



## wwPDB EM Validation Summary Report ⓘ

Jun 22, 2026 – 06:45 PM JST

PDB ID : 9WCX / pdb\_00009wcx  
EMDB ID : EMD-65878  
Title : Cryo-EM structure of the Mycobacterium abscessus cytochrome bcc:aa3 supercomplex  
Authors : Mathiyazakan, V.; Gruber, G.  
Deposited on : 2025-08-18  
Resolution : 2.66 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](mailto: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>.

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

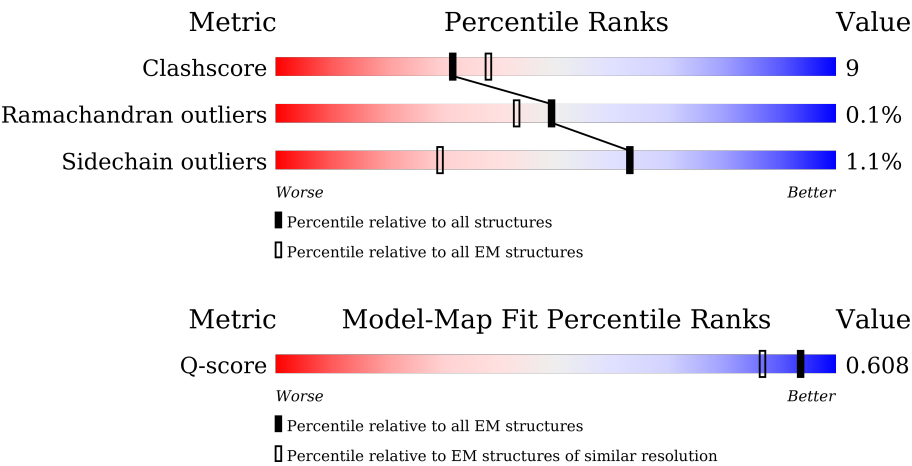
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.66 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	9119 ( 2.16 - 3.16 )

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  $\geq 3$ , 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	G	99	
1	b	99	
2	I	564	
2	L	564	

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Mol	Chain	Length	Quality of chain
3	J	86	
3	h	86	
4	U	295	
4	o	295	
5	V	391	
5	p	391	
6	X	238	
6	a	238	
7	d	349	
7	e	349	
8	f	206	
8	g	206	
9	i	546	
9	j	546	
10	k	175	
10	l	175	
11	m	139	
11	n	139	
12	q	227	
12	r	227	

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
14	CDL	b	103	-	-	X	-
23	MQ9	i	610	-	-	X	-

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 46750 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 Prokaryotic respiratory supercomplex associate factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	76	Total	C	N	O	S	0	0
			575	372	103	98	2		
1	b	76	Total	C	N	O	S	0	0
			575	372	103	98	2		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	551	Total	C	N	O	S	0	0
			4363	2936	696	707	24		
2	L	551	Total	C	N	O	S	0	0
			4363	2936	696	707	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	68	Total	C	N	O	S	0	0
			509	333	86	87	3		
3	h	68	Total	C	N	O	S	0	0
			509	333	86	87	3		

- Molecule 4 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	221	Total	C	N	O	S	0	0
			1639	1015	296	318	10		
4	o	221	Total	C	N	O	S	0	0
			1639	1015	296	318	10		

- Molecule 5 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	381	Total	C	N	O	S	0	0
			2957	1900	511	534	12		
5	p	381	Total	C	N	O	S	0	0
			2957	1900	511	534	12		

- Molecule 6 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	25	Total	C	N	O	S	0	0
			171	104	28	38	1		
6	a	25	Total	C	N	O	S	0	0
			171	104	28	38	1		

- Molecule 7 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	312	Total	C	N	O	S	0	0
			2476	1604	418	445	9		
7	e	312	Total	C	N	O	S	0	0
			2476	1604	418	445	9		

- Molecule 8 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	206	Total	C	N	O	S	0	0
			1595	1053	259	275	8		
8	g	206	Total	C	N	O	S	0	0
			1595	1053	259	275	8		

- Molecule 9 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	527	Total	C	N	O	S	0	0
			4127	2716	693	696	22		
9	j	527	Total	C	N	O	S	0	0
			4127	2716	693	696	22		

- Molecule 10 is a protein called DUF5130 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	144	Total	C	N	O	S	0	0
			1063	669	184	209	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	144	Total	C	N	O	S	0	0
			1063	669	184	209	1		

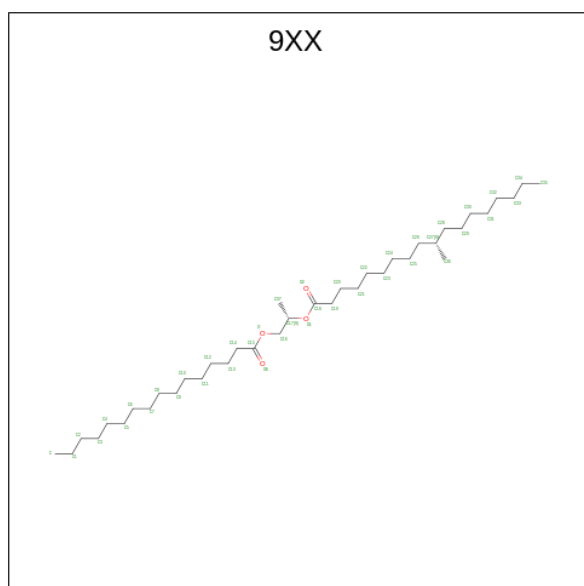
- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	139	Total	C	N	O	S	0	0
			1066	704	169	188	5		
11	n	139	Total	C	N	O	S	0	0
			1066	704	169	188	5		

- Molecule 12 is a protein called Lipoprotein lpqE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	156	Total	C	N	O	S	0	0
			1129	696	201	231	1		
12	r	156	Total	C	N	O	S	0	0
			1129	696	201	231	1		

- Molecule 13 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C<sub>38</sub>H<sub>74</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



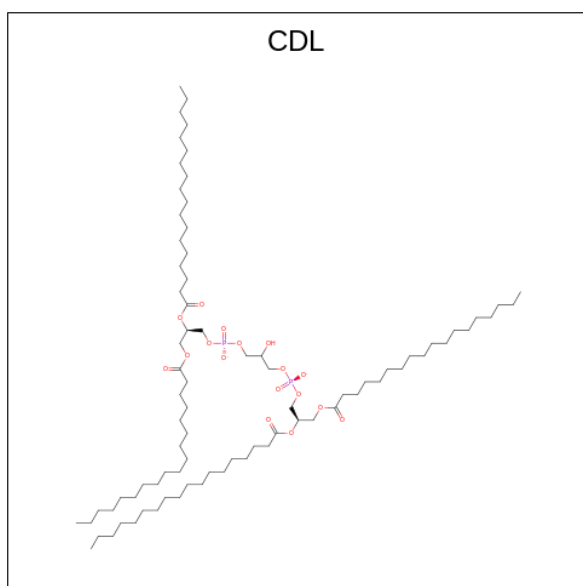
Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	C	O	0
			42	38	4	

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Mol	Chain	Residues	Atoms			AltConf
13	b	1	Total	C	O	0
			42	38	4	
13	i	1	Total	C	O	0
			32	28	4	
13	j	1	Total	C	O	0
			32	28	4	

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



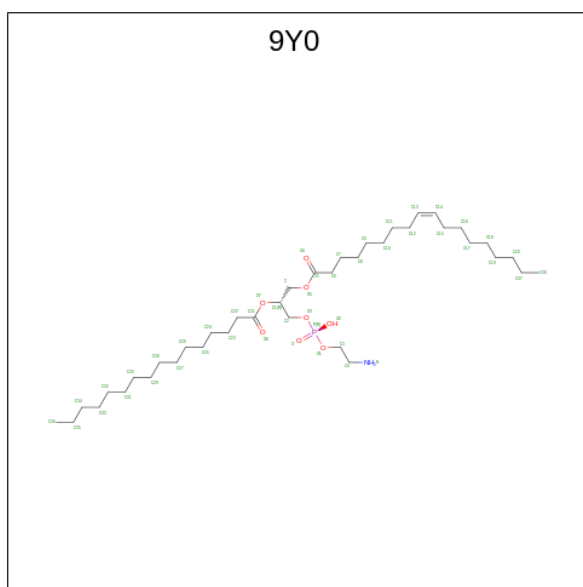
Mol	Chain	Residues	Atoms				AltConf
14	G	1	Total	C	O	P	0
			88	69	17	2	
14	I	1	Total	C	O	P	0
			76	57	17	2	
14	I	1	Total	C	O	P	0
			81	62	17	2	
14	L	1	Total	C	O	P	0
			76	57	17	2	
14	L	1	Total	C	O	P	0
			81	62	17	2	
14	U	1	Total	C	O	P	0
			79	60	17	2	
14	b	1	Total	C	O	P	0
			88	69	17	2	
14	g	1	Total	C	O	P	0
			95	76	17	2	

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Mol	Chain	Residues	Atoms				AltConf
14	i	1	Total	C	O	P	0
			66	47	17	2	
14	i	1	Total	C	O	P	0
			74	55	17	2	
14	i	1	Total	C	O	P	0
			77	58	17	2	
14	i	1	Total	C	O	P	0
			79	60	17	2	
14	i	1	Total	C	O	P	0
			74	55	17	2	
14	j	1	Total	C	O	P	0
			77	58	17	2	
14	j	1	Total	C	O	P	0
			79	60	17	2	
14	j	1	Total	C	O	P	0
			66	47	17	2	
14	m	1	Total	C	O	P	0
			79	60	17	2	
14	p	1	Total	C	O	P	0
			95	76	17	2	

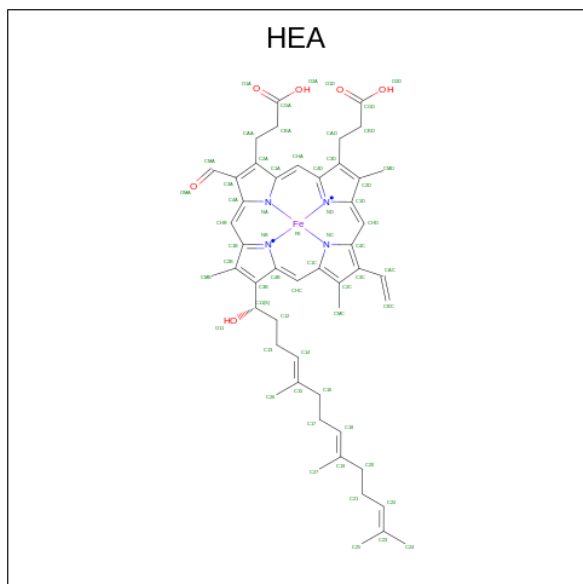
- Molecule 15 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	b	1	Total	C	N	O	P	0
			38	28	1	8	1	
15	b	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	f	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	q	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 16 is HEME-A (CCD ID: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).

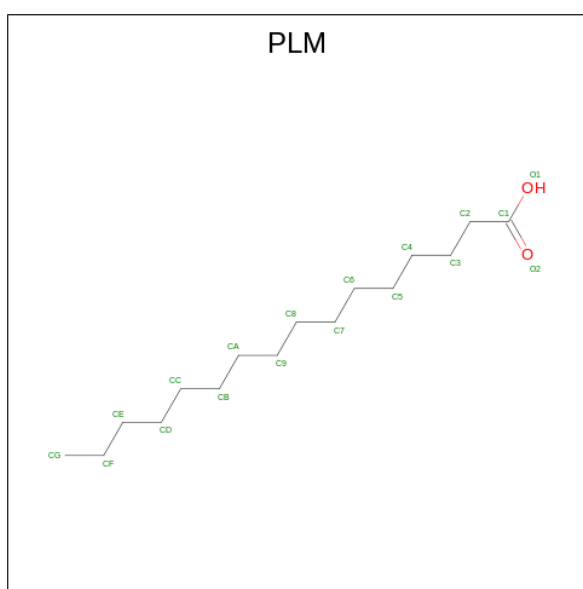


Mol	Chain	Residues	Atoms					AltConf
16	I	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
16	I	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
16	L	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
16	L	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 17 is COPPER (II) ION (CCD ID: CU) (formula:  $Cu$ ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	I	2	Total 2	Cu 2	0
17	L	2	Total 2	Cu 2	0
17	d	2	Total 2	Cu 2	0
17	e	2	Total 2	Cu 2	0

- Molecule 18 is PALMITIC ACID (CCD ID: PLM) (formula:  $C_{16}H_{32}O_2$ ) (labeled as "Ligand of Interest" by depositor).

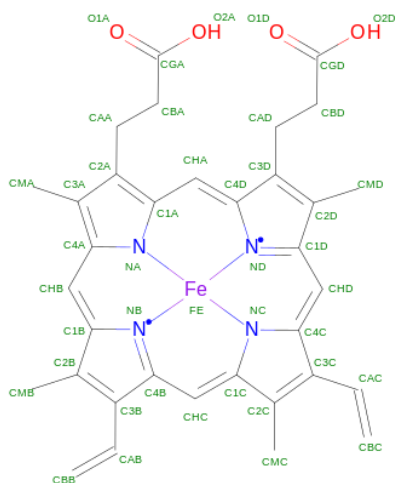


Mol	Chain	Residues	Atoms			AltConf
18	I	1	Total 17	C 16	O 1	0
18	q	1	Total 17	C 16	O 1	0

- Molecule 19 is OXYGEN MOLECULE (CCD ID: OXY) (formula:  $O_2$ ) (labeled as "Ligand of Interest" by depositor).



- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ) (labeled as "Ligand of Interest" by depositor).

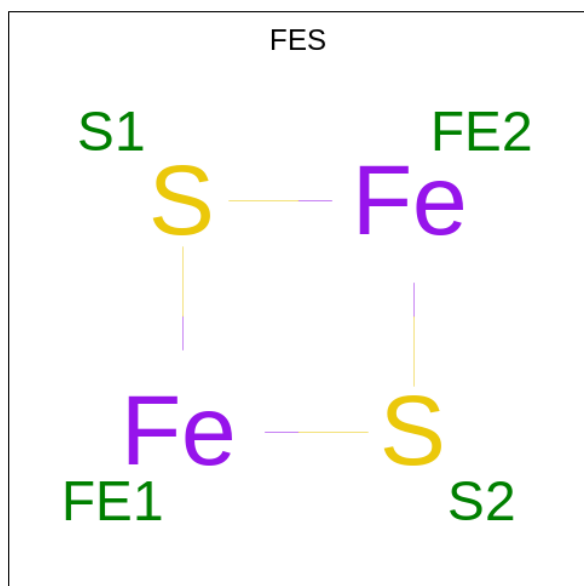


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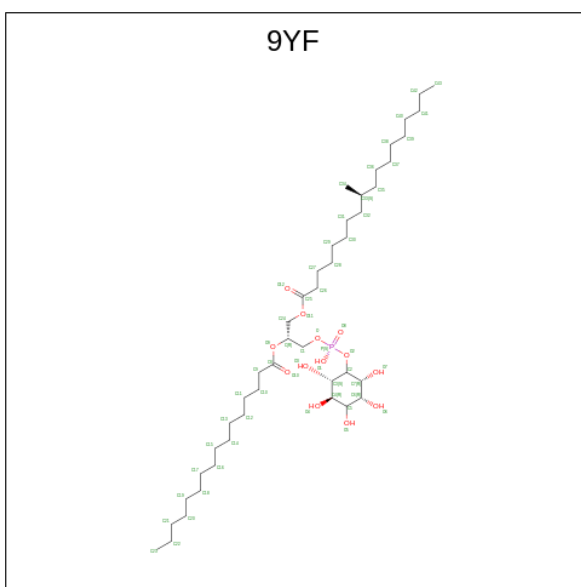
Mol	Chain	Residues	Atoms					AltConf
20	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	i	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
20	i	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	j	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
20	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



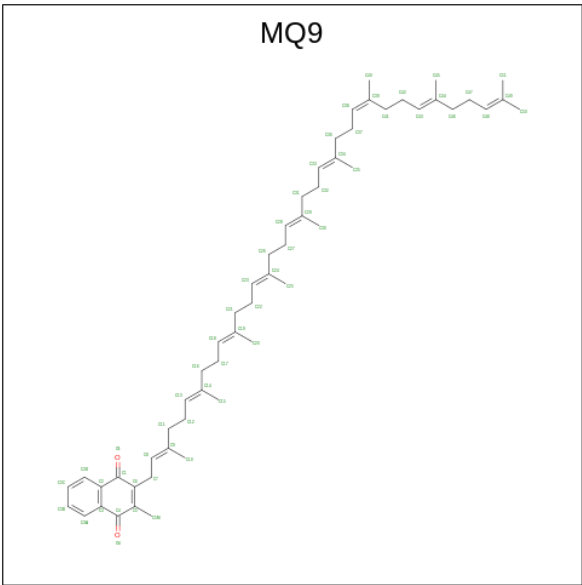
Mol	Chain	Residues	Atoms			AltConf
21	V	1	Total	Fe	S	0
			4	2	2	
21	p	1	Total	Fe	S	0
			4	2	2	

- Molecule 22 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula:  $\text{C}_{44}\text{H}_{85}\text{O}_{13}\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	V	1	Total	C	O	P	0
			58	44	13	1	
22	i	1	Total	C	O	P	0
			58	44	13	1	
22	j	1	Total	C	O	P	0
			58	44	13	1	
22	n	1	Total	C	O	P	0
			58	44	13	1	
22	o	1	Total	C	O	P	0
			58	44	13	1	
22	p	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 23 is MENAQUINONE-9 (CCD ID: MQ9) (formula:  $C_{56}H_{80}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	i	1	Total	C	O	0
			58	56	2	
23	i	1	Total	C	O	0
			58	56	2	
23	i	1	Total	C	O	0
			43	41	2	
23	i	1	Total	C	O	0
			48	46	2	
23	i	1	Total	C	O	0
			58	56	2	
23	j	1	Total	C	O	0
			58	56	2	
23	j	1	Total	C	O	0
			43	41	2	
23	j	1	Total	C	O	0
			58	56	2	
23	j	1	Total	C	O	0
			58	56	2	
23	m	1	Total	C	O	0
			48	46	2	

- Molecule 24 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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Mol	Chain	Residues	Atoms		AltConf
25	o	4	Total	O	0
			4	4	
25	p	3	Total	O	0
			3	3	

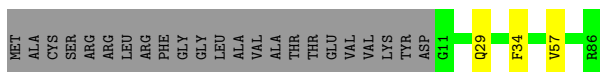


### 3 Residue-property plots [i](#)

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

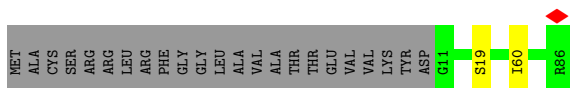
- Molecule 1: Prokaryotic respiratory supercomplex associate factor 1

Chain G:  74% 23%




- Molecule 1: Prokaryotic respiratory supercomplex associate factor 1

Chain b:  75% 23%




- Molecule 2: Cytochrome c oxidase subunit 1

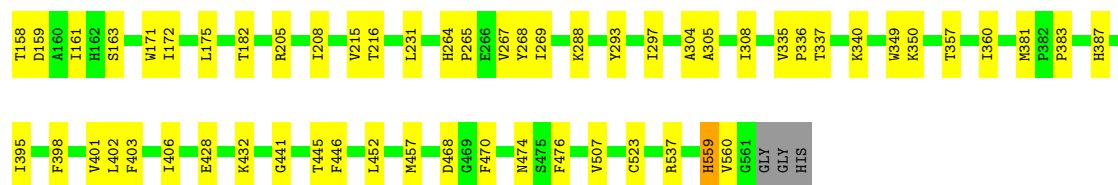
Chain I:  81% 16%



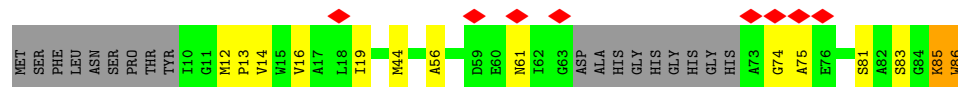
- Molecule 2: Cytochrome c oxidase subunit 1

Chain L:  83% 15%





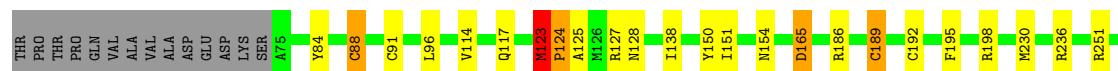
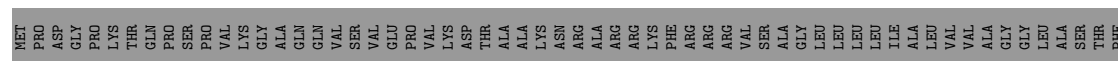
• Molecule 3: Cytochrome c oxidase subunit CtaJ



• Molecule 3: Cytochrome c oxidase subunit CtaJ



• Molecule 4: Cytochrome bc1 complex cytochrome c subunit



• Molecule 4: Cytochrome bc1 complex cytochrome c subunit



• Molecule 5: Cytochrome bc1 complex Rieske iron-sulfur subunit



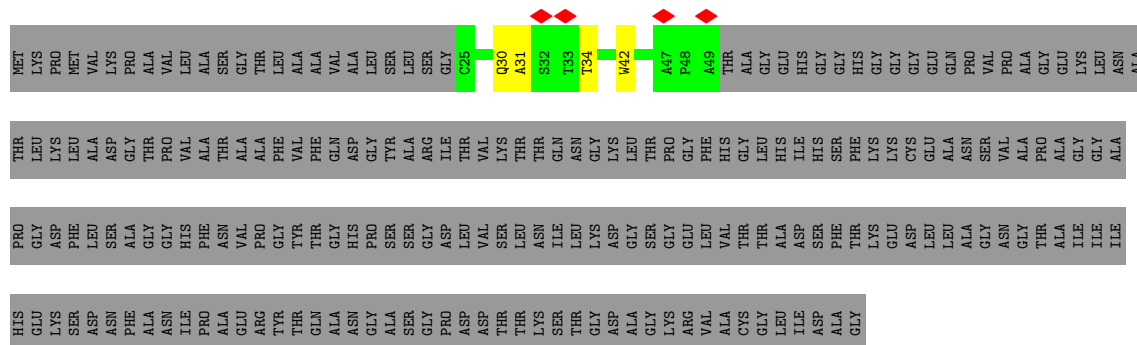
- Molecule 5: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain p:  90% 8%



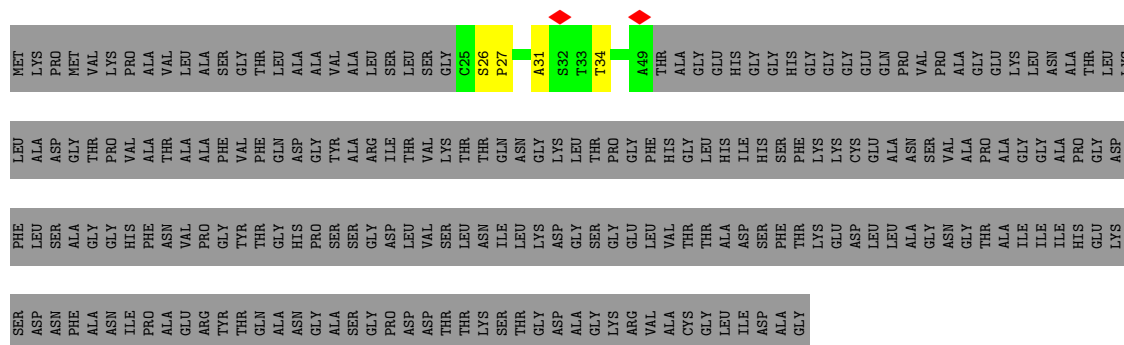
- Molecule 6: Superoxide dismutase [Cu-Zn]

Chain X:  9% 89%




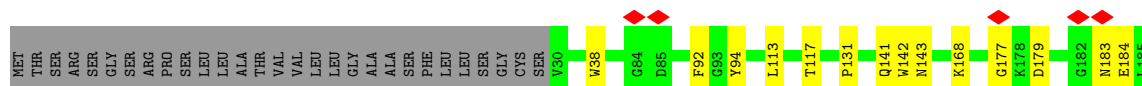
- Molecule 6: Superoxide dismutase [Cu-Zn]

Chain a:  9% 89%



- Molecule 7: cytochrome-c oxidase

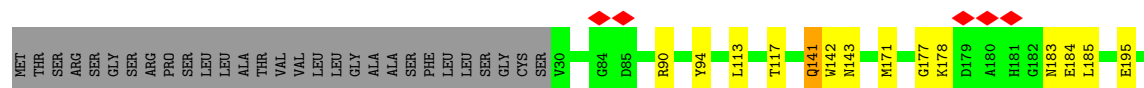
Chain d:  80% 9% 11%





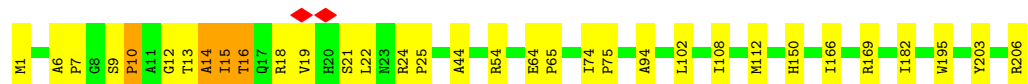
- Molecule 7: cytochrome-c oxidase

Chain e: 82% 7% 11%



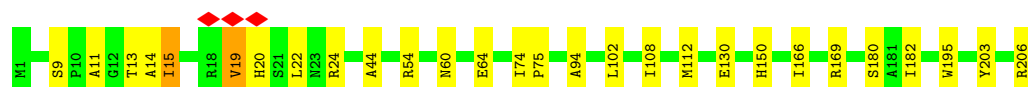
- Molecule 8: Probable cytochrome c oxidase subunit 3

Chain f: 84% 14% 2%



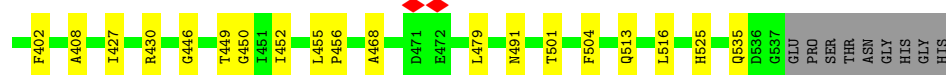
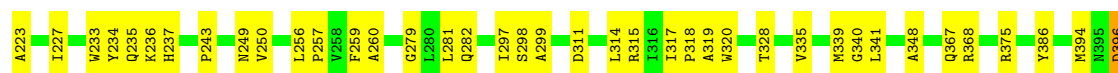
- Molecule 8: Probable cytochrome c oxidase subunit 3

Chain g: 86% 13% 1%



- Molecule 9: Cytochrome bc1 complex cytochrome b subunit

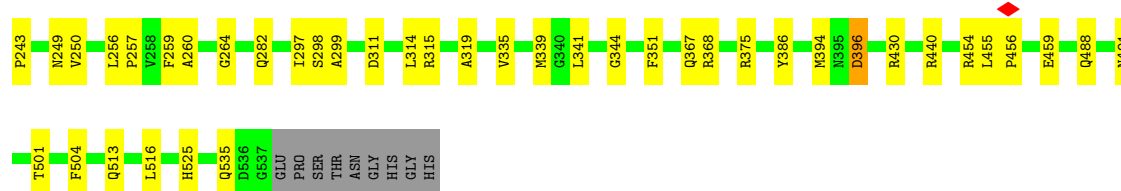
Chain i: 81% 15% 4%



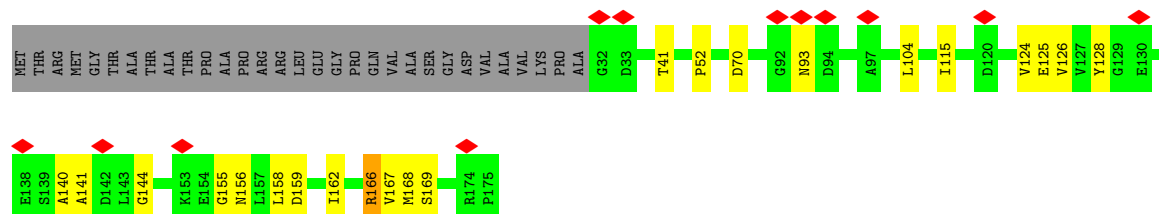
- Molecule 9: Cytochrome bc1 complex cytochrome b subunit

Chain j: 84% 12% 4%

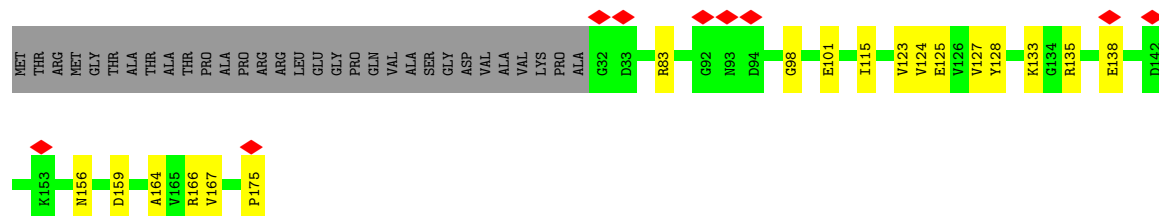




- Molecule 10: DUF5130 domain-containing protein



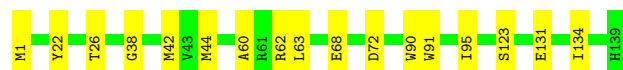
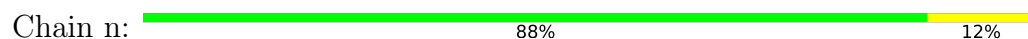
- Molecule 10: DUF5130 domain-containing protein



- Molecule 11: Cytochrome c oxidase polypeptide 4

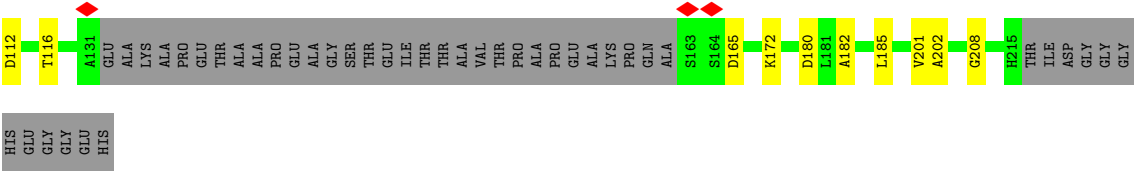


- Molecule 11: Cytochrome c oxidase polypeptide 4

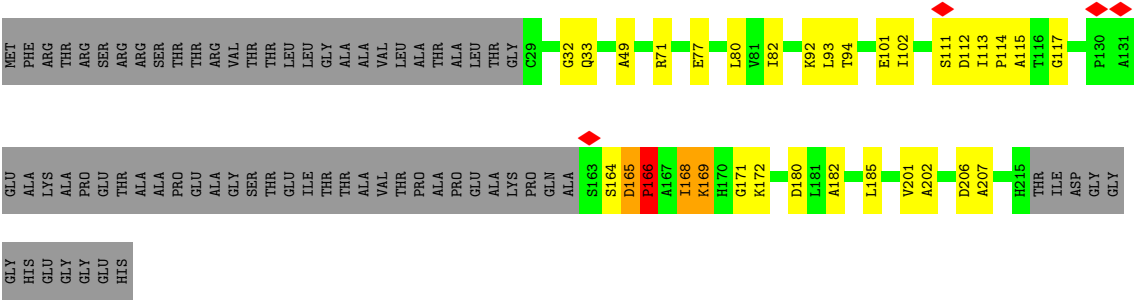


- Molecule 12: Lipoprotein lpqE





● Molecule 12: Lipoprotein lpqE



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194219	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 ( $e^-/\text{\AA}^2$ )	56	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.818	Depositor
Minimum map value	-1.707	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.29	Depositor
Map size ( $\text{\AA}$ )	402.6, 402.6, 402.6	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.671, 0.671, 0.671	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: CDL, CU, 9XX, FES, OXY, HEM, 9YF, 9Y0, HEC, PLM, HEA, 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	G	0.16	0/585	0.25	0/789
1	b	0.16	0/585	0.27	0/789
2	I	0.27	0/4526	0.47	2/6181 (0.0%)
2	L	0.32	1/4526 (0.0%)	0.48	4/6181 (0.1%)
3	J	0.18	0/526	0.35	0/718
3	h	0.14	0/526	0.36	0/718
4	U	0.42	0/1669	0.62	3/2257 (0.1%)
4	o	0.38	0/1669	0.59	4/2257 (0.2%)
5	V	0.17	0/3033	0.33	0/4120
5	p	0.17	0/3033	0.32	0/4120
6	X	0.46	0/177	0.85	1/248 (0.4%)
6	a	0.16	0/177	0.43	0/248
7	d	0.35	1/2547 (0.0%)	0.45	3/3466 (0.1%)
7	e	0.51	2/2547 (0.1%)	0.39	0/3466
8	f	0.35	1/1644 (0.1%)	0.46	2/2244 (0.1%)
8	g	0.31	1/1644 (0.1%)	0.42	2/2244 (0.1%)
9	i	0.26	1/4252 (0.0%)	0.42	3/5785 (0.1%)
9	j	0.19	0/4252	0.34	0/5785
10	k	0.21	0/1083	0.33	0/1474
10	l	0.17	0/1083	0.31	0/1474
11	m	0.16	0/1097	0.29	0/1499
11	n	0.58	2/1097 (0.2%)	0.48	4/1499 (0.3%)
12	q	0.14	0/1144	0.32	0/1551
12	r	0.37	1/1144 (0.1%)	0.54	4/1551 (0.3%)
All	All	0.30	10/44566 (0.0%)	0.43	32/60664 (0.1%)

