



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 02:58 AM EST

PDB ID : 7RH7
EMDB ID : EMD-24457
Title : Mycobacterial CIII2CIV2 supercomplex, Telacebec (Q203) bound
Authors : Di Trani, J.M.; Yanofsky, D.J.; Rubinstein, J.L.
Deposited on : 2021-07-16
Resolution : 3.00 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

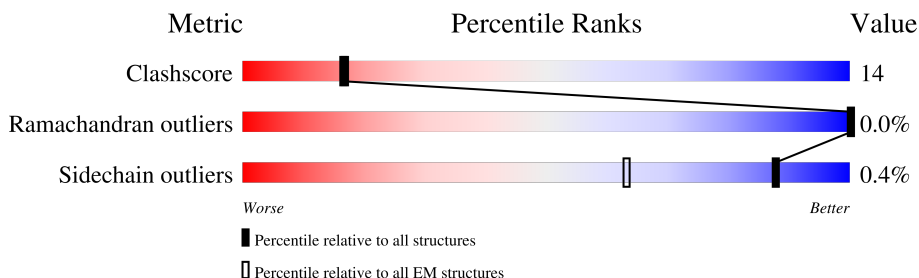
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	W	159	<div> <div>87%</div> <div>80%19%.</div> </div>
1	c	159	<div> <div>88%</div> <div>99%.</div> </div>
2	K	312	<div> <div>49%</div> <div>69%31%</div> </div>
2	Q	312	<div> <div>53%</div> <div>71%29%</div> </div>
3	L	552	<div> <div>9%</div> <div>66%34%</div> </div>
3	R	552	<div> <div>9%</div> <div>66%34%</div> </div>
4	S	203	<div> <div>32%</div> <div>80%20%</div> </div>
4	X	203	<div> <div>34%</div> <div>75%24%.</div> </div>

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Mol	Chain	Length	Quality of chain
5	T	139	
5	Z	139	
6	U	79	
6	a	79	
7	V	145	
7	b	145	
8	J	100	
8	P	100	
9	D	216	
9	G	216	
10	I	223	
10	O	223	
11	E	535	
11	F	535	
12	M	382	
12	Y	382	

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
17	CDL	T	202	-	-	X	-
17	CDL	X	302	-	-	X	-
17	CDL	Z	202	-	-	X	-
24	FES	Y	501	-	-	X	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 95515 atoms, of which 46689 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 LpqE protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	W	158	Total	C	H	N	O	S	0	0
			2259	708	1110	192	248	1		
1	c	158	Total	C	H	N	O	S	0	0
			2259	708	1110	192	248	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Q	312	Total	C	H	N	O	S	0	0
			4857	1592	2392	412	451	10		
2	K	312	Total	C	H	N	O	S	0	0
			4857	1592	2392	412	451	10		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	R	552	Total	C	H	N	O	S	0	0
			8717	2937	4347	695	712	26		
3	L	552	Total	C	H	N	O	S	0	0
			8716	2937	4346	695	712	26		

- Molecule 4 is a protein called Cytochrome aa3 subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	S	203	Total	C	H	N	O	S	0	0
			3108	1039	1548	253	260	8		
4	X	203	Total	C	H	N	O	S	0	0
			3108	1039	1548	253	260	8		

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	T	139	Total	C	H	N	O	S	0	0
			2135	719	1058	167	188	3		
5	Z	139	Total	C	H	N	O	S	0	0
			2135	719	1058	167	188	3		

- Molecule 6 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	U	79	Total	C	H	N	O	S	0	0
			1167	381	576	107	101	2		
6	a	79	Total	C	H	N	O	S	0	0
			1167	381	576	107	101	2		

- Molecule 7 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	V	145	Total	C	H	N	O	S	0	0
			2093	658	1052	176	205	2		
7	b	145	Total	C	H	N	O	S	0	0
			2093	658	1052	176	205	2		

- Molecule 8 is a protein called Conserved transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	92	Total	C	H	N	O	S	0	0
			1452	471	716	136	124	5		
8	J	92	Total	C	H	N	O	S	0	0
			1453	471	717	136	124	5		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	initiating methionine	UNP A0QVH4
P	2	SER	-	expression tag	UNP A0QVH4
P	3	SER	-	expression tag	UNP A0QVH4
P	4	THR	-	expression tag	UNP A0QVH4
P	5	GLN	-	expression tag	UNP A0QVH4
P	6	ASP	-	expression tag	UNP A0QVH4
P	7	ARG	-	expression tag	UNP A0QVH4
P	8	SER	-	expression tag	UNP A0QVH4
P	9	GLN	-	expression tag	UNP A0QVH4
P	10	LEU	-	expression tag	UNP A0QVH4
P	11	ASP	-	expression tag	UNP A0QVH4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	12	PRO	-	expression tag	UNP A0QVH4
P	13	GLU	-	expression tag	UNP A0QVH4
P	14	GLU	-	expression tag	UNP A0QVH4
P	15	GLN	-	expression tag	UNP A0QVH4
P	16	PRO	-	expression tag	UNP A0QVH4
P	17	VAL	-	expression tag	UNP A0QVH4
J	1	MET	-	initiating methionine	UNP A0QVH4
J	2	SER	-	expression tag	UNP A0QVH4
J	3	SER	-	expression tag	UNP A0QVH4
J	4	THR	-	expression tag	UNP A0QVH4
J	5	GLN	-	expression tag	UNP A0QVH4
J	6	ASP	-	expression tag	UNP A0QVH4
J	7	ARG	-	expression tag	UNP A0QVH4
J	8	SER	-	expression tag	UNP A0QVH4
J	9	GLN	-	expression tag	UNP A0QVH4
J	10	LEU	-	expression tag	UNP A0QVH4
J	11	ASP	-	expression tag	UNP A0QVH4
J	12	PRO	-	expression tag	UNP A0QVH4
J	13	GLU	-	expression tag	UNP A0QVH4
J	14	GLU	-	expression tag	UNP A0QVH4
J	15	GLN	-	expression tag	UNP A0QVH4
J	16	PRO	-	expression tag	UNP A0QVH4
J	17	VAL	-	expression tag	UNP A0QVH4

- Molecule 9 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms						AltConf	Trace
9	G	216	Total	C	H	N	O	S	0	0
			1732	645	640	217	229	1		
9	D	216	Total	C	H	N	O	S	0	0
			1732	645	640	217	229	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	O	223	Total	C	H	N	O	S	0	0
			3187	1008	1564	289	314	12		
10	I	223	Total	C	H	N	O	S	0	0
			3186	1008	1563	289	314	12		

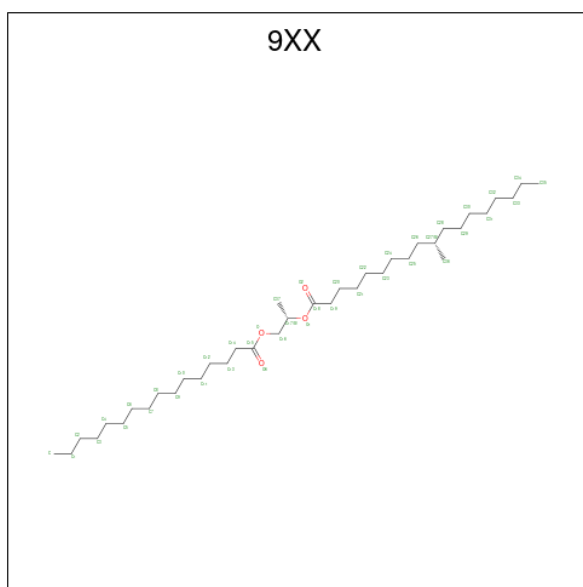
- Molecule 11 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	535	Total	C	H	N	O	S	0	0
			8385	2751	4204	711	701	18		
11	F	535	Total	C	H	N	O	S	0	0
			8385	2751	4204	711	701	18		

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

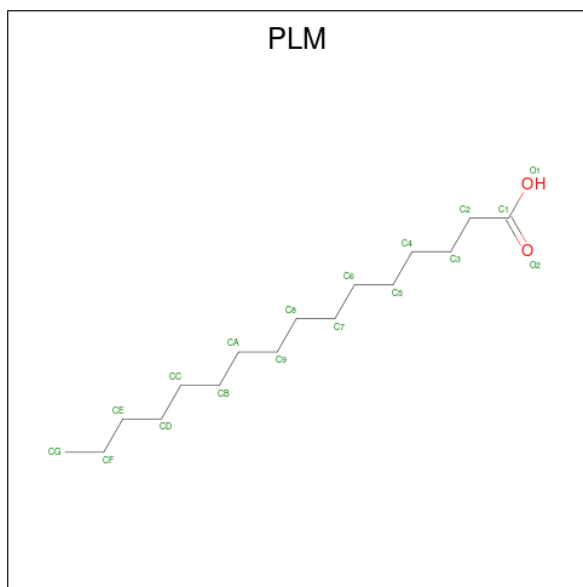
Mol	Chain	Residues	Atoms						AltConf	Trace
12	Y	382	Total	C	H	N	O	S	0	0
			5961	1924	2984	504	538	11		
12	M	382	Total	C	H	N	O	S	0	0
			5961	1924	2984	504	538	11		

- Molecule 13 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (three-letter code: 9XX) (formula: C₃₈H₇₄O₄).



Mol	Chain	Residues	Atoms				AltConf
13	W	1	Total	C	H	O	0
			115	38	73	4	
13	G	1	Total	C	H	O	0
			83	28	51	4	
13	D	1	Total	C	H	O	0
			83	28	51	4	
13	c	1	Total	C	H	O	0
			115	38	73	4	

- Molecule 14 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).

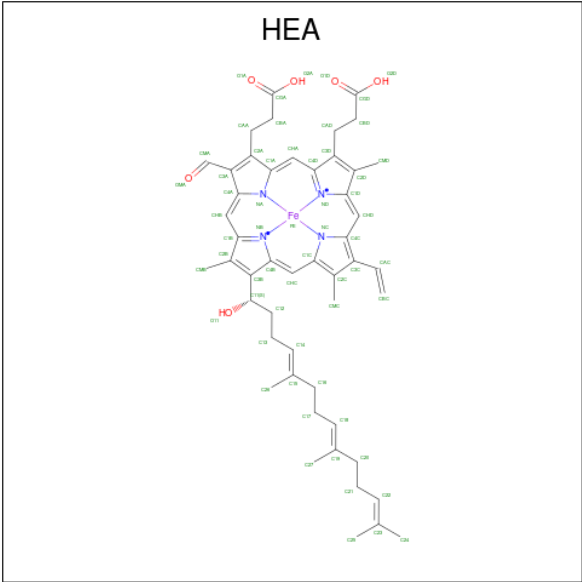


Mol	Chain	Residues	Atoms				AltConf
14	W	1	Total	C	H	O	0
			48	16	31	1	
14	G	1	Total	C	H	O	0
			27	10	16	1	
14	D	1	Total	C	H	O	0
			27	10	16	1	
14	c	1	Total	C	H	O	0
			48	16	31	1	

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

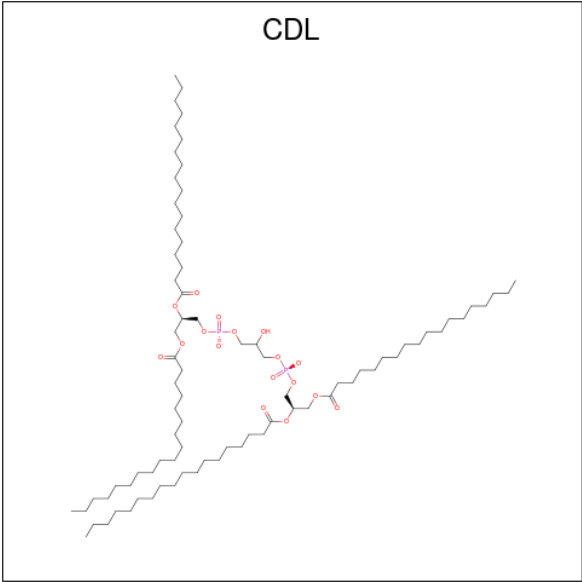
Mol	Chain	Residues	Atoms		AltConf
15	Q	2	Total	Cu	0
			2	2	
15	R	1	Total	Cu	0
			1	1	
15	K	2	Total	Cu	0
			2	2	
15	L	1	Total	Cu	0
			1	1	

- Molecule 16 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



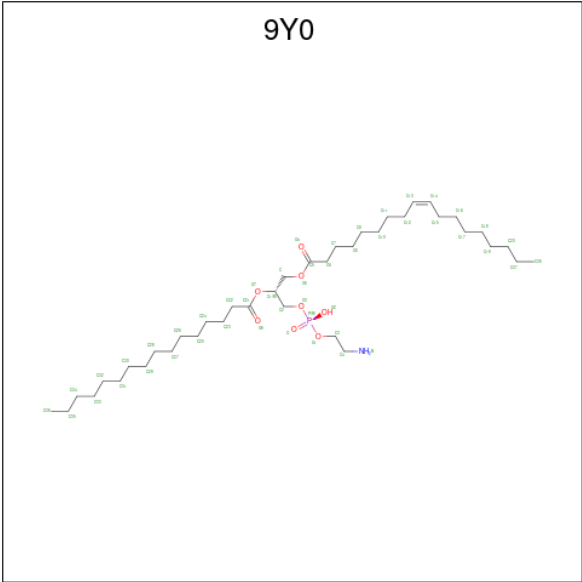
Mol	Chain	Residues	Atoms						AltConf
16	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
16	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
16	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
16	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 17 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



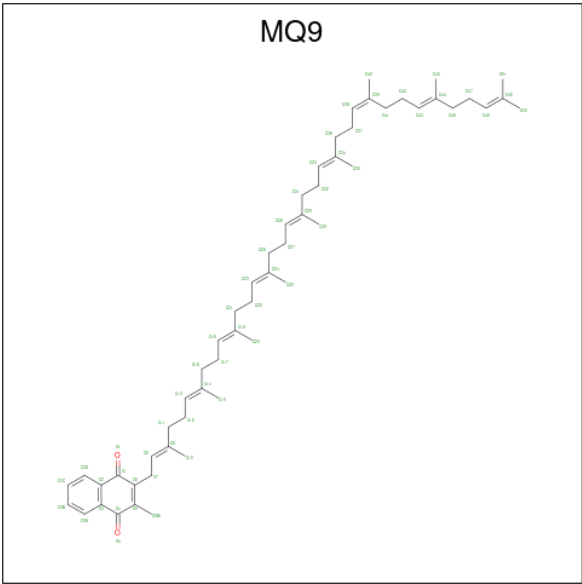
Mol	Chain	Residues	Atoms				AltConf
17	R	1	Total	C	O	P	0
			76	57	17	2	
17	S	1	Total	C	O	P	0
			76	57	17	2	
17	S	1	Total	C	O	P	0
			76	57	17	2	
17	T	1	Total	C	O	P	0
			76	57	17	2	
17	P	1	Total	C	O	P	0
			76	57	17	2	
17	E	1	Total	C	O	P	0
			76	57	17	2	
17	E	1	Total	C	O	P	0
			76	57	17	2	
17	E	1	Total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

- Molecule 18 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (three-letter code: 9Y0) (formula: C₃₉H₇₆NO₈P).



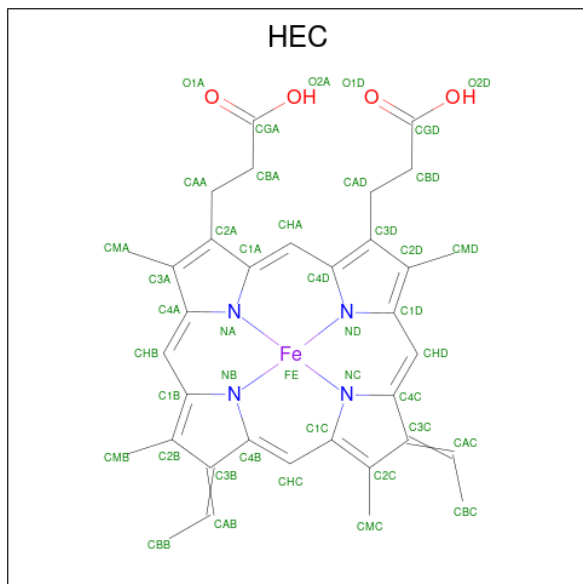
Mol	Chain	Residues	Atoms						AltConf
18	S	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
18	P	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
18	L	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
18	X	1	Total 124	C 39	H 75	N 1	O 8	P 1	0

- Molecule 19 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C₅₆H₈₀O₂).



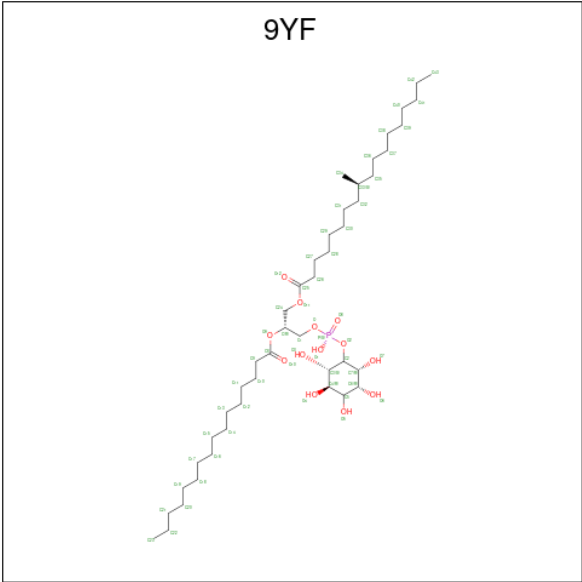
Mol	Chain	Residues	Atoms				AltConf
19	T	1	Total	C	H	O	0
			138	56	80	2	
19	E	1	Total	C	H	O	0
			138	56	80	2	
19	E	1	Total	C	H	O	0
			138	56	80	2	
19	Z	1	Total	C	H	O	0
			138	56	80	2	
19	F	1	Total	C	H	O	0
			138	56	80	2	
19	F	1	Total	C	H	O	0
			138	56	80	2	

- Molecule 20 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



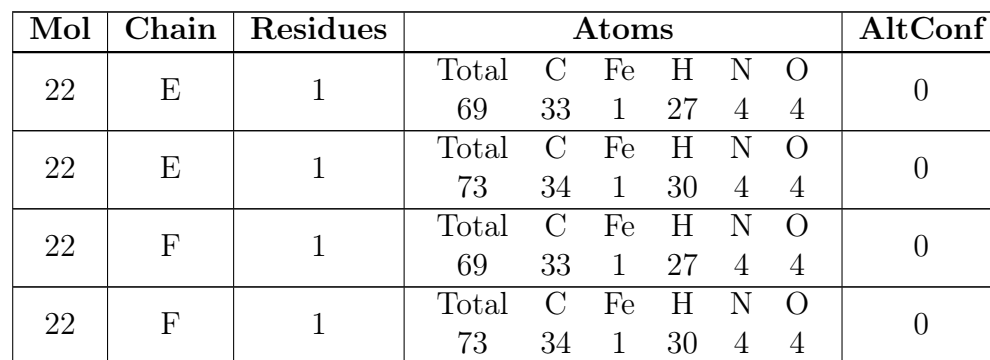
Mol	Chain	Residues	Atoms						AltConf
20	O	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
20	O	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
20	I	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
20	I	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

- Molecule 21 is (2R)-2-(hexadecanoyloxy)-3-[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (three-letter code: 9YF) (formula: $C_{44}H_{85}O_{13}P$).

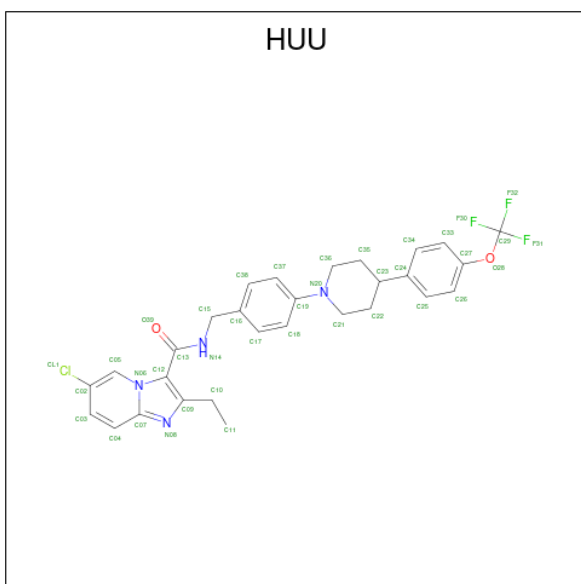


Mol	Chain	Residues	Atoms					AltConf
21	O	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	E	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	I	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	F	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	M	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	M	1	Total	C	H	O	P	0
			142	44	84	13	1	

- Molecule 22 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).

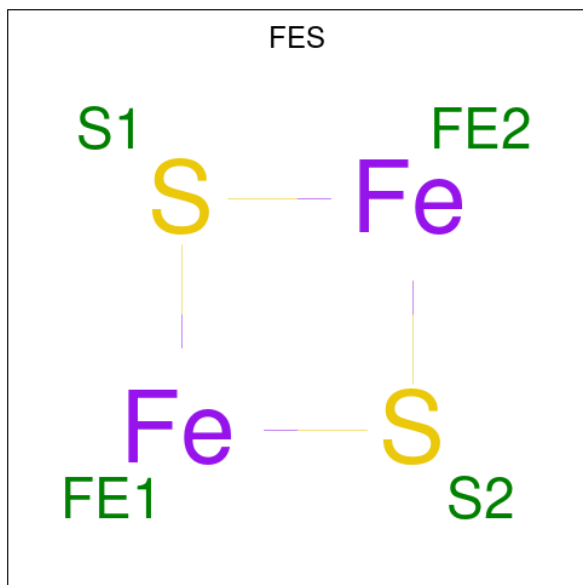


- Molecule 23 is 6-chloranyl-2-ethyl-N-[[4-[4-[4-(trifluoromethoxy)phenyl]piperidin-1-yl]phenyl]methyl]imidazo[1,2-a]pyridine-3-carboxamide (three-letter code: HUU) (formula: C₂₉H₂₈ClF₃N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
23	E	1	Total	C	Cl	F	H	N	O	0
			67	29	1	3	28	4	2	
23	F	1	Total	C	Cl	F	H	N	O	0
			67	29	1	3	28	4	2	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

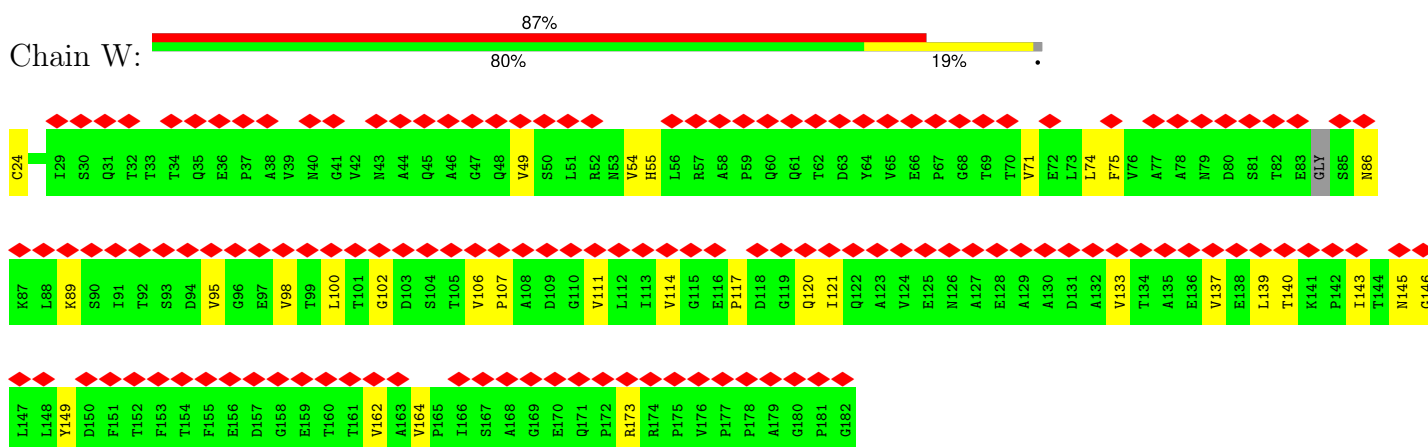


Mol	Chain	Residues	Atoms			AltConf
24	Y	1	Total	Fe	S	0
			4	2	2	
24	M	1	Total	Fe	S	0
			4	2	2	

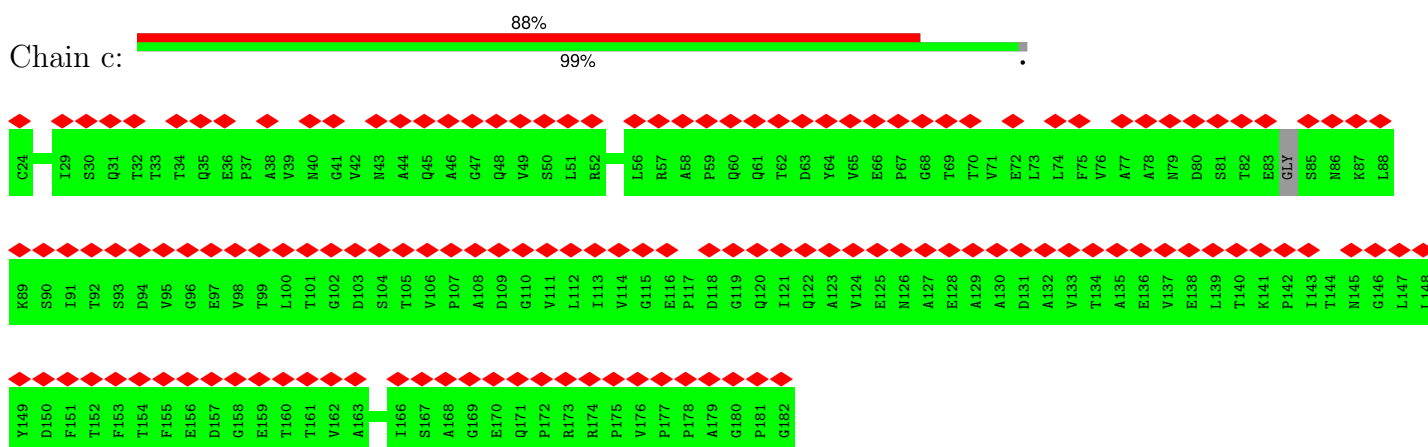
3 Residue-property plots

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.

