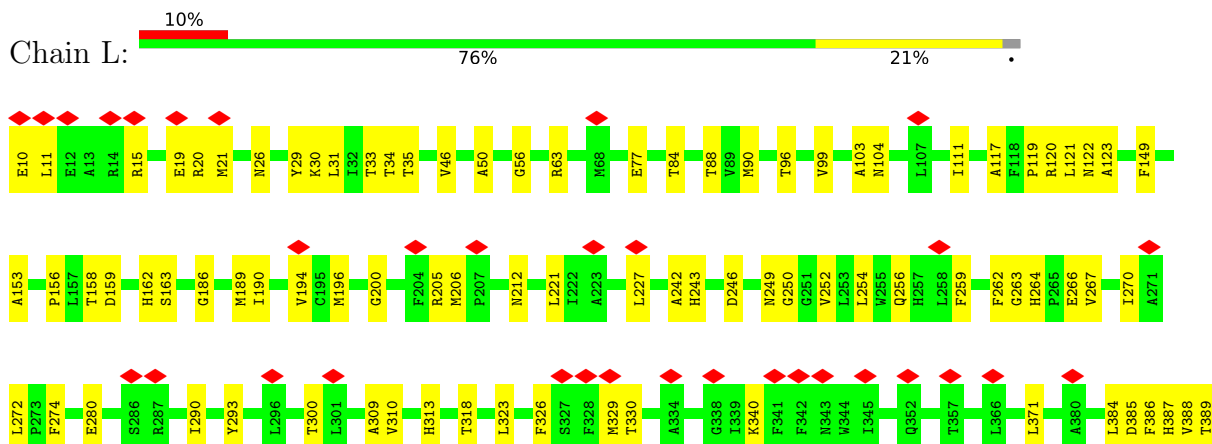
3 Residue-property plots

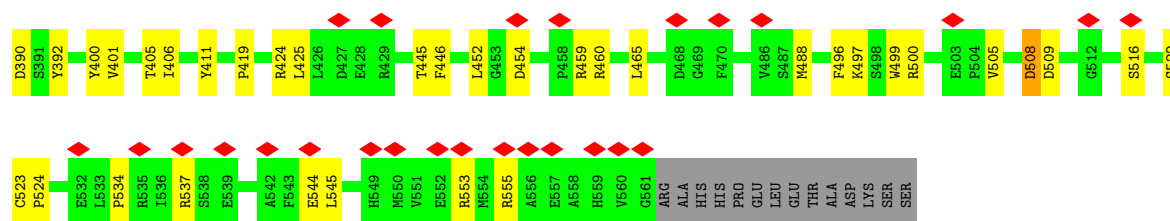
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Cytochrome c oxidase subunit 1

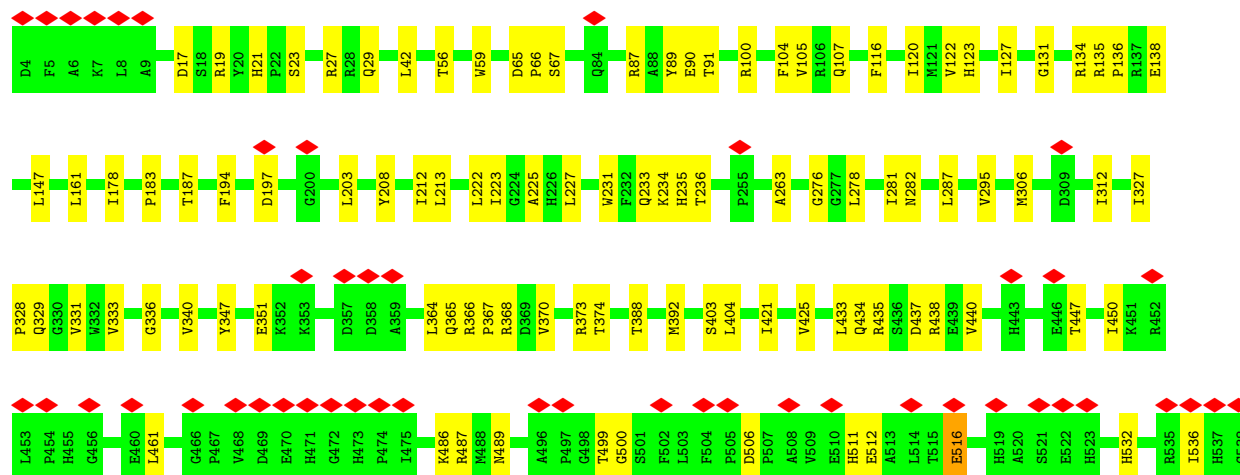
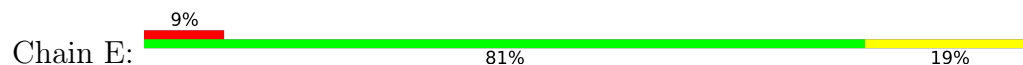


• Molecule 1: Cytochrome c oxidase subunit 1

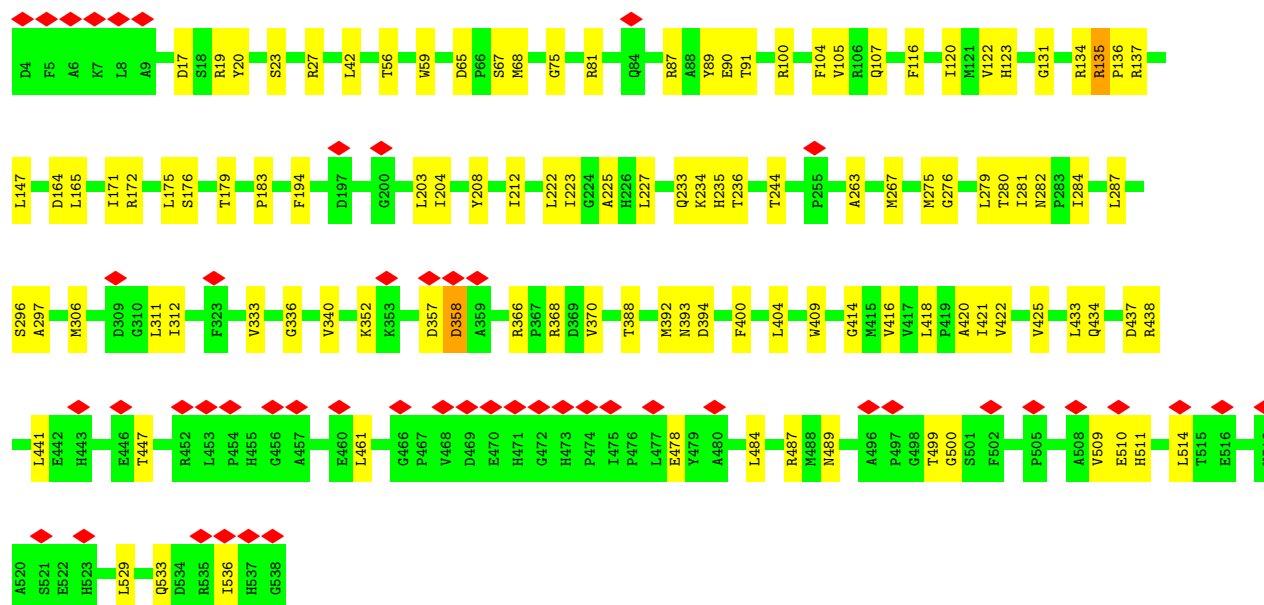
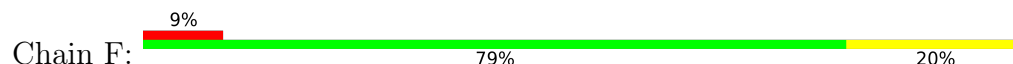




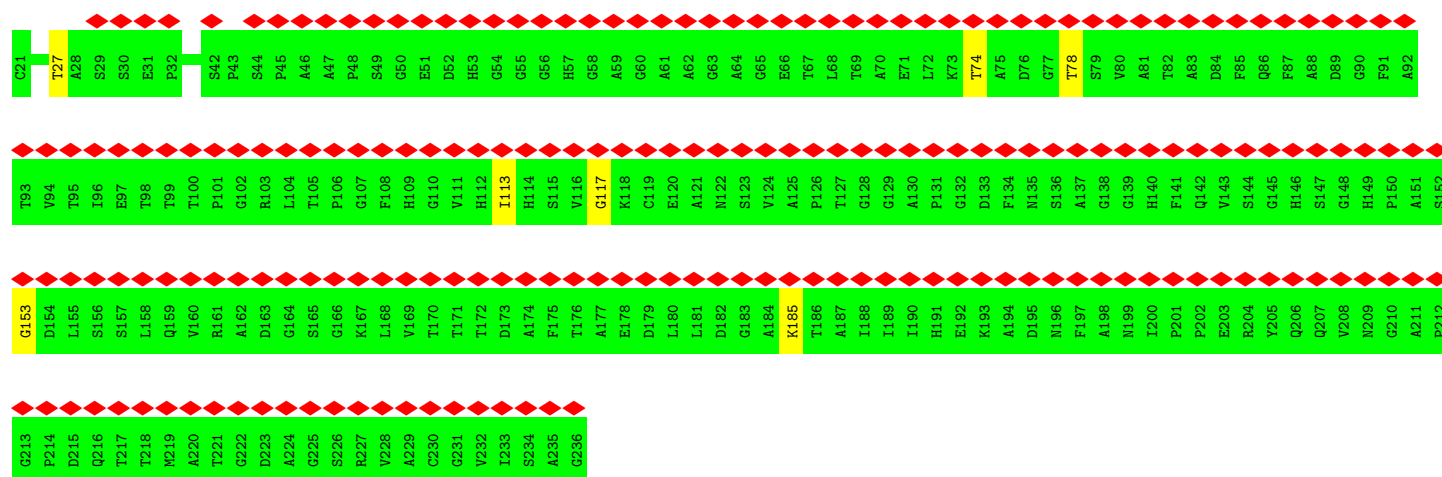
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit



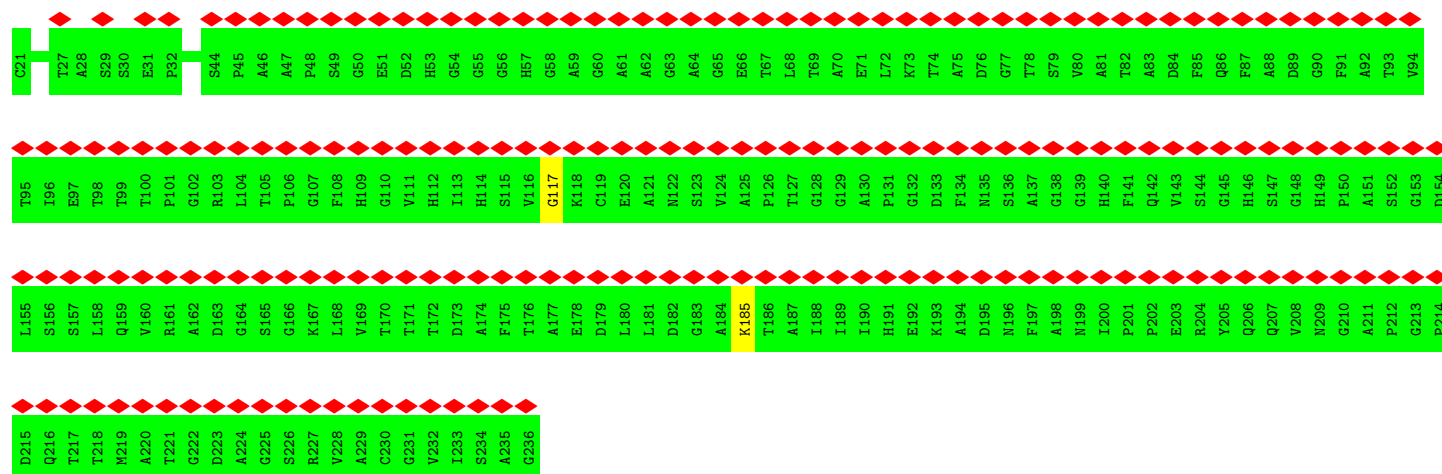
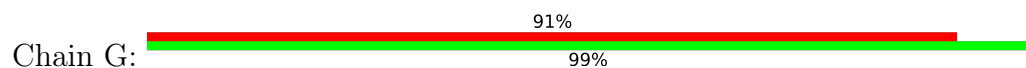
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit



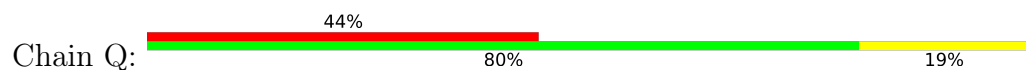
• Molecule 3: Superoxide dismutase [Cu-Zn]

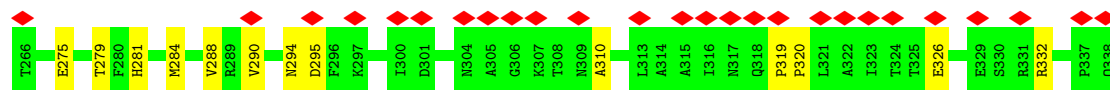


• Molecule 3: Superoxide dismutase [Cu-Zn]



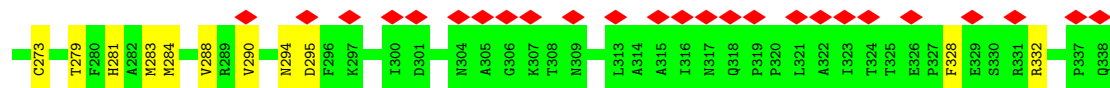
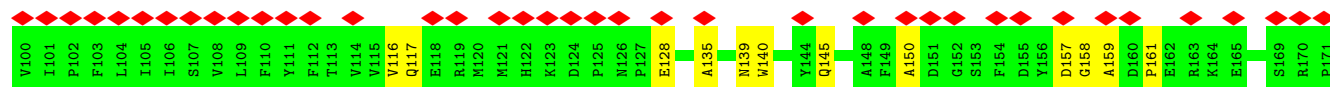
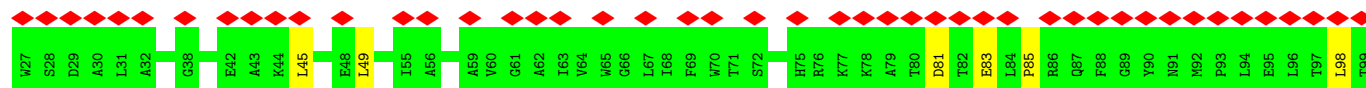
• Molecule 4: Cytochrome aa3 subunit 2





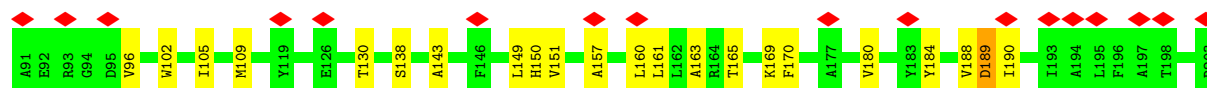
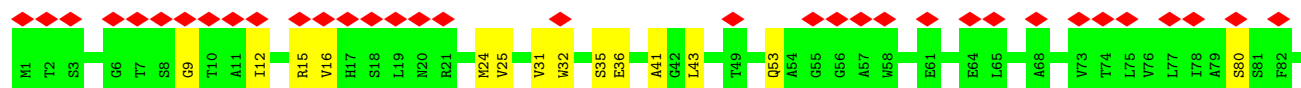
• Molecule 4: Cytochrome aa3 subunit 2

Chain K:



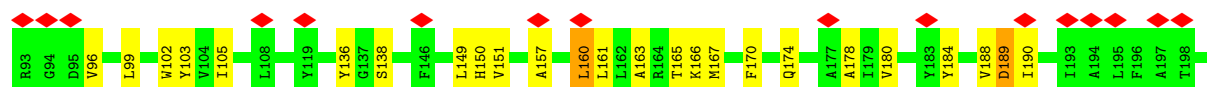
• Molecule 5: Cytochrome aa3 subunit 3

Chain S:

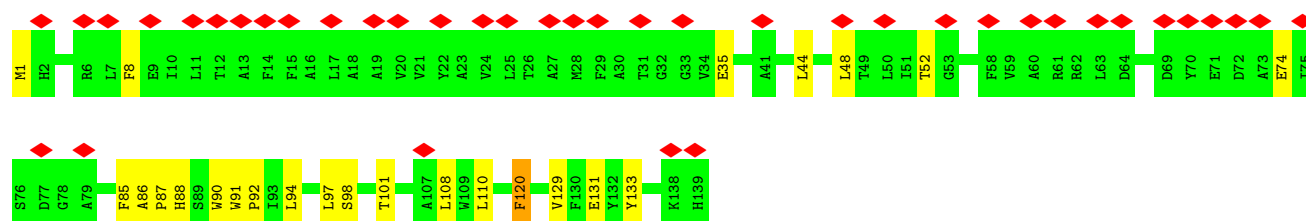
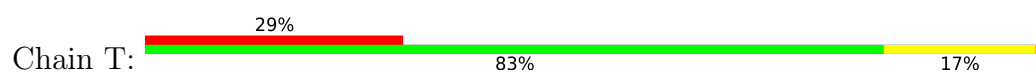


• Molecule 5: Cytochrome aa3 subunit 3

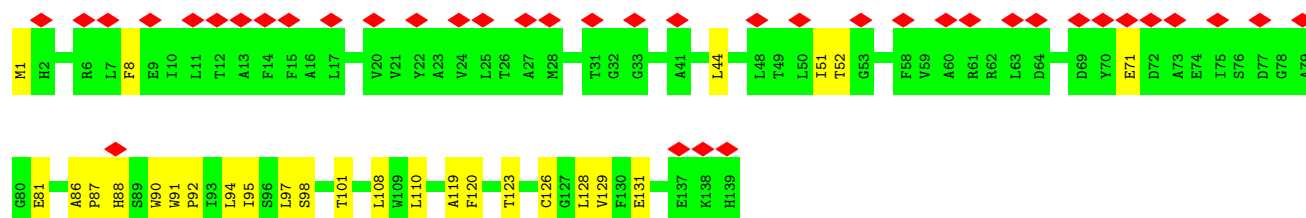
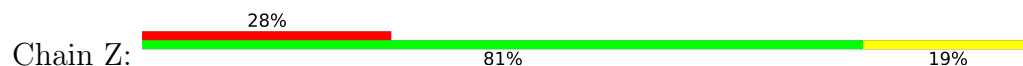
Chain X:



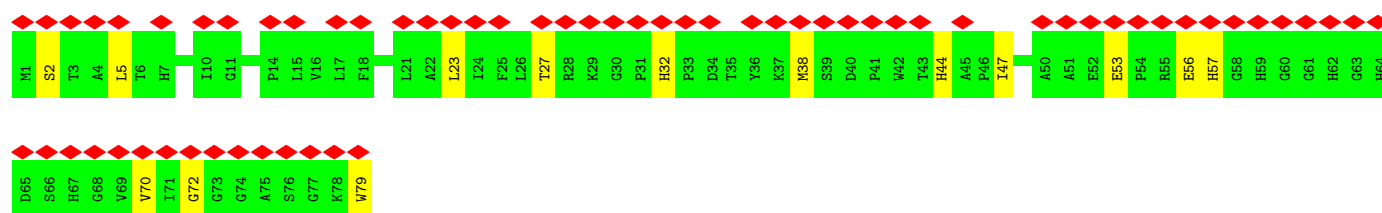
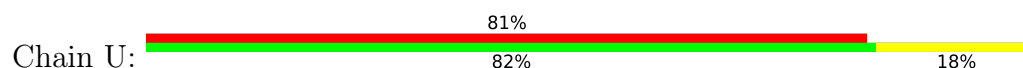
• Molecule 6: Cytochrome c oxidase polypeptide 4



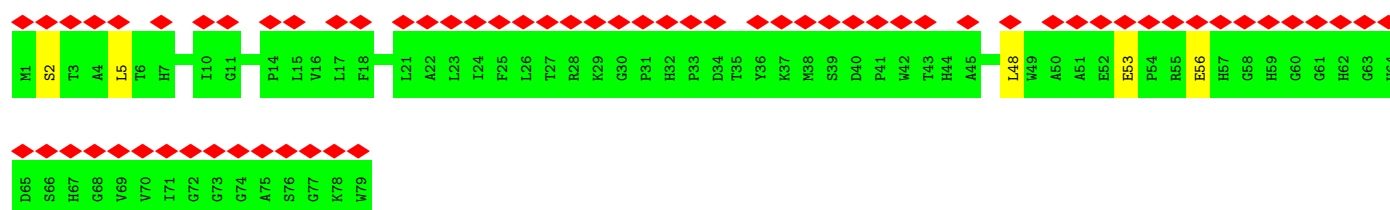
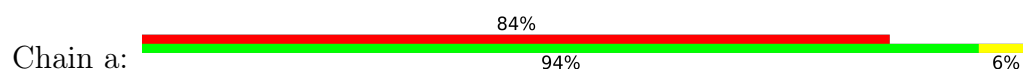
• Molecule 6: Cytochrome c oxidase polypeptide 4



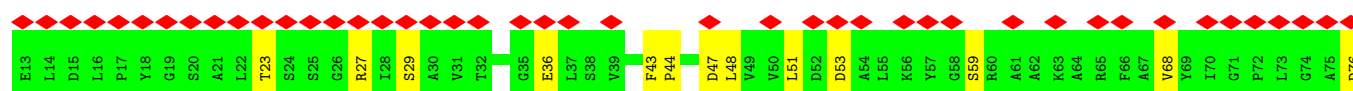
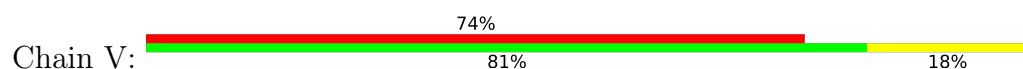
• Molecule 7: Cytochrome c oxidase subunit CtaJ

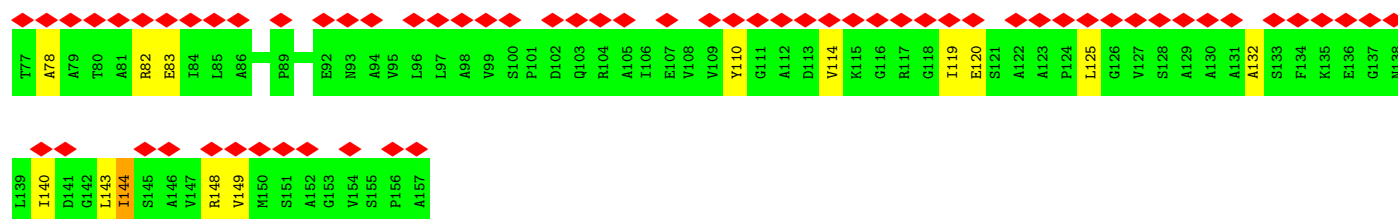


• Molecule 7: Cytochrome c oxidase subunit CtaJ

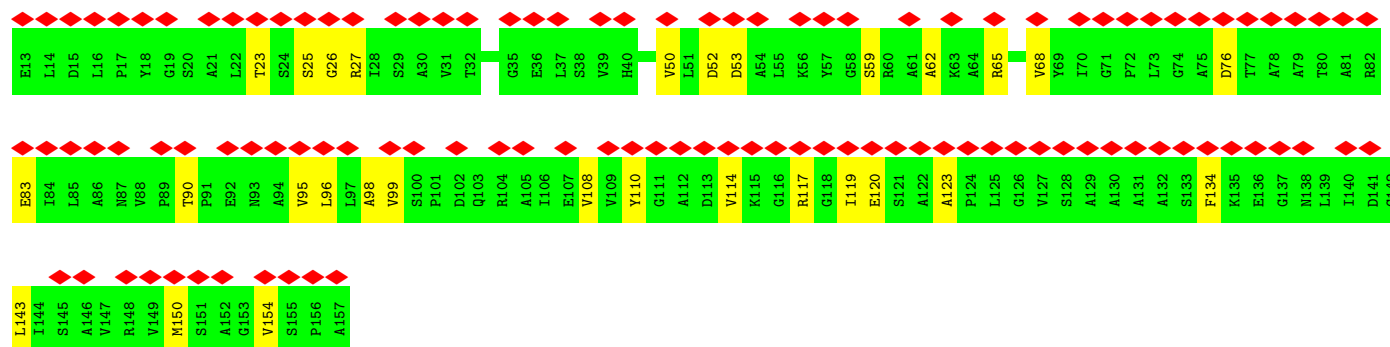
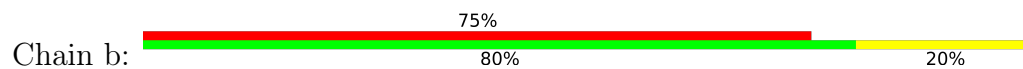


• Molecule 8: Uncharacterized protein MSMEG_4692/MSMEI_4575

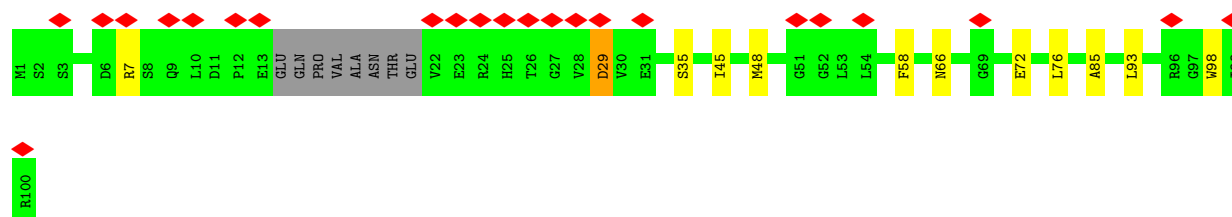
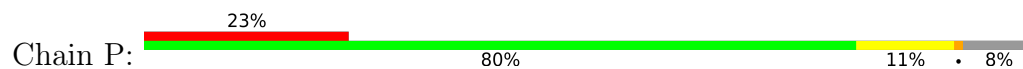




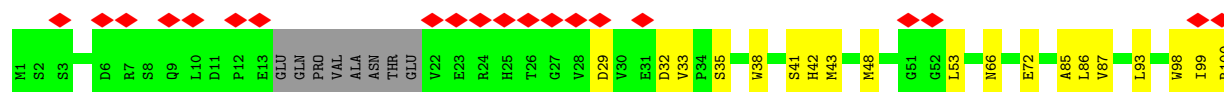
• Molecule 8: Uncharacterized protein MSMEG_4692/MSMEI_4575



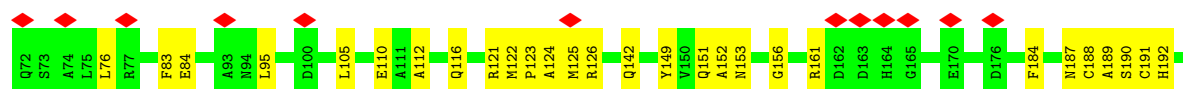
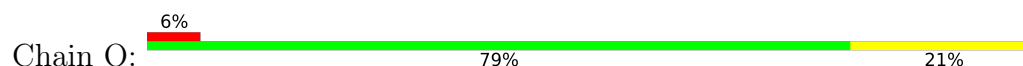
• Molecule 9: Conserved transmembrane protein



• Molecule 9: Conserved transmembrane protein

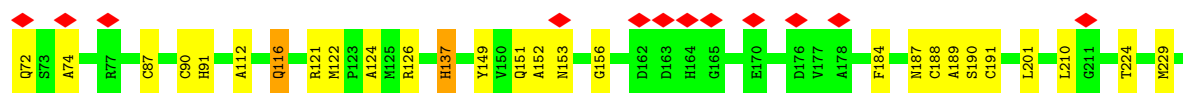
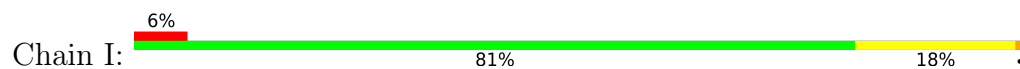


• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

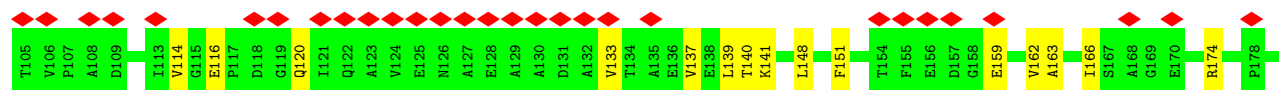
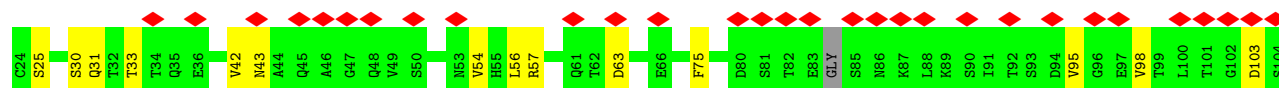
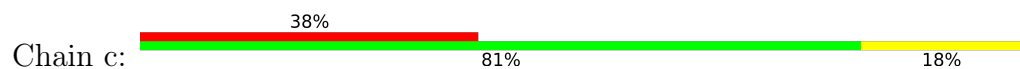




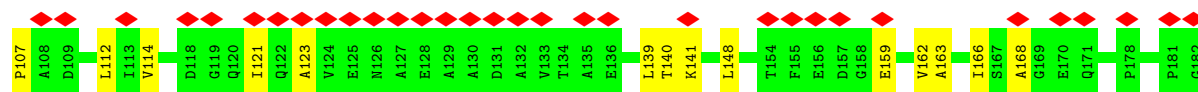
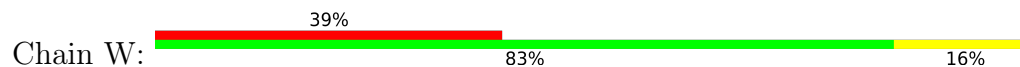
- Molecule 10: Cytochrome bc1 complex cytochrome c subunit



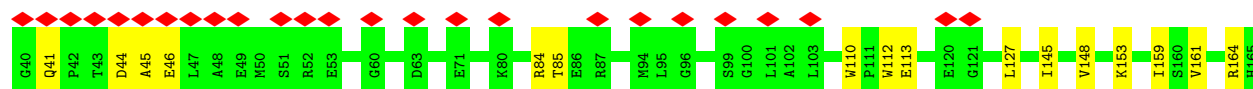
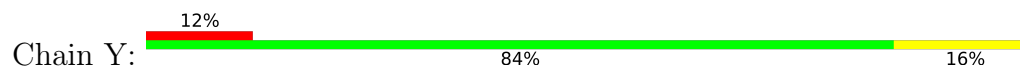
- Molecule 11: LpqE protein

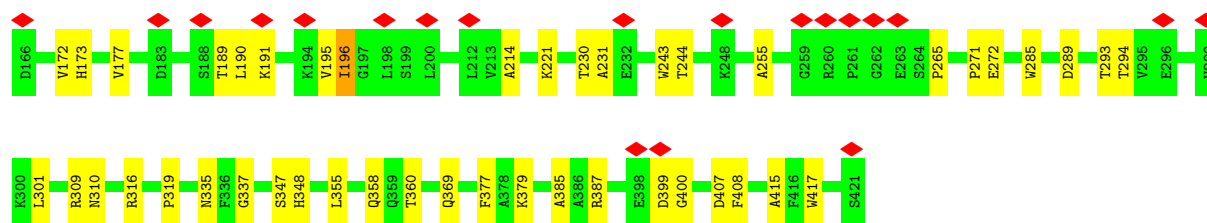


- Molecule 11: LpqE protein

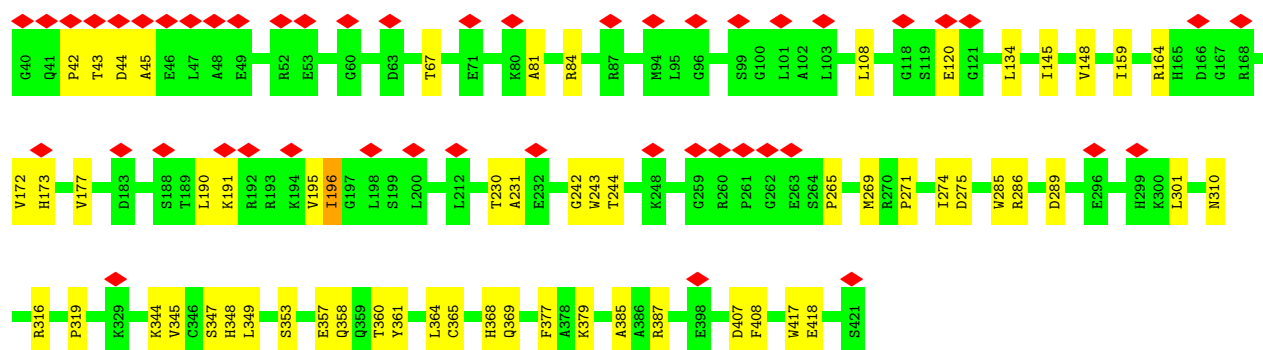
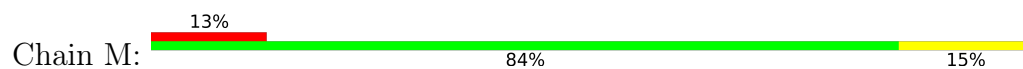


- Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit

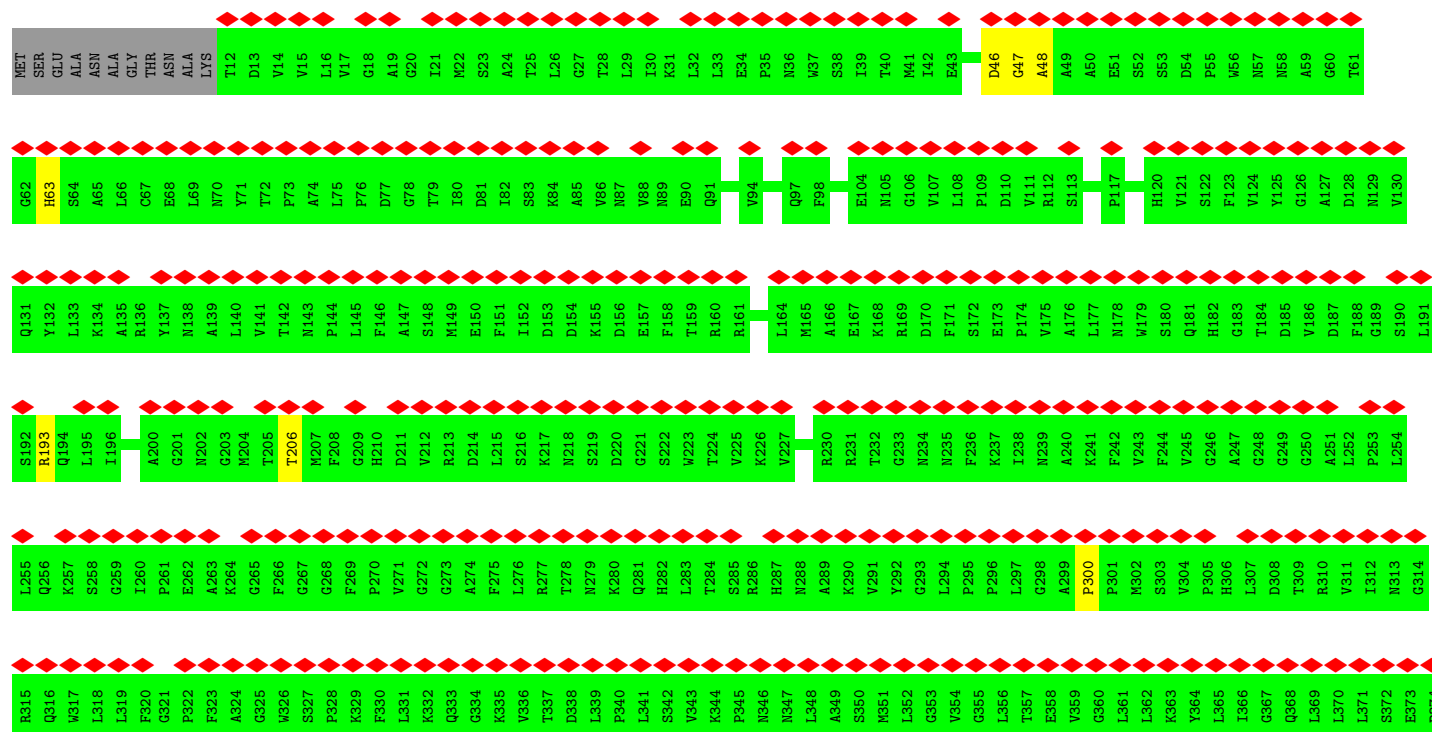
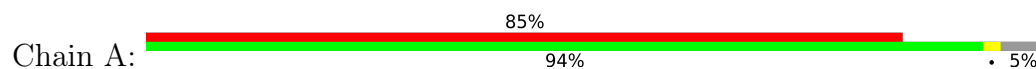




• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit



• Molecule 13: Probable malate:quinone oxidoreductase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145585	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 ($e^-/\text{\AA}^2$)	41.5	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.130	Depositor
Minimum map value	-1.579	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.335	Depositor
Map size (Å)	374.91998, 374.91998, 374.91998	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: 9YF, PLM, FES, CDL, 9XX, HEA, HEM, HEC, CU, 9Y0, MQ9

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	L	0.18	0/4530	0.34	0/6188
1	R	0.17	0/4530	0.33	0/6188
2	E	0.21	0/4314	0.38	0/5882
2	F	0.23	0/4314	0.40	0/5882
3	D	0.14	0/1099	0.33	0/1519
3	G	0.14	0/1099	0.34	0/1519
4	K	0.18	0/2534	0.37	0/3451
4	Q	0.17	0/2534	0.34	0/3451
5	S	0.18	0/1608	0.32	0/2195
5	X	0.19	0/1608	0.32	0/2195
6	T	0.40	1/1112 (0.1%)	0.64	4/1524 (0.3%)
6	Z	0.18	0/1112	0.31	0/1524
7	U	0.15	0/613	0.27	0/836
7	a	0.15	0/613	0.28	0/836
8	V	0.16	0/1059	0.34	0/1446
8	b	0.16	0/1059	0.35	0/1446
9	J	0.16	0/757	0.29	0/1027
9	P	0.25	0/757	0.33	0/1027
10	I	0.18	0/1660	0.39	0/2250
10	O	0.38	0/1660	0.64	2/2250 (0.1%)
11	W	0.14	0/1166	0.32	0/1599
11	c	0.14	0/1166	0.33	0/1599
12	M	0.27	0/3056	0.47	0/4142
12	Y	0.20	0/3056	0.38	1/4142 (0.0%)
13	A	0.66	0/2376	1.18	1/3296 (0.0%)
All	All	0.25	1/49392 (0.0%)	0.46	8/67414 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	120	PHE	C-O	-7.69	1.15	1.24

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	120	PHE	CA-C-O	-9.20	111.05	120.90
6	T	120	PHE	CA-C-N	5.99	128.66	120.46
6	T	120	PHE	C-N-CA	5.99	128.66	120.46
13	A	300	PRO	N-CA-CB	5.61	106.33	103.19
10	O	197	LYS	N-CA-C	-5.45	103.43	110.19

There are no chirality outliers.

There are no planarity outliers.

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	L	4370	0	4346	100	0
1	R	4370	0	4345	105	0
2	E	4181	0	4202	87	0
2	F	4181	0	4199	88	0
3	D	1092	0	640	3	0
3	G	1092	0	640	1	0
4	K	2465	0	2392	36	0
4	Q	2465	0	2392	52	0
5	S	1560	0	1547	66	0
5	X	1560	0	1547	84	0
6	T	1077	0	1058	52	0
6	Z	1077	0	1058	66	0
7	U	591	0	576	10	0
7	a	591	0	576	4	0
8	V	1041	0	1052	49	0
8	b	1041	0	1052	20	0
9	J	736	0	717	14	0
9	P	736	0	717	12	0
10	I	1623	0	1564	42	0
10	O	1623	0	1564	45	0
11	W	1149	0	1110	22	0
11	c	1149	0	1110	22	0
12	M	2977	0	2984	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Y	2977	0	2984	45	0
13	A	2377	0	1117	31	0
14	K	2	0	0	0	0
14	L	1	0	0	0	0
14	Q	2	0	0	0	0
14	R	1	0	0	0	0
15	L	120	0	108	5	0
15	R	120	0	108	4	0
16	E	152	0	192	13	0
16	F	152	0	192	20	0
16	J	76	0	96	11	0
16	L	76	0	96	18	0
16	P	76	0	96	10	0
16	R	76	0	96	22	0
16	S	76	0	96	49	0
16	T	228	0	288	49	0
16	X	152	0	192	97	0
16	Z	152	0	192	80	0
17	E	85	0	57	4	0
17	F	85	0	57	5	0
18	E	116	0	160	6	0
18	F	232	0	320	6	0
18	I	58	0	80	1	0
18	Z	58	0	80	5	0
19	F	49	0	0	0	0
19	J	98	0	0	0	0
19	P	49	0	0	0	0
19	S	49	0	0	0	0
19	X	49	0	0	0	0
20	D	11	0	16	0	0
20	G	11	0	16	0	0
20	W	17	0	31	2	0
20	c	17	0	31	0	0
21	D	32	0	0	0	0
21	G	32	0	0	0	0
21	W	42	0	0	0	0
21	c	42	0	0	0	0
22	I	86	0	64	13	0
22	O	86	0	64	16	0
23	I	58	0	0	5	0
23	M	116	0	0	0	0
23	O	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	W	58	0	0	1	0
23	Y	116	0	0	5	0
23	c	58	0	0	1	0
24	M	4	0	0	1	0
24	Y	4	0	0	1	0
All	All	51339	0	48217	1055	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 11.

The worst 5 of 1055 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)
8:V:125:LEU:CD2	13:A:48:ALA:HB3	1.39	1.50
5:X:166:LYS:NZ	16:X:301:CDL:H112	1.28	1.48
16:Z:203:CDL:H631	23:I:304:9YF:C23	1.48	1.42
8:V:149:VAL:HG22	13:A:46:ASP:C	1.02	1.41
6:Z:120:PHE:CB	16:Z:202:CDL:H612	1.53	1.38

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	550/566 (97%)	516 (94%)	34 (6%)	0	100	100
1	R	550/566 (97%)	518 (94%)	32 (6%)	0	100	100
2	E	533/535 (100%)	490 (92%)	43 (8%)	0	100	100
2	F	533/535 (100%)	489 (92%)	43 (8%)	1 (0%)	43	73
3	D	214/216 (99%)	193 (90%)	20 (9%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	214/216 (99%)	187 (87%)	27 (13%)	0	100	100
4	K	310/312 (99%)	282 (91%)	28 (9%)	0	100	100
4	Q	310/312 (99%)	282 (91%)	28 (9%)	0	100	100
5	S	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
5	X	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
6	T	137/139 (99%)	129 (94%)	8 (6%)	0	100	100
6	Z	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
7	U	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9	40
7	a	77/79 (98%)	70 (91%)	7 (9%)	0	100	100
8	V	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
8	b	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
9	J	88/100 (88%)	85 (97%)	3 (3%)	0	100	100
9	P	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
10	I	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
10	O	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
11	W	154/159 (97%)	137 (89%)	17 (11%)	0	100	100
11	c	154/159 (97%)	135 (88%)	19 (12%)	0	100	100
12	M	380/382 (100%)	344 (90%)	36 (10%)	0	100	100
12	Y	380/382 (100%)	348 (92%)	31 (8%)	1 (0%)	36	68
13	A	483/510 (95%)	474 (98%)	7 (1%)	2 (0%)	30	62
All	All	6499/6628 (98%)	6023 (93%)	470 (7%)	6 (0%)	49	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	135	ARG
13	A	63	HIS
12	Y	113	GLU
3	D	27	THR
13	A	436	GLY

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	L	452/465 (97%)	445 (98%)	7 (2%)	57	76
1	R	452/465 (97%)	447 (99%)	5 (1%)	65	79
2	E	429/429 (100%)	423 (99%)	6 (1%)	59	77
2	F	429/429 (100%)	423 (99%)	6 (1%)	59	77
3	D	20/151 (13%)	20 (100%)	0	100	100
3	G	20/151 (13%)	20 (100%)	0	100	100
4	K	260/266 (98%)	257 (99%)	3 (1%)	63	79
4	Q	260/266 (98%)	258 (99%)	2 (1%)	73	82
5	S	155/161 (96%)	153 (99%)	2 (1%)	61	78
5	X	155/161 (96%)	152 (98%)	3 (2%)	50	73
6	T	106/106 (100%)	106 (100%)	0	100	100
6	Z	106/106 (100%)	106 (100%)	0	100	100
7	U	59/59 (100%)	59 (100%)	0	100	100
7	a	59/59 (100%)	59 (100%)	0	100	100
8	V	107/107 (100%)	105 (98%)	2 (2%)	50	73
8	b	107/107 (100%)	106 (99%)	1 (1%)	70	81
9	J	76/83 (92%)	73 (96%)	3 (4%)	28	62
9	P	76/83 (92%)	75 (99%)	1 (1%)	61	78
10	I	163/163 (100%)	160 (98%)	3 (2%)	51	74
10	O	163/163 (100%)	162 (99%)	1 (1%)	78	84
11	W	127/127 (100%)	127 (100%)	0	100	100
11	c	127/127 (100%)	125 (98%)	2 (2%)	55	75
12	M	312/312 (100%)	310 (99%)	2 (1%)	78	84
12	Y	312/312 (100%)	309 (99%)	3 (1%)	68	80
All	All	4532/4858 (93%)	4480 (99%)	52 (1%)	63	79

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	V	83	GLU
5	X	160	LEU

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Mol	Chain	Res	Type
12	Y	196	ILE
8	V	144	ILE
4	K	139	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
11	c	31	GLN
10	I	137	HIS
10	I	94	ASN
10	I	142	GLN
1	L	249	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 6 are monoatomic - leaving 60 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	$\# Z > 2$
15	HEA	L	603	1	67,67,67	1.38	9 (13%)	81,103,103	1.93	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	9YF	M	501	-	58,58,58	1.08	6 (10%)	68,71,71	1.30	7 (10%)
16	CDL	T	202	-	75,75,99	0.33	0	81,87,111	0.40	0
18	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.63	16 (21%)
18	MQ9	F	707	-	59,59,59	2.25	21 (35%)	73,75,75	1.73	21 (28%)
22	HEC	O	302	10	46,50,50	1.85	5 (10%)	58,82,82	1.68	5 (8%)
19	9Y0	S	302	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
22	HEC	I	301	-	46,50,50	1.83	5 (10%)	58,82,82	1.83	4 (6%)
23	9YF	M	502	-	58,58,58	1.09	5 (8%)	68,71,71	1.33	5 (7%)
16	CDL	L	604	-	75,75,99	0.34	0	81,87,111	0.71	3 (3%)
16	CDL	F	705	-	75,75,99	0.37	0	81,87,111	0.46	1 (1%)
21	9XX	W	202	-	41,41,41	1.10	4 (9%)	44,44,44	1.19	3 (6%)
19	9Y0	J	203	-	48,48,48	1.16	3 (6%)	51,53,53	0.77	2 (3%)
16	CDL	E	606	-	75,75,99	0.37	0	81,87,111	0.42	0
16	CDL	E	605	-	75,75,99	0.34	0	81,87,111	0.42	0
17	HEM	E	601	2	49,49,50	1.39	7 (14%)	67,81,82	1.05	2 (2%)
18	MQ9	F	701	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	15 (20%)
16	CDL	T	201	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
17	HEM	E	602	2	50,50,50	1.42	7 (14%)	67,82,82	1.14	5 (7%)
20	PLM	D	301	3	9,10,17	0.53	0	8,9,17	0.43	0
21	9XX	G	302	3	31,31,41	1.12	3 (9%)	34,34,44	1.47	5 (14%)
19	9Y0	J	202	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)
15	HEA	L	602	1	67,67,67	1.43	11 (16%)	81,103,103	2.38	30 (37%)
15	HEA	R	602	1	67,67,67	1.44	10 (14%)	81,103,103	2.33	30 (37%)
22	HEC	I	302	10	46,50,50	1.84	6 (13%)	58,82,82	1.68	6 (10%)
20	PLM	c	201	11	15,16,17	0.47	0	14,15,17	0.34	0
16	CDL	J	201	-	75,75,99	0.33	0	81,87,111	0.45	0
23	9YF	O	303	-	58,58,58	1.05	5 (8%)	68,71,71	1.01	3 (4%)
16	CDL	X	301	-	75,75,99	0.33	0	81,87,111	0.40	0
17	HEM	F	702	2	49,49,50	1.37	6 (12%)	67,81,82	1.03	2 (2%)
19	9Y0	X	303	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)
18	MQ9	I	303	-	59,59,59	2.39	23 (38%)	73,75,75	1.43	18 (24%)
16	CDL	F	704	-	75,75,99	0.34	0	81,87,111	0.42	0
16	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.60	2 (2%)
17	HEM	F	703	2	50,50,50	1.41	7 (14%)	67,82,82	1.12	3 (4%)
18	MQ9	F	709	-	59,59,59	2.43	22 (37%)	73,75,75	1.54	15 (20%)
19	9Y0	P	202	-	48,48,48	1.19	3 (6%)	51,53,53	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PLM	W	201	11	15,16,17	0.49	0	14,15,17	0.33	0
23	9YF	Y	502	-	58,58,58	1.08	7 (12%)	68,71,71	1.30	7 (10%)
15	HEA	R	603	1	67,67,67	1.37	10 (14%)	81,103,103	2.04	18 (22%)
21	9XX	c	202	11	41,41,41	0.96	3 (7%)	44,44,44	1.18	4 (9%)
24	FES	M	503	12	0,4,4	-	-	-	-	-
23	9YF	c	203	-	58,58,58	1.01	5 (8%)	68,71,71	1.13	3 (4%)
18	MQ9	E	604	-	59,59,59	2.41	22 (37%)	73,75,75	1.53	16 (21%)
23	9YF	W	203	-	58,58,58	1.02	5 (8%)	68,71,71	1.13	3 (4%)
16	CDL	Z	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
20	PLM	G	301	3	9,10,17	0.54	0	8,9,17	0.43	0
22	HEC	O	301	10	46,50,50	1.85	6 (13%)	58,82,82	1.67	4 (6%)
23	9YF	Y	503	-	58,58,58	1.09	5 (8%)	68,71,71	1.33	5 (7%)
24	FES	Y	501	12	0,4,4	-	-	-	-	-
23	9YF	I	304	-	58,58,58	1.04	5 (8%)	68,71,71	1.01	3 (4%)
19	9Y0	F	706	-	48,48,48	1.17	3 (6%)	51,53,53	0.87	2 (3%)
16	CDL	S	301	-	75,75,99	1.32	7 (9%)	81,87,111	1.99	9 (11%)
16	CDL	Z	202	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
16	CDL	T	203	-	75,75,99	0.37	0	81,87,111	0.45	0
16	CDL	P	201	-	75,75,99	0.33	0	81,87,111	0.45	0
21	9XX	D	302	-	31,31,41	1.11	3 (9%)	34,34,44	1.44	4 (11%)
18	MQ9	F	708	-	59,59,59	2.30	22 (37%)	73,75,75	1.43	9 (12%)
18	MQ9	E	603	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	13 (17%)
16	CDL	X	302	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)

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
15	HEA	L	603	1	-	3/36/76/76	-
23	9YF	M	501	-	-	23/54/78/78	0/1/1/1
16	CDL	T	202	-	-	46/86/86/110	-
18	MQ9	Z	201	-	-	11/53/73/73	0/2/2/2
18	MQ9	F	707	-	-	17/53/73/73	0/2/2/2
22	HEC	O	302	10	-	6/14/54/54	-
19	9Y0	S	302	-	-	19/52/52/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	HEC	I	301	-	-	4/14/54/54	-
23	9YF	M	502	-	-	27/54/78/78	0/1/1/1
16	CDL	L	604	-	-	48/86/86/110	-
16	CDL	F	705	-	-	44/86/86/110	-
21	9XX	W	202	-	-	15/43/43/43	-
19	9Y0	J	203	-	-	25/52/52/52	-
16	CDL	E	606	-	-	40/86/86/110	-
16	CDL	E	605	-	-	49/86/86/110	-
17	HEM	E	601	2	-	2/12/52/54	-
18	MQ9	F	701	-	-	6/53/73/73	0/2/2/2
16	CDL	T	201	-	-	34/86/86/110	-
17	HEM	E	602	2	-	2/14/54/54	-
20	PLM	D	301	3	-	3/8/8/15	-
21	9XX	G	302	3	-	10/33/33/43	-
19	9Y0	J	202	-	-	19/52/52/52	-
15	HEA	L	602	1	-	12/36/76/76	-
15	HEA	R	602	1	-	7/36/76/76	-
22	HEC	I	302	10	-	3/14/54/54	-
20	PLM	c	201	11	-	5/14/14/15	-
16	CDL	J	201	-	-	48/86/86/110	-
23	9YF	O	303	-	-	28/54/78/78	0/1/1/1
16	CDL	X	301	-	-	46/86/86/110	-
17	HEM	F	702	2	-	4/12/52/54	-
19	9Y0	X	303	-	-	17/52/52/52	-
18	MQ9	I	303	-	-	8/53/73/73	0/2/2/2
16	CDL	F	704	-	-	49/86/86/110	-
16	CDL	R	604	-	-	47/86/86/110	-
17	HEM	F	703	2	-	0/14/54/54	-
18	MQ9	F	709	-	-	12/53/73/73	0/2/2/2
19	9Y0	P	202	-	-	22/52/52/52	-
20	PLM	W	201	11	-	4/14/14/15	-
23	9YF	Y	502	-	-	23/54/78/78	0/1/1/1
15	HEA	R	603	1	-	3/36/76/76	-
21	9XX	c	202	11	-	16/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	FES	M	503	12	-	-	0/1/1/1
23	9YF	c	203	-	-	22/54/78/78	0/1/1/1
18	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
23	9YF	W	203	-	-	22/54/78/78	0/1/1/1
16	CDL	Z	203	-	-	38/86/86/110	-
20	PLM	G	301	3	-	2/8/8/15	-
22	HEC	O	301	10	-	5/14/54/54	-
23	9YF	Y	503	-	-	27/54/78/78	0/1/1/1
24	FES	Y	501	12	-	-	0/1/1/1
23	9YF	I	304	-	-	27/54/78/78	0/1/1/1
19	9Y0	F	706	-	-	16/52/52/52	-
16	CDL	S	301	-	-	43/86/86/110	-
16	CDL	Z	202	-	-	34/86/86/110	-
16	CDL	T	203	-	-	47/86/86/110	-
16	CDL	P	201	-	-	48/86/86/110	-
21	9XX	D	302	-	-	9/33/33/43	-
18	MQ9	F	708	-	-	11/53/73/73	0/2/2/2
18	MQ9	E	603	-	-	6/53/73/73	0/2/2/2
16	CDL	X	302	-	-	43/86/86/110	-

The worst 5 of 380 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	E	604	MQ9	C6-C5	8.80	1.51	1.35
18	F	709	MQ9	C6-C5	8.77	1.50	1.35
18	F	708	MQ9	C6-C5	8.60	1.50	1.35
18	F	701	MQ9	C6-C5	8.58	1.50	1.35
18	I	303	MQ9	C6-C5	8.52	1.50	1.35

The worst 5 of 378 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Z	203	CDL	CB6-CB4-CB3	-9.90	88.70	111.78
16	X	302	CDL	CB6-CB4-CB3	-9.67	89.24	111.78
16	S	301	CDL	CB6-CB4-CB3	-9.67	89.25	111.78
16	T	201	CDL	OB6-CB4-CB6	9.23	141.47	108.34
16	Z	202	CDL	OB6-CB4-CB6	9.23	141.45	108.34

There are no chirality outliers.

5 of 1218 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	R	602	HEA	C2D-C3D-CAD-CBD
15	R	602	HEA	C4D-C3D-CAD-CBD
15	L	602	HEA	C12-C11-C3B-C2B
16	R	604	CDL	CA3-OA5-PA1-OA2
16	R	604	CDL	CA3-OA5-PA1-OA3

There are no ring outliers.

42 monomers are involved in 403 short contacts:

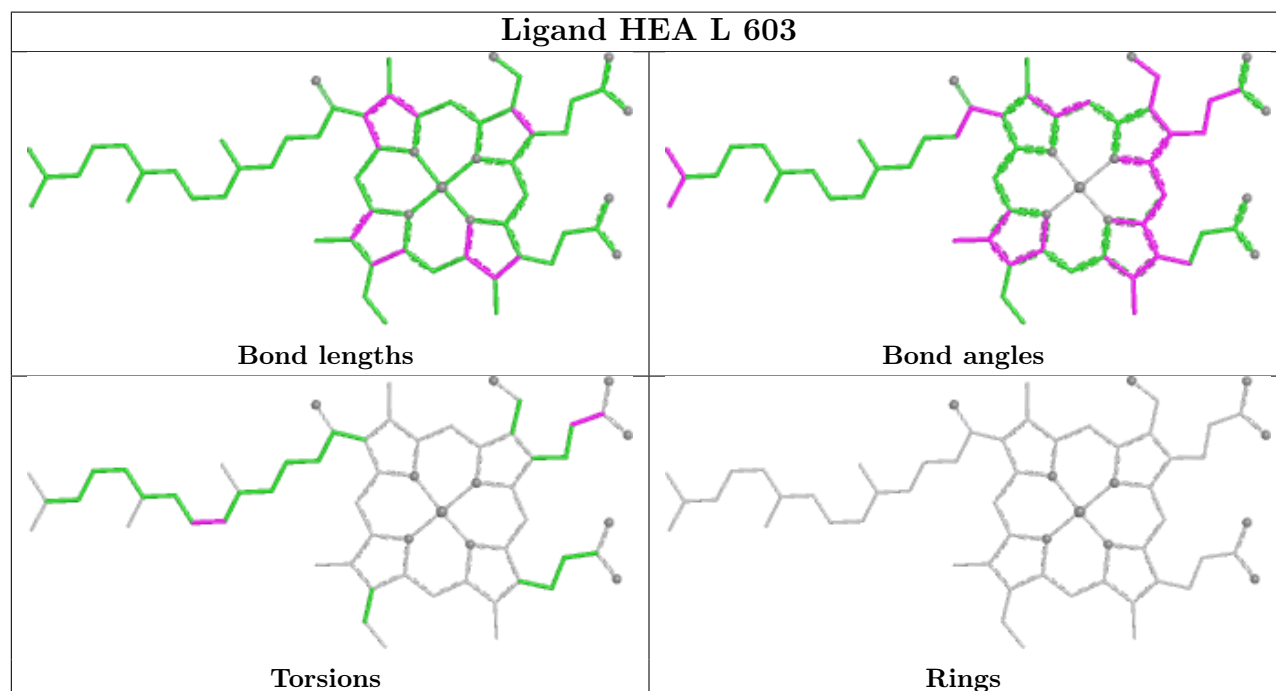
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	L	603	HEA	3	0
16	T	202	CDL	9	0
18	Z	201	MQ9	5	0
22	O	302	HEC	11	0
22	I	301	HEC	4	0
16	L	604	CDL	18	0
16	F	705	CDL	10	0
16	E	606	CDL	3	0
16	E	605	CDL	10	0
17	E	601	HEM	2	0
18	F	701	MQ9	1	0
16	T	201	CDL	33	0
17	E	602	HEM	2	0
15	L	602	HEA	2	0
22	I	302	HEC	9	0
16	J	201	CDL	11	0
16	X	301	CDL	43	0
17	F	702	HEM	1	0
18	I	303	MQ9	1	0
16	F	704	CDL	10	0
16	R	604	CDL	22	0
17	F	703	HEM	4	0
18	F	709	MQ9	4	0
20	W	201	PLM	2	0
23	Y	502	9YF	2	0
15	R	603	HEA	4	0
24	M	503	FES	1	0
23	c	203	9YF	1	0
18	E	604	MQ9	5	0
23	W	203	9YF	1	0

