



## wwPDB EM Validation Summary Report ⓘ

Jan 16, 2023 – 05:09 pm GMT

PDB ID : 7ZYV  
EMDB ID : EMD-15027  
Title : Cryo-EM structure of catalytically active *Spinacia oleracea* cytochrome b6f in complex with endogenous plastoquinones at 2.13 Å resolution  
Authors : Sarewicz, M.; Szwalec, M.; Pintscher, S.; Indyka, P.; Rawski, M.; Pietras, R.; Mielecki, B.; Koziej, L.; Jaciuk, M.; Glatt, S.; Osyczka, A.  
Deposited on : 2022-05-25  
Resolution : 2.13 Å (reported)  
Based on initial model : 7QRM

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.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

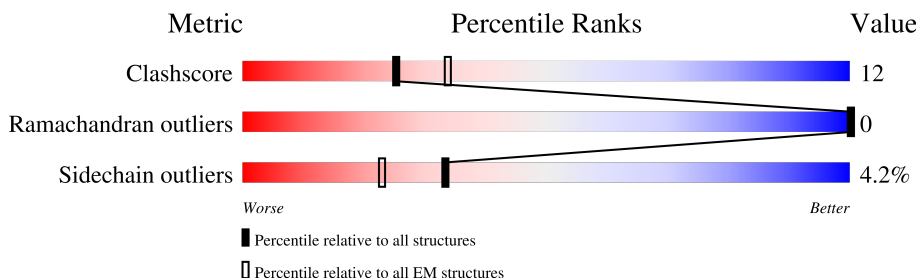
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.13 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	215	86% 13%
1	I	215	85% 14%
2	B	160	85% 13% ..
2	J	160	86% 12% ..
3	C	320	66% 18% • 13%
3	K	320	67% 18% • 13%
4	D	230	60% 11% • 28%
4	L	230	59% 12% • 28%

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Mol	Chain	Length	Quality of chain
5	E	31	87% 13%
5	M	31	87% 13%
6	F	131	27% 72%
6	N	131	25% 73%
7	G	37	89% 8%
7	O	37	76% 11% 11%
8	H	29	97%
8	P	29	93% 7%
9	Q	103	17% 7% 75%
9	R	103	17% 8% 75%

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
12	CLA	A	304	X	-	-	-
12	CLA	I	304	X	-	-	-

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 16892 atoms, of which 440 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	214	Total	C	N	O	S	0	0
			1697	1126	271	289	11		
1	I	214	Total	C	N	O	S	0	0
			1697	1126	271	289	11		

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	159	Total	C	N	O	S	0	0
			1225	820	193	208	4		
2	J	159	Total	C	N	O	S	0	0
			1226	820	193	209	4		

- Molecule 3 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	278	Total	C	N	O	S	0	0
			2158	1391	365	396	6		
3	K	279	Total	C	N	O	S	0	0
			2167	1396	366	399	6		

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	166	Total	C	N	O	S	0	0
			1259	807	212	233	7		
4	L	165	Total	C	N	O	S	0	0
			1254	804	211	232	7		

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	31	Total	C	N	O	S	0	0
			243	167	36	39	1		
5	M	31	Total	C	N	O	S	0	0
			243	167	36	39	1		

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	37	Total	C	N	O	S	0	0
			269	174	45	49	1		
6	N	36	Total	C	N	O	S	0	0
			264	171	44	48	1		

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	34	Total	C	N	O	S	0	0
			266	181	41	43	1		
7	O	33	Total	C	N	O	S	0	0
			261	178	40	42	1		

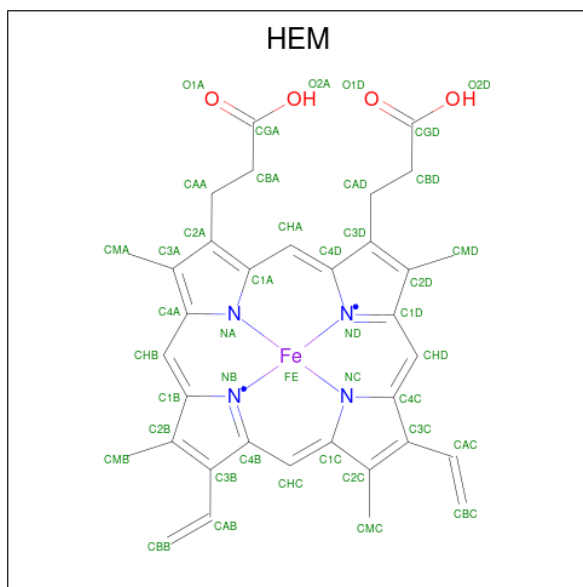
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	29	Total	C	N	O	S	0	0
			222	150	34	36	2		
8	P	29	Total	C	N	O	S	0	0
			223	150	34	37	2		

- Molecule 9 is a protein called Thylakoid soluble phosphoprotein.

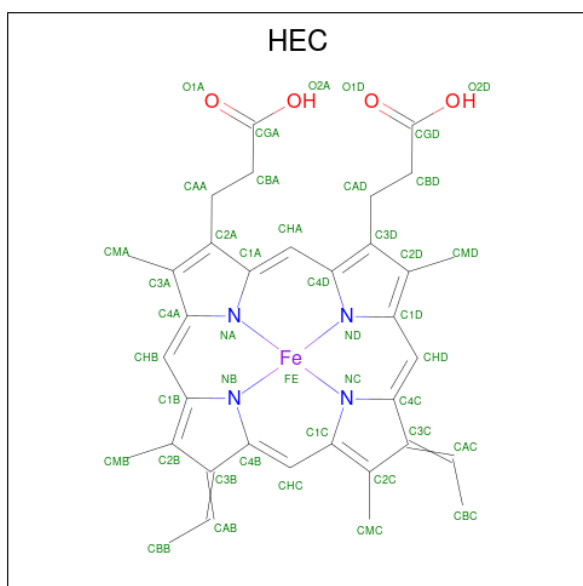
Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	26	Total	C	N	O	0	0
			219	144	34	41		
9	Q	26	Total	C	N	O	0	0
			219	144	34	41		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



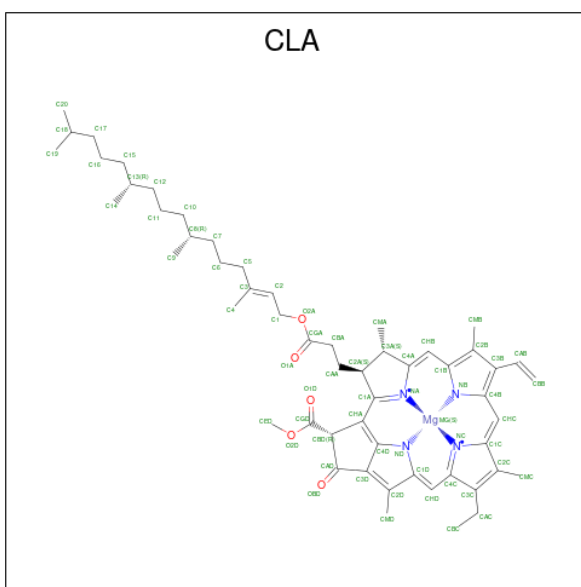
Mol	Chain	Residues	Atoms				AltConf		
			Total	C	Fe	N		O	
10	A	1	Total	86	68	2	8	8	0
10	A	1	Total	86	68	2	8	8	0
10	I	1	Total	86	68	2	8	8	0
10	I	1	Total	86	68	2	8	8	0

- Molecule 11 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



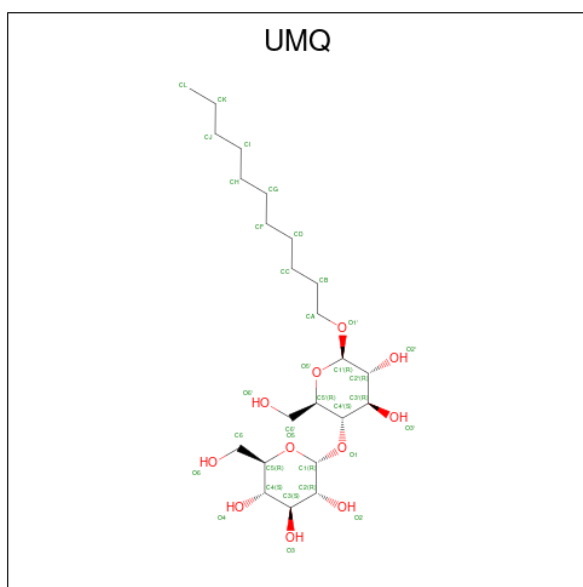
Mol	Chain	Residues	Atoms				AltConf	
11	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

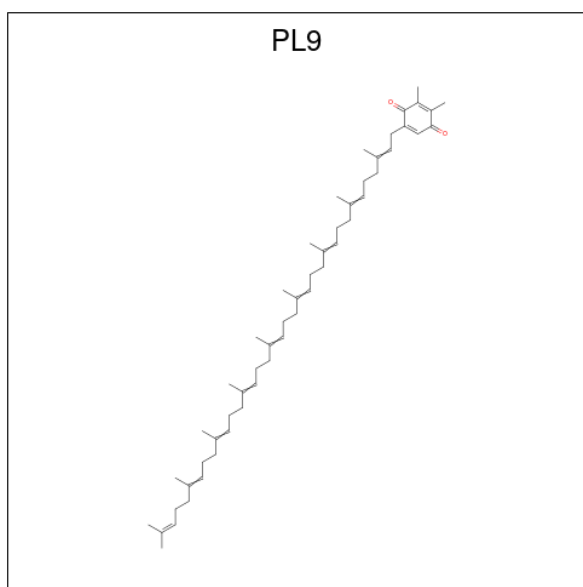
- Molecule 13 is UNDECYL-MALTOSE (three-letter code: UMQ) (formula:  $C_{23}H_{44}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
13	A	1	156	46	88	22	0
13	A	1	156	46	88	22	0
13	B	1	156	46	88	22	0
13	B	1	156	46	88	22	0
13	H	1	78	23	44	11	0
13	I	1	156	46	88	22	0
13	I	1	156	46	88	22	0
13	J	1	156	46	88	22	0
13	J	1	156	46	88	22	0
13	P	1	78	23	44	11	0

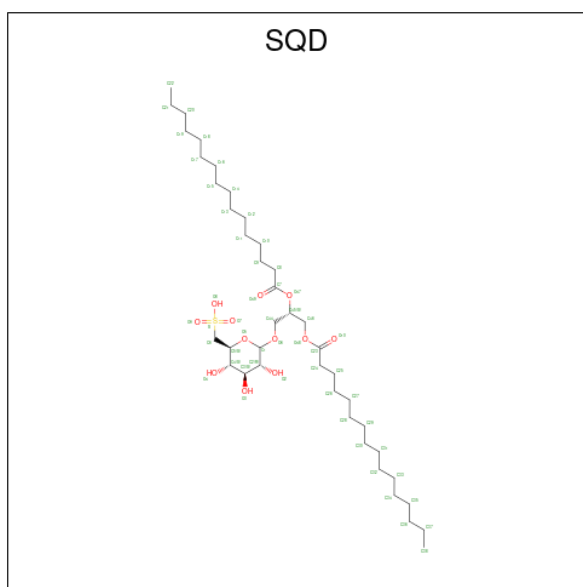
- Molecule 14 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ) (labeled as "Ligand of Interest" by depositor).





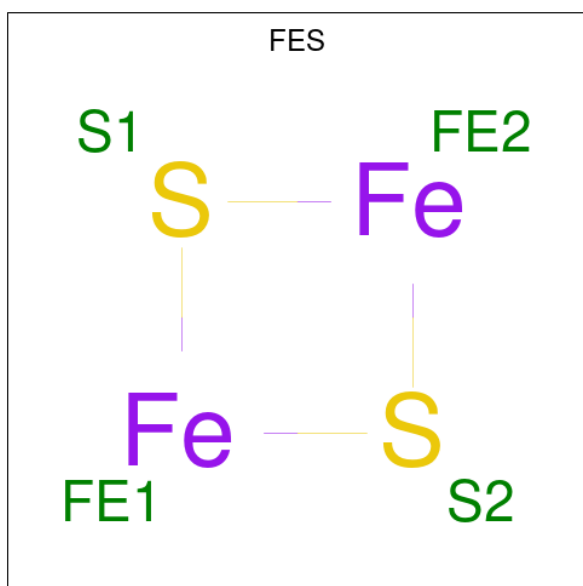
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	A	1	55	53	2	0
14	B	1	110	106	4	0
14	B	1	110	106	4	0
14	J	1	110	106	4	0
14	J	1	110	106	4	0
14	K	1	55	53	2	0

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		S
15	D	1	54	41	12	1	0
15	L	1	54	41	12	1	0

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



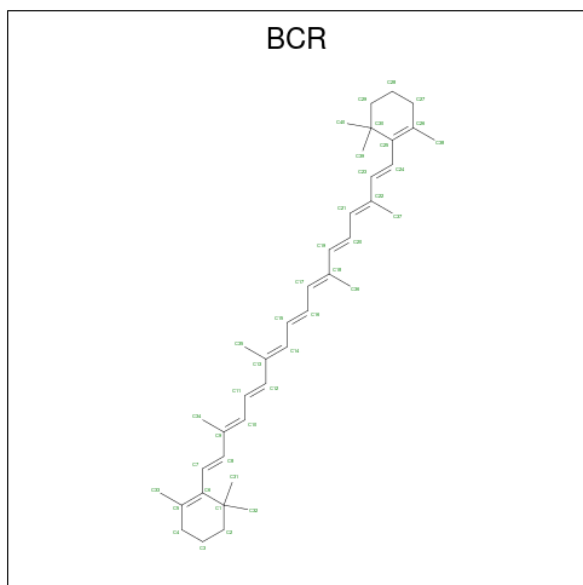
Mol	Chain	Residues	Atoms		AltConf	
			Total	Fe		S
16	D	1	4	2	2	0

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

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).