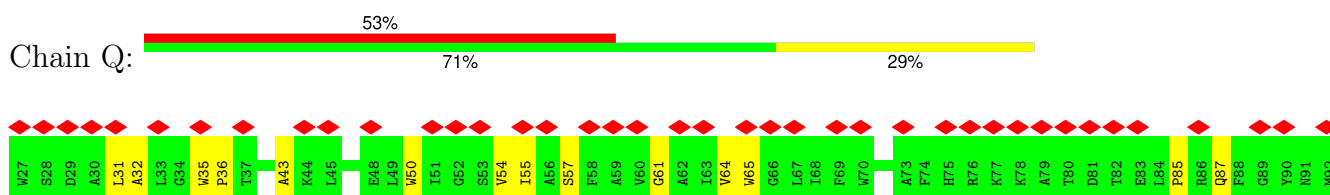
- Molecule 1: LpqE protein

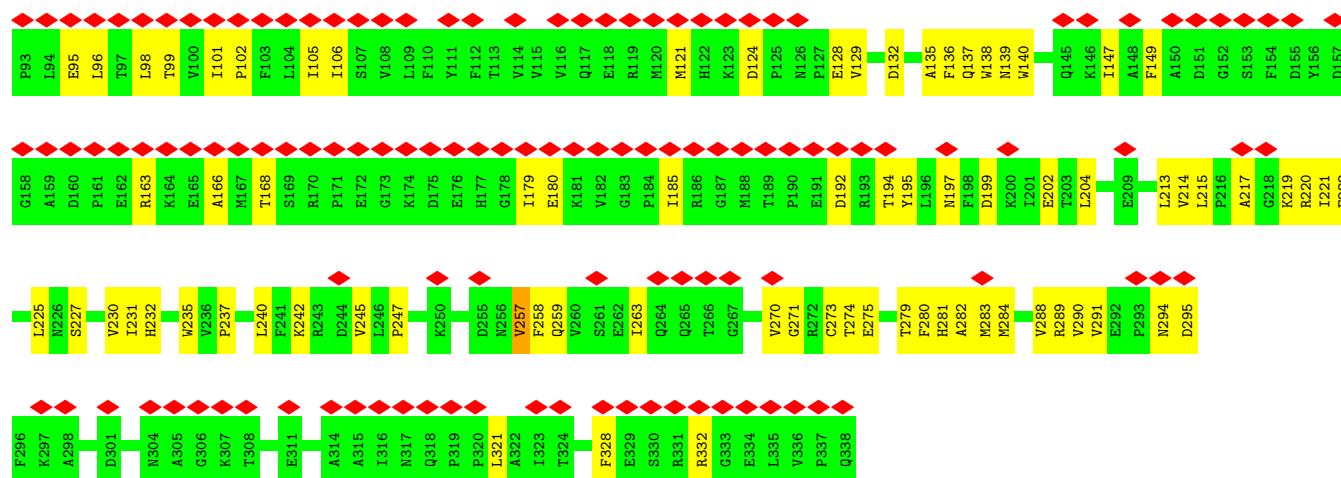


- Molecule 1: LpqE protein

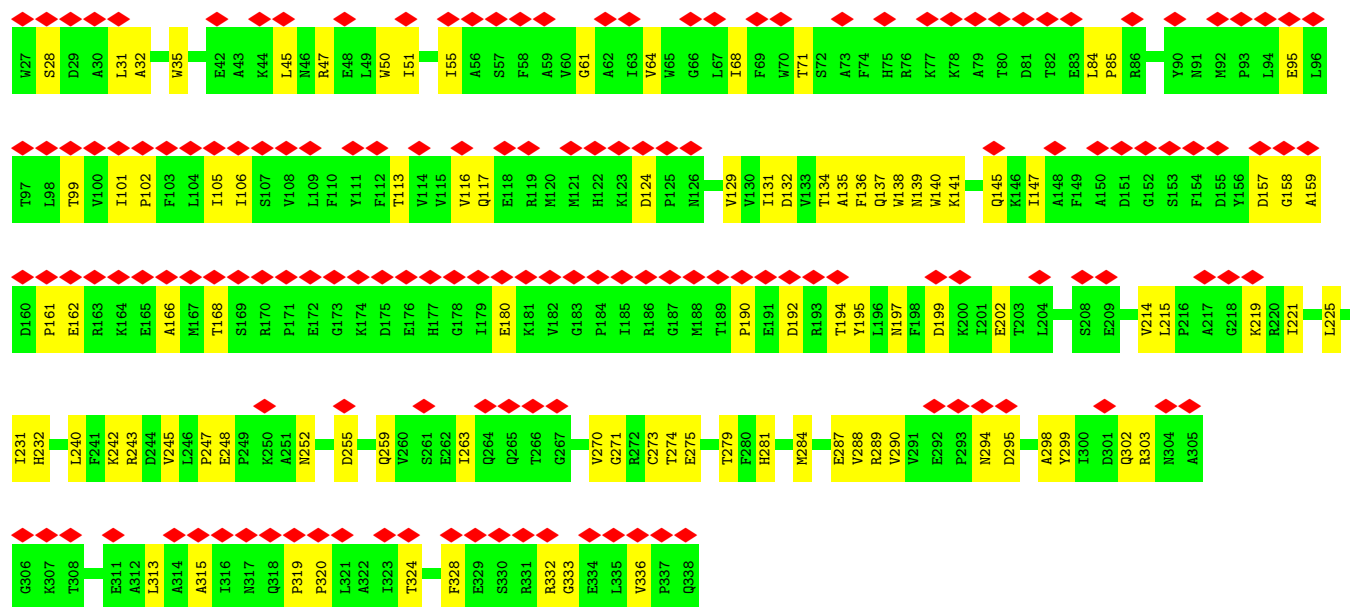


- Molecule 2: Cytochrome aa3 subunit 2

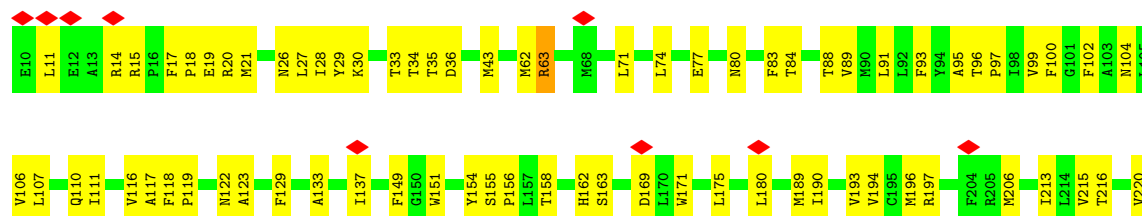


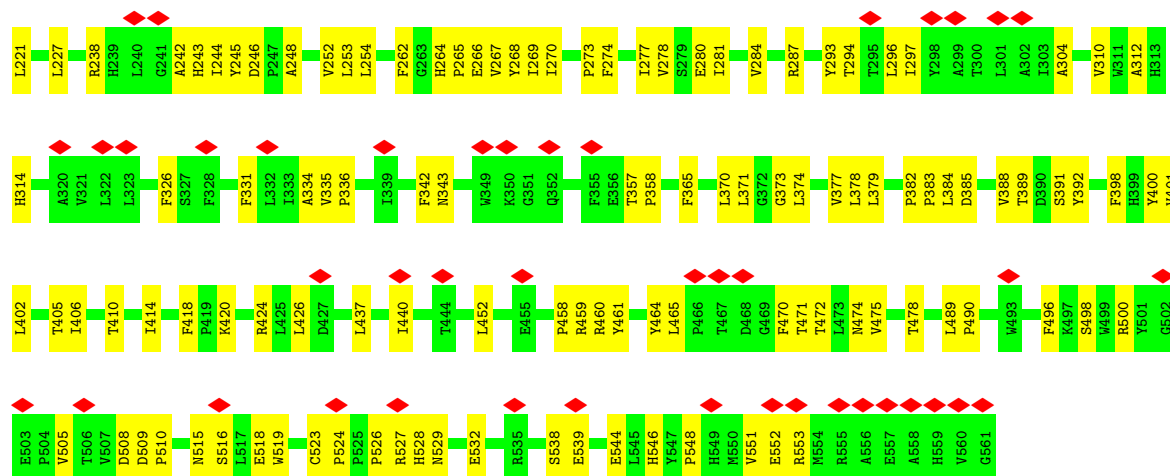


• Molecule 2: Cytochrome aa3 subunit 2

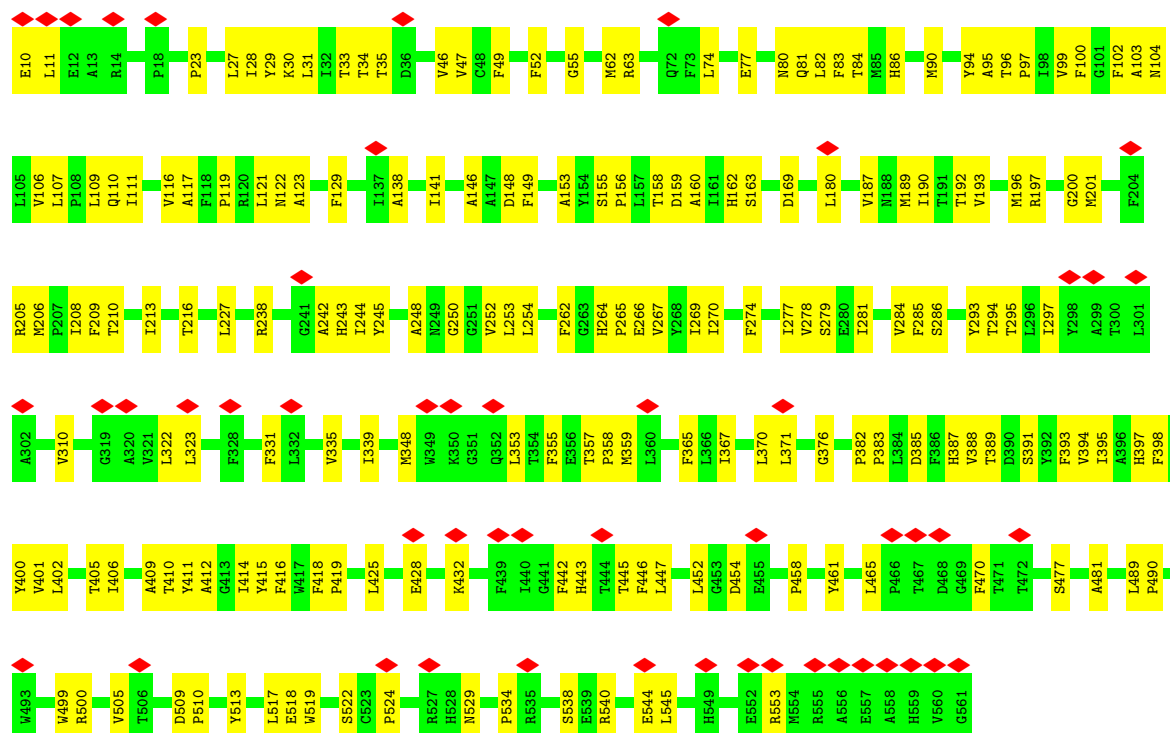


• Molecule 3: Cytochrome c oxidase subunit 1

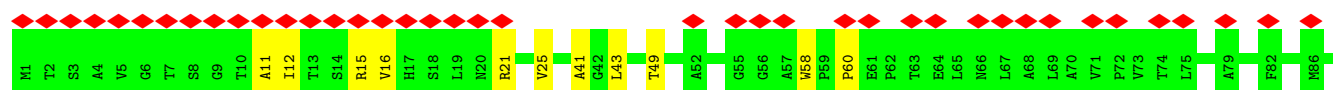


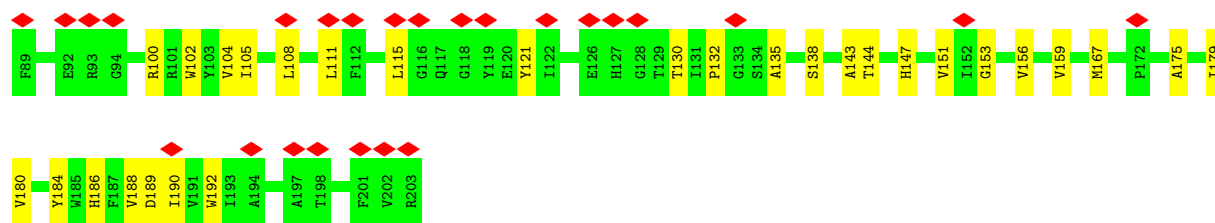


• Molecule 3: Cytochrome c oxidase subunit 1

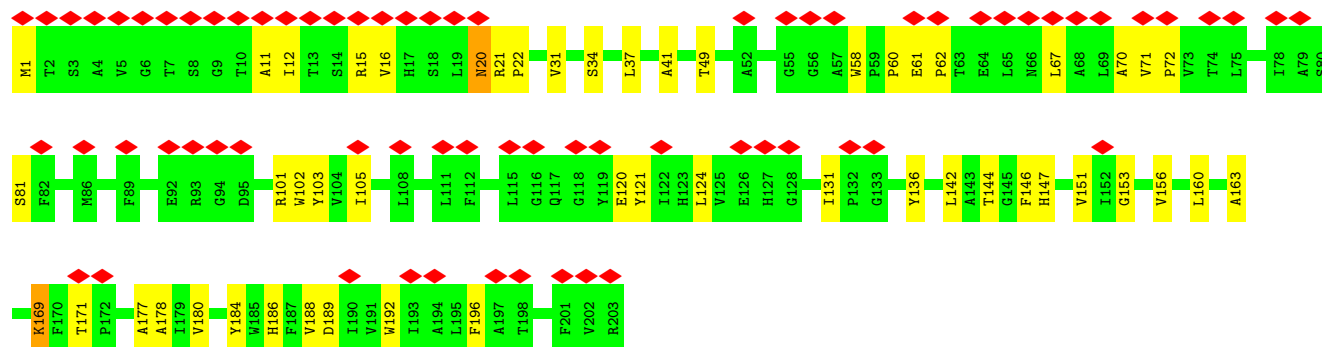
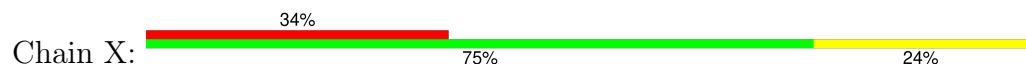


• Molecule 4: Cytochrome aa3 subunit 3

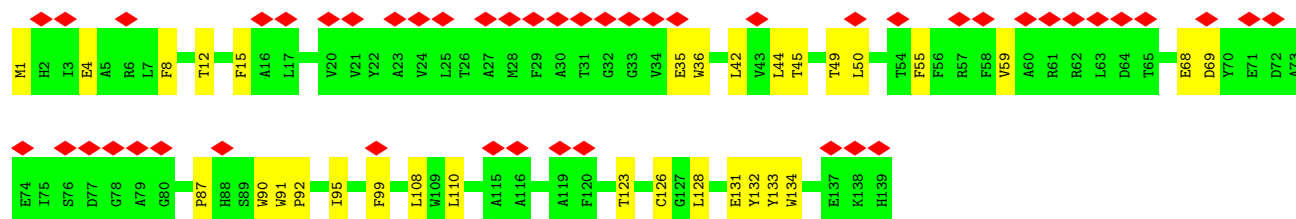
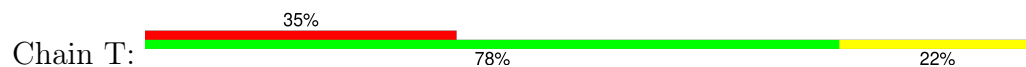




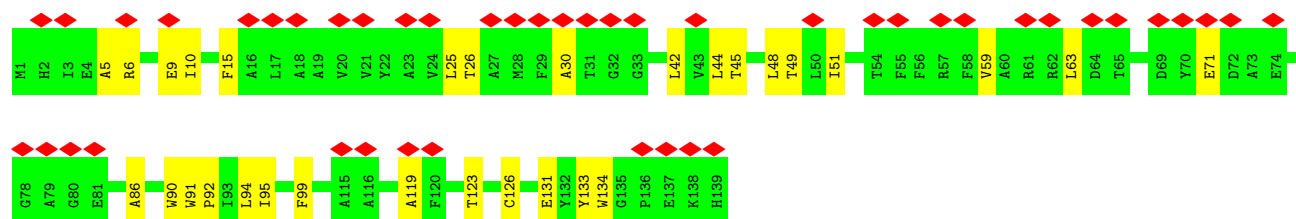
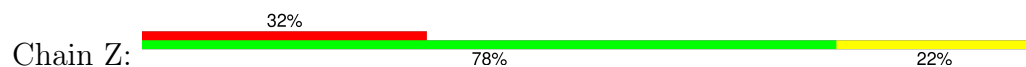
• Molecule 4: Cytochrome aa3 subunit 3



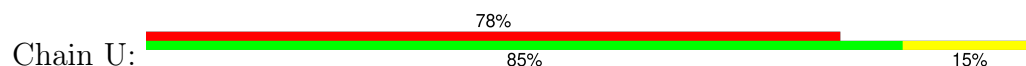
• Molecule 5: Cytochrome c oxidase polypeptide 4

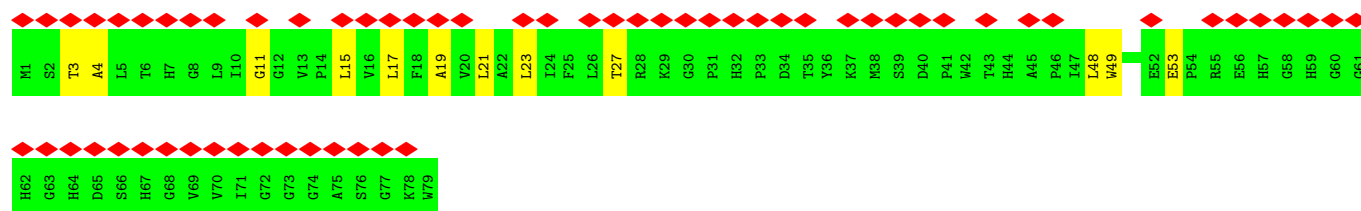


• Molecule 5: Cytochrome c oxidase polypeptide 4

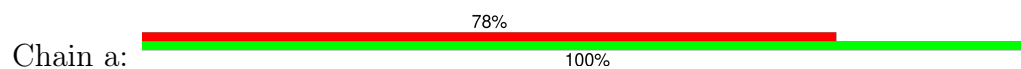


• Molecule 6: Cytochrome c oxidase subunit CtaJ

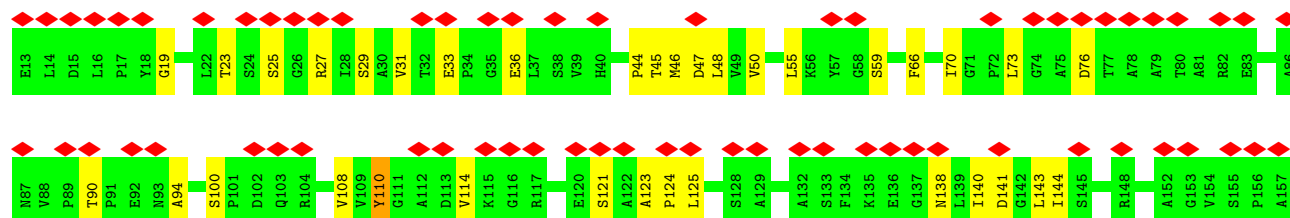
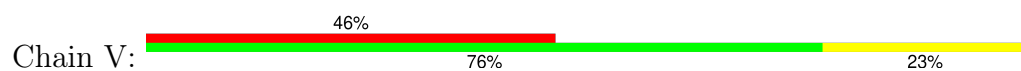




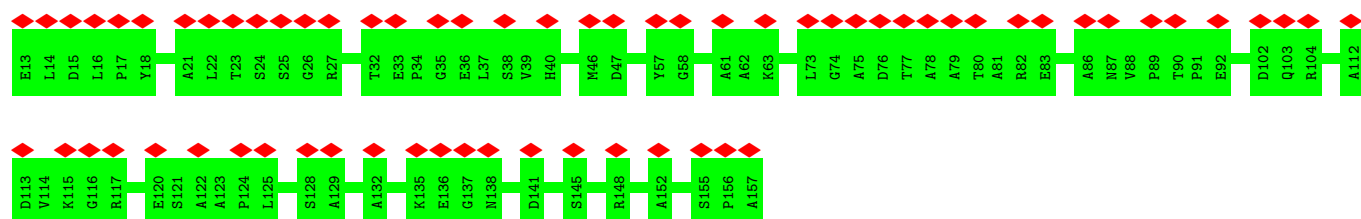
• Molecule 6: Cytochrome c oxidase subunit CtaJ



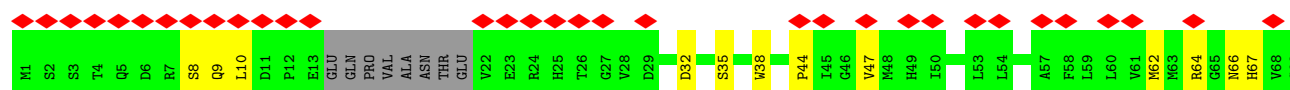
• Molecule 7: Uncharacterized protein MSMEG_4692/MSMEI_4575



• Molecule 7: Uncharacterized protein MSMEG_4692/MSMEI_4575

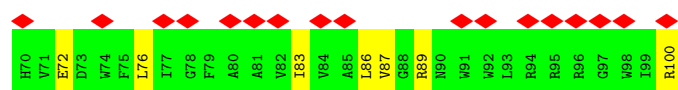
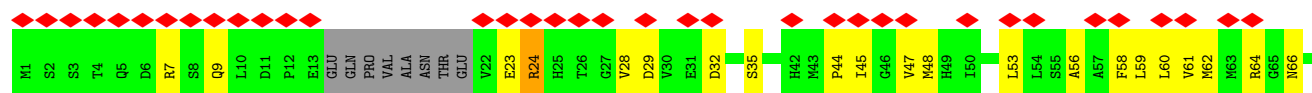


• Molecule 8: Conserved transmembrane protein

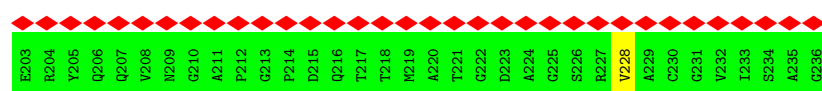
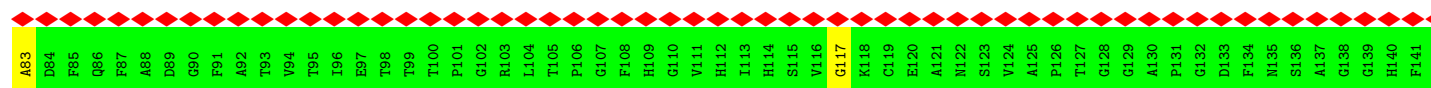
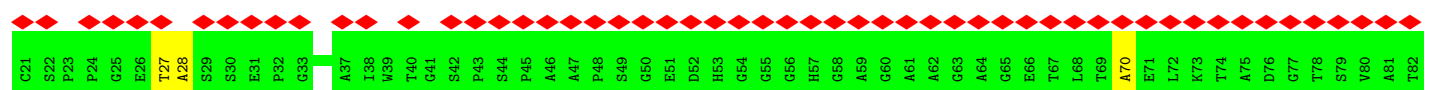




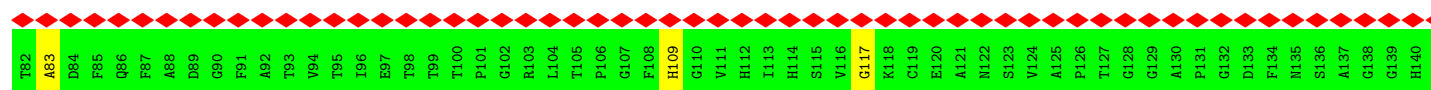
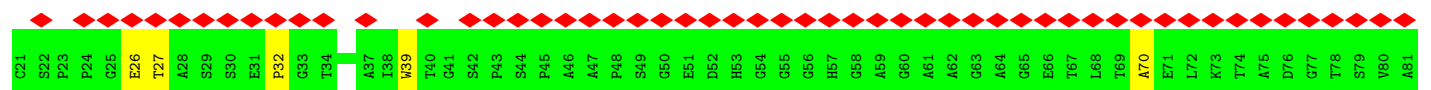
• Molecule 8: Conserved transmembrane protein

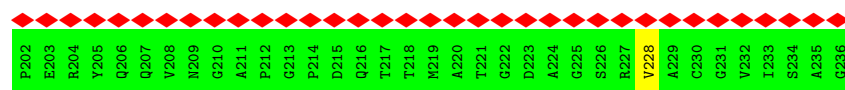


• Molecule 9: Superoxide dismutase [Cu-Zn]

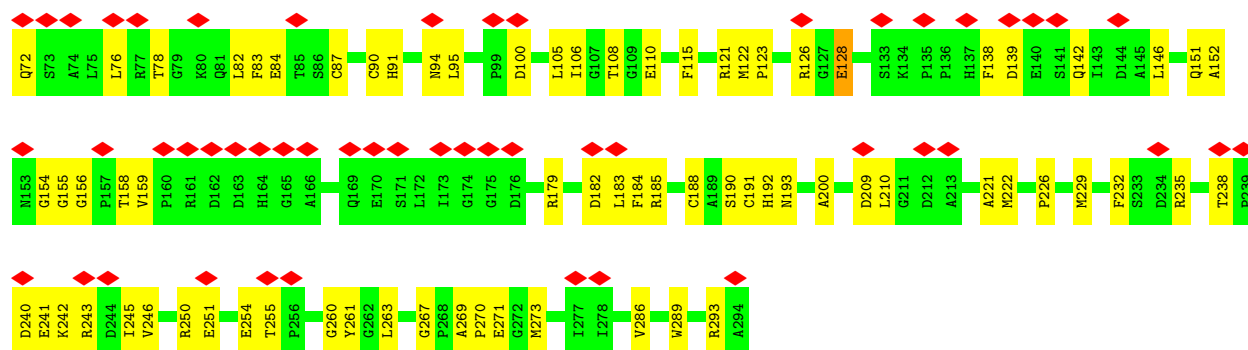


• Molecule 9: Superoxide dismutase [Cu-Zn]

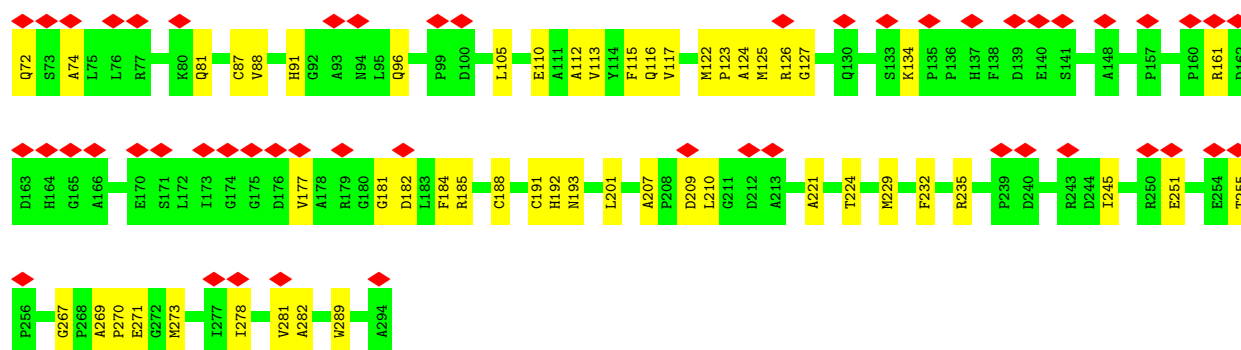
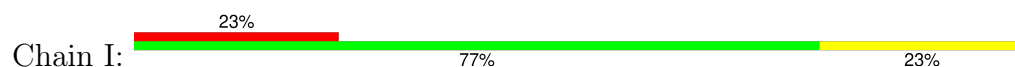




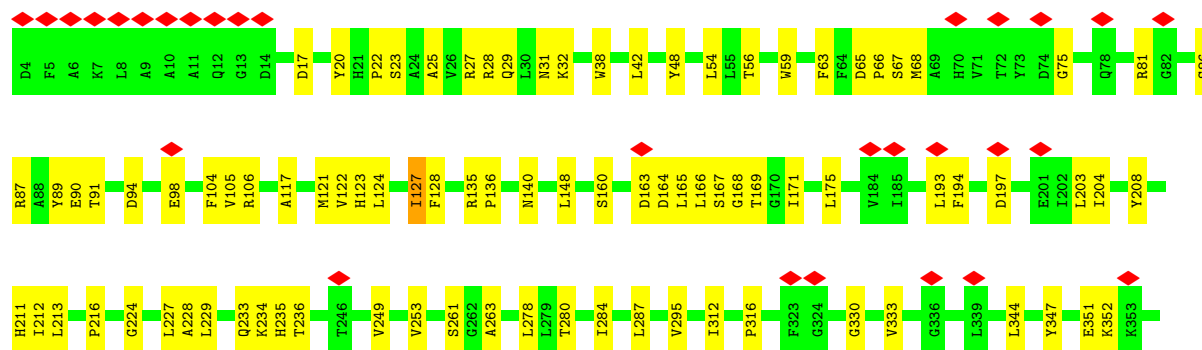
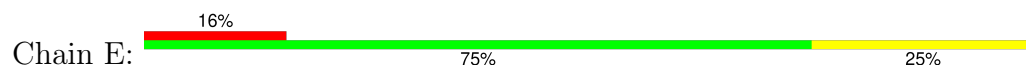
• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

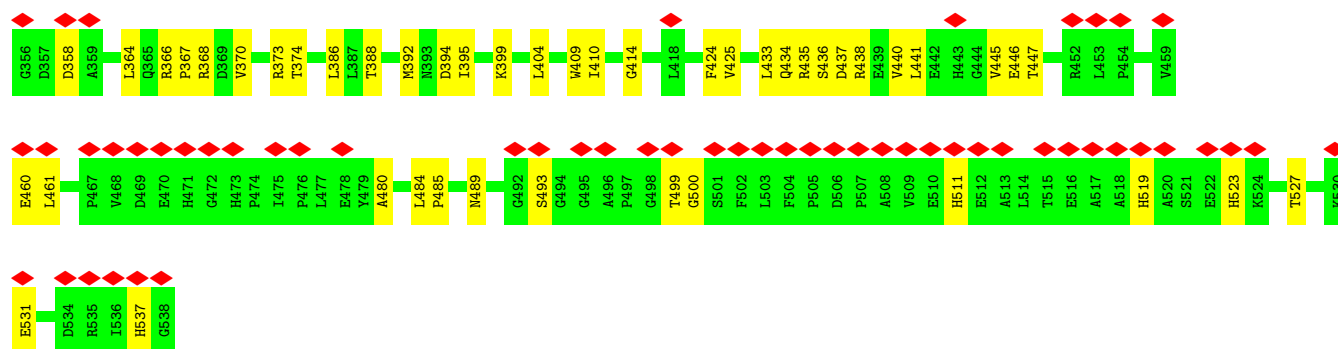


• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

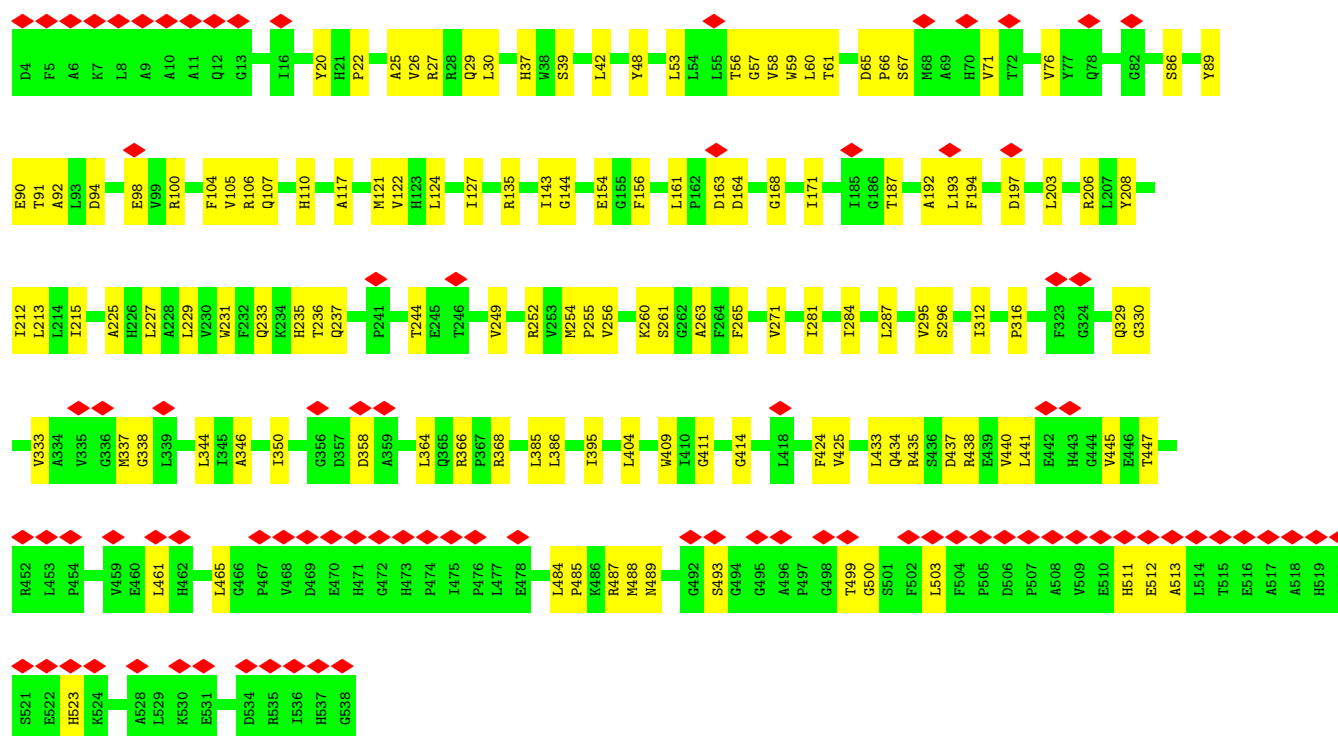


• Molecule 11: Cytochrome bc1 complex cytochrome b subunit

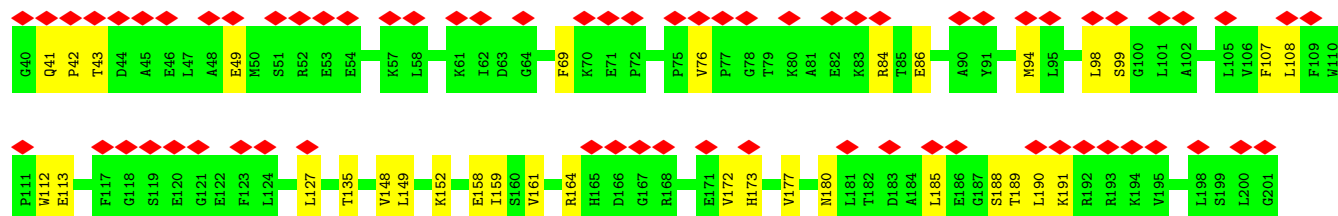


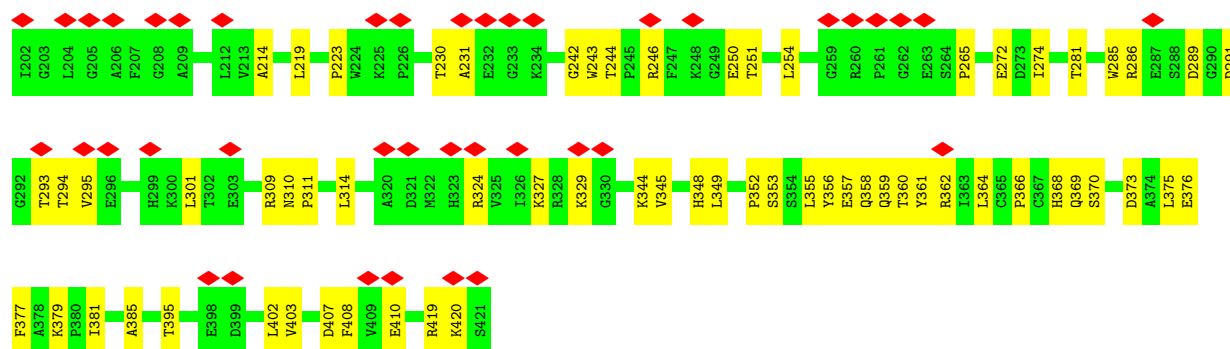


• Molecule 11: Cytochrome bc1 complex cytochrome b subunit

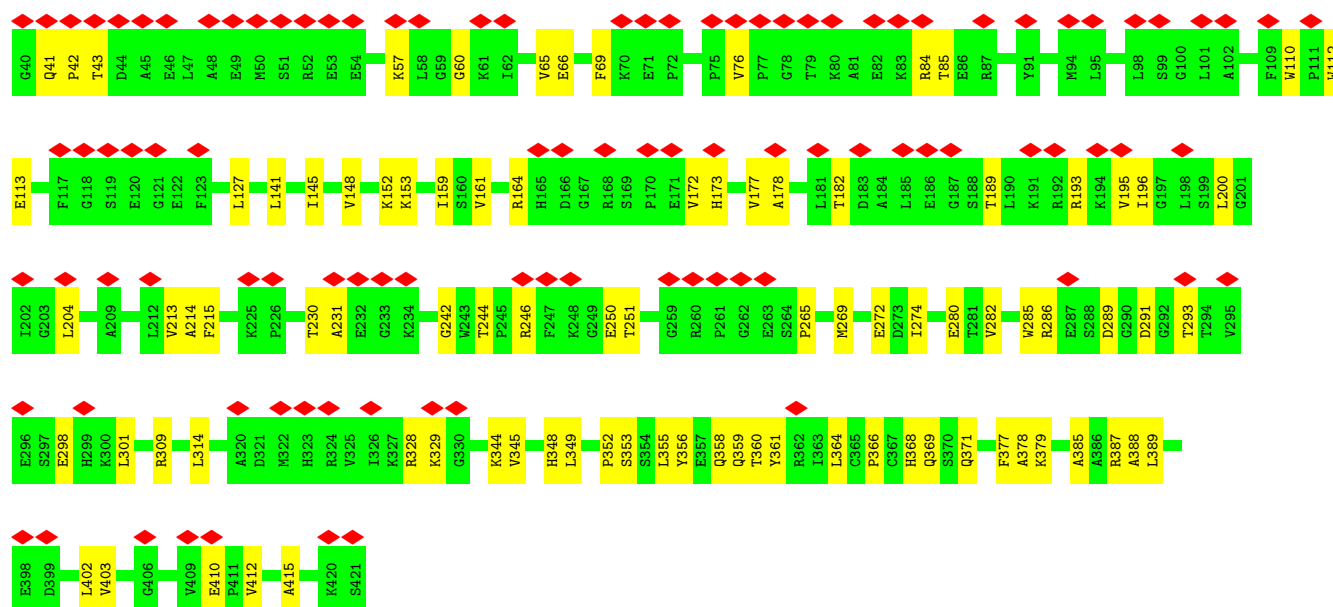
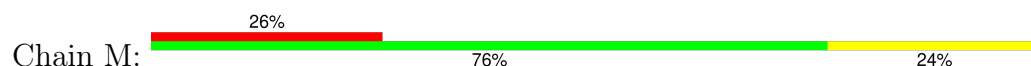


• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70818	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 ($e^-/\text{\AA}^2$)	43.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.407	Depositor
Minimum map value	-4.052	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.82	Depositor
Map size (Å)	339.9, 339.9, 339.9	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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	W	0.25	0/1166	0.51	0/1599
1	c	0.25	0/1166	0.50	0/1599
2	K	0.27	0/2534	0.49	0/3451
2	Q	0.31	0/2534	0.54	0/3451
3	L	0.32	0/4530	0.49	0/6188
3	R	0.31	0/4530	0.50	0/6188
4	S	0.29	0/1608	0.47	0/2195
4	X	0.29	0/1608	0.47	0/2195
5	T	0.28	0/1112	0.46	0/1524
5	Z	0.28	0/1112	0.46	0/1524
6	U	0.36	0/613	0.63	0/836
6	a	0.26	0/613	0.45	0/836
7	V	0.30	0/1059	0.55	0/1446
7	b	0.29	0/1059	0.52	0/1446
8	J	0.25	0/757	0.54	0/1027
8	P	0.25	0/757	0.51	0/1027
9	D	0.26	0/1099	0.46	0/1519
9	G	0.26	0/1099	0.47	0/1519
10	I	0.28	0/1660	0.50	0/2250
10	O	0.38	0/1660	0.68	3/2250 (0.1%)
11	E	0.36	0/4314	0.59	2/5882 (0.0%)
11	F	0.29	0/4314	0.49	0/5882
12	M	0.29	0/3056	0.51	0/4142
12	Y	0.28	0/3056	0.50	0/4142
All	All	0.30	0/47016	0.51	5/64118 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	O	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	136	PRO	N-CA-C	-7.17	93.45	112.10
11	E	140	ASN	CB-CA-C	6.46	123.31	110.40
10	O	121	ARG	CB-CA-C	-5.09	100.22	110.40
10	O	121	ARG	NE-CZ-NH1	5.06	122.83	120.30
10	O	123	PRO	N-CA-C	-5.03	99.03	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	O	128	GLU	Mainchain

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	W	1149	1110	1110	26	0
1	c	1149	1110	1110	0	0
2	K	2465	2392	2392	84	0
2	Q	2465	2392	2392	84	0
3	L	4370	4346	4346	172	0
3	R	4370	4347	4345	179	0
4	S	1560	1548	1547	41	0
4	X	1560	1548	1547	50	0
5	T	1077	1058	1058	30	0
5	Z	1077	1058	1058	40	0
6	U	591	576	576	9	0
6	a	591	576	576	0	0
7	V	1041	1052	1052	25	0
7	b	1041	1052	1052	0	0
8	J	736	717	717	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	P	736	716	717	18	0
9	D	1092	640	640	8	0
9	G	1092	640	640	5	0
10	I	1623	1563	1563	52	0
10	O	1623	1564	1564	64	0
11	E	4181	4204	4202	115	0
11	F	4181	4204	4202	122	0
12	M	2977	2984	2984	76	0
12	Y	2977	2984	2984	89	0
13	D	32	51	0	0	0
13	G	32	51	0	0	0
13	W	42	73	0	1	0
13	c	42	73	0	0	0
14	D	11	16	16	1	0
14	G	11	16	16	0	0
14	W	17	31	31	0	0
14	c	17	31	31	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	1	0	0	0	0
16	L	120	108	108	13	0
16	R	120	108	108	12	0
17	E	228	0	288	17	0
17	F	228	0	288	25	0
17	J	76	0	96	11	0
17	L	76	0	96	14	0
17	P	76	0	96	8	0
17	R	76	0	96	10	0
17	S	152	0	190	34	0
17	T	76	0	96	21	0
17	X	152	0	192	34	0
17	Z	76	0	96	26	0
18	L	49	75	0	0	0
18	P	49	75	0	0	0
18	S	49	75	0	0	0
18	X	49	75	0	1	0
19	E	116	160	160	11	0
19	F	116	160	160	13	0
19	T	58	80	80	5	0
19	Z	58	80	80	3	0
20	I	86	64	64	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	O	86	64	64	21	0
21	E	58	84	0	0	0
21	F	58	84	0	0	0
21	I	58	84	0	1	0
21	M	116	168	0	0	0
21	O	58	84	0	0	0
21	Y	116	168	0	0	0
22	E	85	57	57	14	0
22	F	85	57	57	9	0
23	E	39	28	0	0	0
23	F	39	28	0	0	0
24	M	4	0	0	1	0
24	Y	4	0	0	3	0
All	All	48826	46689	46940	1240	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 14.