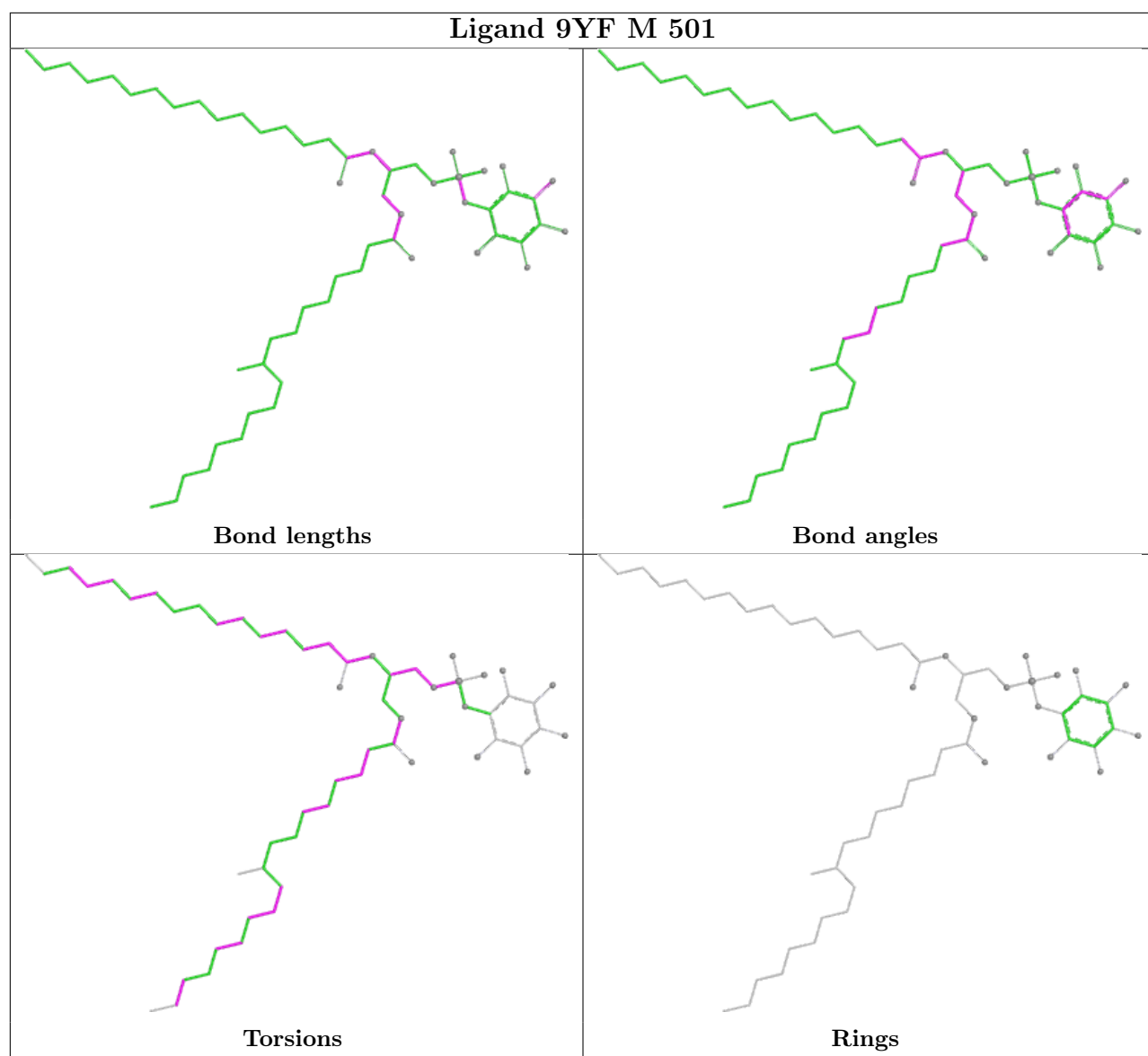
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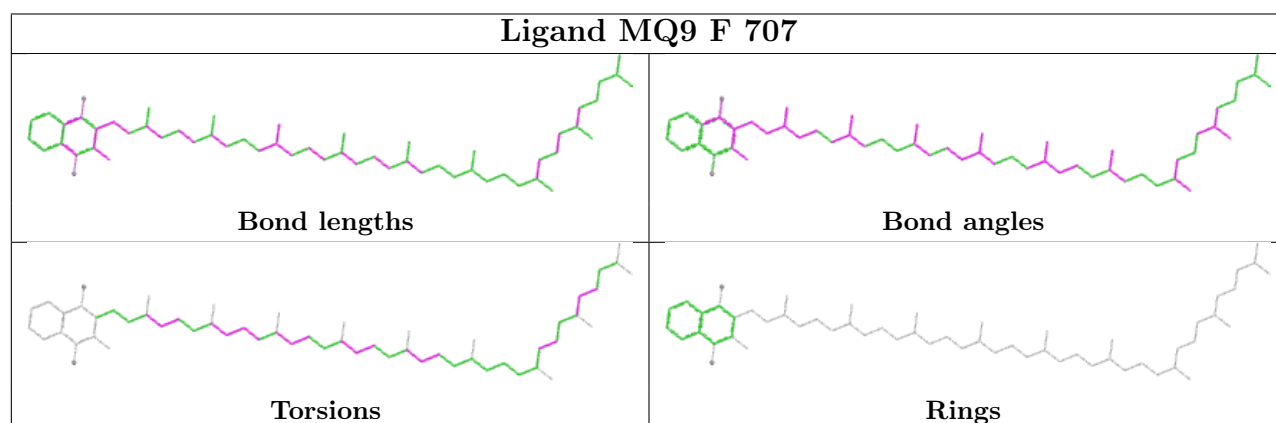
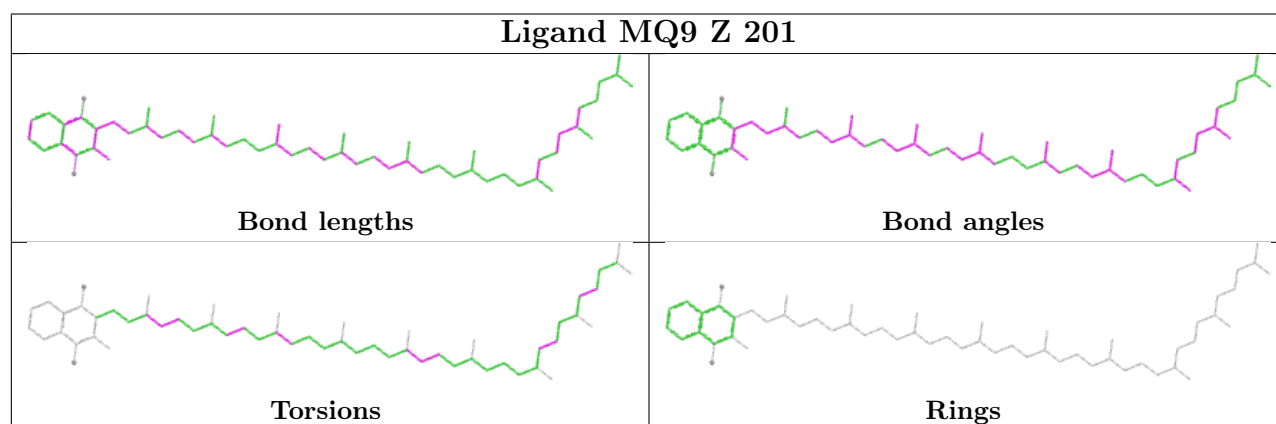
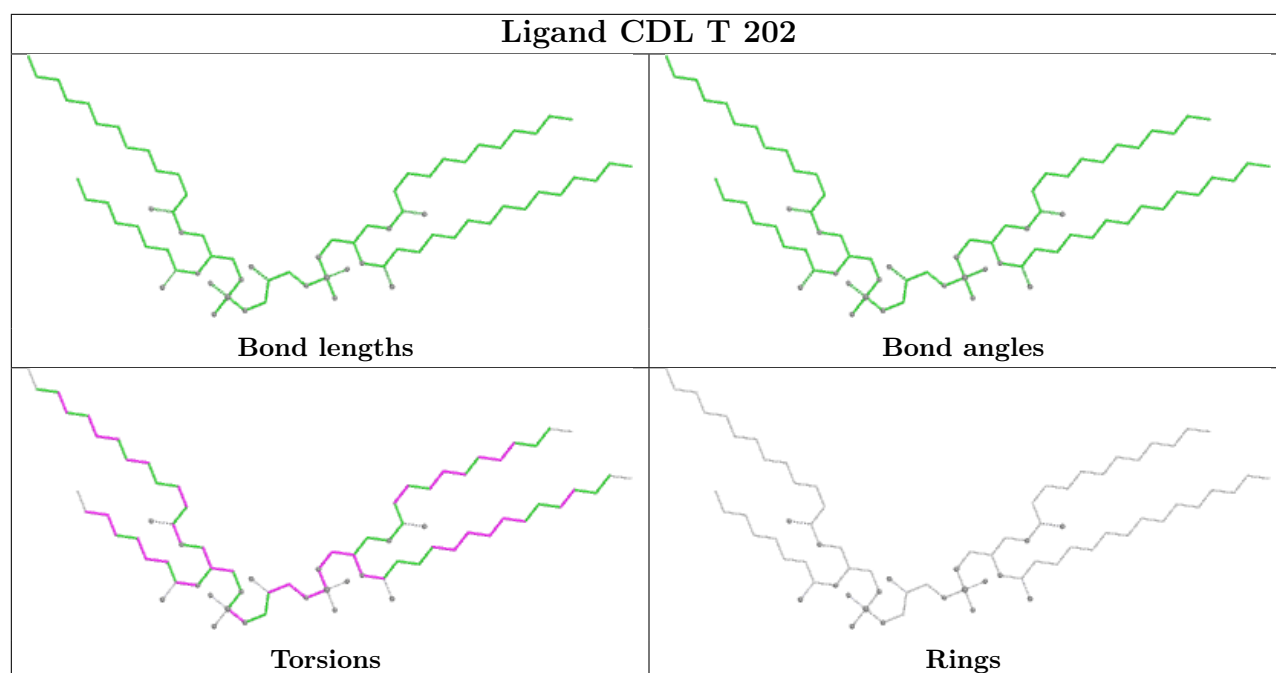
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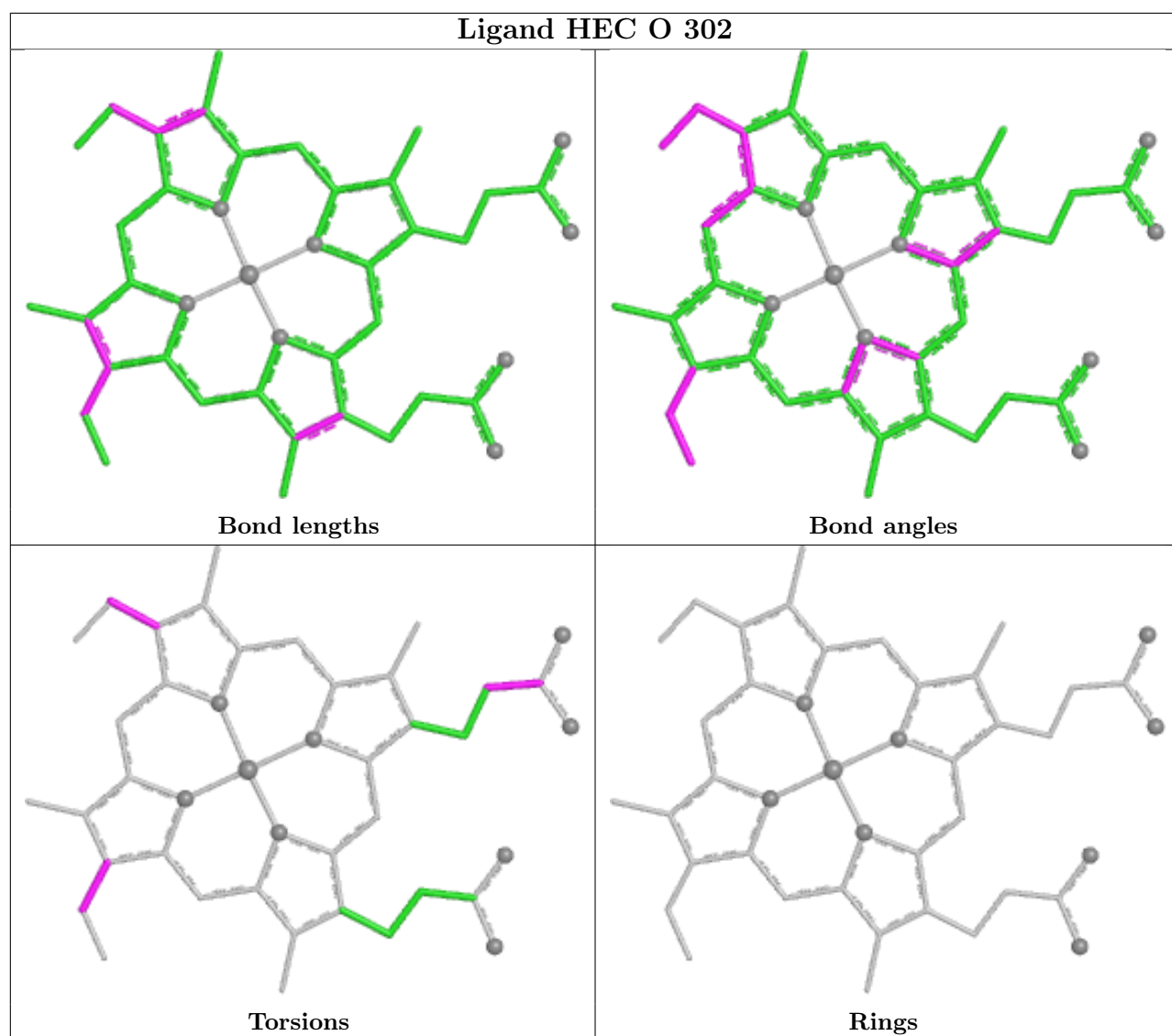
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Z	203	CDL	44	0
22	O	301	HEC	5	0
23	Y	503	9YF	3	0
24	Y	501	FES	1	0
23	I	304	9YF	5	0
16	S	301	CDL	49	0
16	Z	202	CDL	36	0
16	T	203	CDL	9	0
16	P	201	CDL	10	0
18	F	708	MQ9	1	0
18	E	603	MQ9	1	0
16	X	302	CDL	54	0

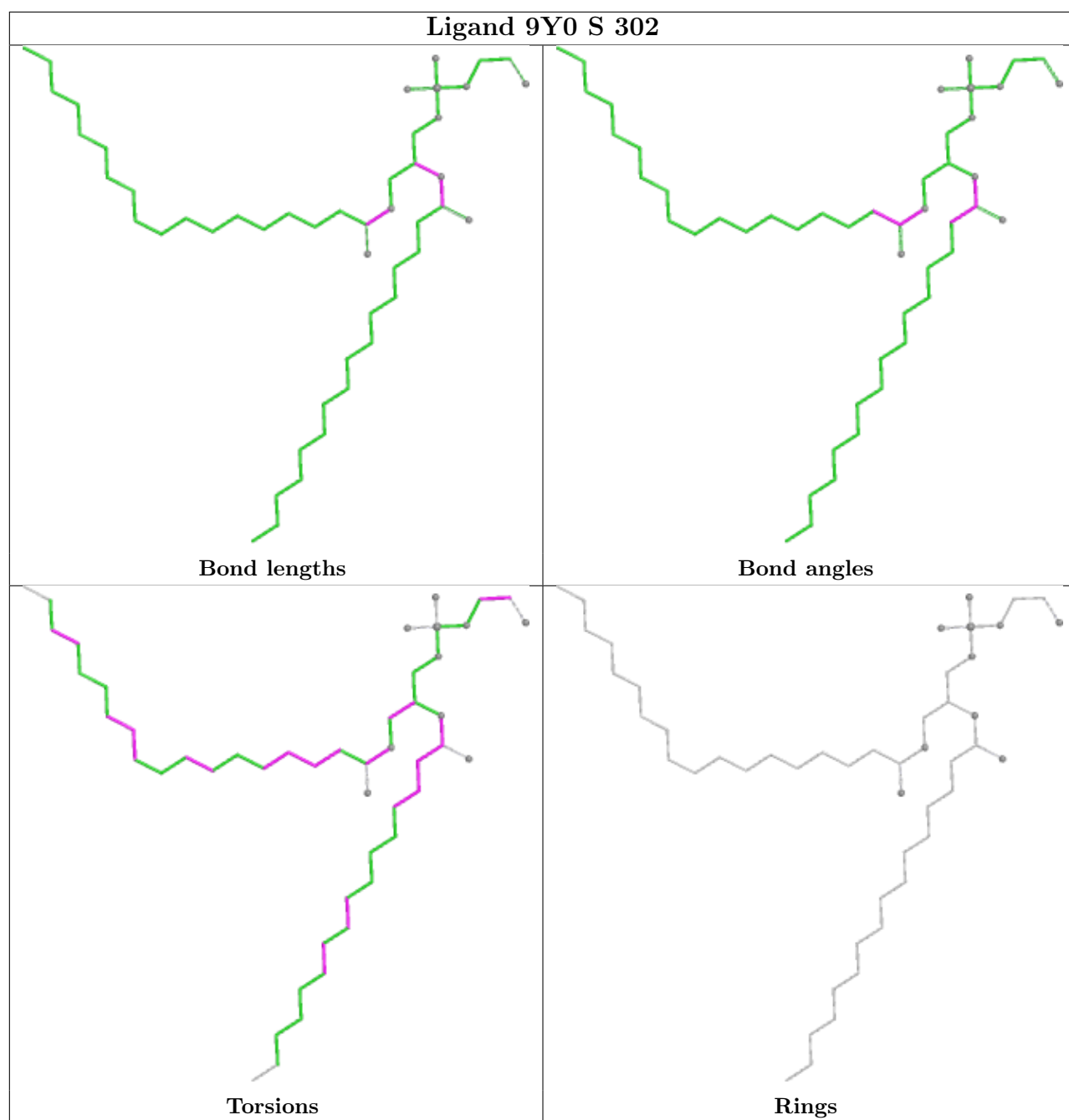
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



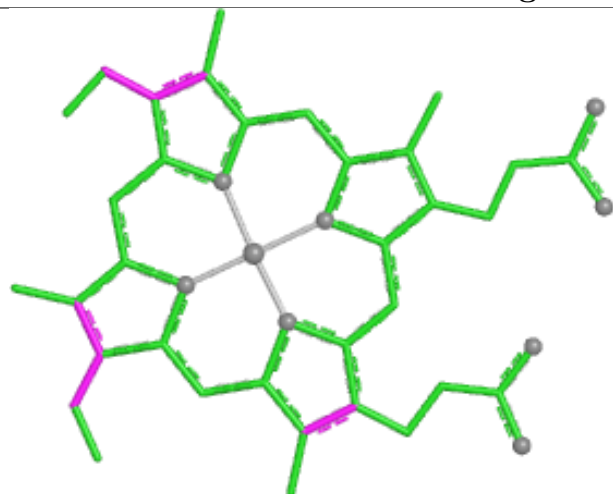




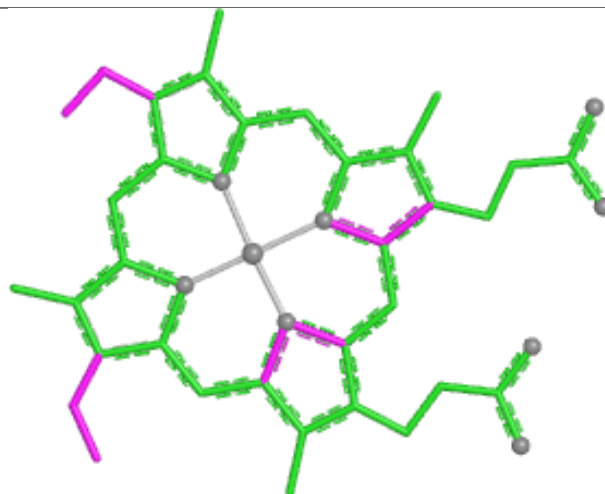




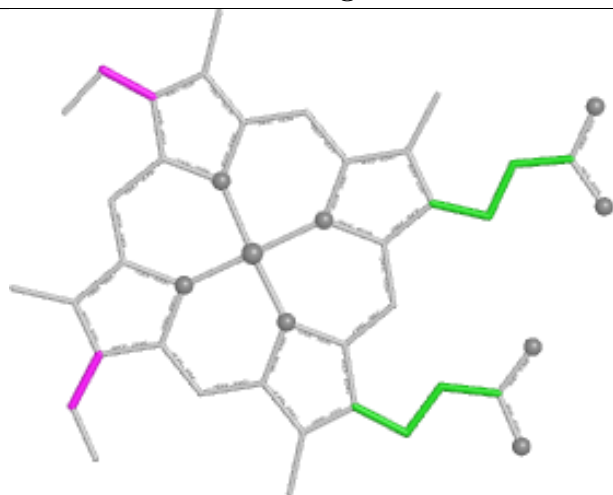
Ligand HEC I 301



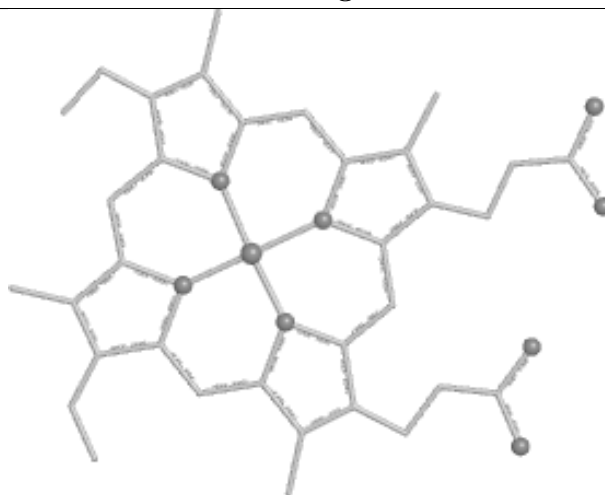
Bond lengths



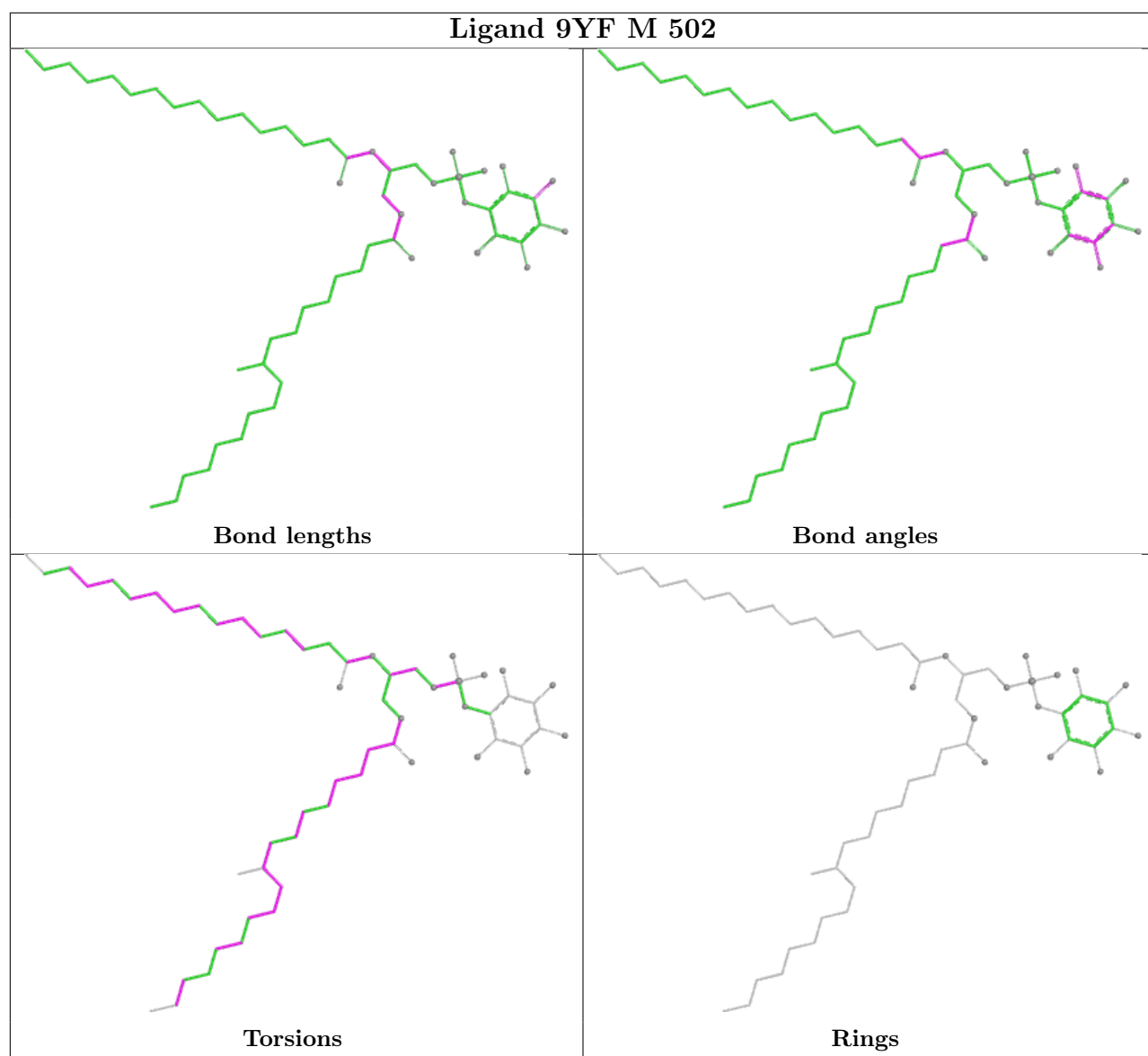
Bond angles

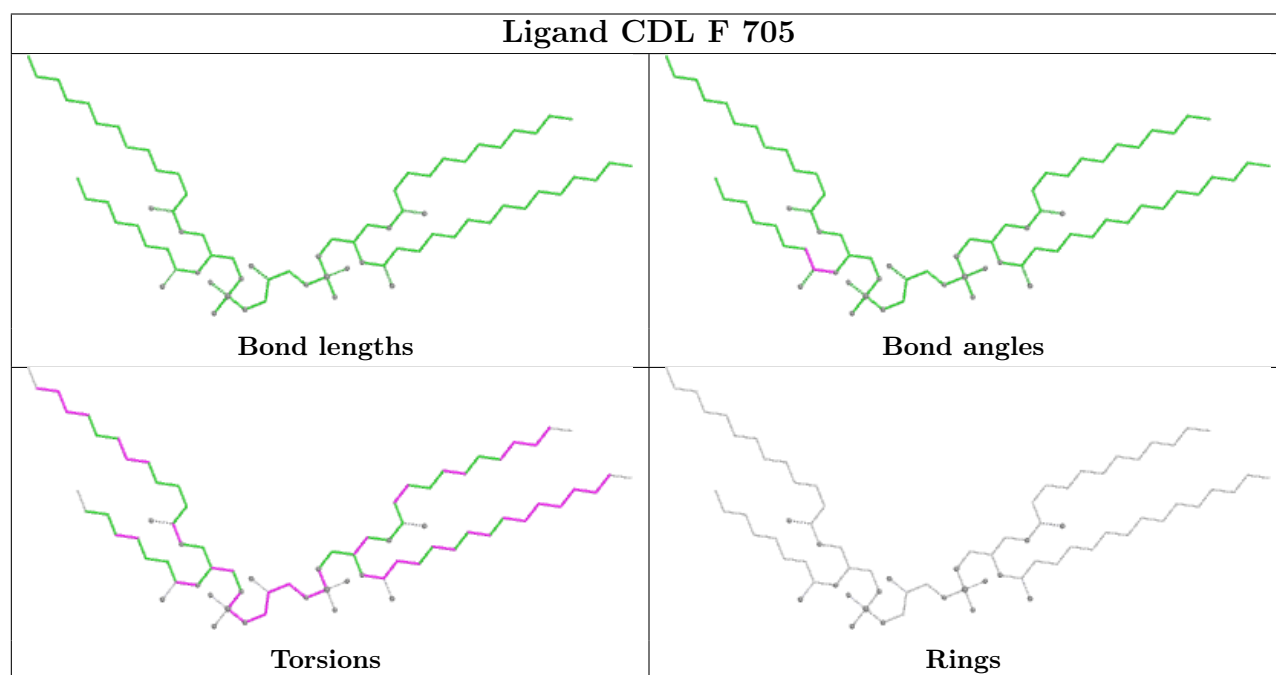
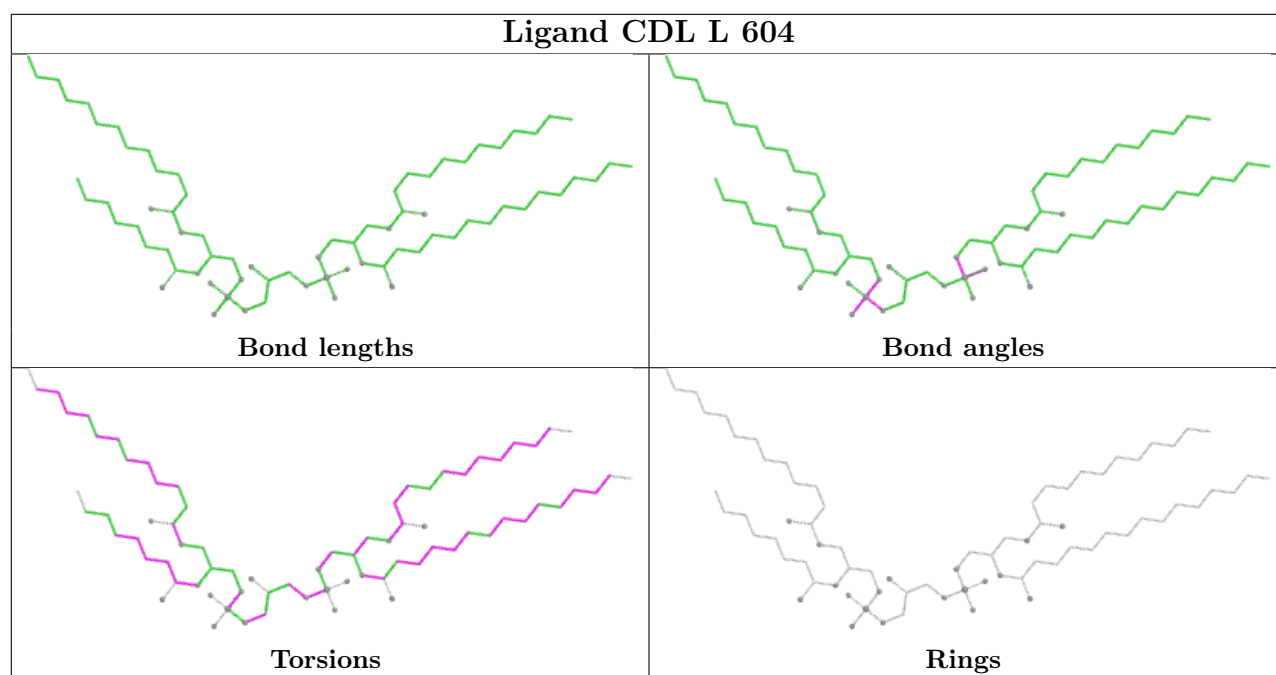