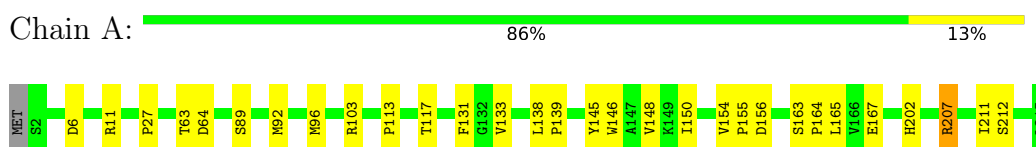


Mol	Chain	Residues	Atoms		AltConf
17	F	1	Total	C	0
			40	40	
17	P	1	Total	C	0
			40	40	

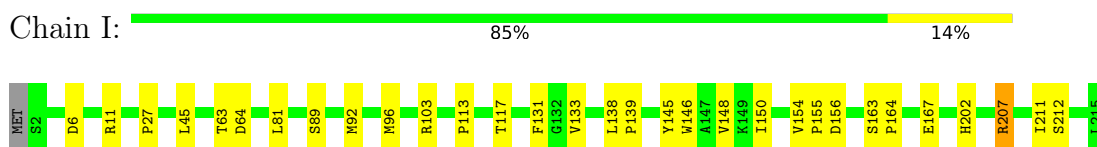
### 3 Residue-property plots

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

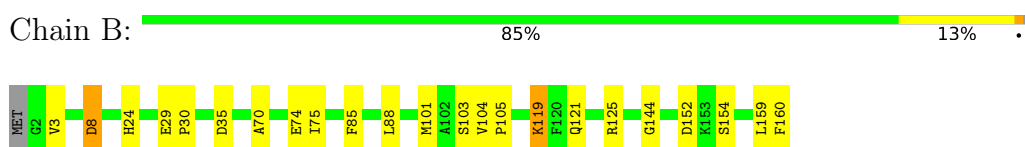
- Molecule 1: Cytochrome b6



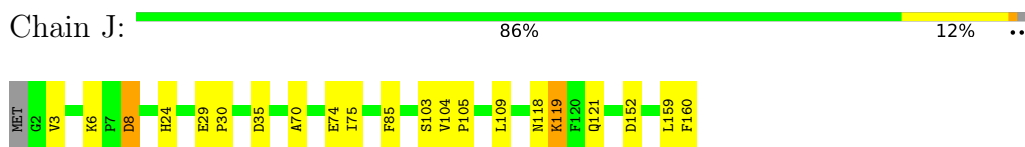
- Molecule 1: Cytochrome b6



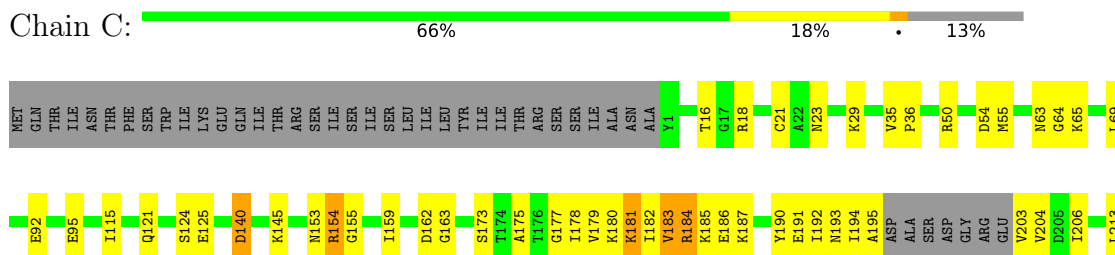
- Molecule 2: Cytochrome b6-f complex subunit 4

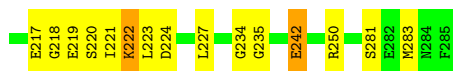


- Molecule 2: Cytochrome b6-f complex subunit 4

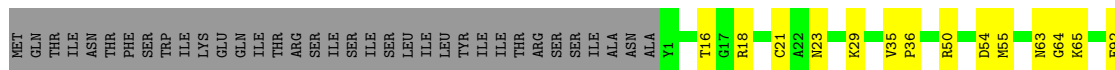


- Molecule 3: Cytochrome f

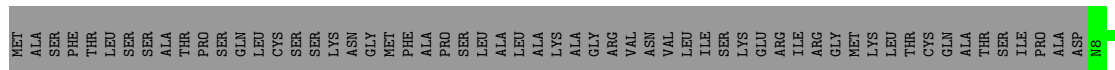




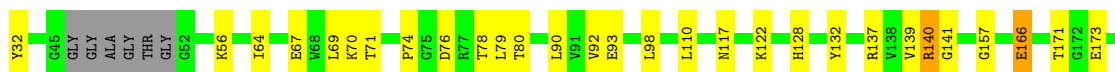
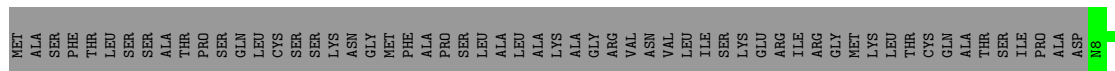
• Molecule 3: Cytochrome f



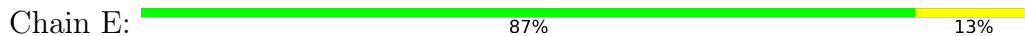
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic



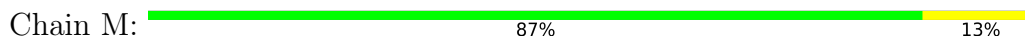
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

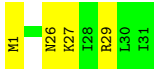


• Molecule 5: Cytochrome b6-f complex subunit 6

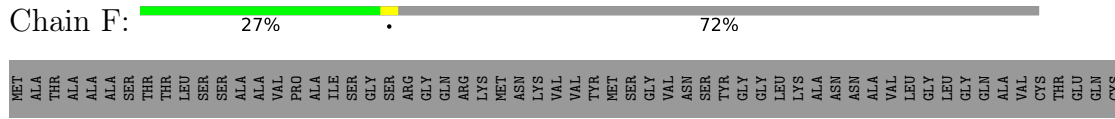


• Molecule 5: Cytochrome b6-f complex subunit 6

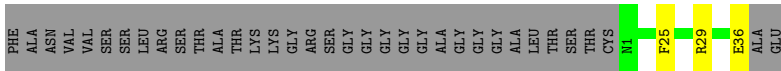
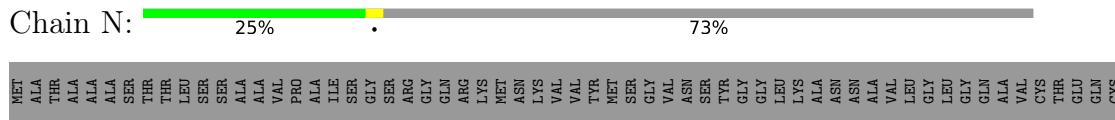




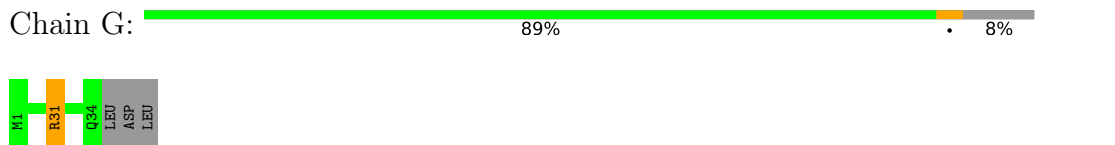
• Molecule 6: Cytochrome b6-f complex subunit 7



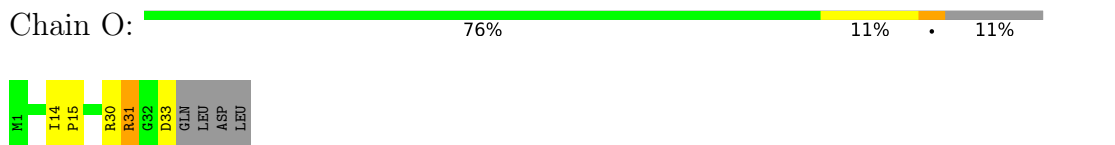
• Molecule 6: Cytochrome b6-f complex subunit 7



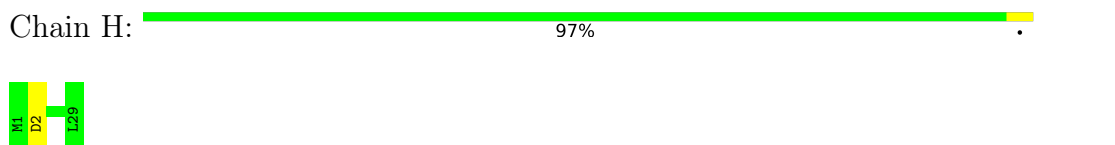
• Molecule 7: Cytochrome b6-f complex subunit 5



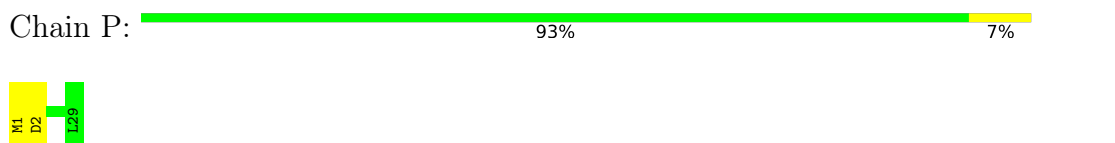
• Molecule 7: Cytochrome b6-f complex subunit 5



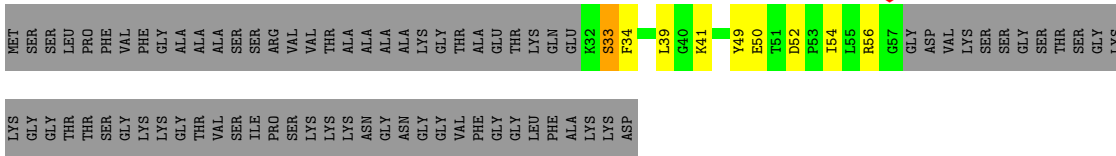
• Molecule 8: Cytochrome b6-f complex subunit 8



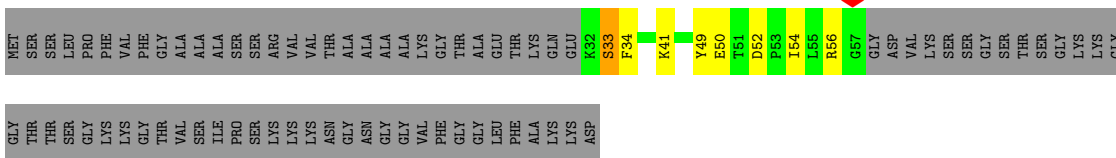
• Molecule 8: Cytochrome b6-f complex subunit 8



• Molecule 9: Thylakoid soluble phosphoprotein



• Molecule 9: Thylakoid soluble phosphoprotein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	685979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Non-uniform Refinement with iterative global CTF refinement and anisotropic magnification fitting	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.455	Depositor
Minimum map value	-0.577	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.208	Depositor
Map size ( $\text{\AA}$ )	319.92, 319.92, 319.92	wwPDB
Map dimensions	372, 372, 372	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.86, 0.86, 0.86	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, SQD, UMQ, PL9, BCR, HEM, HEC, CLA

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	A	0.26	0/1747	0.42	0/2382
1	I	0.26	0/1747	0.42	0/2382
2	B	0.25	0/1262	0.43	0/1733
2	J	0.25	0/1263	0.43	0/1733
3	C	0.26	0/2204	0.44	0/2987
3	K	0.27	0/2213	0.44	0/2999
4	D	0.24	0/1293	0.44	0/1769
4	L	0.24	0/1288	0.44	0/1762
5	E	0.26	0/247	0.41	0/333
5	M	0.26	0/247	0.40	0/333
6	F	0.28	0/270	0.40	0/366
6	N	0.29	0/265	0.41	0/359
7	G	0.27	0/271	0.41	0/367
7	O	0.27	0/266	0.40	0/360
8	H	0.26	0/227	0.39	0/309
8	P	0.27	0/228	0.40	0/309
9	Q	0.24	0/224	0.35	0/301
9	R	0.23	0/224	0.35	0/301
All	All	0.26	0/15486	0.43	0/21085

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	0	1724	18	0
1	I	1697	0	1724	20	0
2	B	1225	0	1276	28	0
2	J	1226	0	1276	23	0
3	C	2158	0	2212	84	0
3	K	2167	0	2218	78	0
4	D	1259	0	1232	23	0
4	L	1254	0	1227	23	0
5	E	243	0	268	1	0
5	M	243	0	268	4	0
6	F	269	0	287	2	0
6	N	264	0	282	2	0
7	G	266	0	282	1	0
7	O	261	0	280	3	0
8	H	222	0	234	1	0
8	P	223	0	234	1	0
9	Q	219	0	216	7	0
9	R	219	0	216	8	0
10	A	86	0	60	9	0
10	I	86	0	60	10	0
11	A	43	0	31	2	0
11	C	43	0	31	6	0
11	I	43	0	31	2	0
11	K	43	0	31	5	0
12	A	65	0	72	4	0
12	I	65	0	72	5	0
13	A	68	88	88	0	0
13	B	68	88	88	3	0
13	H	34	44	44	1	0
13	I	68	88	88	2	0
13	J	68	88	88	1	0
13	P	34	44	44	1	0
14	A	55	0	80	10	0
14	B	110	0	158	27	0
14	J	110	0	160	28	0
14	K	55	0	77	4	0
15	D	54	0	77	5	0
15	L	54	0	77	1	0
16	D	4	0	0	0	0
16	L	4	0	0	0	0
17	F	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	P	40	0	56	5	0
All	All	16452	440	17025	386	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 12.