The worst 5 of 1240 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)
17:S:303:CDL:OA9	17:S:303:CDL:H332	1.37	1.14
17:X:302:CDL:HB62	17:X:302:CDL:C51	1.73	1.10
4:S:15:ARG:NH1	17:S:303:CDL:CA2	2.20	1.04
17:L:605:CDL:H512	17:L:605:CDL:H721	1.40	1.04
11:E:425:VAL:HG11	17:E:608:CDL:H371	1.40	1.04

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	W	154/159 (97%)	137 (89%)	17 (11%)	0	100	100
1	c	154/159 (97%)	143 (93%)	11 (7%)	0	100	100
2	K	310/312 (99%)	279 (90%)	31 (10%)	0	100	100
2	Q	310/312 (99%)	279 (90%)	31 (10%)	0	100	100
3	L	550/552 (100%)	512 (93%)	38 (7%)	0	100	100
3	R	550/552 (100%)	512 (93%)	38 (7%)	0	100	100
4	S	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
4	X	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
5	T	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
5	Z	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
6	U	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
6	a	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
7	V	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
7	b	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
8	J	88/100 (88%)	82 (93%)	6 (7%)	0	100	100
8	P	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
9	D	214/216 (99%)	193 (90%)	21 (10%)	0	100	100
9	G	214/216 (99%)	190 (89%)	24 (11%)	0	100	100
10	I	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
10	O	221/223 (99%)	193 (87%)	28 (13%)	0	100	100
11	E	533/535 (100%)	489 (92%)	43 (8%)	1 (0%)	44	77
11	F	533/535 (100%)	486 (91%)	47 (9%)	0	100	100
12	M	380/382 (100%)	348 (92%)	32 (8%)	0	100	100
12	Y	380/382 (100%)	350 (92%)	30 (8%)	0	100	100
All	All	6016/6090 (99%)	5531 (92%)	484 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	E	135	ARG

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	W	127/127 (100%)	127 (100%)	0	100	100
1	c	127/127 (100%)	127 (100%)	0	100	100
2	K	260/266 (98%)	260 (100%)	0	100	100
2	Q	260/266 (98%)	257 (99%)	3 (1%)	67	86
3	L	452/453 (100%)	452 (100%)	0	100	100
3	R	452/453 (100%)	450 (100%)	2 (0%)	89	95
4	S	155/161 (96%)	155 (100%)	0	100	100
4	X	155/161 (96%)	153 (99%)	2 (1%)	65	85
5	T	106/106 (100%)	106 (100%)	0	100	100
5	Z	106/106 (100%)	106 (100%)	0	100	100
6	U	59/59 (100%)	59 (100%)	0	100	100
6	a	59/59 (100%)	59 (100%)	0	100	100
7	V	107/107 (100%)	106 (99%)	1 (1%)	75	89
7	b	107/107 (100%)	107 (100%)	0	100	100
8	J	76/83 (92%)	74 (97%)	2 (3%)	41	72
8	P	76/83 (92%)	75 (99%)	1 (1%)	65	85
9	D	20/151 (13%)	20 (100%)	0	100	100
9	G	20/151 (13%)	20 (100%)	0	100	100
10	I	163/163 (100%)	163 (100%)	0	100	100
10	O	163/163 (100%)	160 (98%)	3 (2%)	54	80
11	E	429/429 (100%)	426 (99%)	3 (1%)	81	91
11	F	429/429 (100%)	428 (100%)	1 (0%)	92	97
12	M	312/312 (100%)	312 (100%)	0	100	100
12	Y	312/312 (100%)	312 (100%)	0	100	100
All	All	4532/4834 (94%)	4514 (100%)	18 (0%)	88	95

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	X	169	LYS
11	F	523	HIS
8	J	64	ARG
10	O	126	ARG
4	X	20	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	R	104	ASN
11	E	325	HIS
10	I	116	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 [i](#)

Of 64 ligands modelled in this entry, 6 are monoatomic - leaving 58 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	HUU	E	603	-	39,43,43	2.12	10 (25%)	50,62,62	2.14	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	9Y0	S	301	-	48,48,48	1.18	3 (6%)	51,53,53	0.86	2 (3%)
17	CDL	T	202	-	75,75,99	0.34	0	81,87,111	0.42	0
18	9Y0	L	604	-	48,48,48	1.18	3 (6%)	51,53,53	0.81	2 (3%)
17	CDL	Z	202	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
13	9XX	D	301	-	31,31,41	1.10	4 (12%)	34,34,44	1.31	3 (8%)
13	9XX	W	201	-	41,41,41	0.98	4 (9%)	44,44,44	1.26	3 (6%)
14	PLM	G	302	9	9,10,17	0.55	0	8,9,17	0.43	0
21	9YF	E	609	-	58,58,58	1.00	4 (6%)	68,71,71	1.42	8 (11%)
21	9YF	Y	503	-	58,58,58	1.13	7 (12%)	68,71,71	1.49	9 (13%)
17	CDL	P	202	-	75,75,99	0.32	0	81,87,111	0.42	0
21	9YF	O	303	-	58,58,58	1.07	6 (10%)	68,71,71	1.07	4 (5%)
24	FES	M	501	12	0,4,4	-	-	-	-	-
21	9YF	M	503	-	58,58,58	1.12	5 (8%)	68,71,71	1.40	10 (14%)
22	HEM	E	602	11	42,50,50	1.48	4 (9%)	46,82,82	1.34	4 (8%)
14	PLM	D	302	9	9,10,17	0.53	0	8,9,17	0.43	0
13	9XX	c	202	1	41,41,41	0.95	4 (9%)	44,44,44	1.22	3 (6%)
16	HEA	L	603	3	58,67,67	1.54	9 (15%)	63,103,103	2.05	20 (31%)
16	HEA	R	603	3	58,67,67	1.52	9 (15%)	63,103,103	2.04	18 (28%)
22	HEM	F	602	11	42,50,50	1.49	4 (9%)	46,82,82	1.29	6 (13%)
17	CDL	F	606	-	75,75,99	0.36	0	81,87,111	0.61	2 (2%)
17	CDL	L	605	-	75,75,99	0.33	0	81,87,111	0.70	2 (2%)
19	MQ9	F	604	-	59,59,59	2.37	22 (37%)	73,75,75	1.51	19 (26%)
16	HEA	L	602	3	58,67,67	1.58	9 (15%)	63,103,103	2.32	24 (38%)
17	CDL	F	607	-	75,75,99	0.38	0	81,87,111	0.48	0
17	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.66	2 (2%)
22	HEM	F	601	11	41,49,50	1.22	2 (4%)	47,81,82	1.25	5 (10%)
23	HUU	F	603	-	39,43,43	2.11	10 (25%)	50,62,62	2.12	6 (12%)
14	PLM	W	202	1	15,16,17	0.49	0	14,15,17	0.33	0
21	9YF	I	303	-	58,58,58	1.06	6 (10%)	68,71,71	1.18	4 (5%)
17	CDL	J	201	-	75,75,99	0.31	0	81,87,111	0.42	0
19	MQ9	T	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.58	16 (21%)
20	HEC	O	301	10	32,50,50	2.11	3 (9%)	30,82,82	2.44	7 (23%)
18	9Y0	P	201	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
17	CDL	E	606	-	75,75,99	0.35	0	81,87,111	0.46	0
19	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.56	16 (21%)
20	HEC	I	301	10	32,50,50	2.10	3 (9%)	30,82,82	2.16	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CDL	X	303	-	75,75,99	0.33	0	81,87,111	0.69	2 (2%)
17	CDL	S	302	-	75,75,99	0.32	0	81,87,111	0.43	0
16	HEA	R	602	3	58,67,67	1.58	9 (15%)	63,103,103	2.25	23 (36%)
21	9YF	F	609	-	58,58,58	1.00	5 (8%)	68,71,71	1.47	8 (11%)
14	PLM	c	201	1	15,16,17	0.45	0	14,15,17	0.34	0
17	CDL	E	608	-	75,75,99	0.36	0	81,87,111	0.45	0
19	MQ9	E	605	-	59,59,59	2.39	22 (37%)	73,75,75	1.53	17 (23%)
20	HEC	I	302	10	32,50,50	2.12	3 (9%)	30,82,82	2.32	5 (16%)
19	MQ9	E	604	-	59,59,59	2.37	22 (37%)	73,75,75	1.50	19 (26%)
13	9XX	G	301	-	31,31,41	1.08	4 (12%)	34,34,44	1.44	3 (8%)
21	9YF	Y	502	-	58,58,58	1.09	6 (10%)	68,71,71	1.35	8 (11%)
17	CDL	E	607	-	75,75,99	0.38	0	81,87,111	0.55	1 (1%)
18	9Y0	X	301	-	48,48,48	1.18	3 (6%)	51,53,53	0.87	2 (3%)
20	HEC	O	302	10	32,50,50	2.11	3 (9%)	30,82,82	2.29	5 (16%)
17	CDL	X	302	-	75,75,99	0.30	0	81,87,111	0.36	0
22	HEM	E	601	11	41,49,50	1.22	2 (4%)	47,81,82	1.31	5 (10%)
17	CDL	S	303	-	75,75,99	0.34	0	81,87,111	0.51	0
17	CDL	F	608	-	75,75,99	0.38	0	81,87,111	0.42	0
21	9YF	M	502	-	58,58,58	1.09	6 (10%)	68,71,71	1.31	7 (10%)
24	FES	Y	501	12	0,4,4	-	-	-	-	-
19	MQ9	F	605	-	59,59,59	2.39	23 (38%)	73,75,75	1.50	18 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	HUU	E	603	-	-	6/20/34/34	0/5/5/5
18	9Y0	S	301	-	-	20/52/52/52	-
17	CDL	T	202	-	-	41/86/86/110	-
18	9Y0	L	604	-	-	24/52/52/52	-
17	CDL	Z	202	-	-	38/86/86/110	-
13	9XX	D	301	-	-	13/33/33/43	-
13	9XX	W	201	-	-	16/43/43/43	-
14	PLM	G	302	9	-	2/8/8/15	-
21	9YF	E	609	-	-	19/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	9YF	Y	503	-	-	26/54/78/78	0/1/1/1
17	CDL	P	202	-	-	46/86/86/110	-
21	9YF	O	303	-	-	30/54/78/78	0/1/1/1
24	FES	M	501	12	-	-	0/1/1/1
21	9YF	M	503	-	-	24/54/78/78	0/1/1/1
22	HEM	E	602	11	-	3/12/54/54	-
14	PLM	D	302	9	-	3/8/8/15	-
13	9XX	c	202	1	-	13/43/43/43	-
16	HEA	L	603	3	-	3/32/76/76	-
16	HEA	R	603	3	-	4/32/76/76	-
22	HEM	F	602	11	-	4/12/54/54	-
17	CDL	F	606	-	-	51/86/86/110	-
17	CDL	L	605	-	-	48/86/86/110	-
19	MQ9	F	604	-	-	9/53/73/73	0/2/2/2
16	HEA	L	602	3	-	9/32/76/76	-
17	CDL	F	607	-	-	40/86/86/110	-
17	CDL	R	604	-	-	39/86/86/110	-
22	HEM	F	601	11	-	2/12/52/54	-
23	HUU	F	603	-	-	2/20/34/34	0/5/5/5
14	PLM	W	202	1	-	4/14/14/15	-
21	9YF	I	303	-	-	25/54/78/78	0/1/1/1
17	CDL	J	201	-	-	55/86/86/110	-
19	MQ9	T	201	-	-	11/53/73/73	0/2/2/2
20	HEC	O	301	10	-	3/10/54/54	-
18	9Y0	P	201	-	-	24/52/52/52	-
17	CDL	E	606	-	-	51/86/86/110	-
19	MQ9	Z	201	-	-	14/53/73/73	0/2/2/2
20	HEC	I	301	10	-	1/10/54/54	-
17	CDL	X	303	-	-	44/86/86/110	-
17	CDL	S	302	-	-	52/86/86/110	-
16	HEA	R	602	3	-	8/32/76/76	-
21	9YF	F	609	-	-	22/54/78/78	0/1/1/1
14	PLM	c	201	1	-	3/14/14/15	-
17	CDL	E	608	-	-	45/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MQ9	E	605	-	-	11/53/73/73	0/2/2/2
20	HEC	I	302	10	-	0/10/54/54	-
19	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
13	9XX	G	301	-	-	11/33/33/43	-
21	9YF	Y	502	-	-	23/54/78/78	0/1/1/1
17	CDL	E	607	-	-	47/86/86/110	-
18	9Y0	X	301	-	-	18/52/52/52	-
20	HEC	O	302	10	-	0/10/54/54	-
17	CDL	X	302	-	-	52/86/86/110	-
22	HEM	E	601	11	-	3/12/52/54	-
17	CDL	S	303	-	-	47/86/86/110	-
17	CDL	F	608	-	-	37/86/86/110	-
21	9YF	M	502	-	-	23/54/78/78	0/1/1/1
24	FES	Y	501	12	-	-	0/1/1/1
19	MQ9	F	605	-	-	8/53/73/73	0/2/2/2

The worst 5 of 293 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	605	MQ9	C6-C5	8.56	1.50	1.35
19	E	604	MQ9	C6-C5	8.53	1.50	1.35
19	E	605	MQ9	C6-C5	8.50	1.50	1.35
19	F	604	MQ9	C6-C5	8.43	1.50	1.35
19	Z	201	MQ9	C6-C5	8.37	1.50	1.35

The worst 5 of 340 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	E	603	HUU	C22-C23-C24	-10.69	87.34	112.67
23	F	603	HUU	C22-C23-C24	-10.13	88.69	112.67
17	Z	202	CDL	CB6-CB4-CB3	-9.90	88.70	111.78
17	Z	202	CDL	OB6-CB4-CB3	-8.35	78.39	108.34
23	E	603	HUU	C35-C23-C24	8.29	132.31	112.67

There are no chirality outliers.

5 of 1188 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	301	9XX	O2-C18-O1-C17

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Mol	Chain	Res	Type	Atoms
13	c	202	9XX	O-C16-C17-O1
13	c	202	9XX	C37-C17-O1-C18
13	c	202	9XX	C19-C18-O1-C17
16	R	602	HEA	C2D-C3D-CAD-CBD

There are no ring outliers.

40 monomers are involved in 296 short contacts:

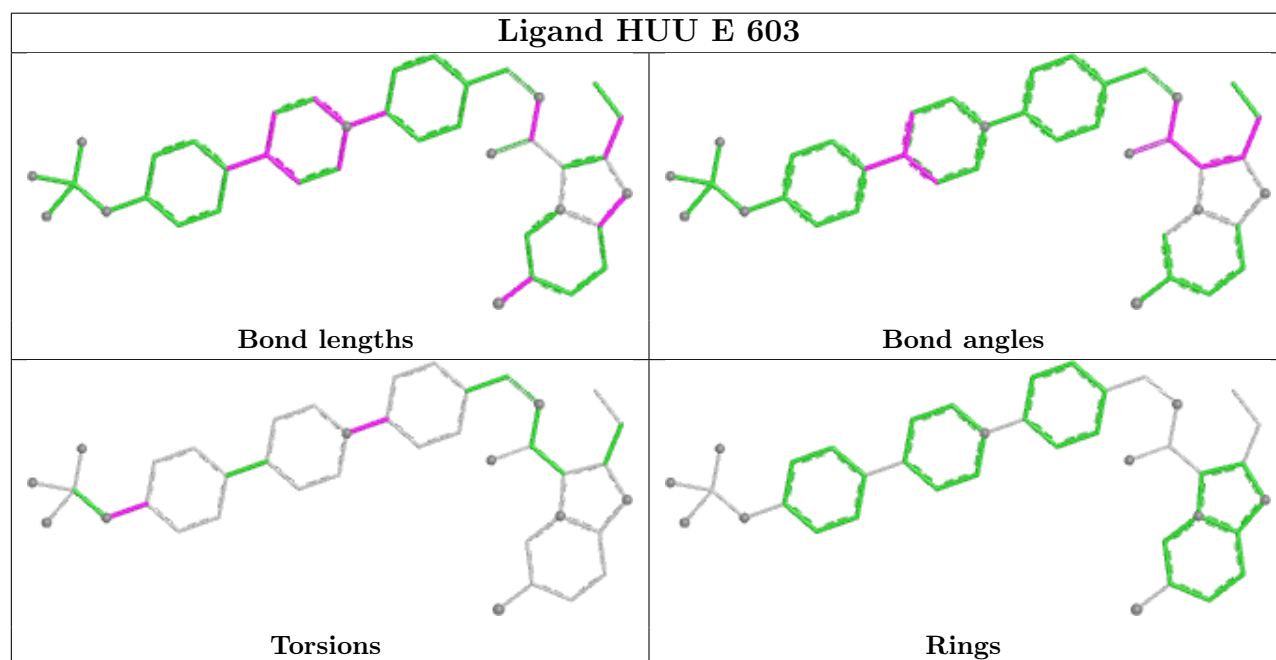
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	202	CDL	21	0
17	Z	202	CDL	26	0
13	W	201	9XX	1	0
17	P	202	CDL	8	0
24	M	501	FES	1	0
22	E	602	HEM	9	0
14	D	302	PLM	1	0
16	L	603	HEA	7	0
16	R	603	HEA	6	0
22	F	602	HEM	3	0
17	F	606	CDL	7	0
17	L	605	CDL	14	0
19	F	604	MQ9	2	0
16	L	602	HEA	6	0
17	F	607	CDL	10	0
17	R	604	CDL	10	0
22	F	601	HEM	6	0
21	I	303	9YF	1	0
17	J	201	CDL	11	0
19	T	201	MQ9	5	0
20	O	301	HEC	12	0
17	E	606	CDL	6	0
19	Z	201	MQ9	3	0
20	I	301	HEC	6	0
17	X	303	CDL	8	0
17	S	302	CDL	18	0
16	R	602	HEA	6	0
17	E	608	CDL	7	0
19	E	605	MQ9	6	0
20	I	302	HEC	7	0
19	E	604	MQ9	5	0
17	E	607	CDL	4	0
18	X	301	9Y0	1	0

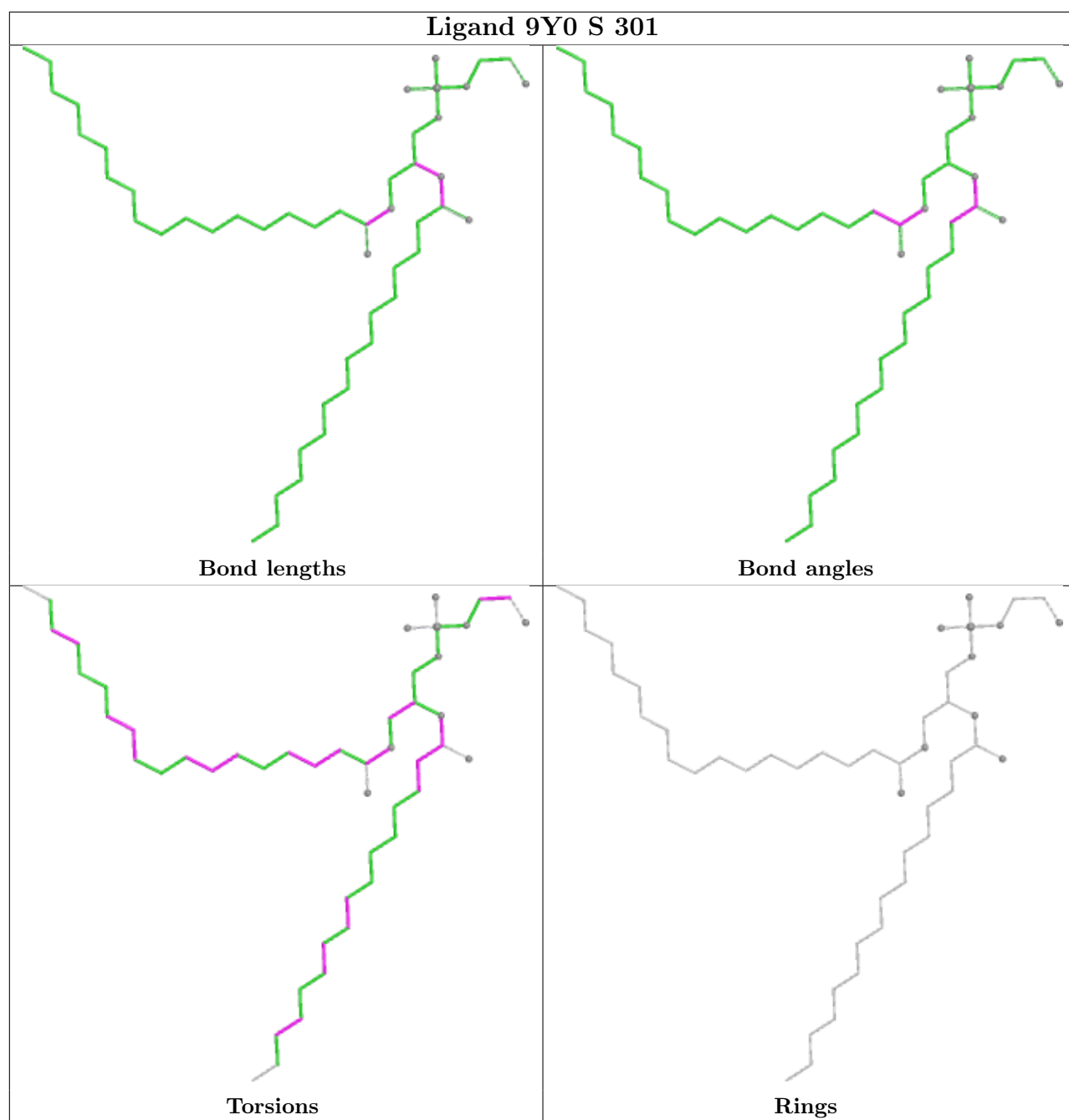
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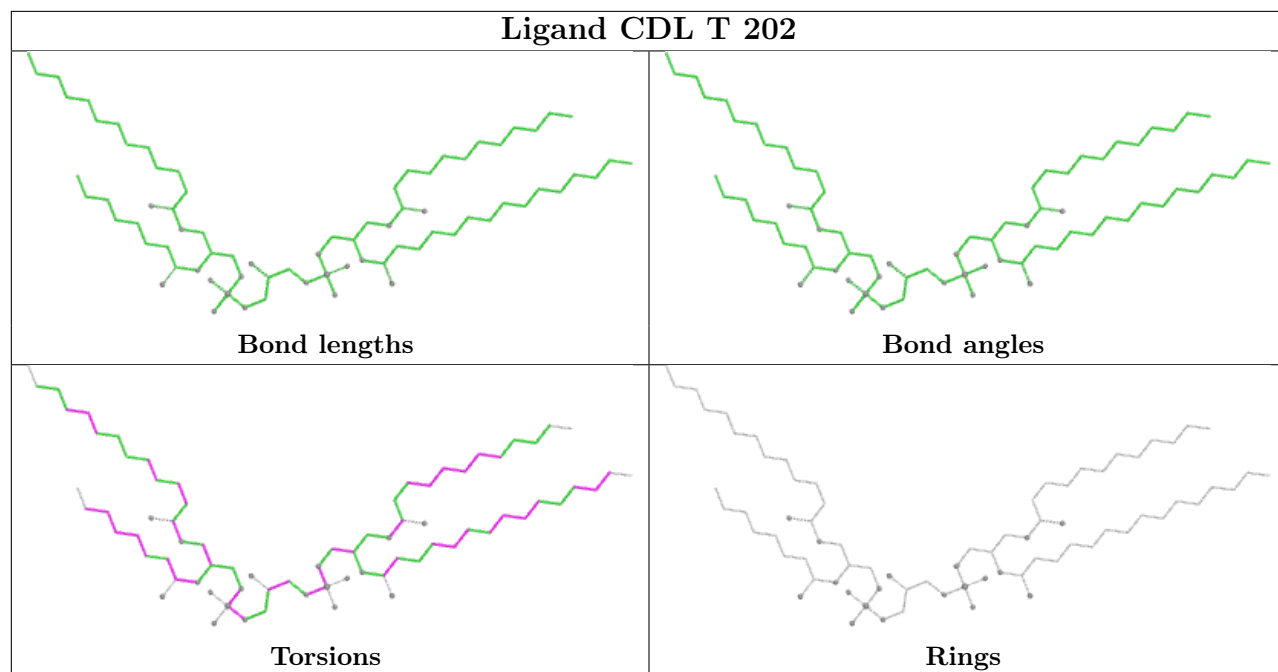
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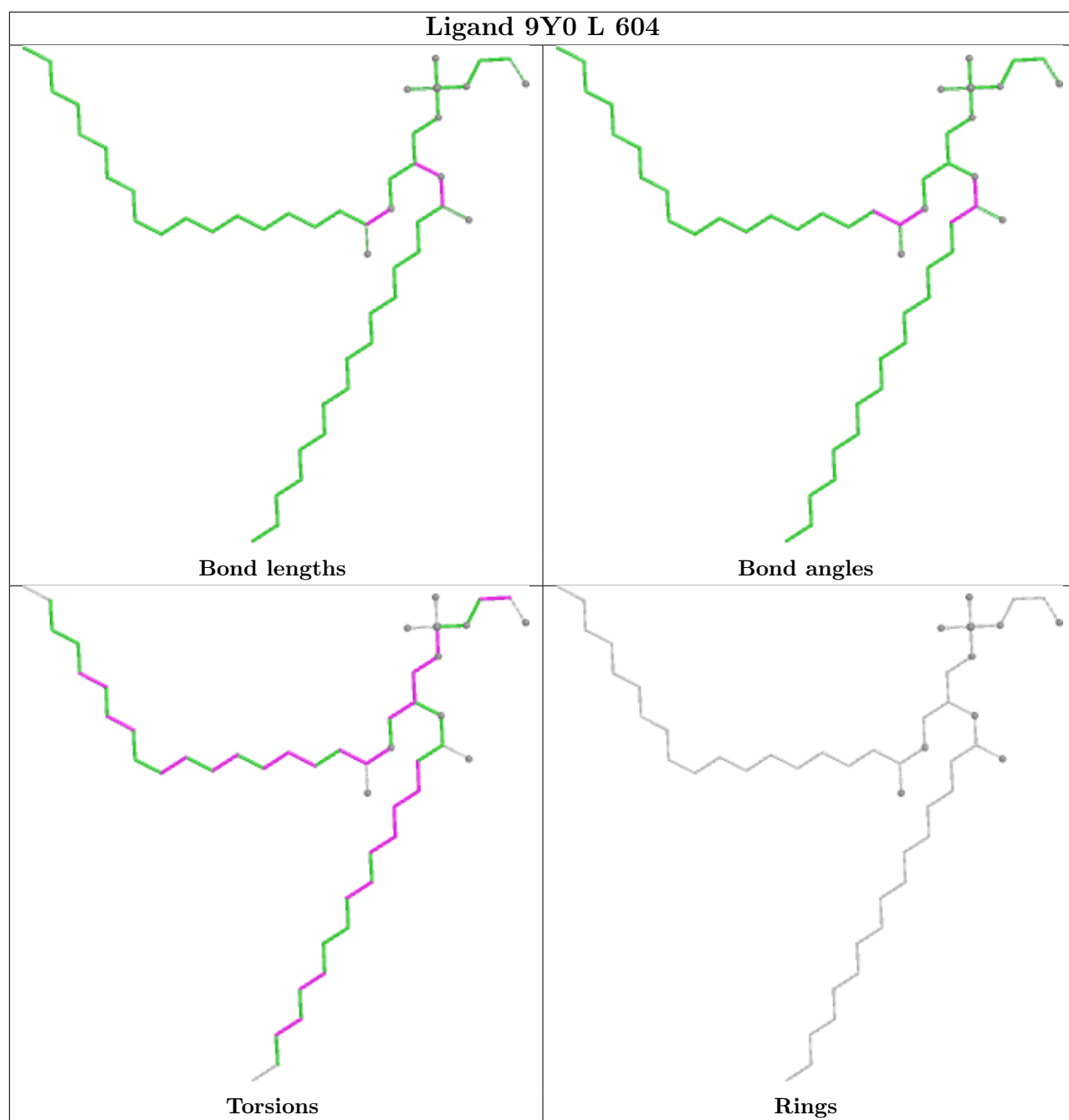
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	O	302	HEC	9	0
17	X	302	CDL	26	0
22	E	601	HEM	5	0
17	S	303	CDL	16	0
17	F	608	CDL	9	0
24	Y	501	FES	3	0
19	F	605	MQ9	11	0