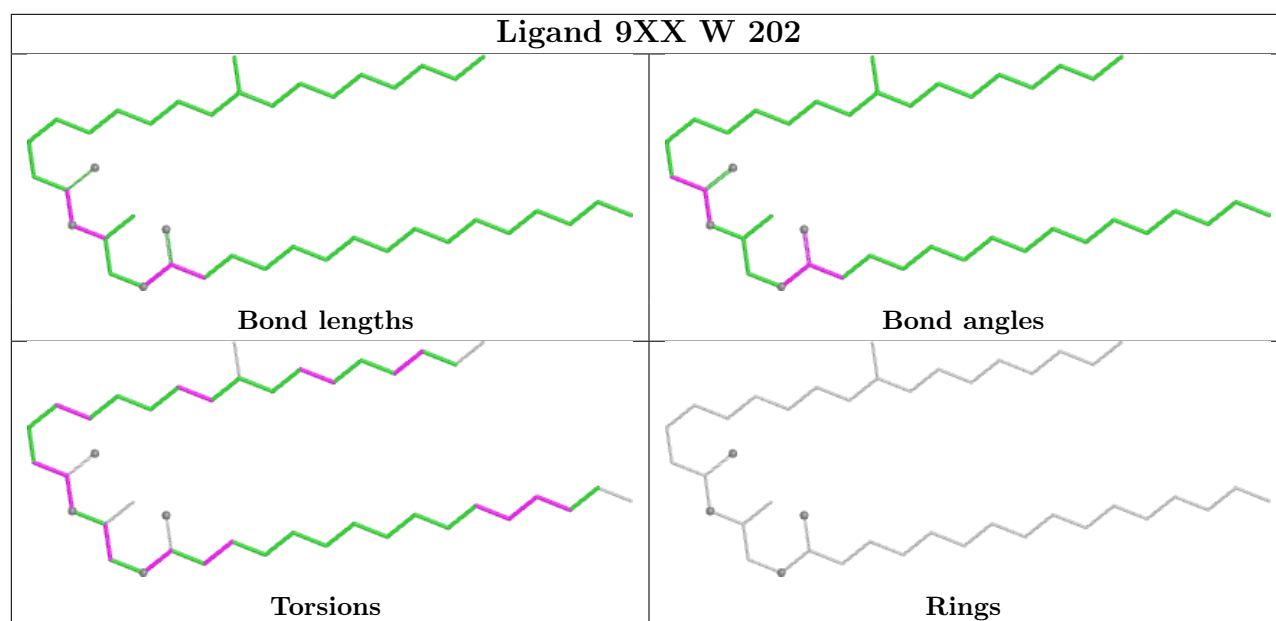
Torsions

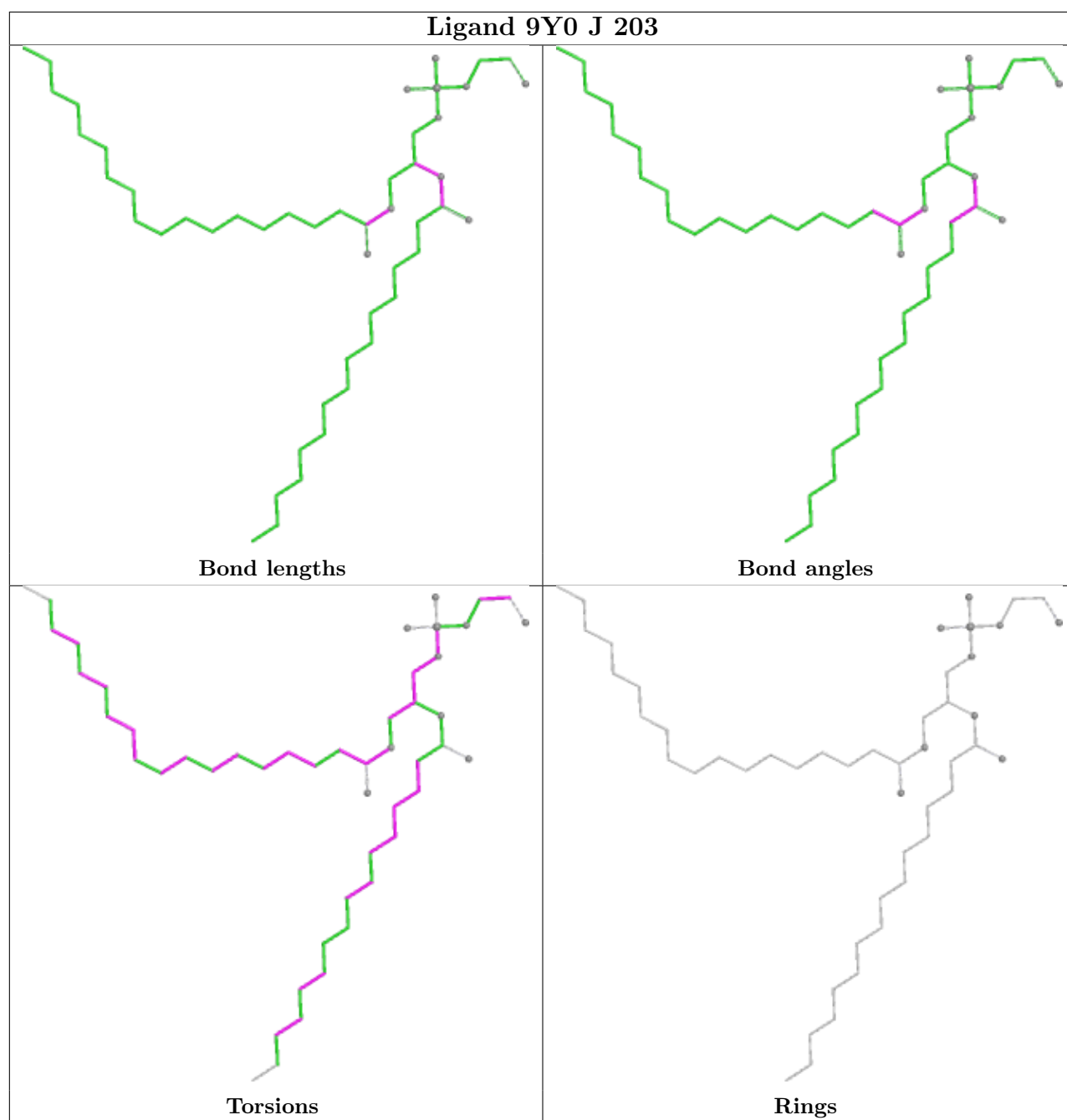


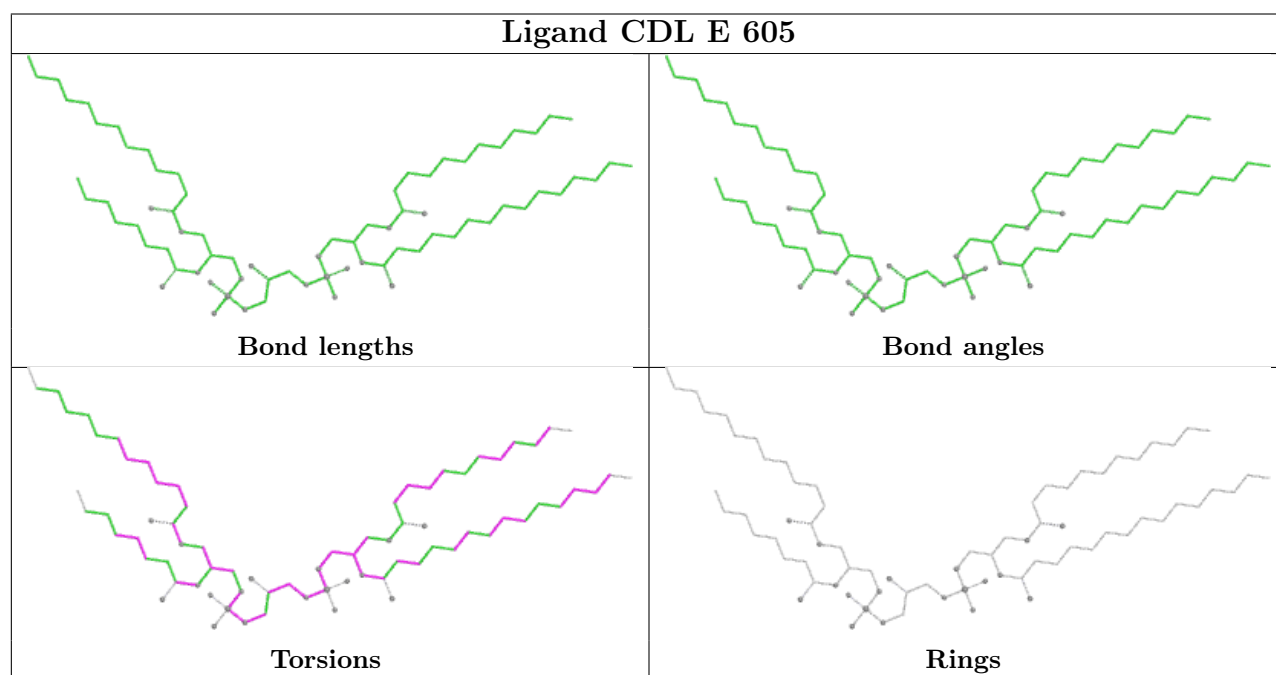
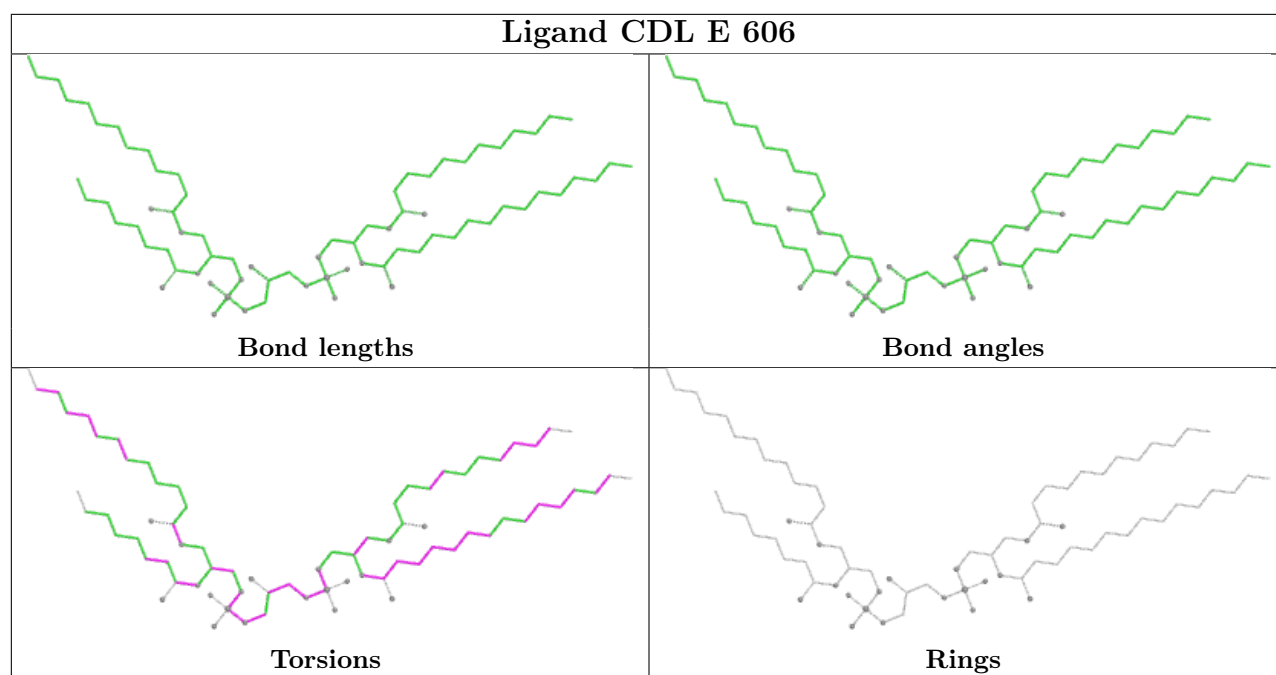
Rings

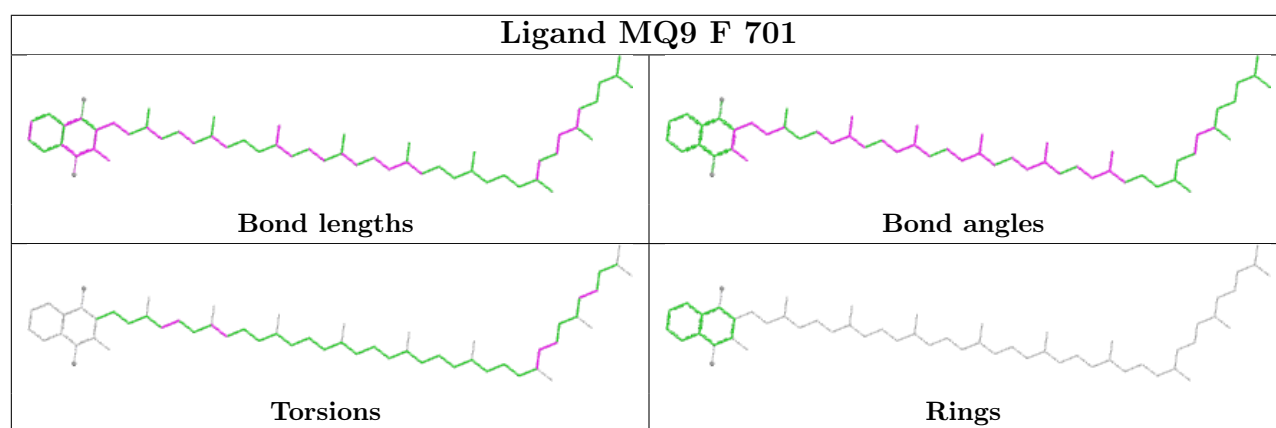
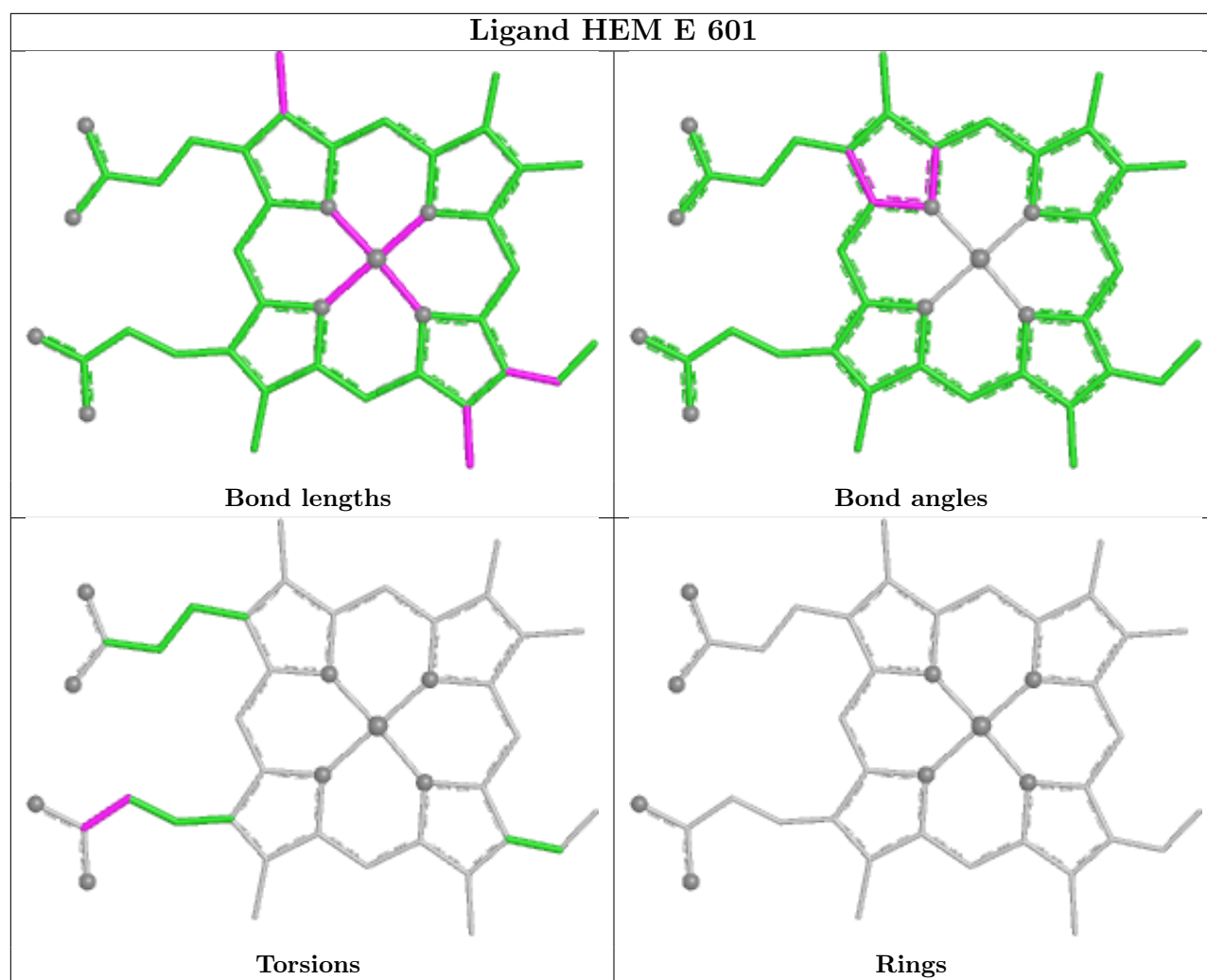


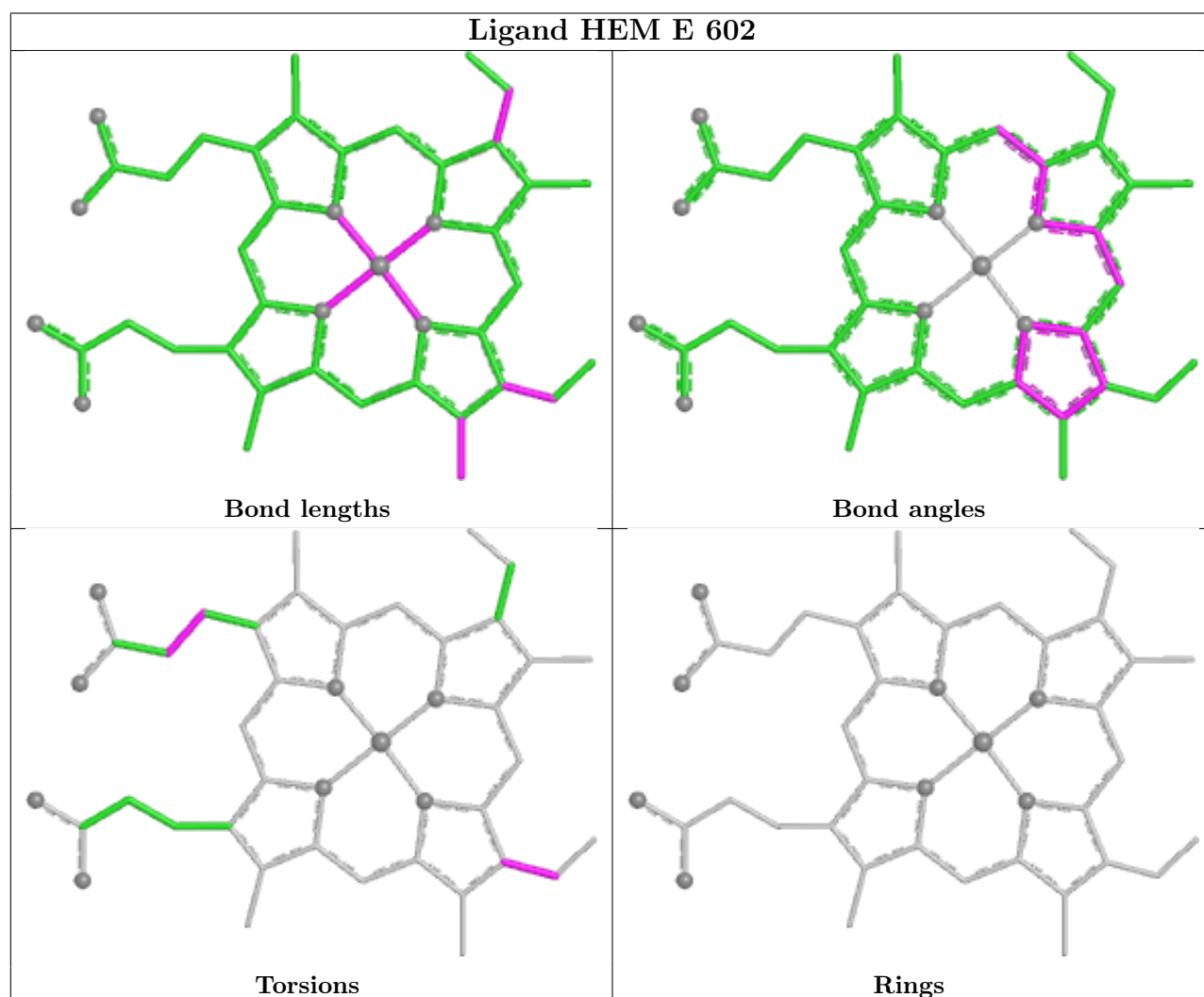
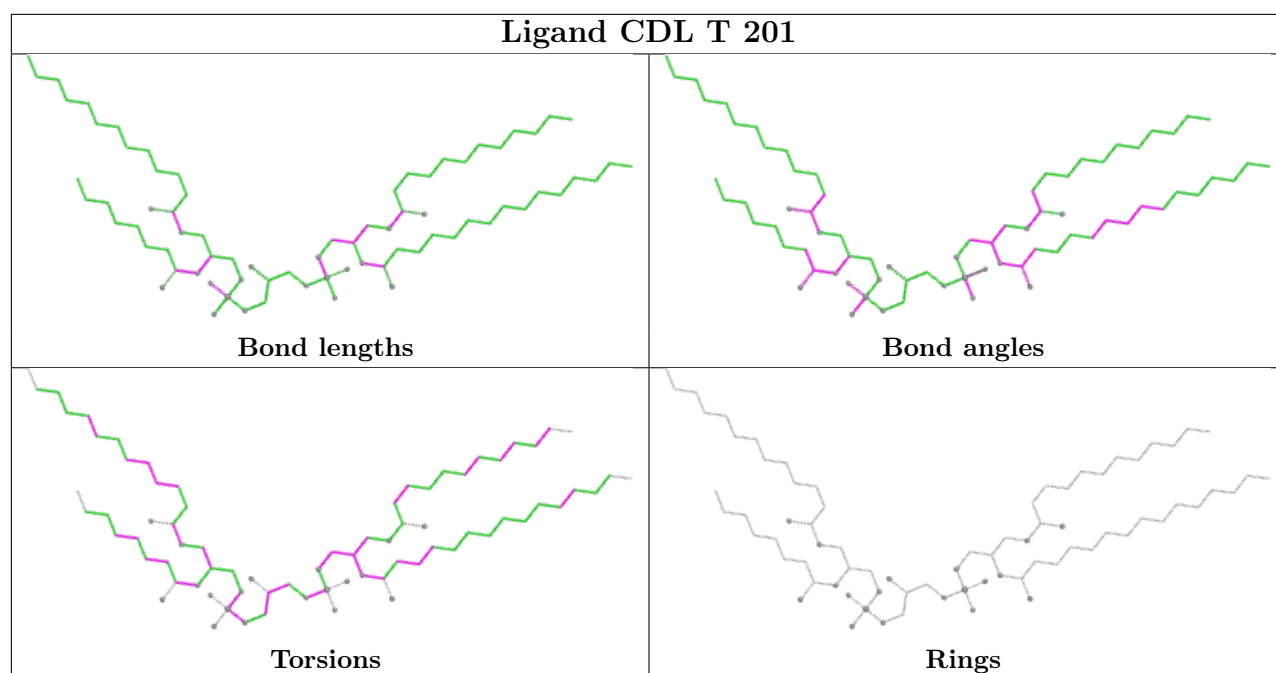


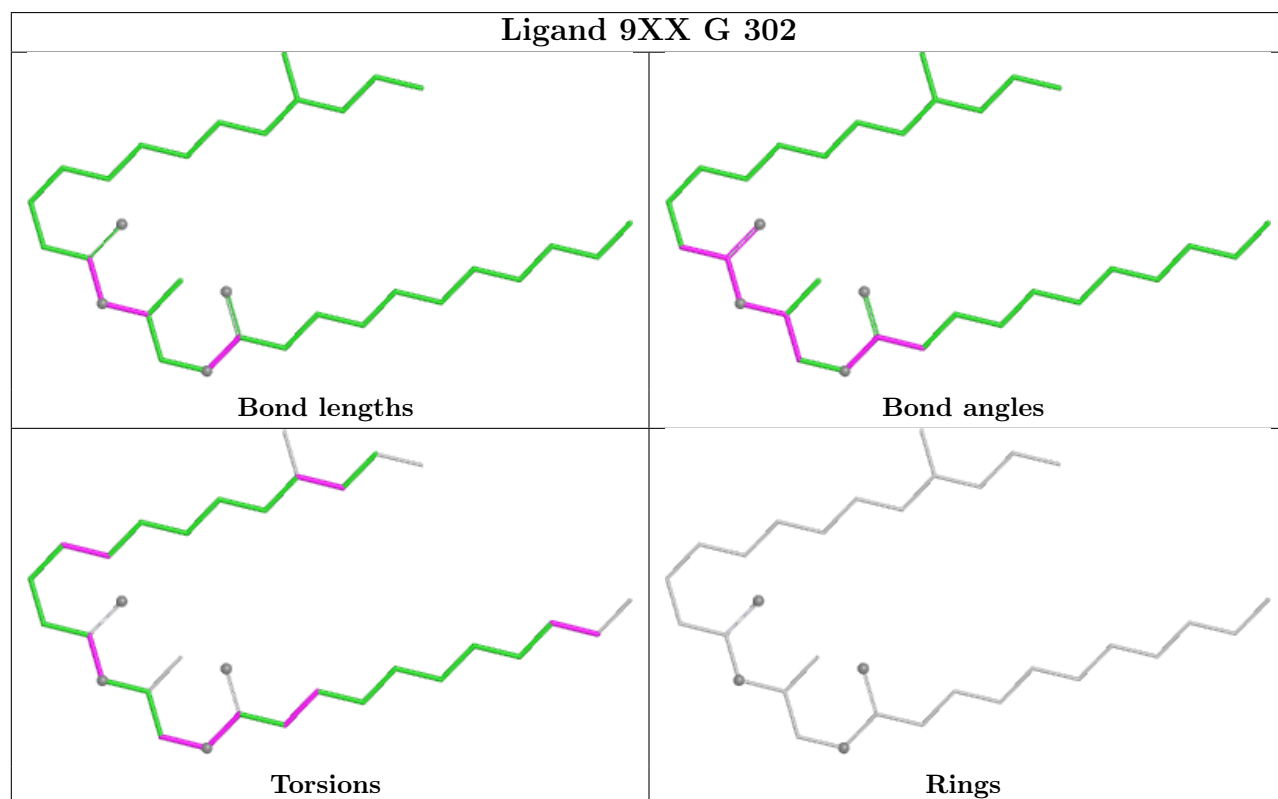
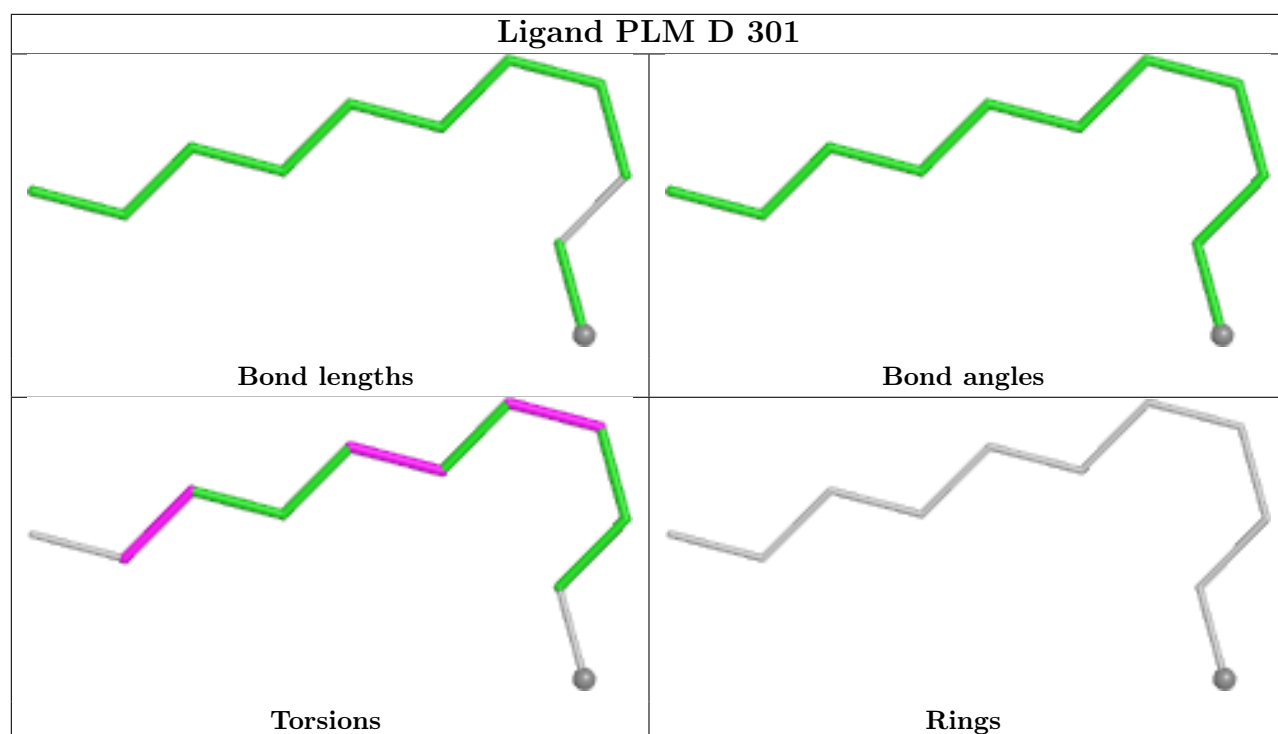