The worst 5 of 386 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)
3:K:180:LYS:HG2	3:K:194:ILE:HA	1.39	1.04
3:K:180:LYS:HE2	3:K:195:ALA:H	1.22	1.03
3:C:180:LYS:HE2	3:C:195:ALA:H	1.22	1.01
3:C:180:LYS:HG2	3:C:194:ILE:HA	1.39	1.00
3:C:179:VAL:HA	3:C:194:ILE:HG22	1.44	0.99

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	A	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
1	I	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
2	J	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
3	C	274/320 (86%)	263 (96%)	11 (4%)	0	100	100
3	K	275/320 (86%)	264 (96%)	11 (4%)	0	100	100
4	D	162/230 (70%)	151 (93%)	11 (7%)	0	100	100
4	L	161/230 (70%)	152 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
5	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	F	35/131 (27%)	35 (100%)	0	0	100	100
6	N	34/131 (26%)	34 (100%)	0	0	100	100
7	G	32/37 (86%)	31 (97%)	1 (3%)	0	100	100
7	O	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	27 (100%)	0	0	100	100
9	Q	24/103 (23%)	23 (96%)	1 (4%)	0	100	100
9	R	24/103 (23%)	23 (96%)	1 (4%)	0	100	100
All	All	1902/2512 (76%)	1828 (96%)	74 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	A	185/186 (100%)	178 (96%)	7 (4%)	33	30
1	I	185/186 (100%)	178 (96%)	7 (4%)	33	30
2	B	134/135 (99%)	128 (96%)	6 (4%)	27	23
2	J	134/135 (99%)	128 (96%)	6 (4%)	27	23
3	C	237/275 (86%)	228 (96%)	9 (4%)	33	30
3	K	238/275 (86%)	231 (97%)	7 (3%)	42	40
4	D	135/183 (74%)	130 (96%)	5 (4%)	34	31
4	L	135/183 (74%)	130 (96%)	5 (4%)	34	31
5	E	26/26 (100%)	23 (88%)	3 (12%)	5	2
5	M	26/26 (100%)	24 (92%)	2 (8%)	13	7
6	F	26/90 (29%)	25 (96%)	1 (4%)	33	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	N	26/90 (29%)	25 (96%)	1 (4%)	33	30
7	G	27/31 (87%)	26 (96%)	1 (4%)	34	31
7	O	27/31 (87%)	25 (93%)	2 (7%)	13	8
8	H	24/24 (100%)	24 (100%)	0	100	100
8	P	24/24 (100%)	23 (96%)	1 (4%)	30	26
9	Q	24/78 (31%)	21 (88%)	3 (12%)	4	1
9	R	24/78 (31%)	21 (88%)	3 (12%)	4	1
All	All	1637/2056 (80%)	1568 (96%)	69 (4%)	33	26

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	M	1	MET
6	N	29	ARG
9	R	56	ARG
4	D	137	ARG
4	D	76	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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	UMQ	I	305	-	35,35,35	1.15	1 (2%)	46,46,46	0.96	3 (6%)
16	FES	D	202	4	0,4,4	-	-	-		
17	BCR	F	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	7 (12%)
13	UMQ	A	306	-	35,35,35	1.15	1 (2%)	46,46,46	0.96	3 (6%)
13	UMQ	I	306	-	35,35,35	1.13	1 (2%)	46,46,46	0.97	1 (2%)
10	HEM	A	301	1	41,50,50	1.47	3 (7%)	45,82,82	1.41	6 (13%)
12	CLA	A	304	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	9 (11%)
13	UMQ	H	201	-	35,35,35	1.12	1 (2%)	46,46,46	0.94	3 (6%)
14	PL9	B	402	-	55,55,55	1.08	4 (7%)	68,69,69	1.53	16 (23%)
12	CLA	I	304	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	9 (11%)
13	UMQ	B	404	-	35,35,35	1.14	2 (5%)	46,46,46	1.05	4 (8%)
14	PL9	A	307	-	55,55,55	1.03	4 (7%)	68,69,69	1.54	10 (14%)
16	FES	L	402	4	0,4,4	-	-	-		
11	HEC	I	303	1	32,50,50	2.28	3 (9%)	24,82,82	1.37	2 (8%)
14	PL9	J	401	-	55,55,55	1.03	4 (7%)	68,69,69	1.55	12 (17%)
10	HEM	I	302	1	41,50,50	1.47	3 (7%)	45,82,82	1.33	6 (13%)
10	HEM	I	301	1	41,50,50	1.46	3 (7%)	45,82,82	1.40	6 (13%)
13	UMQ	J	403	-	35,35,35	1.18	3 (8%)	46,46,46	0.92	2 (4%)
14	PL9	K	302	14	55,55,55	1.02	3 (5%)	68,69,69	1.52	10 (14%)
13	UMQ	P	102	-	35,35,35	1.12	1 (2%)	46,46,46	1.09	3 (6%)
15	SQD	L	401	-	53,54,54	0.98	5 (9%)	62,65,65	1.46	8 (12%)
11	HEC	K	301	3	32,50,50	2.26	3 (9%)	24,82,82	1.32	1 (4%)
11	HEC	C	301	3	32,50,50	2.25	3 (9%)	24,82,82	1.32	1 (4%)
13	UMQ	A	305	-	35,35,35	1.15	2 (5%)	46,46,46	0.85	0
14	PL9	B	401	14	55,55,55	1.03	4 (7%)	68,69,69	1.55	13 (19%)
17	BCR	P	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	9 (16%)
13	UMQ	B	403	-	35,35,35	1.23	3 (8%)	46,46,46	1.40	7 (15%)
14	PL9	J	402	-	55,55,55	1.05	4 (7%)	68,69,69	1.53	11 (16%)
10	HEM	A	302	1	41,50,50	1.47	3 (7%)	45,82,82	1.33	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	SQD	D	201	-	53,54,54	0.97	5 (9%)	62,65,65	1.53	8 (12%)
13	UMQ	J	404	-	35,35,35	1.23	4 (11%)	46,46,46	1.40	7 (15%)
11	HEC	A	303	1	32,50,50	2.27	3 (9%)	24,82,82	1.36	2 (8%)

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	UMQ	I	305	-	-	9/20/60/60	0/2/2/2
16	FES	D	202	4	-	-	0/1/1/1
17	BCR	F	101	-	-	4/29/63/63	0/2/2/2
13	UMQ	A	306	-	-	9/20/60/60	0/2/2/2
13	UMQ	I	306	-	-	12/20/60/60	0/2/2/2
12	CLA	A	304	-	1/1/15/20	16/37/115/115	-
10	HEM	A	301	1	-	3/12/54/54	-
13	UMQ	H	201	-	-	5/20/60/60	0/2/2/2
14	PL9	B	402	-	-	24/53/73/73	0/1/1/1
12	CLA	I	304	-	1/1/15/20	16/37/115/115	-
13	UMQ	B	404	-	-	11/20/60/60	0/2/2/2
14	PL9	A	307	-	-	19/53/73/73	0/1/1/1
16	FES	L	402	4	-	-	0/1/1/1
11	HEC	I	303	1	-	4/10/54/54	-
14	PL9	J	401	-	-	21/53/73/73	0/1/1/1
10	HEM	I	301	1	-	3/12/54/54	-
10	HEM	I	302	1	-	2/12/54/54	-
13	UMQ	J	403	-	-	12/20/60/60	0/2/2/2
14	PL9	K	302	14	-	21/53/73/73	0/1/1/1
13	UMQ	P	102	-	-	8/20/60/60	0/2/2/2
15	SQD	L	401	-	-	20/49/69/69	0/1/1/1
11	HEC	K	301	3	-	2/10/54/54	-
11	HEC	C	301	3	-	2/10/54/54	-
13	UMQ	A	305	-	-	7/20/60/60	0/2/2/2
14	PL9	B	401	14	-	18/53/73/73	0/1/1/1
17	BCR	P	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	UMQ	B	403	-	-	8/20/60/60	0/2/2/2
14	PL9	J	402	-	-	21/53/73/73	0/1/1/1
10	HEM	A	302	1	-	2/12/54/54	-
15	SQD	D	201	-	-	15/49/69/69	0/1/1/1
13	UMQ	J	404	-	-	8/20/60/60	0/2/2/2
11	HEC	A	303	1	-	4/10/54/54	-

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	304	CLA	C4B-NB	7.39	1.41	1.35
12	I	304	CLA	C4B-NB	7.34	1.41	1.35
11	I	303	HEC	C2B-C3B	-6.94	1.33	1.40
11	A	303	HEC	C2B-C3B	-6.88	1.33	1.40
11	I	303	HEC	C3C-C2C	-6.76	1.33	1.40

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	304	CLA	C4A-NA-C1A	6.36	109.56	106.71
12	I	304	CLA	C4A-NA-C1A	6.30	109.54	106.71
14	J	401	PL9	C7-C3-C4	5.60	121.43	116.88
14	A	307	PL9	C7-C3-C4	5.55	121.39	116.88
14	B	401	PL9	C7-C3-C4	5.39	121.25	116.88

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	304	CLA	ND
12	I	304	CLA	ND

5 of 308 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	302	HEM	C1A-C2A-CAA-CBA
10	A	302	HEM	C3A-C2A-CAA-CBA
10	I	302	HEM	C1A-C2A-CAA-CBA
10	I	302	HEM	C3A-C2A-CAA-CBA
11	A	303	HEC	C1A-C2A-CAA-CBA

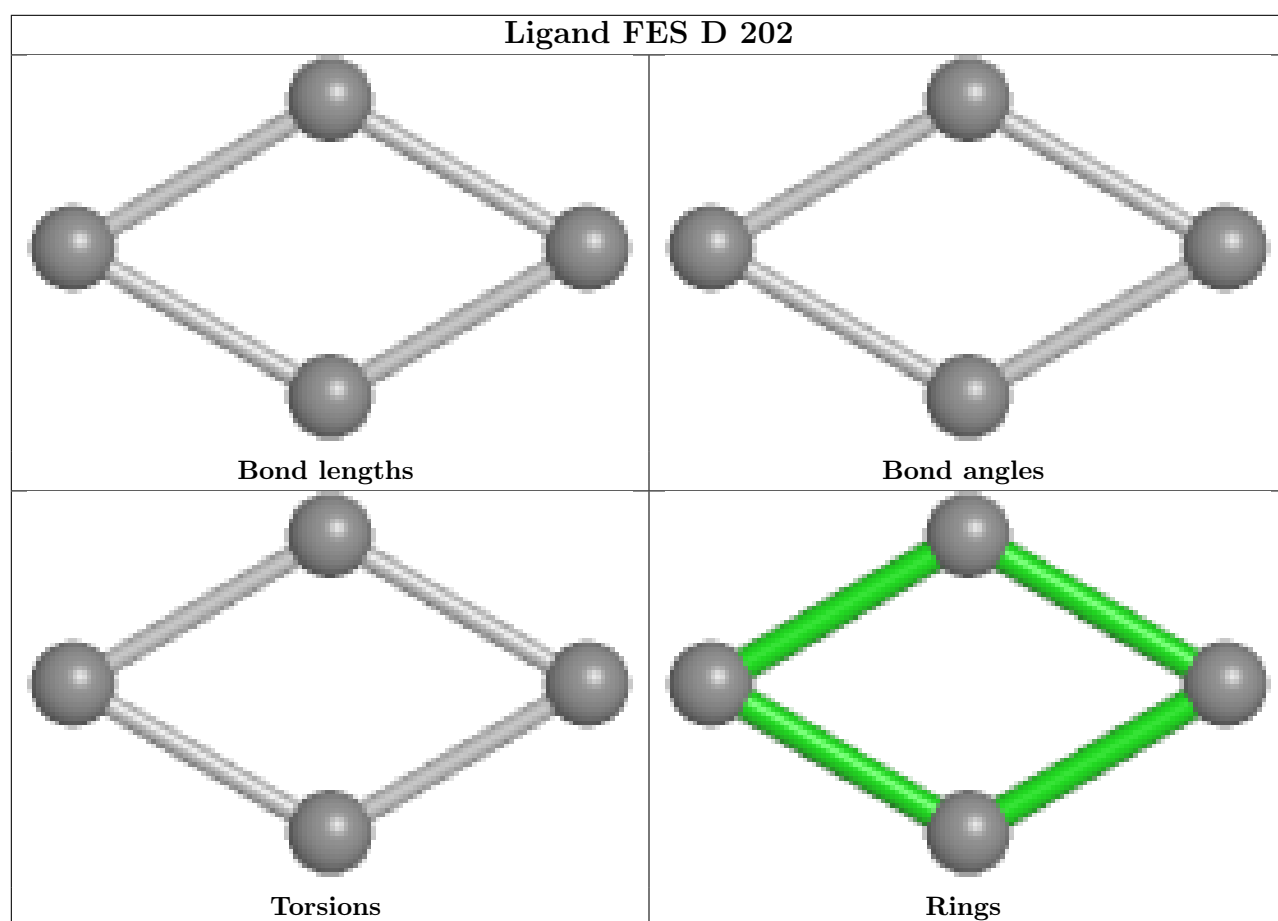
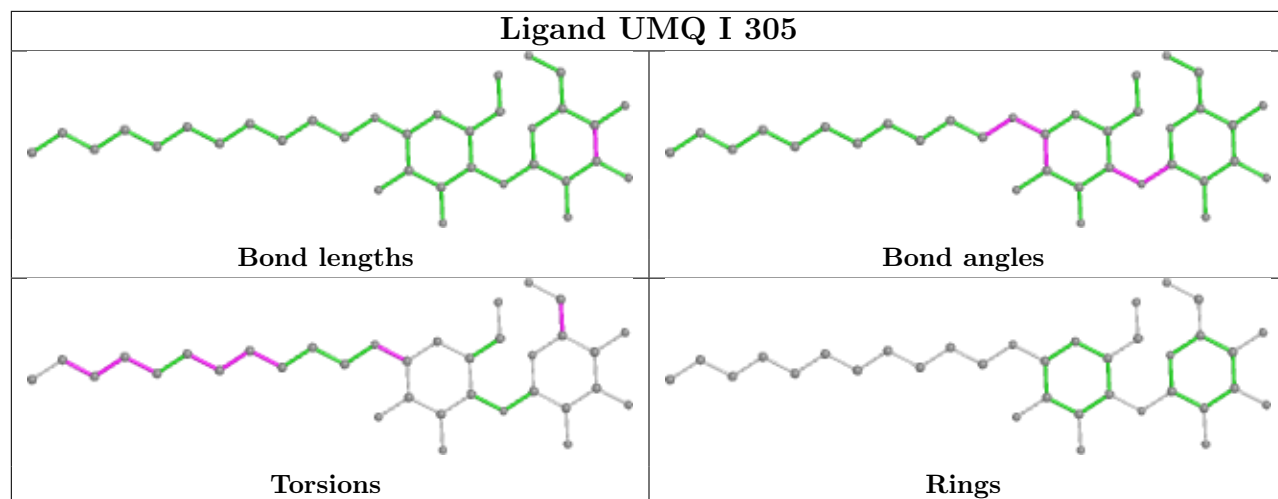