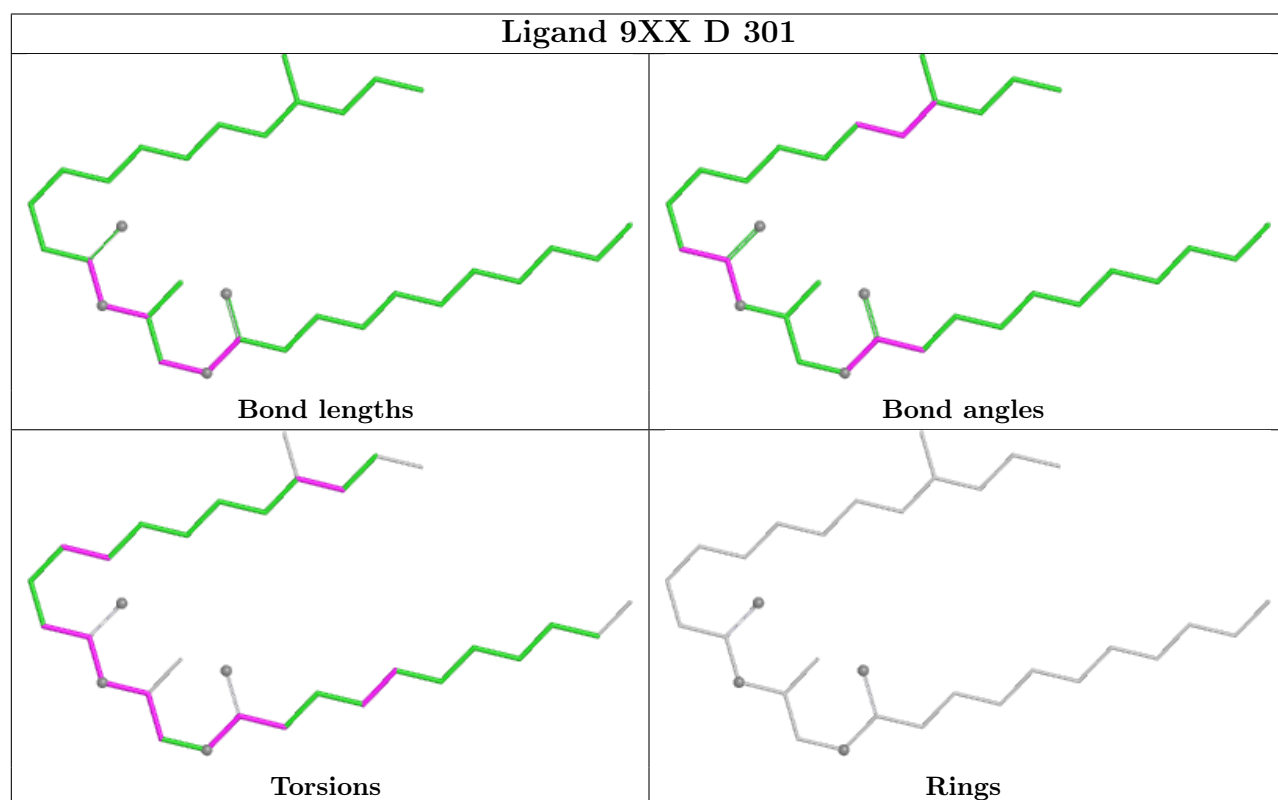
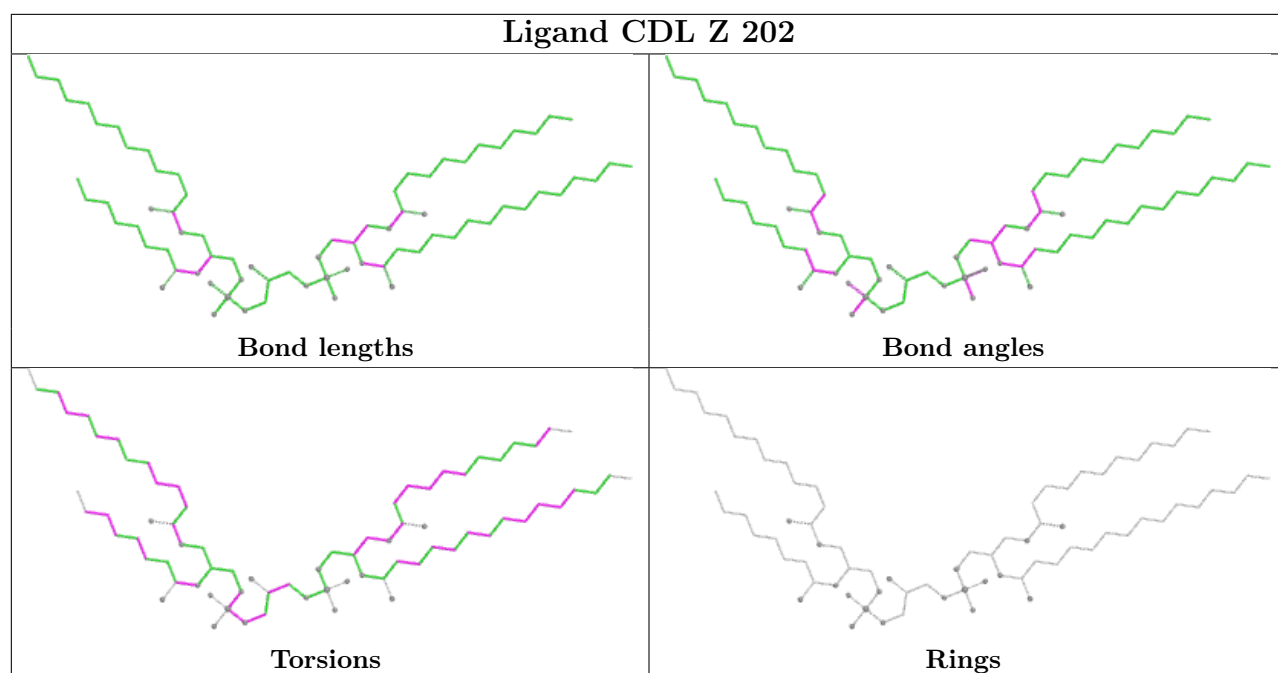
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

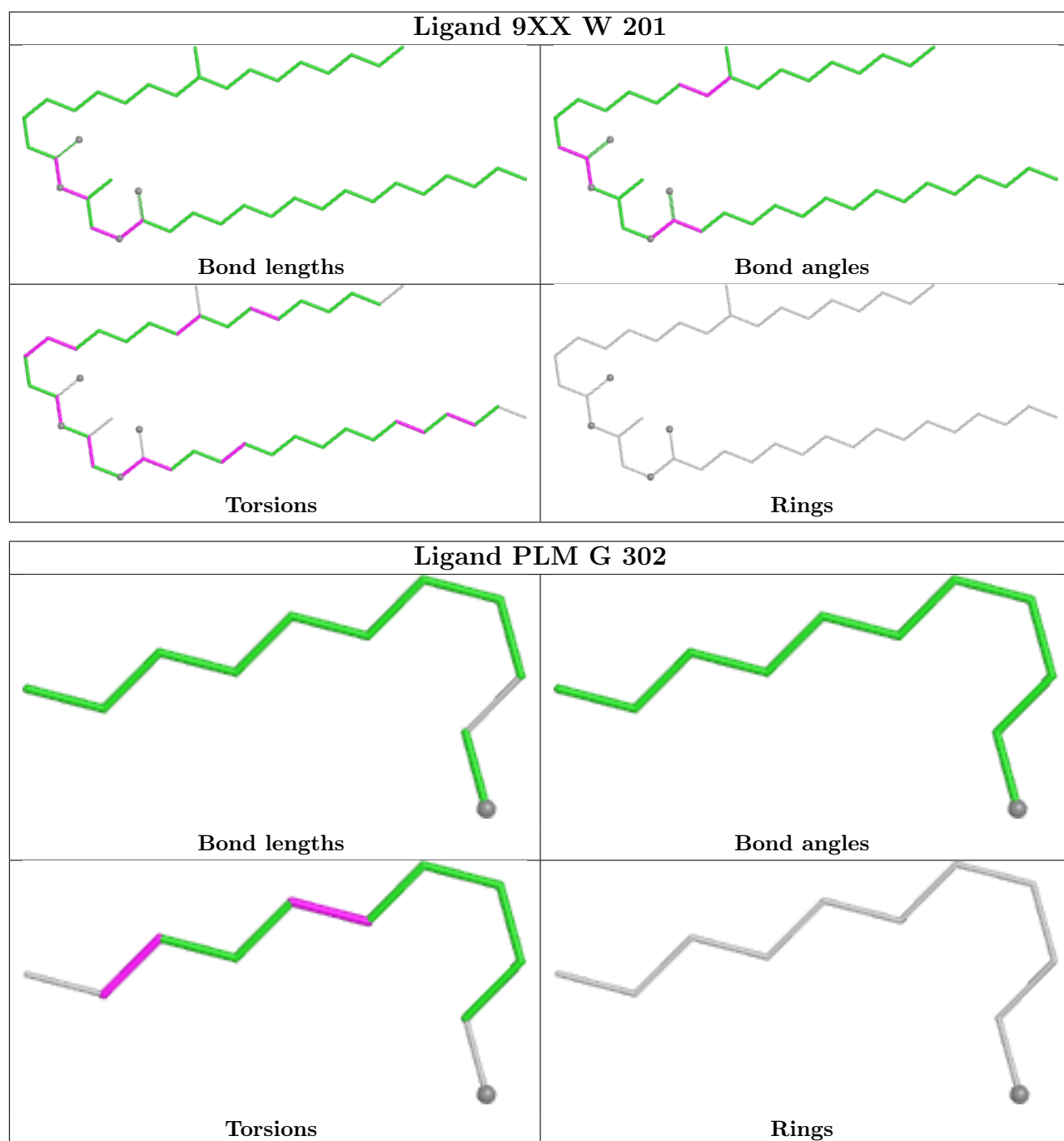


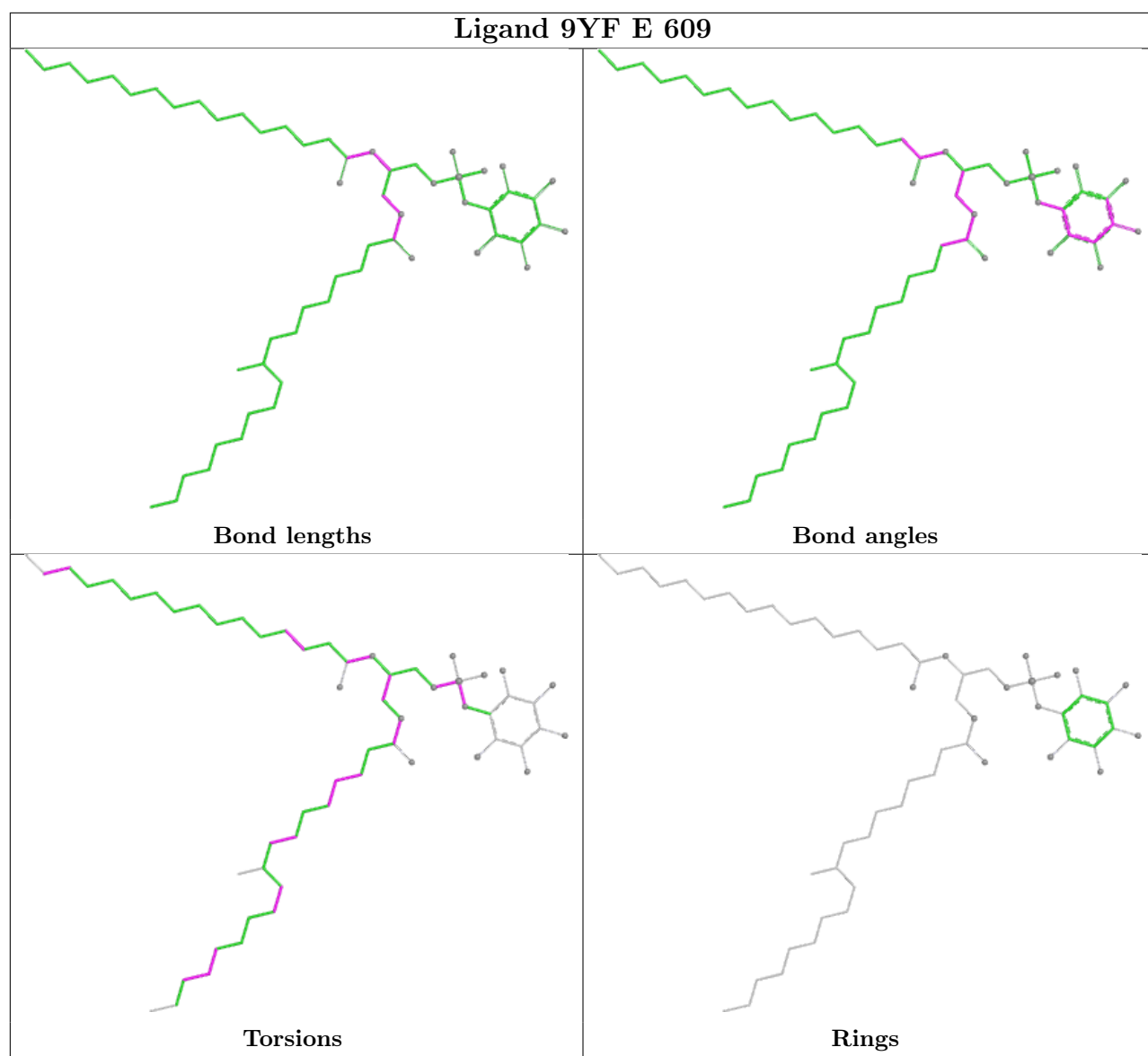


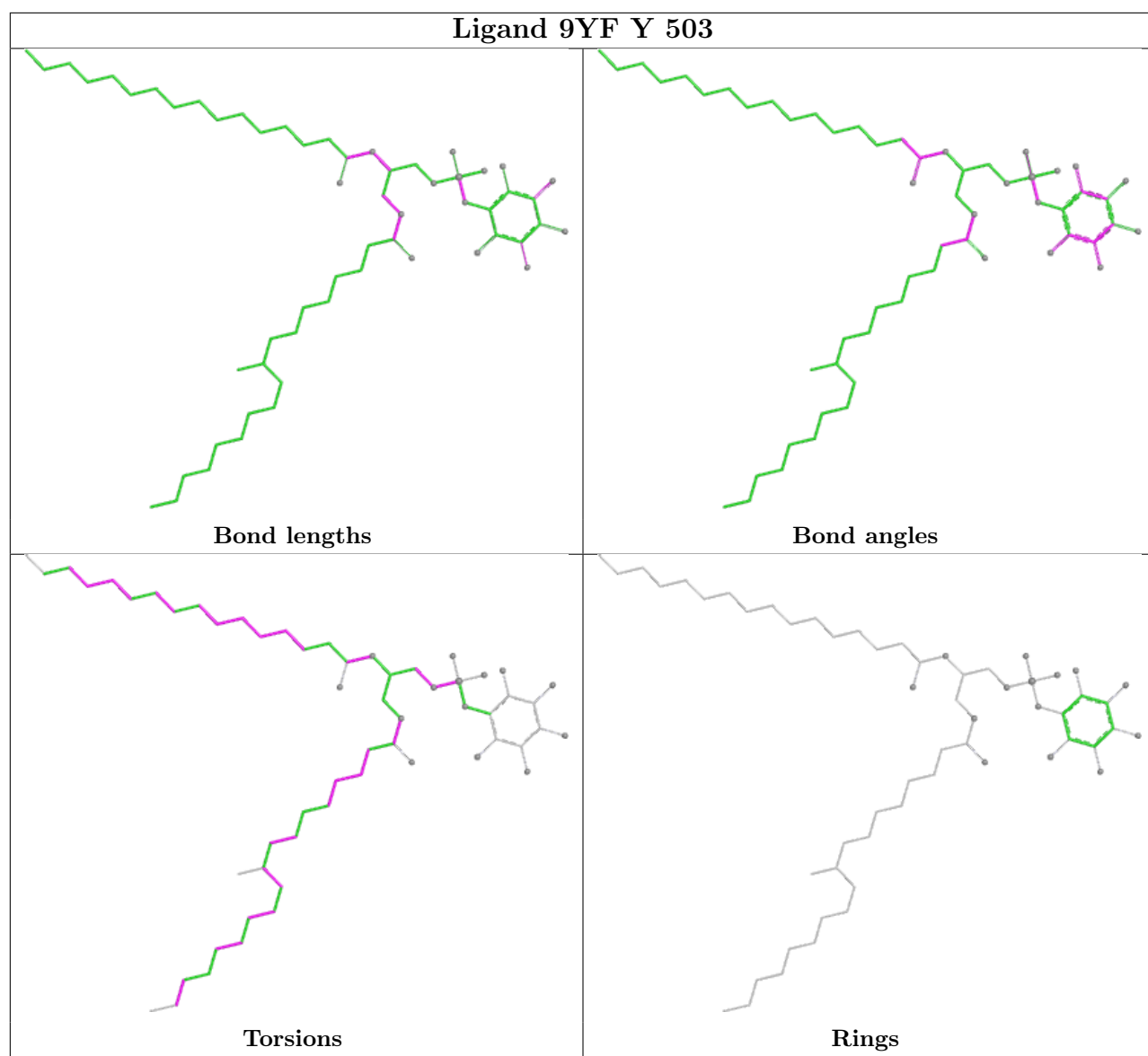


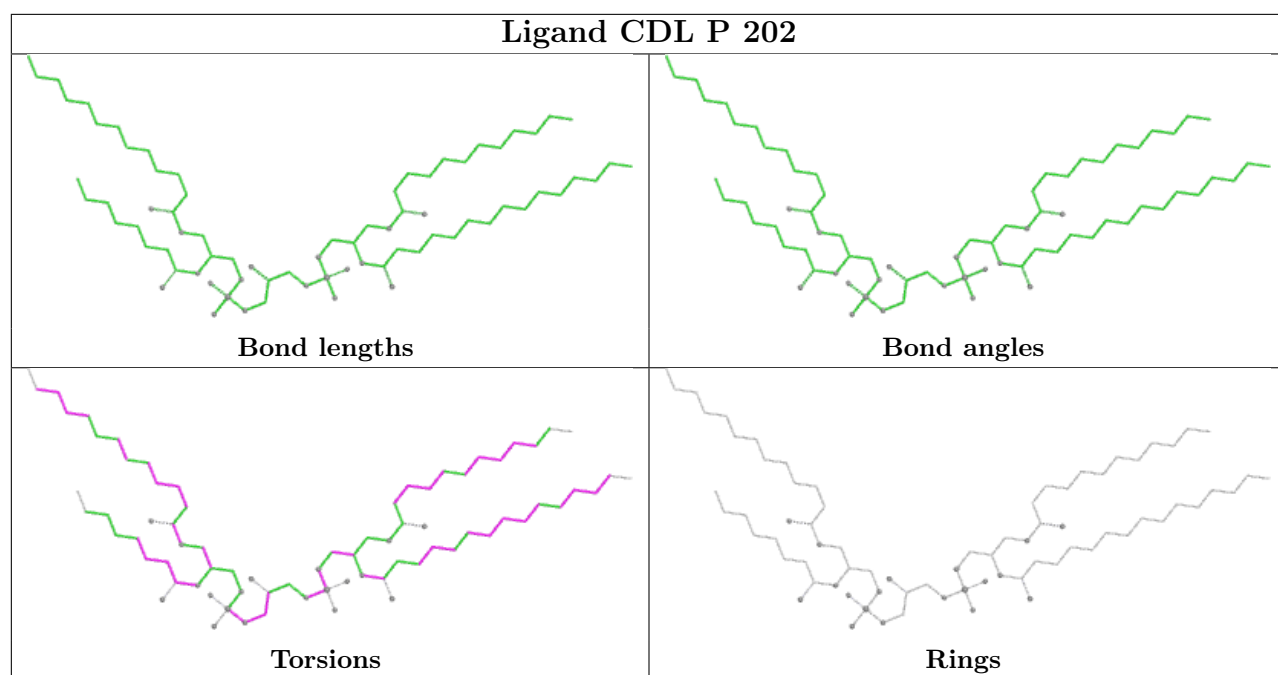


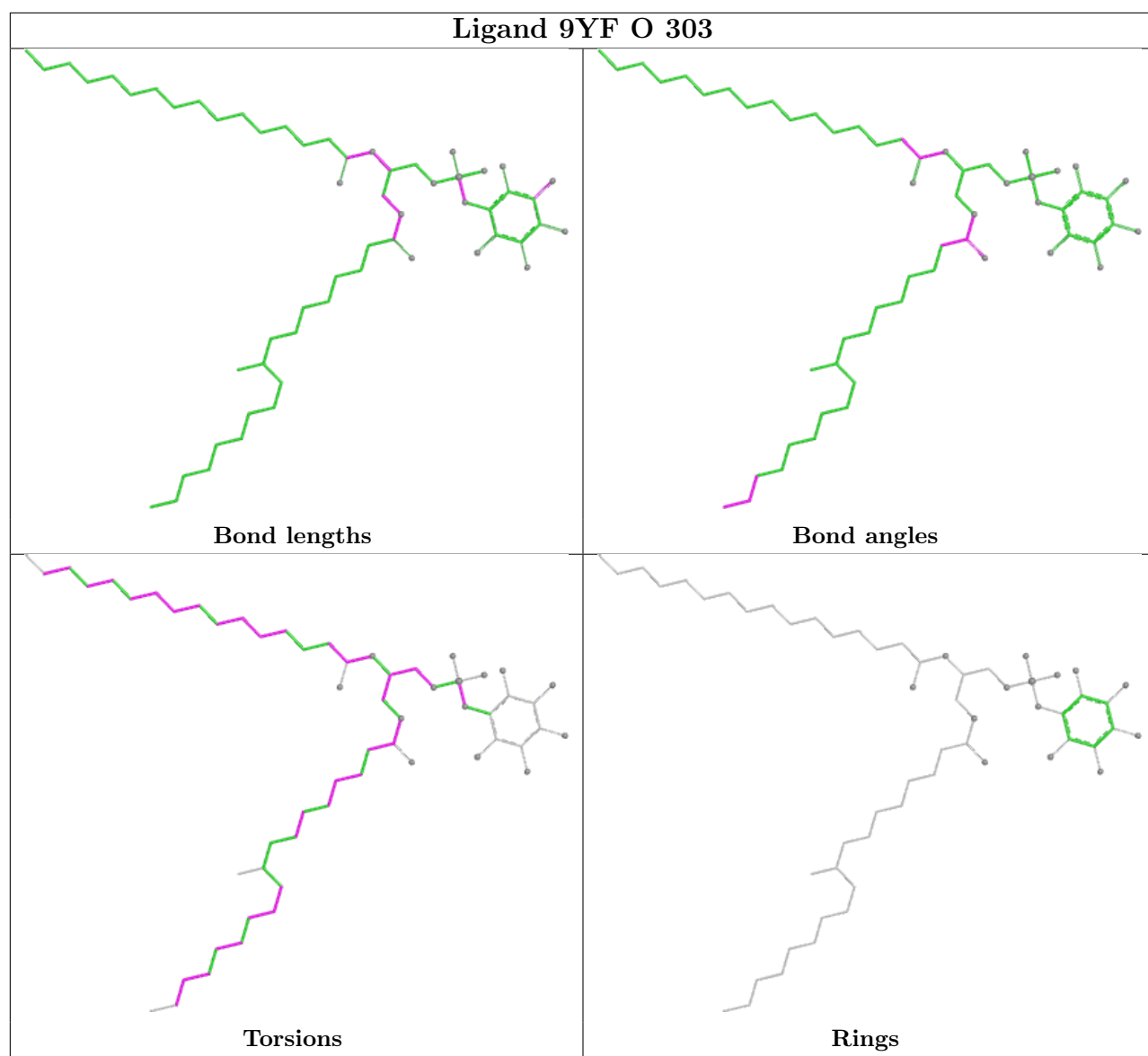


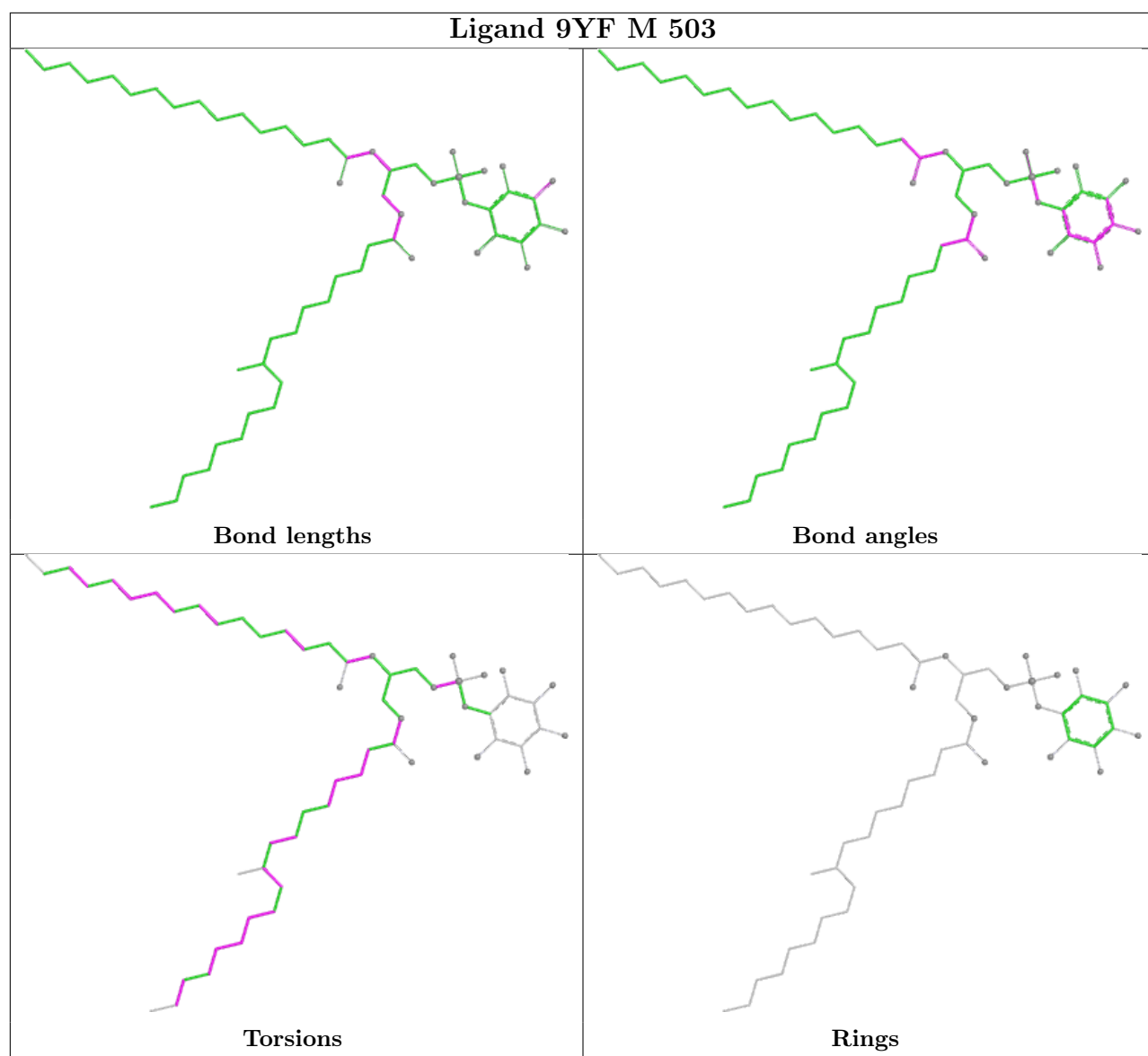


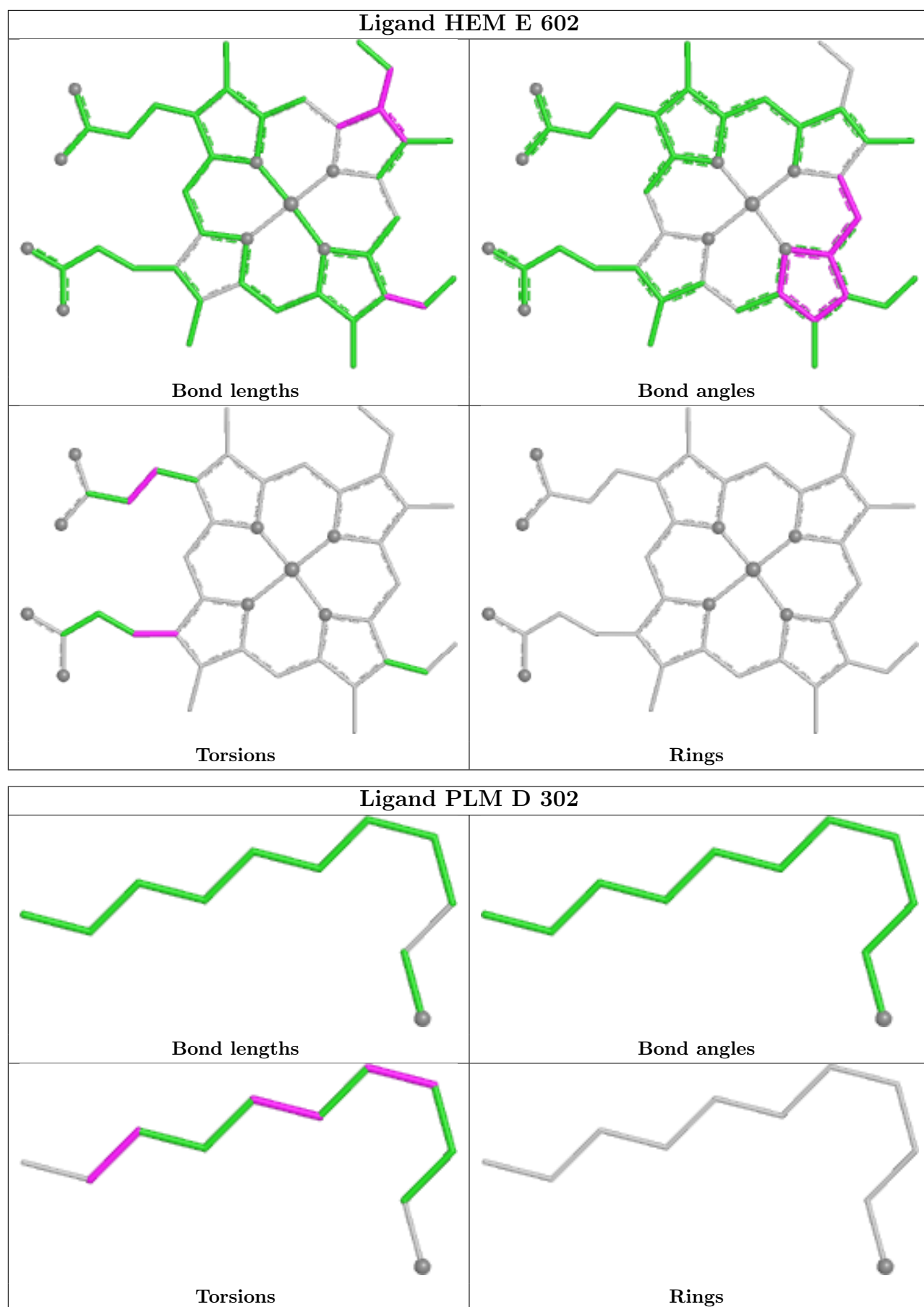


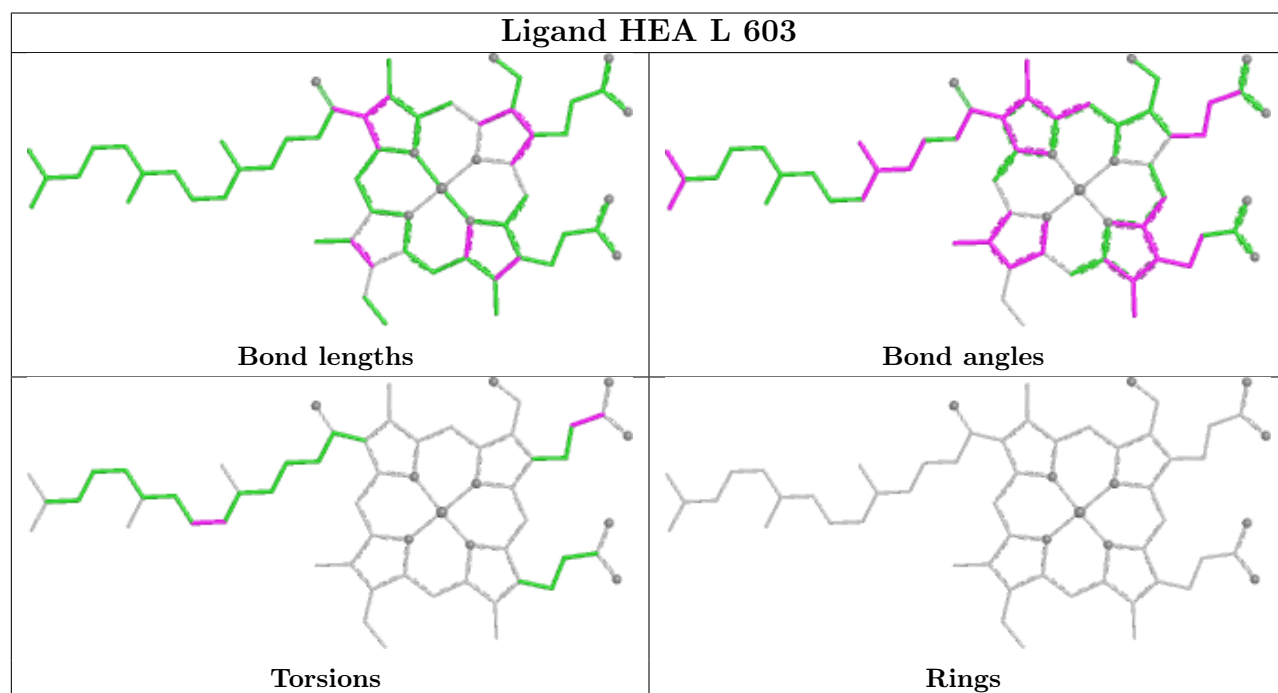
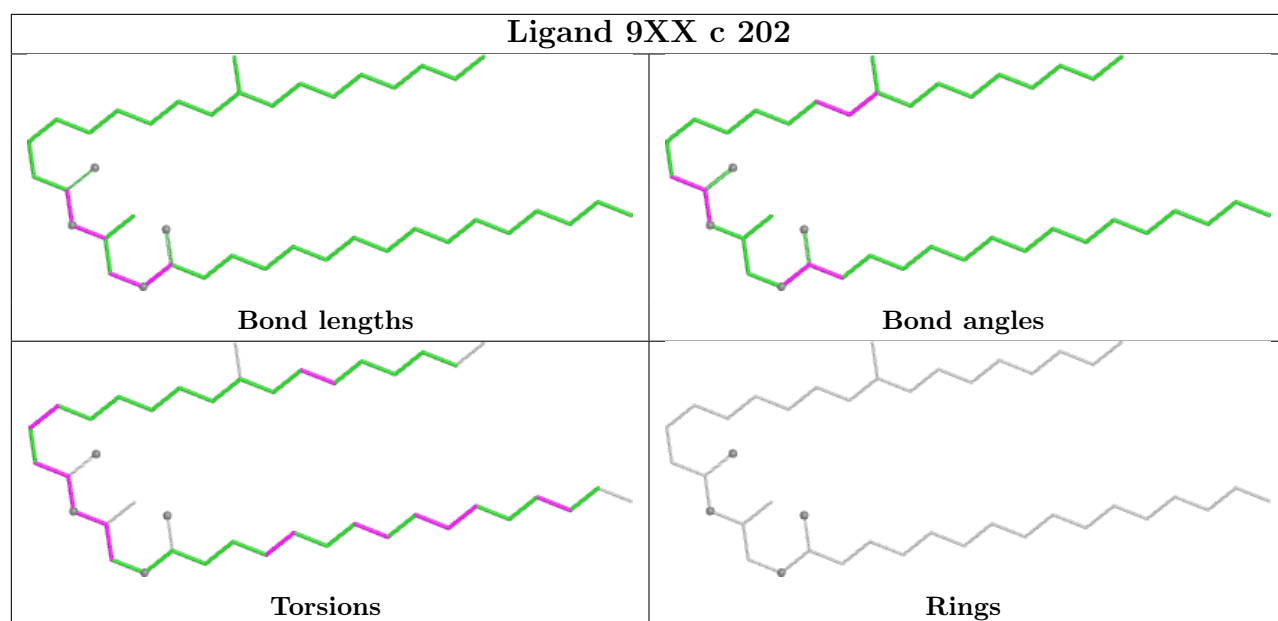