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
4	U	0	1
7	d	0	1
10	k	0	1
10	l	0	1
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	n	131	GLU	C-O	17.25	1.44	1.24
7	e	336	ARG	CA-CB	16.80	1.79	1.53
7	e	336	ARG	C-N	14.64	1.49	1.33
7	d	336	ARG	CA-CB	13.09	1.75	1.53
2	L	559	HIS	CA-C	-11.38	1.38	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	n	131	GLU	O-C-N	-11.07	109.53	122.15
4	o	124	PRO	N-CA-C	-10.25	91.35	112.47
4	U	124	PRO	N-CA-C	-9.07	93.78	112.47
2	L	559	HIS	CB-CA-C	7.65	122.46	109.53
4	U	124	PRO	CB-CA-C	7.09	123.26	111.56

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	U	186	ARG	Sidechain
7	d	276	ARG	Sidechain
10	k	166	ARG	Sidechain
10	l	166	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	575	0	591	5	0
1	b	575	0	591	2	0
2	I	4363	0	4322	80	0
2	L	4363	0	4322	64	0
3	J	509	0	500	17	0
3	h	509	0	500	15	0
4	U	1639	0	1600	41	0
4	o	1639	0	1598	24	0
5	V	2957	0	2964	30	0
5	p	2957	0	2964	25	0
6	X	171	0	156	4	0
6	a	171	0	156	4	0
7	d	2476	0	2445	34	0
7	e	2476	0	2445	28	0
8	f	1595	0	1581	40	0
8	g	1595	0	1581	40	0
9	i	4127	0	4158	84	0
9	j	4127	0	4158	77	0
10	k	1063	0	1049	28	0
10	l	1063	0	1049	18	0
11	m	1066	0	1052	15	0
11	n	1066	0	1052	14	0
12	q	1129	0	1126	22	0
12	r	1129	0	1126	31	0
13	G	42	0	0	1	0
13	b	42	0	0	1	0
13	i	32	0	0	2	0
13	j	32	0	0	0	0
14	G	88	0	126	13	0
14	I	157	0	208	14	0
14	L	157	0	208	11	0
14	U	79	0	105	3	0
14	b	88	0	126	33	0
14	g	95	0	143	13	0
14	i	370	0	463	34	0
14	j	222	0	279	11	0
14	m	79	0	105	8	0
14	p	95	0	143	19	0
15	G	41	0	0	0	0
15	b	79	0	0	0	0
15	f	43	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	g	43	0	0	0	0
15	q	38	0	0	1	0
16	I	120	0	108	9	0
16	L	120	0	108	8	0
17	I	2	0	0	0	0
17	L	2	0	0	0	0
17	d	2	0	0	1	0
17	e	2	0	0	0	0
18	I	17	0	31	0	0
18	q	17	0	31	5	0
19	I	2	0	0	0	0
19	L	2	0	0	0	0
20	U	86	0	60	12	0
20	i	85	0	57	1	0
20	j	85	0	57	4	0
21	V	4	0	0	0	0
21	p	4	0	0	0	0
22	V	58	0	0	1	0
22	i	58	0	0	1	0
22	j	58	0	0	0	0
22	n	58	0	0	1	0
22	o	58	0	0	4	0
22	p	58	0	0	1	0
23	i	265	0	349	71	0
23	j	217	0	293	37	0
23	m	48	0	61	9	0
24	o	86	0	62	10	0
25	I	18	0	0	2	0
25	L	18	0	0	3	0
25	U	3	0	0	0	0
25	V	2	0	0	0	0
25	d	1	0	0	0	0
25	e	1	0	0	0	0
25	i	9	0	0	0	0
25	j	10	0	0	0	0
25	m	2	0	0	0	0
25	n	3	0	0	0	0
25	o	4	0	0	0	0
25	p	3	0	0	0	0
All	All	46750	0	46209	812	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 812 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:336:ARG:CA	7:d:336:ARG:CB	1.75	1.60
23:i:610:MQ9:C26	23:i:610:MQ9:C20	1.74	1.54
7:e:336:ARG:CB	7:e:336:ARG:CA	1.80	1.54
23:i:610:MQ9:C27	23:i:610:MQ9:C19	1.99	1.40
8:g:169:ARG:HD3	9:j:504:PHE:CE1	1.55	1.39

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	G	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
1	b	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
2	I	549/564 (97%)	520 (95%)	29 (5%)	0	100	100
2	L	549/564 (97%)	521 (95%)	28 (5%)	0	100	100
3	J	64/86 (74%)	61 (95%)	3 (5%)	0	100	100
3	h	64/86 (74%)	61 (95%)	3 (5%)	0	100	100
4	U	219/295 (74%)	205 (94%)	14 (6%)	0	100	100
4	o	219/295 (74%)	204 (93%)	15 (7%)	0	100	100
5	V	379/391 (97%)	370 (98%)	9 (2%)	0	100	100
5	p	379/391 (97%)	367 (97%)	12 (3%)	0	100	100
6	X	23/238 (10%)	20 (87%)	3 (13%)	0	100	100
6	a	23/238 (10%)	20 (87%)	3 (13%)	0	100	100
7	d	310/349 (89%)	295 (95%)	15 (5%)	0	100	100
7	e	310/349 (89%)	296 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	f	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	24	39
8	g	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	12	20
9	i	525/546 (96%)	494 (94%)	31 (6%)	0	100	100
9	j	525/546 (96%)	497 (95%)	28 (5%)	0	100	100
10	k	142/175 (81%)	139 (98%)	3 (2%)	0	100	100
10	l	142/175 (81%)	137 (96%)	5 (4%)	0	100	100
11	m	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
11	n	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
12	q	152/227 (67%)	144 (95%)	8 (5%)	0	100	100
12	r	152/227 (67%)	140 (92%)	11 (7%)	1 (1%)	18	30
All	All	5556/6630 (84%)	5282 (95%)	270 (5%)	4 (0%)	49	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	f	10	PRO
8	g	19	VAL
8	g	15	ILE
12	r	166	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	59/77 (77%)	59 (100%)	0	100	100
1	b	59/77 (77%)	59 (100%)	0	100	100
2	I	448/455 (98%)	441 (98%)	7 (2%)	55	74
2	L	448/455 (98%)	443 (99%)	5 (1%)	65	80
3	J	49/63 (78%)	47 (96%)	2 (4%)	27	46
3	h	49/63 (78%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	U	164/223 (74%)	159 (97%)	5 (3%)	36	57
4	o	164/223 (74%)	162 (99%)	2 (1%)	63	79
5	V	312/321 (97%)	312 (100%)	0	100	100
5	p	312/321 (97%)	311 (100%)	1 (0%)	86	94
6	X	20/173 (12%)	20 (100%)	0	100	100
6	a	20/173 (12%)	20 (100%)	0	100	100
7	d	269/298 (90%)	264 (98%)	5 (2%)	50	71
7	e	269/298 (90%)	265 (98%)	4 (2%)	57	75
8	f	163/163 (100%)	160 (98%)	3 (2%)	51	72
8	g	163/163 (100%)	163 (100%)	0	100	100
9	i	421/437 (96%)	415 (99%)	6 (1%)	59	76
9	j	421/437 (96%)	417 (99%)	4 (1%)	68	81
10	k	108/130 (83%)	107 (99%)	1 (1%)	70	82
10	l	108/130 (83%)	107 (99%)	1 (1%)	70	82
11	m	103/103 (100%)	103 (100%)	0	100	100
11	n	103/103 (100%)	103 (100%)	0	100	100
12	q	121/171 (71%)	121 (100%)	0	100	100
12	r	121/171 (71%)	119 (98%)	2 (2%)	53	73
All	All	4474/5228 (86%)	4426 (99%)	48 (1%)	63	80

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	f	1	MET
9	i	452	ILE
8	f	15	ILE
9	i	235	GLN
9	j	235	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
7	d	285	HIS
12	q	64	ASN
9	i	80	GLN

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Mol	Chain	Res	Type
12	q	60	HIS
12	r	60	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 70 ligands modelled in this entry, 8 are monoatomic - leaving 62 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	$\# Z  > 2$
13	9XX	i	613	-	31,31,41	0.32	0	34,34,44	0.33	0
14	CDL	i	604	-	65,65,99	0.33	0	71,77,111	0.39	0
21	FES	V	601	5	0,4,4	-	-	-		
22	9YF	i	601	-	58,58,58	0.32	0	69,71,71	0.42	0
16	HEA	L	601	2	66,67,67	2.37	22 (33%)	78,103,103	2.60	31 (39%)
23	MQ9	j	611	-	59,59,59	0.36	0	72,75,75	0.39	0
15	9Y0	f	601	-	42,42,48	0.34	0	44,47,53	0.39	0
14	CDL	U	603	-	78,78,99	0.97	3 (3%)	84,90,111	0.45	0
14	CDL	I	605	-	80,80,99	0.31	0	86,92,111	0.41	0
22	9YF	V	602	-	58,58,58	1.61	6 (10%)	69,71,71	1.63	9 (13%)
15	9Y0	b	104	-	40,40,48	0.35	0	43,45,53	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	HEM	j	604	9	50,50,50	1.71	12 (24%)	66,82,82	1.94	16 (24%)
16	HEA	I	601	2	66,67,67	2.38	22 (33%)	78,103,103	2.59	31 (39%)
15	9Y0	b	101	-	37,37,48	0.35	0	40,42,53	0.41	0
14	CDL	j	606	-	78,78,99	0.35	0	84,90,111	0.47	0
23	MQ9	j	602	-	59,59,59	0.32	0	72,75,75	0.45	0
15	9Y0	q	301	-	37,37,48	0.37	0	40,42,53	0.38	0
18	PLM	q	302	-	16,16,17	0.35	0	15,15,17	0.39	0
14	CDL	i	609	-	78,78,99	0.36	0	84,90,111	0.38	0
14	CDL	i	614	-	73,73,99	0.34	0	79,85,111	0.42	0
14	CDL	I	604	-	75,75,99	0.33	0	81,87,111	0.40	0
14	CDL	j	609	-	65,65,99	0.34	0	71,77,111	0.39	0
15	9Y0	g	302	-	42,42,48	0.35	0	44,47,53	0.42	0
23	MQ9	j	608	-	59,59,59	0.34	0	72,75,75	0.40	0
22	9YF	o	603	-	58,58,58	0.29	0	69,71,71	0.41	0
16	HEA	L	602	2	66,67,67	2.40	23 (34%)	78,103,103	2.53	35 (44%)
20	HEM	U	601	4	50,50,50	2.88	25 (50%)	66,82,82	2.29	20 (30%)
23	MQ9	i	612	-	59,59,59	0.35	0	72,75,75	0.51	0
14	CDL	L	606	-	80,80,99	0.31	0	86,92,111	0.39	0
14	CDL	j	605	-	76,76,99	0.35	0	82,88,111	0.37	0
20	HEM	i	605	9	49,49,50	1.68	10 (20%)	66,81,82	1.62	12 (18%)
13	9XX	G	101	-	41,41,41	0.27	0	44,44,44	0.57	1 (2%)
23	MQ9	j	607	-	44,44,59	0.34	0	54,57,75	0.52	0
14	CDL	m	202	-	78,78,99	0.33	0	84,90,111	0.38	0
24	HEC	o	602	4	46,50,50	3.56	3 (6%)	60,82,82	2.07	9 (15%)
20	HEM	j	603	9	49,49,50	1.66	9 (18%)	66,81,82	1.63	12 (18%)
23	MQ9	m	201	-	49,49,59	0.39	0	60,63,75	0.42	0
14	CDL	i	607	-	73,73,99	0.33	0	79,85,111	0.37	0
14	CDL	b	103	-	87,87,99	0.31	0	93,99,111	0.34	0
24	HEC	o	601	4	46,50,50	3.73	23 (50%)	60,82,82	2.10	21 (35%)
16	HEA	I	602	2	66,67,67	2.40	23 (34%)	78,103,103	2.53	36 (46%)
19	OXY	L	607	-	1,1,1	0.15	0	-	-	-
13	9XX	b	102	-	41,41,41	0.28	0	44,44,44	0.22	0
21	FES	p	602	5	0,4,4	-	-	-	-	-
15	9Y0	G	103	-	40,40,48	0.32	0	43,45,53	0.42	0
14	CDL	i	608	-	76,76,99	0.36	0	82,88,111	0.43	0
22	9YF	j	601	-	58,58,58	0.31	0	69,71,71	0.43	0
14	CDL	L	605	-	75,75,99	0.38	0	81,87,111	0.24	0
14	CDL	G	102	-	87,87,99	0.31	0	93,99,111	0.41	0
14	CDL	p	603	-	94,94,99	0.29	0	100,106,111	0.34	0
22	9YF	n	201	-	58,58,58	0.26	0	69,71,71	0.38	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	9YF	p	601	-	58,58,58	0.31	0	69,71,71	0.54	1 (1%)
23	MQ9	i	603	-	59,59,59	0.35	0	72,75,75	0.41	0
20	HEM	U	602	4	50,50,50	2.86	28 (56%)	66,82,82	2.42	22 (33%)
23	MQ9	i	602	-	59,59,59	0.35	0	72,75,75	0.42	0
14	CDL	g	301	-	94,94,99	0.29	0	100,106,111	0.32	0
23	MQ9	i	610	-	44,44,59	0.33	0	54,57,75	0.39	0
20	HEM	i	606	9	50,50,50	1.68	11 (22%)	66,82,82	1.91	18 (27%)
23	MQ9	i	611	-	49,49,59	0.34	0	60,63,75	0.54	1 (1%)
13	9XX	j	610	-	31,31,41	0.31	0	34,34,44	0.40	0
19	OXY	I	607	-	1,1,1	0.15	0	-		
18	PLM	I	606	-	16,16,17	0.34	0	15,15,17	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	9XX	i	613	-	-	6/33/33/43	-
14	CDL	i	604	-	-	17/76/76/110	-
22	9YF	i	601	-	-	9/54/78/78	0/1/1/1
21	FES	V	601	5	-	-	0/1/1/1
16	HEA	L	601	2	-	5/36/76/76	-
23	MQ9	j	611	-	-	31/53/73/73	0/2/2/2
15	9Y0	f	601	-	-	15/46/46/52	-
14	CDL	U	603	-	-	55/89/89/110	-
14	CDL	I	605	-	-	24/91/91/110	-
22	9YF	V	602	-	-	23/54/78/78	0/1/1/1
15	9Y0	b	104	-	-	4/44/44/52	-
20	HEM	j	604	9	-	1/14/54/54	-
16	HEA	I	601	2	-	5/36/76/76	-
15	9Y0	b	101	-	-	9/41/41/52	-
14	CDL	j	606	-	-	27/89/89/110	-
23	MQ9	j	602	-	-	24/53/73/73	0/2/2/2
15	9Y0	q	301	-	-	16/41/41/52	-
18	PLM	q	302	-	-	4/13/14/15	-
14	CDL	i	609	-	-	24/89/89/110	-
14	CDL	i	614	-	-	25/84/84/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	I	604	-	-	22/86/86/110	-
14	CDL	j	609	-	-	22/76/76/110	-
15	9Y0	g	302	-	-	15/46/46/52	-
23	MQ9	j	608	-	-	23/53/73/73	0/2/2/2
22	9YF	o	603	-	-	12/54/78/78	0/1/1/1
16	HEA	L	602	2	-	6/36/76/76	-
20	HEM	U	601	4	-	3/14/54/54	-
23	MQ9	i	612	-	-	36/53/73/73	0/2/2/2
14	CDL	L	606	-	-	21/91/91/110	-
14	CDL	j	605	-	-	17/87/87/110	-
20	HEM	i	605	9	-	6/12/52/54	-
13	9XX	G	101	-	-	10/43/43/43	-
23	MQ9	j	607	-	-	19/35/55/73	0/2/2/2
14	CDL	m	202	-	-	20/89/89/110	-
24	HEC	o	602	4	-	4/14/54/54	-
20	HEM	j	603	9	-	6/12/52/54	-
23	MQ9	m	201	-	-	21/41/61/73	0/2/2/2
14	CDL	i	607	-	-	22/84/84/110	-
14	CDL	b	103	-	-	25/98/98/110	-
24	HEC	o	601	4	-	4/14/54/54	-
16	HEA	I	602	2	-	6/36/76/76	-
13	9XX	b	102	-	-	15/43/43/43	-
21	FES	p	602	5	-	-	0/1/1/1
15	9Y0	G	103	-	-	10/44/44/52	-
14	CDL	i	608	-	-	22/87/87/110	-
22	9YF	j	601	-	-	9/54/78/78	0/1/1/1
14	CDL	L	605	-	-	44/86/86/110	-
14	CDL	G	102	-	-	38/98/98/110	-
14	CDL	p	603	-	-	30/105/105/110	-
22	9YF	n	201	-	-	20/54/78/78	0/1/1/1
22	9YF	p	601	-	-	13/54/78/78	0/1/1/1
23	MQ9	i	603	-	-	24/53/73/73	0/2/2/2
20	HEM	U	602	4	-	2/14/54/54	-
23	MQ9	i	602	-	-	30/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	g	301	-	-	28/105/105/110	-
23	MQ9	i	610	-	-	14/35/55/73	0/2/2/2
20	HEM	i	606	9	-	1/14/54/54	-
23	MQ9	i	611	-	-	15/41/61/73	0/2/2/2
13	9XX	j	610	-	-	6/33/33/43	-
18	PLM	I	606	-	-	1/13/14/15	-

The worst 5 of 220 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	o	602	HEC	CAC-C3C	16.22	1.55	1.34
24	o	602	HEC	CAB-C3B	15.74	1.55	1.34
24	o	601	HEC	CAC-C3C	15.70	1.55	1.34
24	o	601	HEC	CAB-C3B	10.63	1.48	1.34
14	U	603	CDL	CB3-CB4	6.23	1.69	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	602	HEM	C3B-C2B-C1B	-9.55	99.40	106.49
24	o	602	HEC	CBB-CAB-C3B	-8.87	111.56	127.86
20	U	601	HEM	C3B-C2B-C1B	-7.98	100.57	106.49
20	j	604	HEM	CHC-C4B-NB	7.05	132.08	124.42
16	L	601	HEA	C3C-C4C-NC	7.00	114.56	110.25

There are no chirality outliers.

5 of 966 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	b	102	9XX	O-C16-C17-C37
13	b	102	9XX	O-C16-C17-O1
13	b	102	9XX	C36-C27-C28-C29
13	j	610	9XX	O-C16-C17-C37
14	G	102	CDL	CA3-OA5-PA1-OA4

There are no ring outliers.

50 monomers are involved in 323 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	i	613	9XX	2	0

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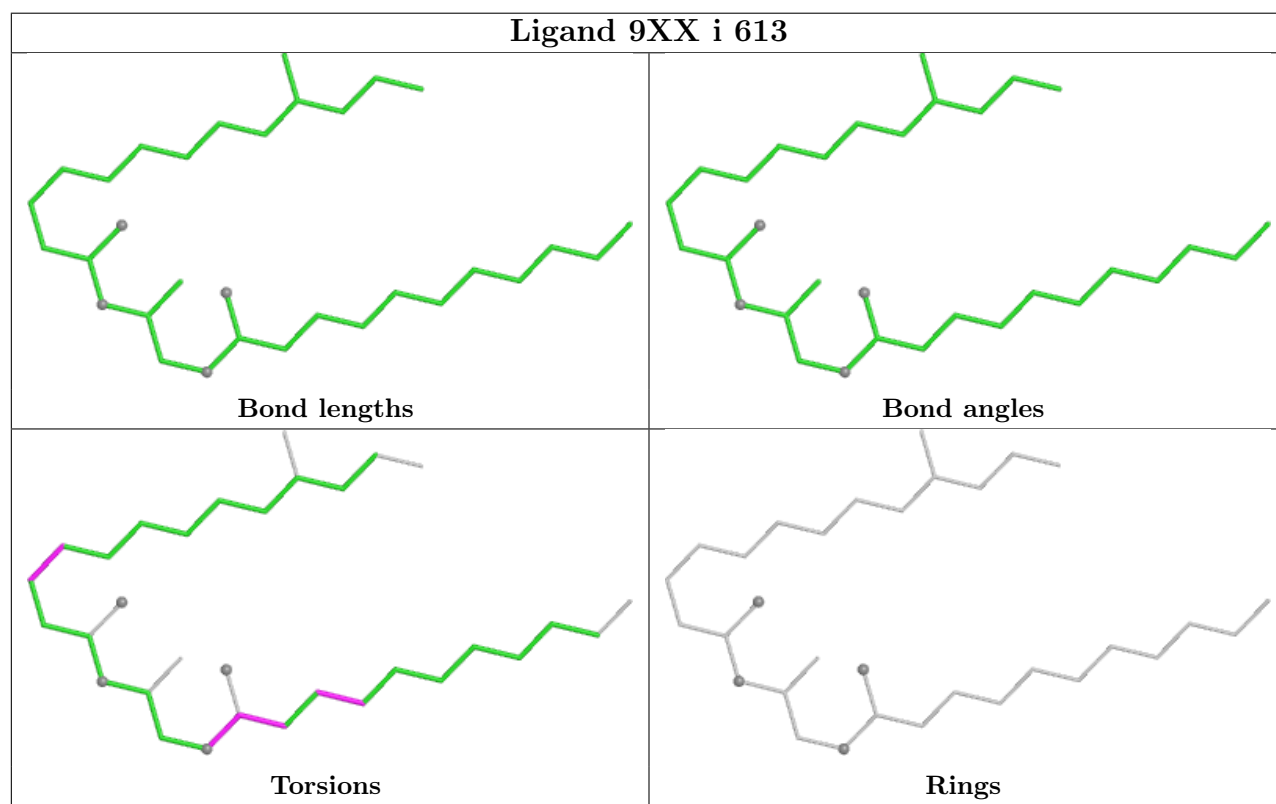
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	i	604	CDL	5	0
22	i	601	9YF	1	0
16	L	601	HEA	3	0
23	j	611	MQ9	6	0
15	f	601	9Y0	1	0
14	U	603	CDL	3	0
14	I	605	CDL	6	0
22	V	602	9YF	1	0
20	j	604	HEM	2	0
16	I	601	HEA	3	0
14	j	606	CDL	5	0
23	j	602	MQ9	9	0
15	q	301	9Y0	1	0
18	q	302	PLM	5	0
14	i	609	CDL	5	0
14	i	614	CDL	10	0
14	I	604	CDL	8	0
14	j	609	CDL	3	0
23	j	608	MQ9	14	0
22	o	603	9YF	4	0
16	L	602	HEA	5	0
20	U	601	HEM	8	0
23	i	612	MQ9	19	0
14	L	606	CDL	8	0
14	j	605	CDL	3	0
20	i	605	HEM	1	0
13	G	101	9XX	1	0
23	j	607	MQ9	11	0
14	m	202	CDL	8	0
24	o	602	HEC	2	0
20	j	603	HEM	2	0
23	m	201	MQ9	9	0
14	i	607	CDL	11	0
14	b	103	CDL	33	0
24	o	601	HEC	8	0
16	I	602	HEA	6	0
13	b	102	9XX	1	0
14	i	608	CDL	3	0
14	L	605	CDL	3	0
14	G	102	CDL	13	0
14	p	603	CDL	19	0
22	n	201	9YF	1	0