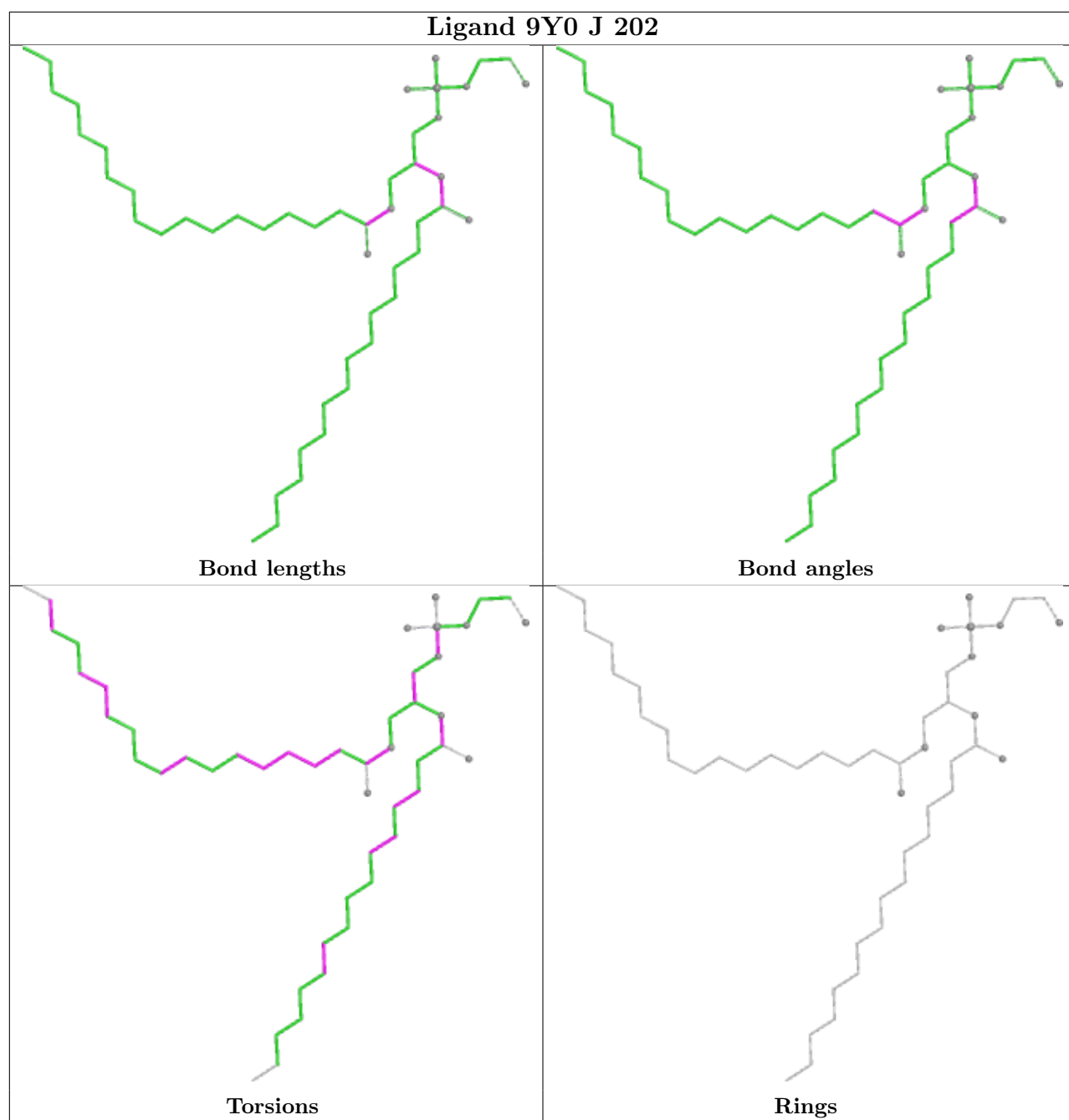


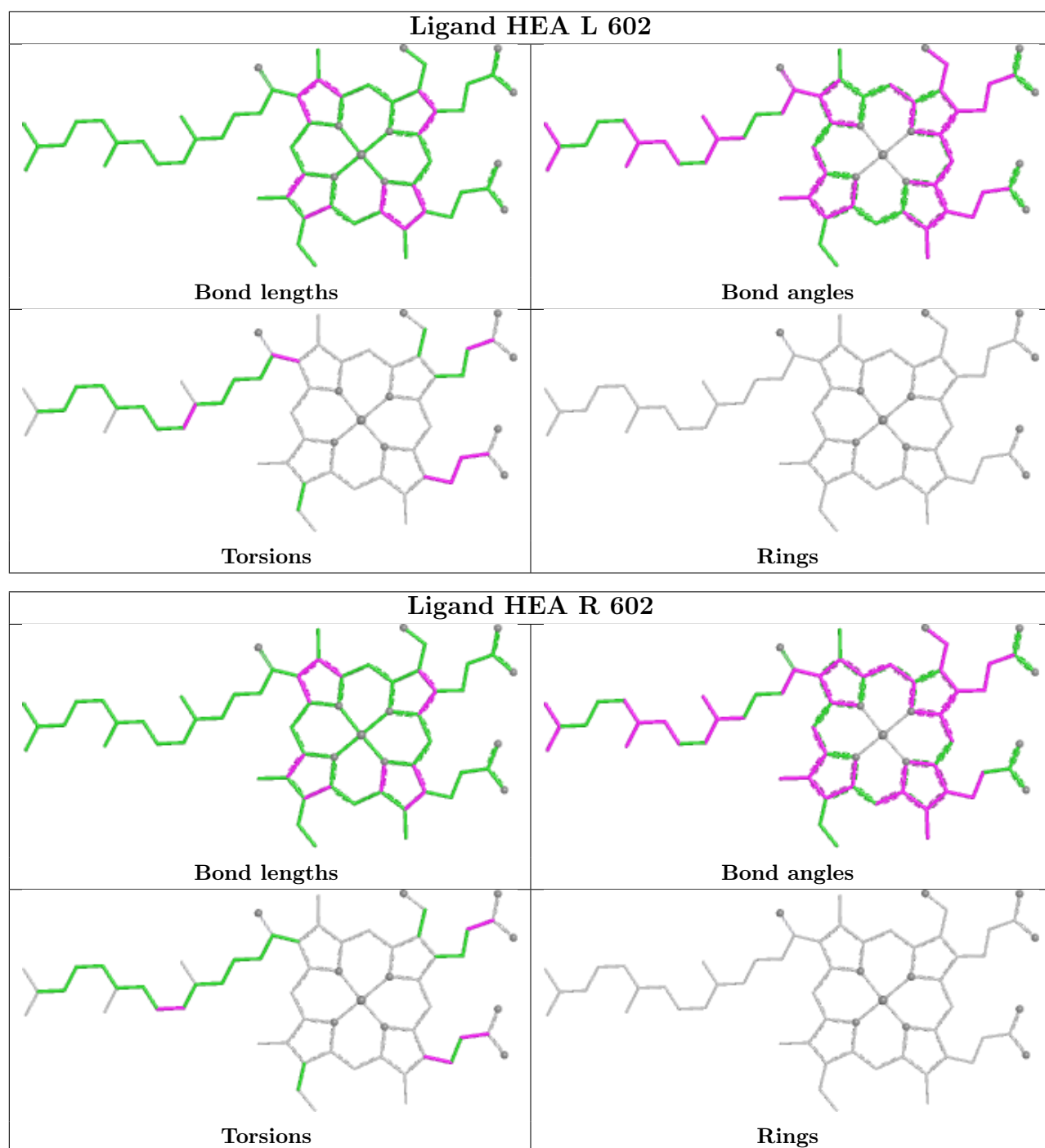




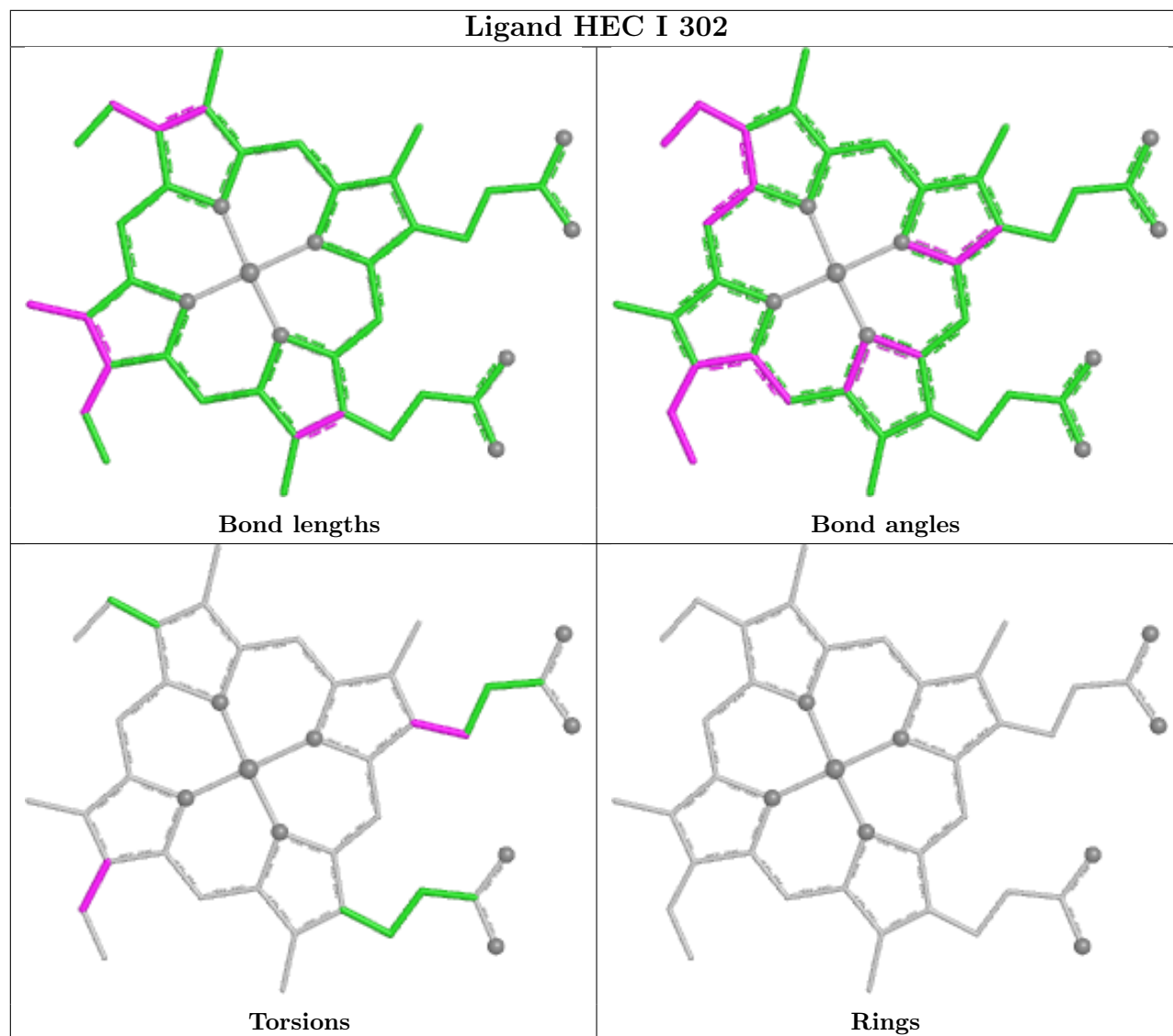




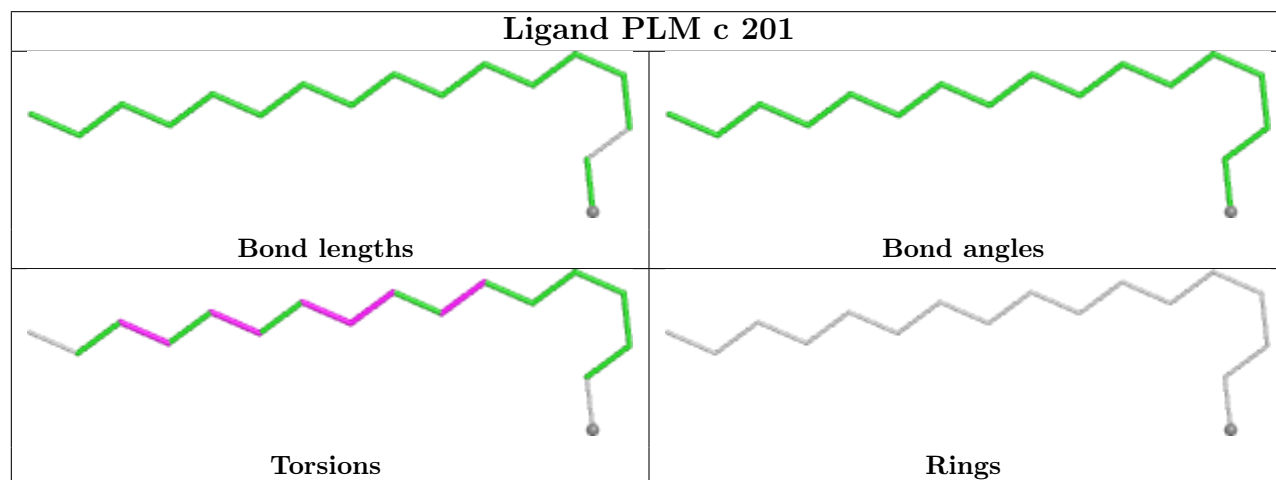


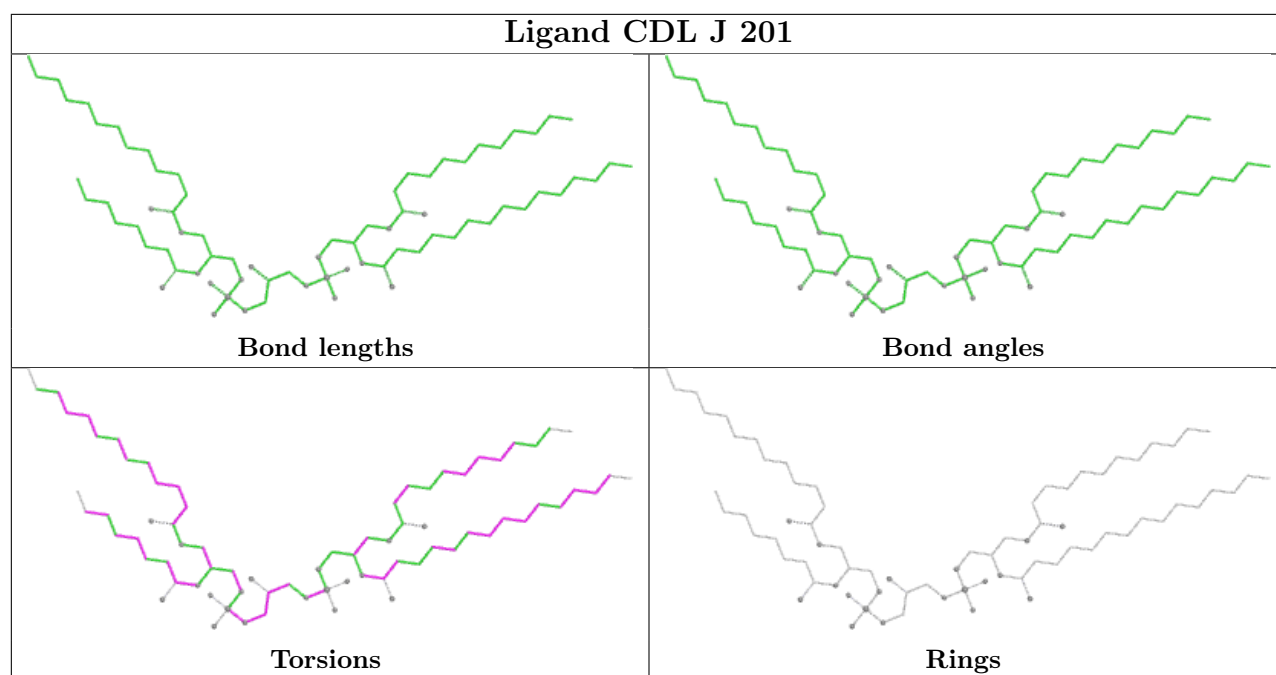


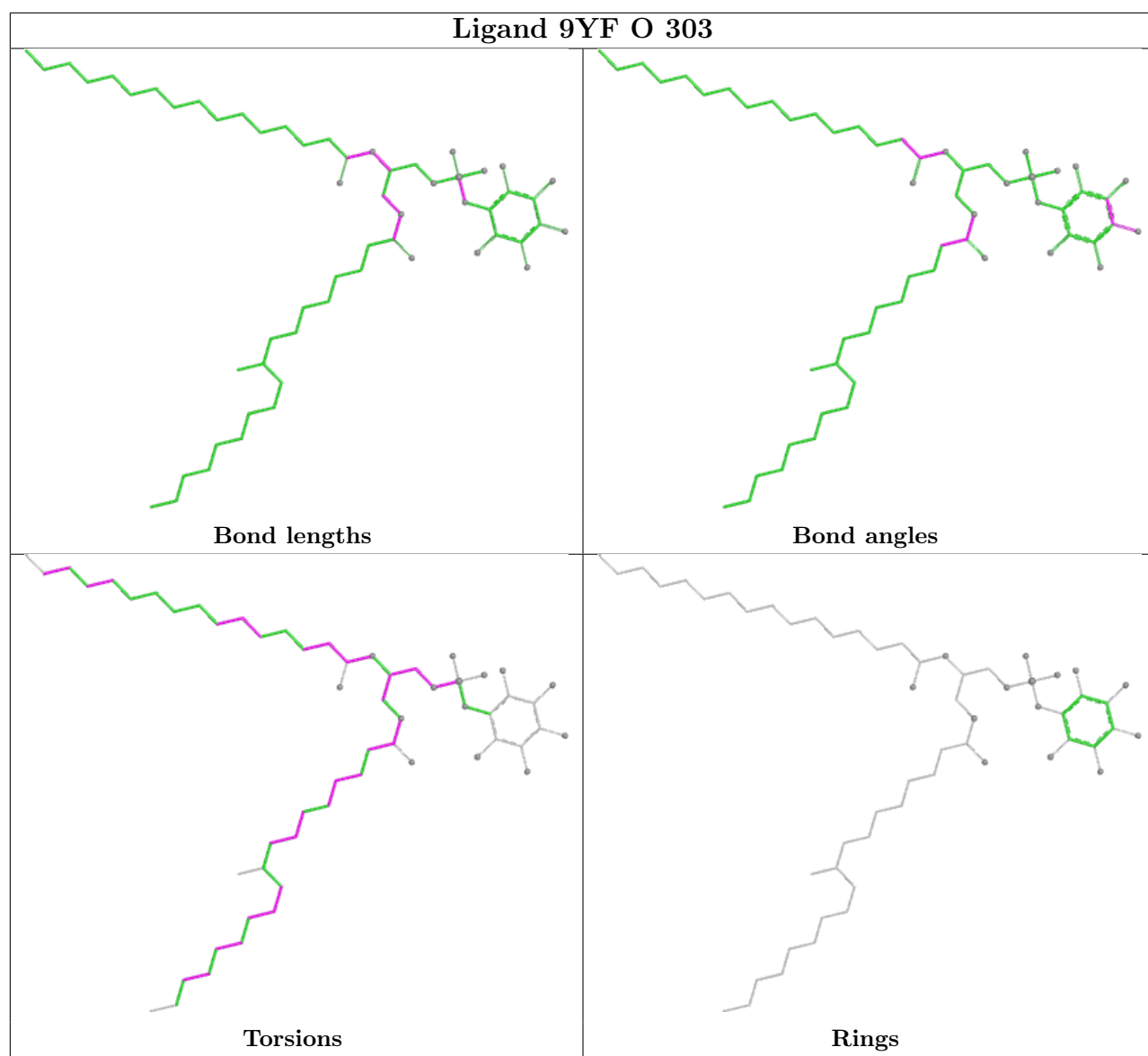
Ligand HEC I 302

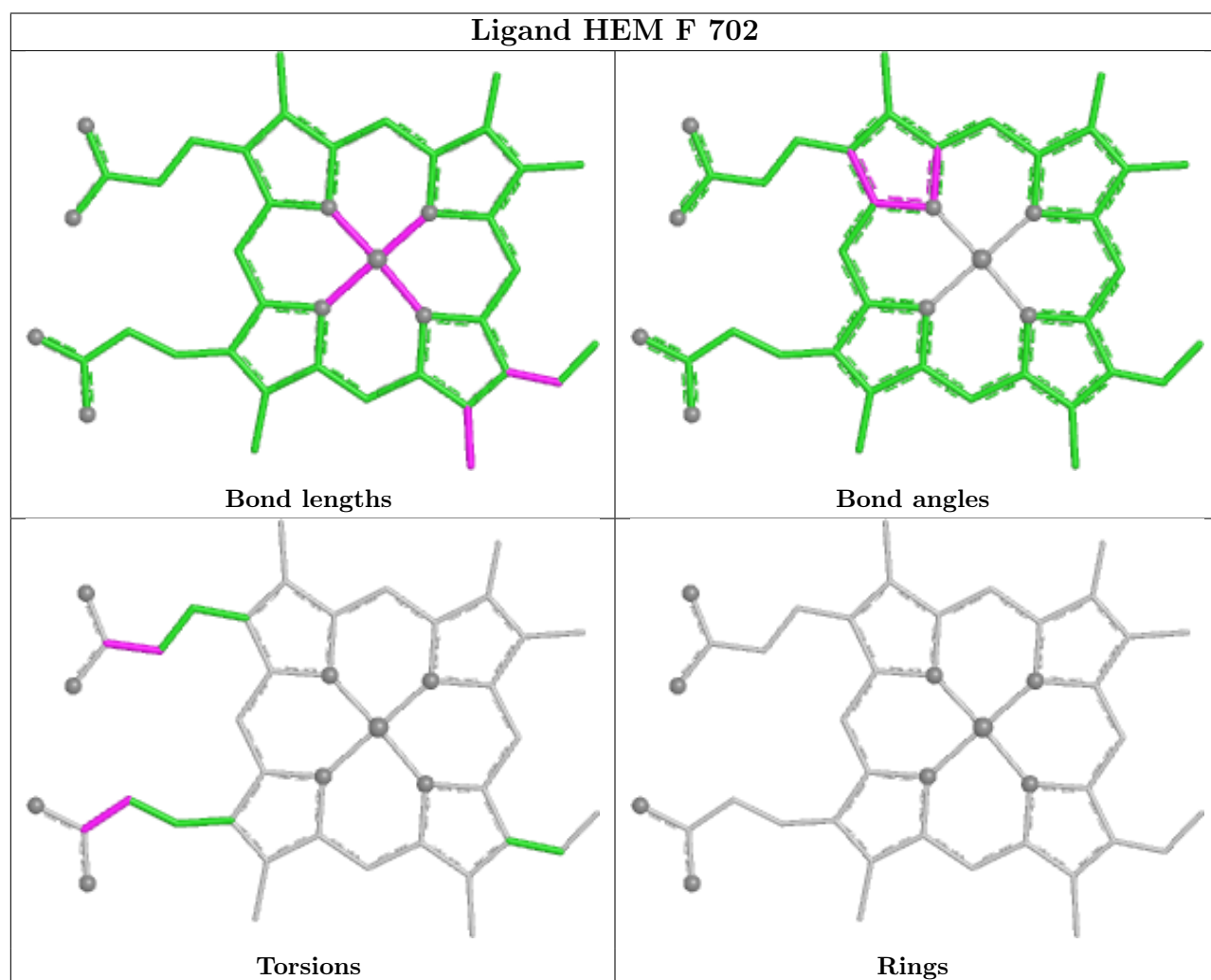
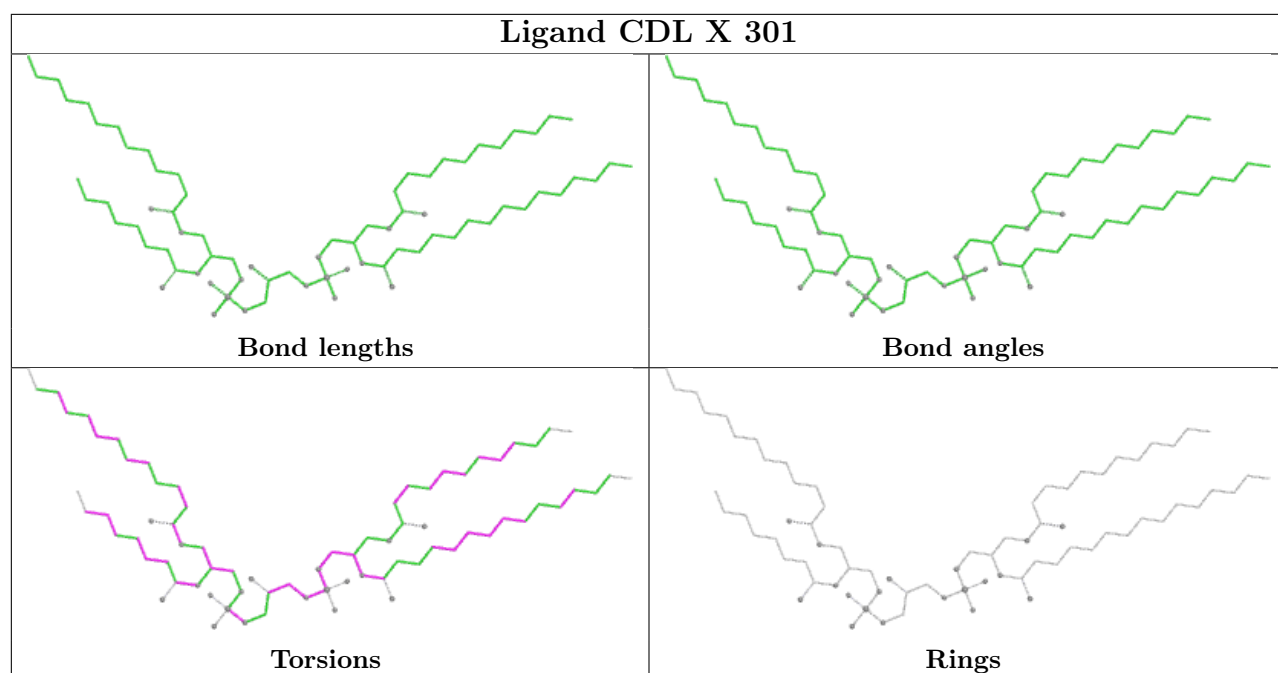


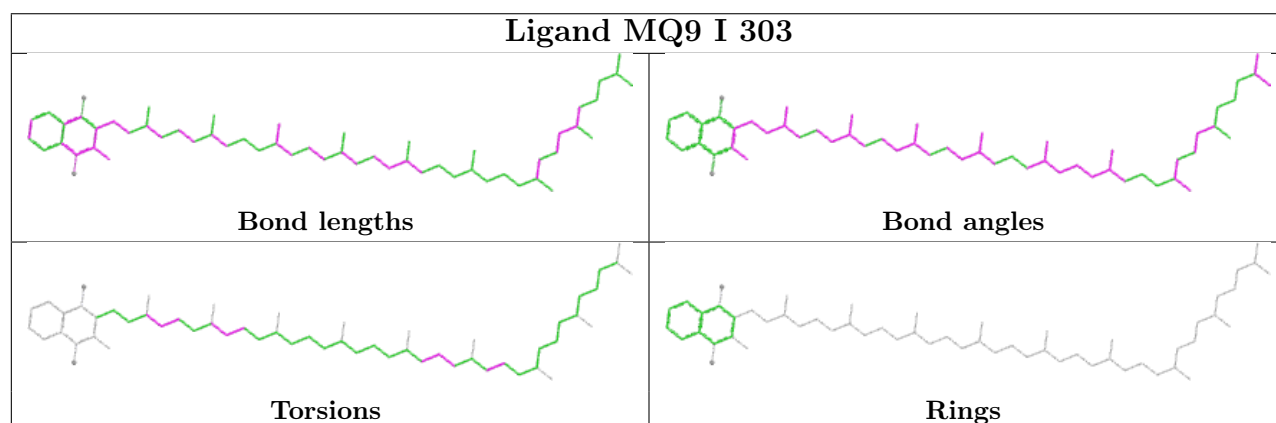
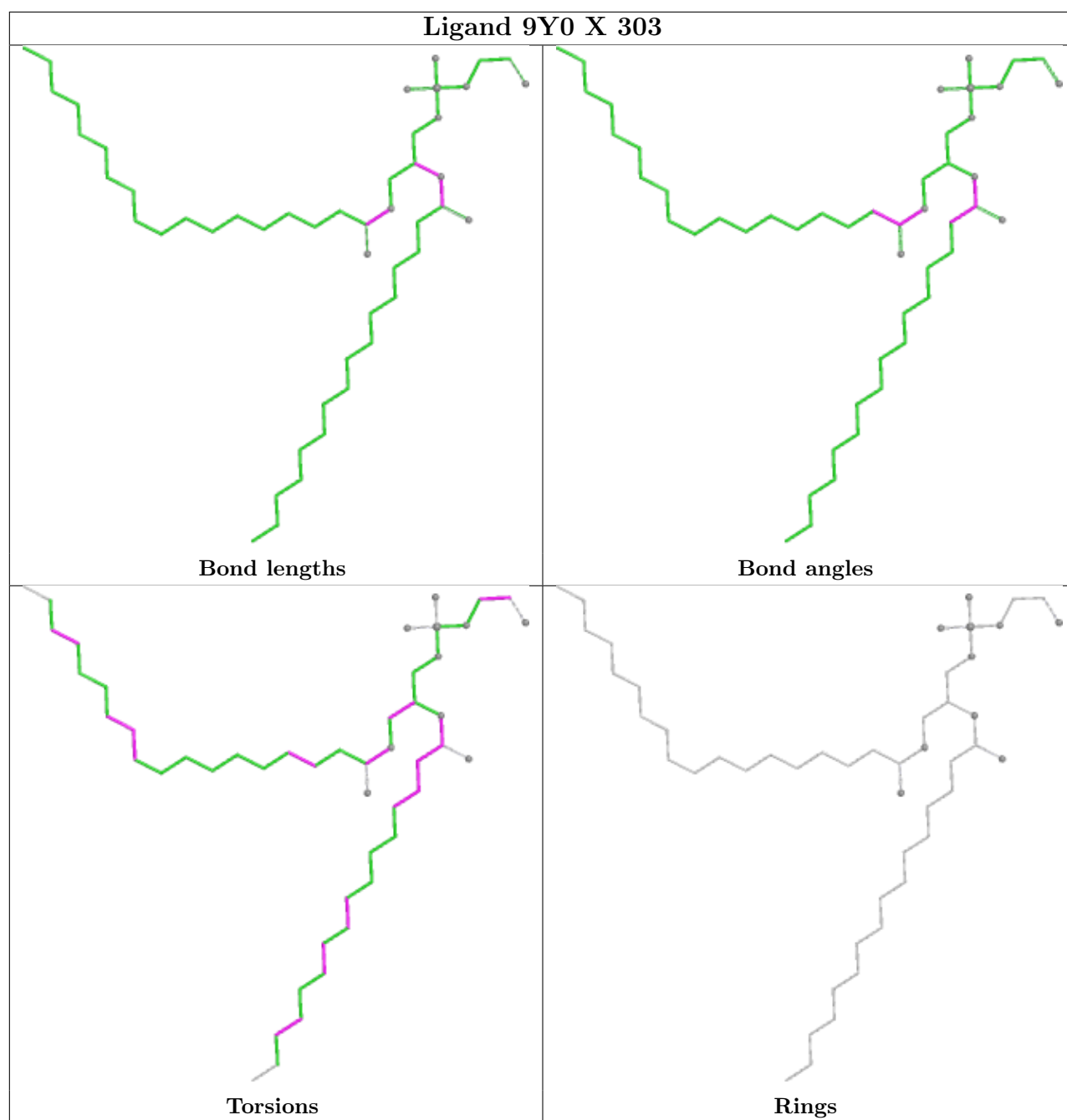
Ligand PLM c 201

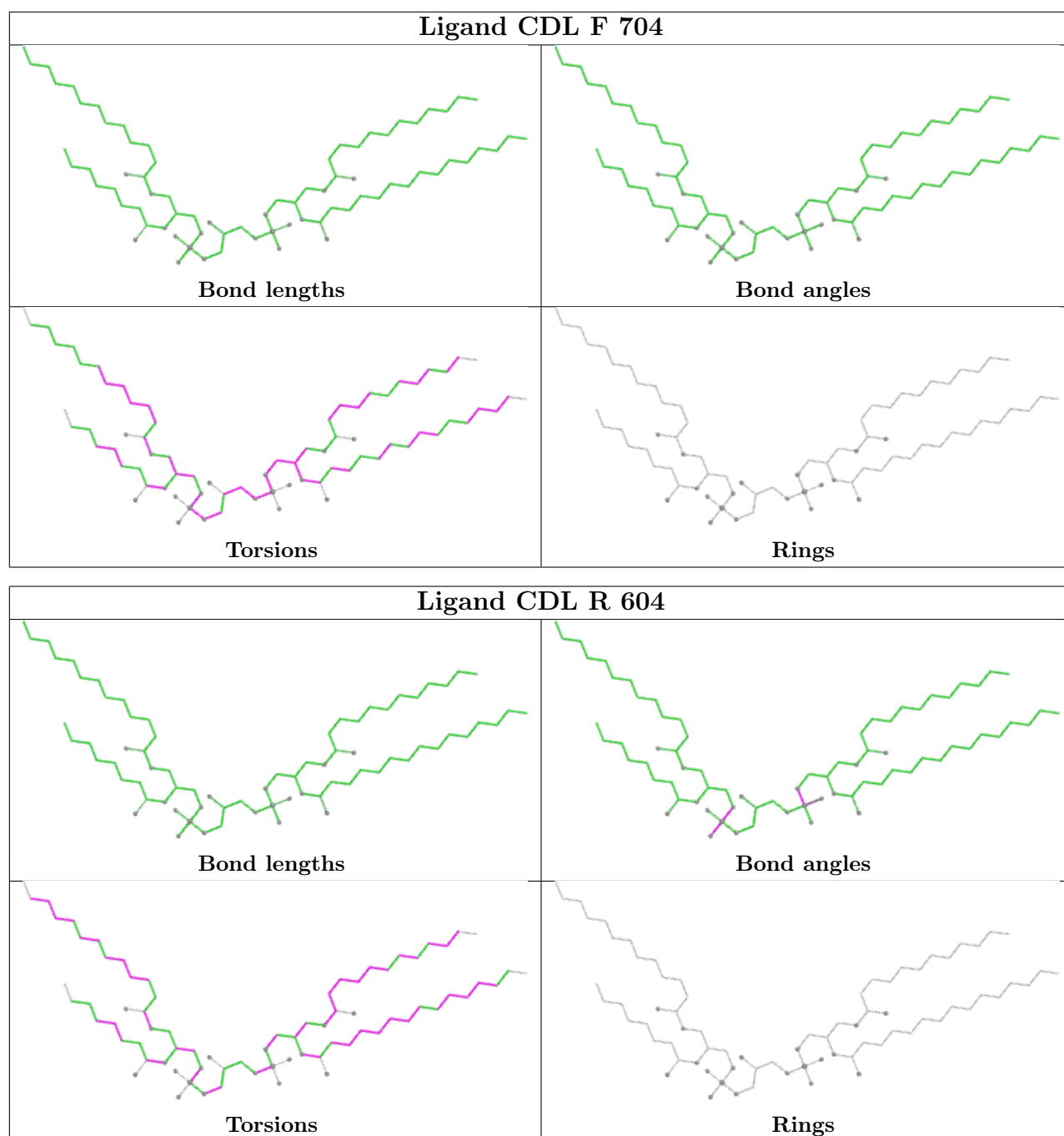


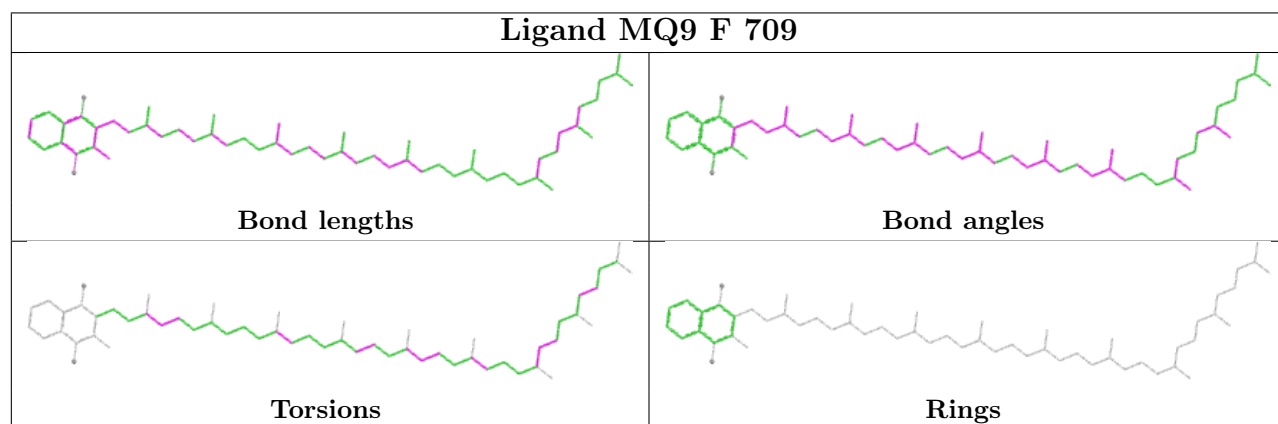
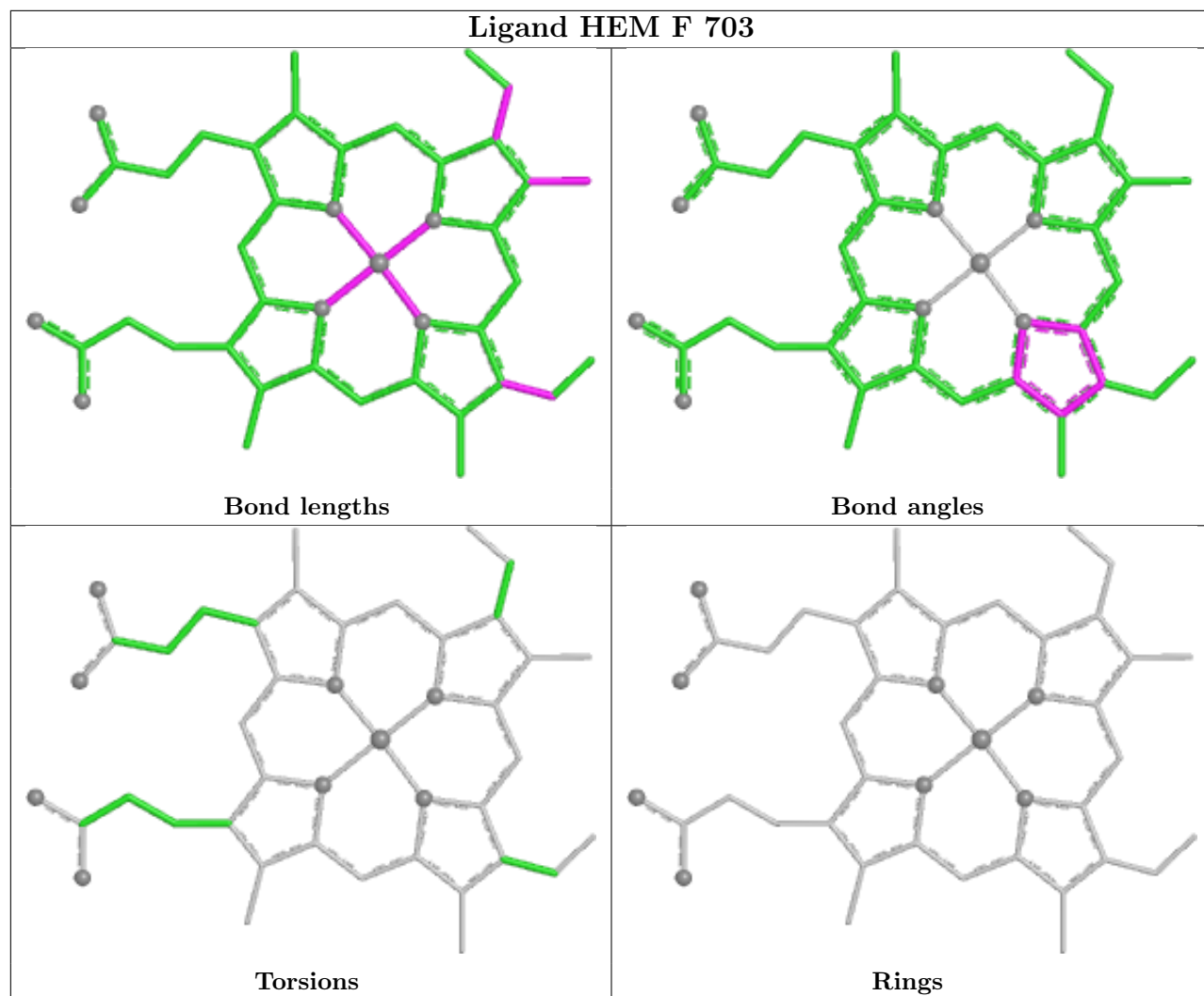