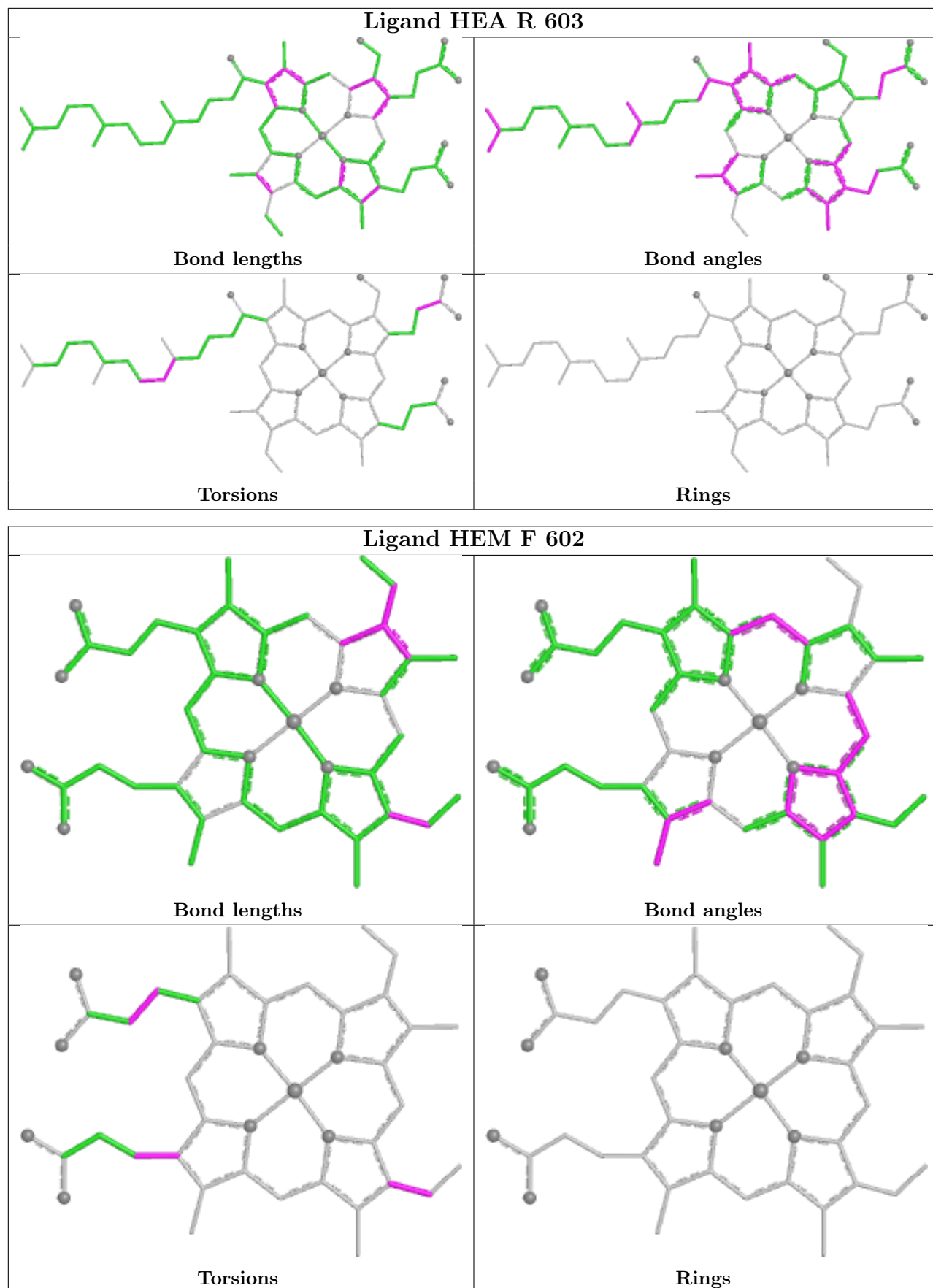


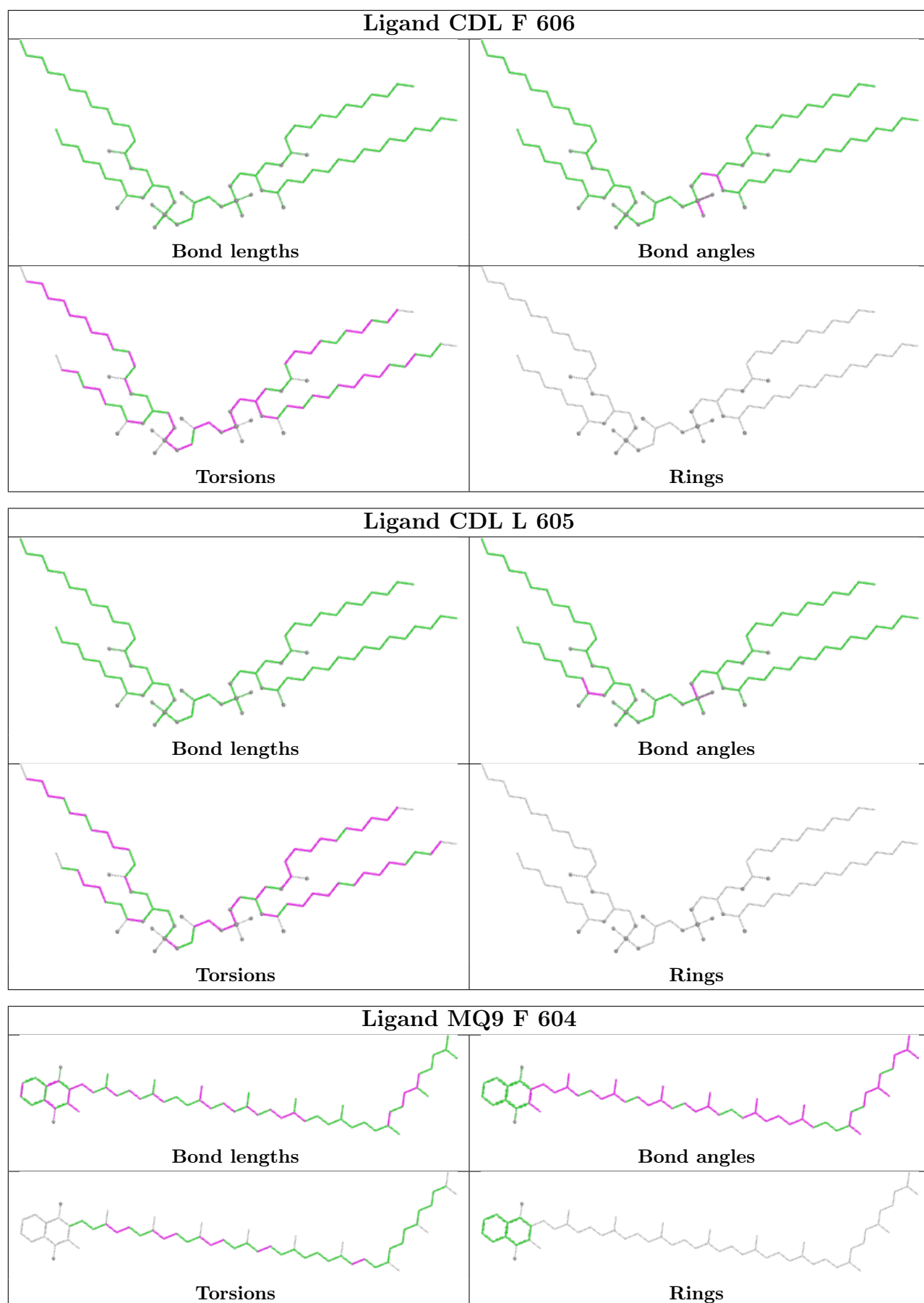


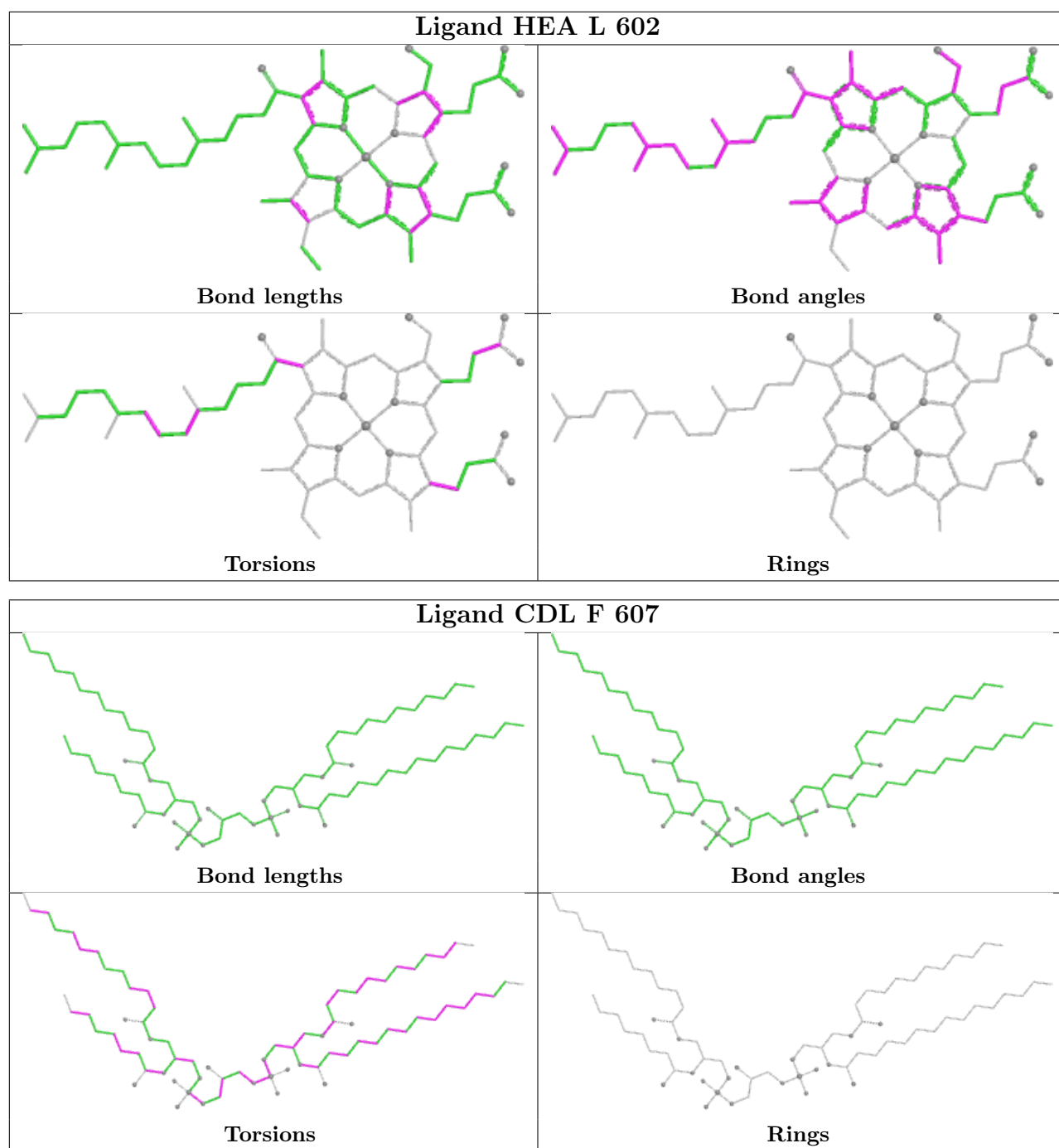


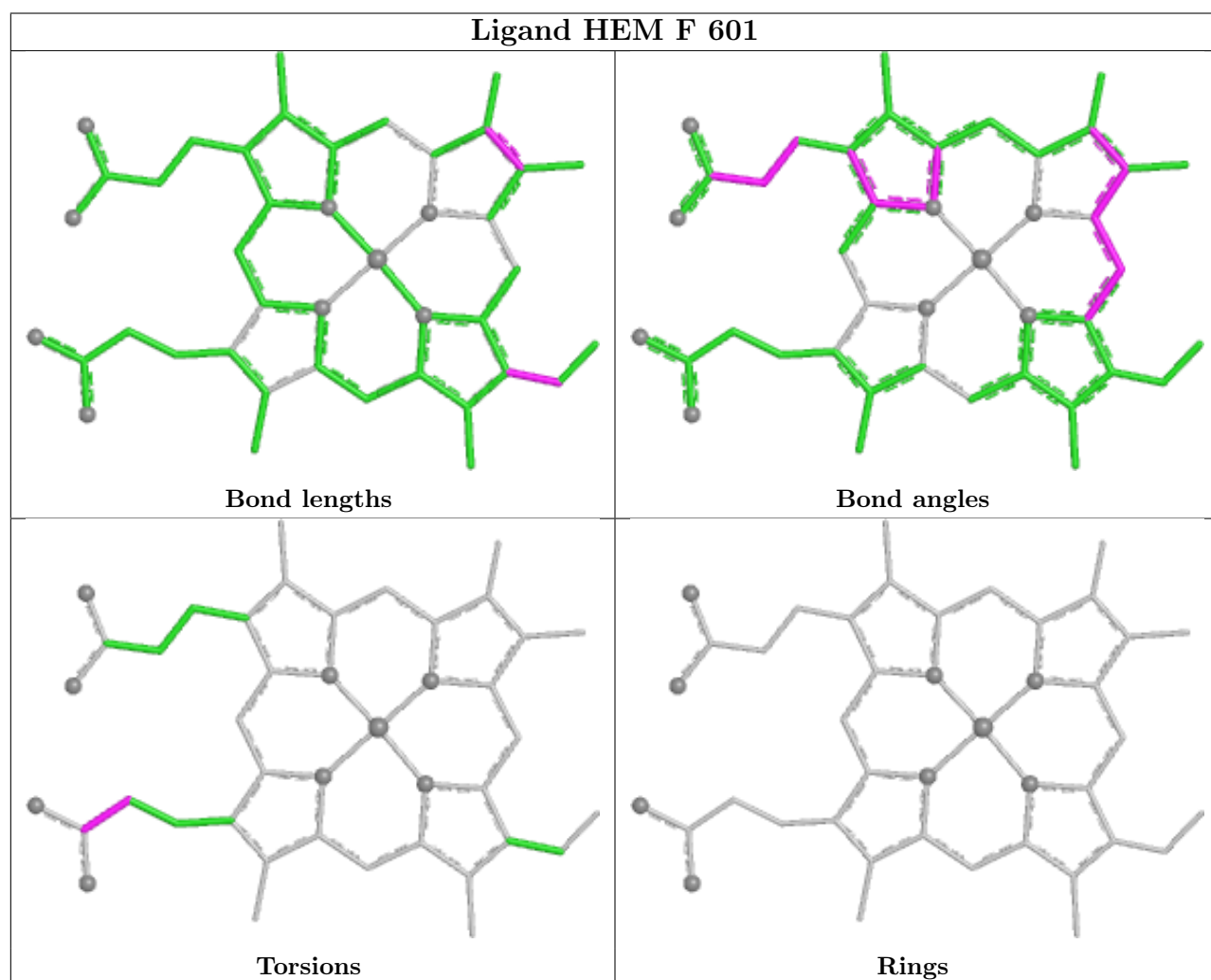
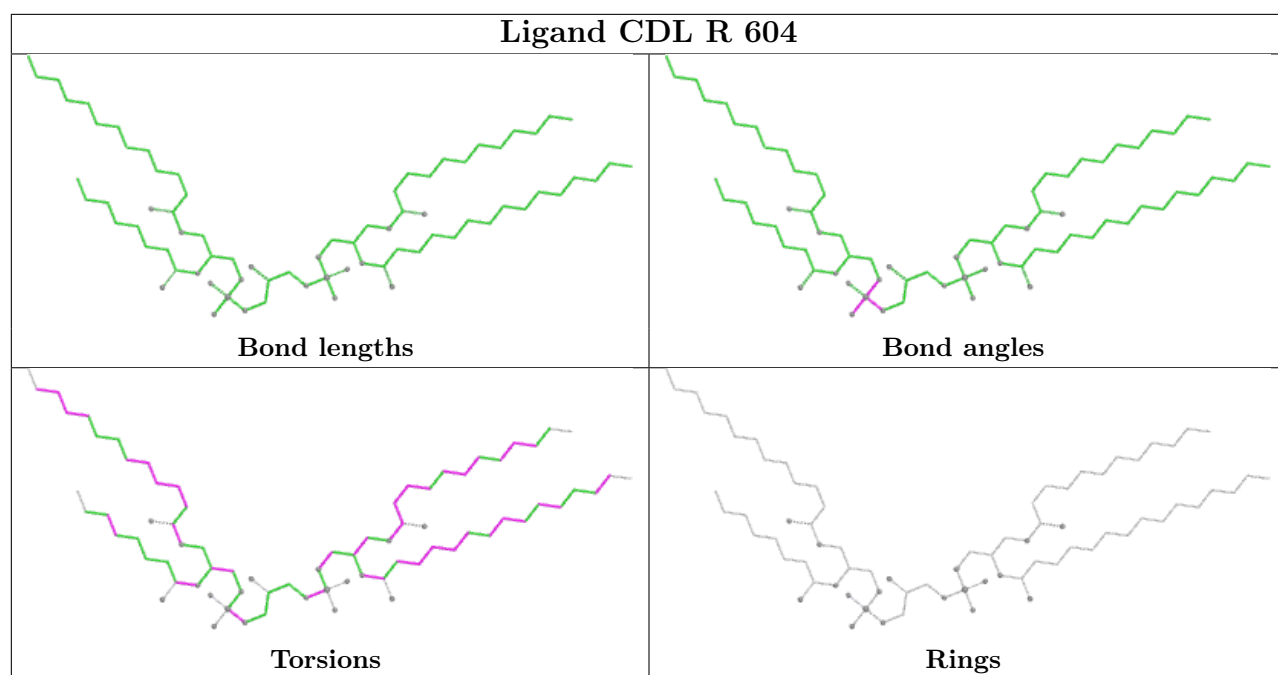


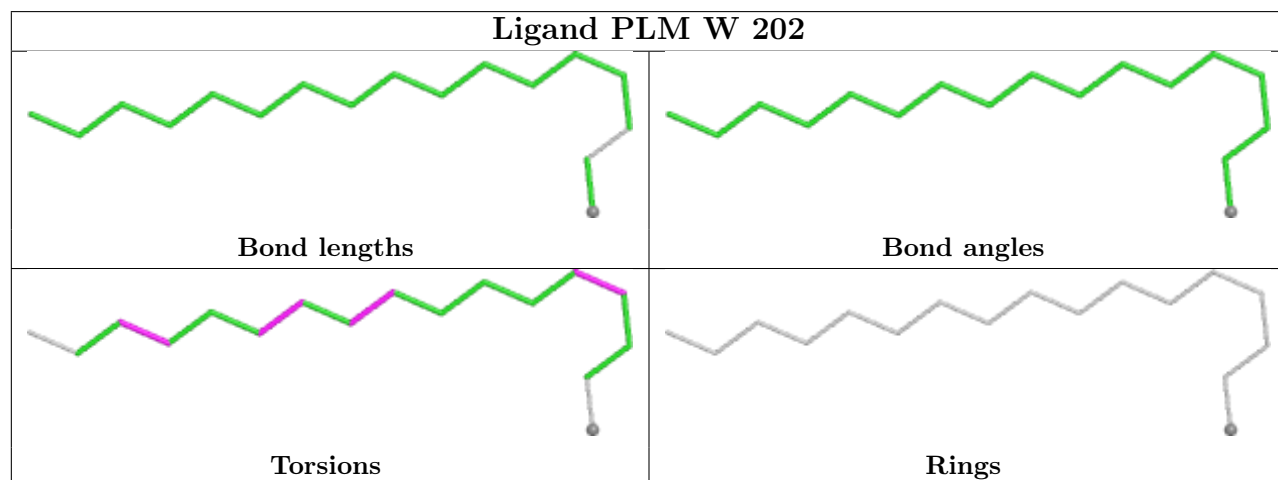
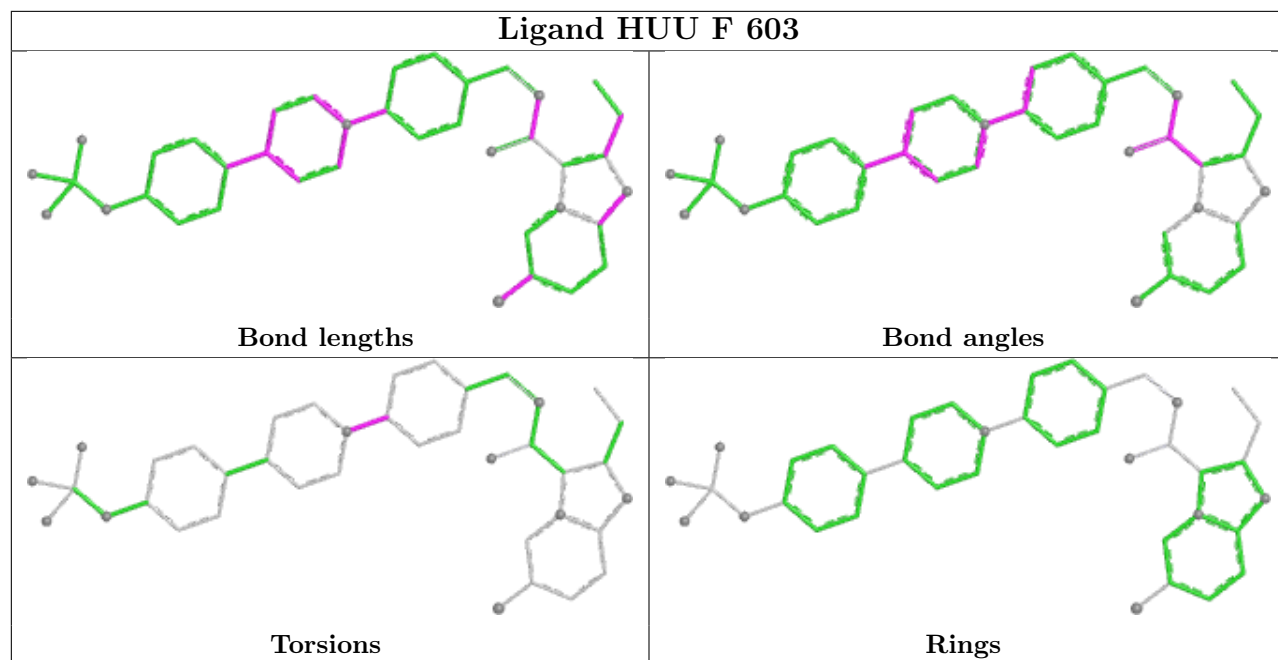