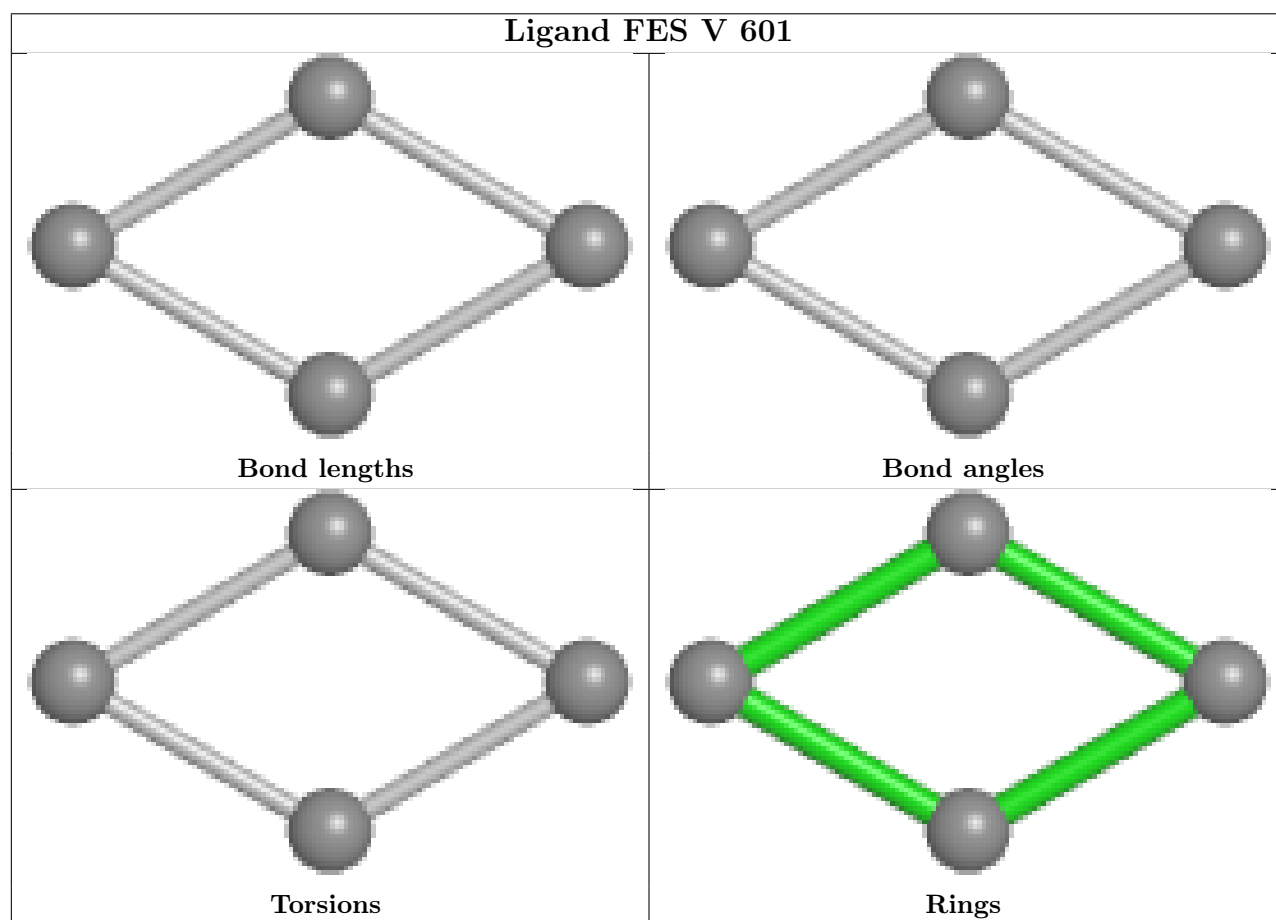
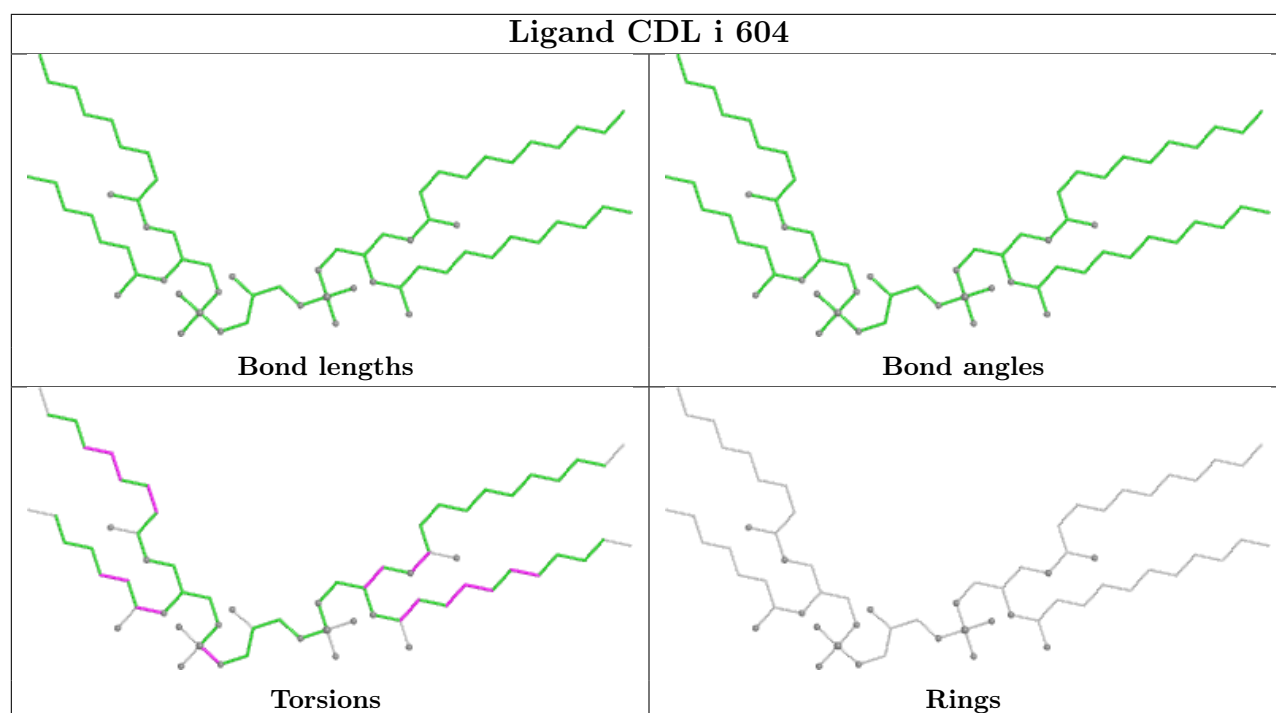
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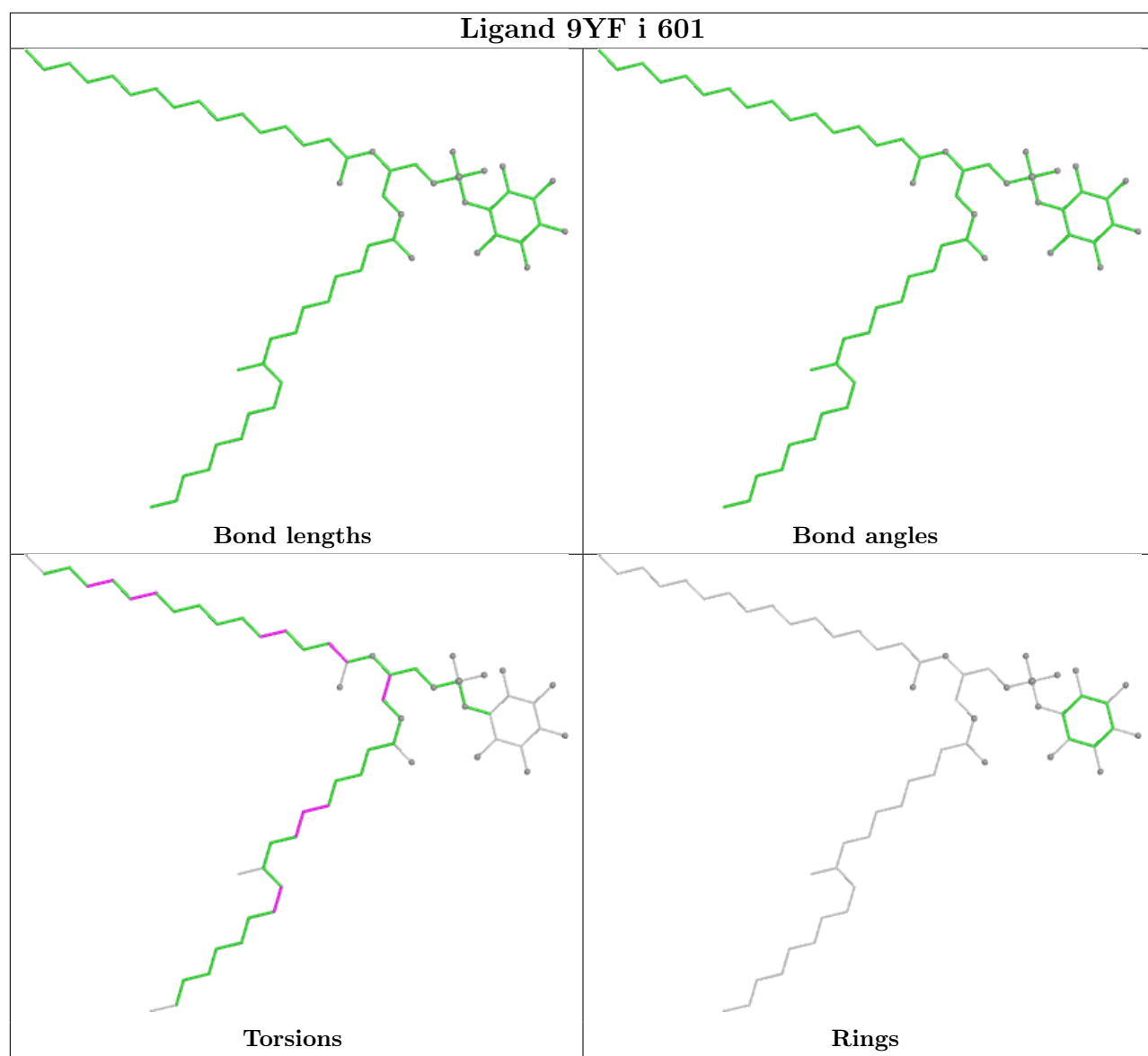
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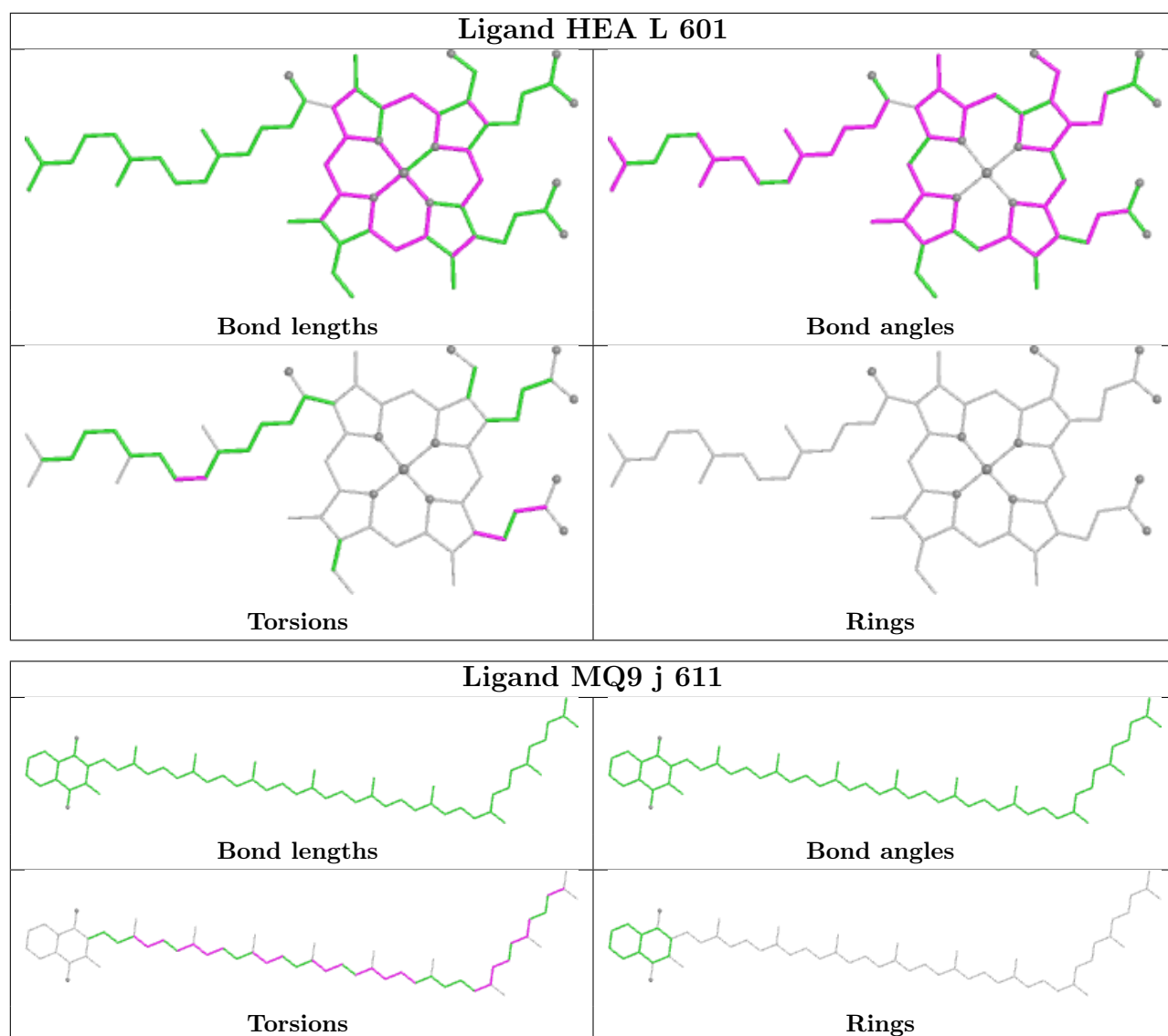
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	p	601	9YF	1	0
23	i	603	MQ9	8	0
20	U	602	HEM	4	0
23	i	602	MQ9	5	0
14	g	301	CDL	13	0
23	i	610	MQ9	21	0
23	i	611	MQ9	18	0

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.

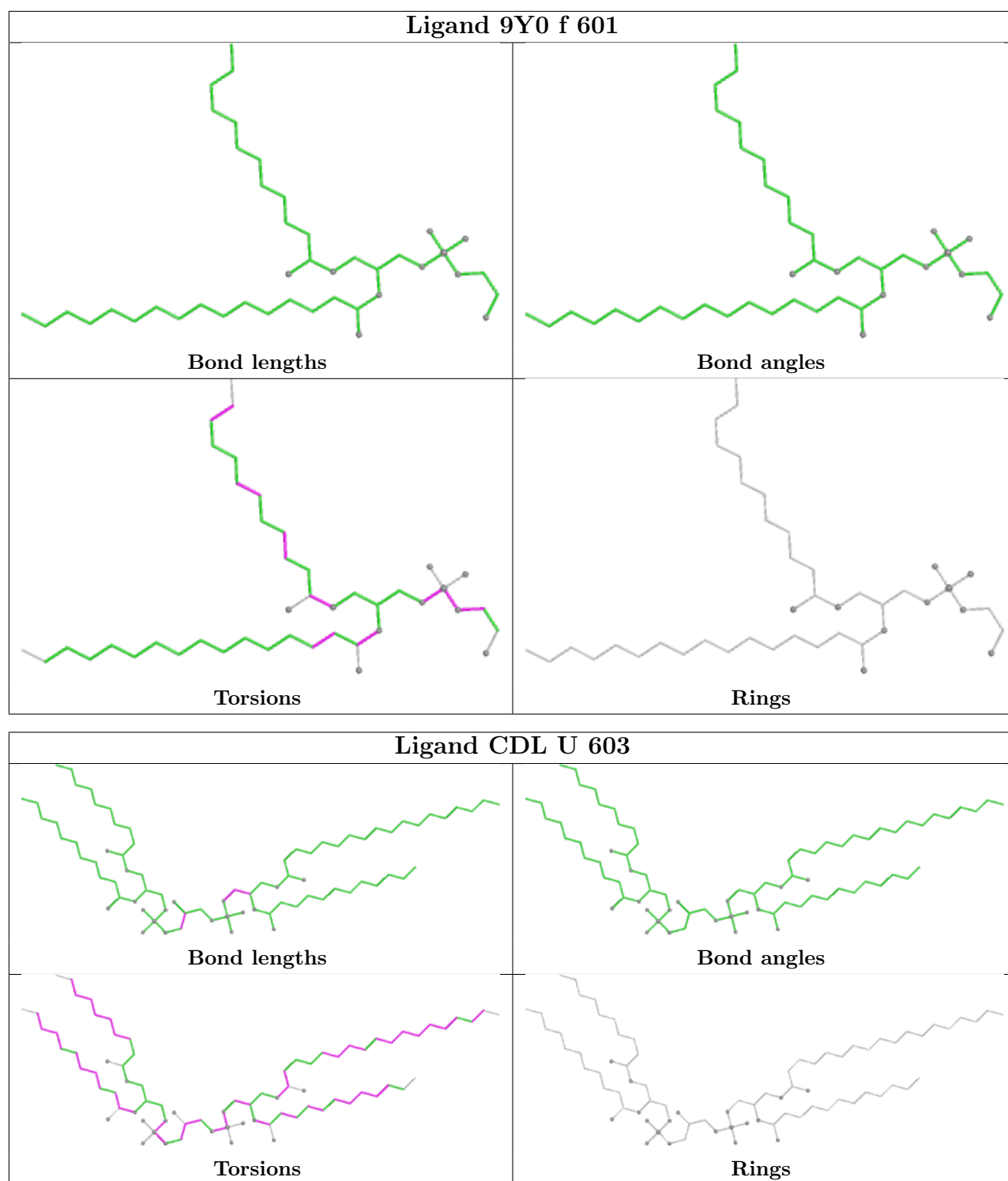


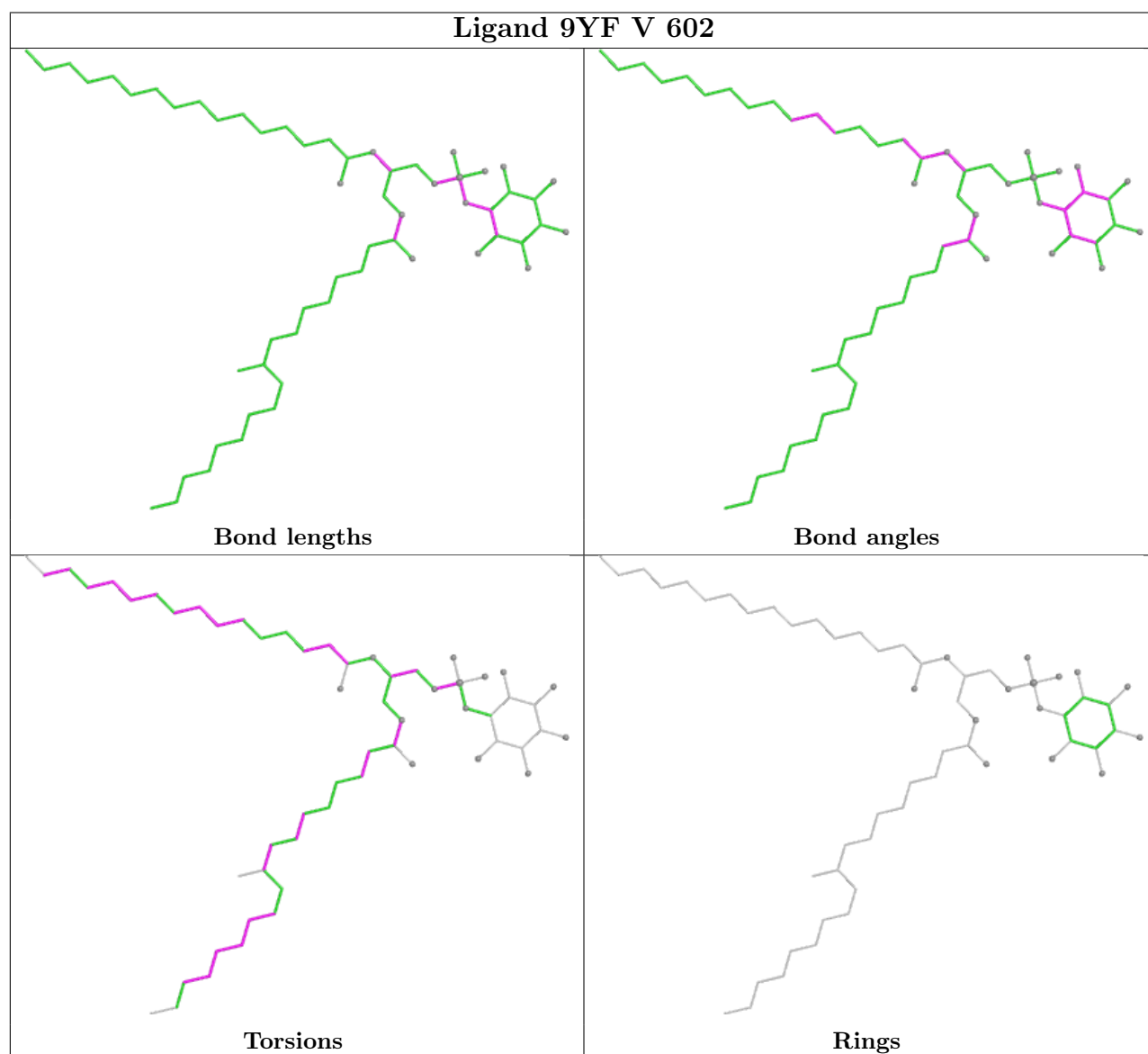
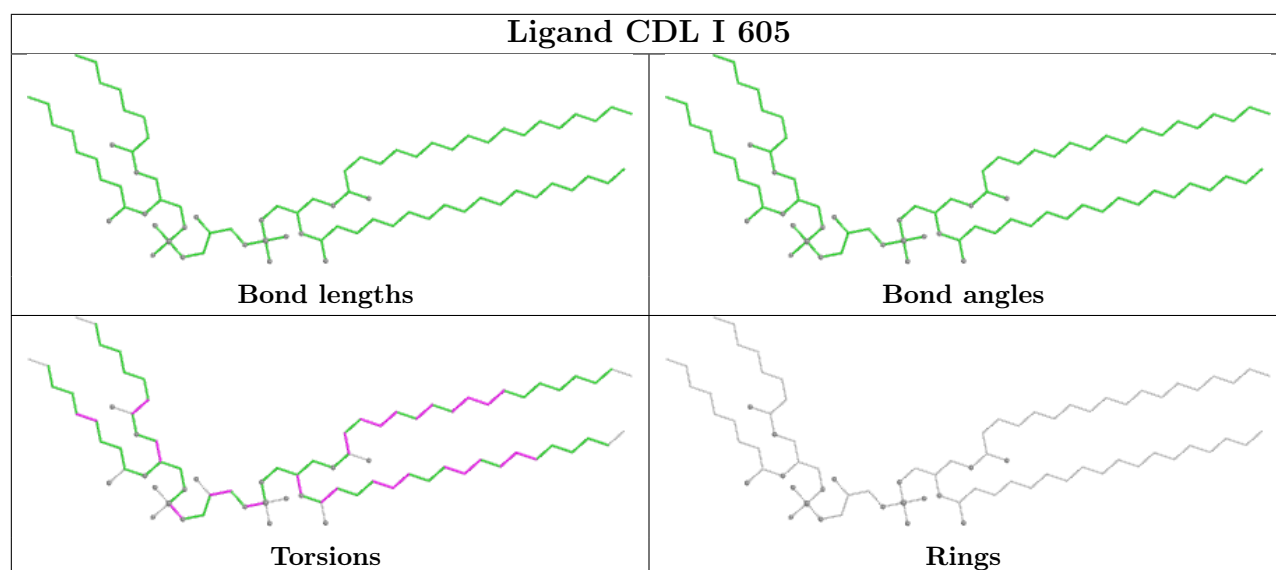


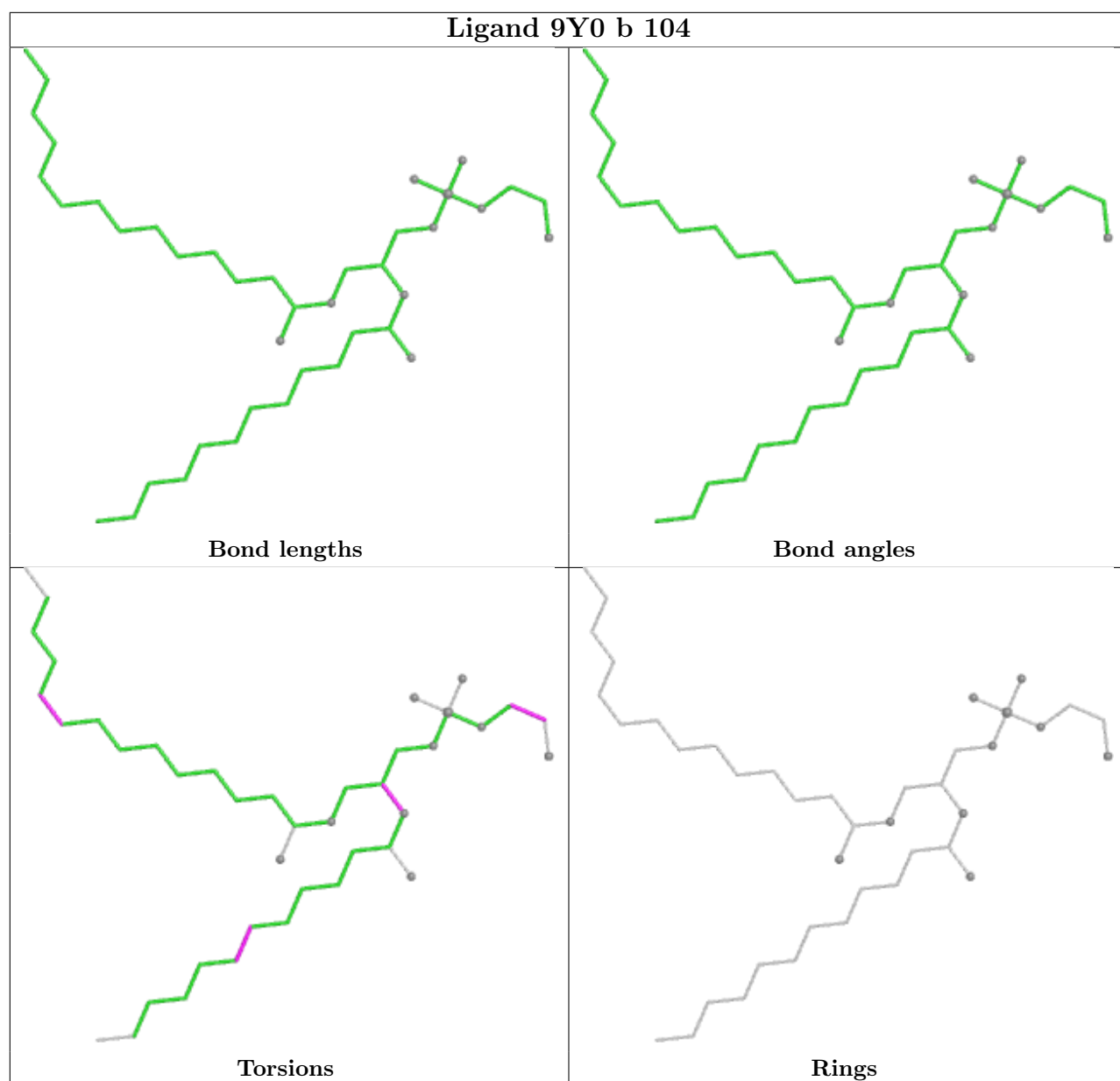


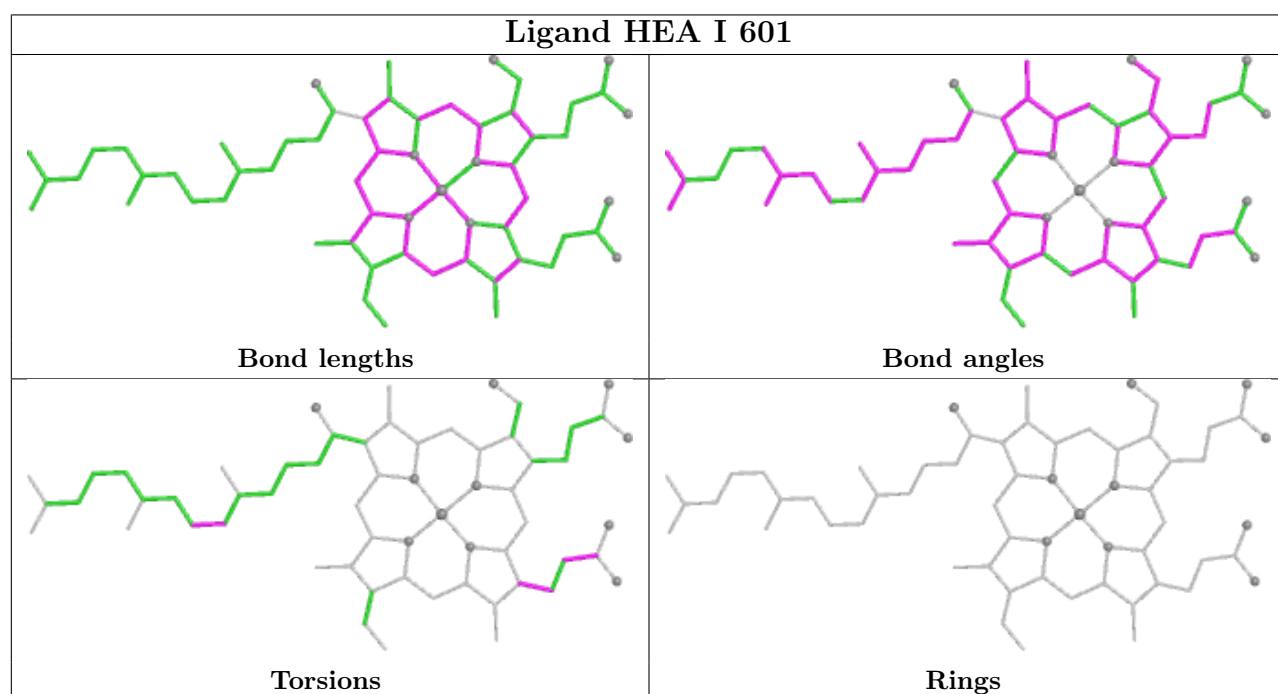
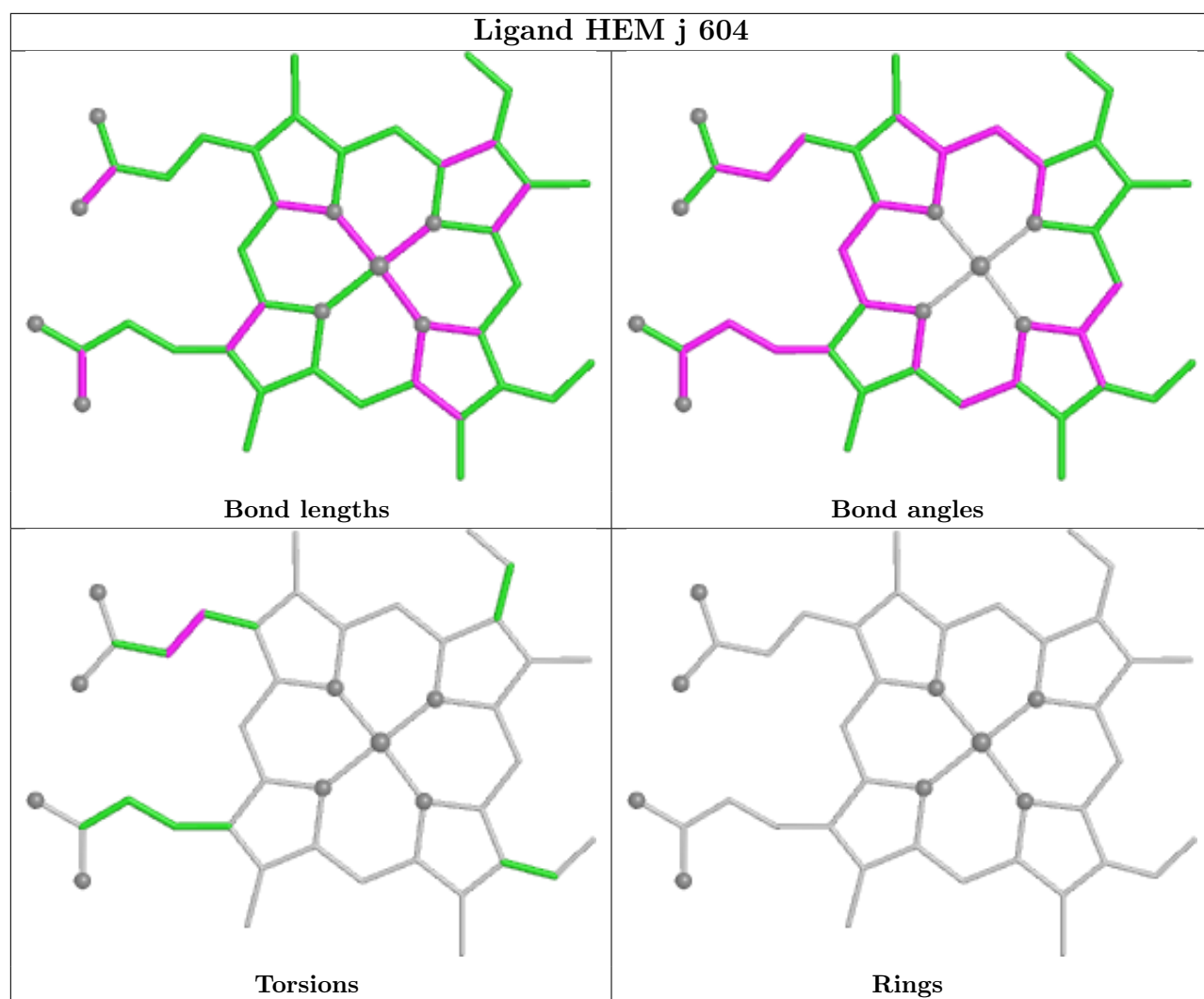


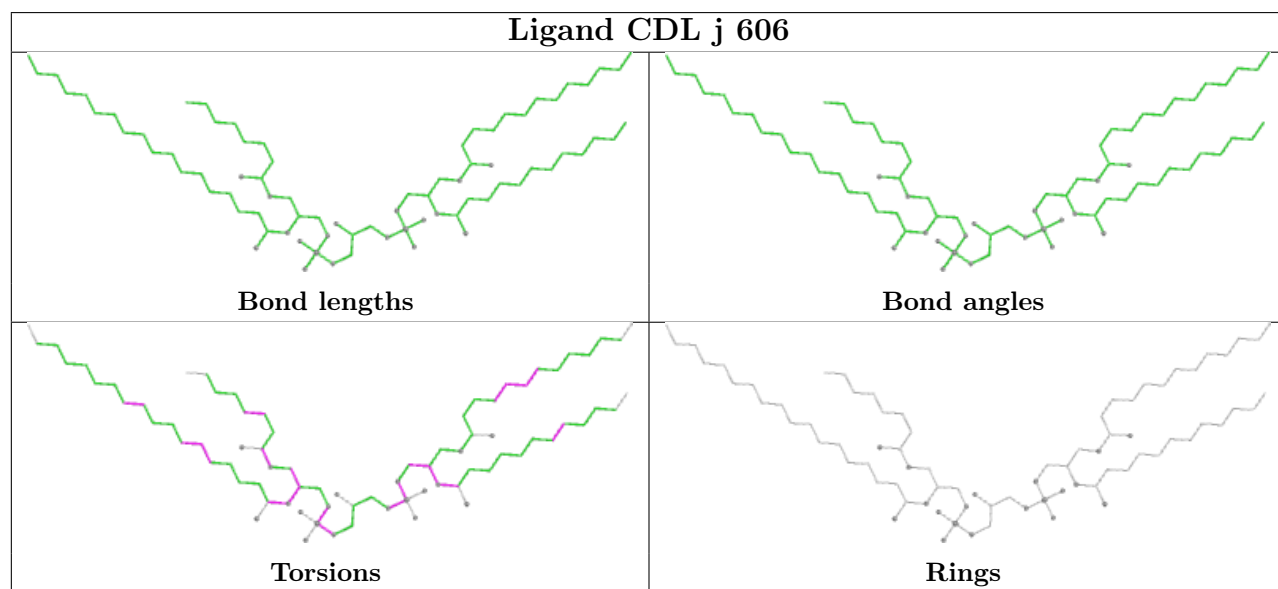
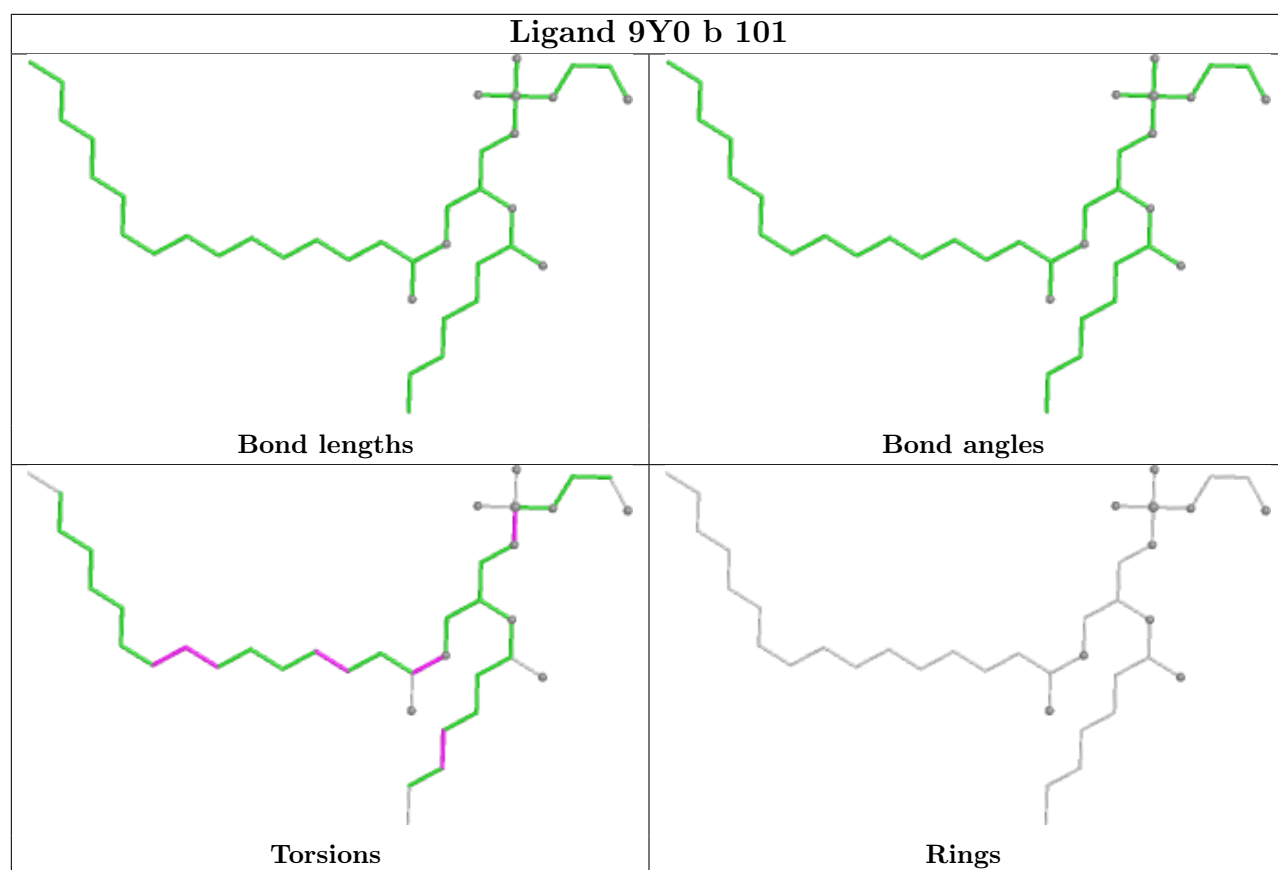