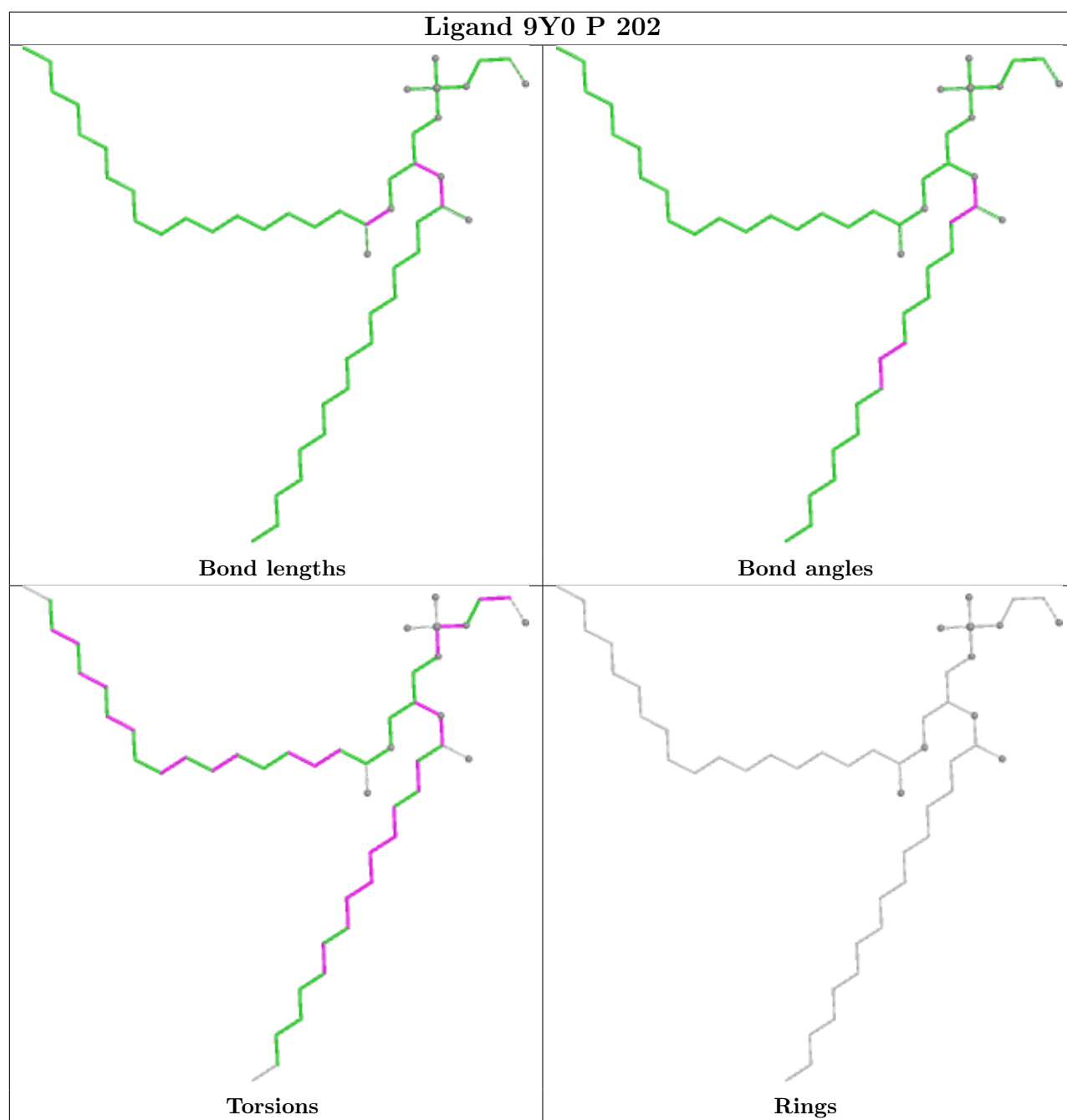


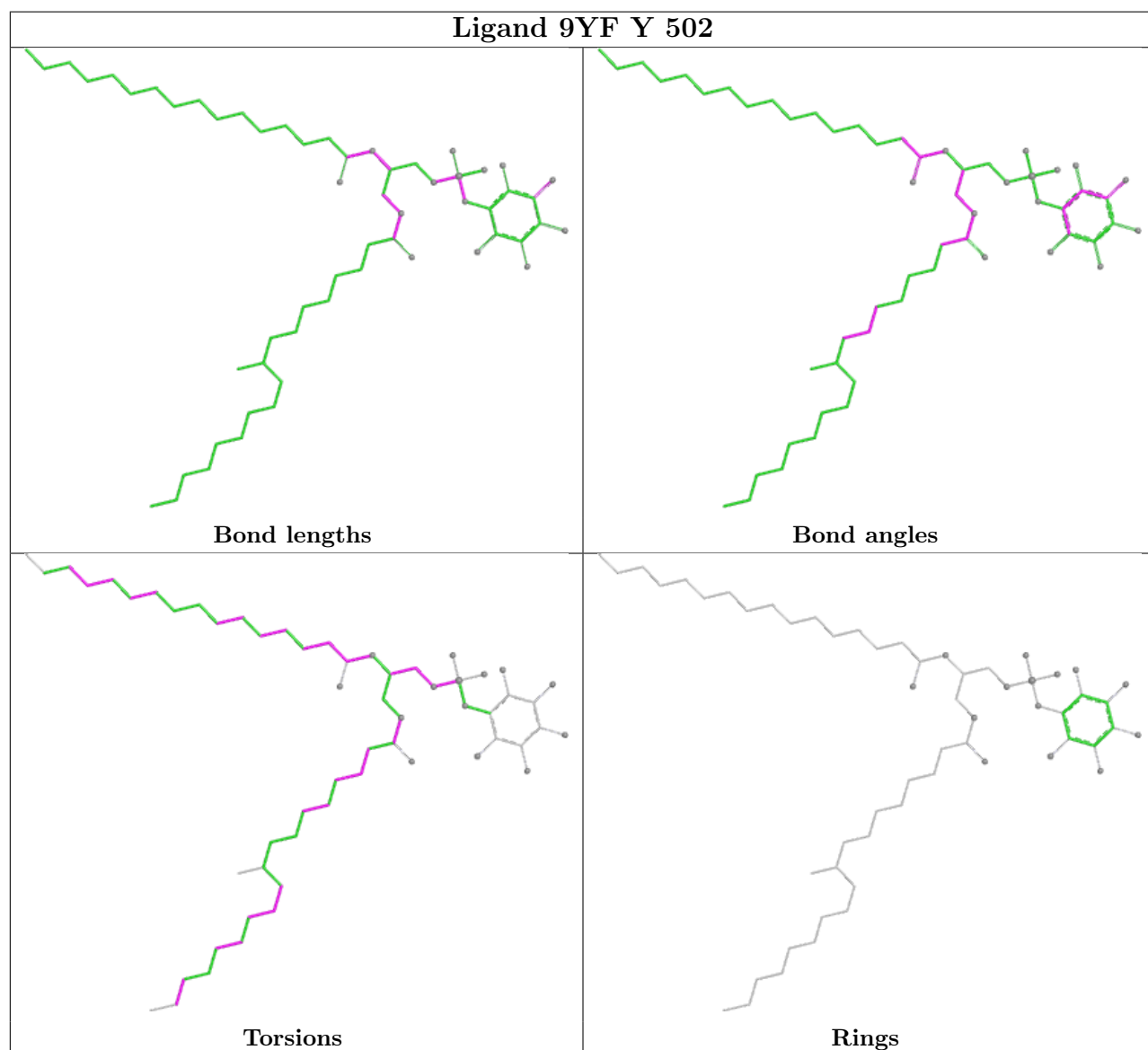
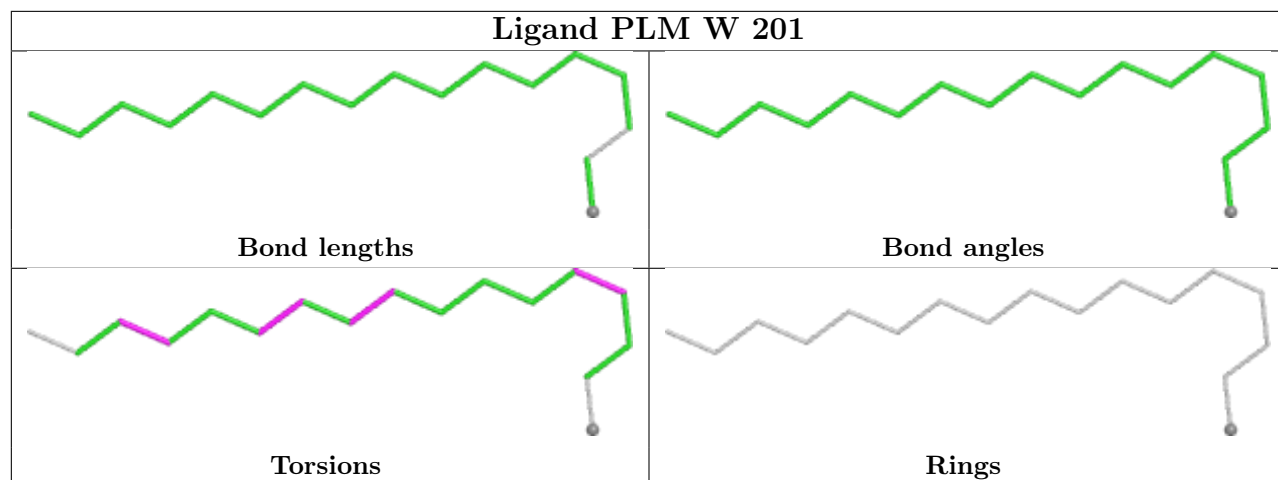


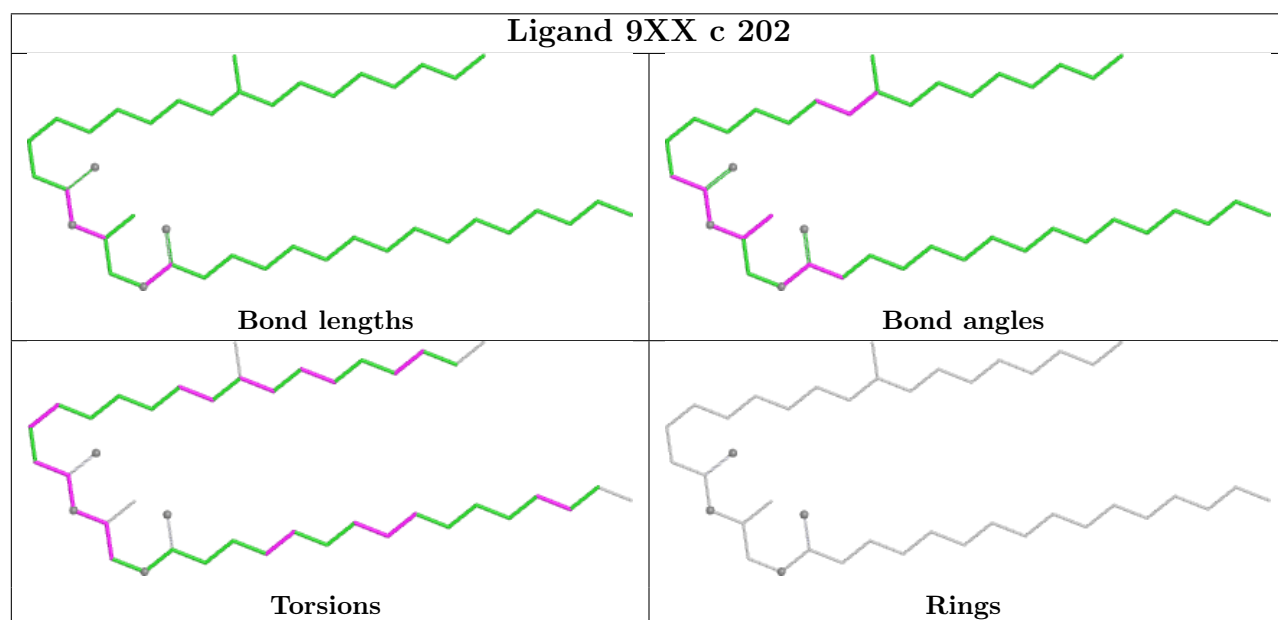
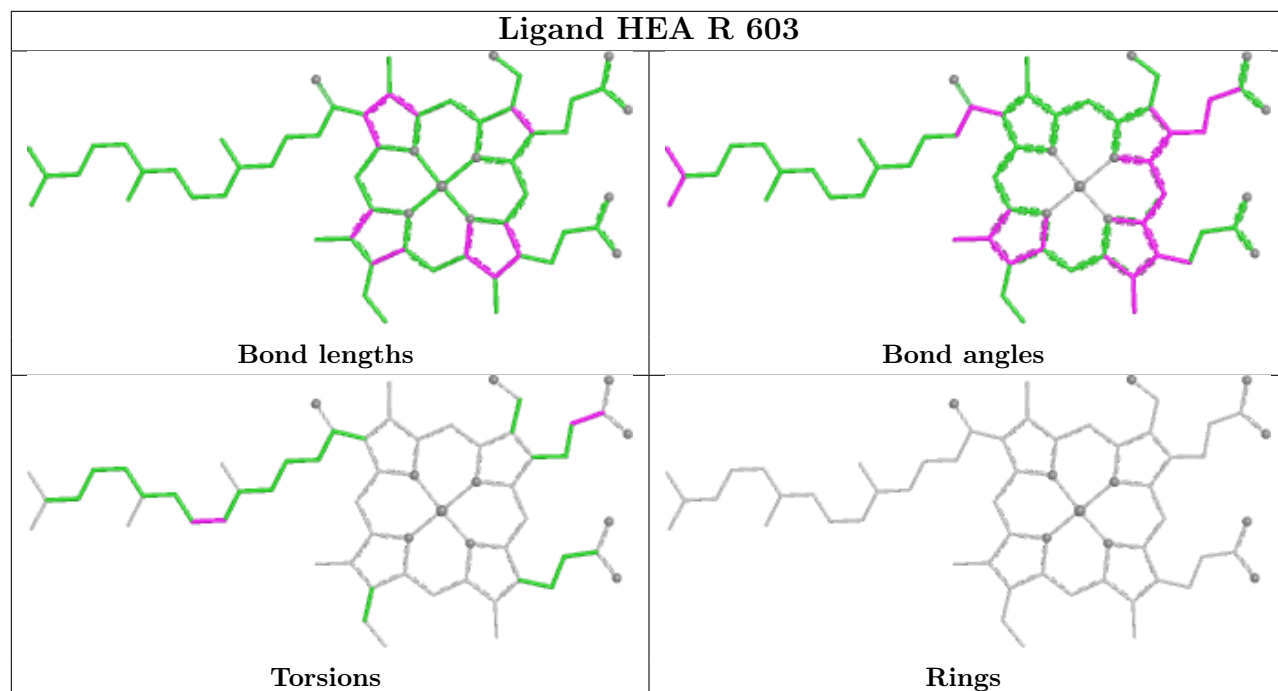


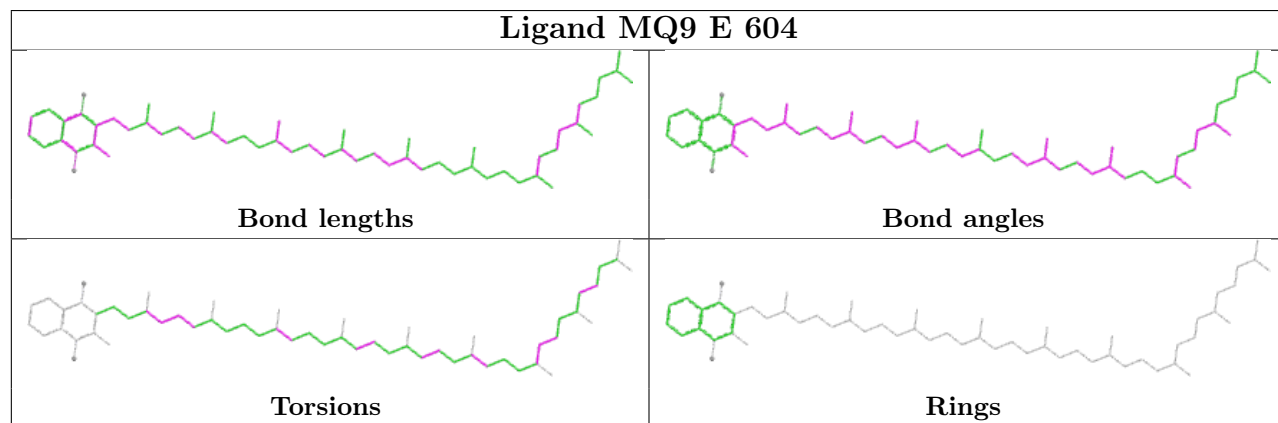
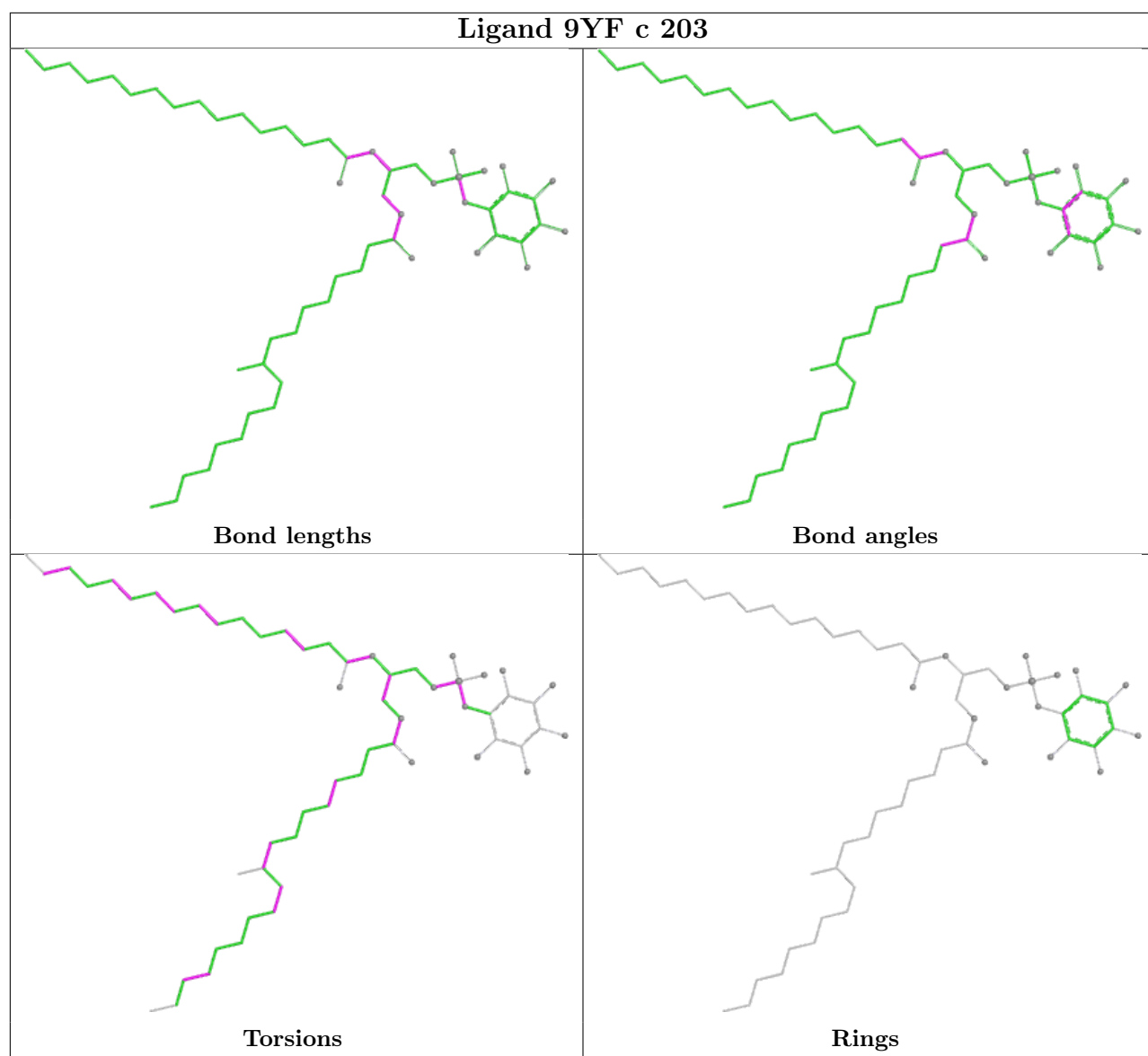


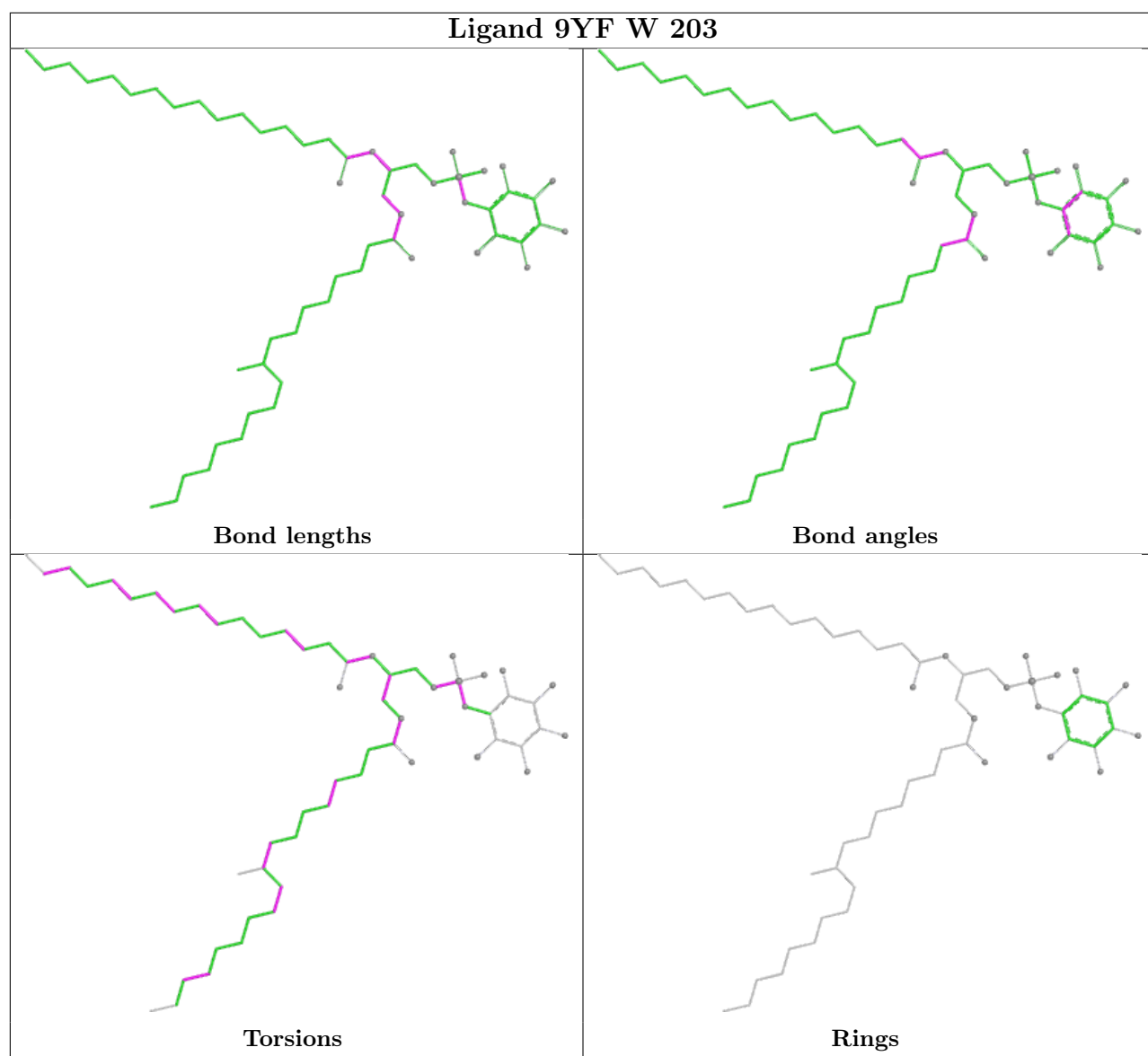


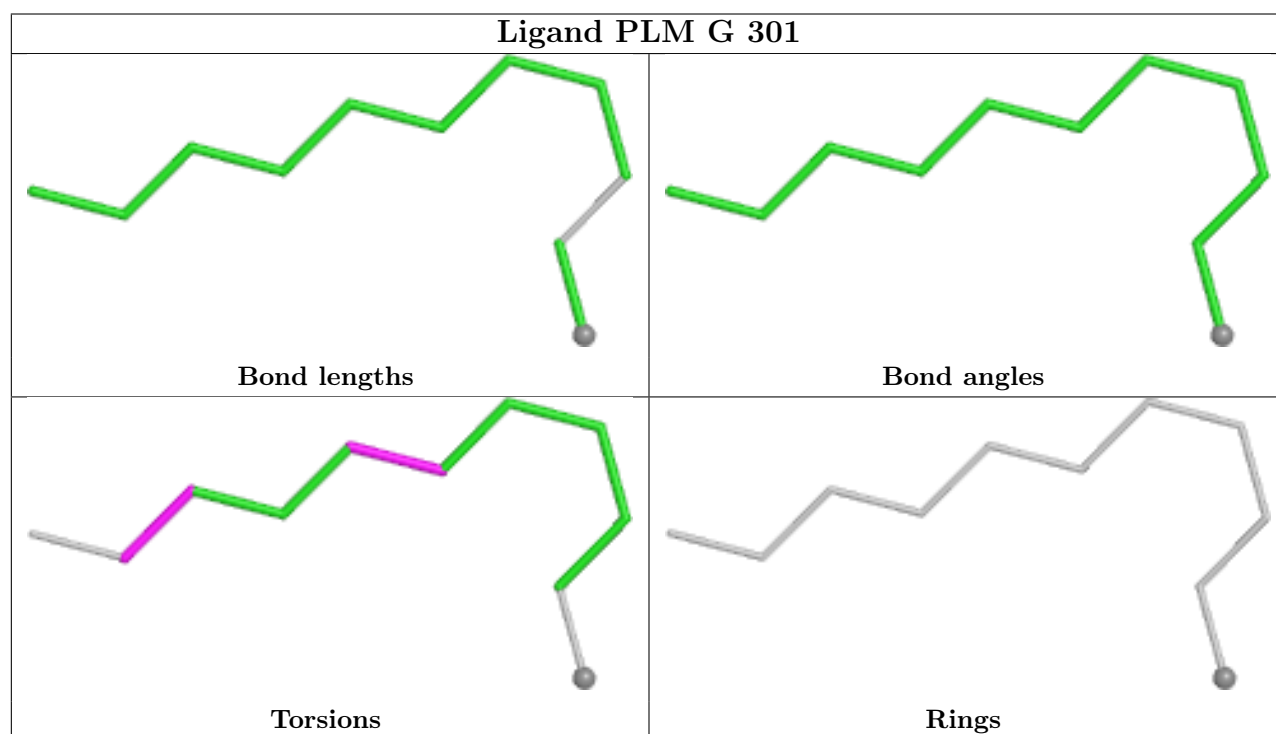
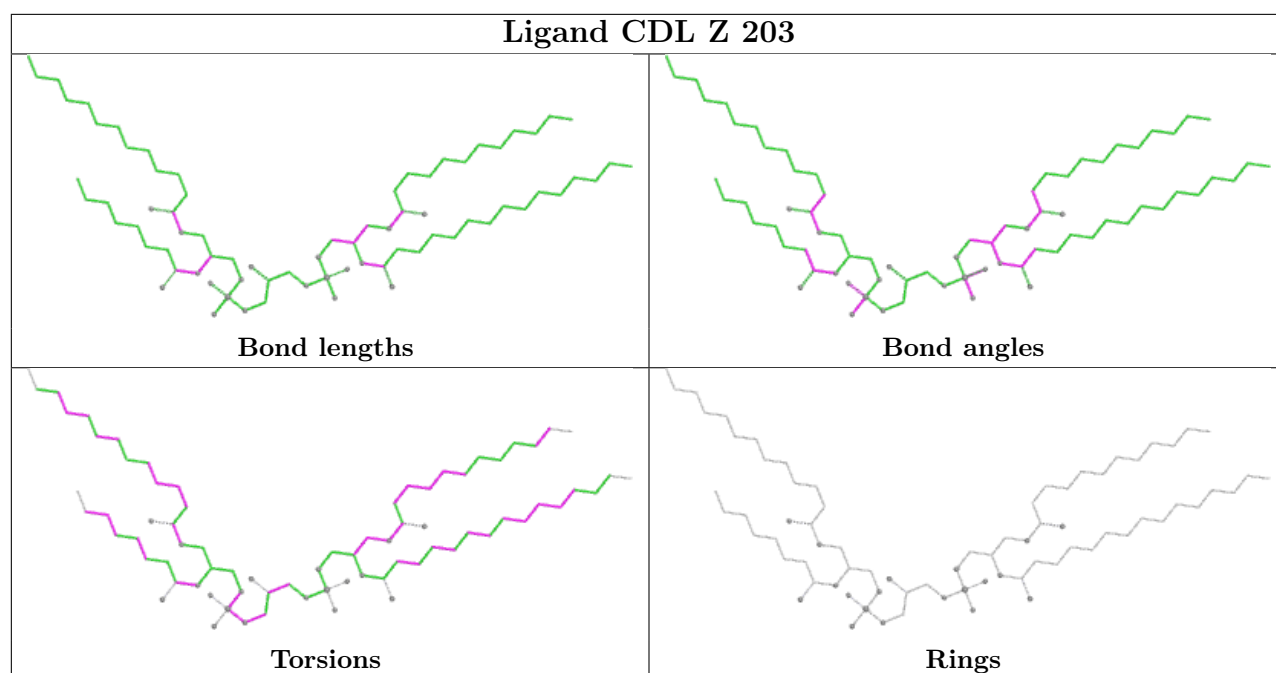