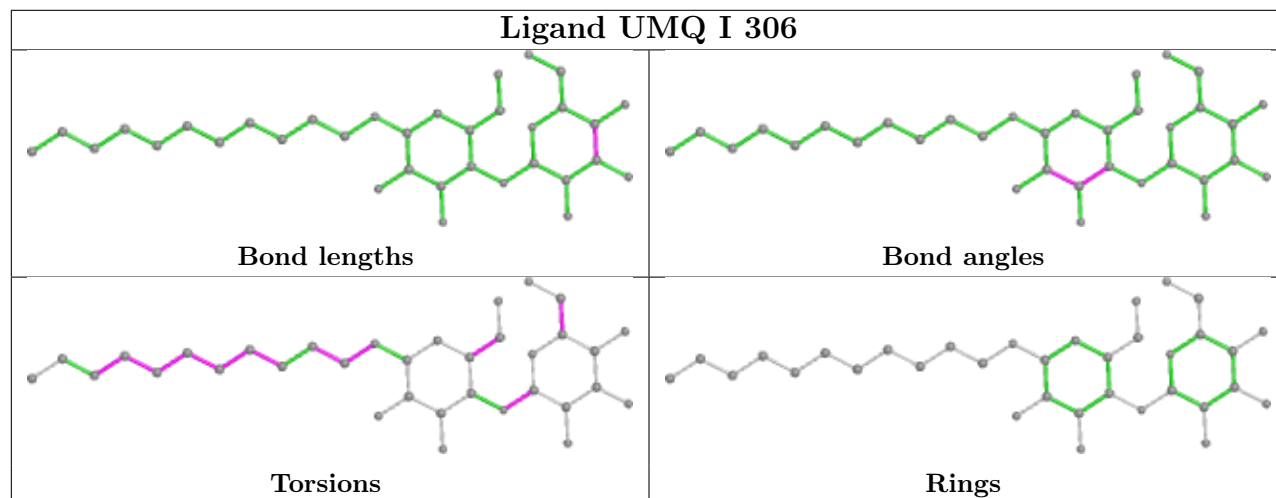
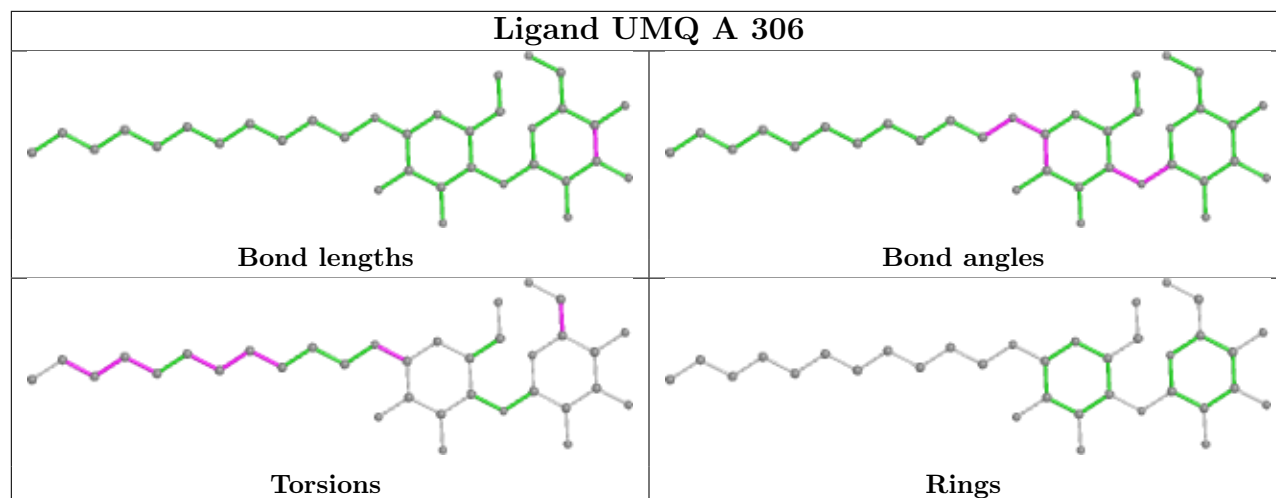
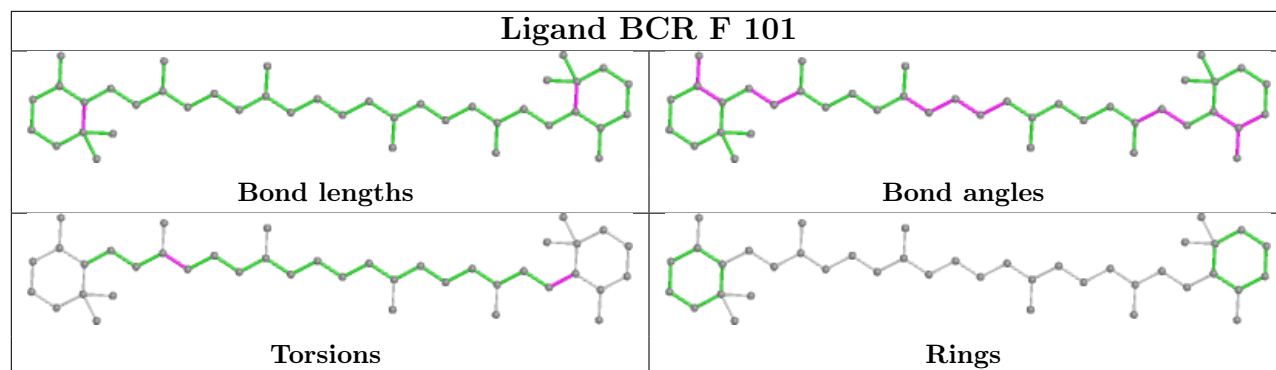
There are no ring outliers.

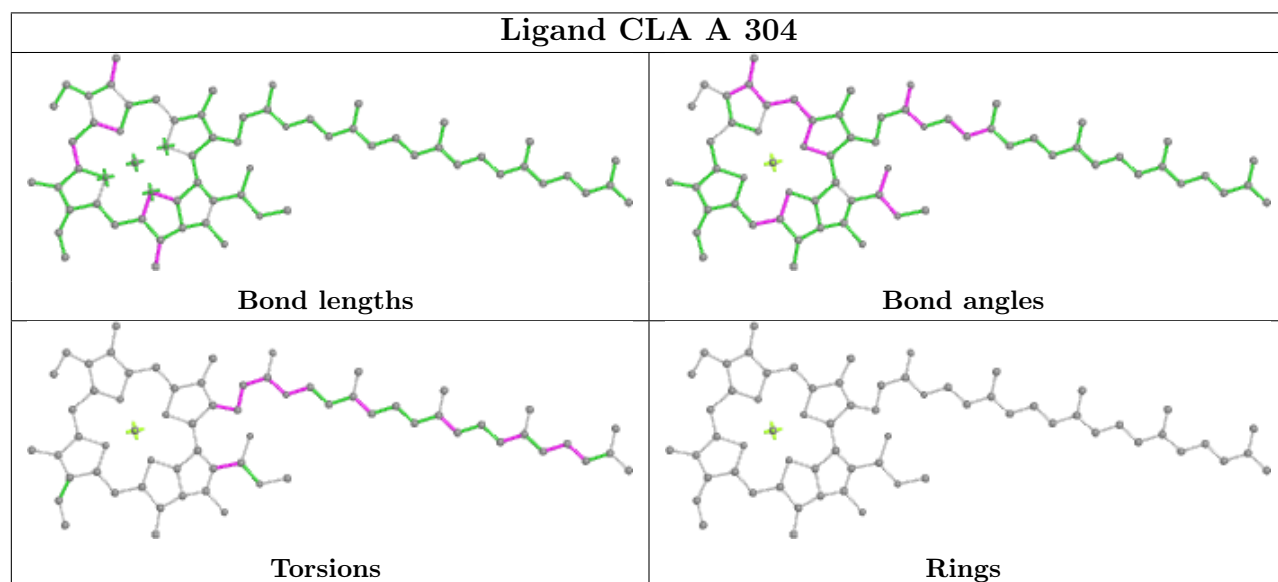
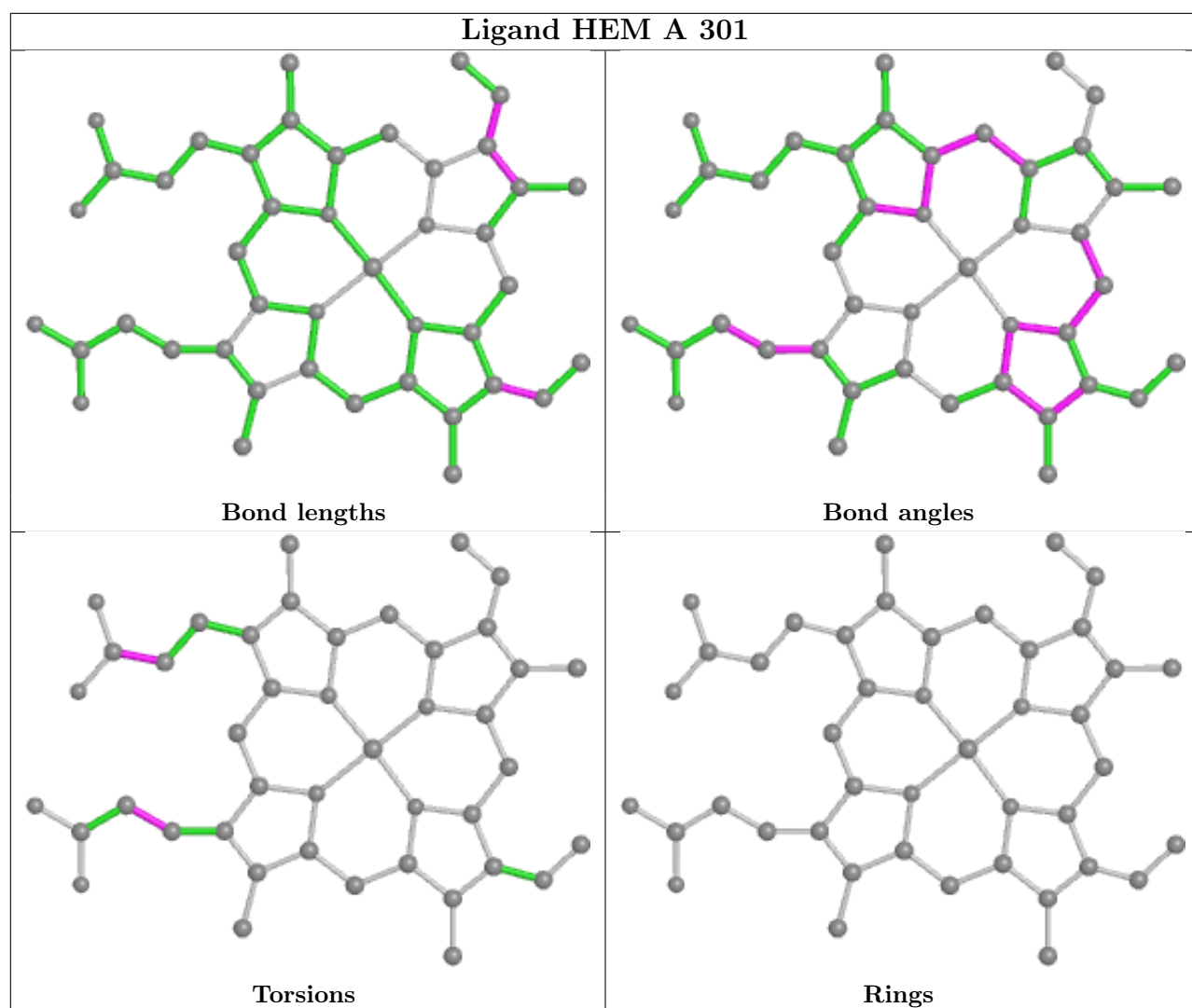
27 monomers are involved in 122 short contacts:

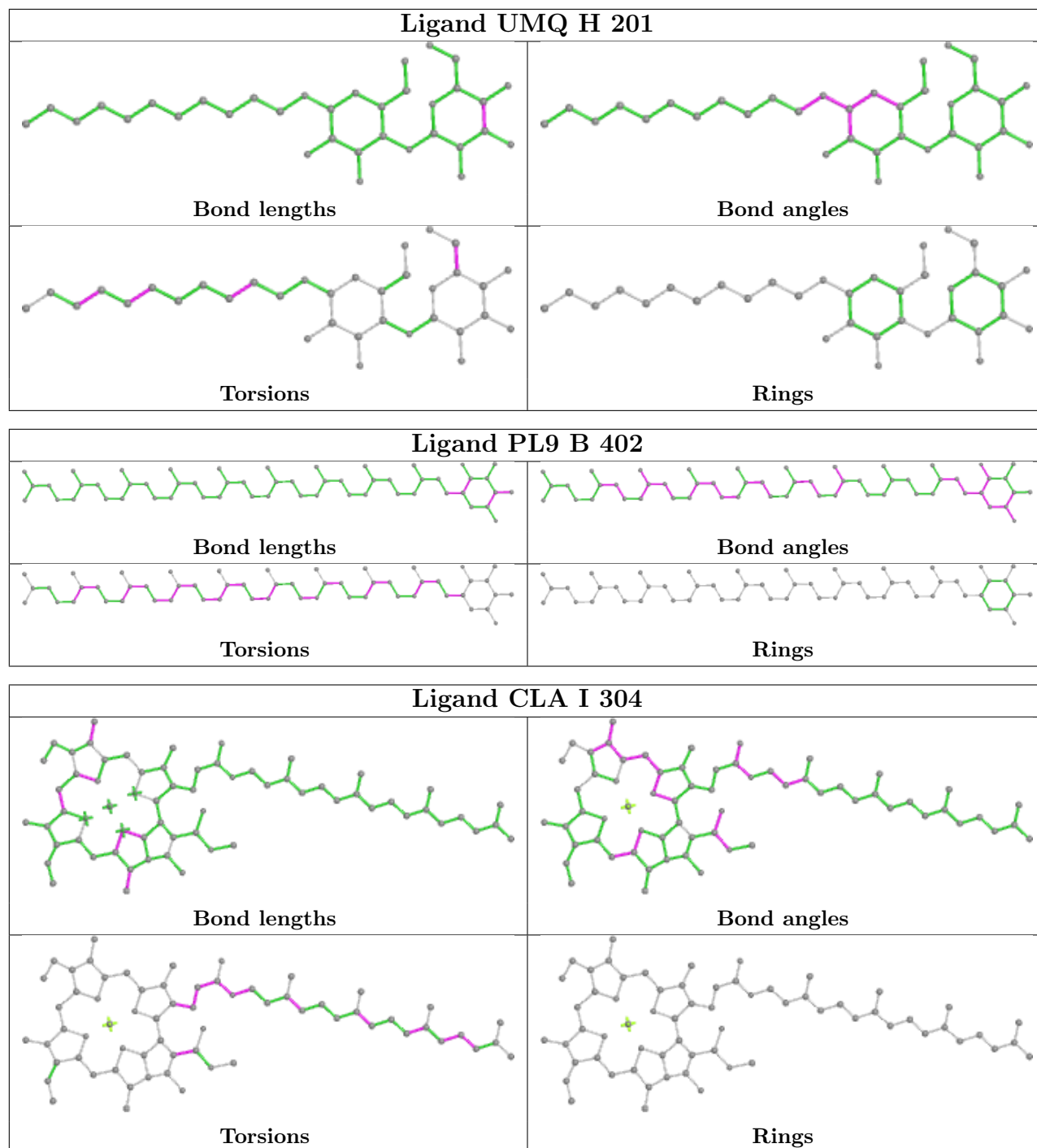
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	305	UMQ	1	0
17	F	101	BCR	2	0
13	I	306	UMQ	1	0
10	A	301	HEM	4	0
12	A	304	CLA	4	0
13	H	201	UMQ	1	0
14	B	402	PL9	17	0
12	I	304	CLA	5	0
13	B	404	UMQ	1	0
14	A	307	PL9	10	0
11	I	303	HEC	2	0
14	J	401	PL9	14	0
10	I	302	HEM	6	0
10	I	301	HEM	4	0
13	J	403	UMQ	1	0
14	K	302	PL9	4	0
13	P	102	UMQ	1	0
15	L	401	SQD	1	0
11	K	301	HEC	5	0
11	C	301	HEC	6	0
14	B	401	PL9	10	0
17	P	101	BCR	5	0
13	B	403	UMQ	2	0
14	J	402	PL9	14	0
10	A	302	HEM	5	0
15	D	201	SQD	5	0
11	A	303	HEC	2	0

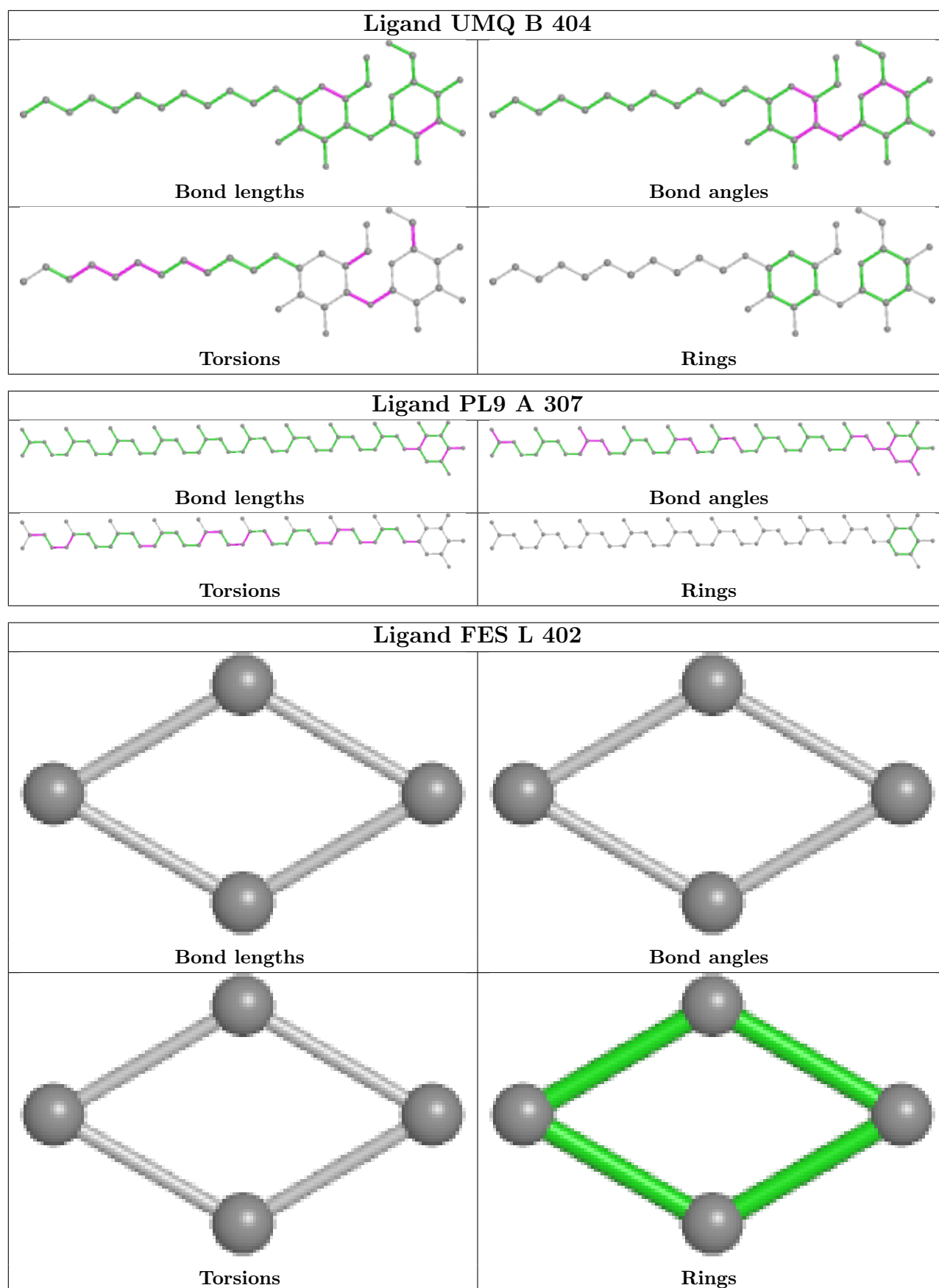
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