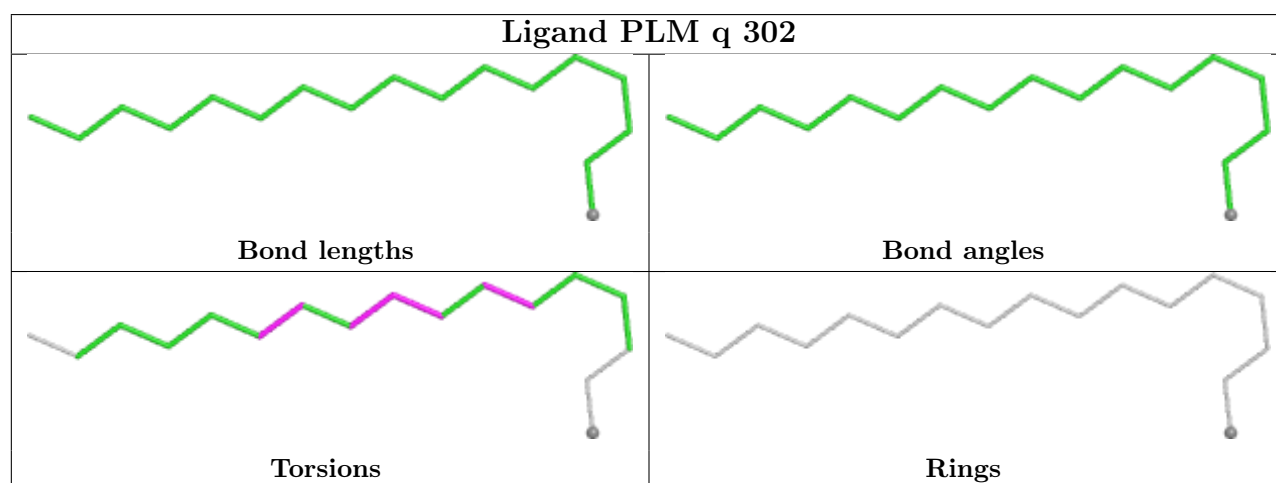
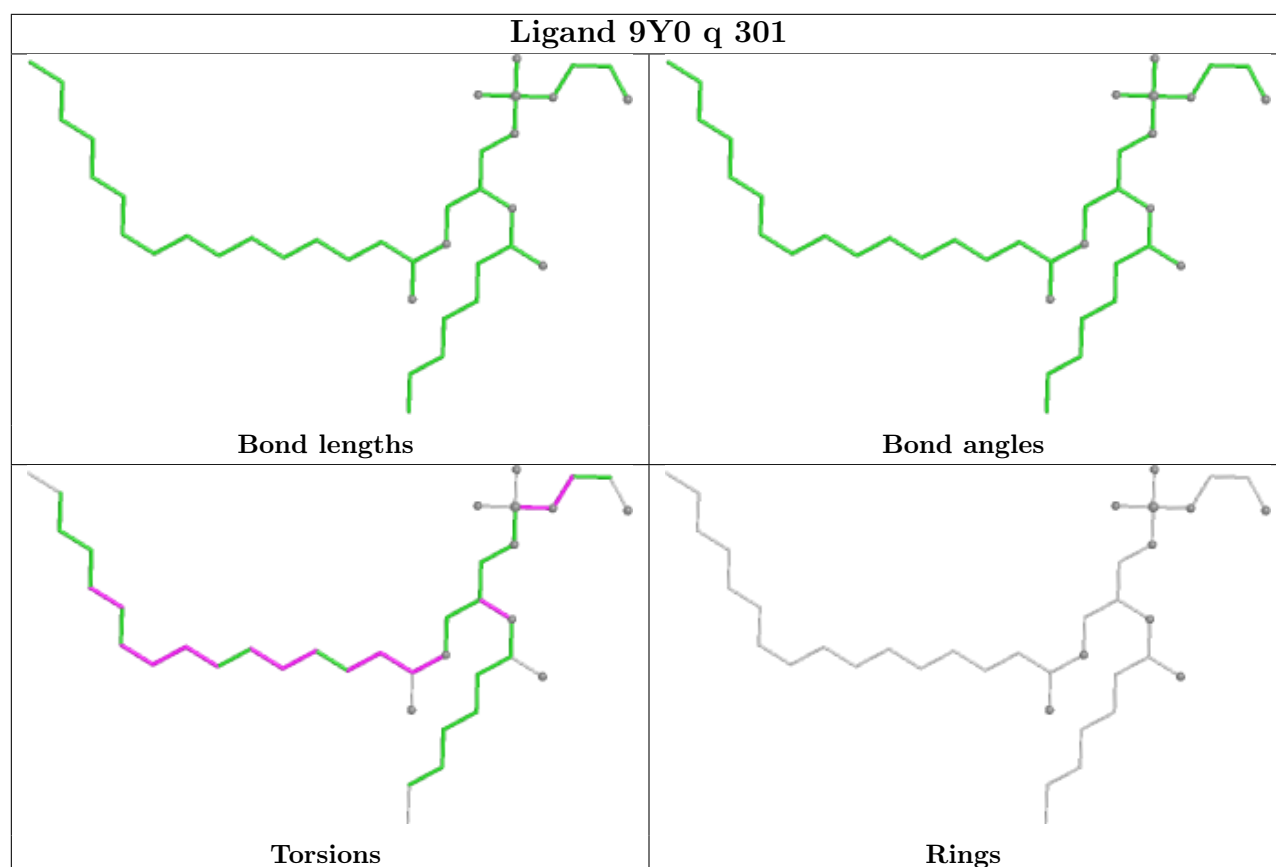
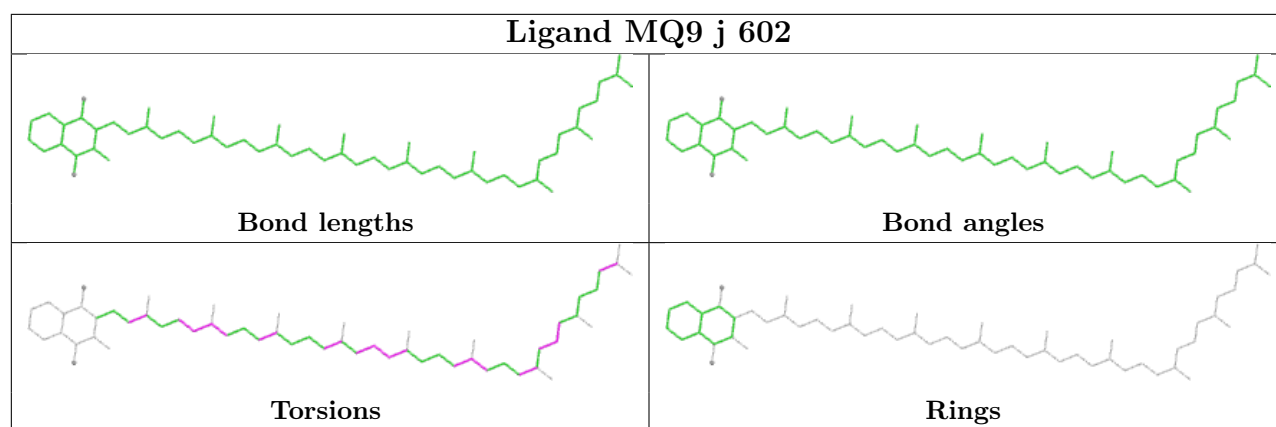


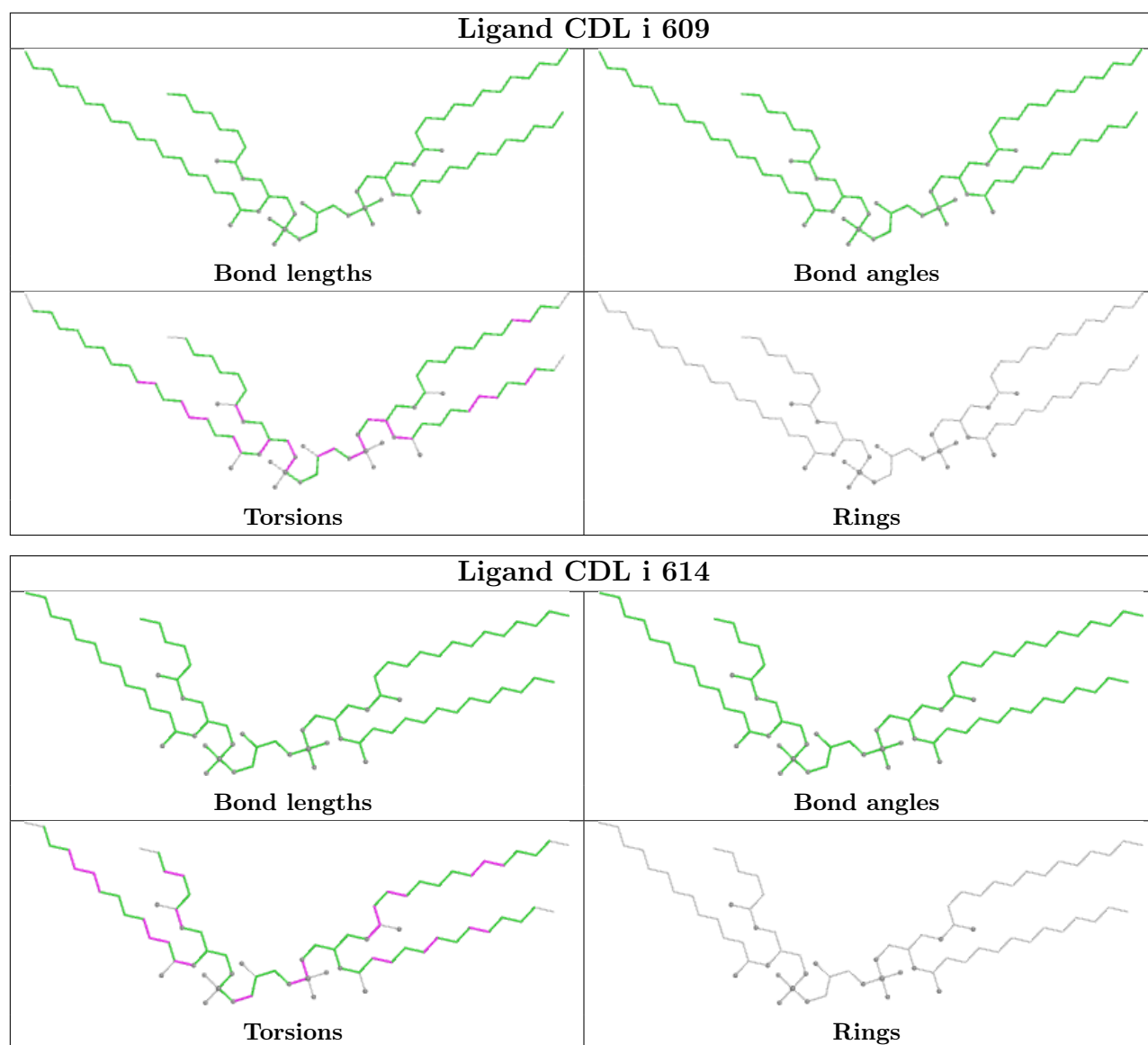


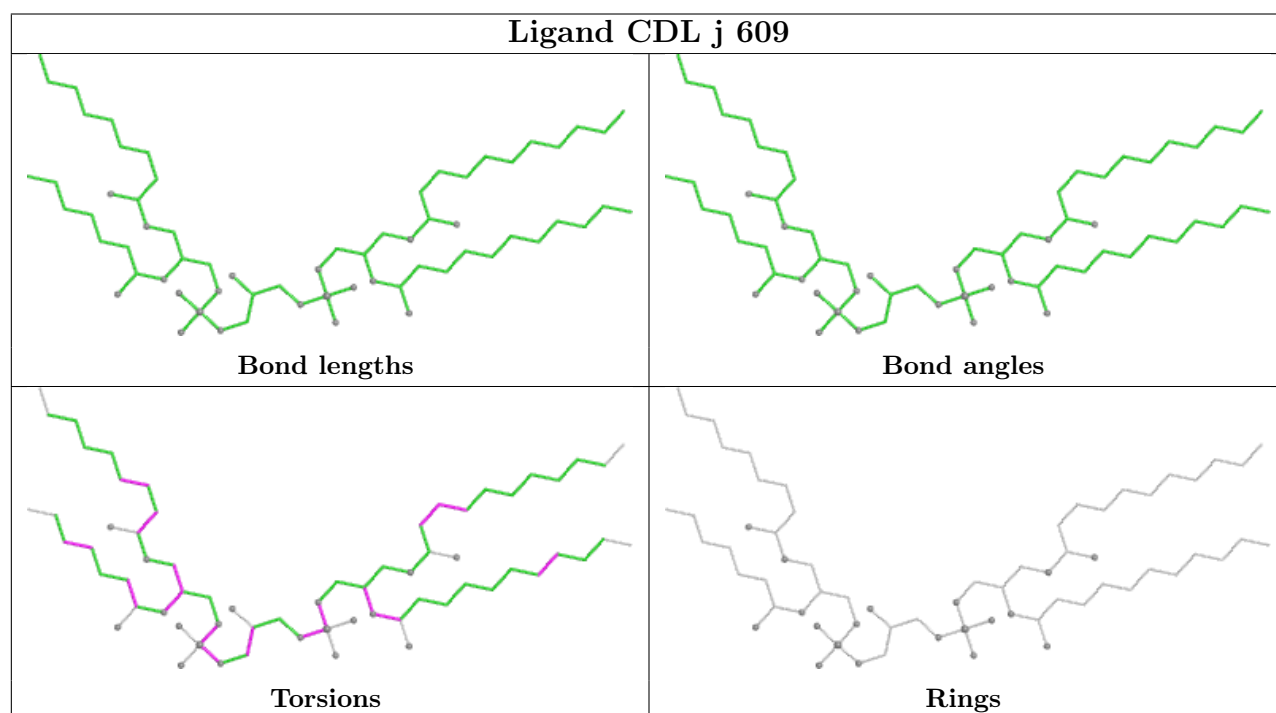
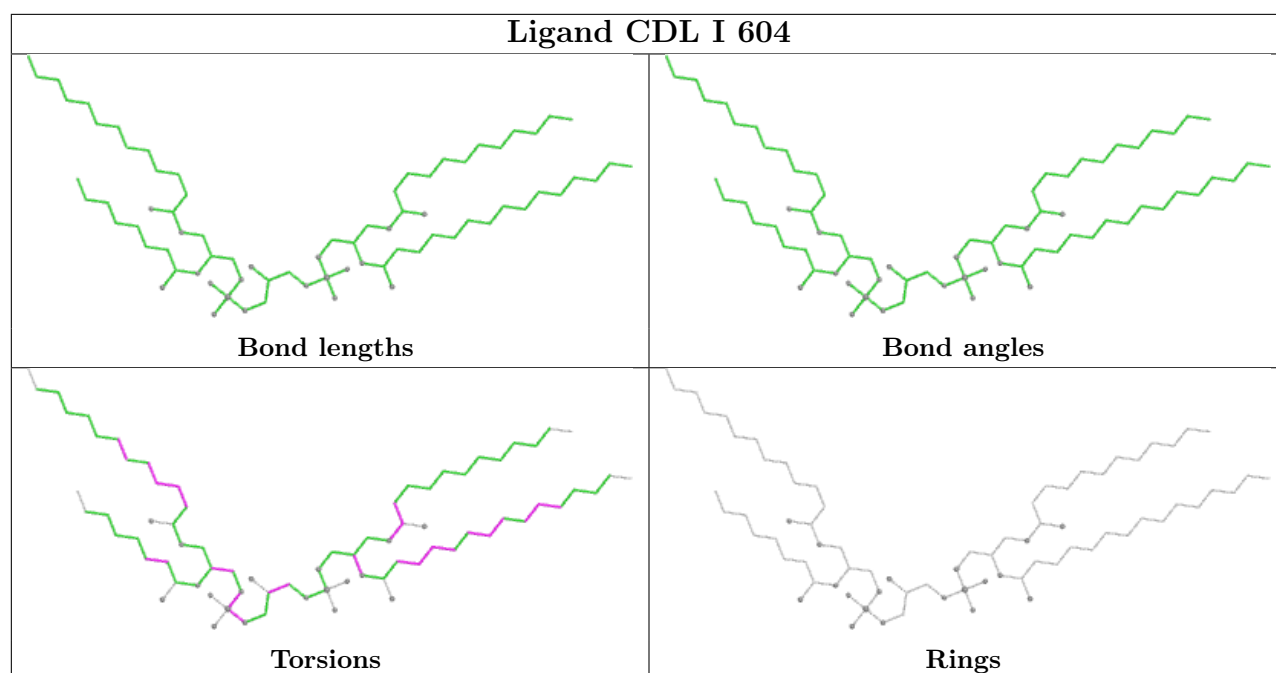