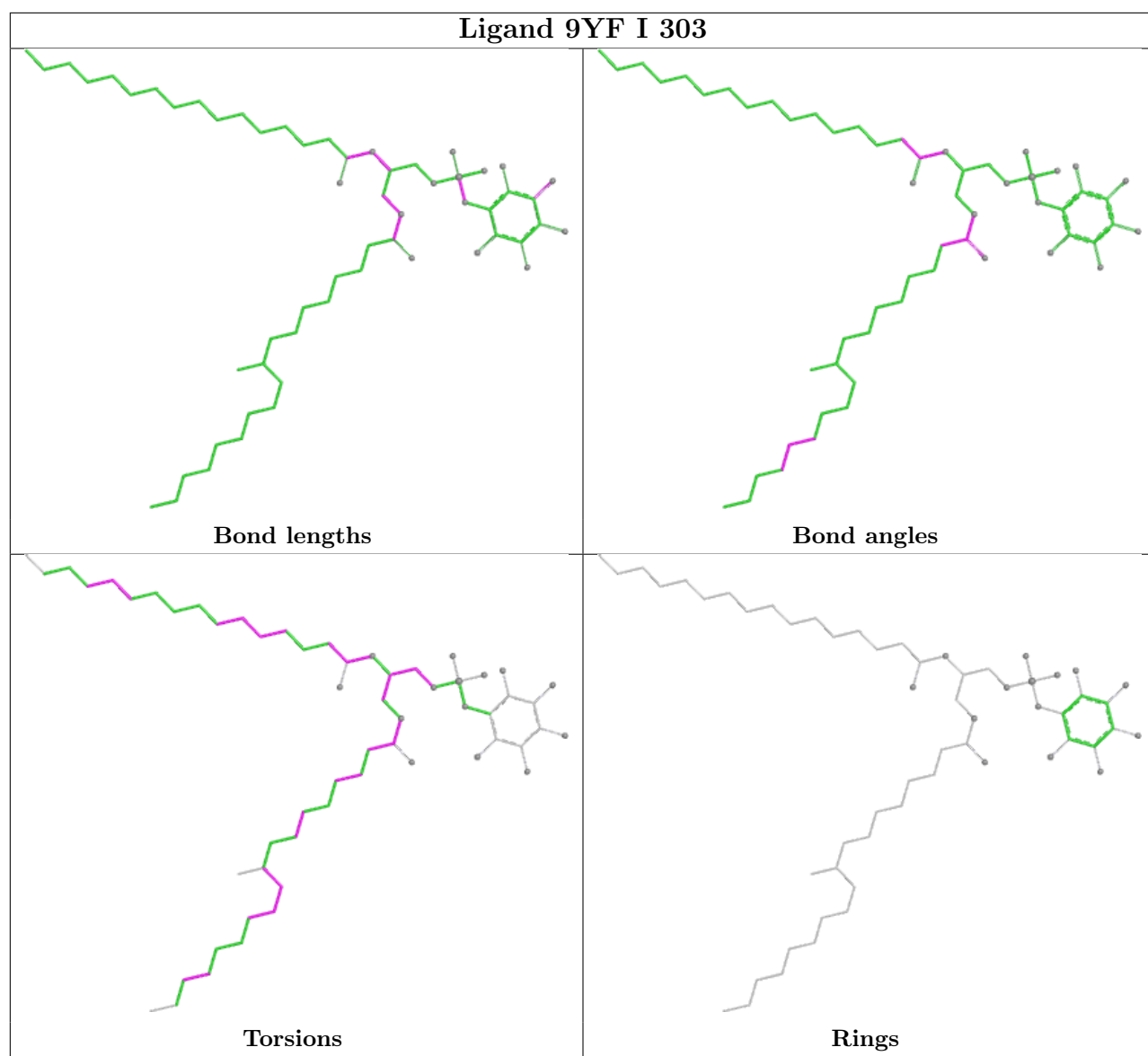


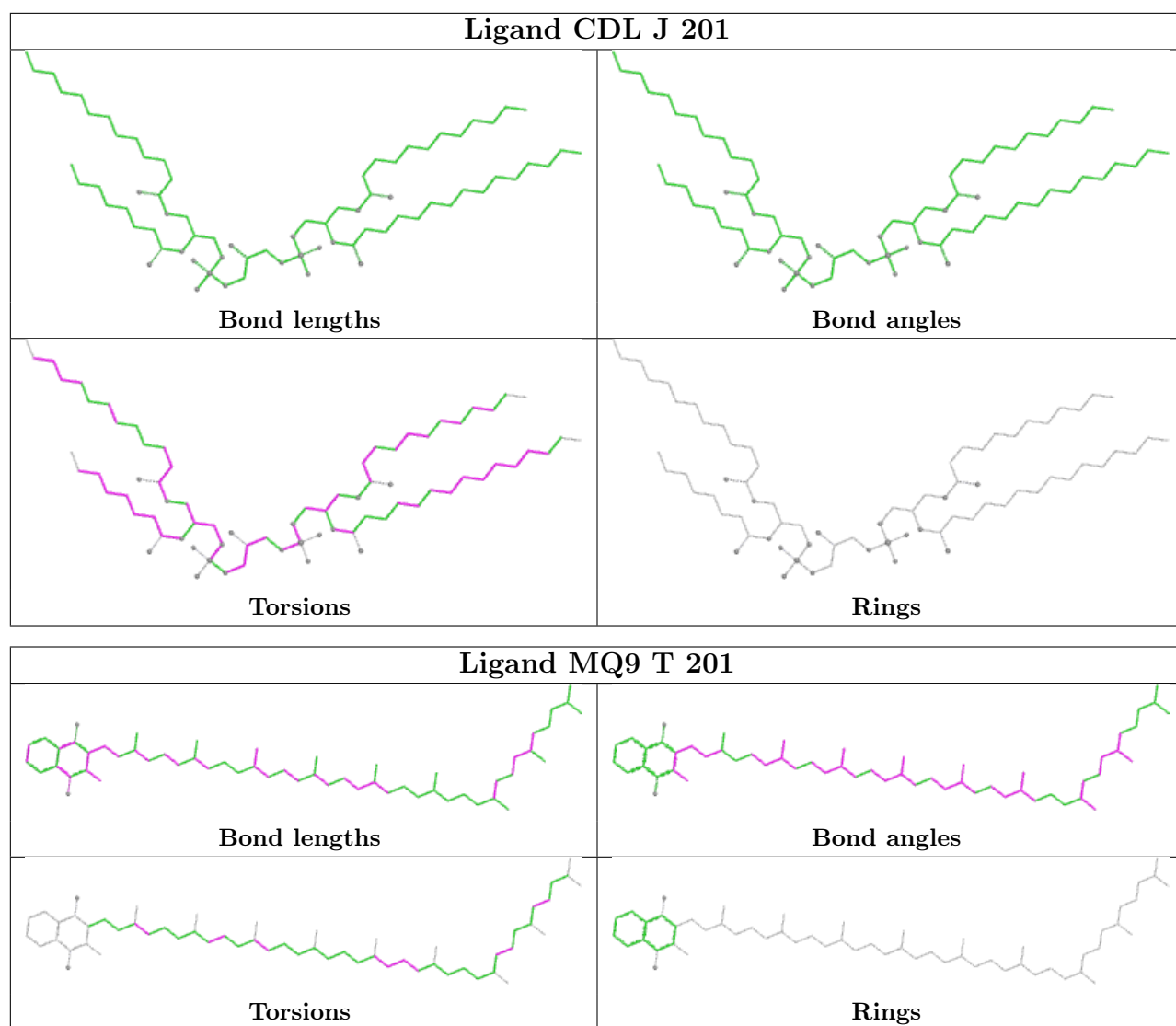


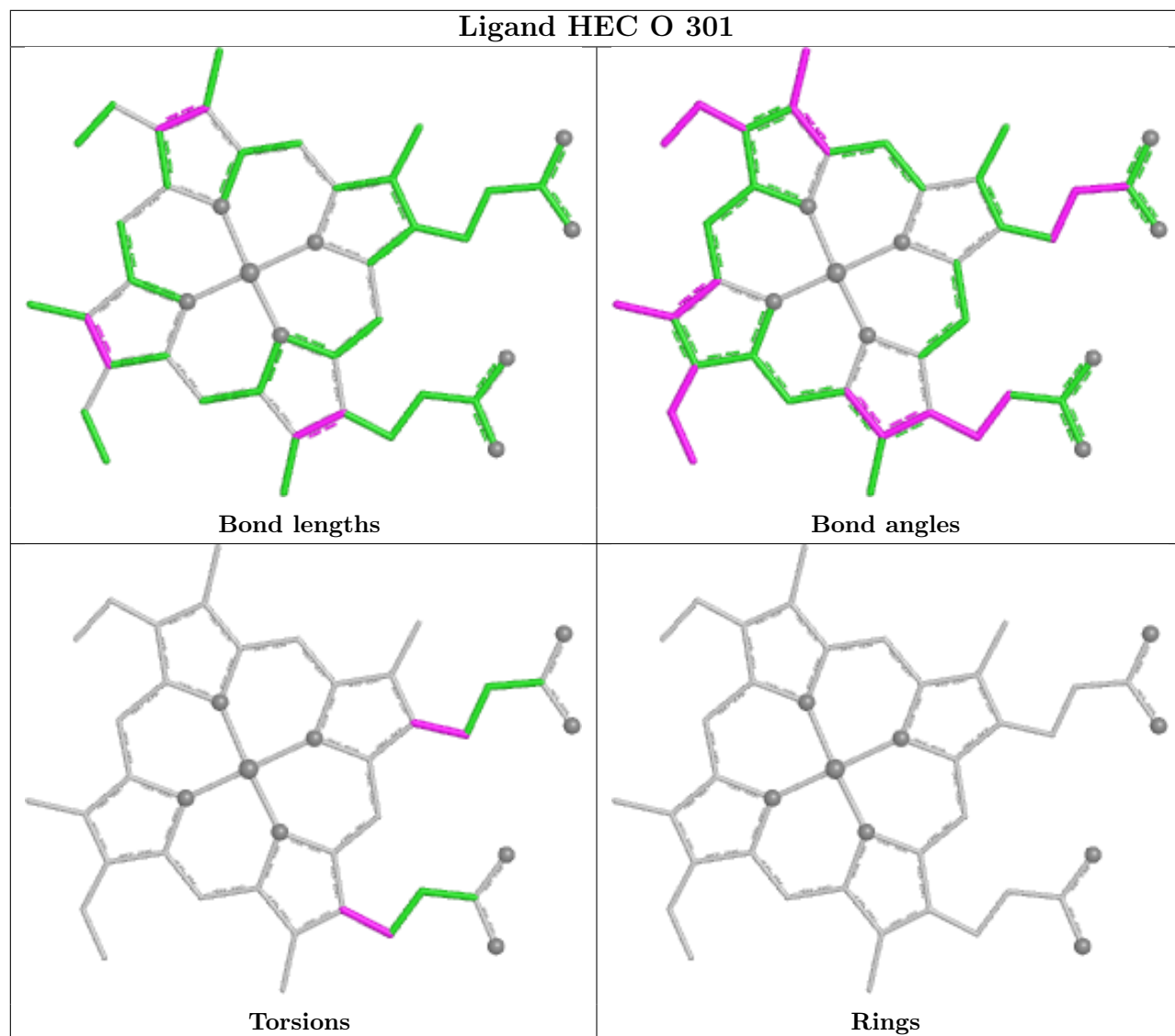


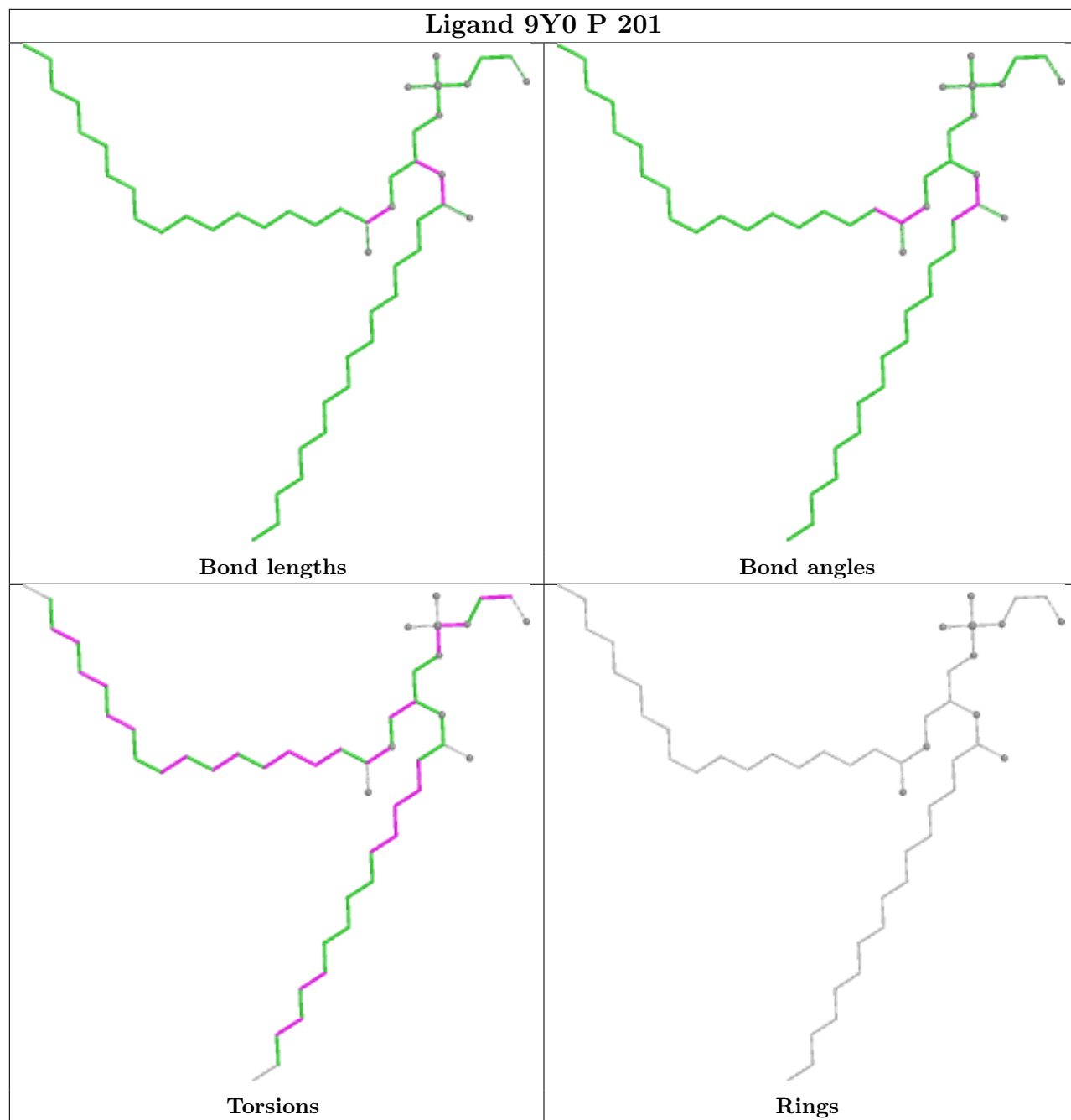


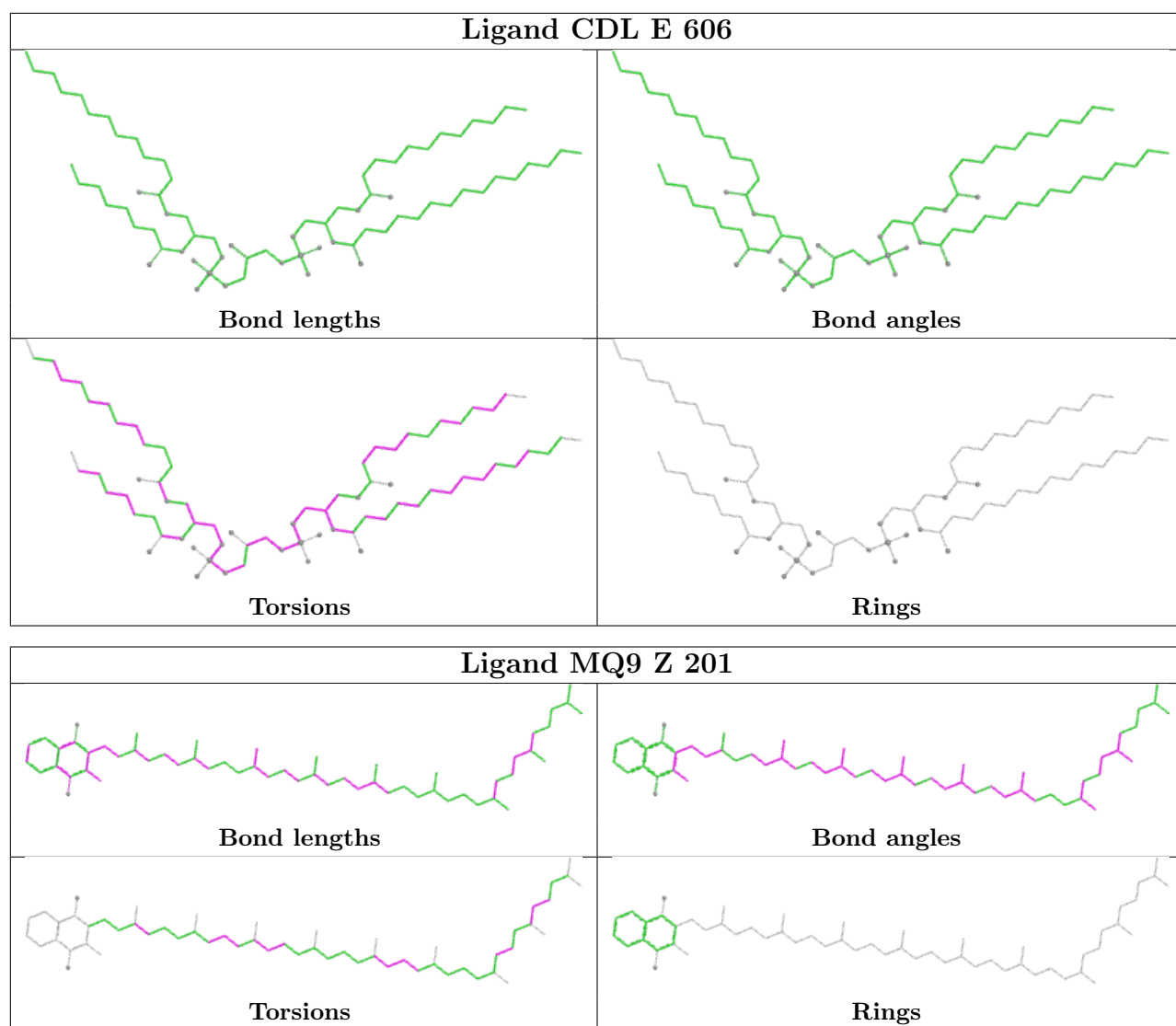




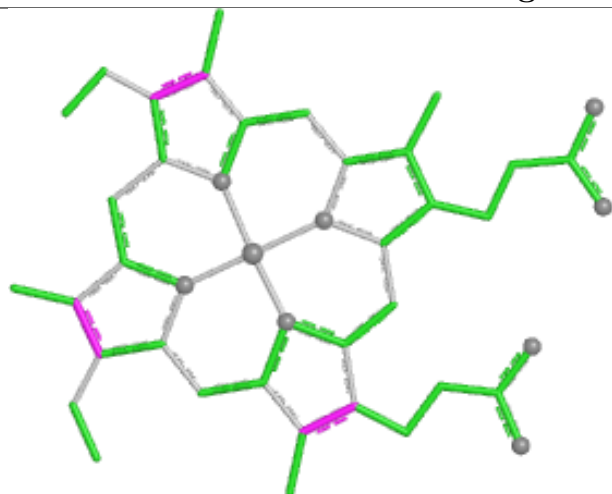




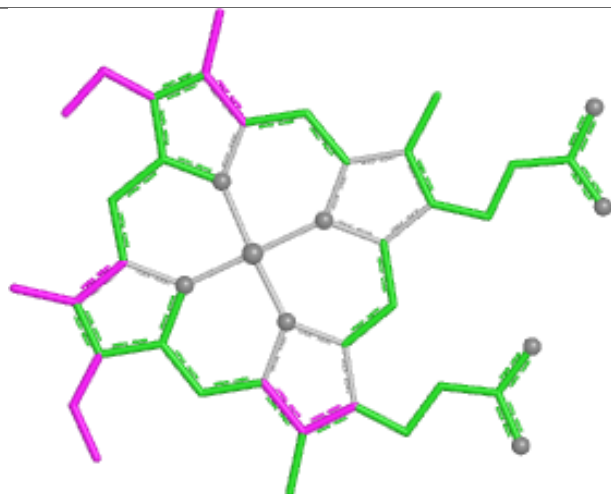




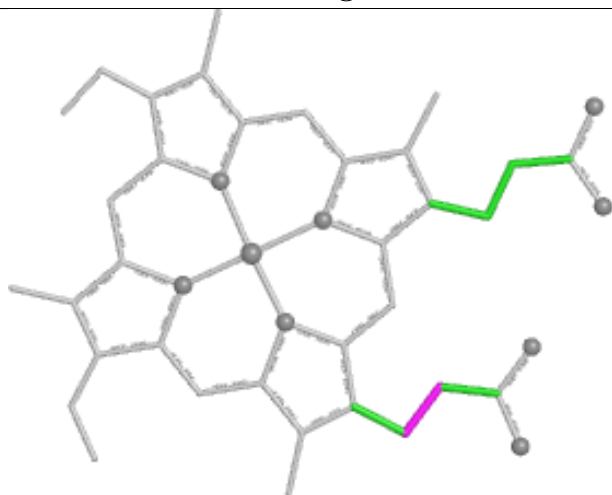
Ligand HEC I 301



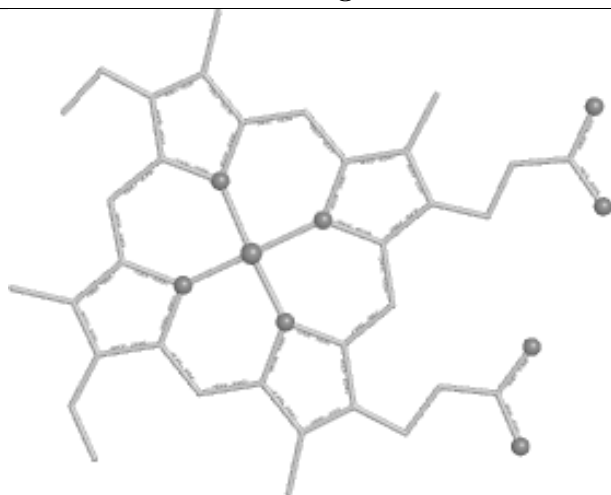
Bond lengths



Bond angles

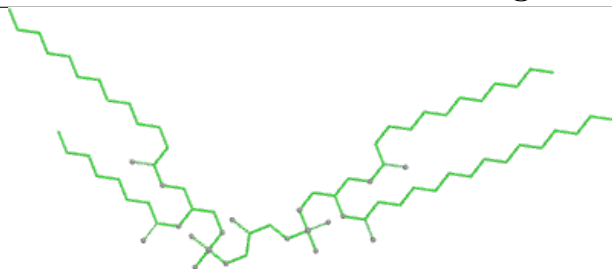


Torsions

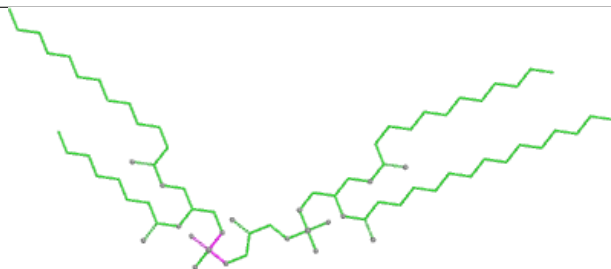


Rings

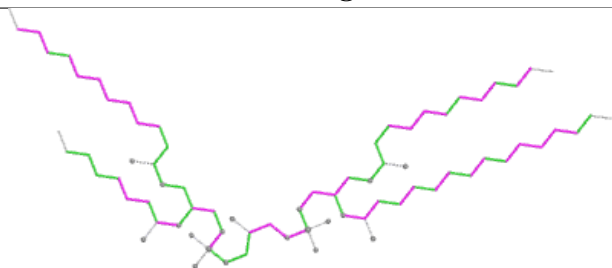
Ligand CDL X 303



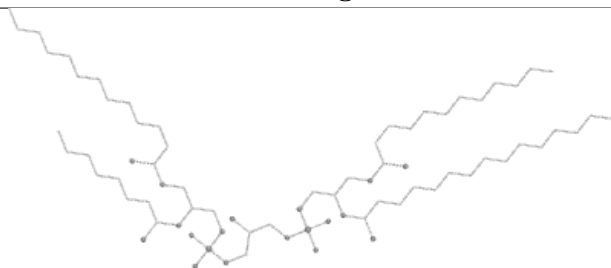
Bond lengths



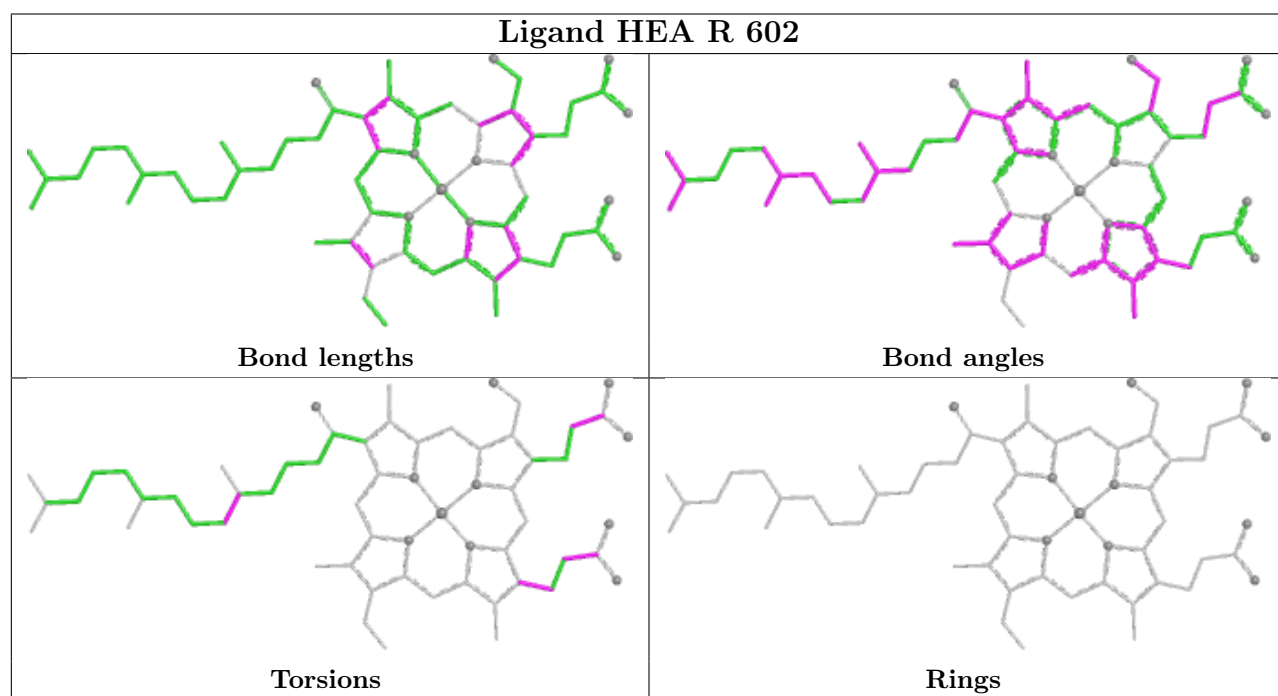
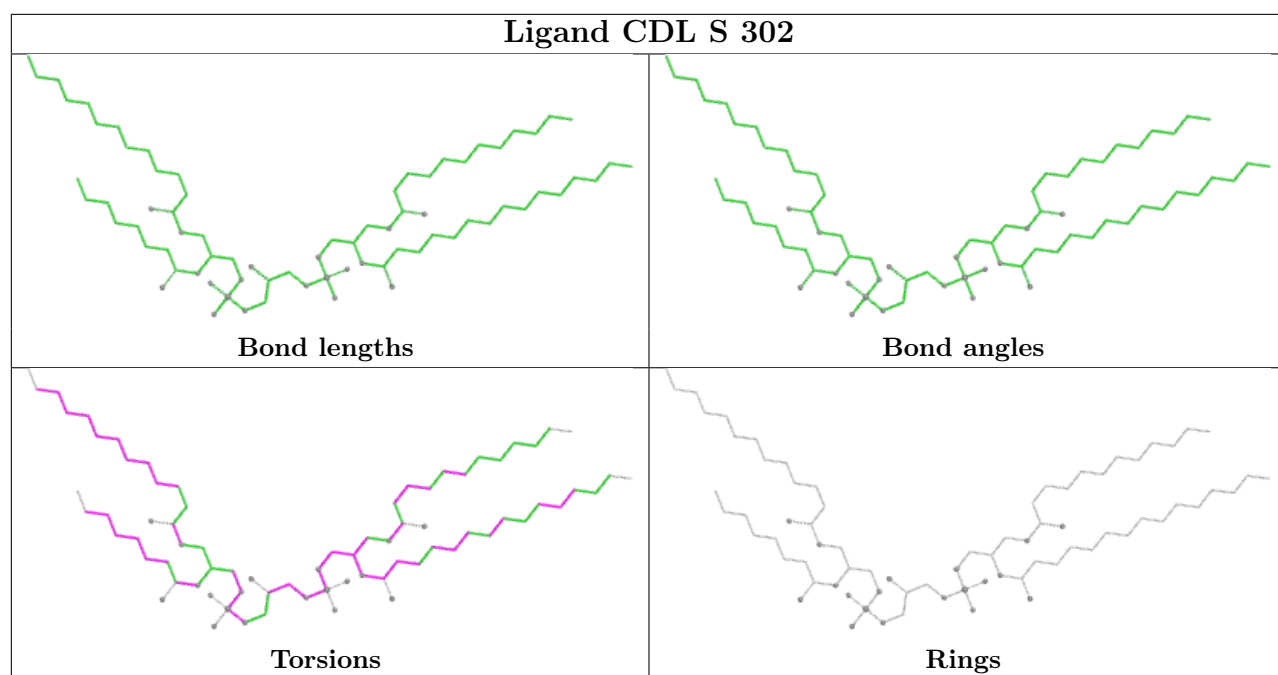
Bond angles

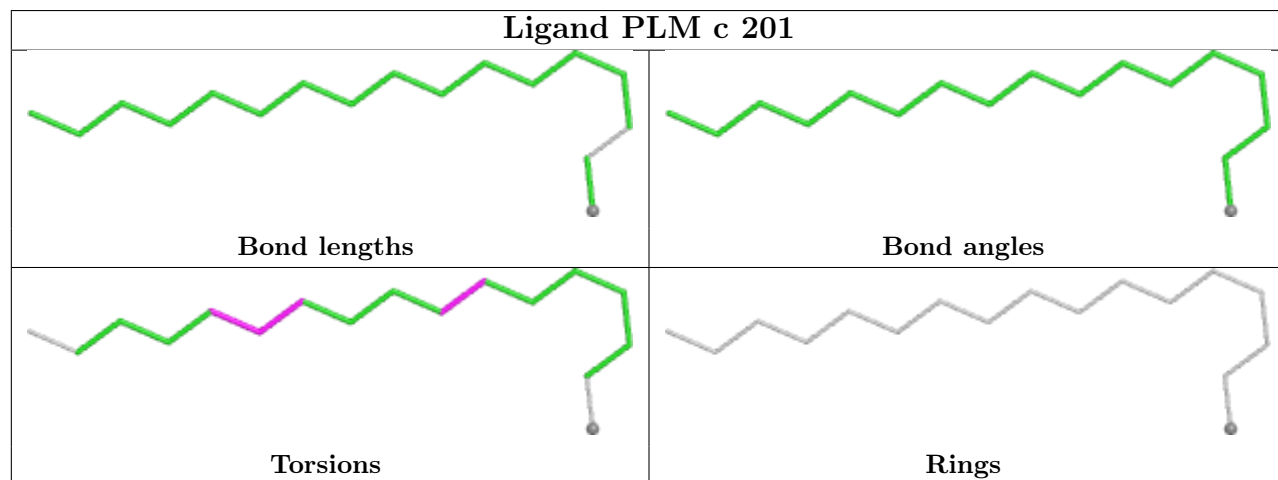
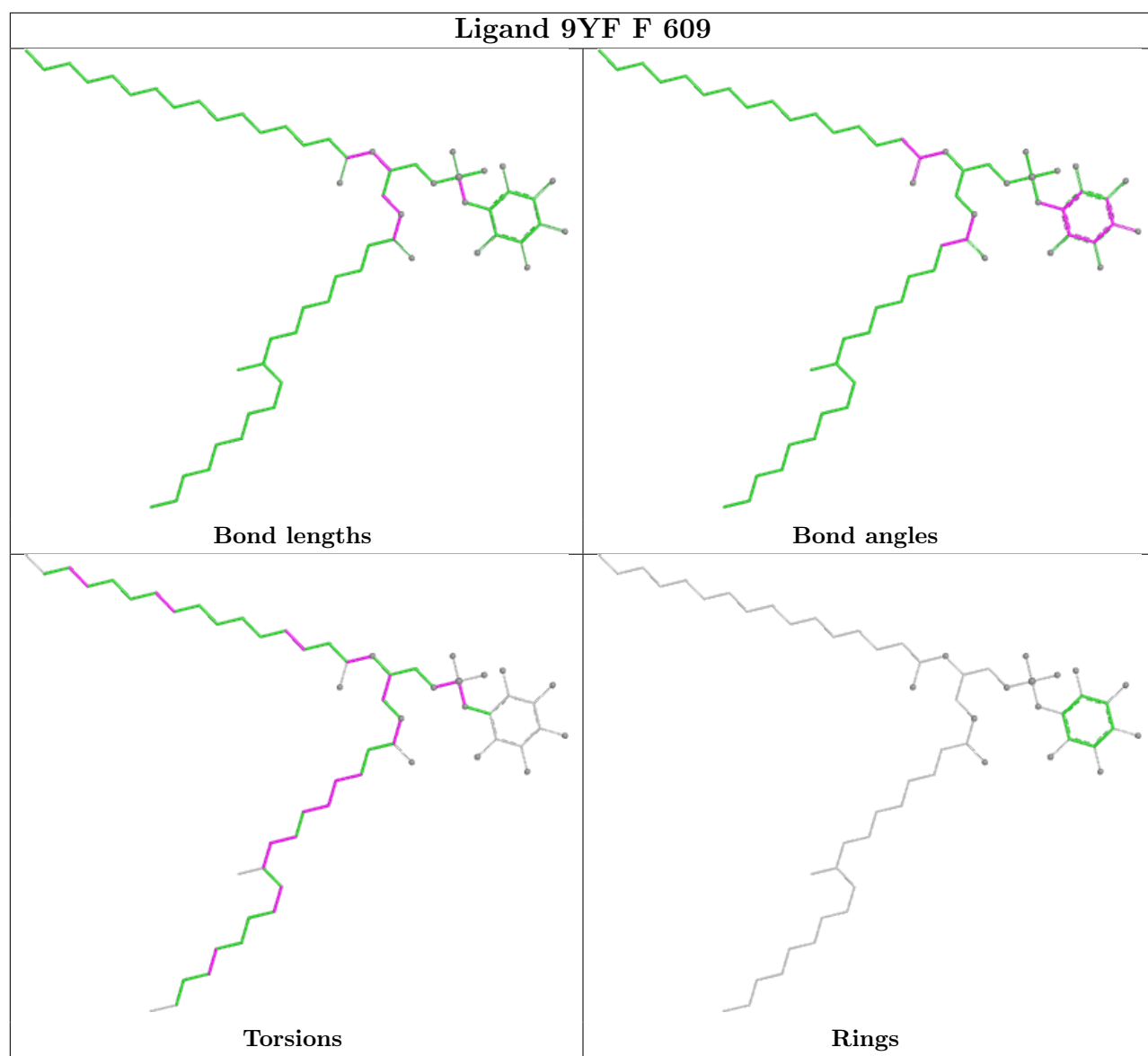