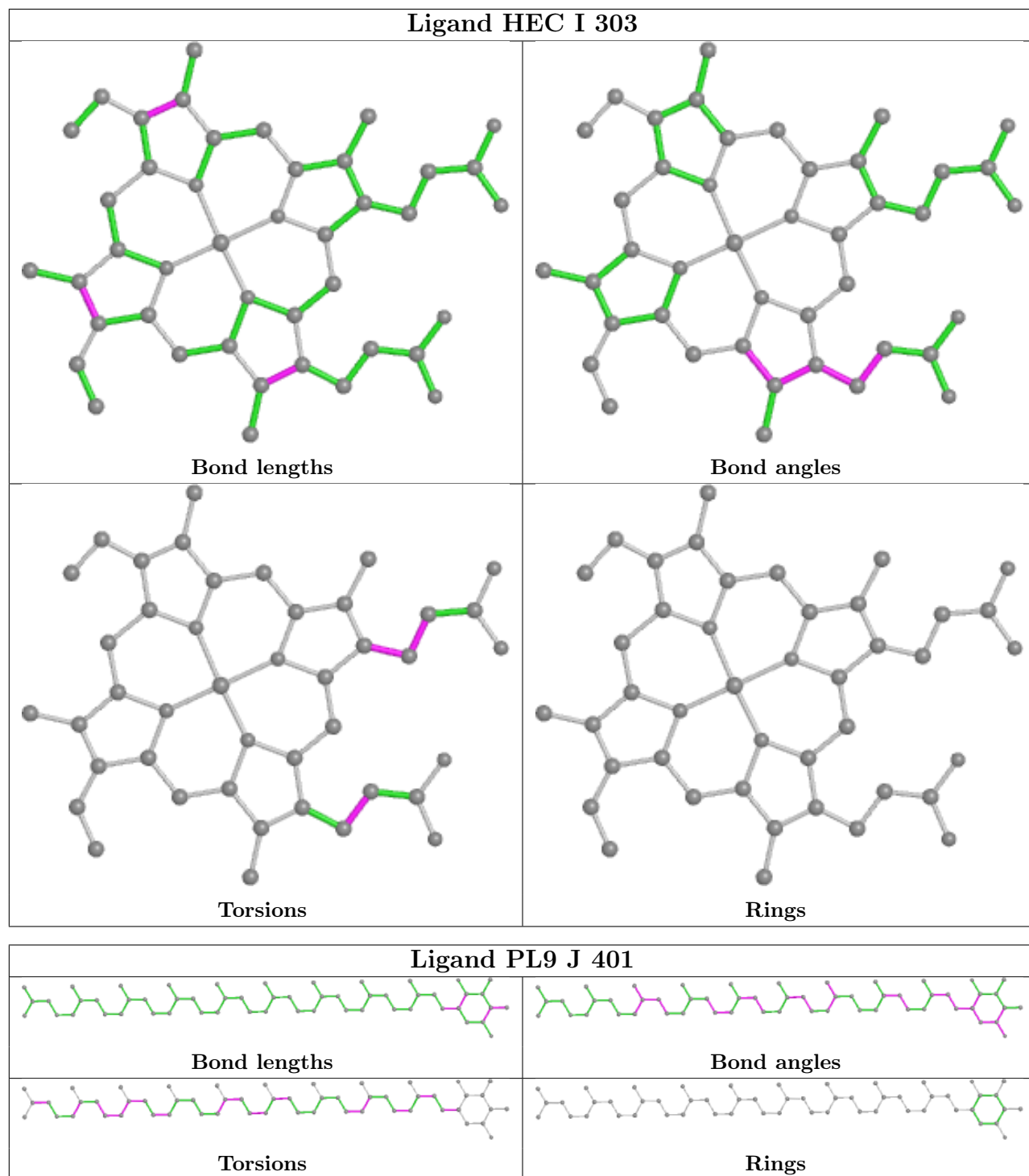


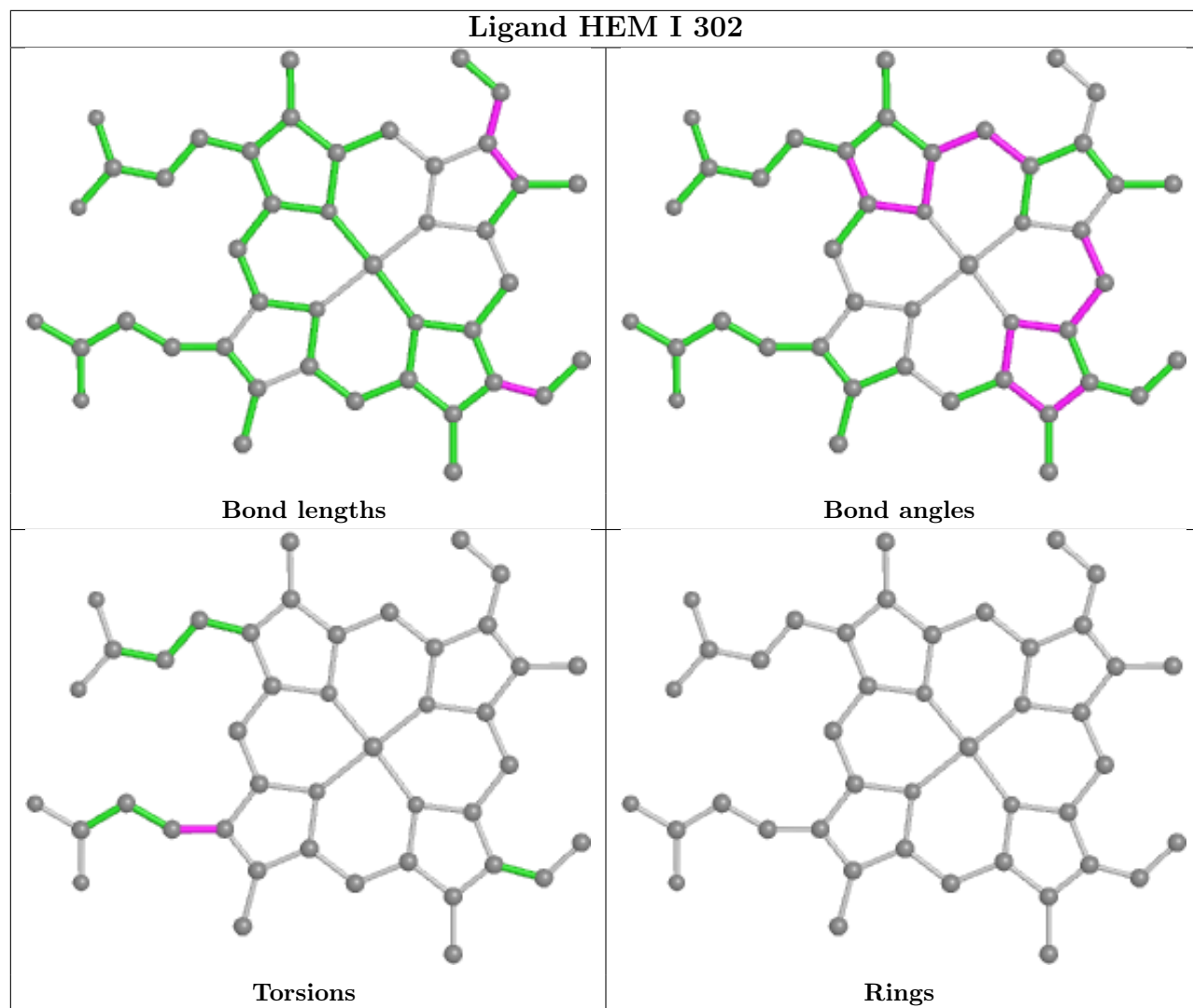




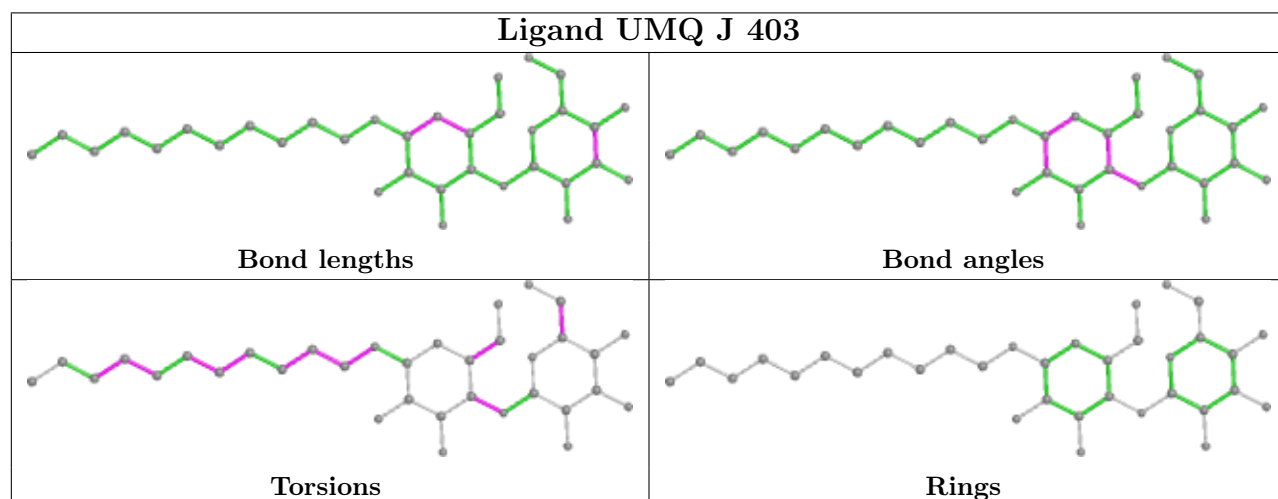
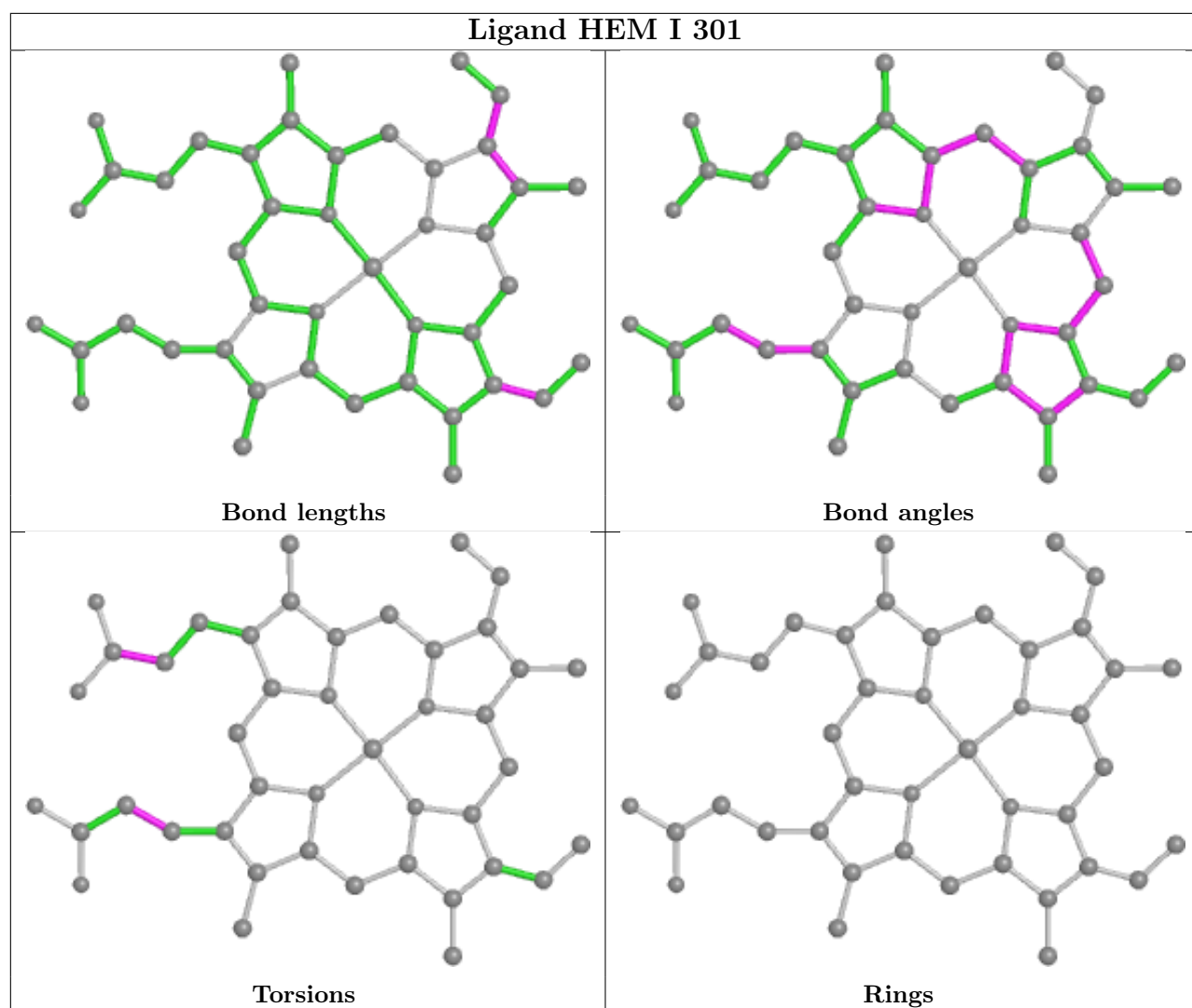


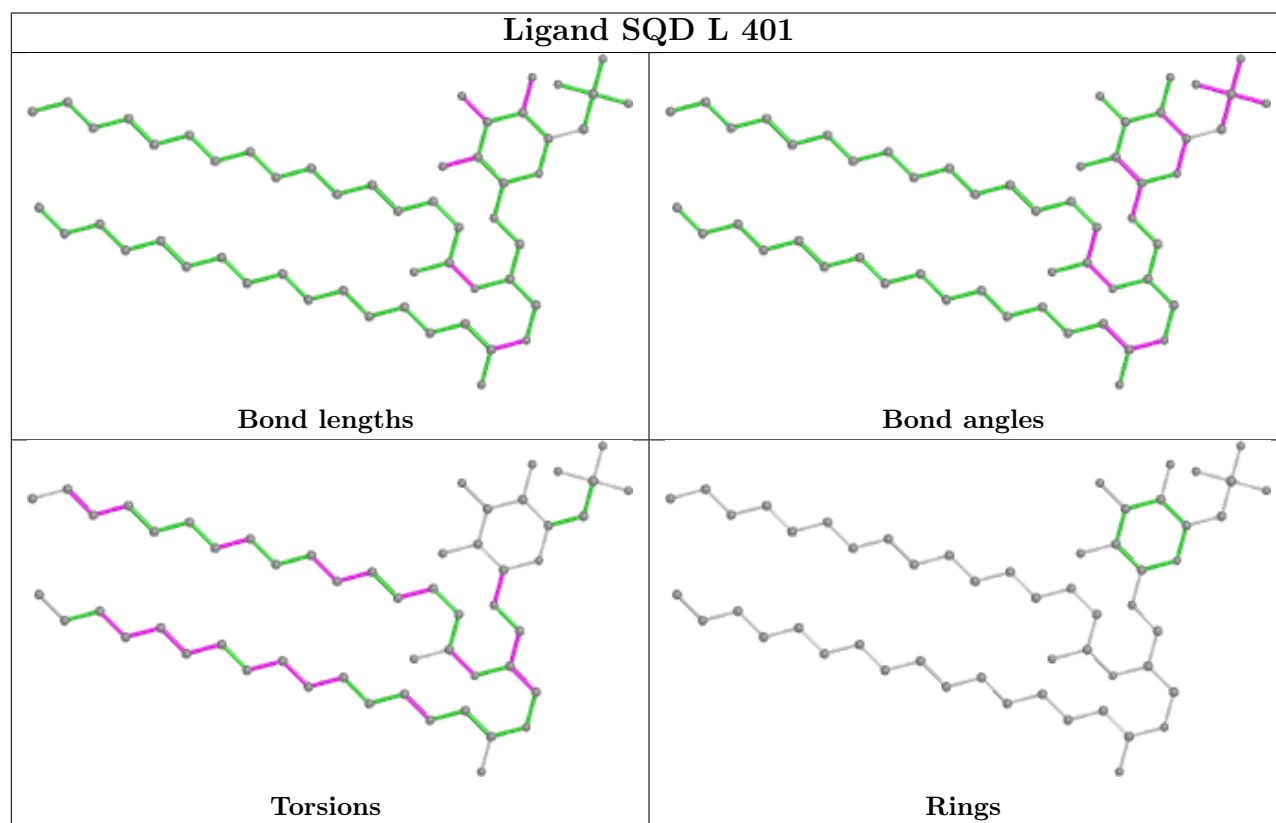
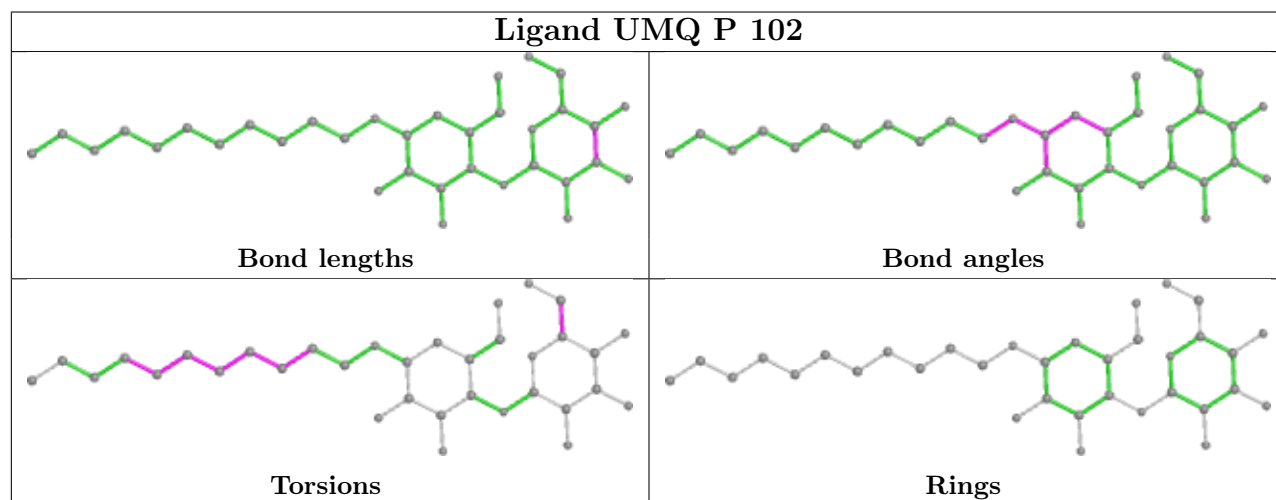
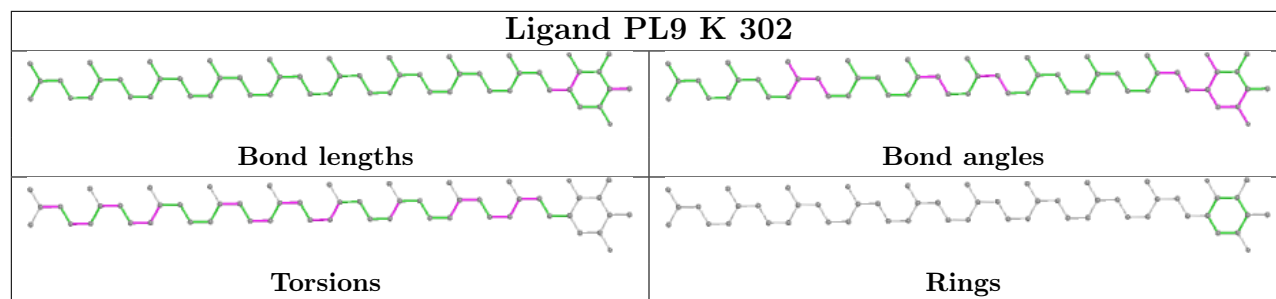