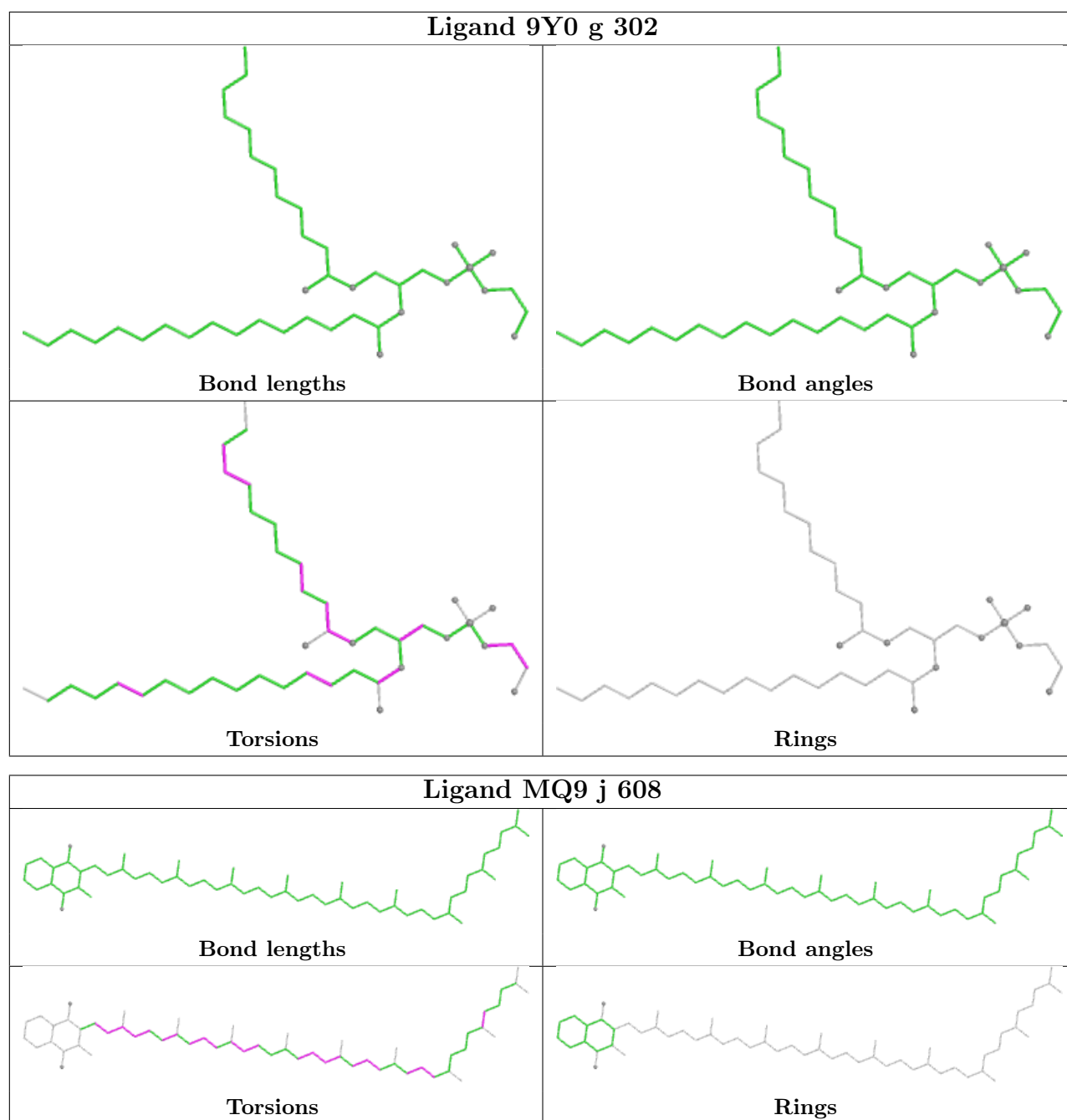


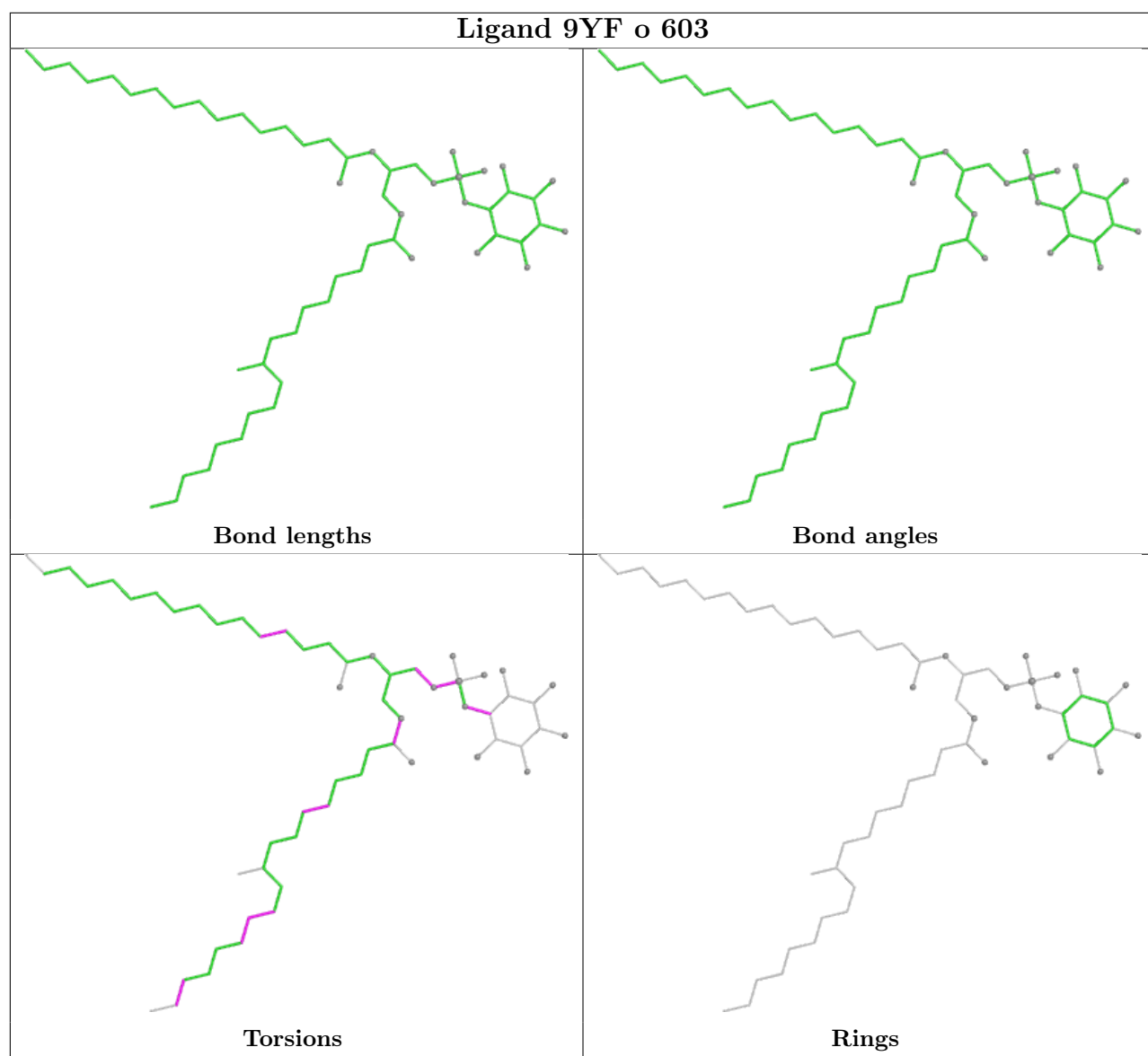




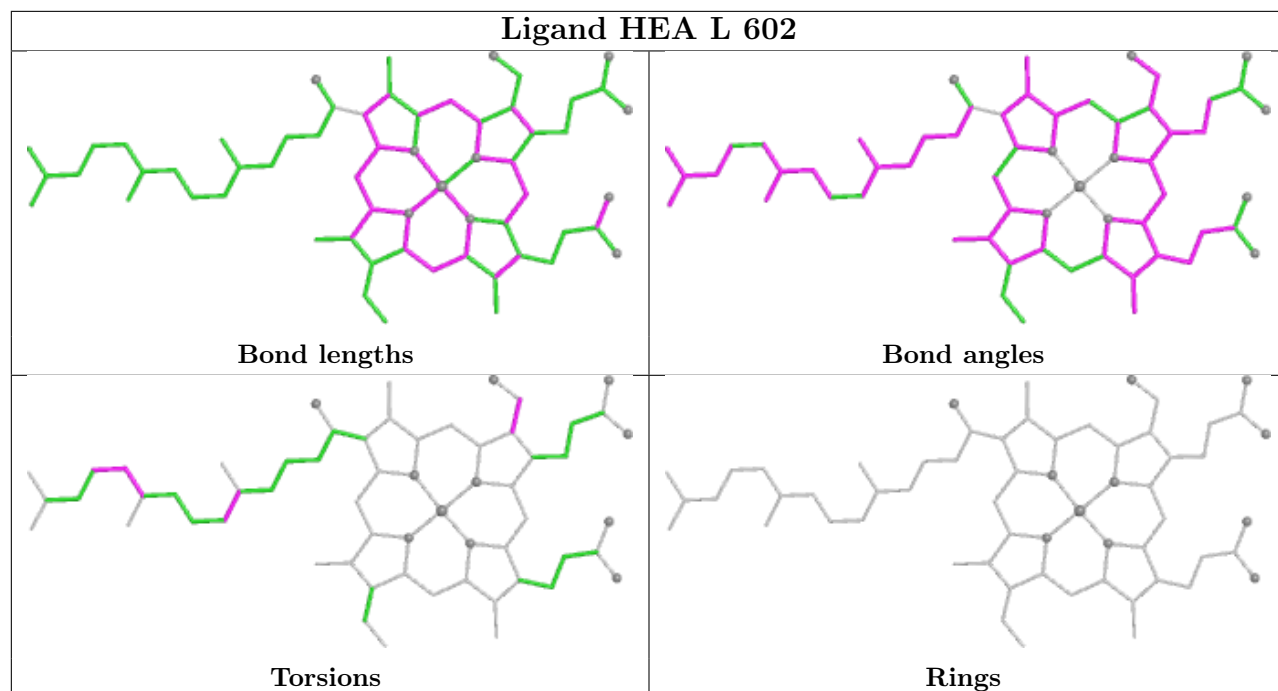




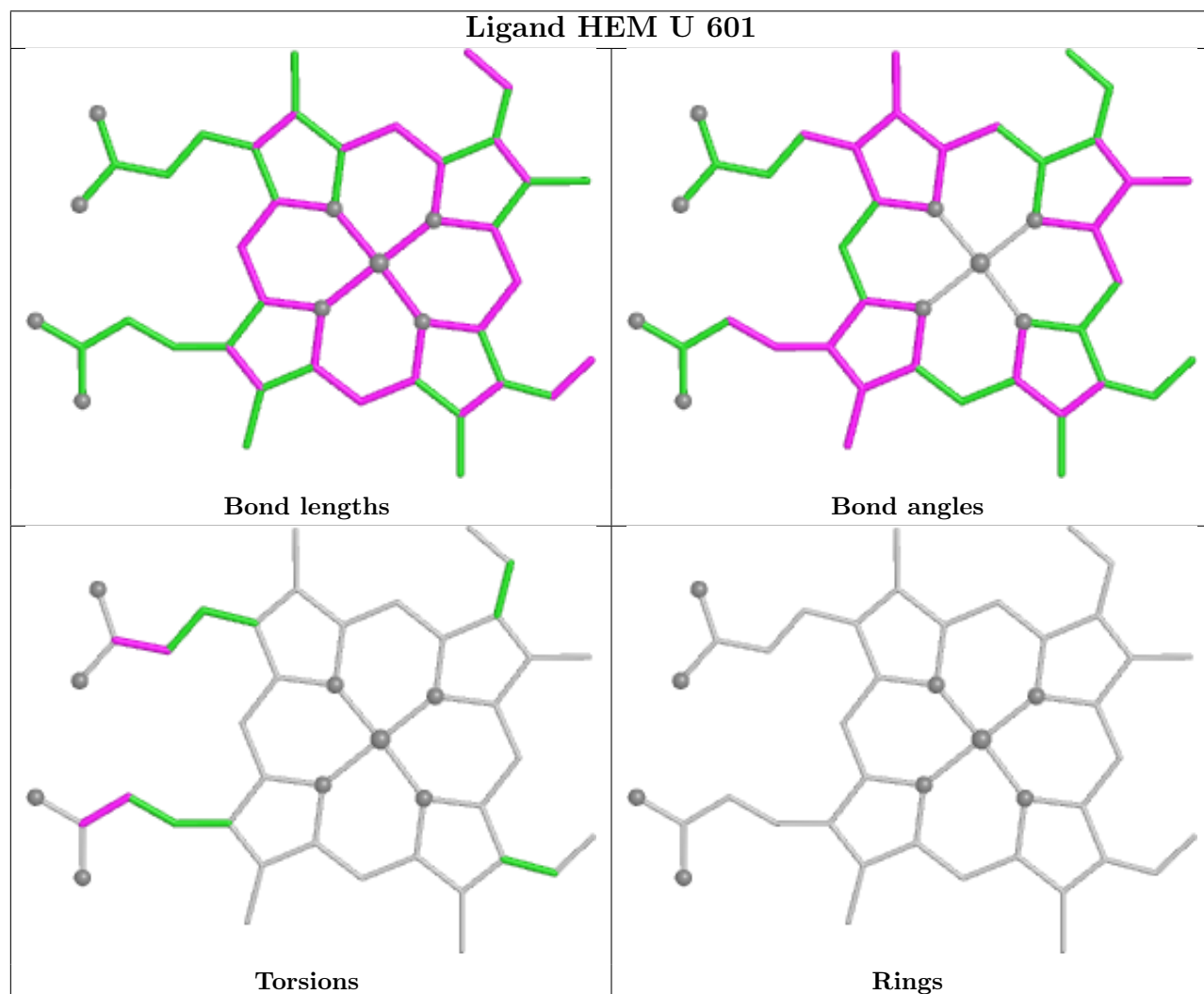


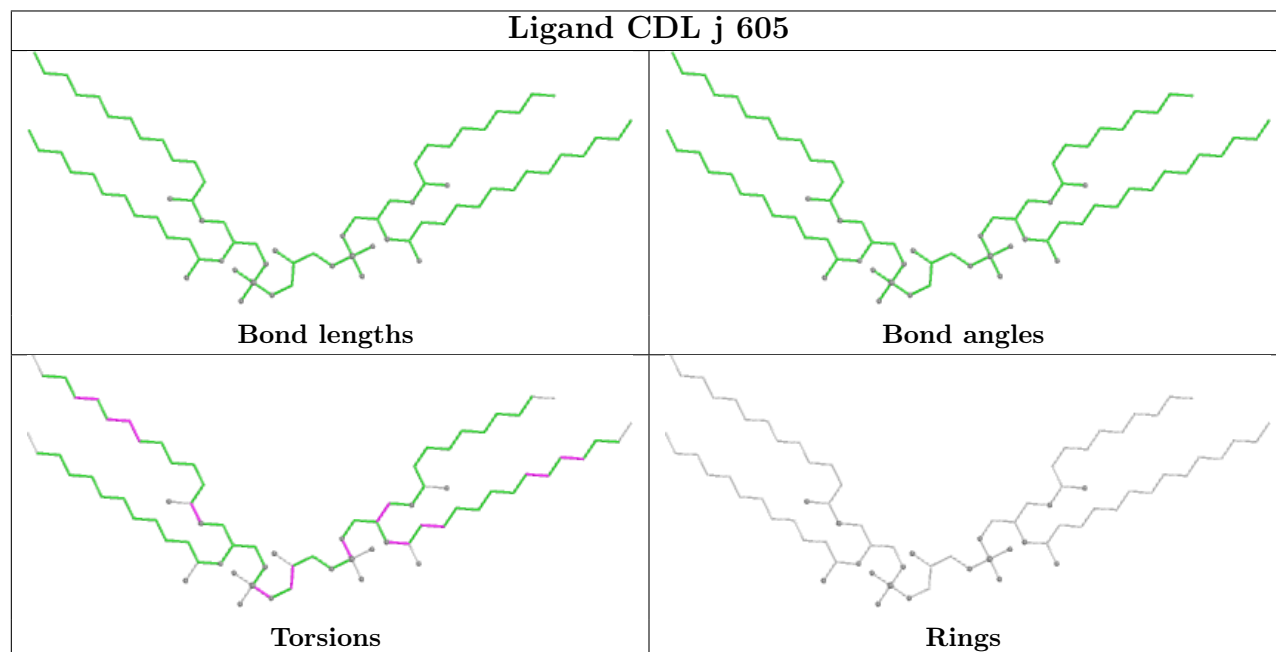
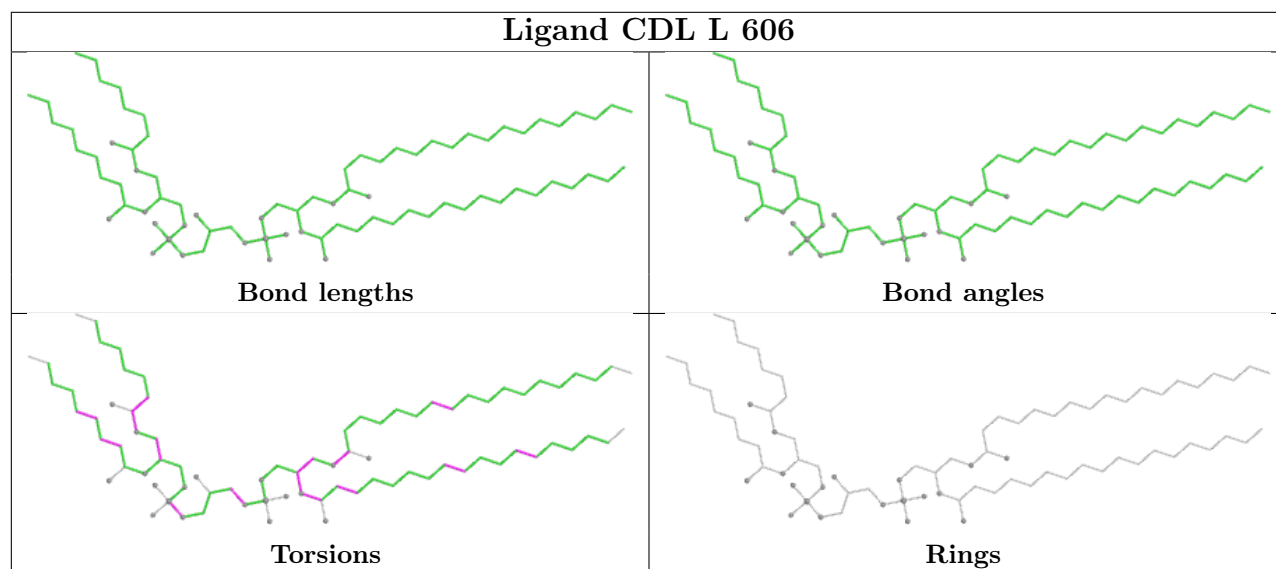
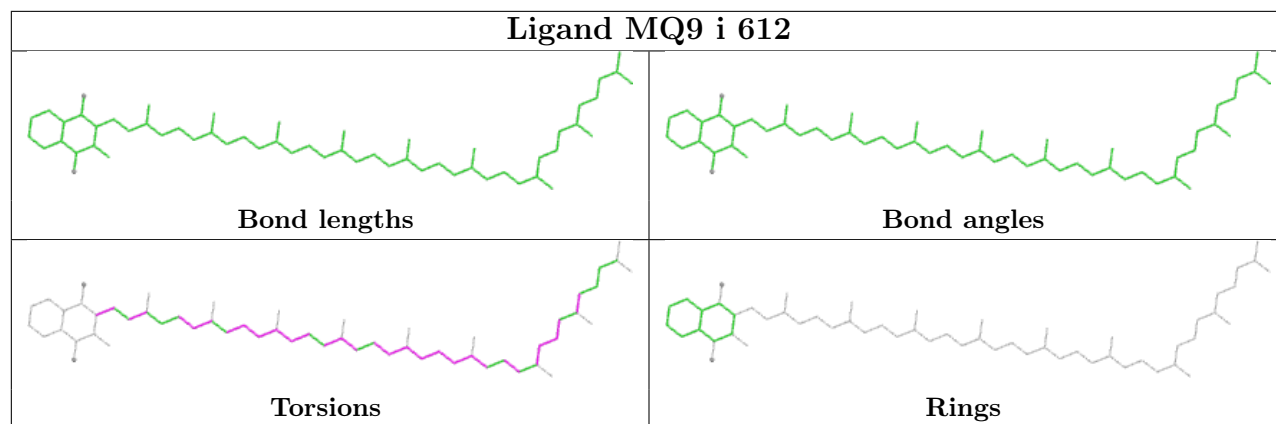


## Ligand HEA L 602

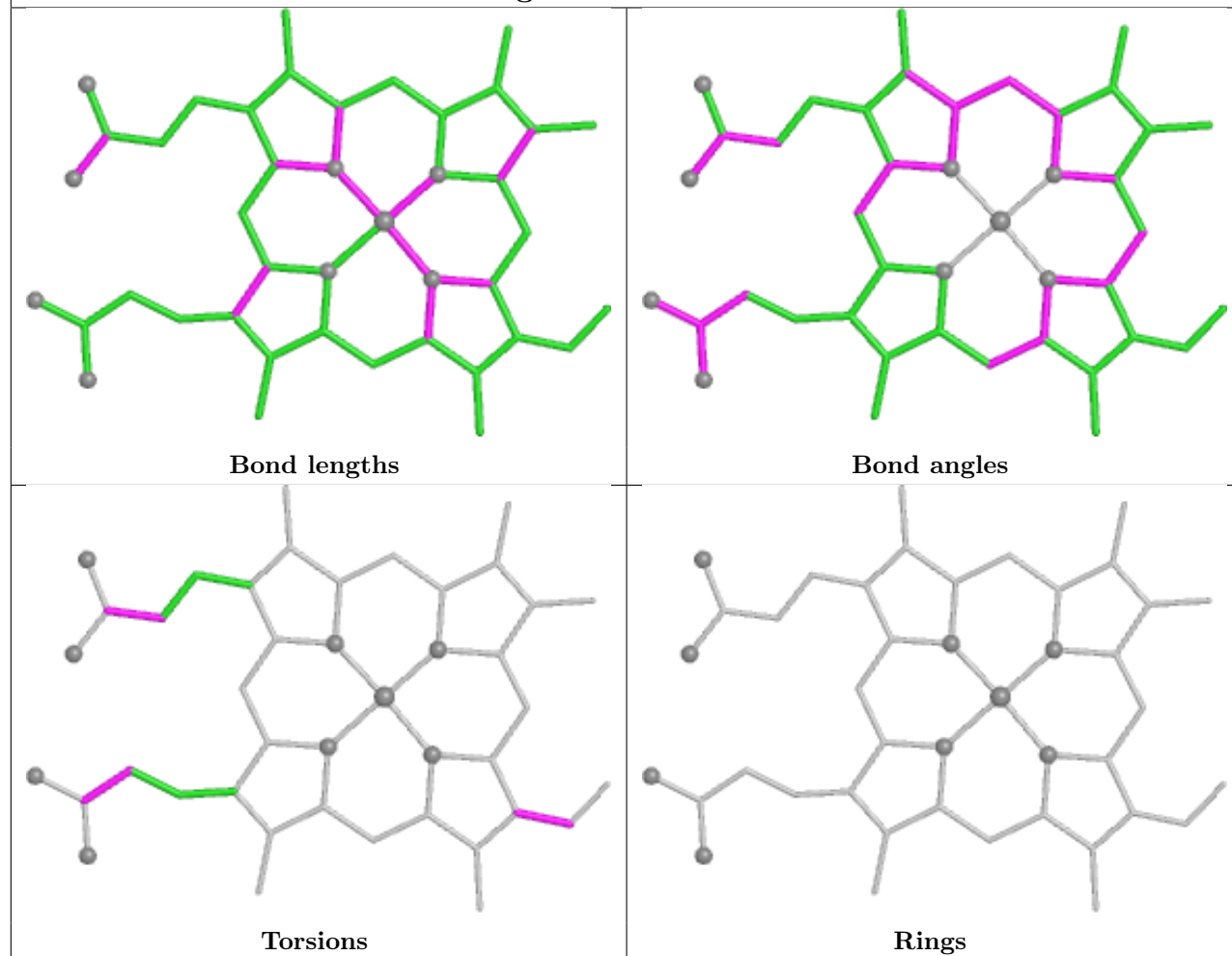


## Ligand HEM U 601

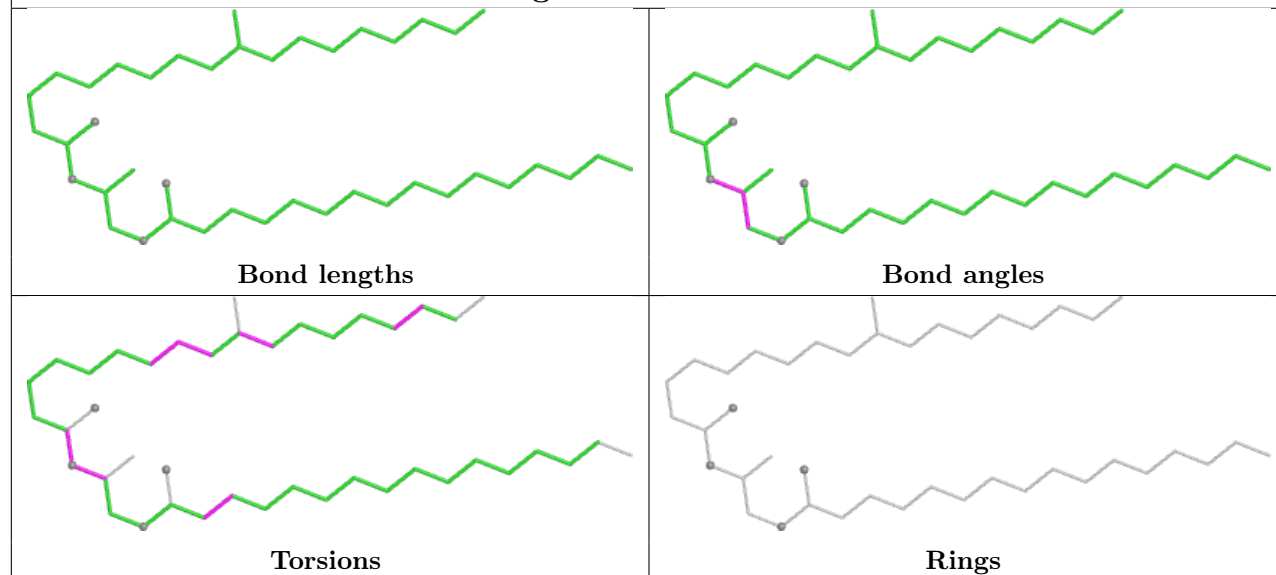


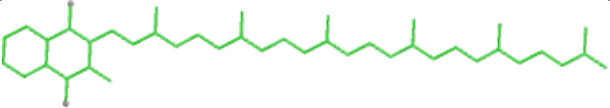
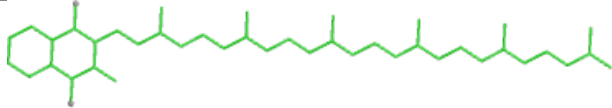
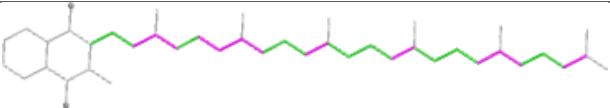
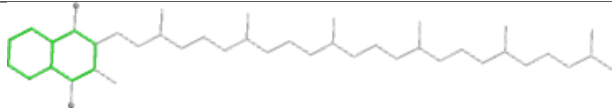


## Ligand HEM i 605

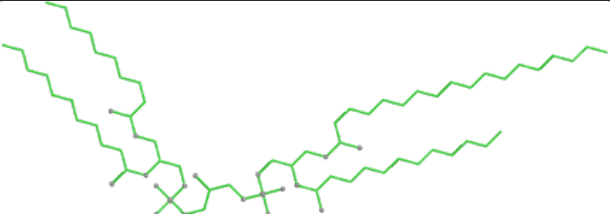
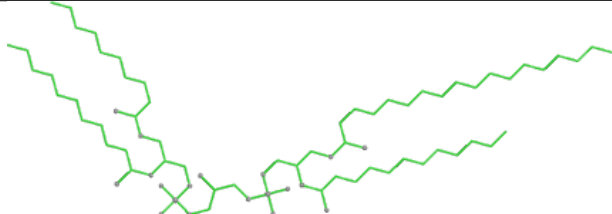
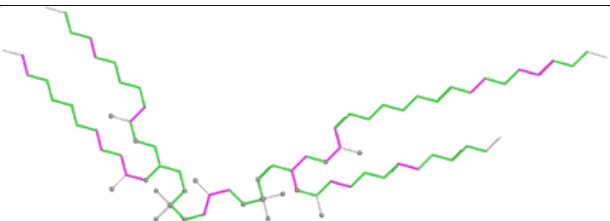
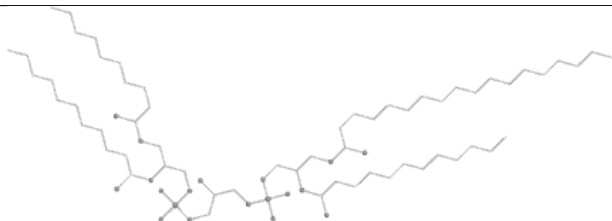


## Ligand 9XX G 101

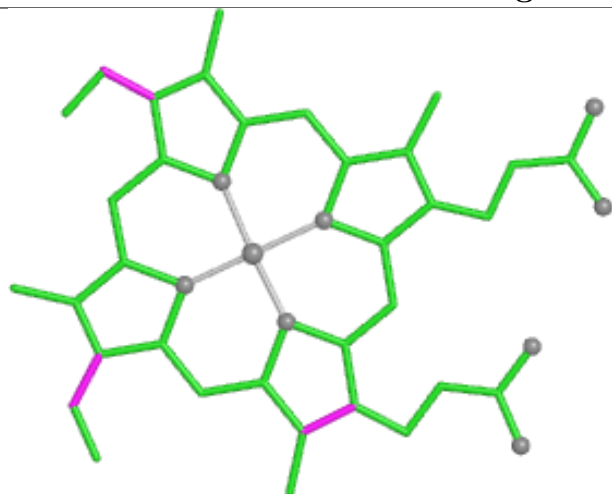


Ligand MQ9 j 607			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

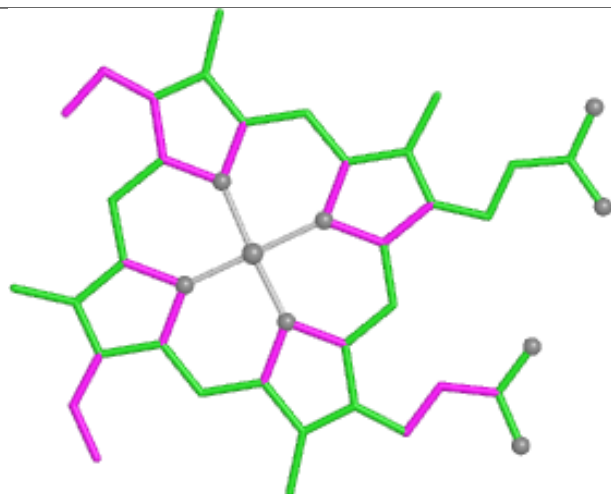
  

Ligand CDL m 202			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

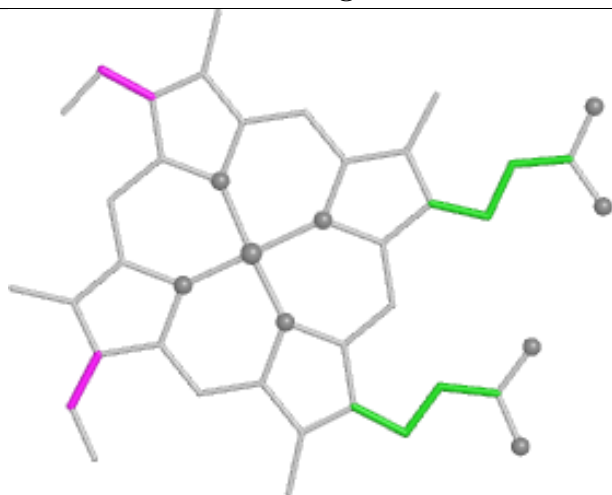
## Ligand HEC o 602



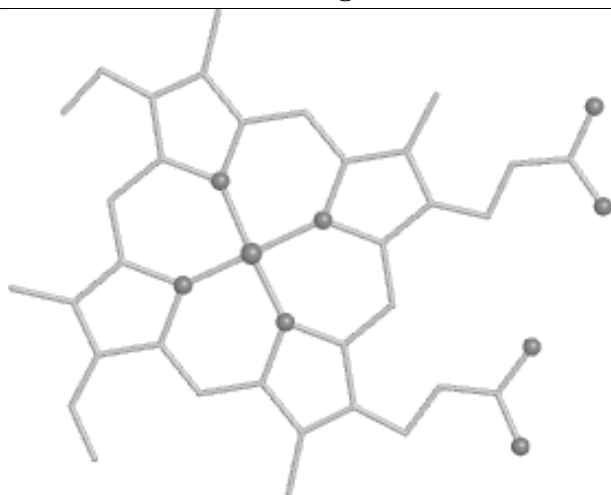
Bond lengths



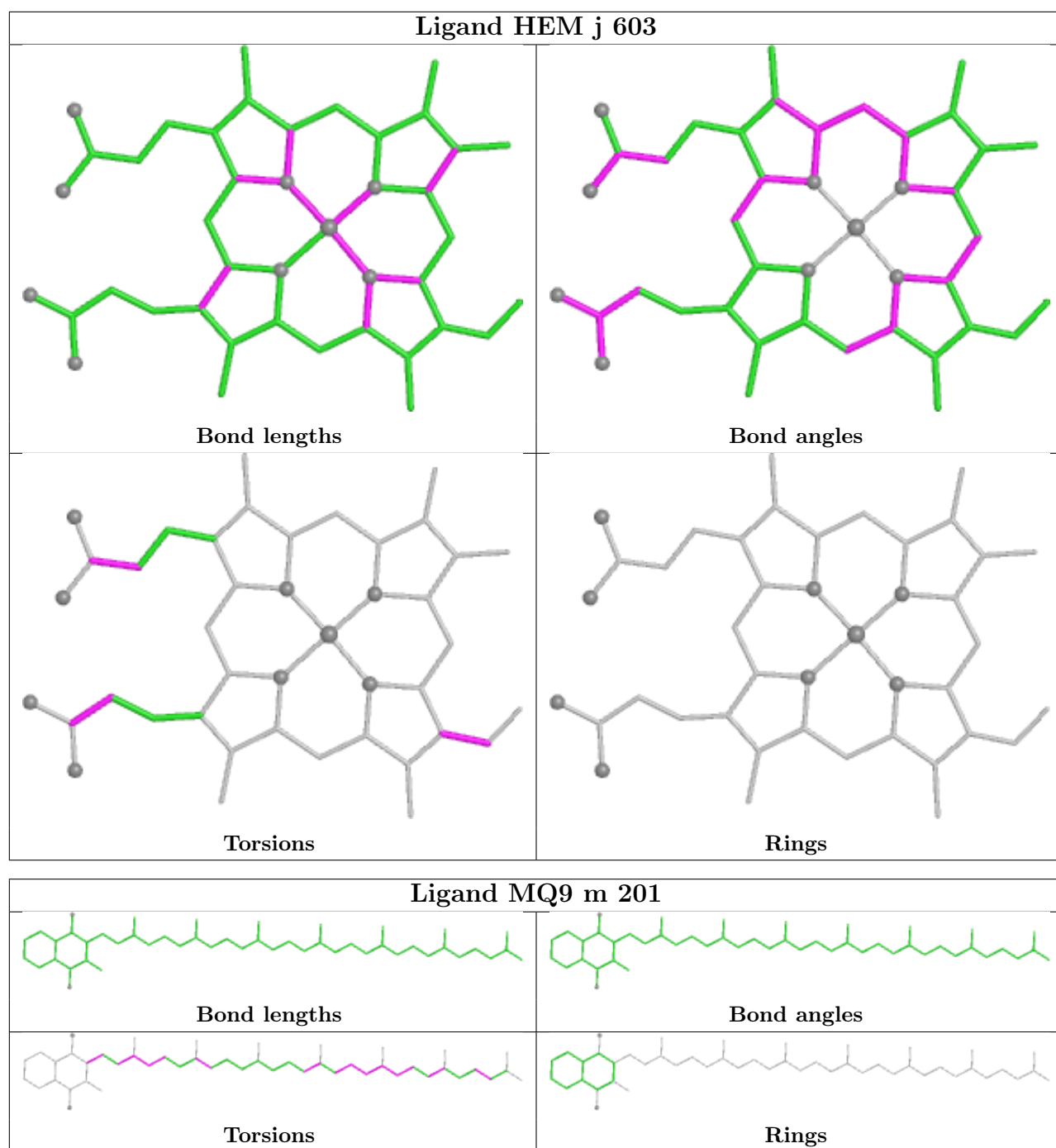
Bond angles



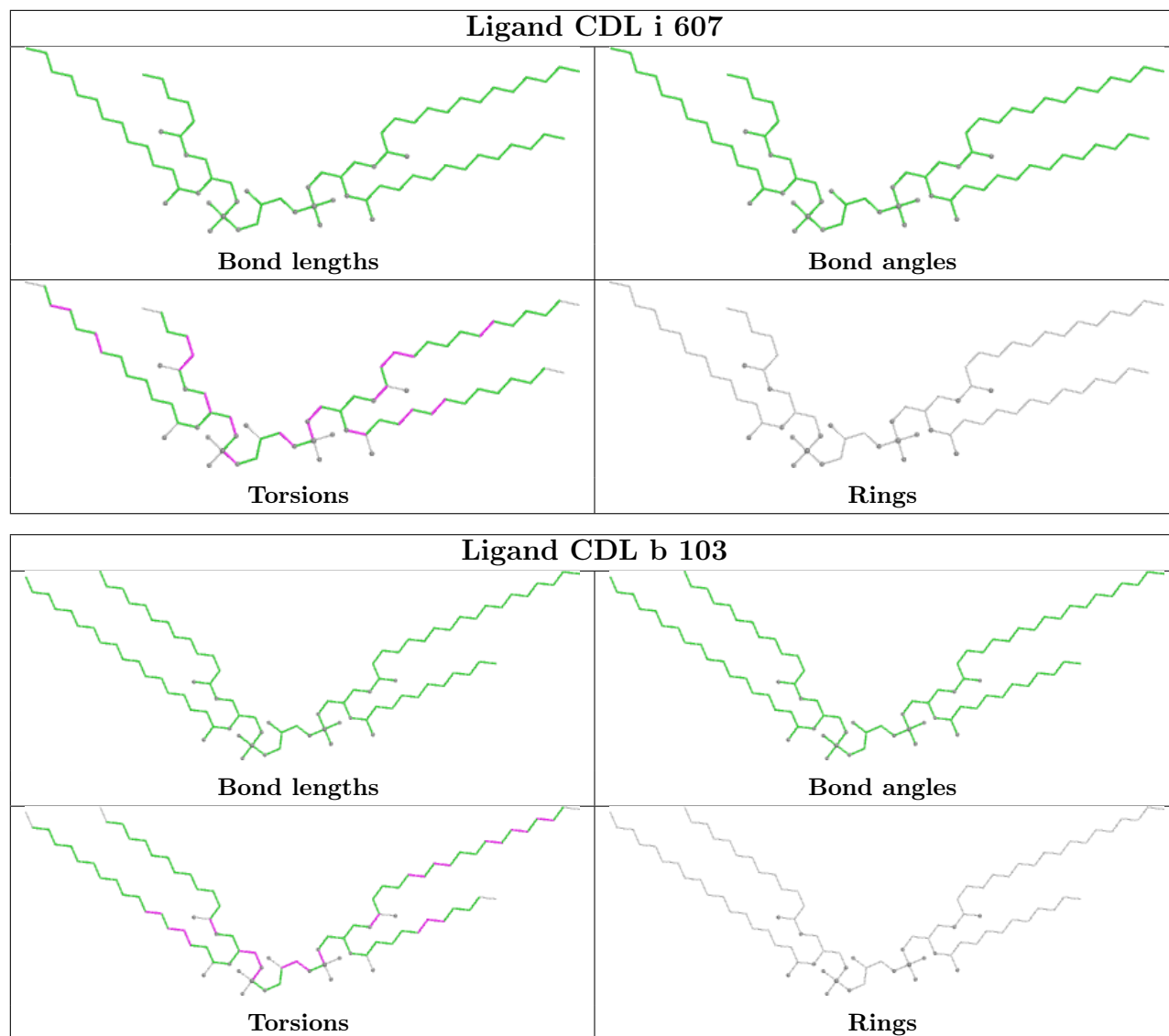
Torsions



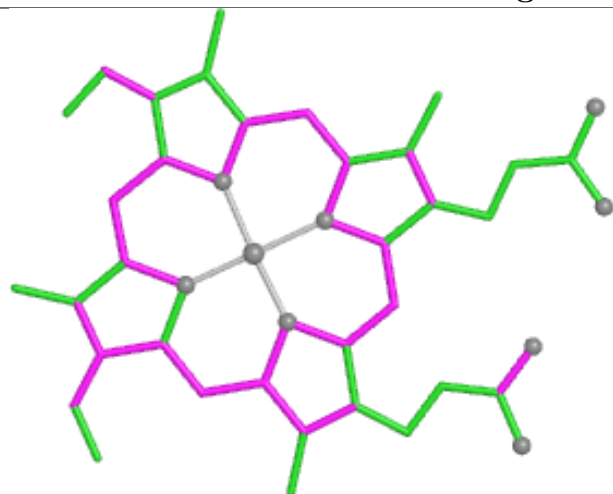
Rings



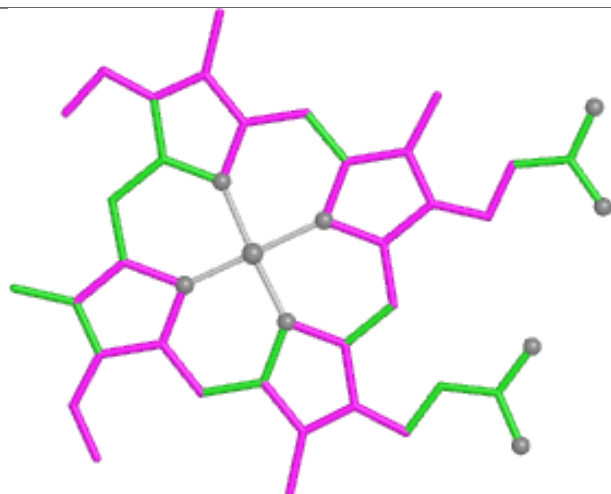




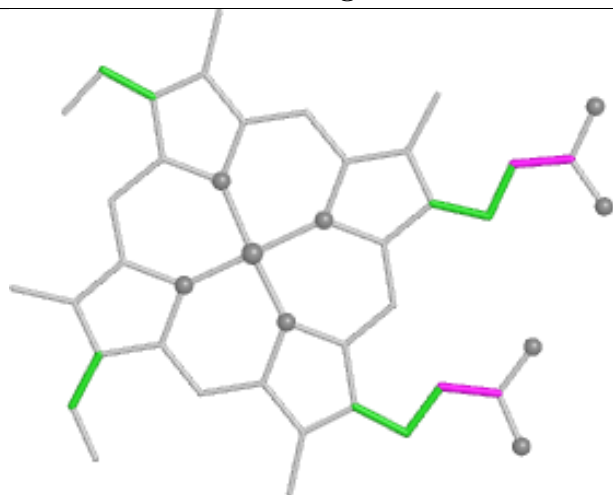
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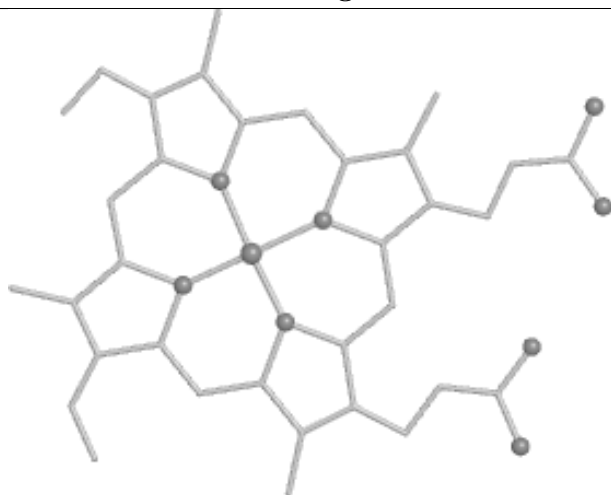
Bond lengths