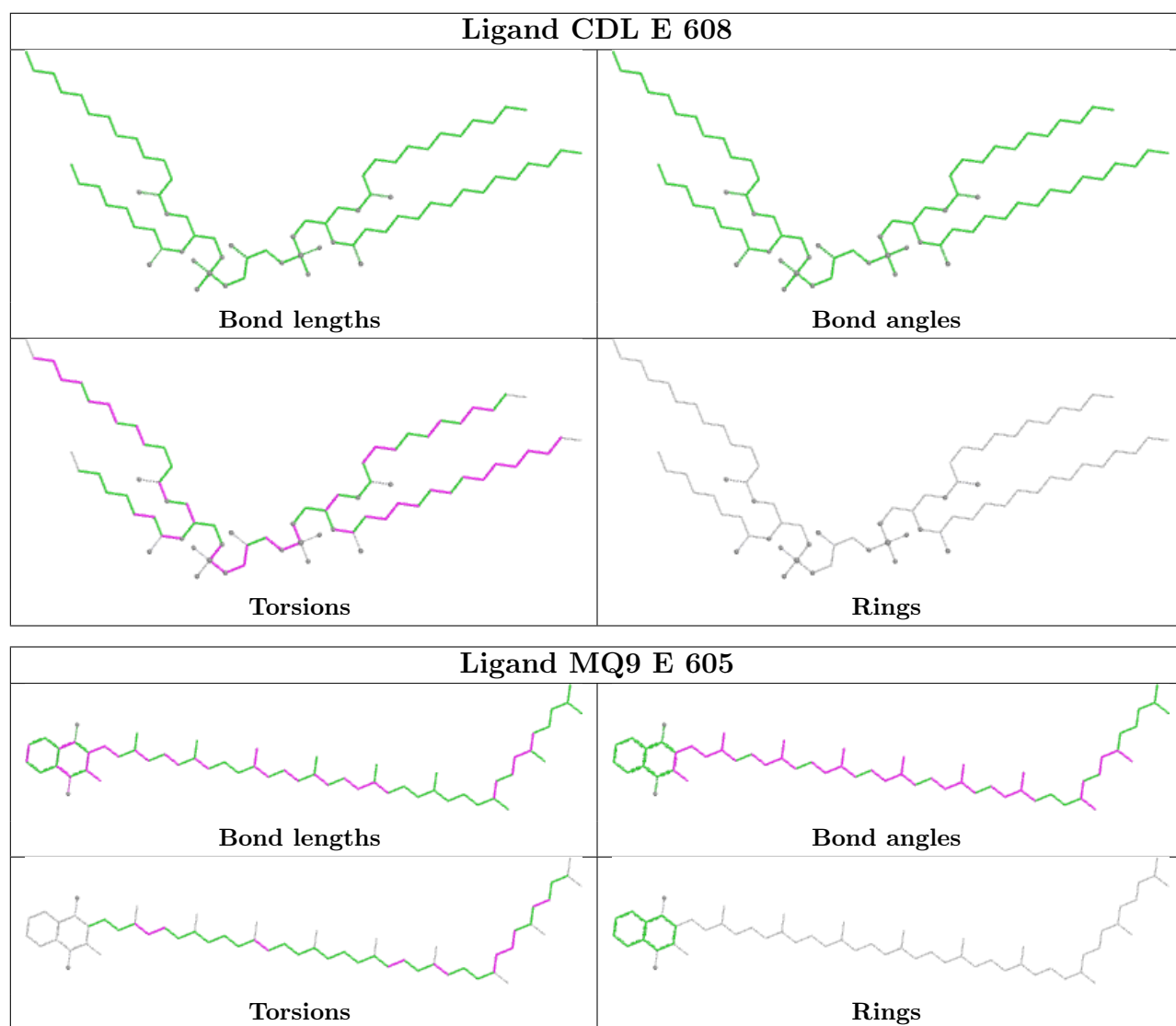
Torsions



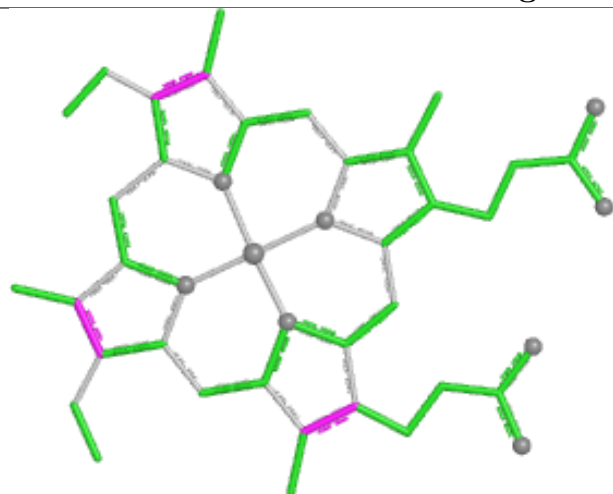
Rings



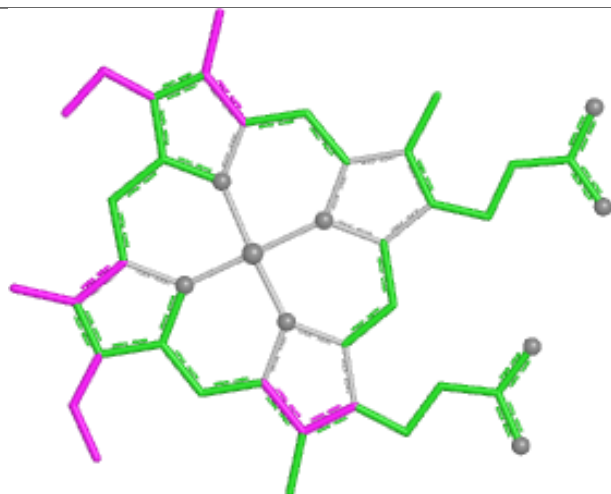




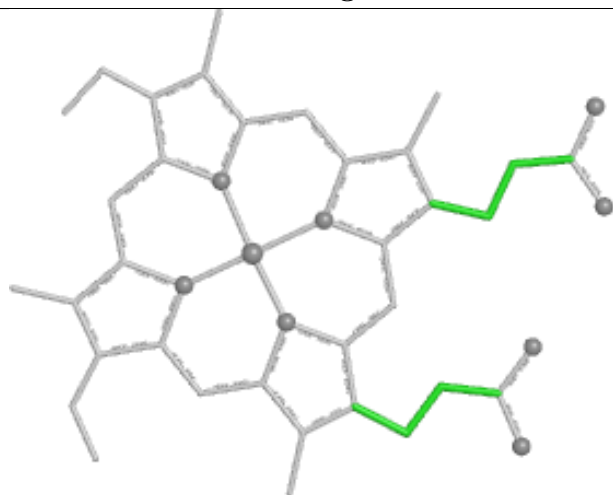
Ligand HEC I 302



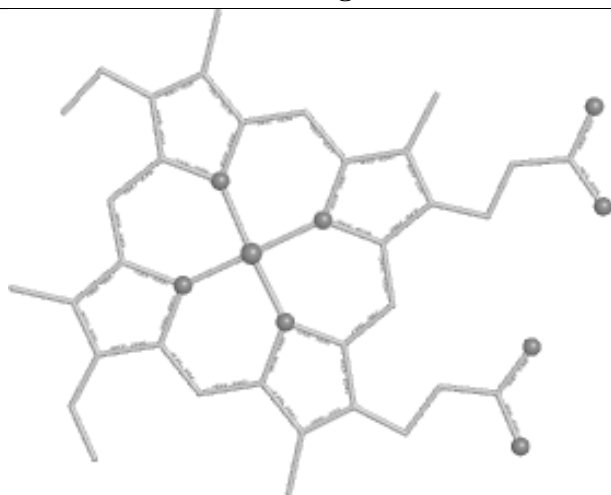
Bond lengths



Bond angles

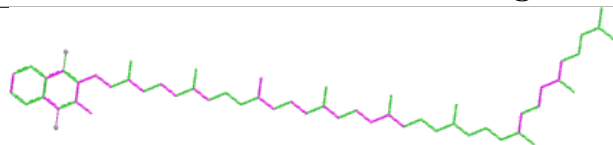


Torsions



Rings

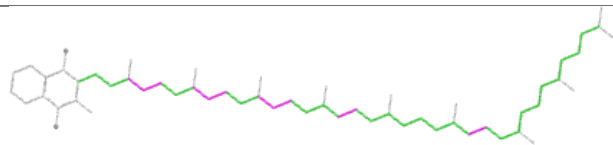
Ligand MQ9 E 604



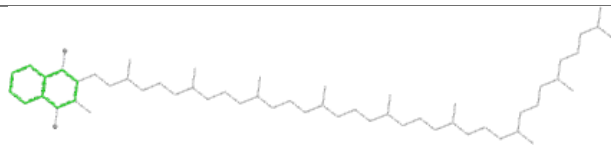
Bond lengths



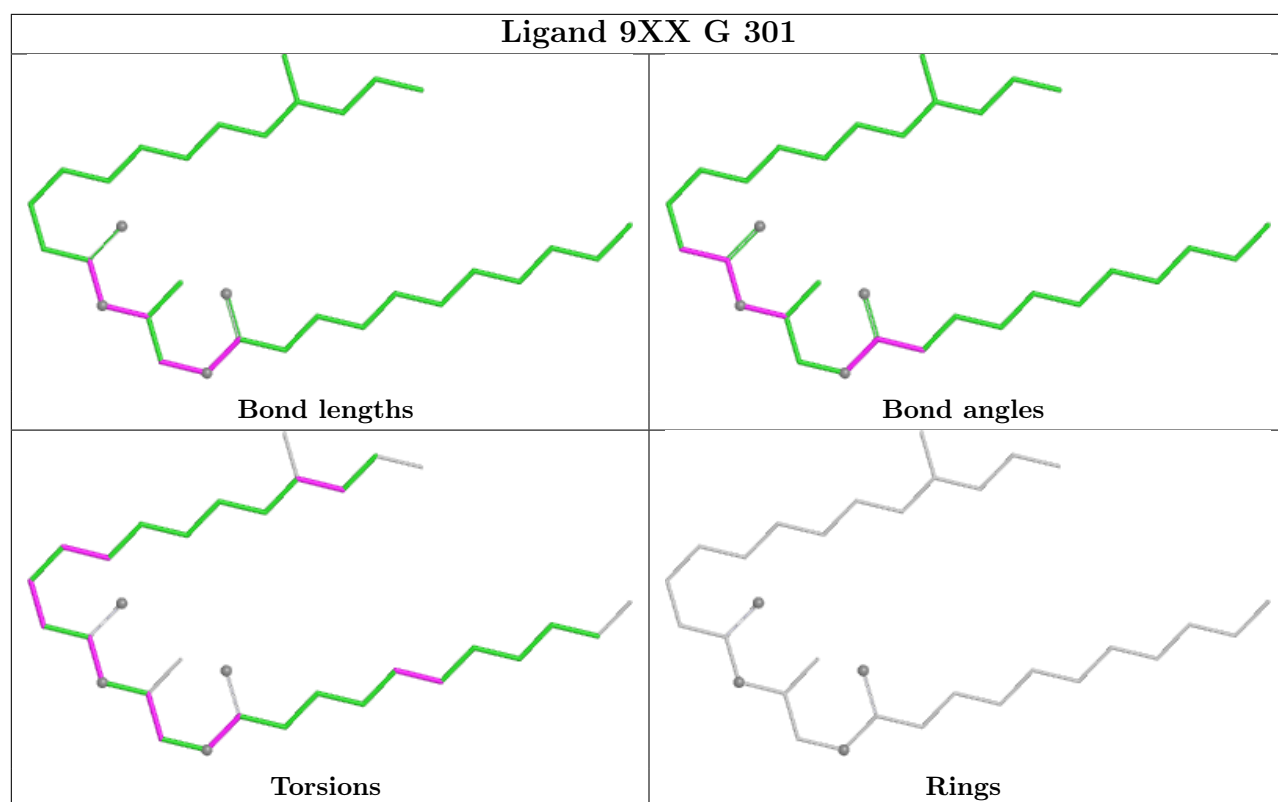
Bond angles

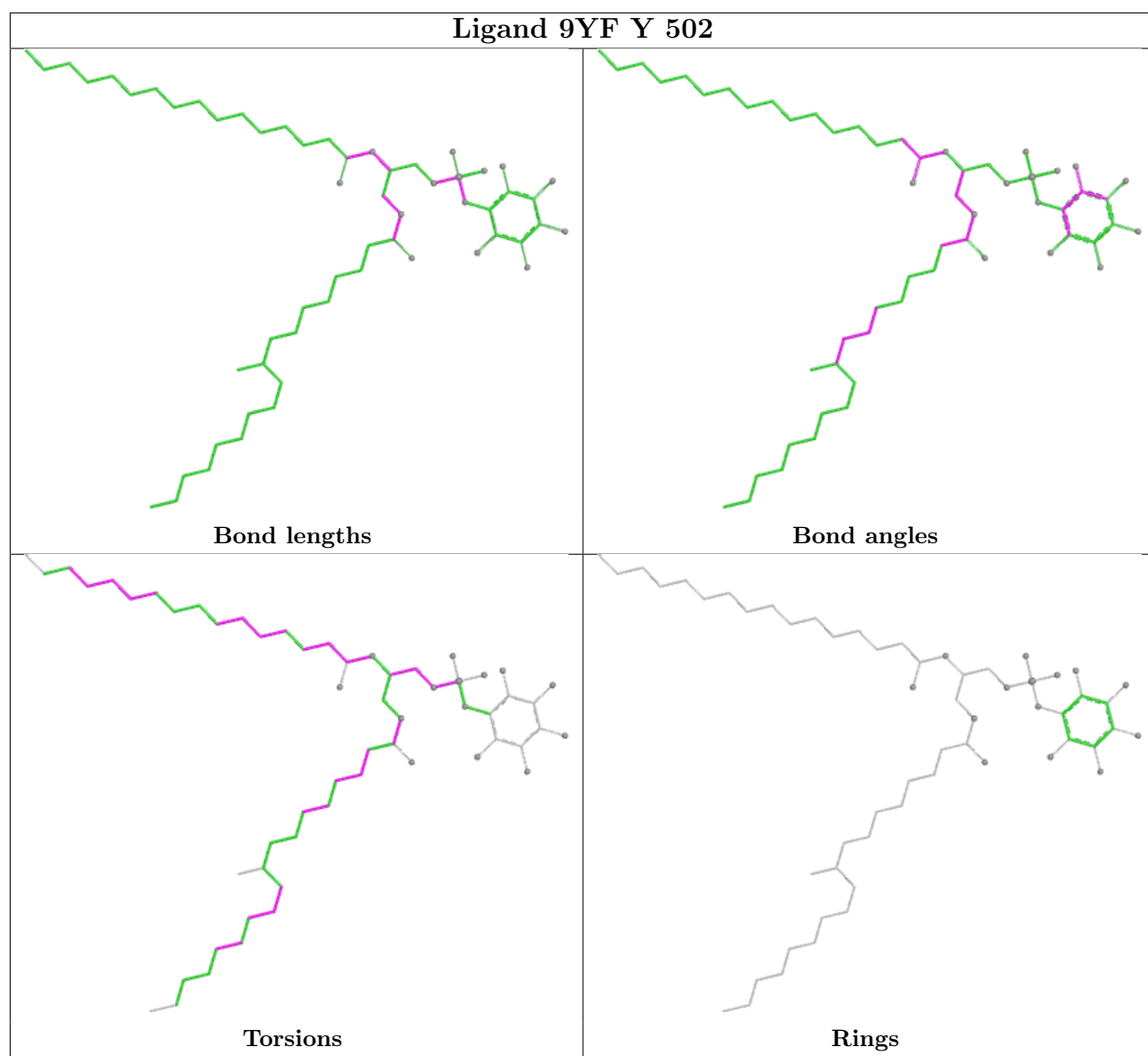


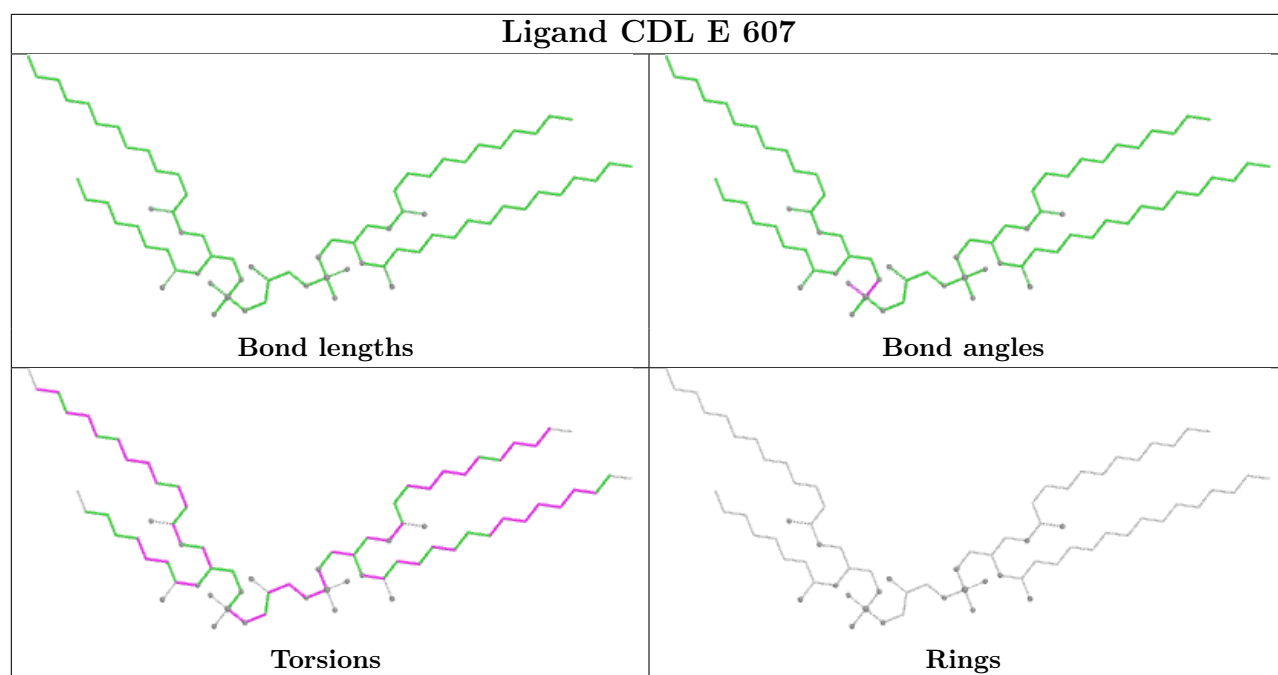
Torsions

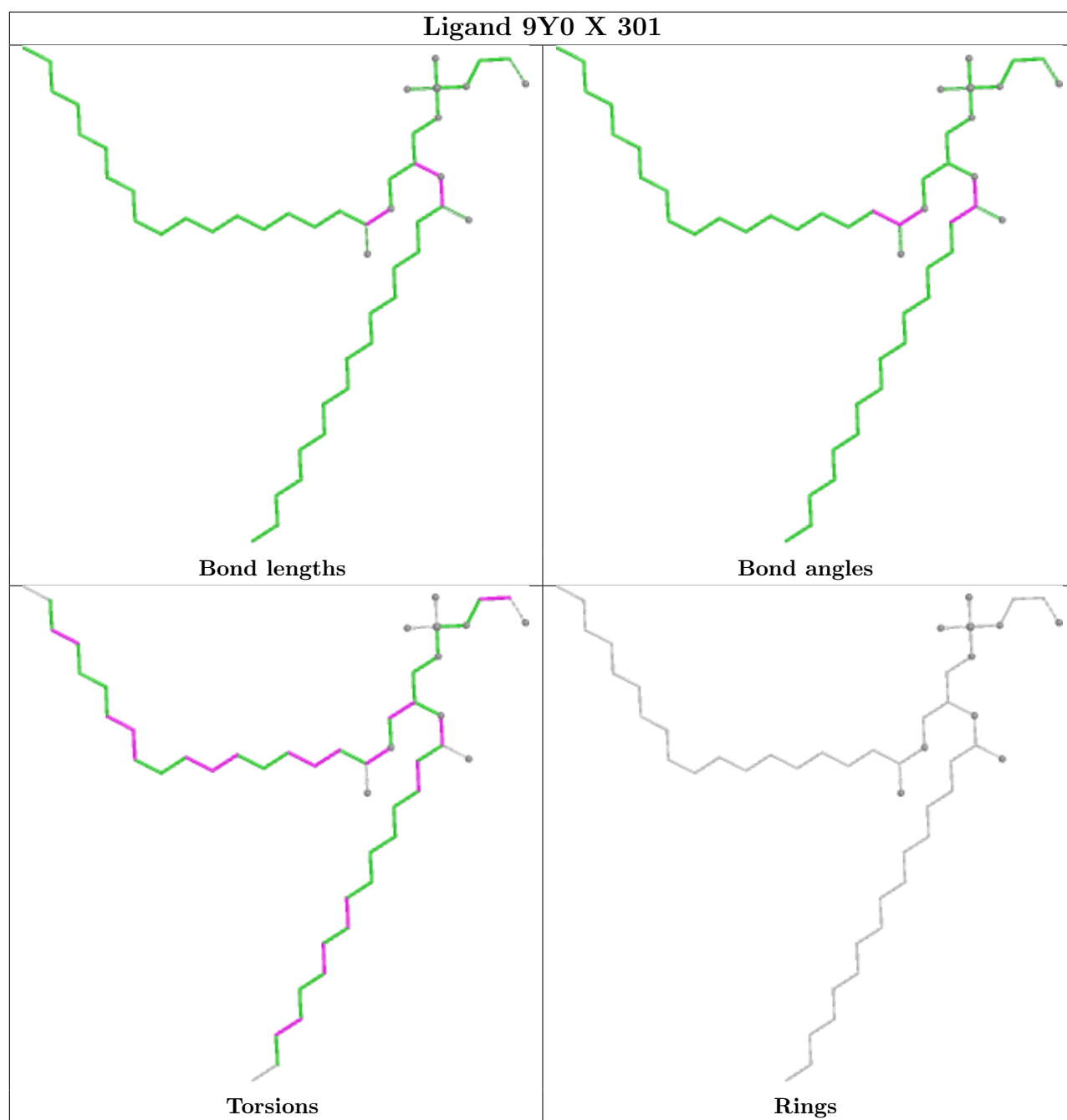


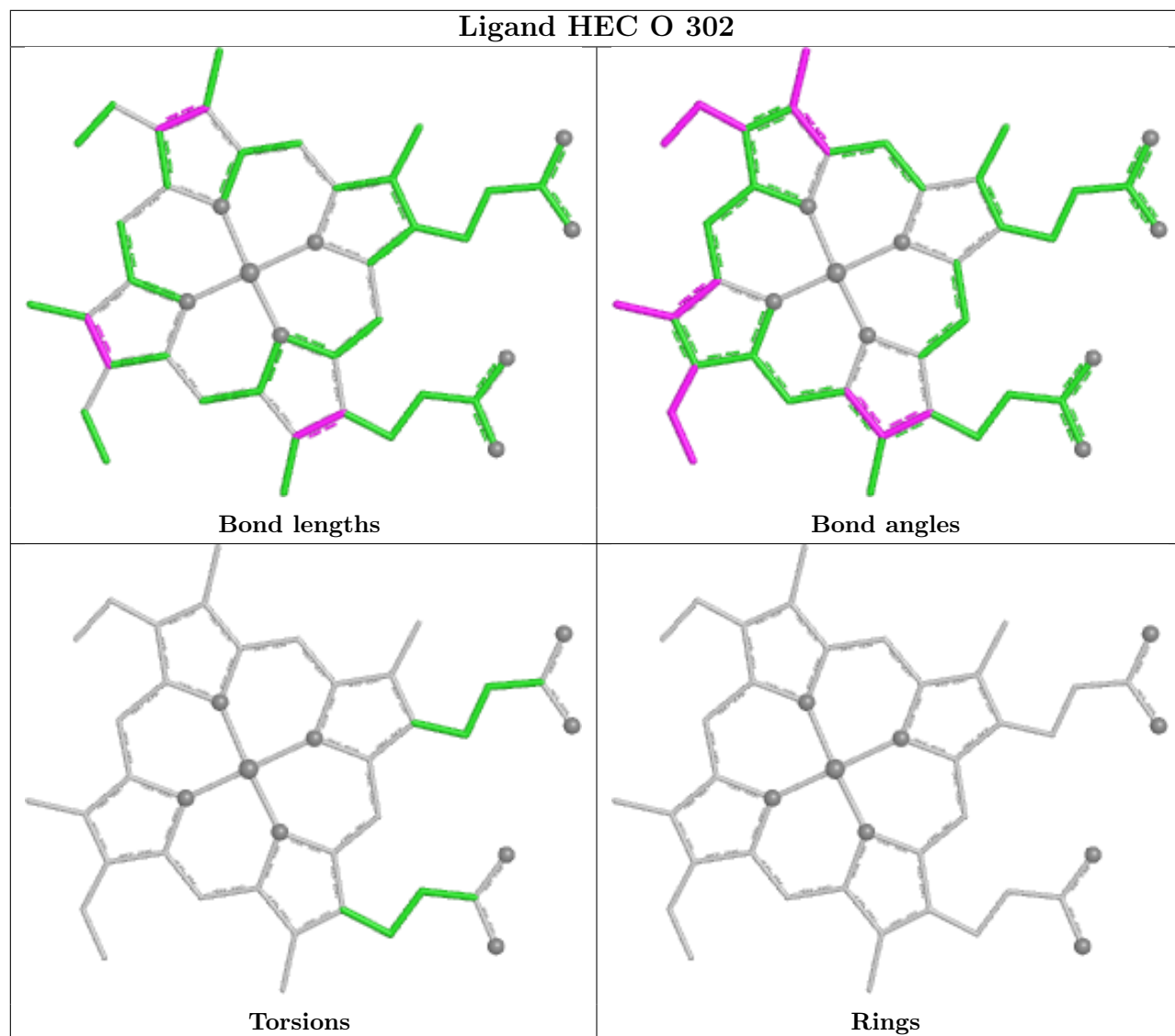
Rings

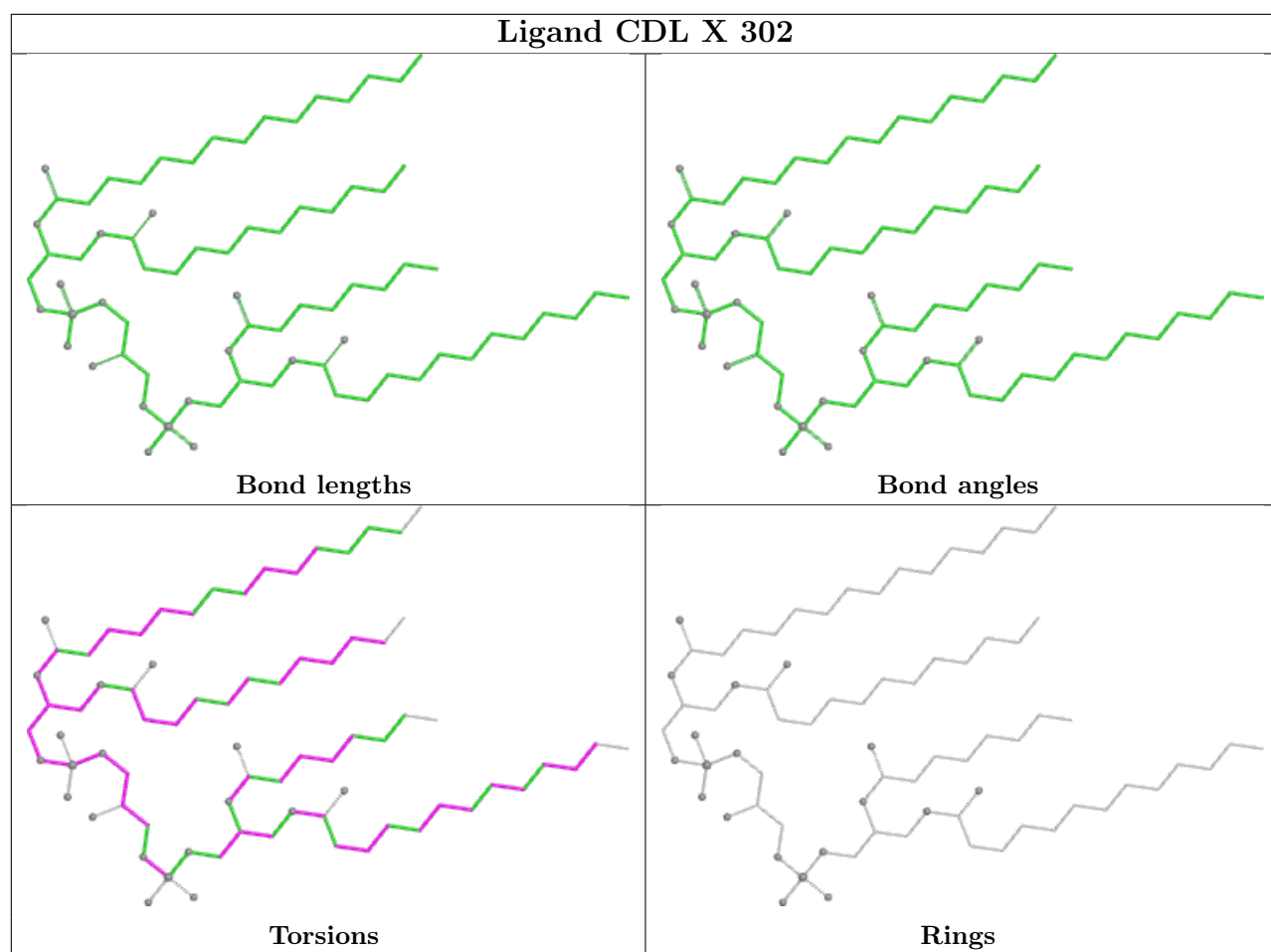


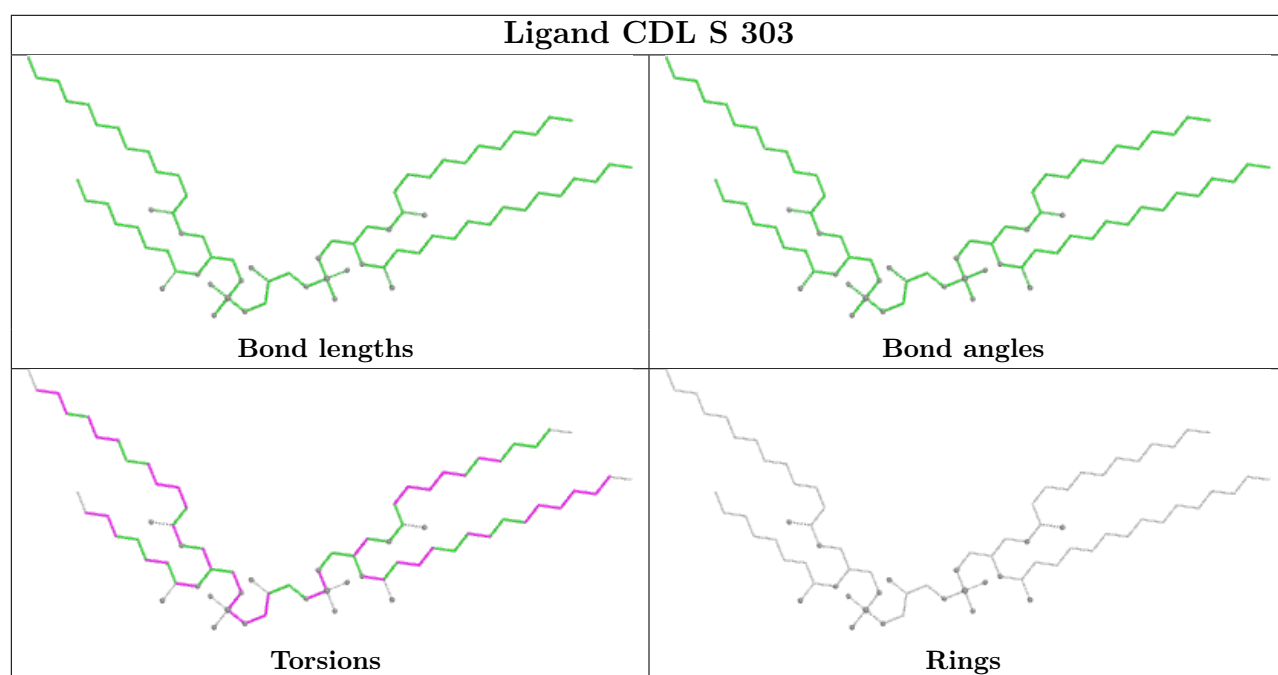
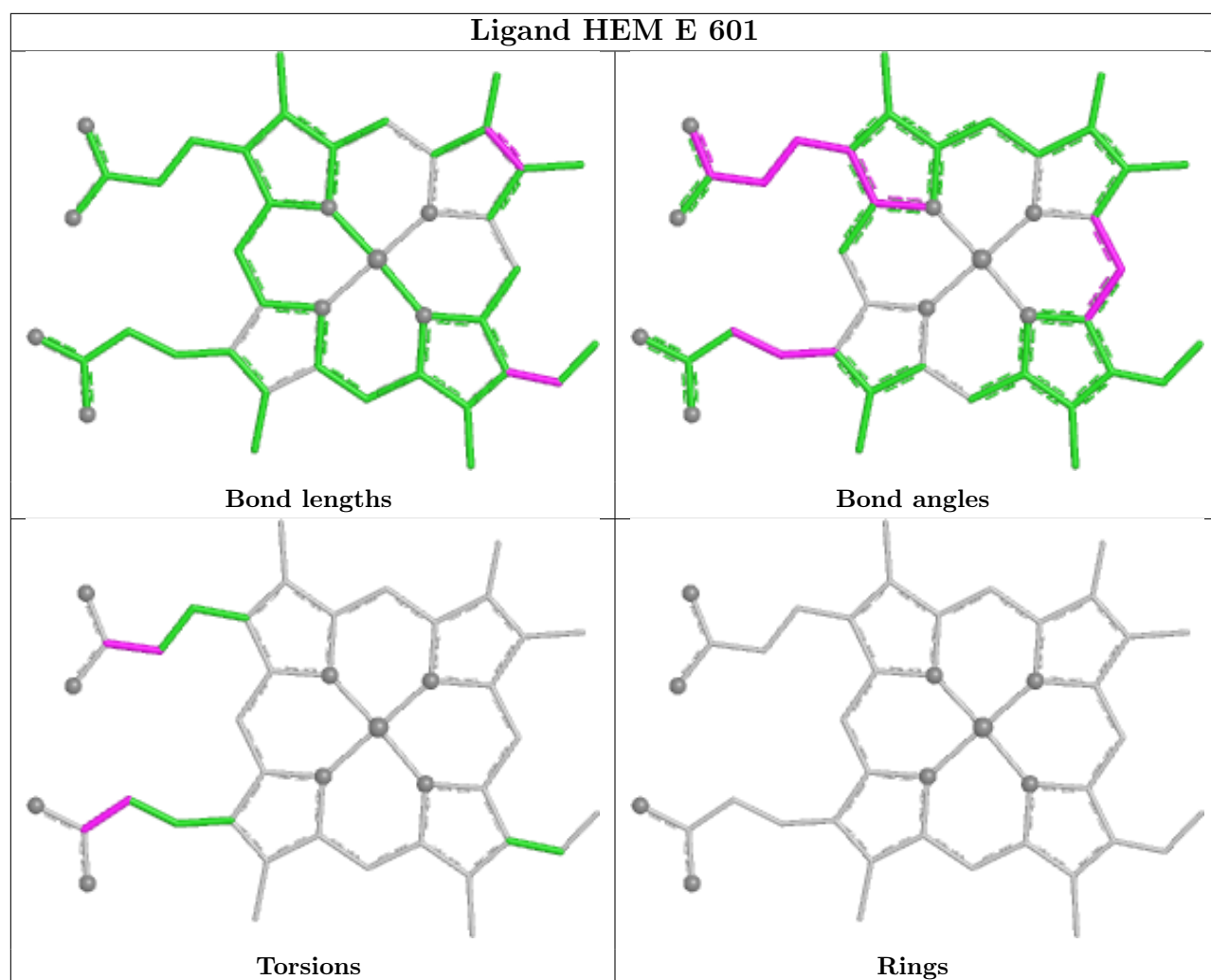