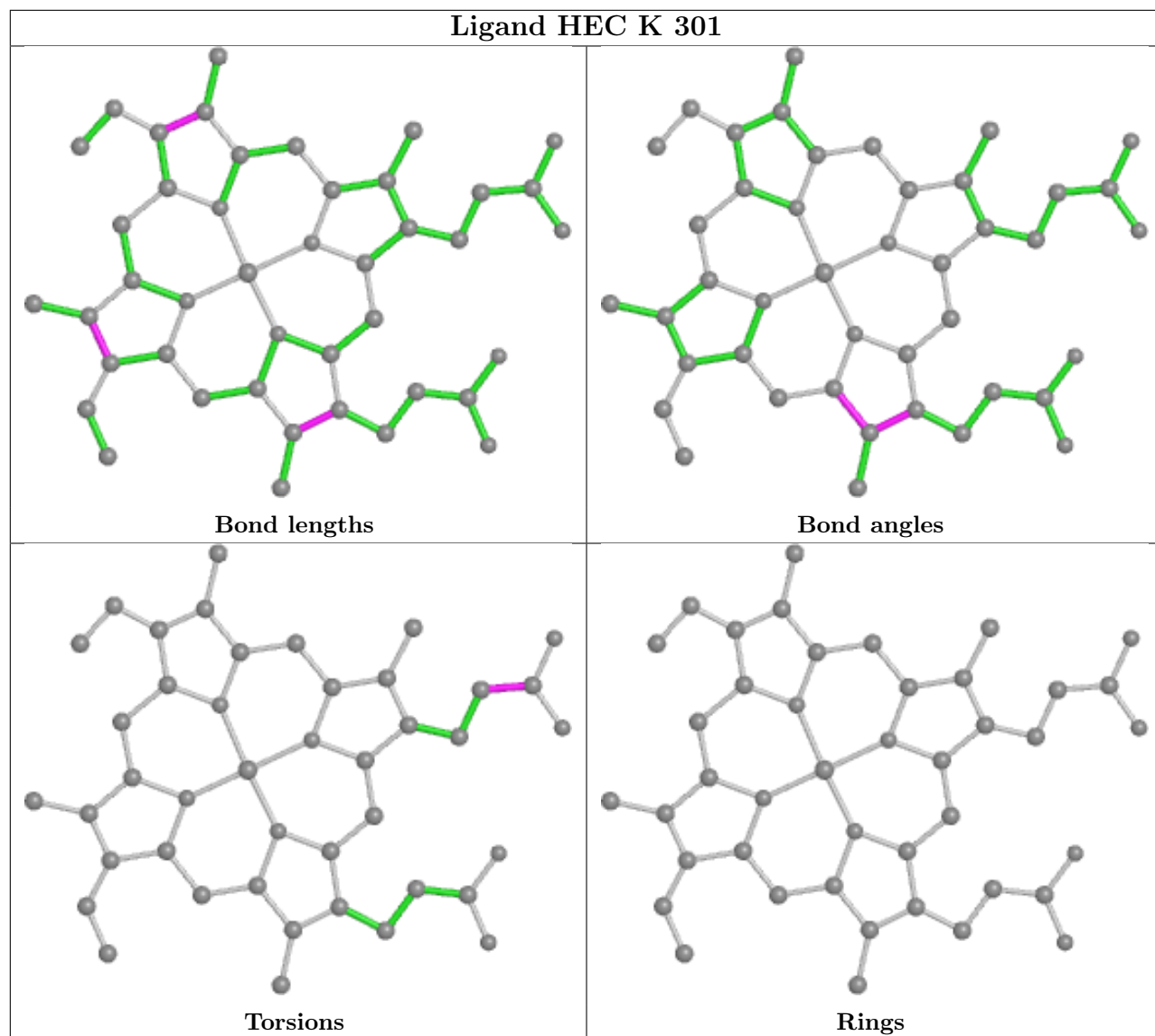


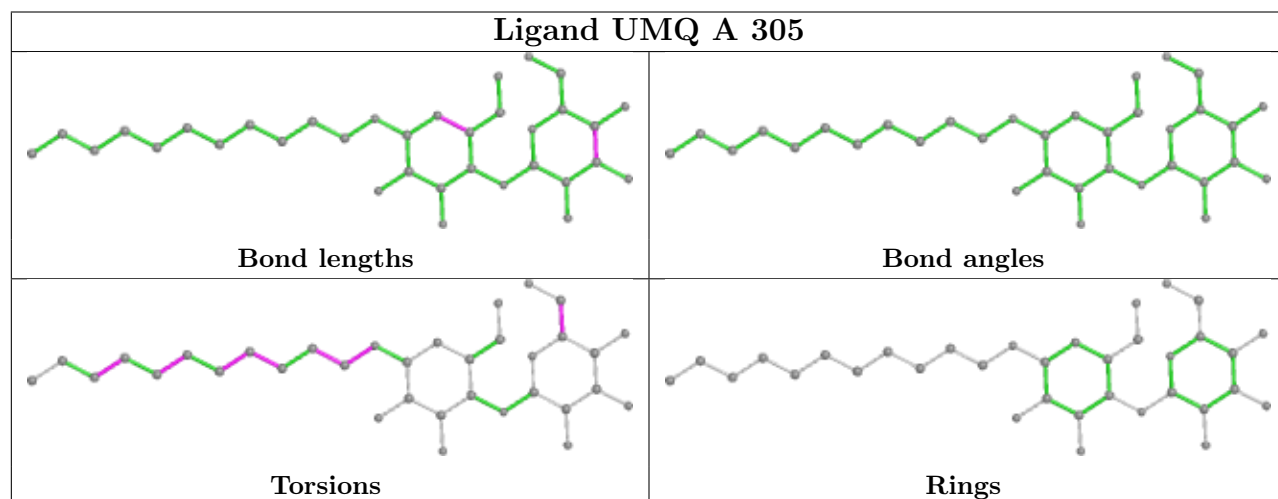
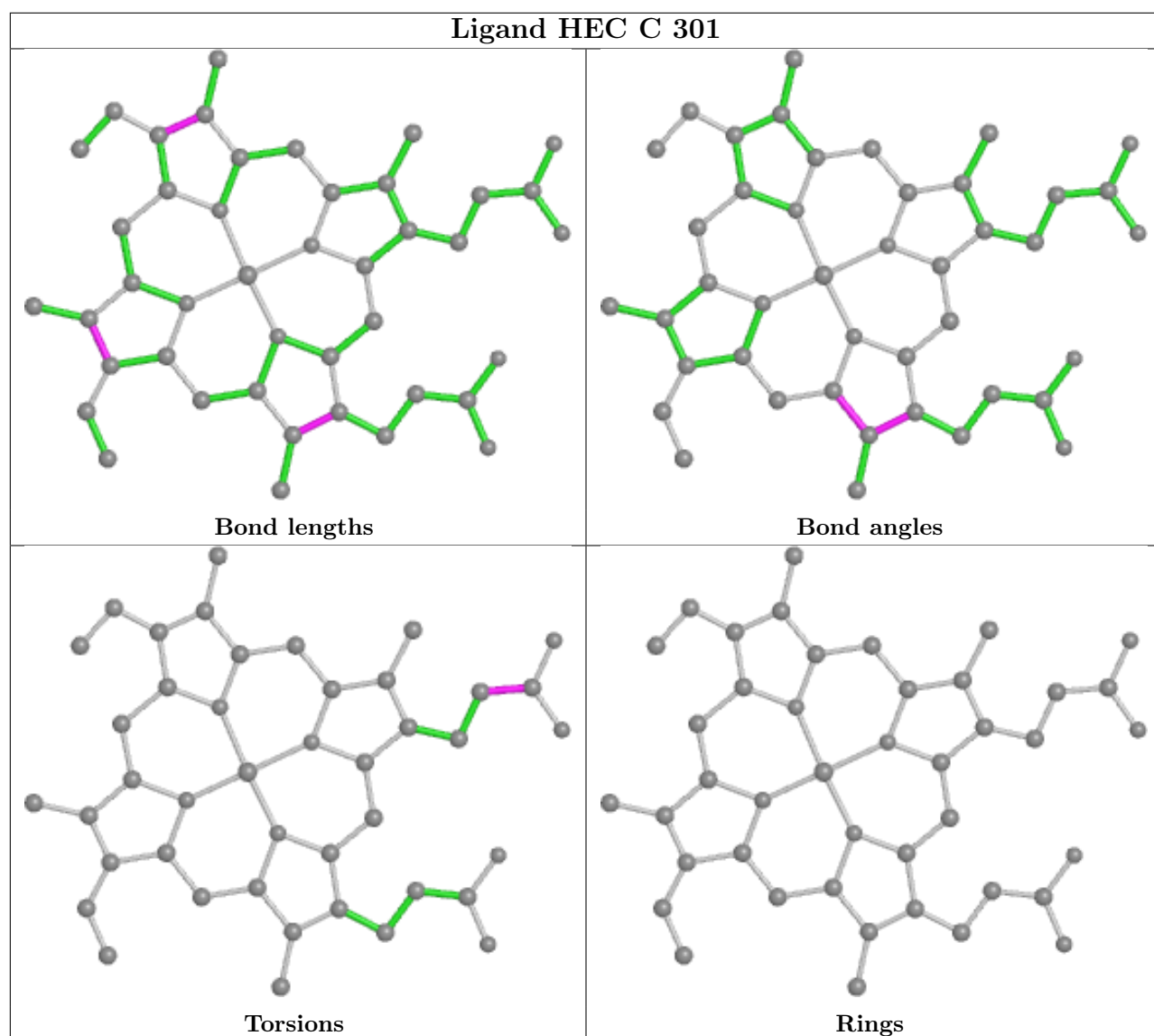