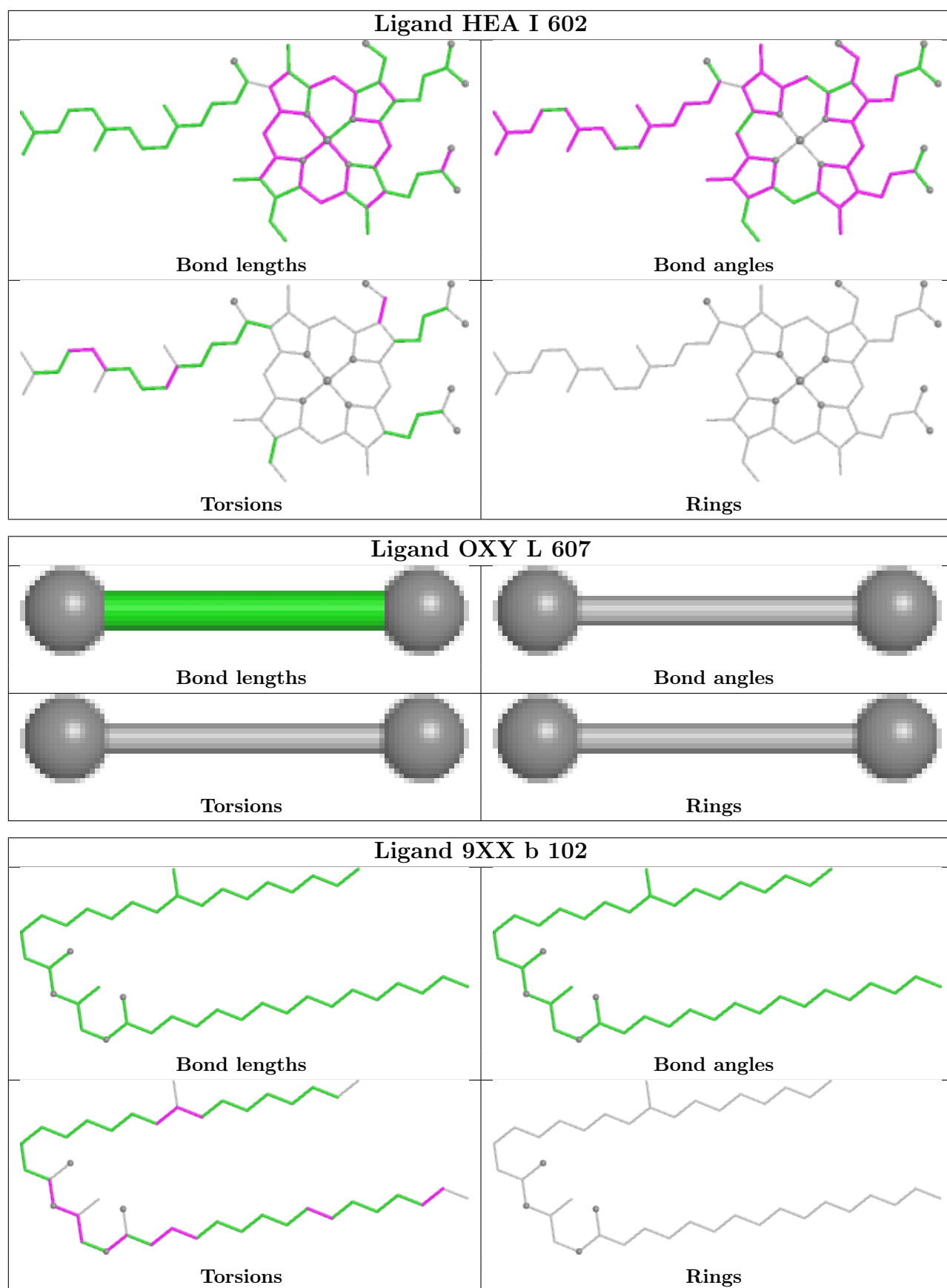
Bond angles

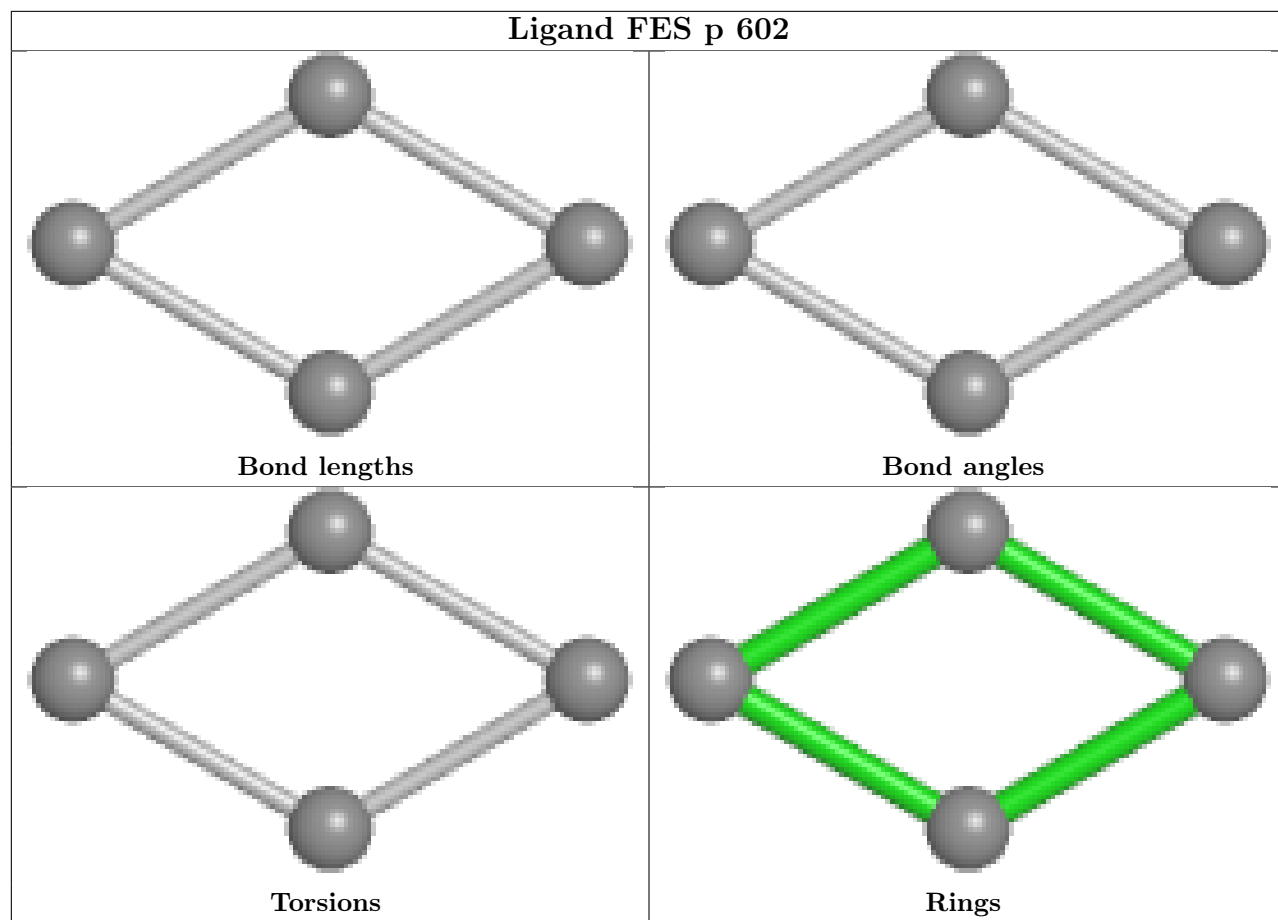


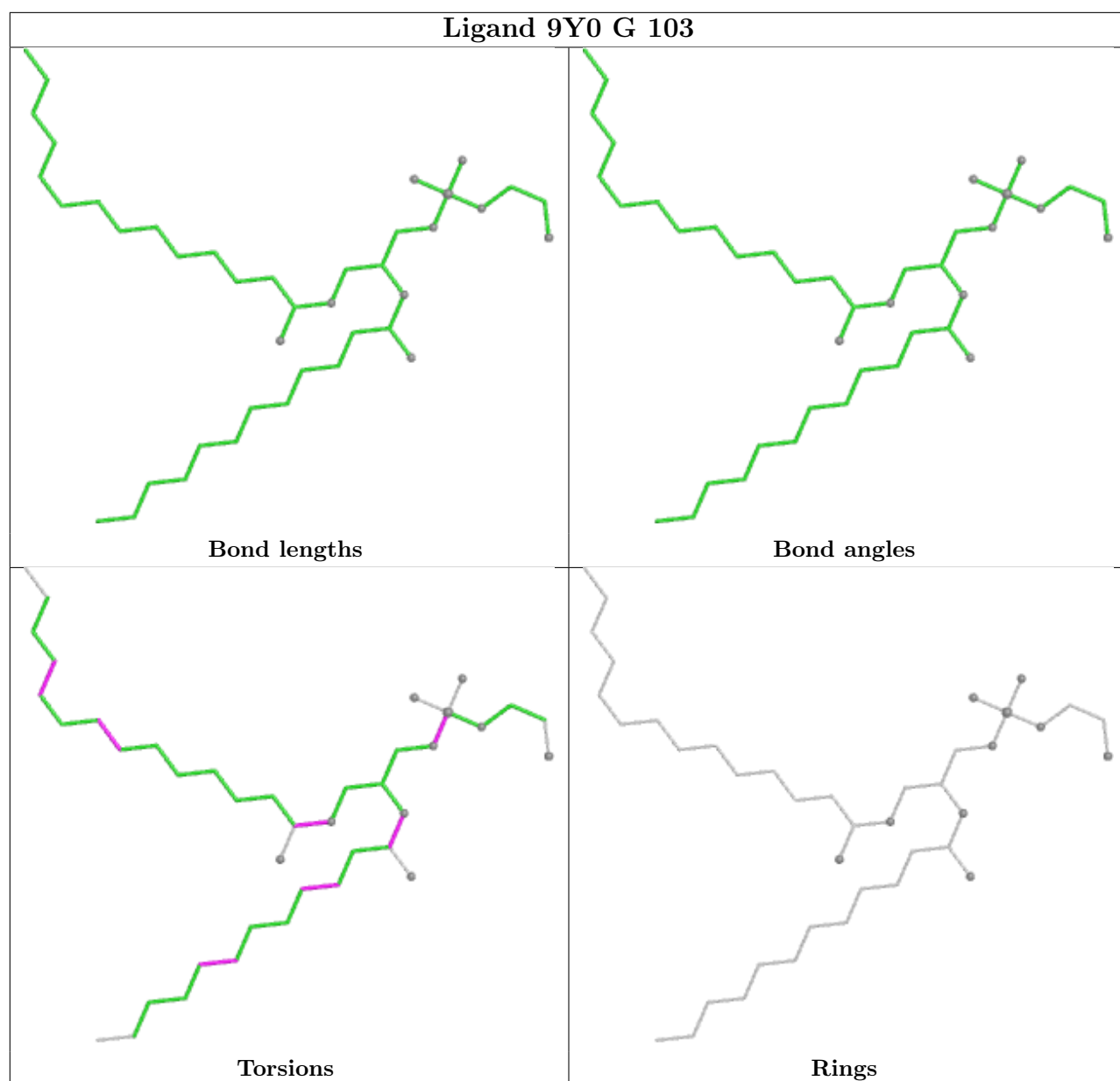
Torsions

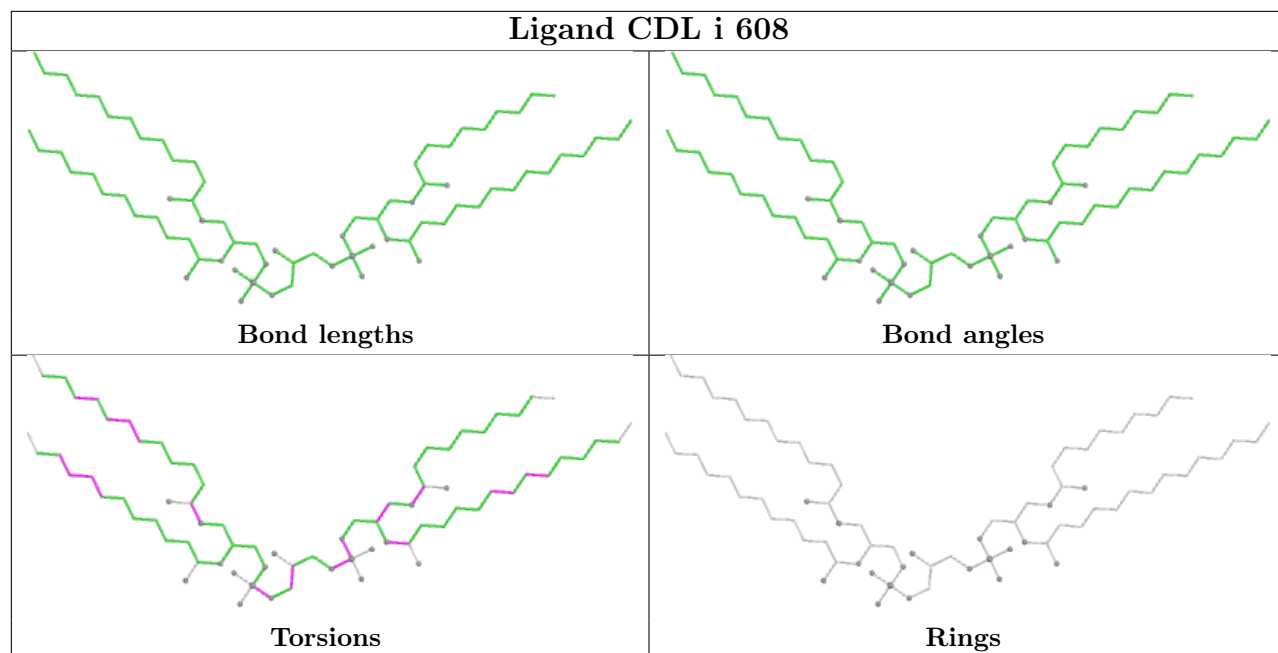


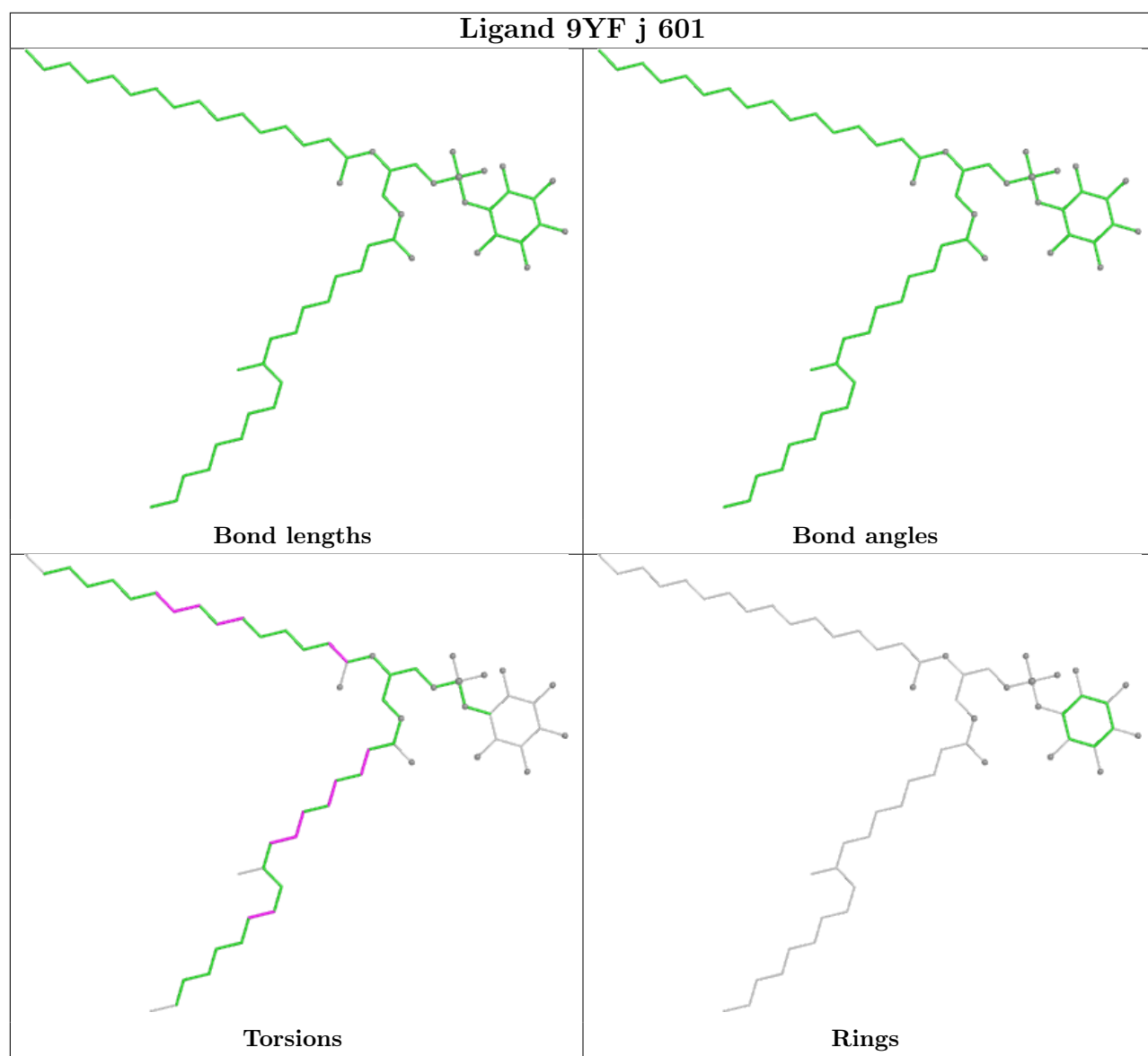
Rings

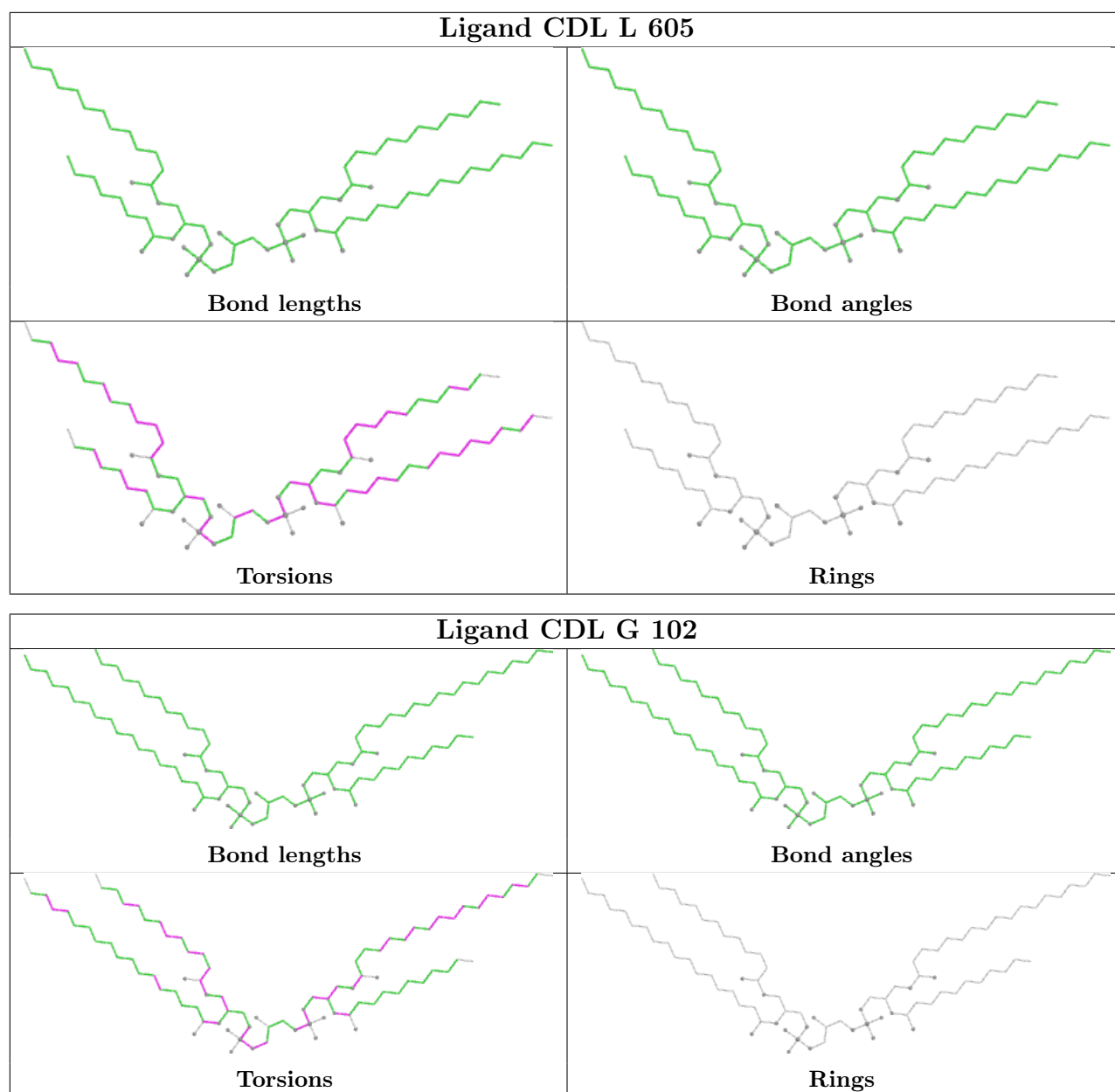




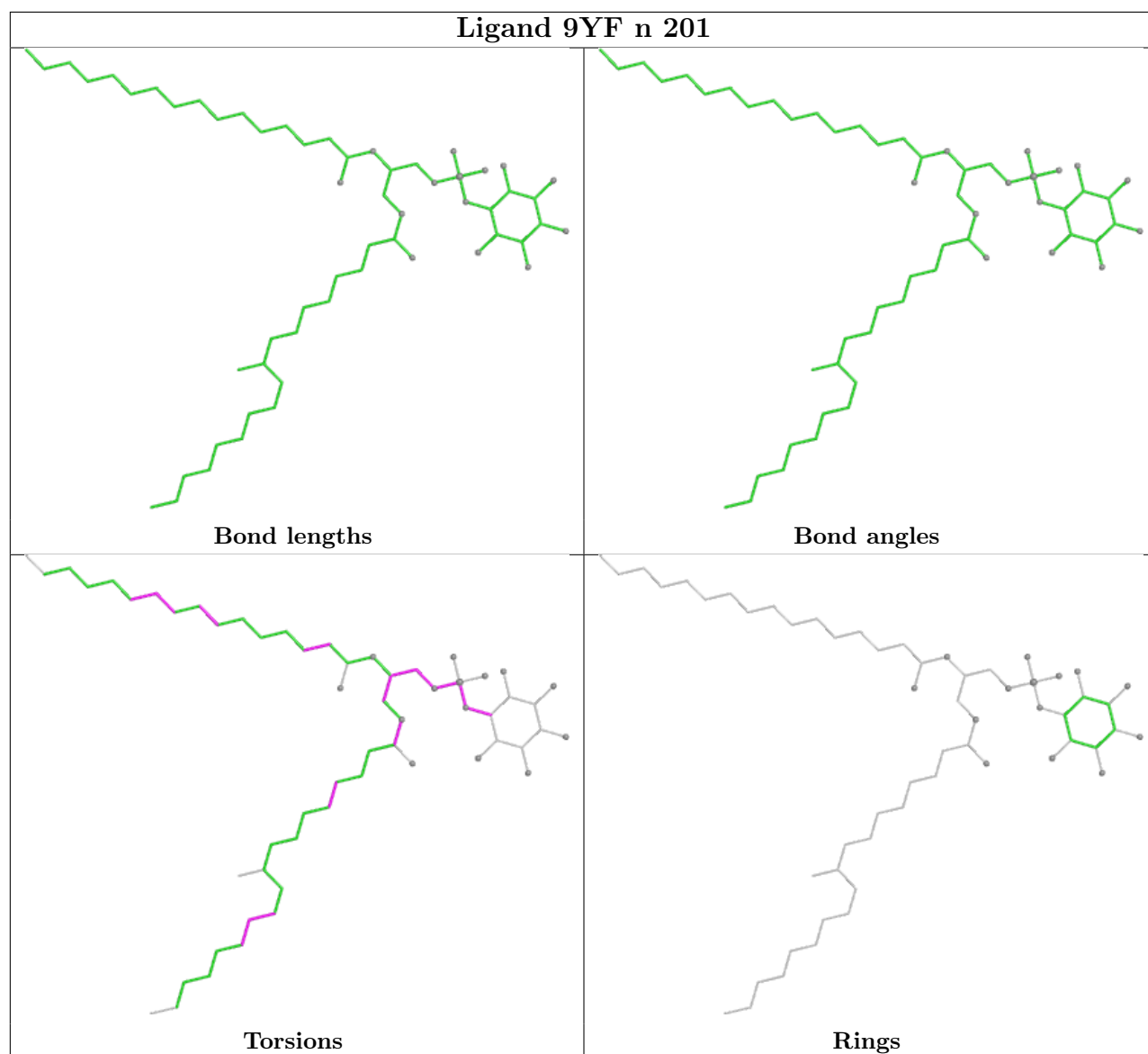
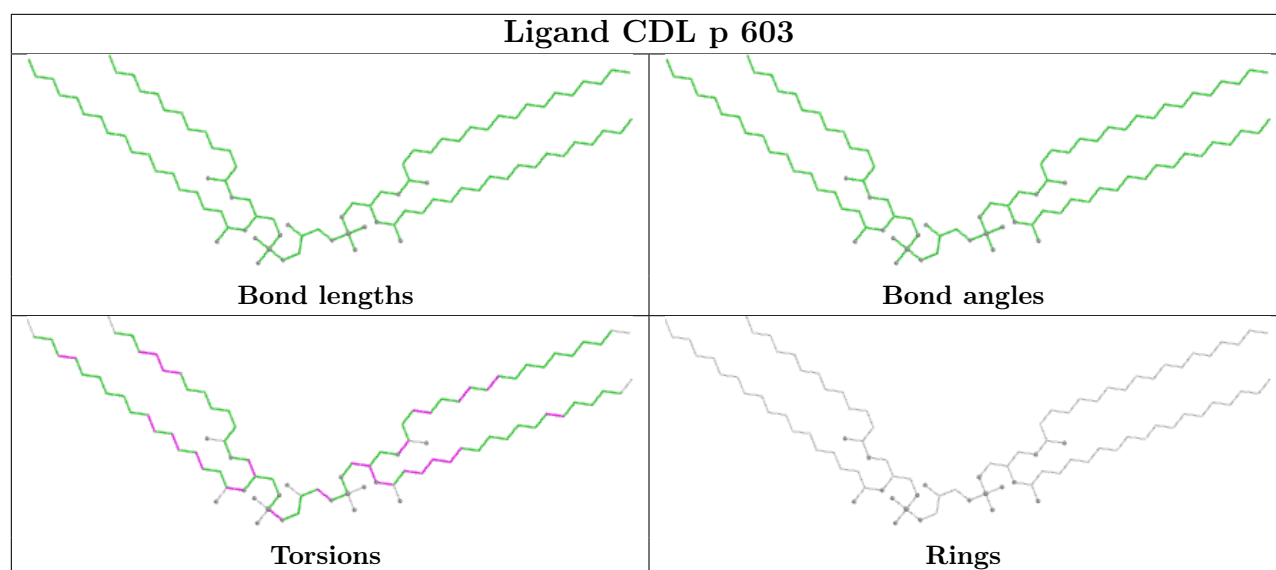


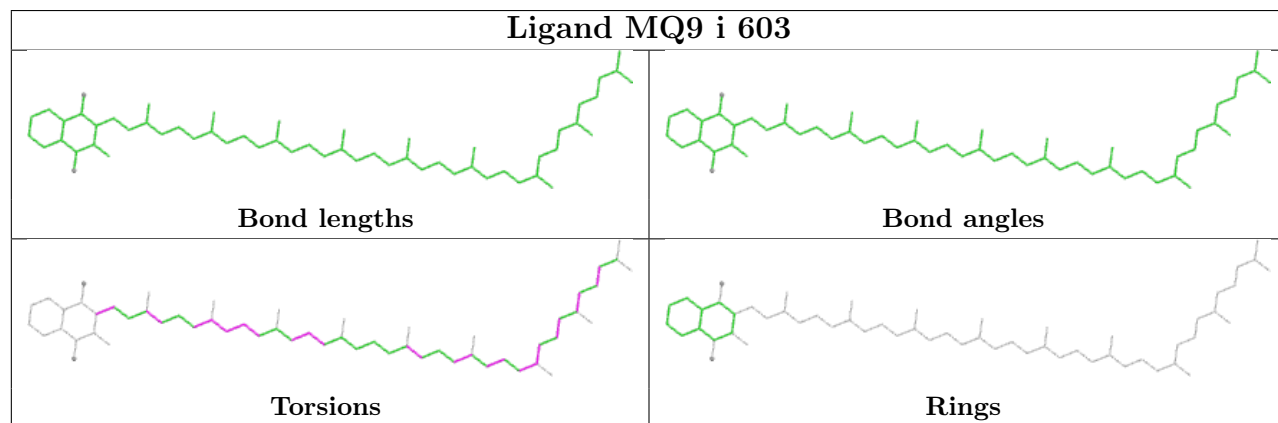
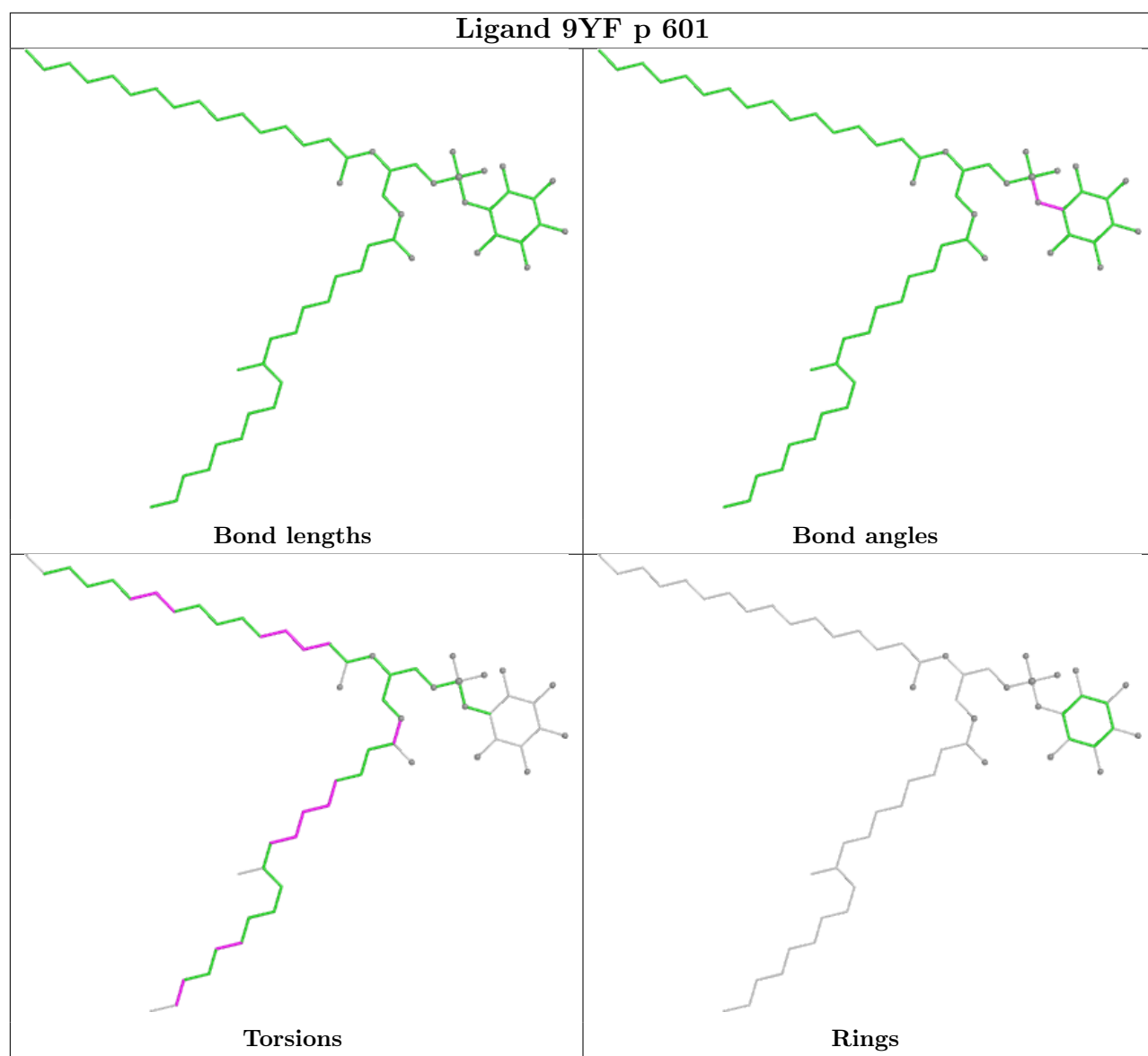