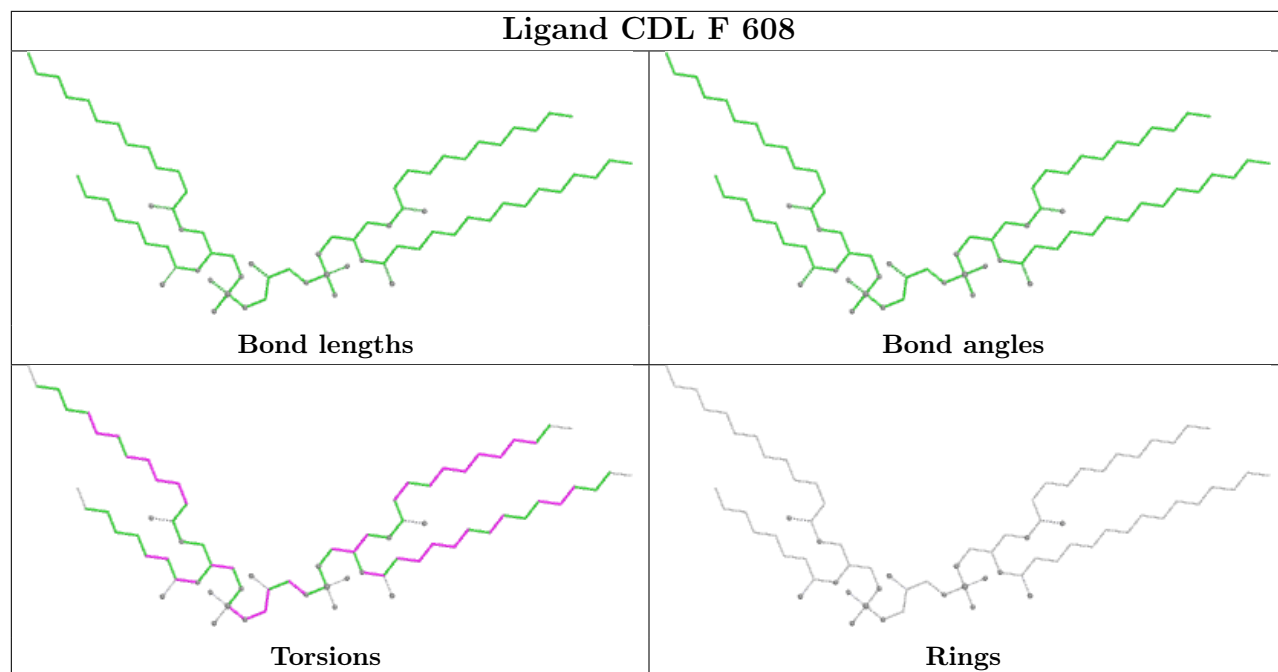


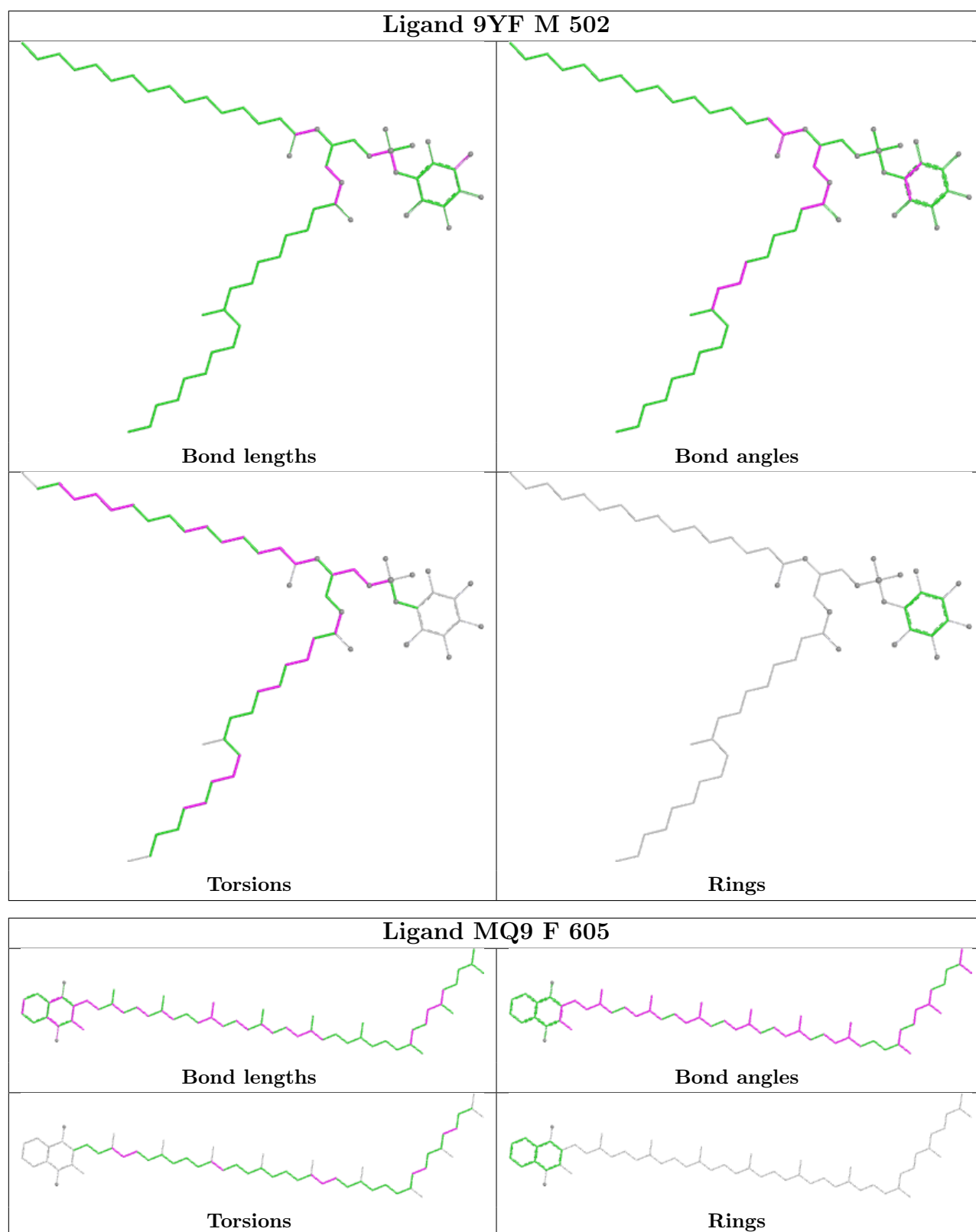












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

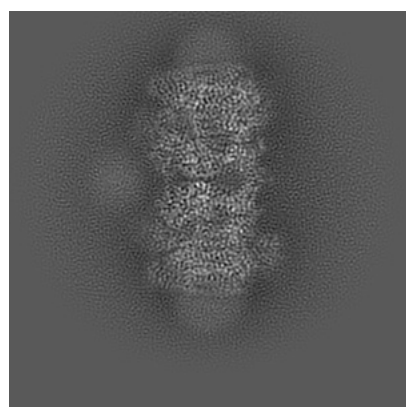
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24457. These allow visual inspection of the internal detail of the map and identification of artifacts.

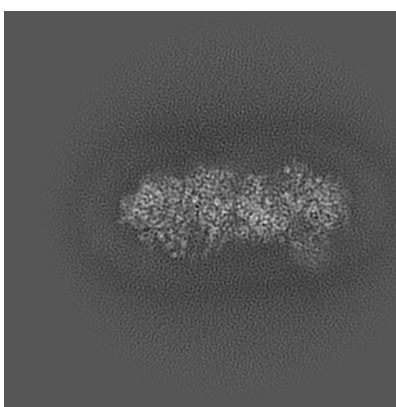
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

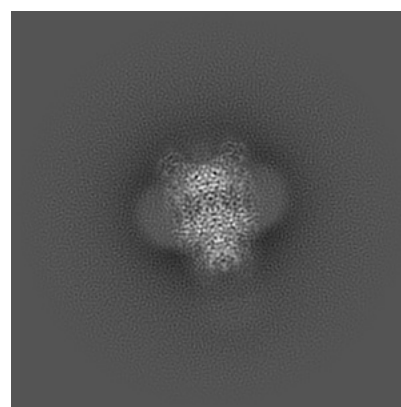
6.1.1 Primary map



X



Y

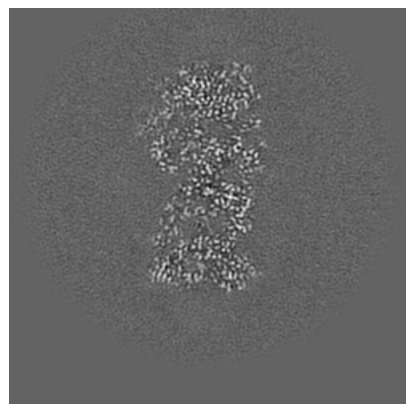


Z

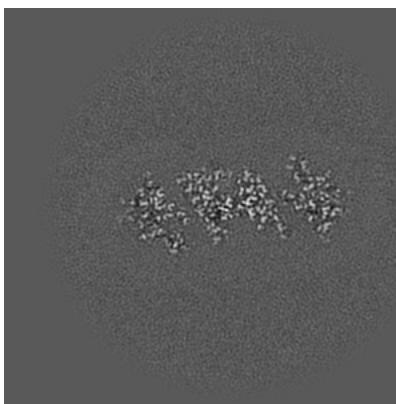
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

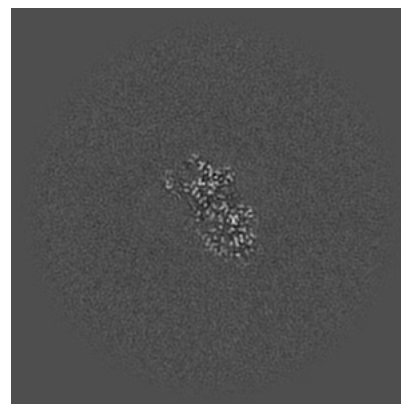
6.2.1 Primary map



X Index: 165



Y Index: 165

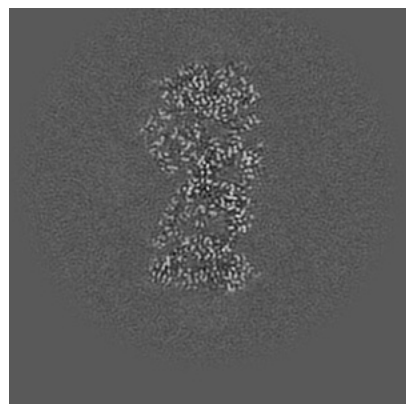


Z Index: 165

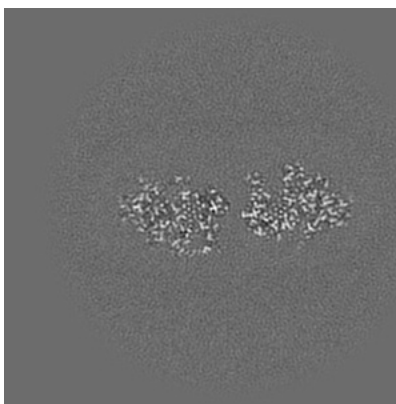
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

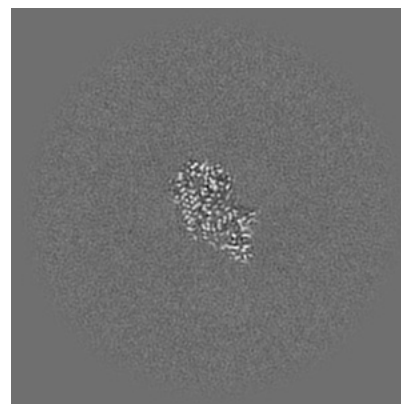
6.3.1 Primary map



X Index: 166



Y Index: 182

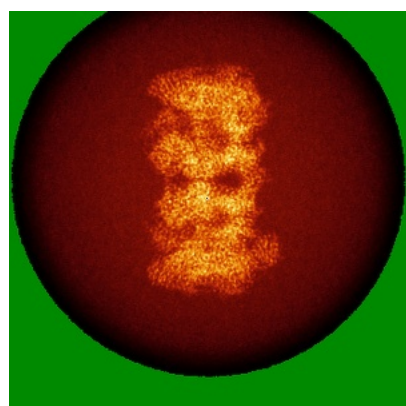


Z Index: 172

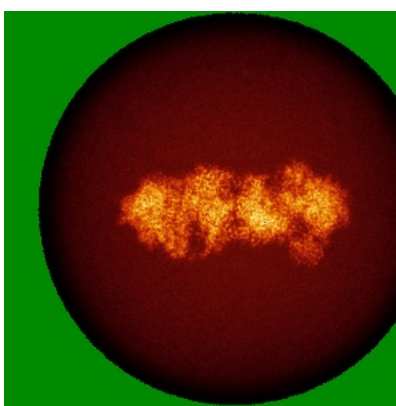
The images above show the largest variance slices of the map in three orthogonal directions.

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

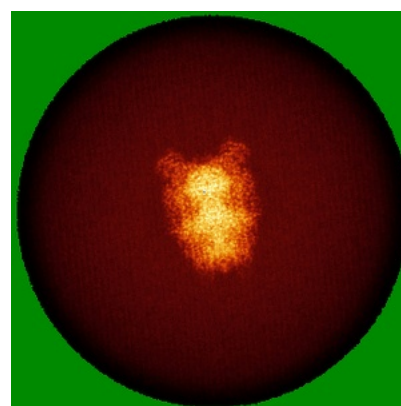
6.4.1 Primary map



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 0.82. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

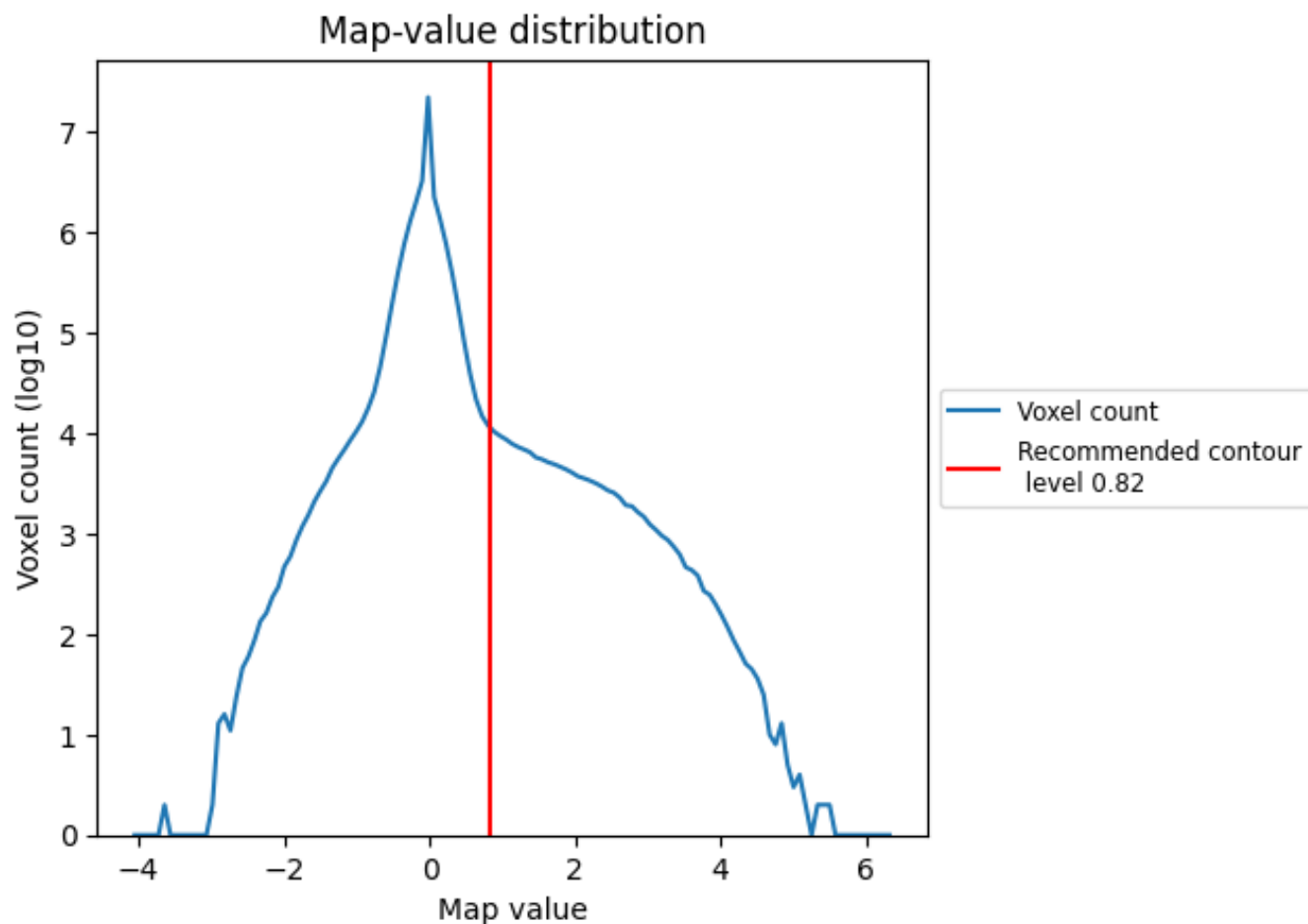
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

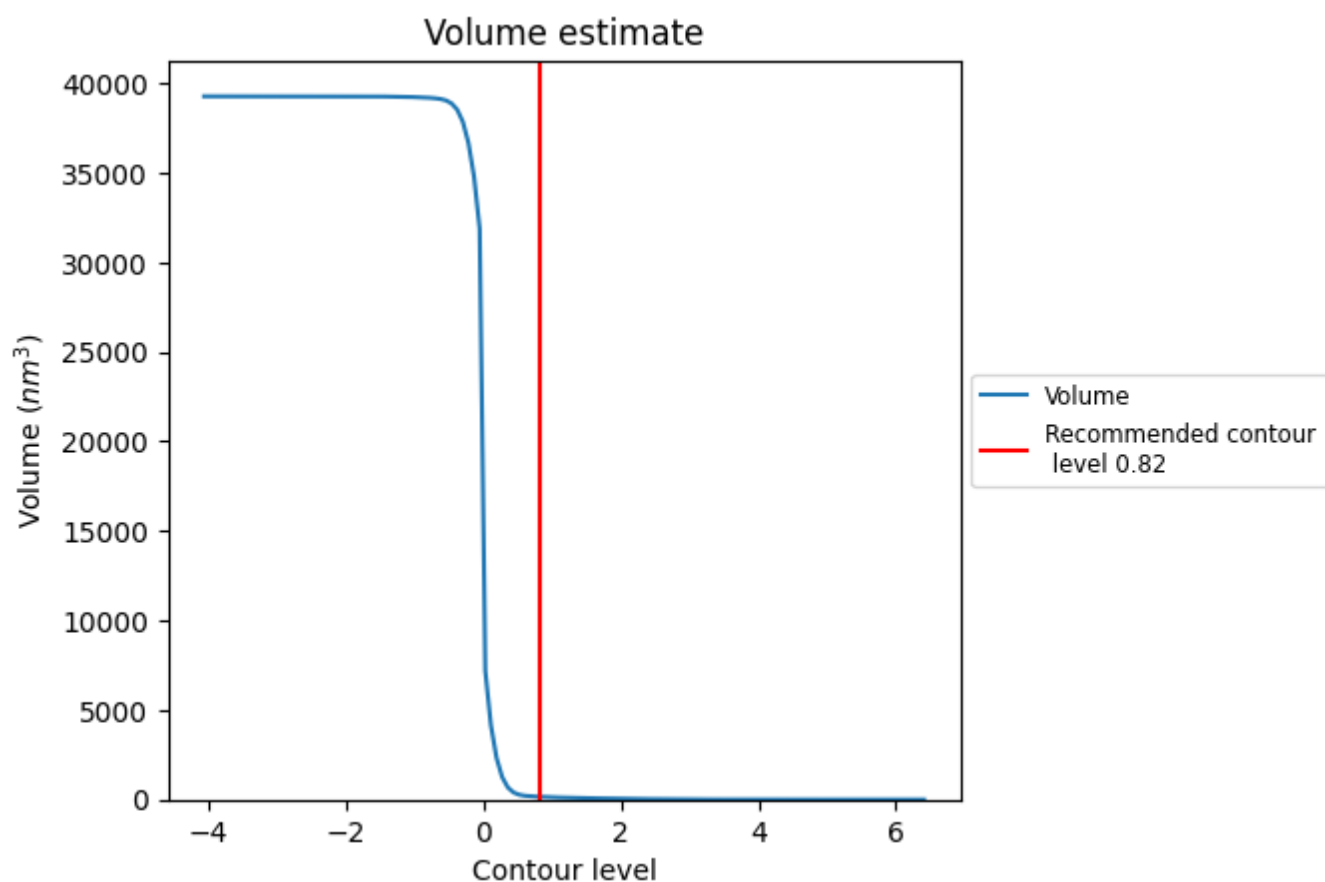
This section contains the results of statistical analysis of the map.

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.

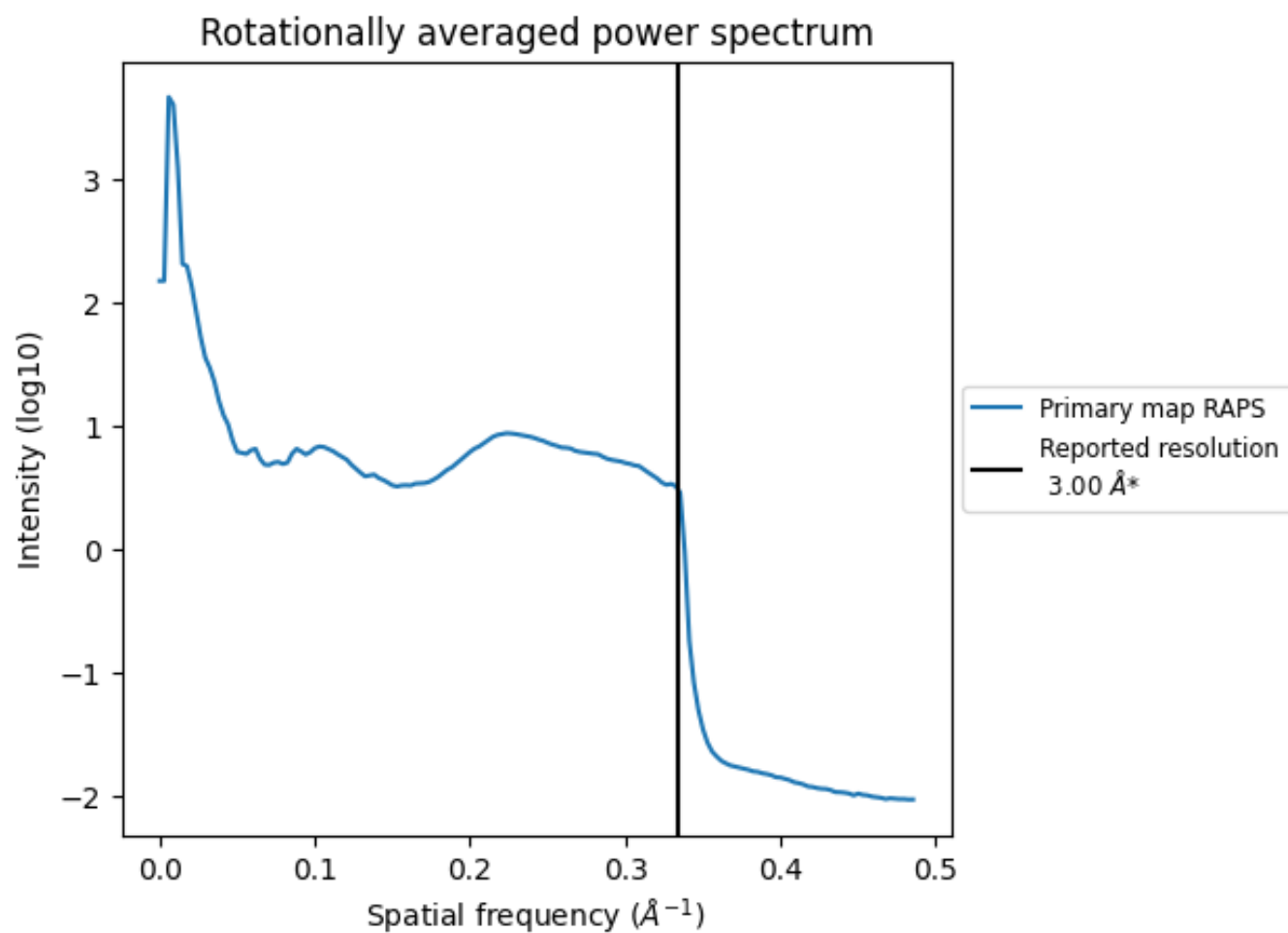
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 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 0.333 Å⁻¹

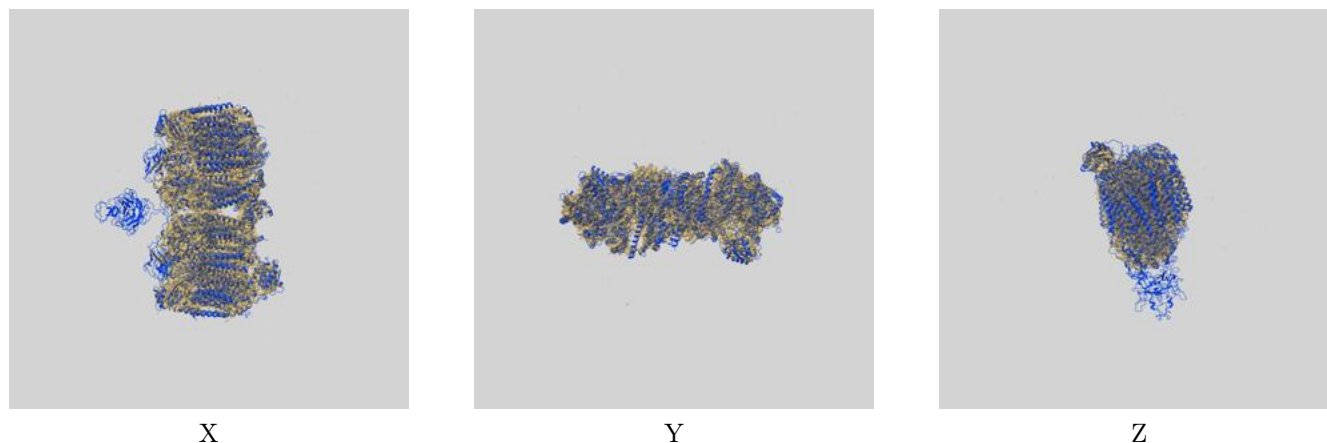
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

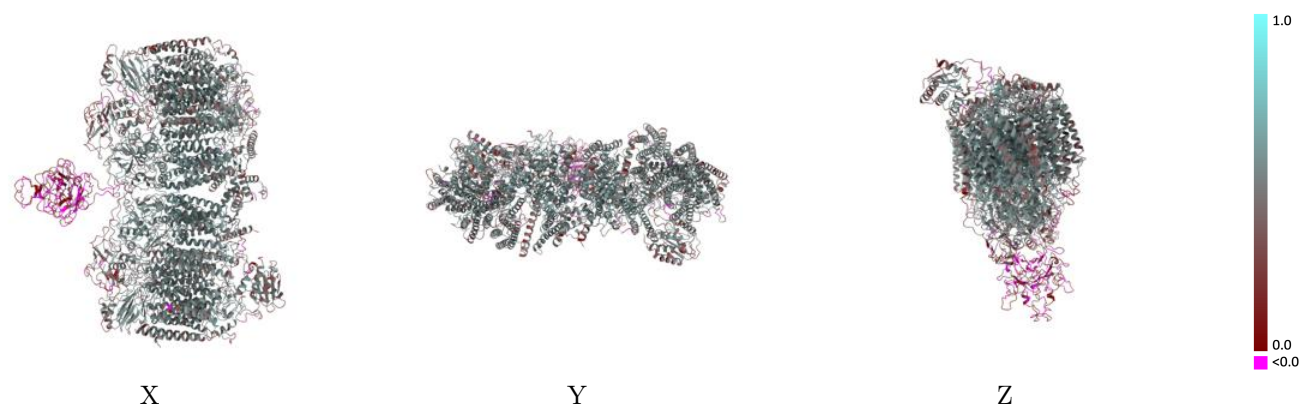
This section contains information regarding the fit between EMDB map EMD-24457 and PDB model 7RH7. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



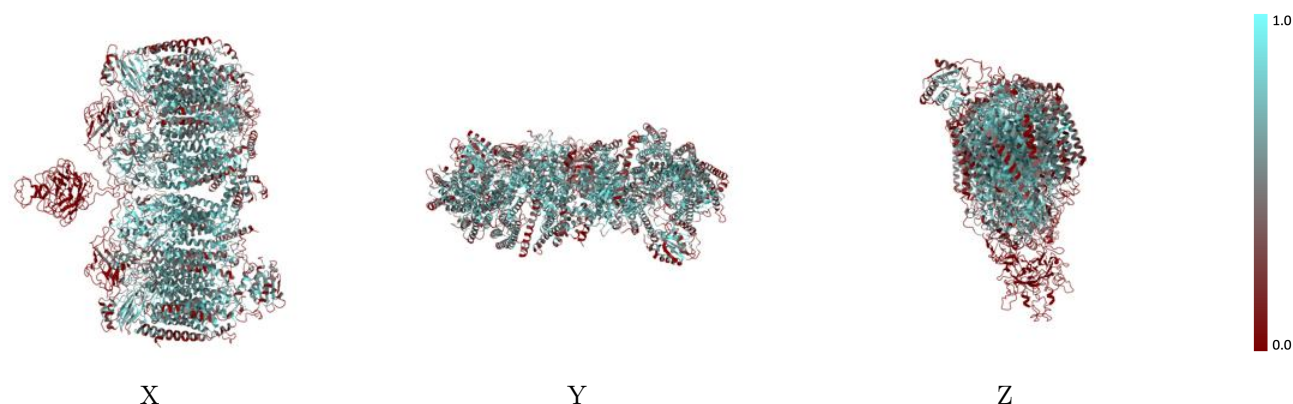
The images above show the 3D surface view of the map at the recommended contour level 0.82 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



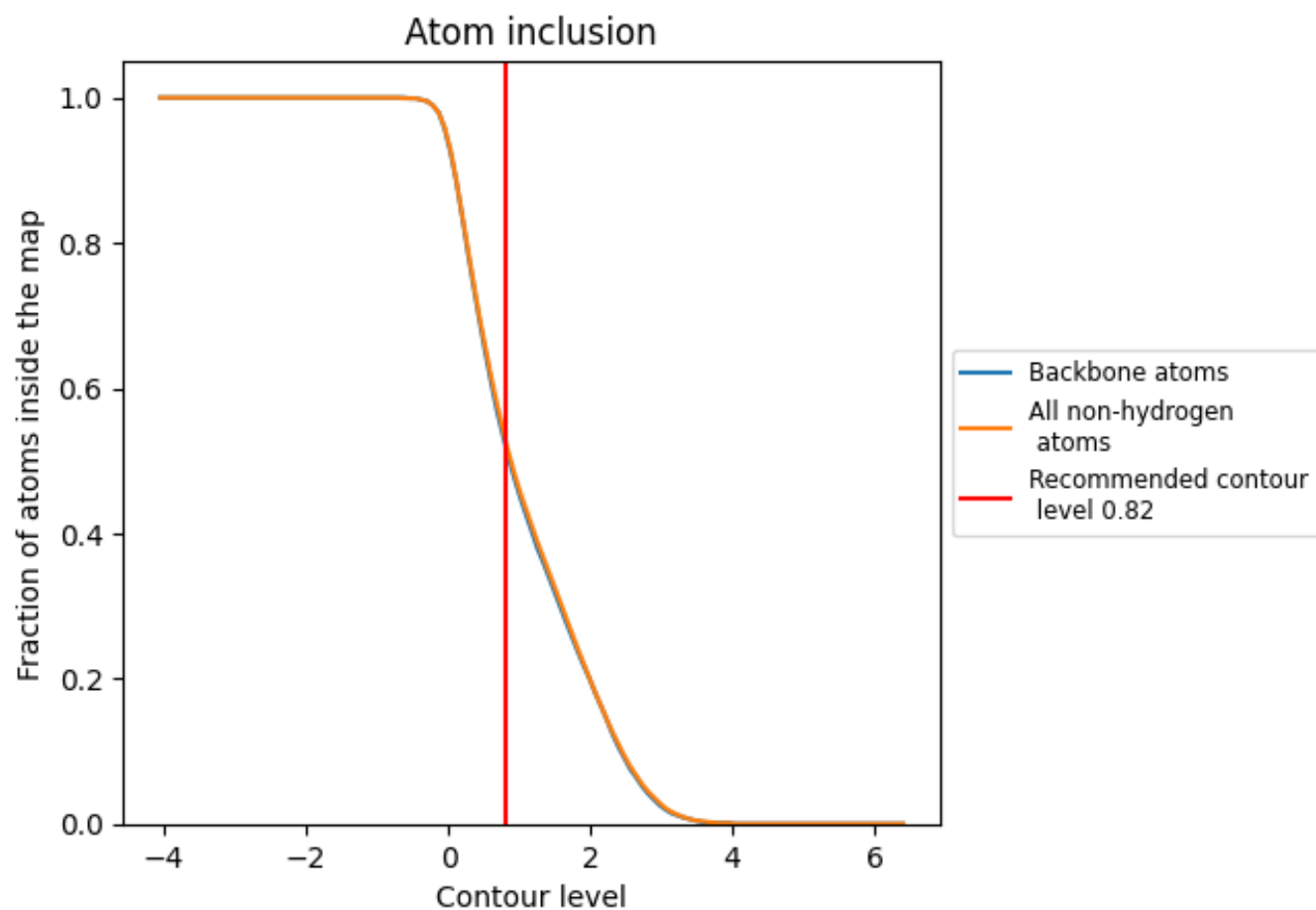
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.82).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 52% 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 (0.82) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5230	 0.4770
D	 0.0440	 0.1470
E	 0.6830	 0.5400
F	 0.6730	 0.5350
G	 0.0400	 0.1360
I	 0.5800	 0.5070
J	 0.3510	 0.4360
K	 0.4340	 0.4440
L	 0.6830	 0.5360
M	 0.5960	 0.5090
O	 0.5830	 0.5100
P	 0.3280	 0.4570
Q	 0.4100	 0.4320
R	 0.6900	 0.5350
S	 0.5000	 0.4820
T	 0.5300	 0.5100
U	 0.2280	 0.3790
V	 0.4510	 0.4300
W	 0.1200	 0.3510
X	 0.5070	 0.4940
Y	 0.5840	 0.5080
Z	 0.5140	 0.4870
a	 0.2330	 0.3590
b	 0.4430	 0.4220
c	 0.1110	 0.3700