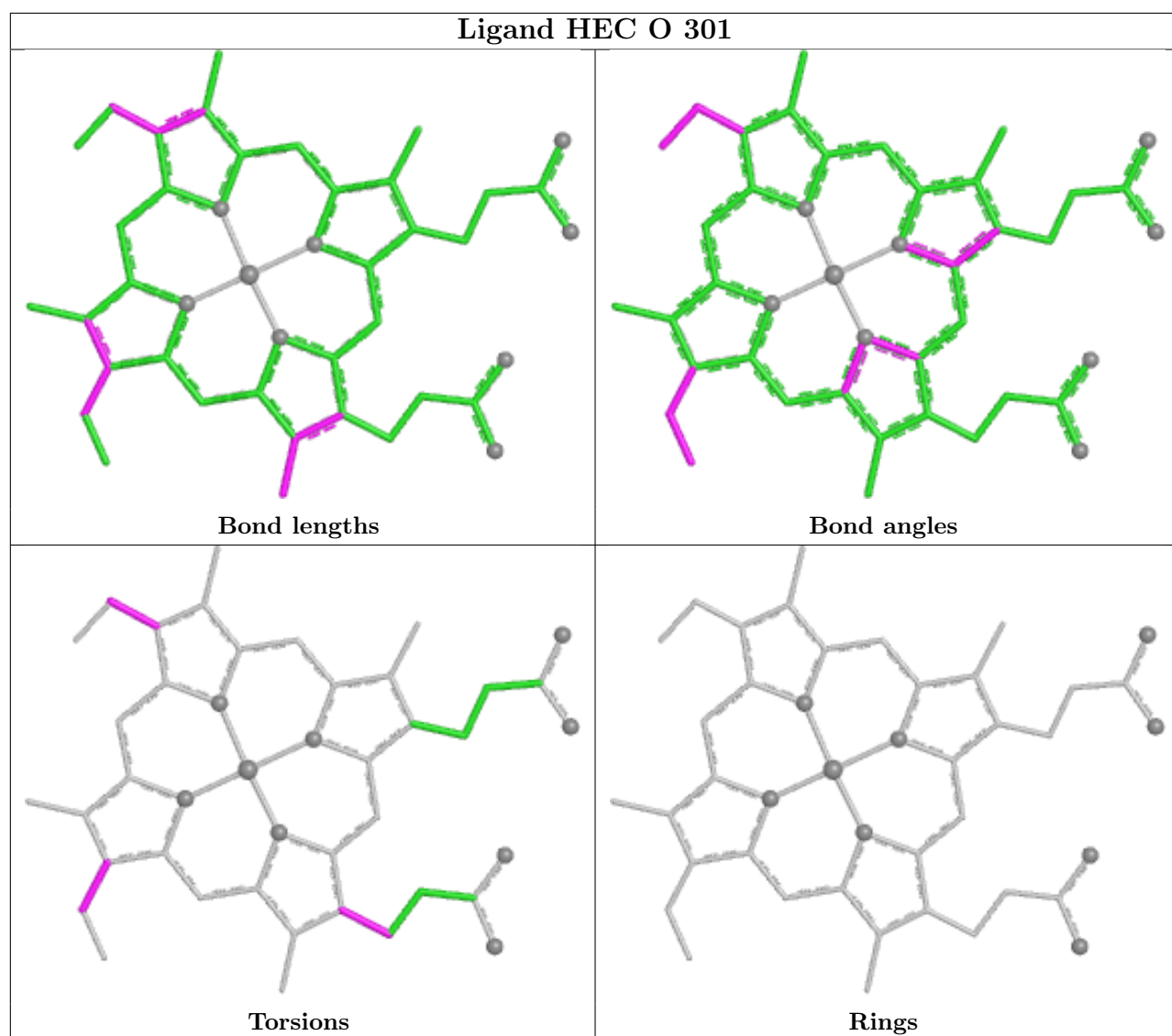


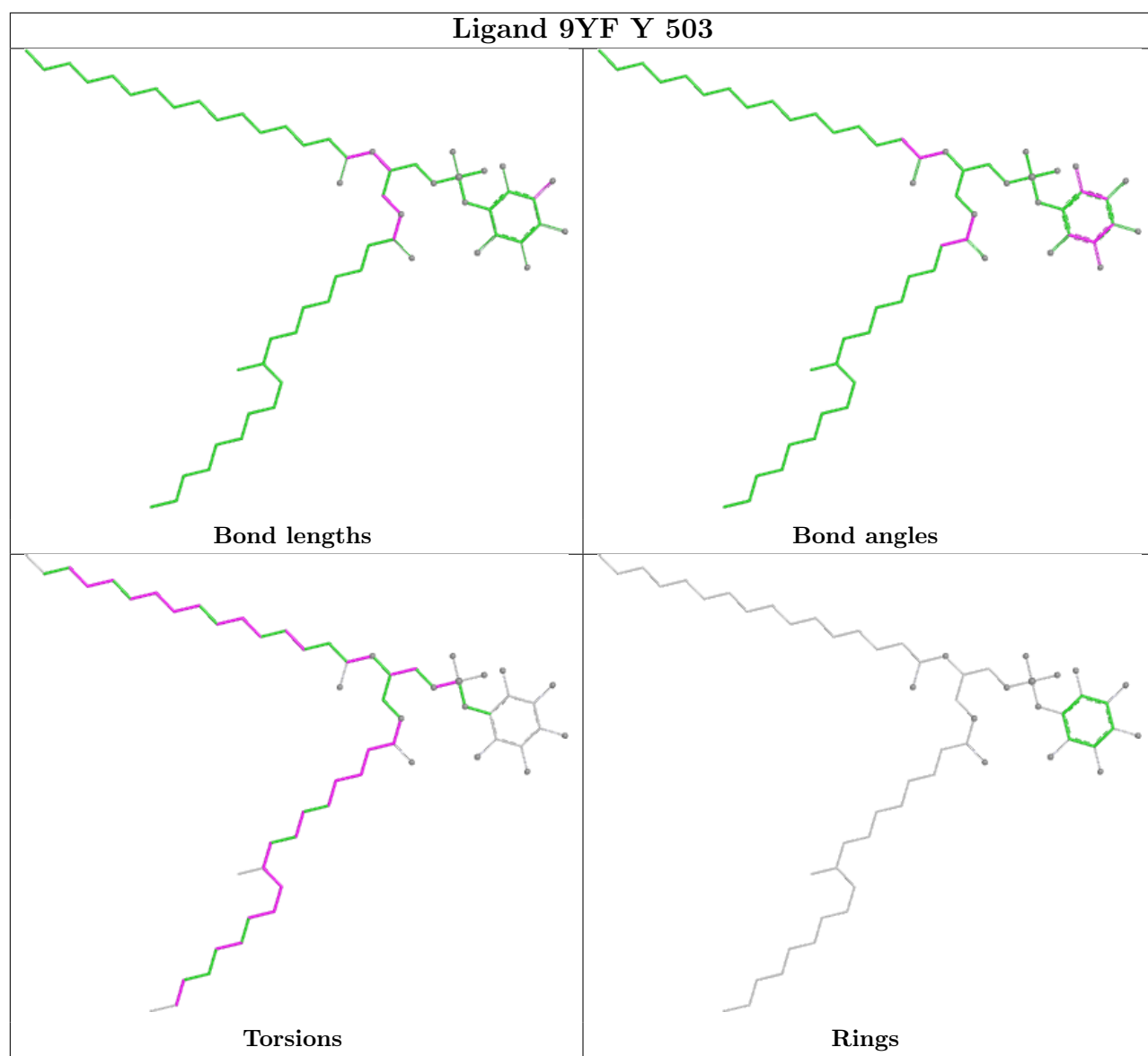


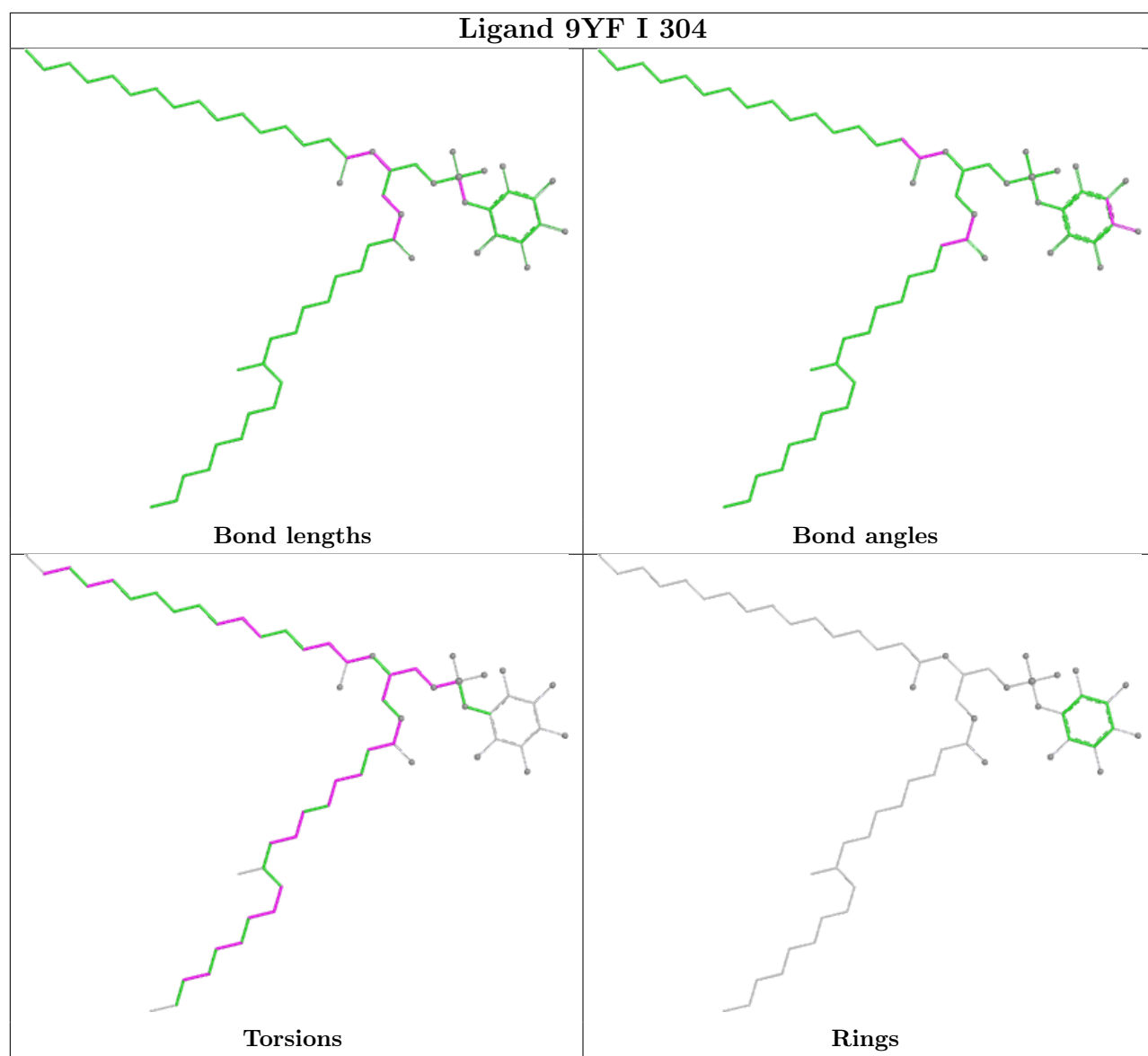


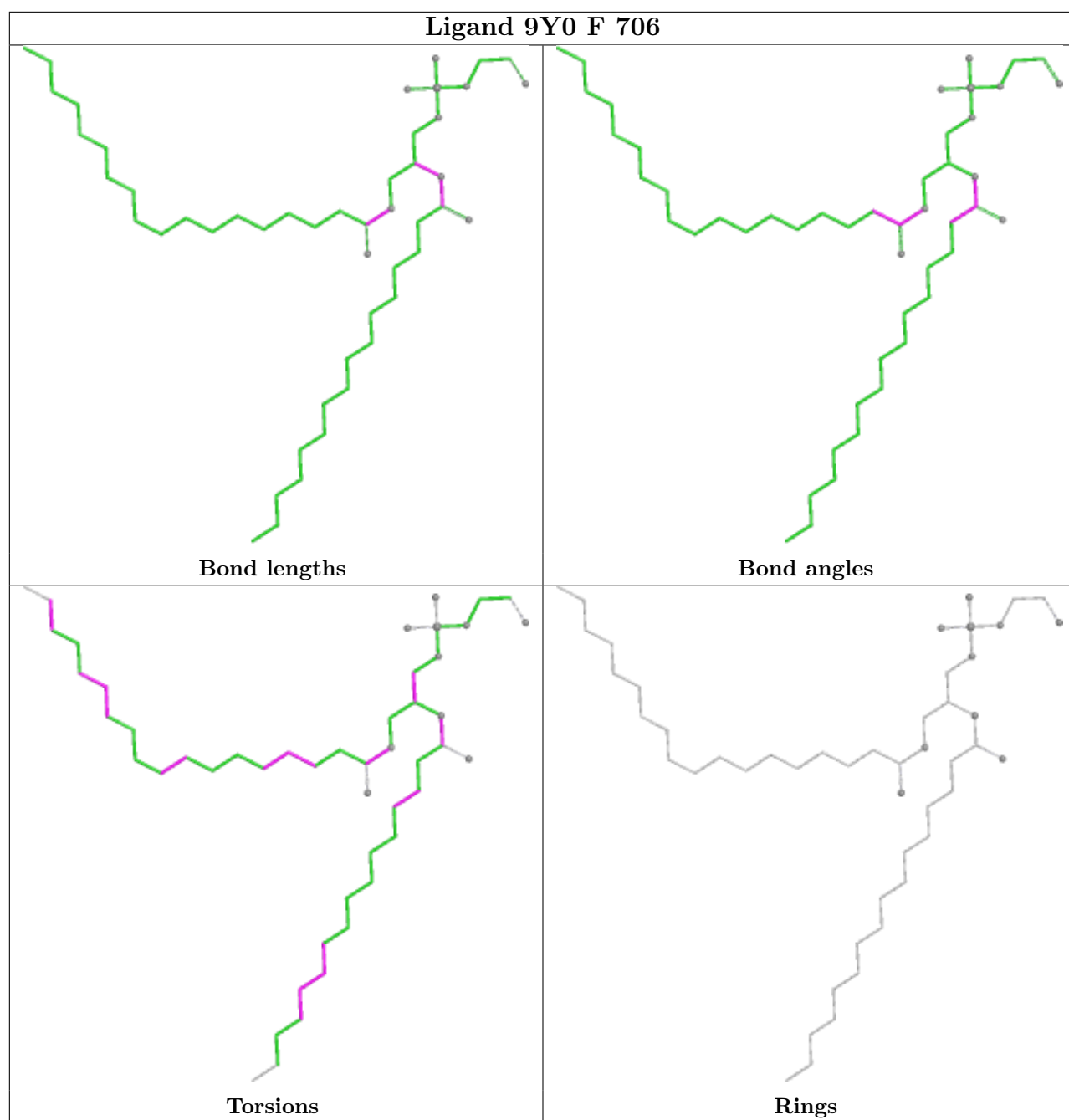


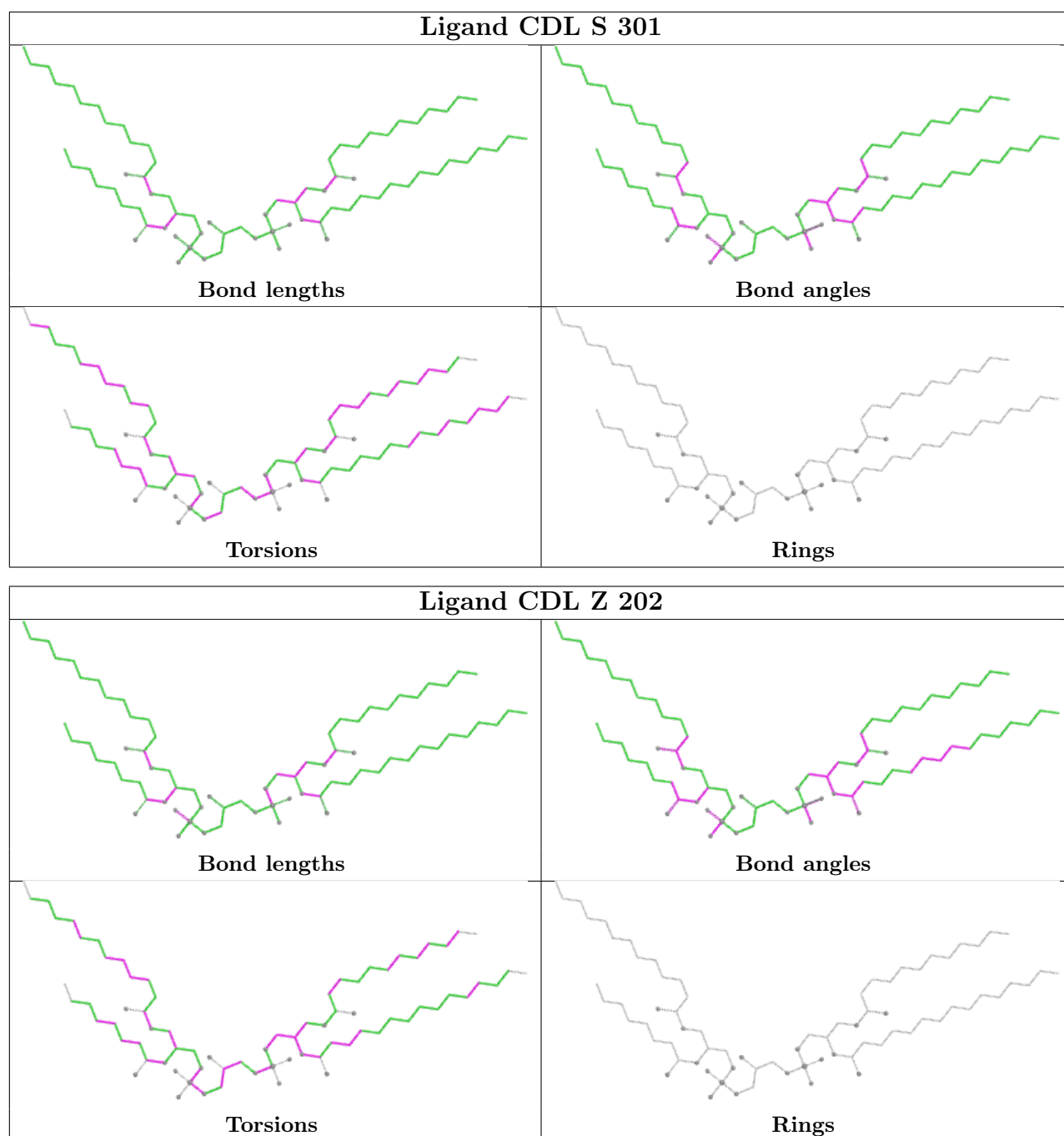


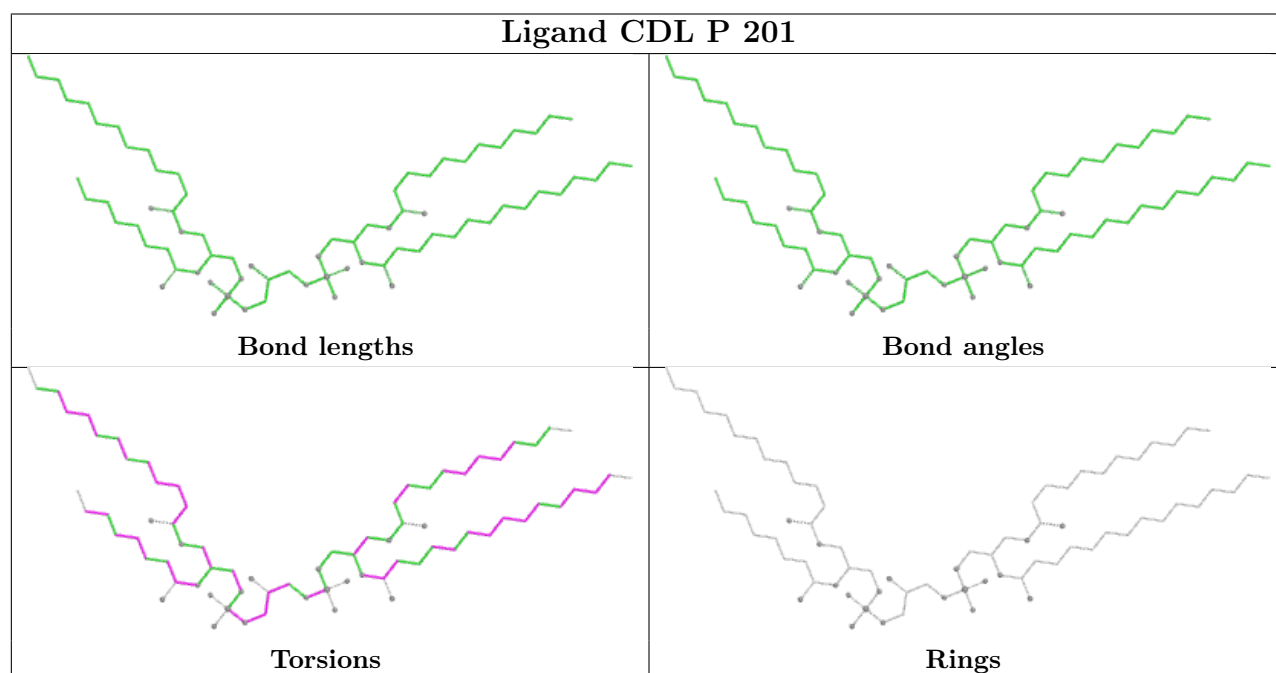
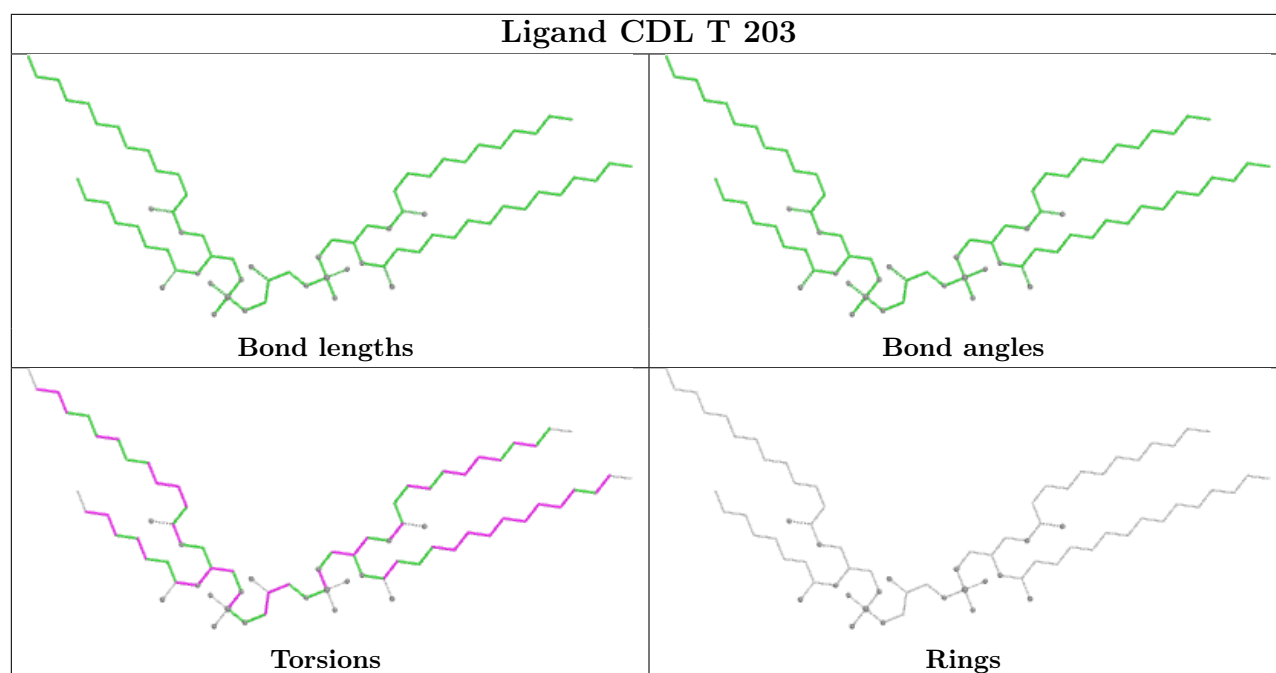


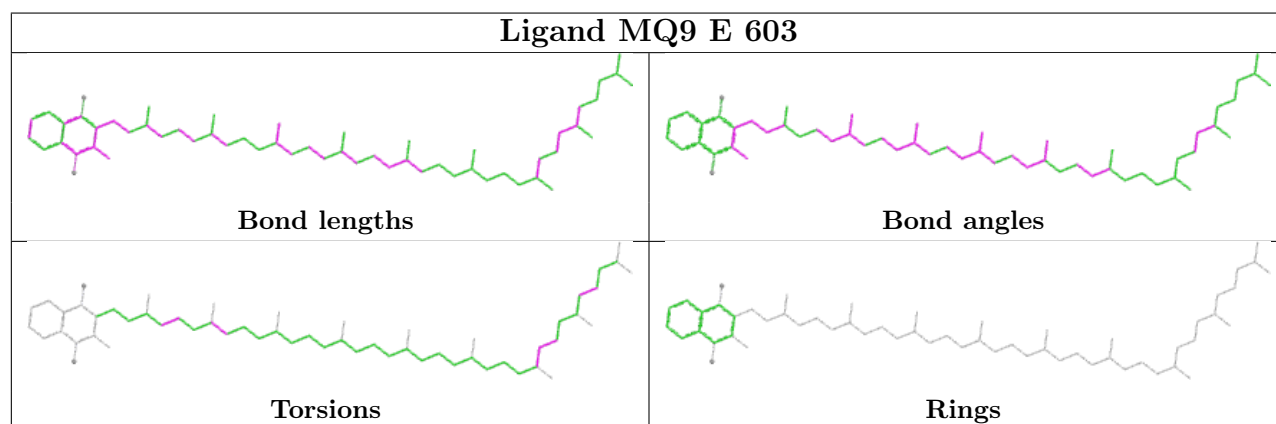
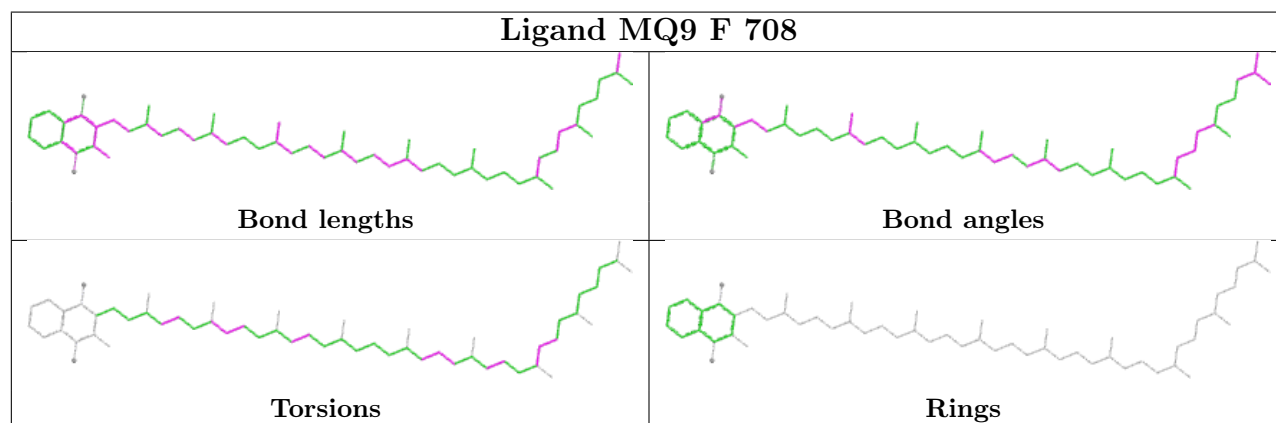
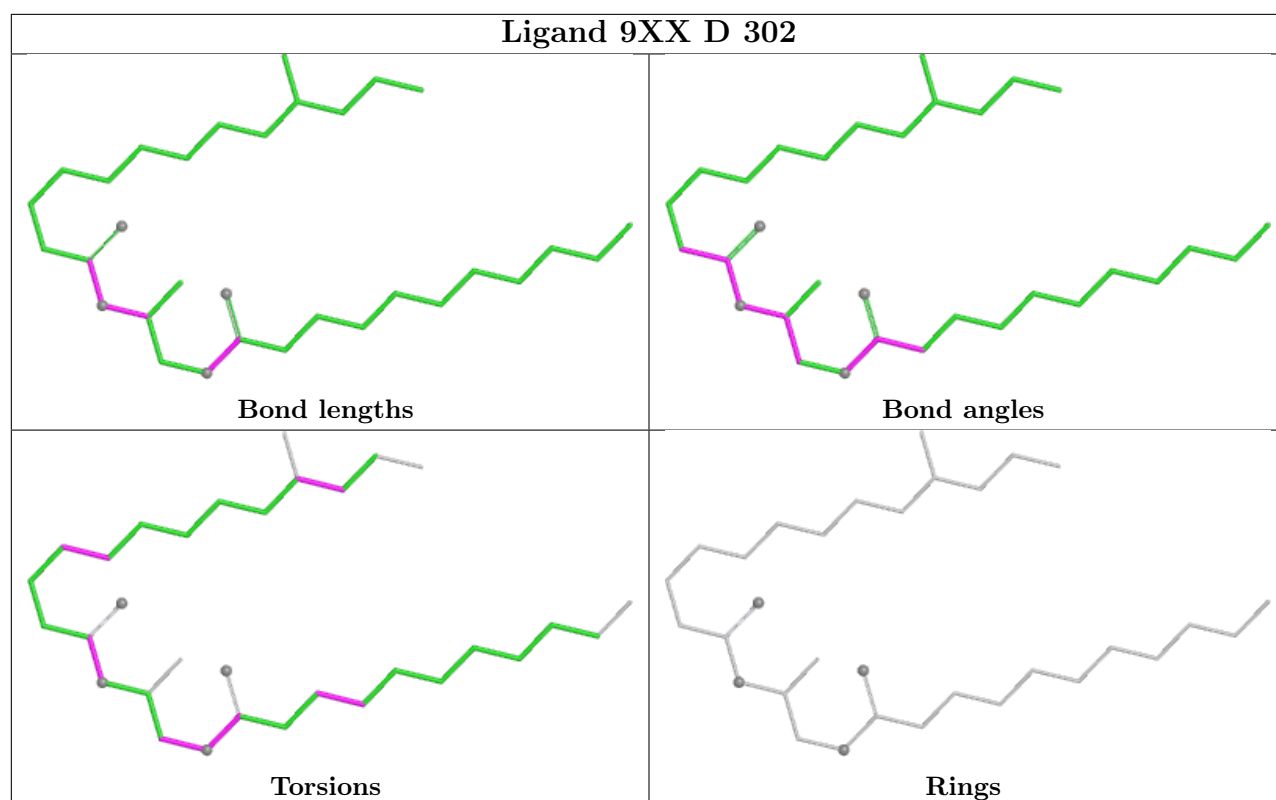


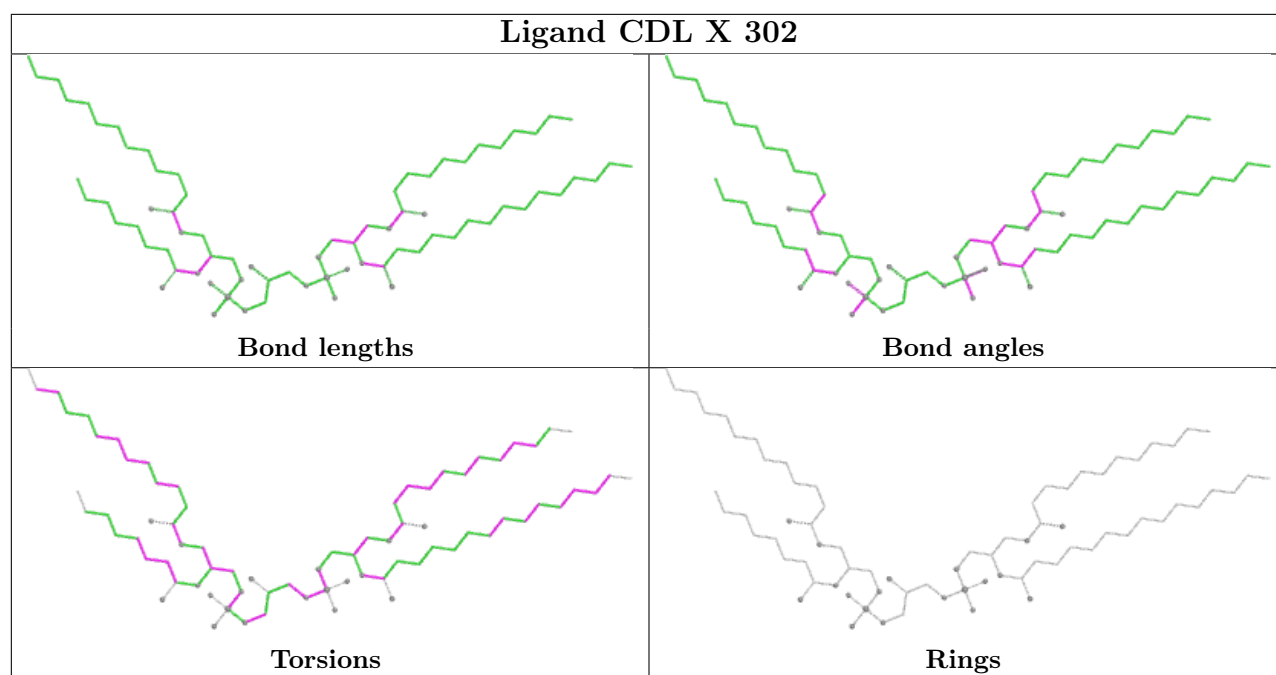












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

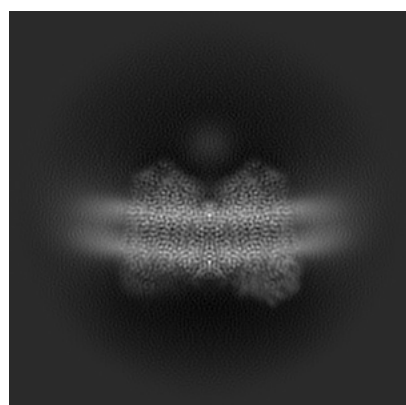
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46995. These allow visual inspection of the internal detail of the map and identification of artifacts.