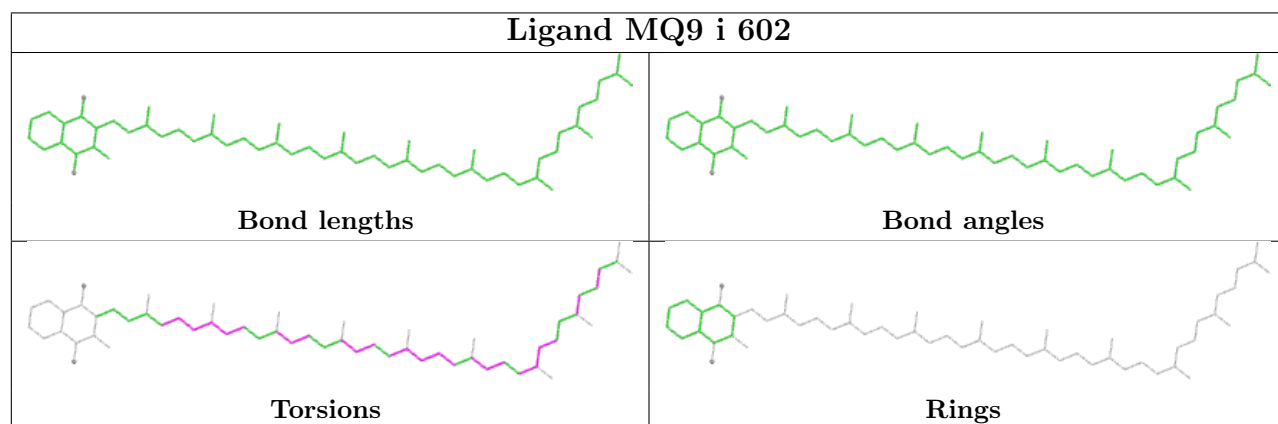
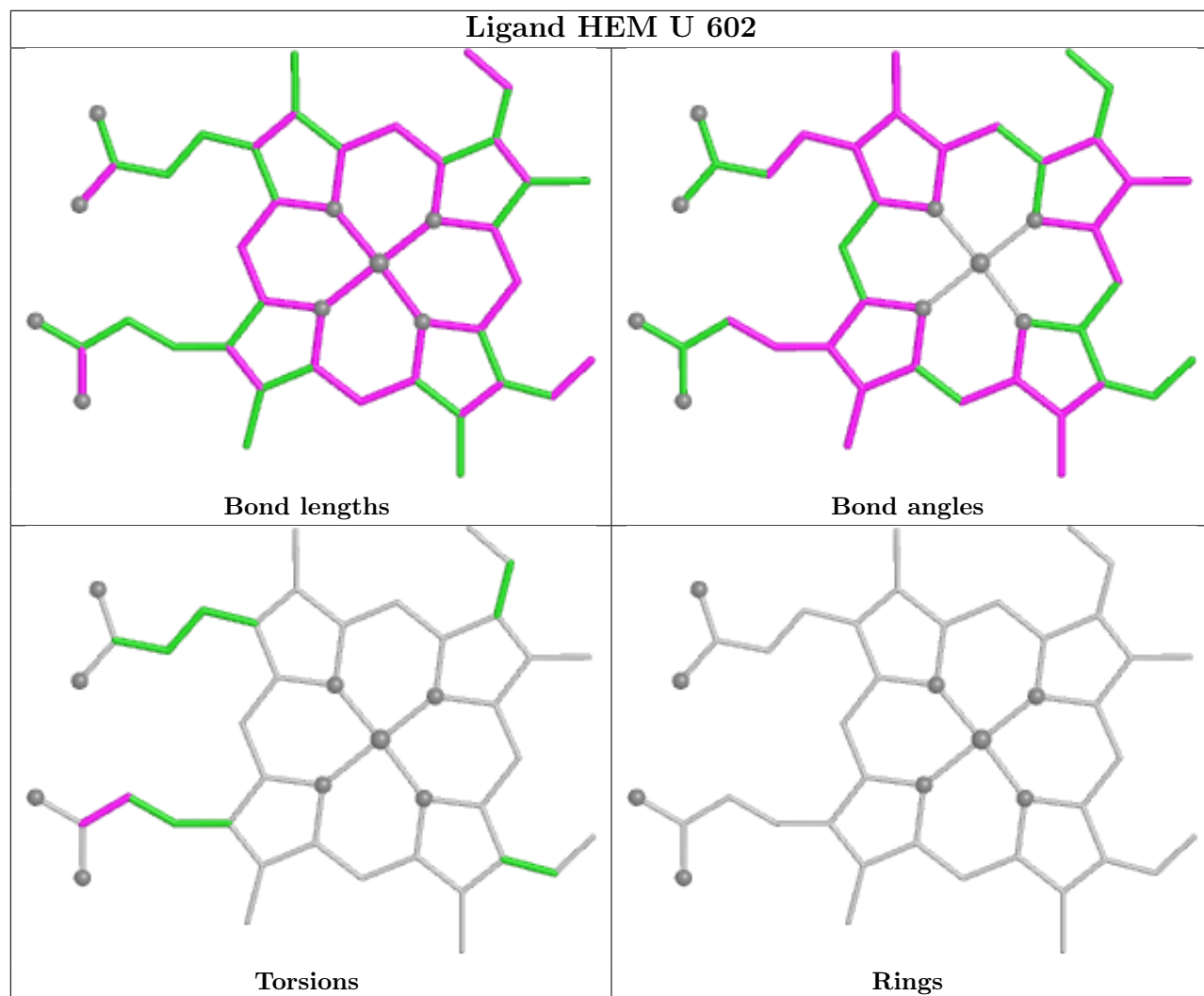


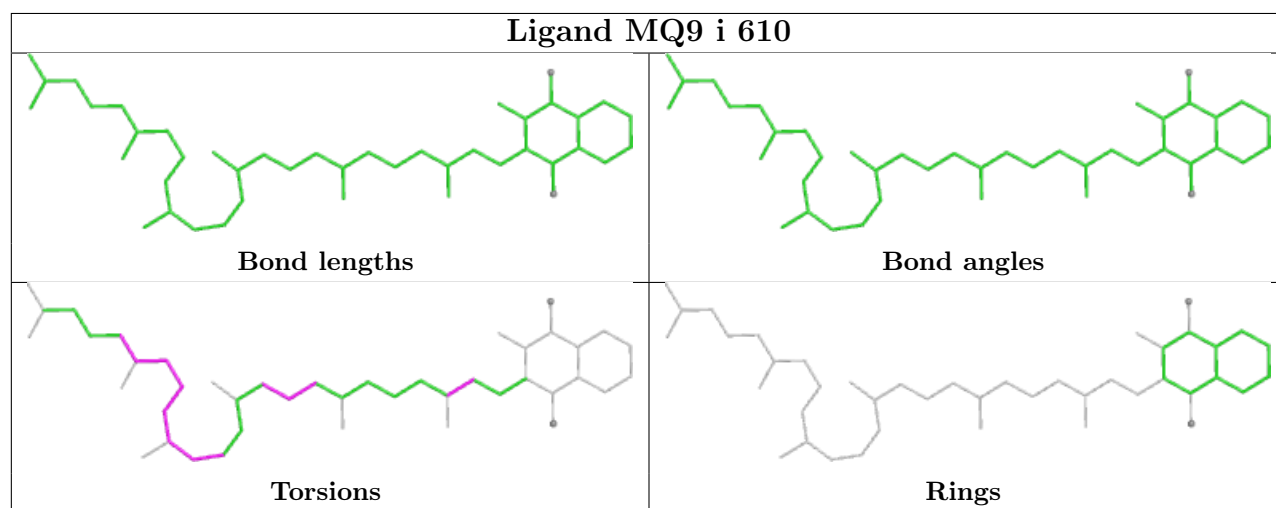
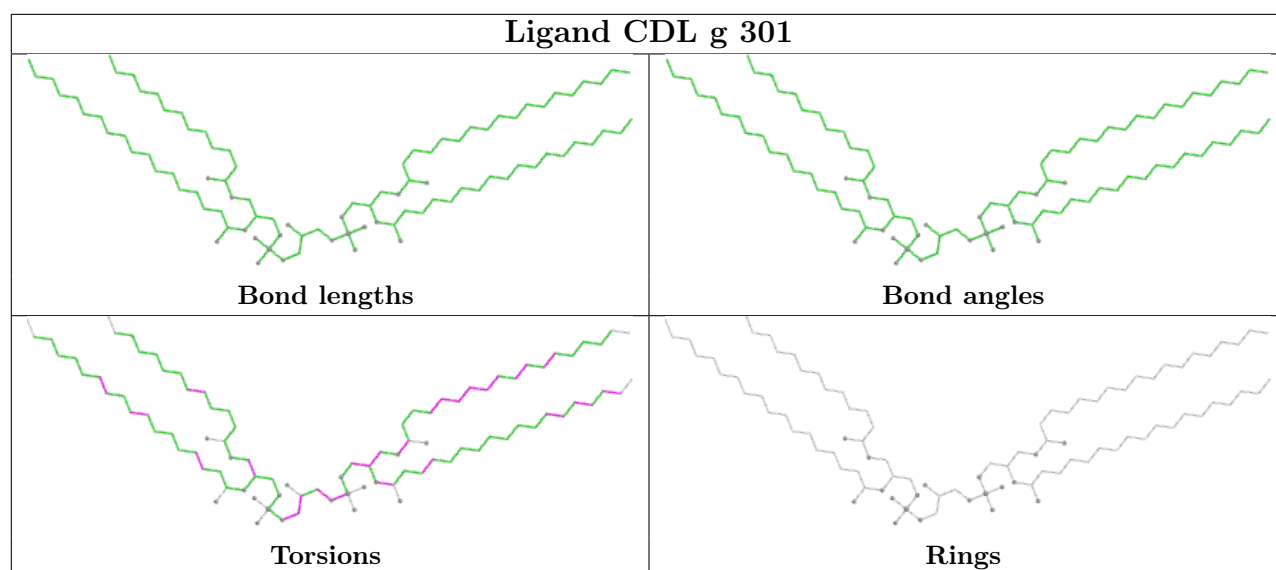


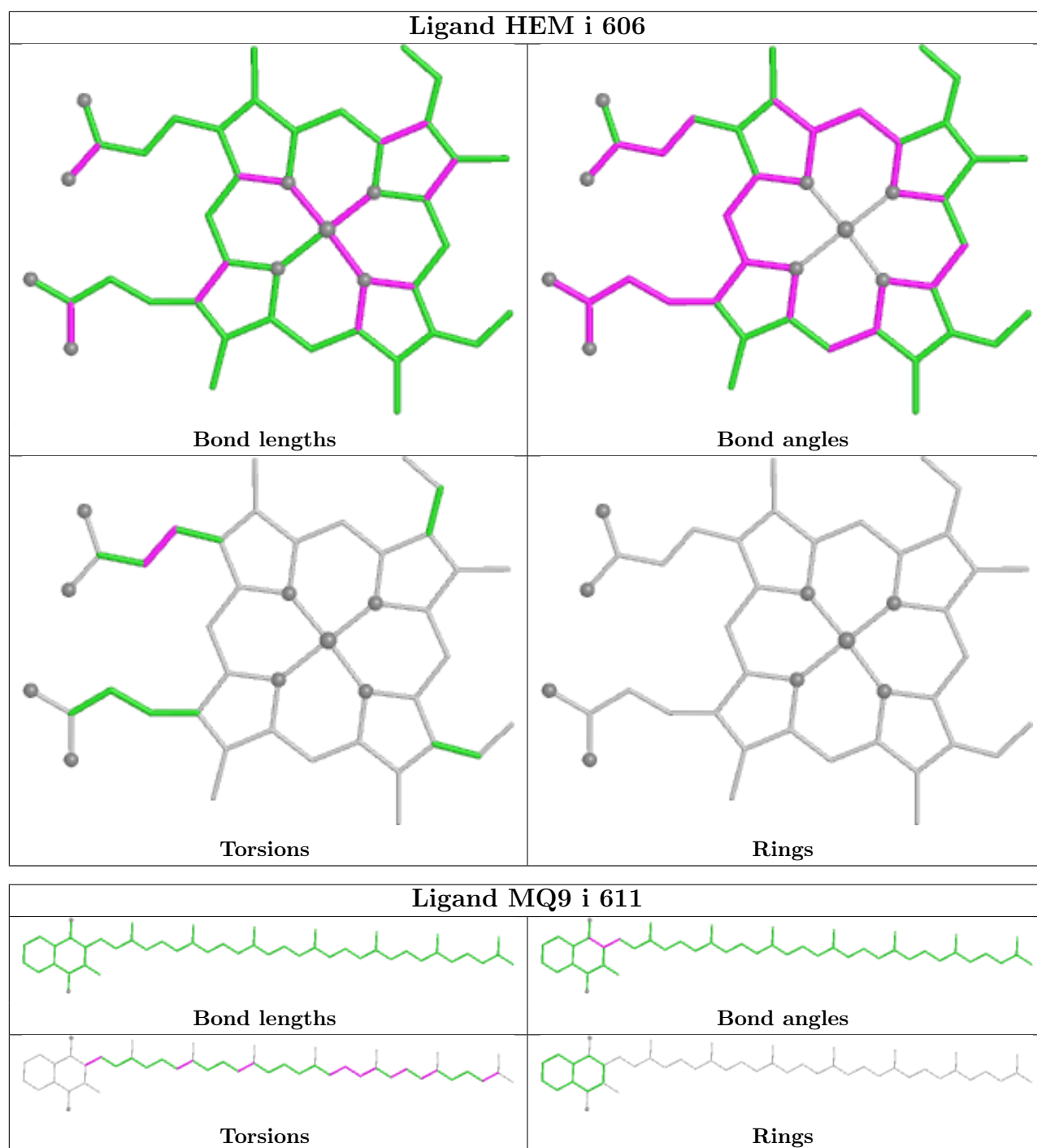


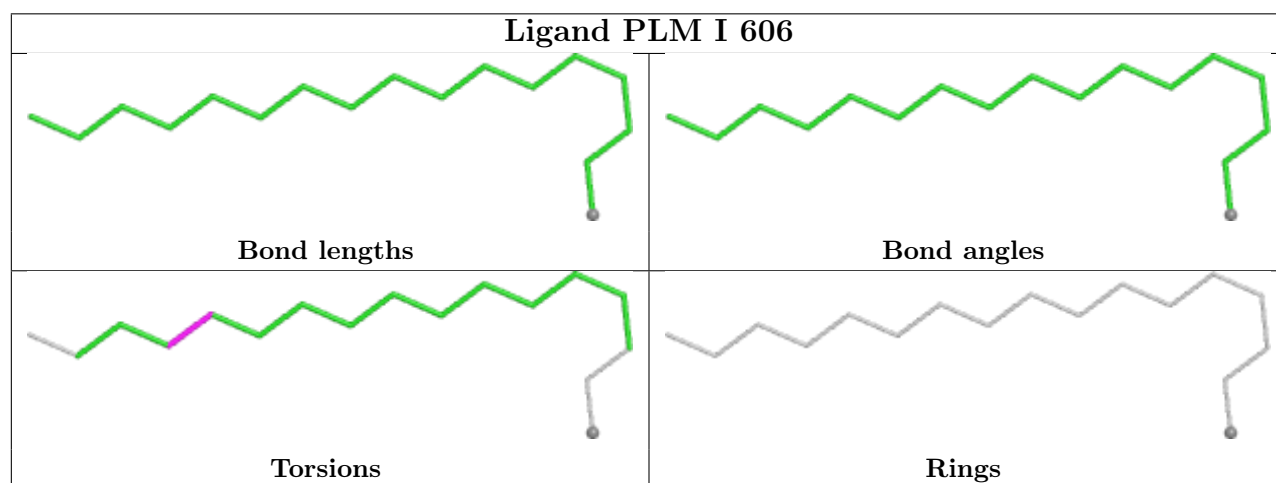
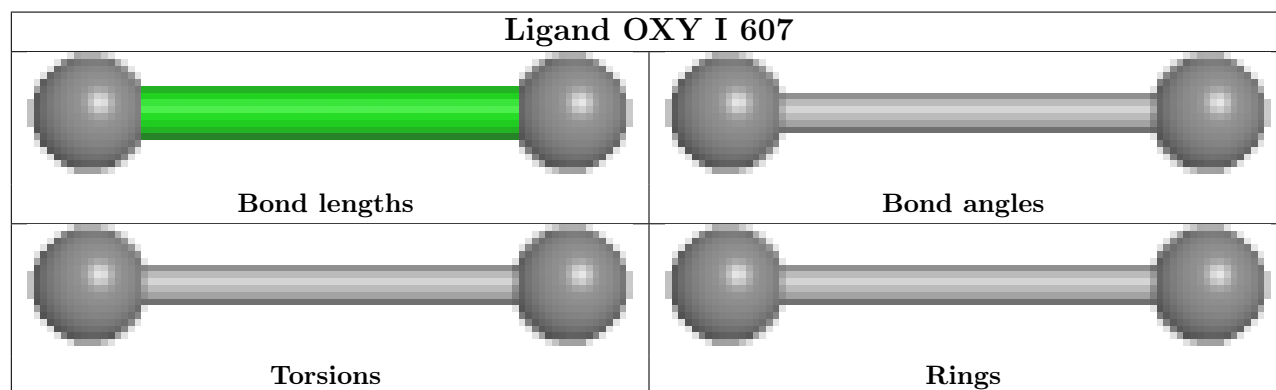
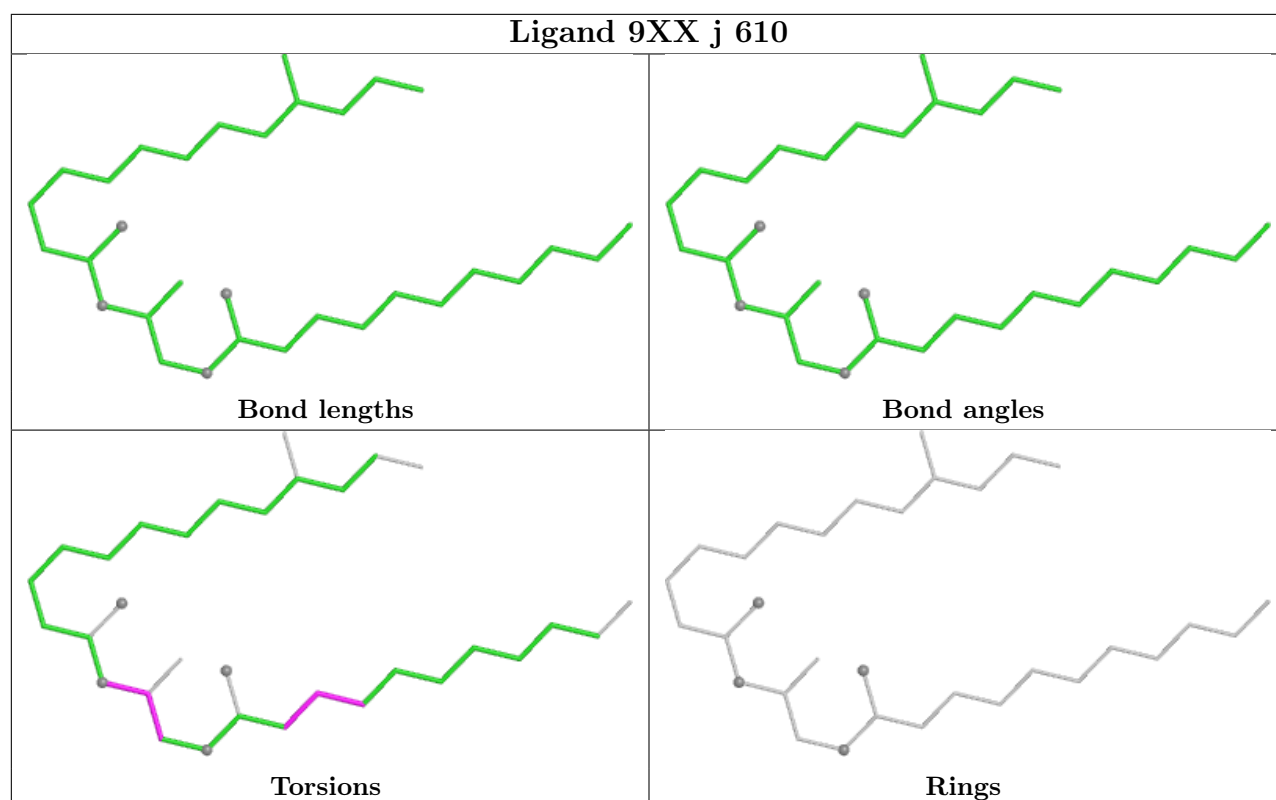












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

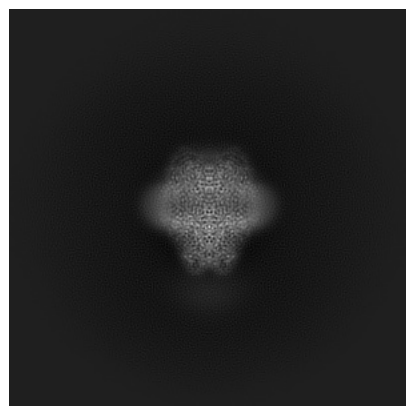
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65878. These allow visual inspection of the internal detail of the map and identification of artifacts.

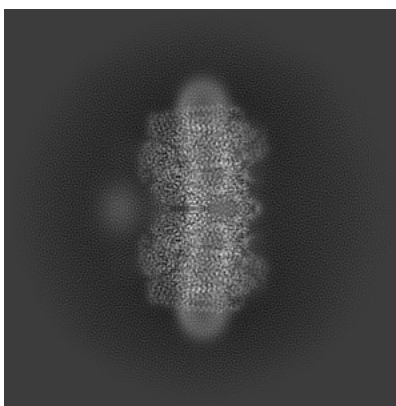
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

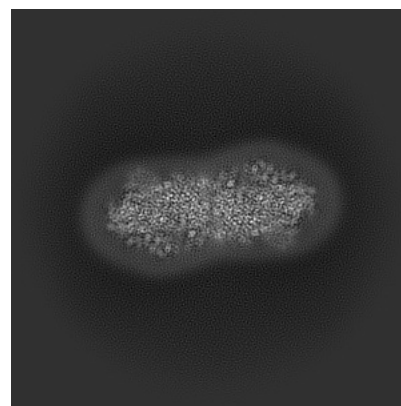
#### 6.1.1 Primary map



X

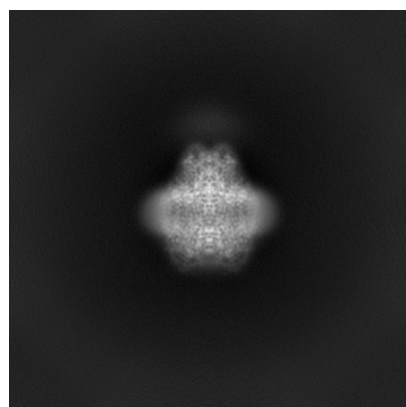


Y

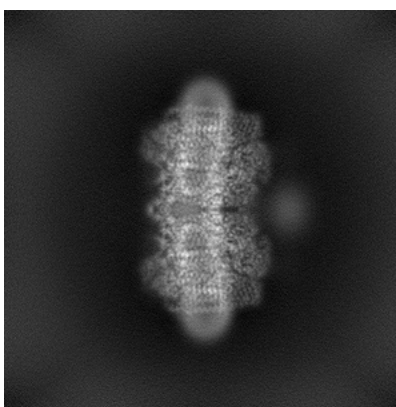


Z

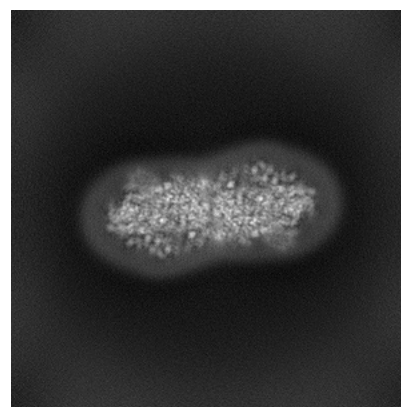
#### 6.1.2 Raw map



X



Y



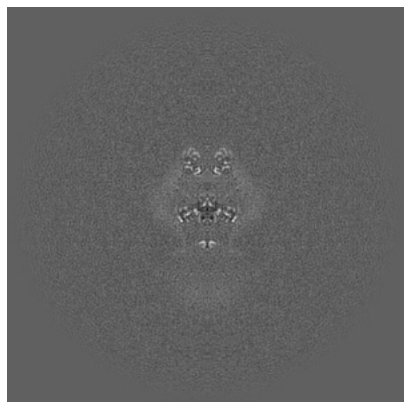
Z

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

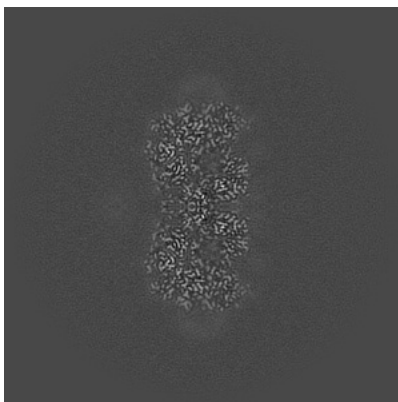


## 6.2 Central slices [i](#)

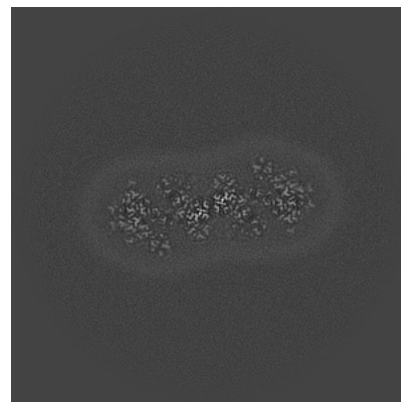
### 6.2.1 Primary map



X Index: 300

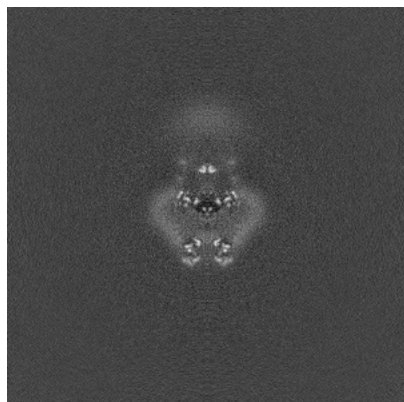


Y Index: 300

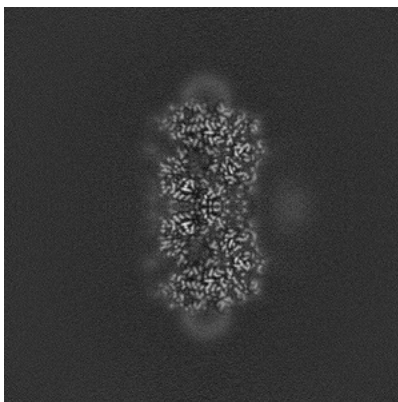


Z Index: 300

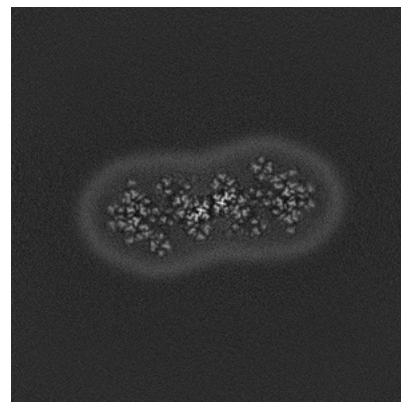
### 6.2.2 Raw map



X Index: 300



Y Index: 300

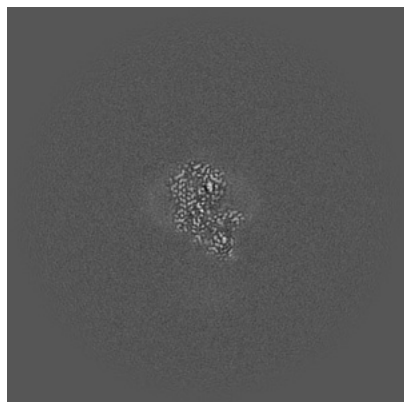


Z Index: 300

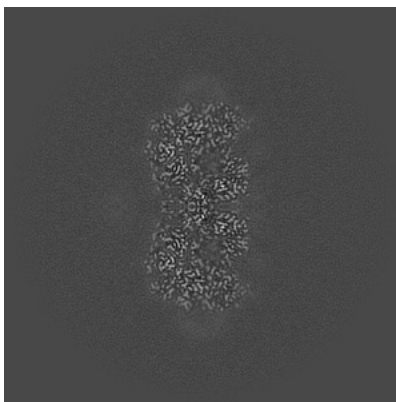
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

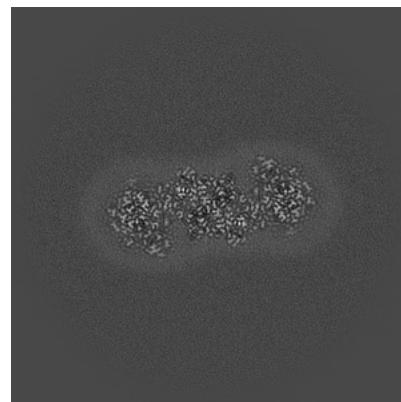
### 6.3.1 Primary map



X Index: 272

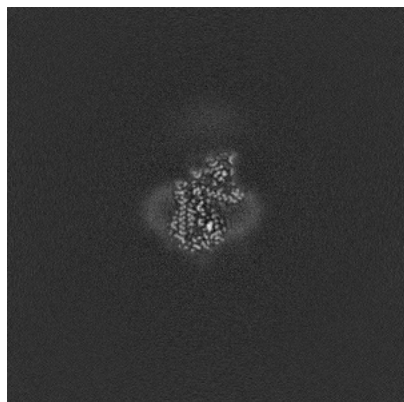


Y Index: 300

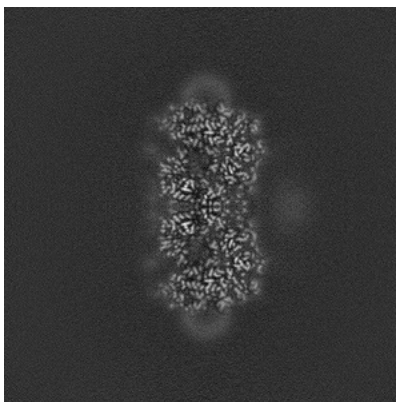


Z Index: 283

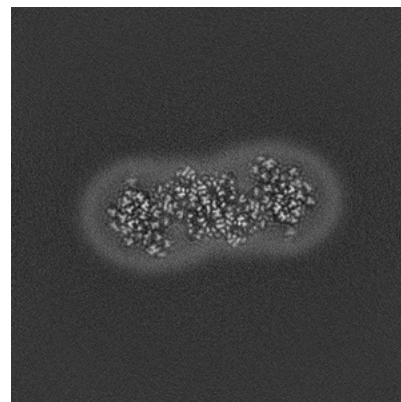
### 6.3.2 Raw map



X Index: 272



Y Index: 300

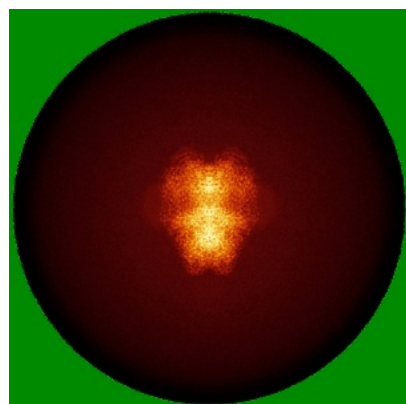


Z Index: 317

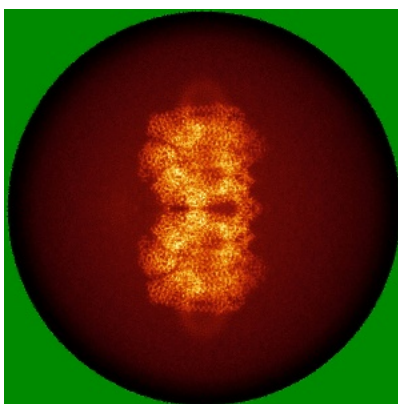
The images above show the largest variance slices of the map in three orthogonal directions.

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

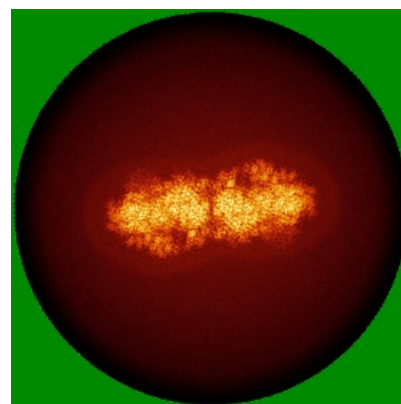
### 6.4.1 Primary map



X

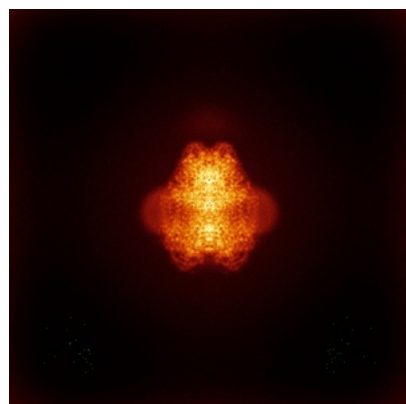


Y

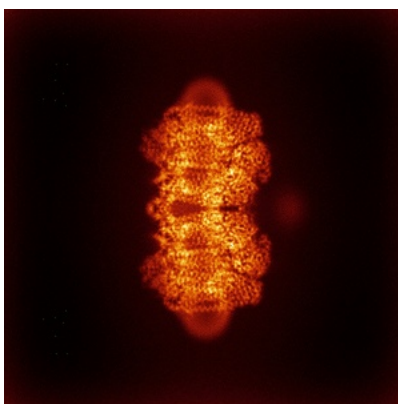


Z

### 6.4.2 Raw map



X



Y

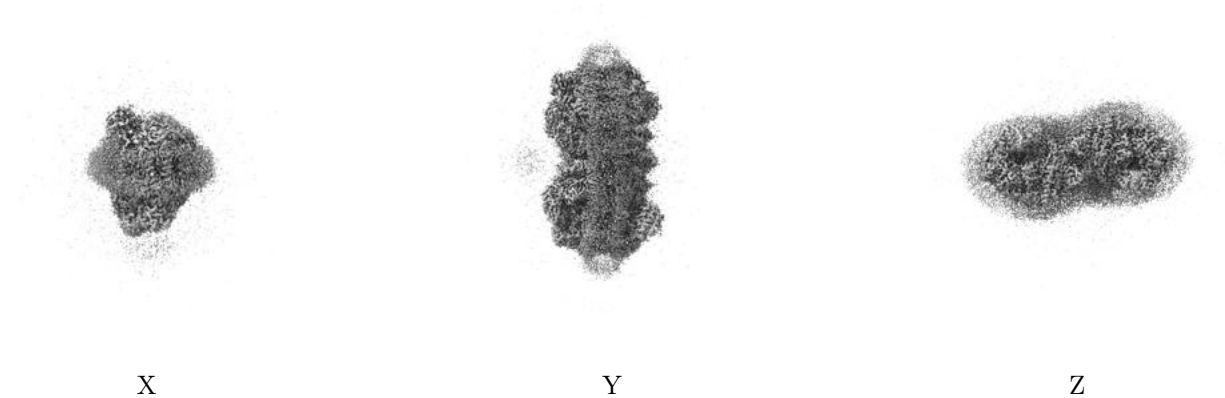


Z

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

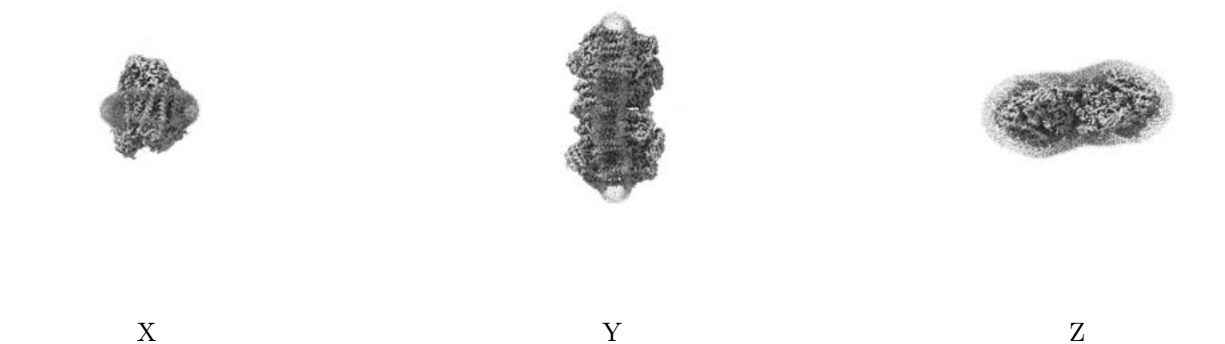
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

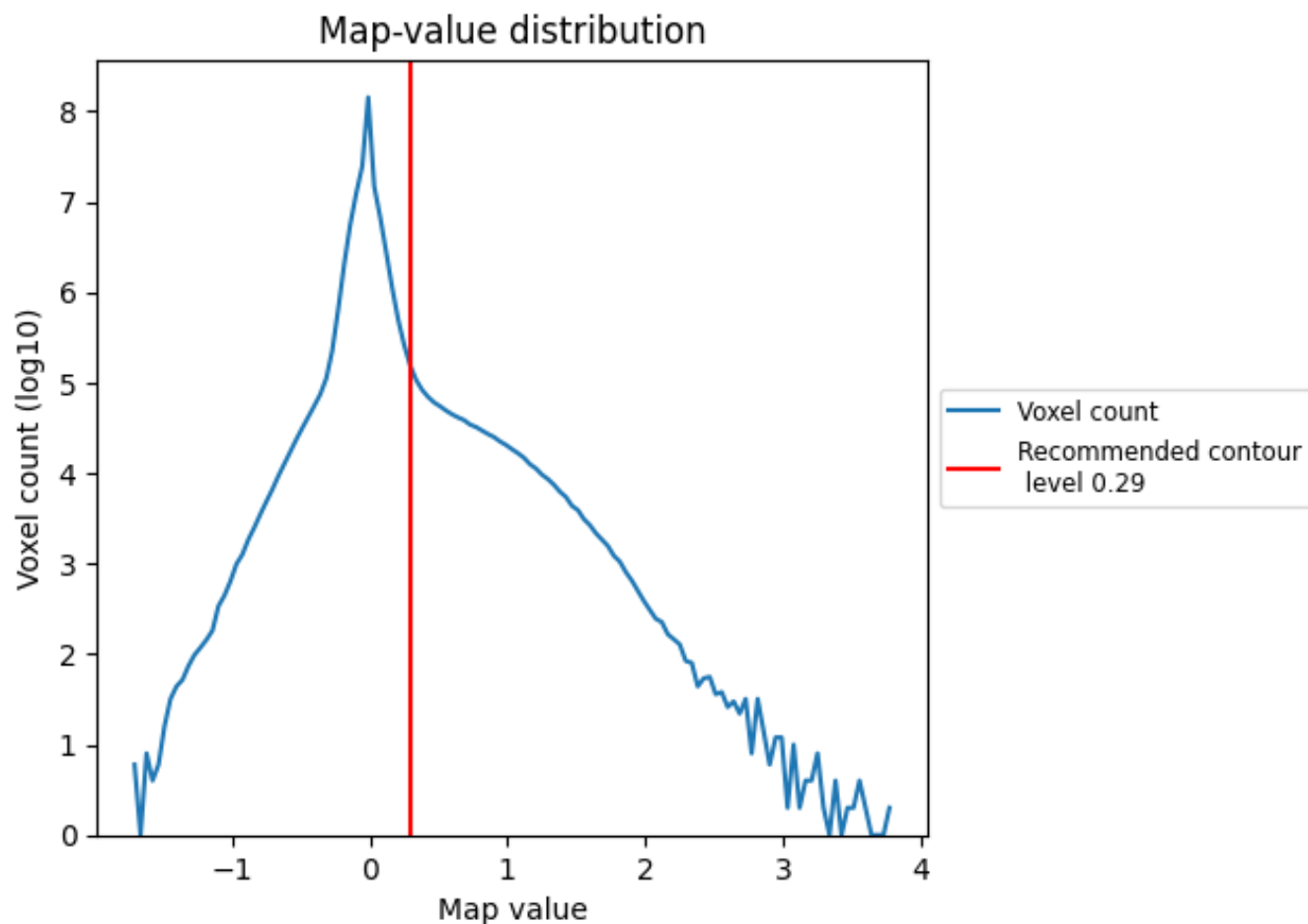
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

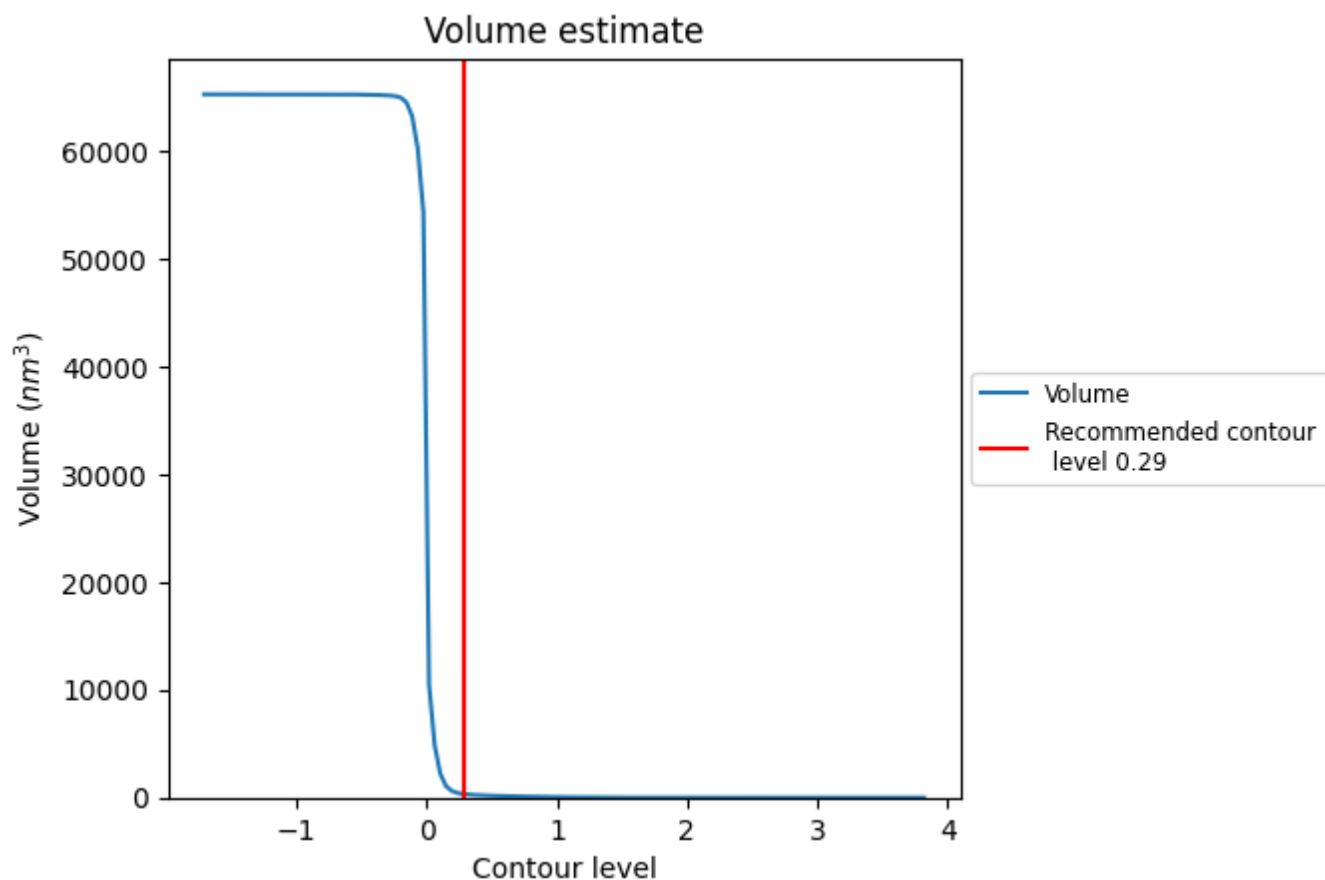
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

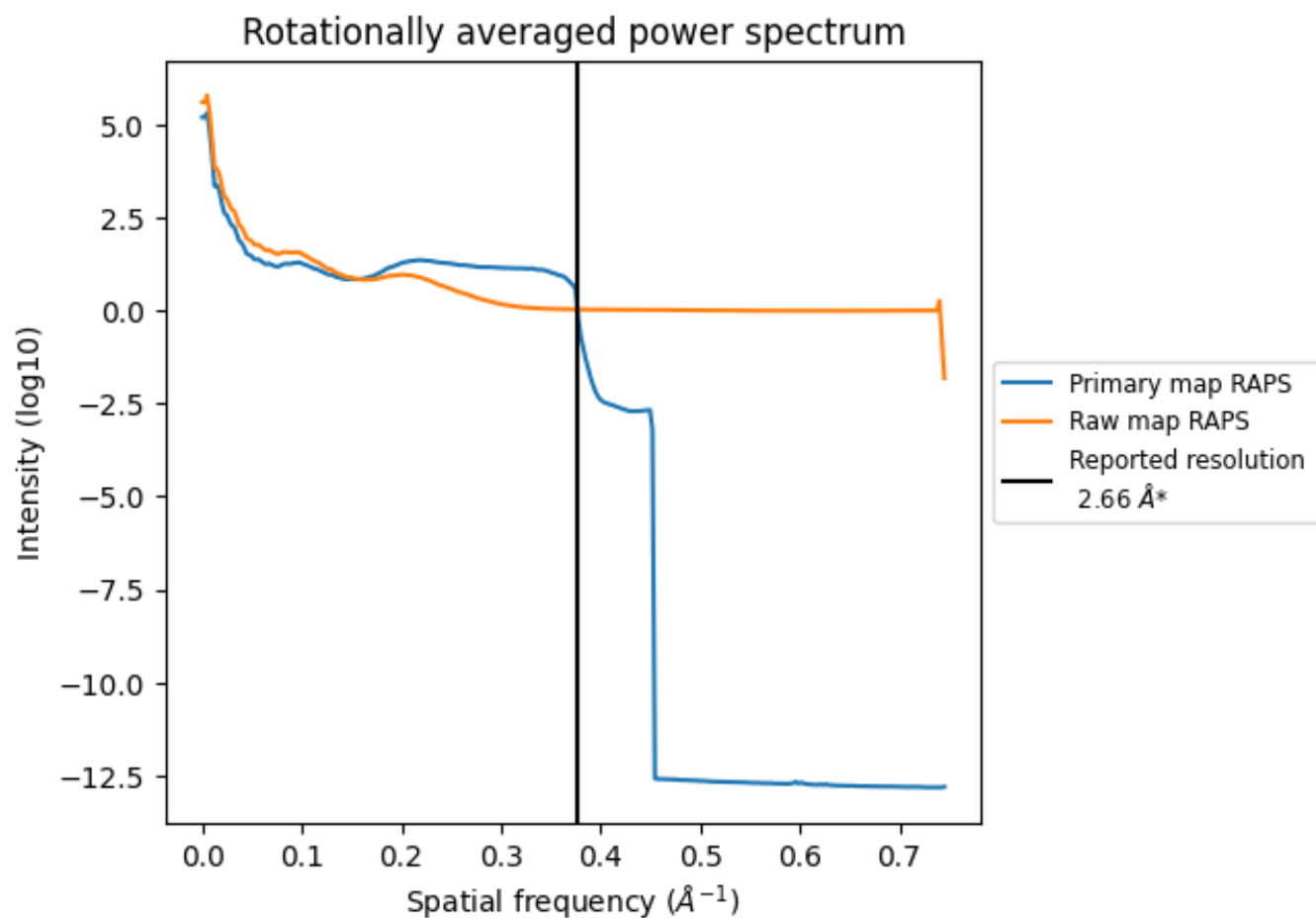
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm<sup>3</sup>; this corresponds to an approximate mass of 289 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 ⓘ



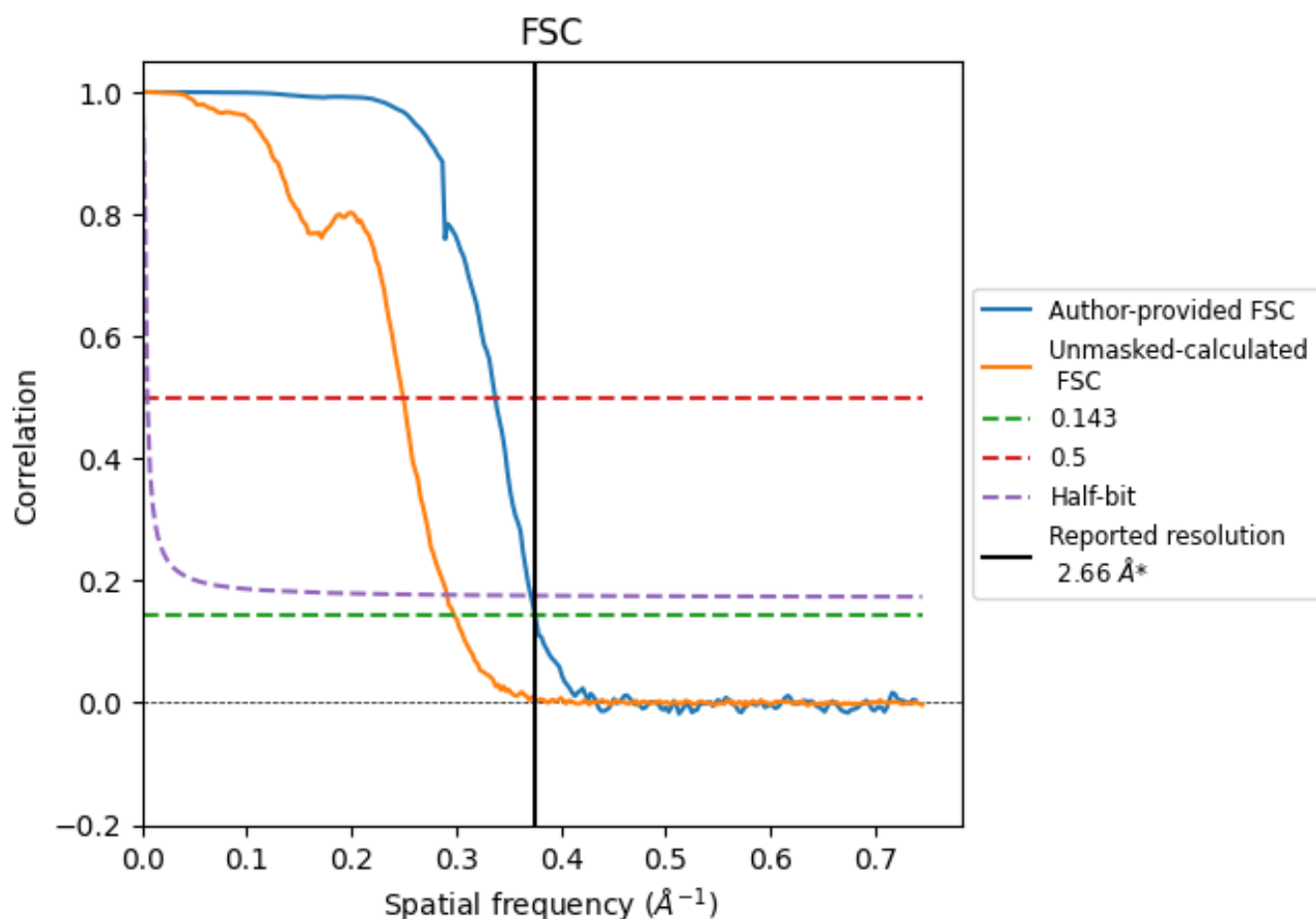
\*Reported resolution corresponds to spatial frequency of 0.376 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.376 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

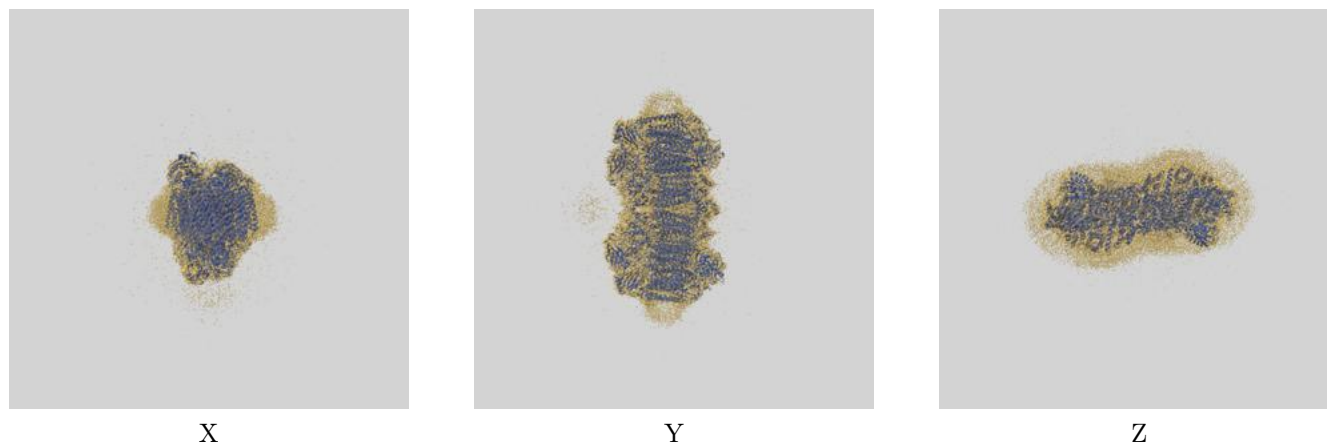
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	2.97	2.69
Unmasked-calculated*	3.36	4.01	3.43

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.66 by more than 10 %

## 9 Map-model fit [i](#)

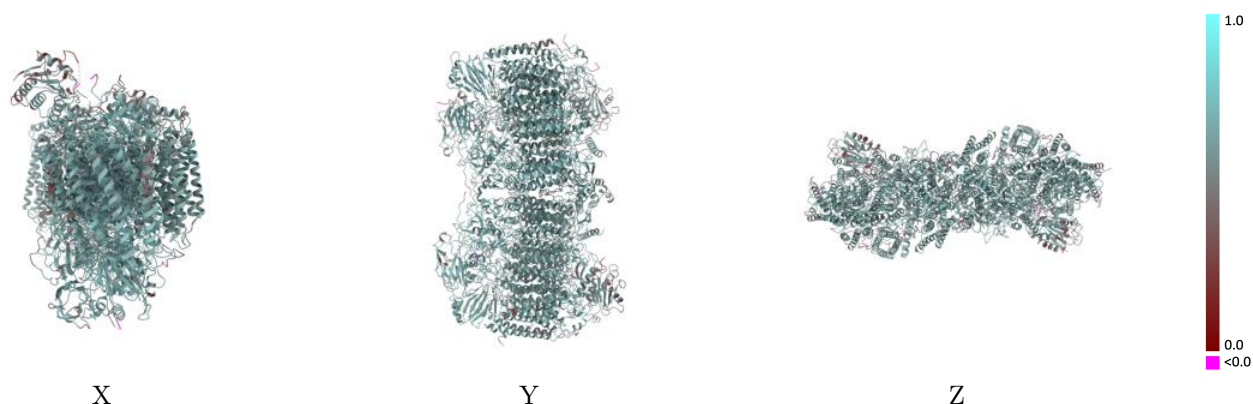
This section contains information regarding the fit between EMDB map EMD-65878 and PDB model 9WCX. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

### 9.1 Map-model overlay [i](#)



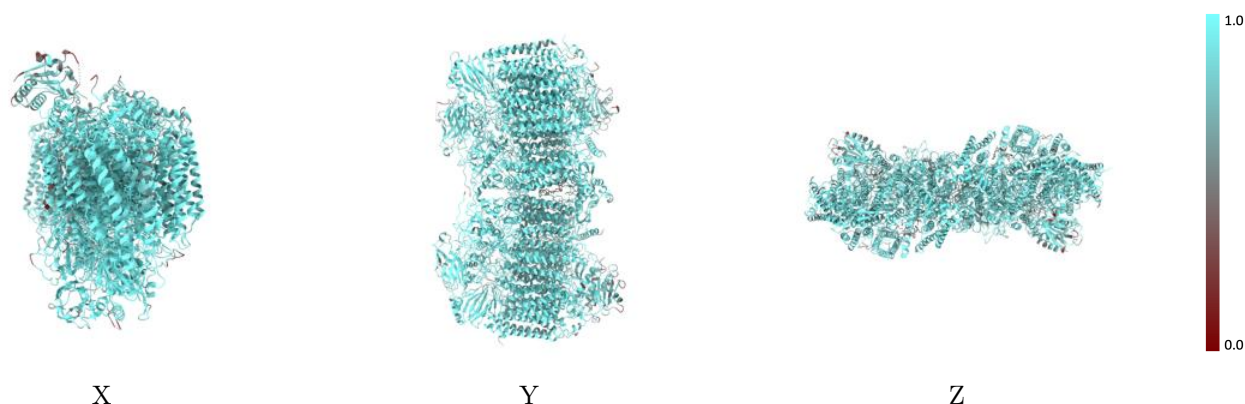
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



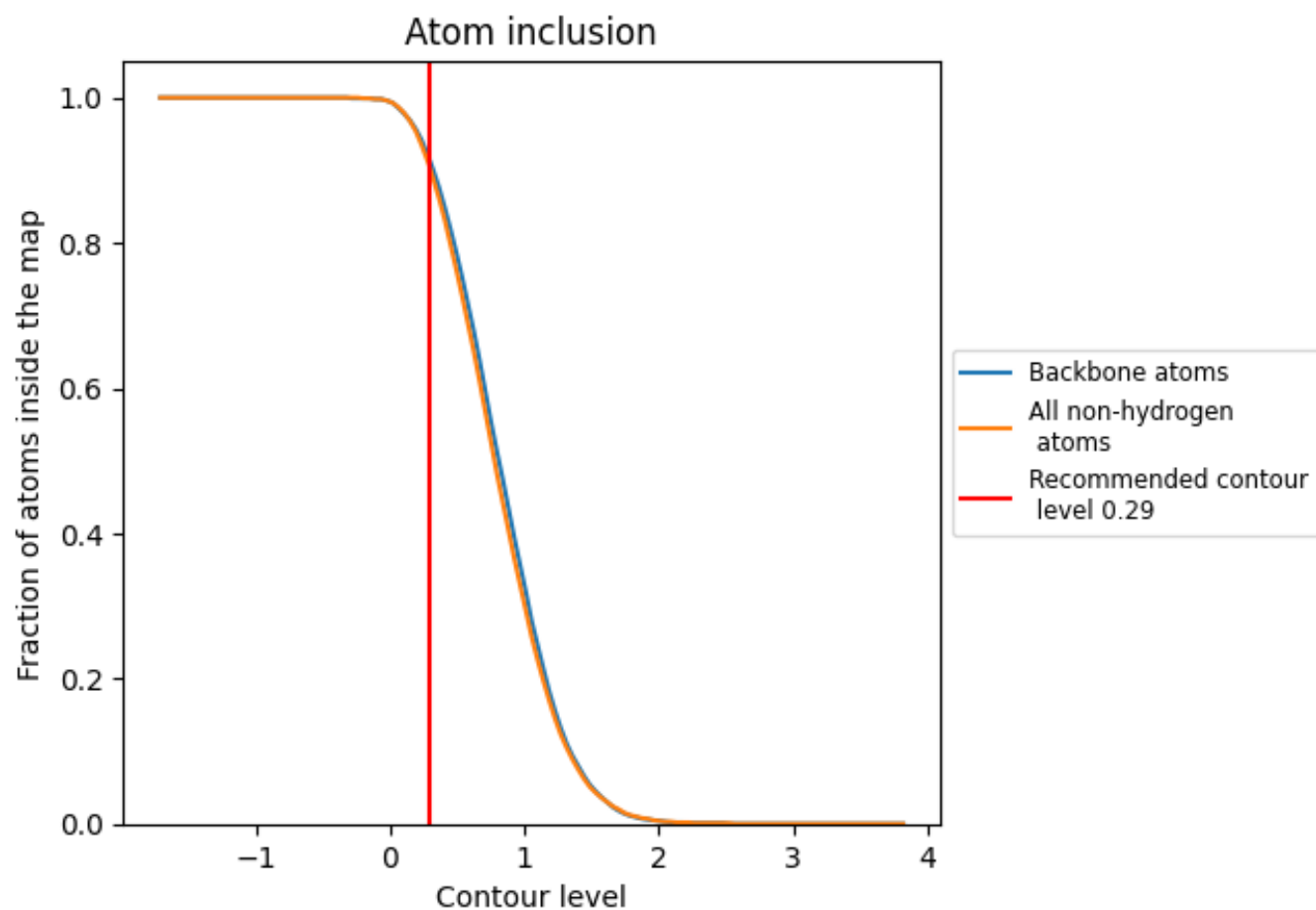
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.6080
G	 0.8600	 0.5990
I	 0.9510	 0.6290
J	 0.6970	 0.4740
L	 0.9500	 0.6280
U	 0.9510	 0.6370
V	 0.9500	 0.6310
X	 0.7820	 0.4980
a	 0.8290	 0.5120
b	 0.8500	 0.5940
d	 0.8910	 0.5920
e	 0.8890	 0.5930
f	 0.9160	 0.5860
g	 0.8870	 0.5800
h	 0.6930	 0.4890
i	 0.9200	 0.6270
j	 0.9340	 0.6290
k	 0.7220	 0.5070
l	 0.7410	 0.5150
m	 0.9080	 0.6010
n	 0.9120	 0.6010
o	 0.9480	 0.6350
p	 0.9360	 0.6280
q	 0.8720	 0.5830
r	 0.8640	 0.5790