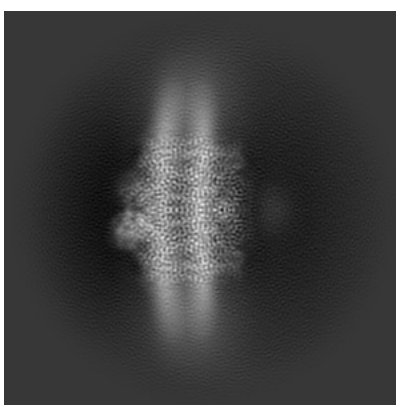
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

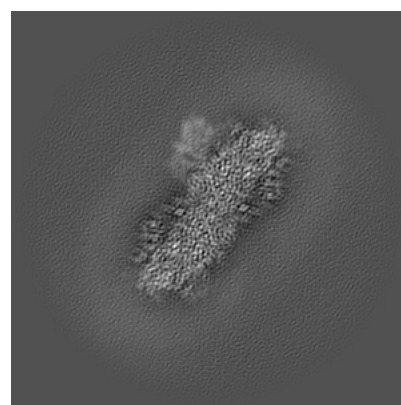
6.1.1 Primary map



X



Y

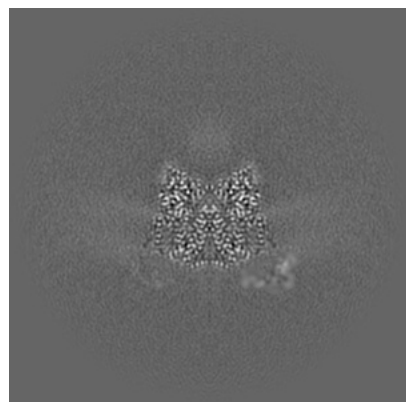


Z

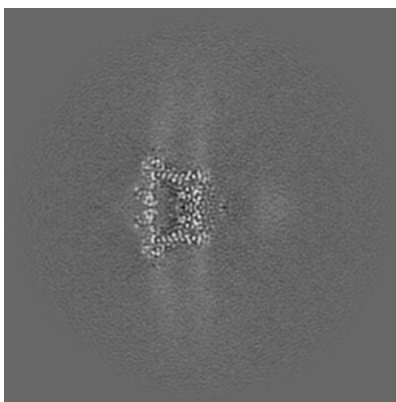
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

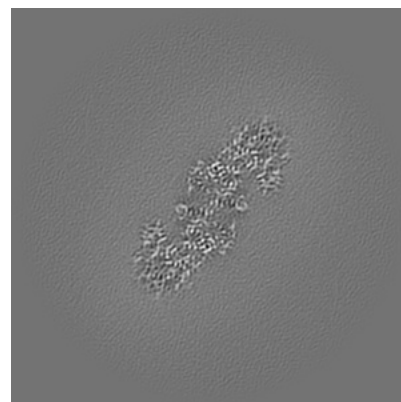
6.2.1 Primary map



X Index: 182



Y Index: 182

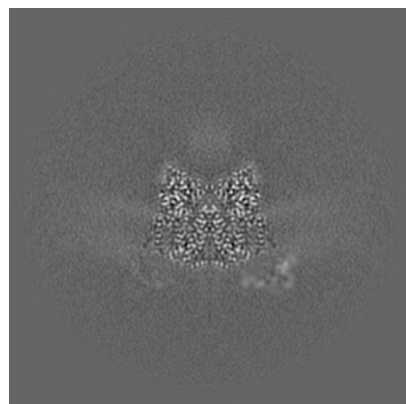


Z Index: 182

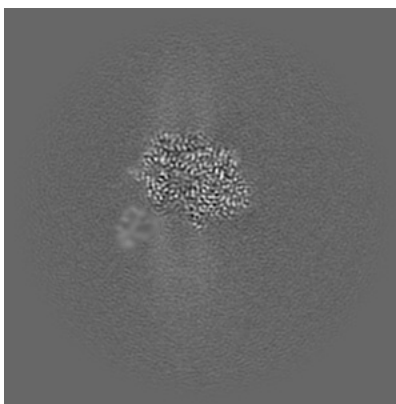
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

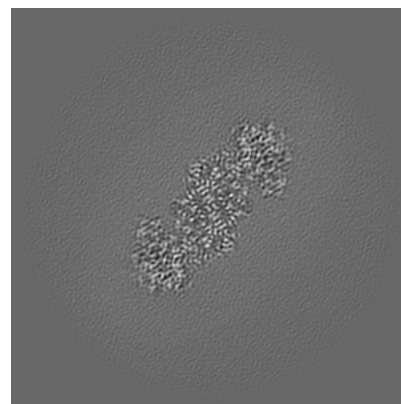
6.3.1 Primary map



X Index: 182



Y Index: 219

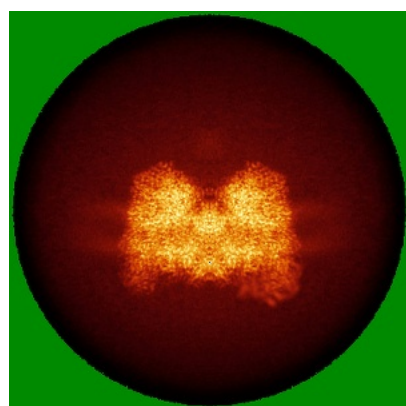


Z Index: 175

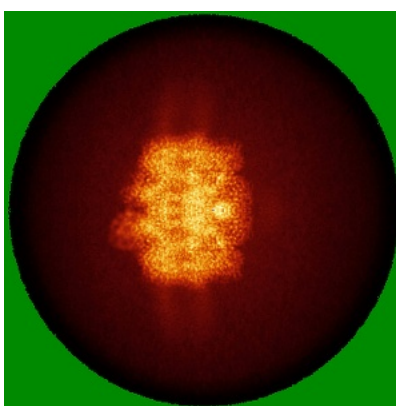
The images above show the largest variance slices of the map in three orthogonal directions.

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

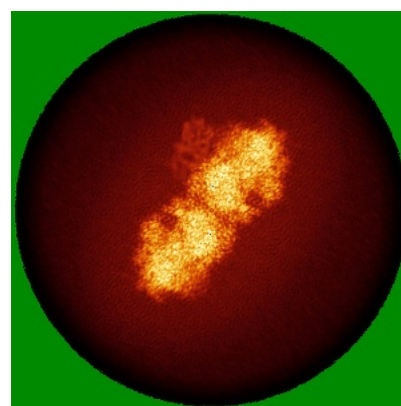
6.4.1 Primary map



X



Y



Z

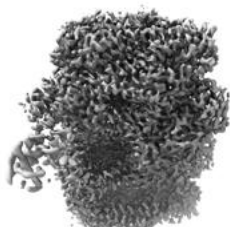
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.335. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

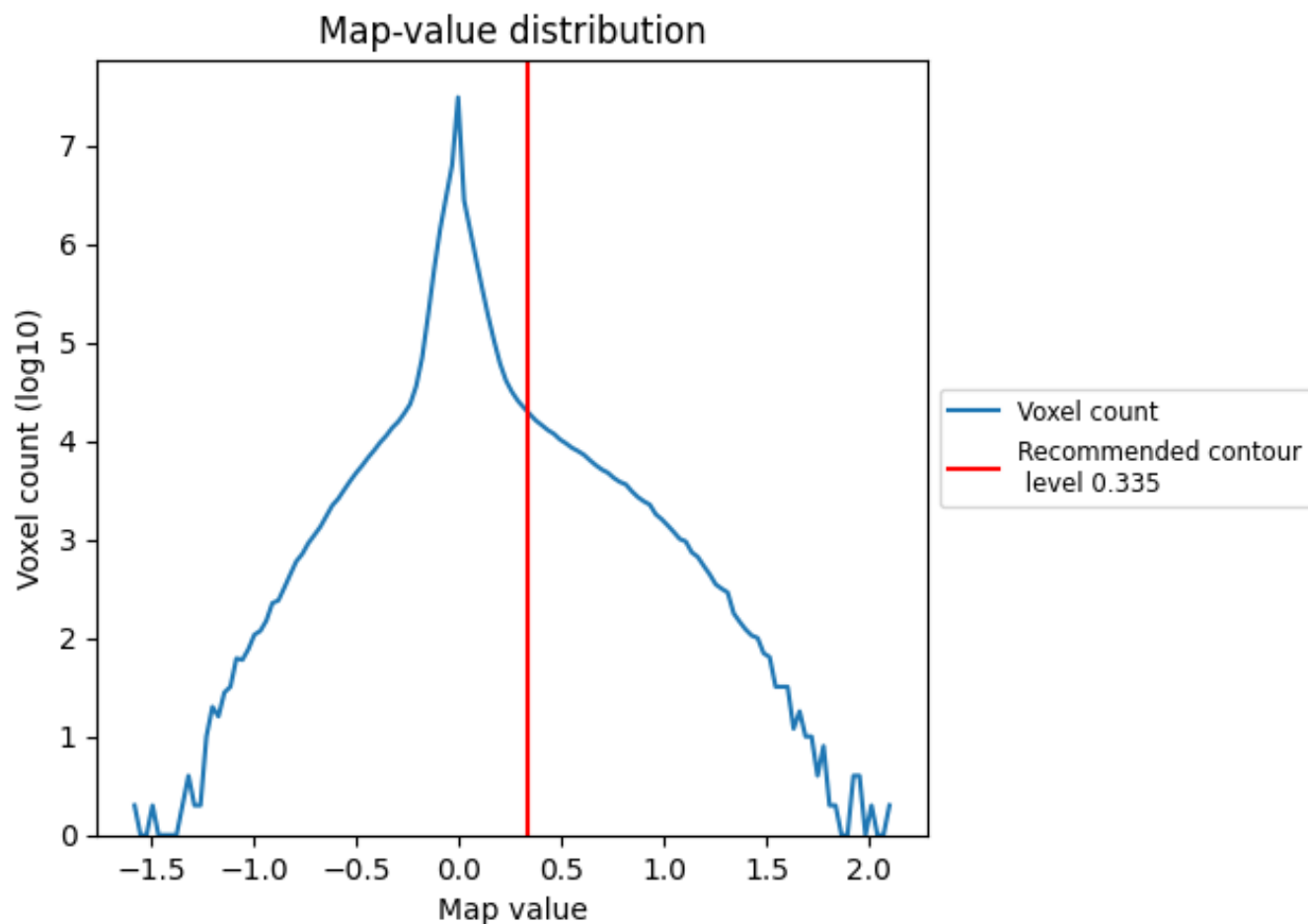
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

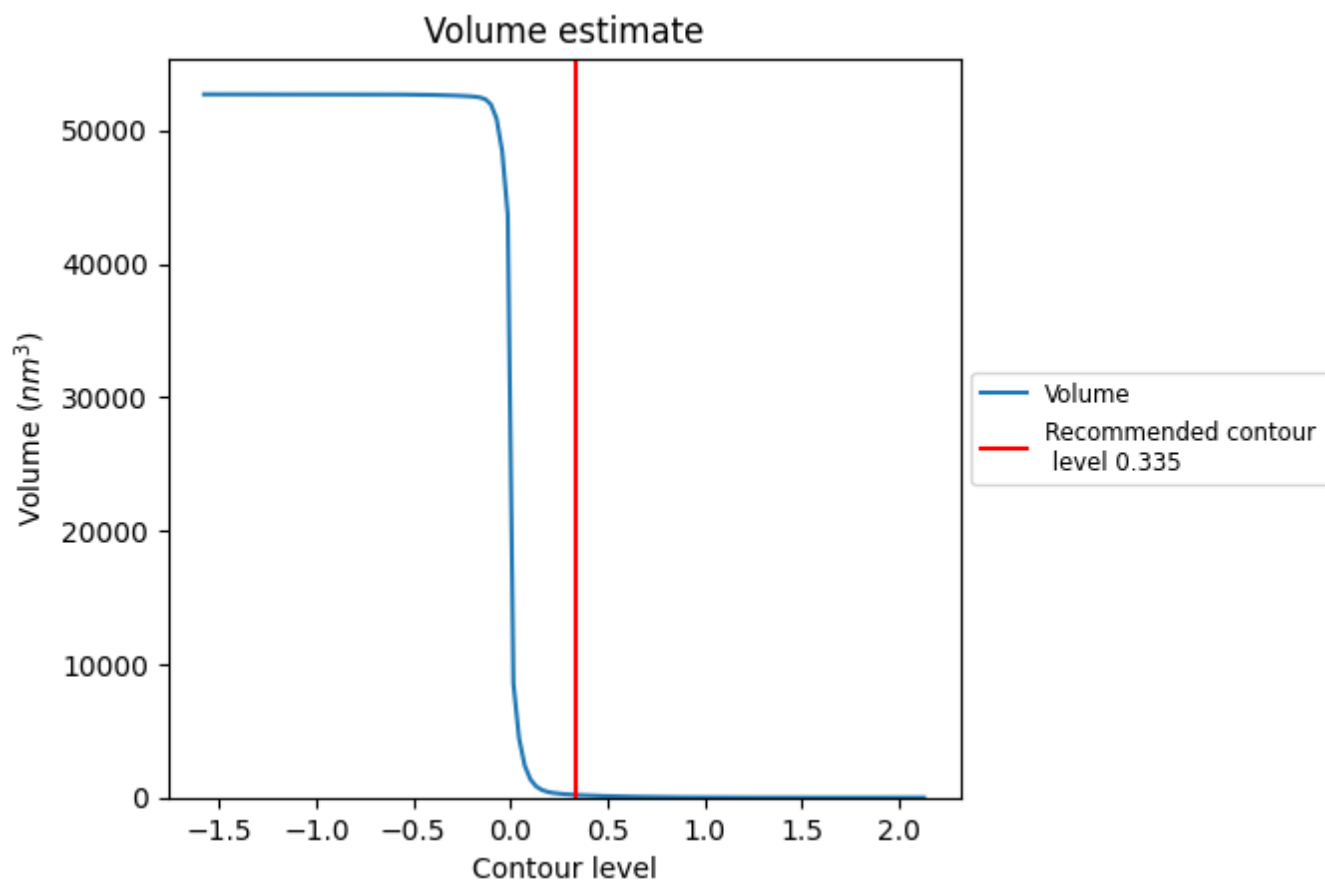
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

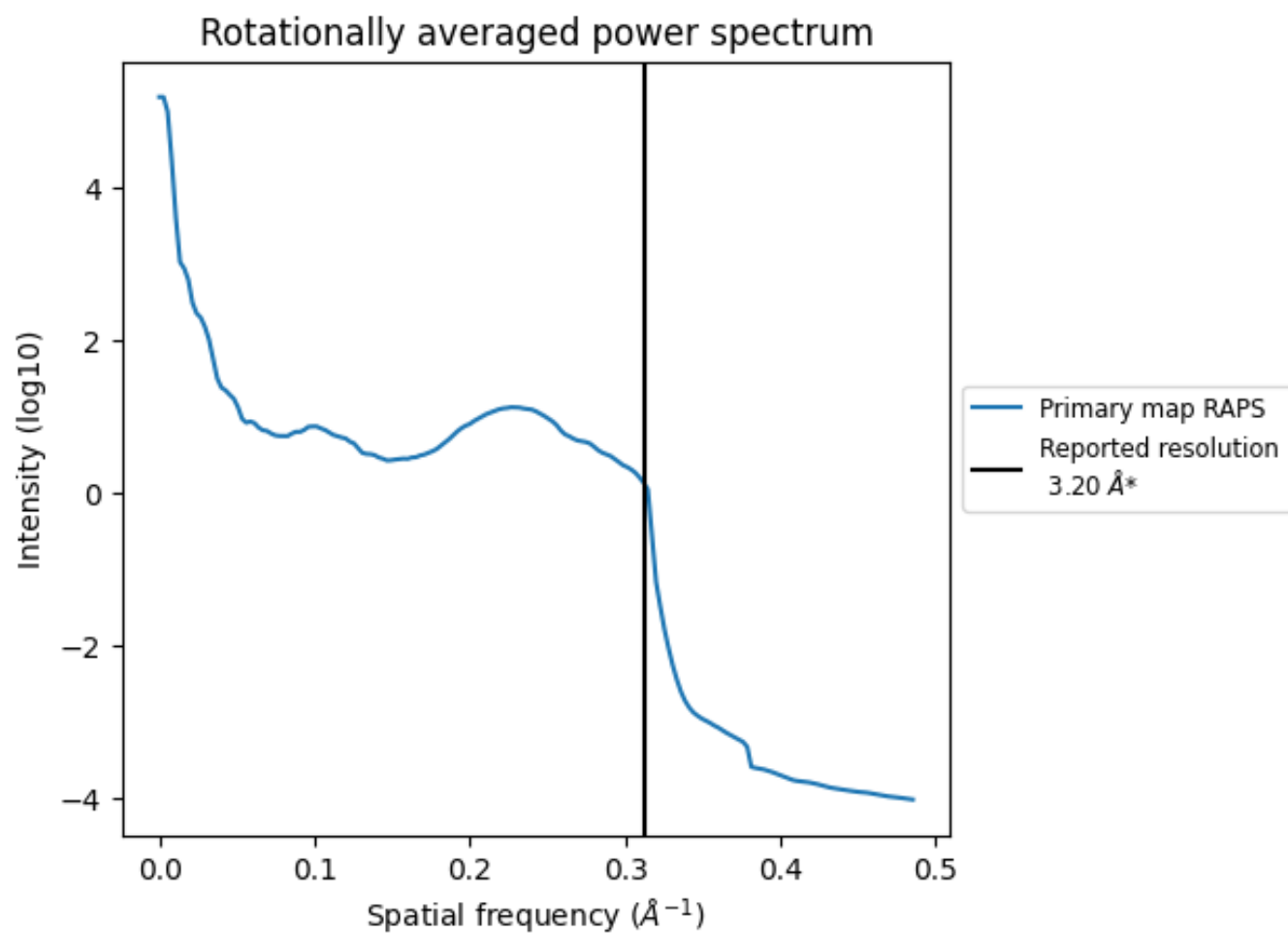
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 200 nm³; this corresponds to an approximate mass of 181 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 0.312 Å⁻¹

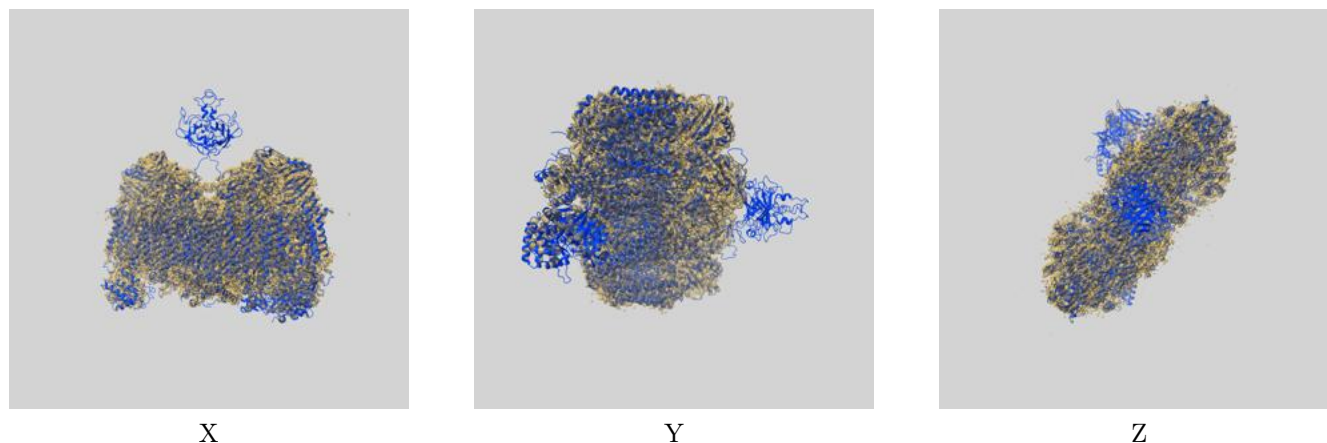
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

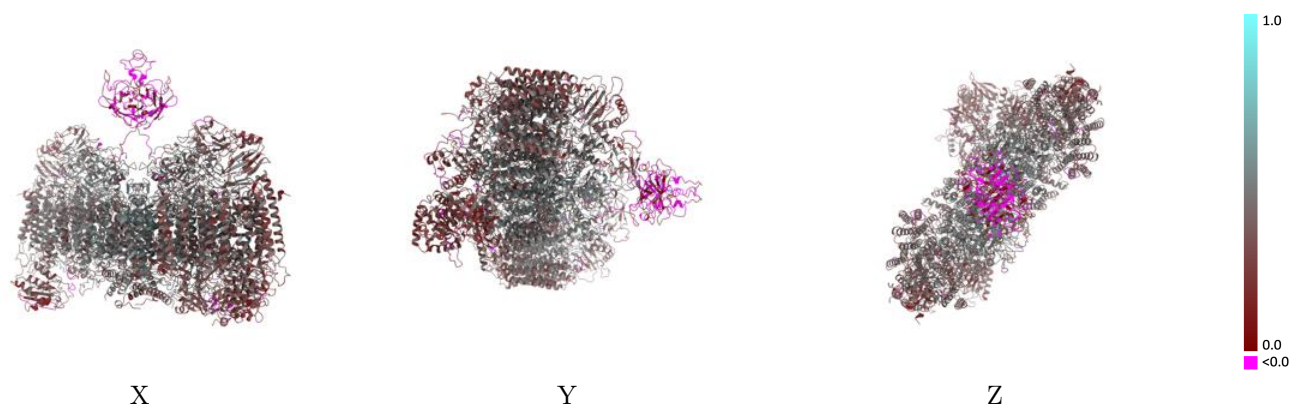
This section contains information regarding the fit between EMDB map EMD-46995 and PDB model 9DM1. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



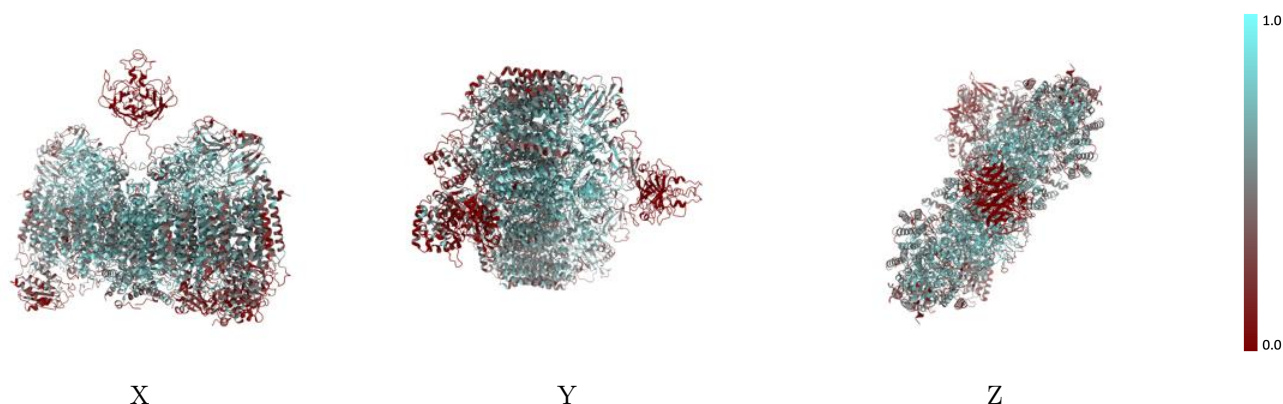
The images above show the 3D surface view of the map at the recommended contour level 0.335 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



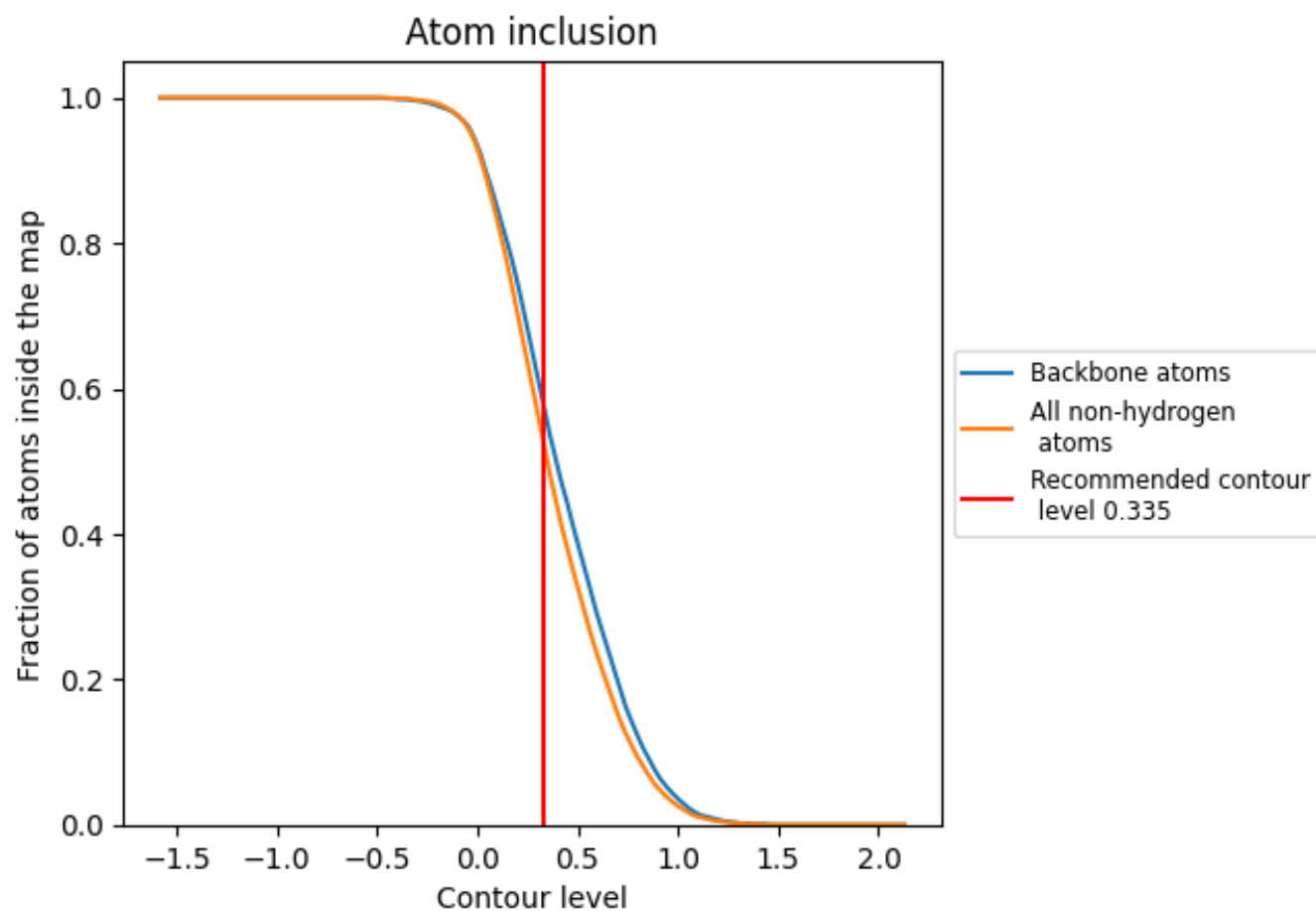
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.335).

9.4 Atom inclusion ⓘ



At the recommended contour level, 57% of all backbone atoms, 52% 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 (0.335) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5180	 0.3800
A	 0.1360	 0.2590
D	 0.0790	 0.0750
E	 0.6770	 0.4710
F	 0.6650	 0.4700
G	 0.0860	 0.0680
I	 0.6890	 0.4580
J	 0.5010	 0.3780
K	 0.4450	 0.3360
L	 0.6040	 0.4050
M	 0.6340	 0.4430
O	 0.6830	 0.4550
P	 0.5030	 0.3780
Q	 0.4460	 0.3330
R	 0.6010	 0.4050
S	 0.5180	 0.3590
T	 0.4840	 0.3780
U	 0.2070	 0.2670
V	 0.2750	 0.2860
W	 0.4470	 0.3430
X	 0.5010	 0.3510
Y	 0.6330	 0.4410
Z	 0.4860	 0.3760
a	 0.2040	 0.2620
b	 0.2730	 0.2940
c	 0.4510	 0.3510