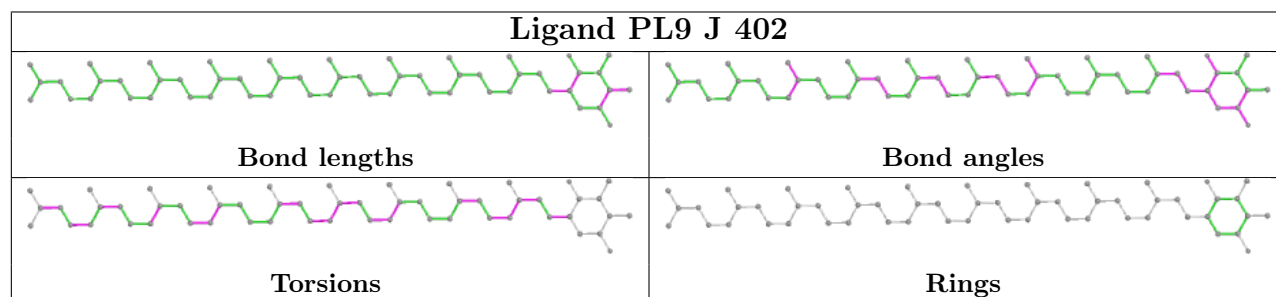
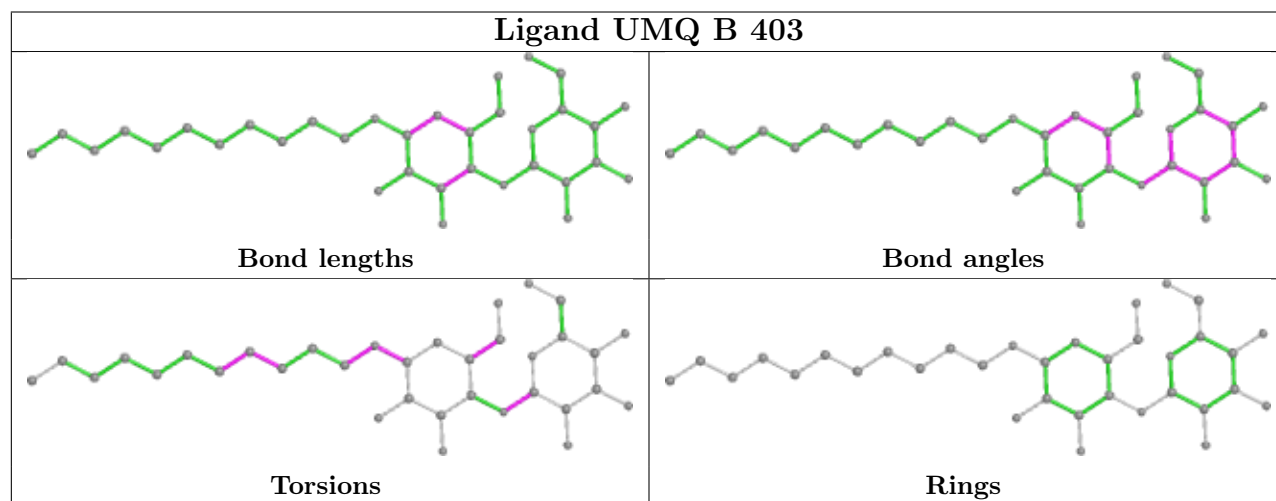
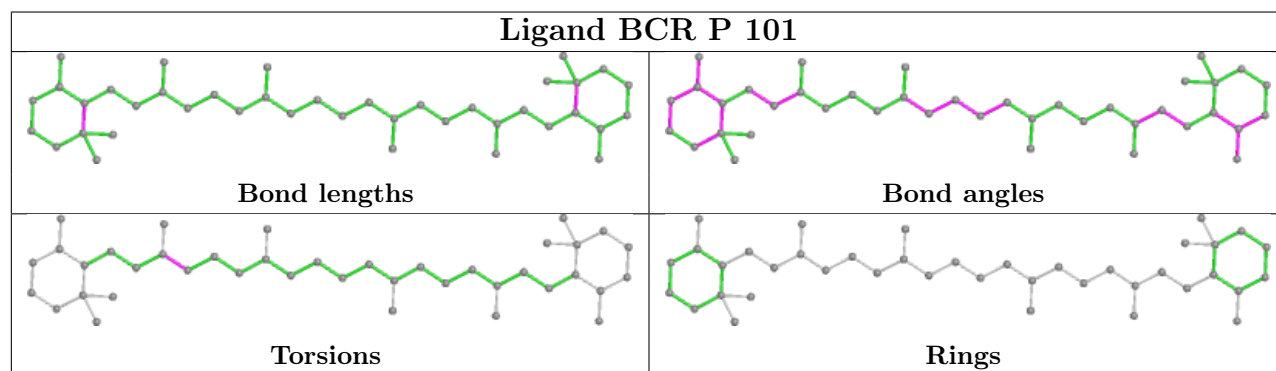
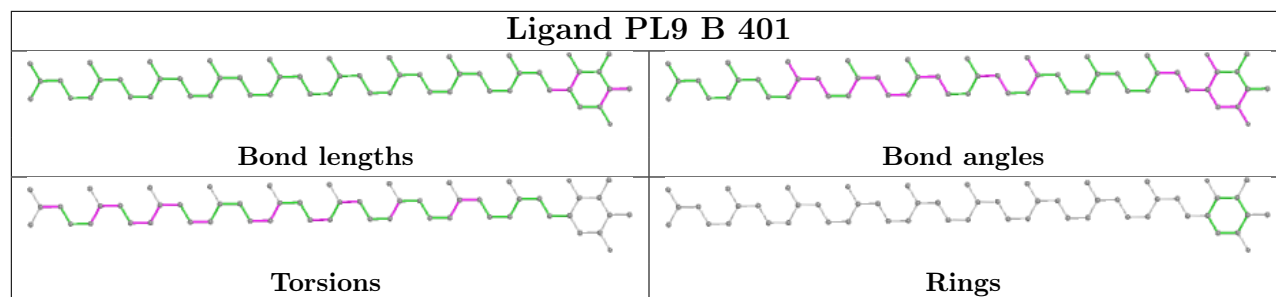


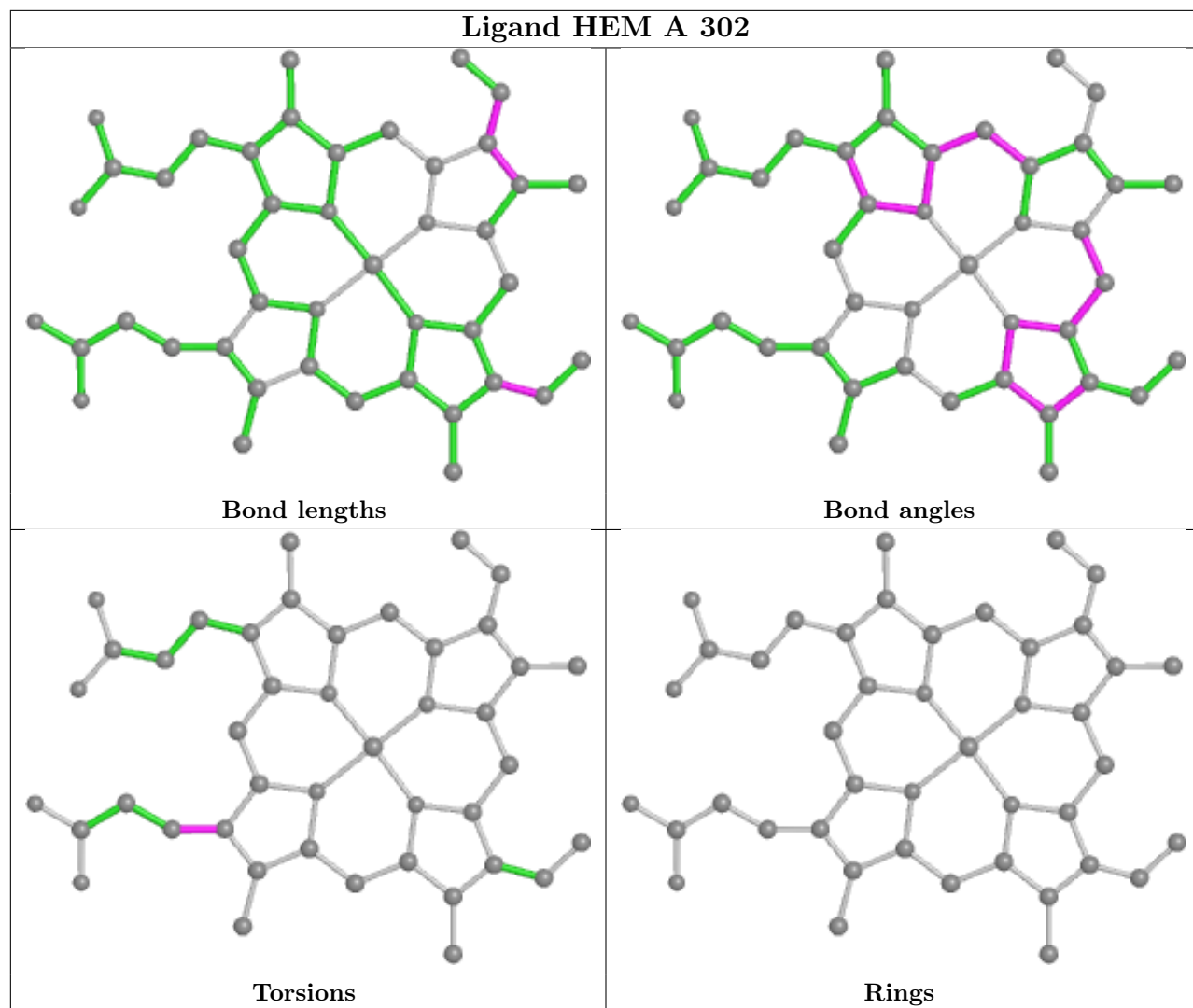


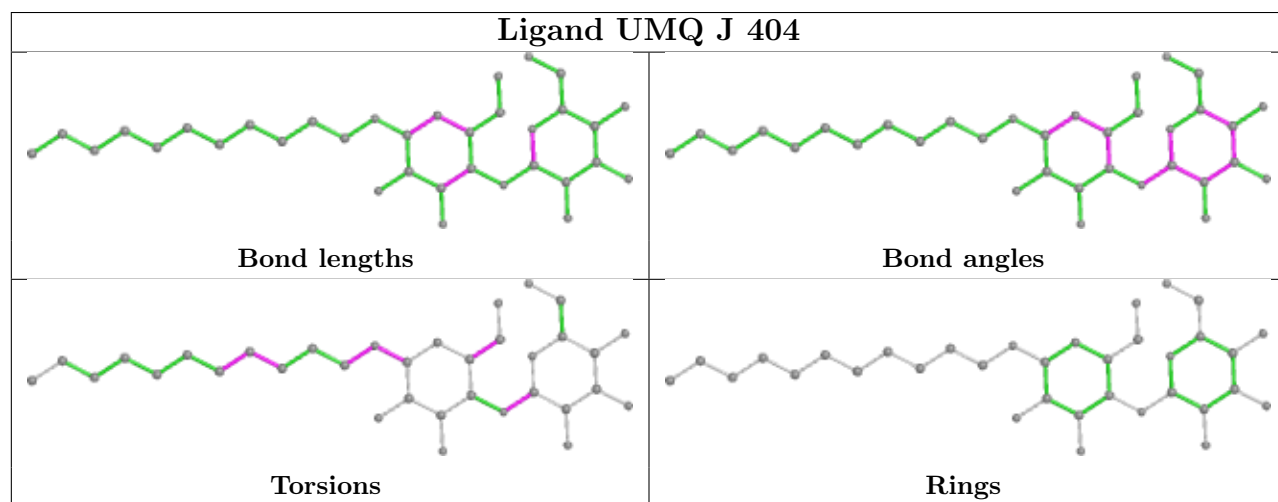
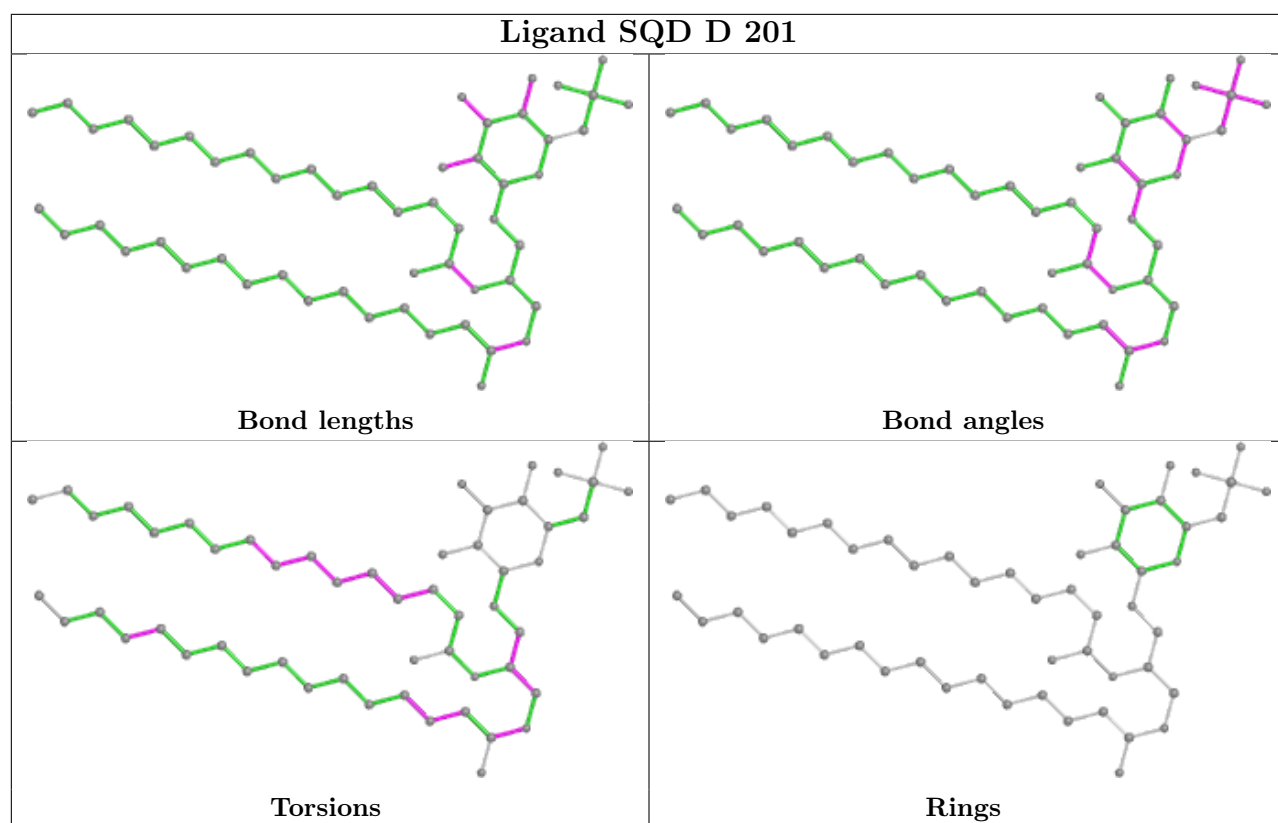


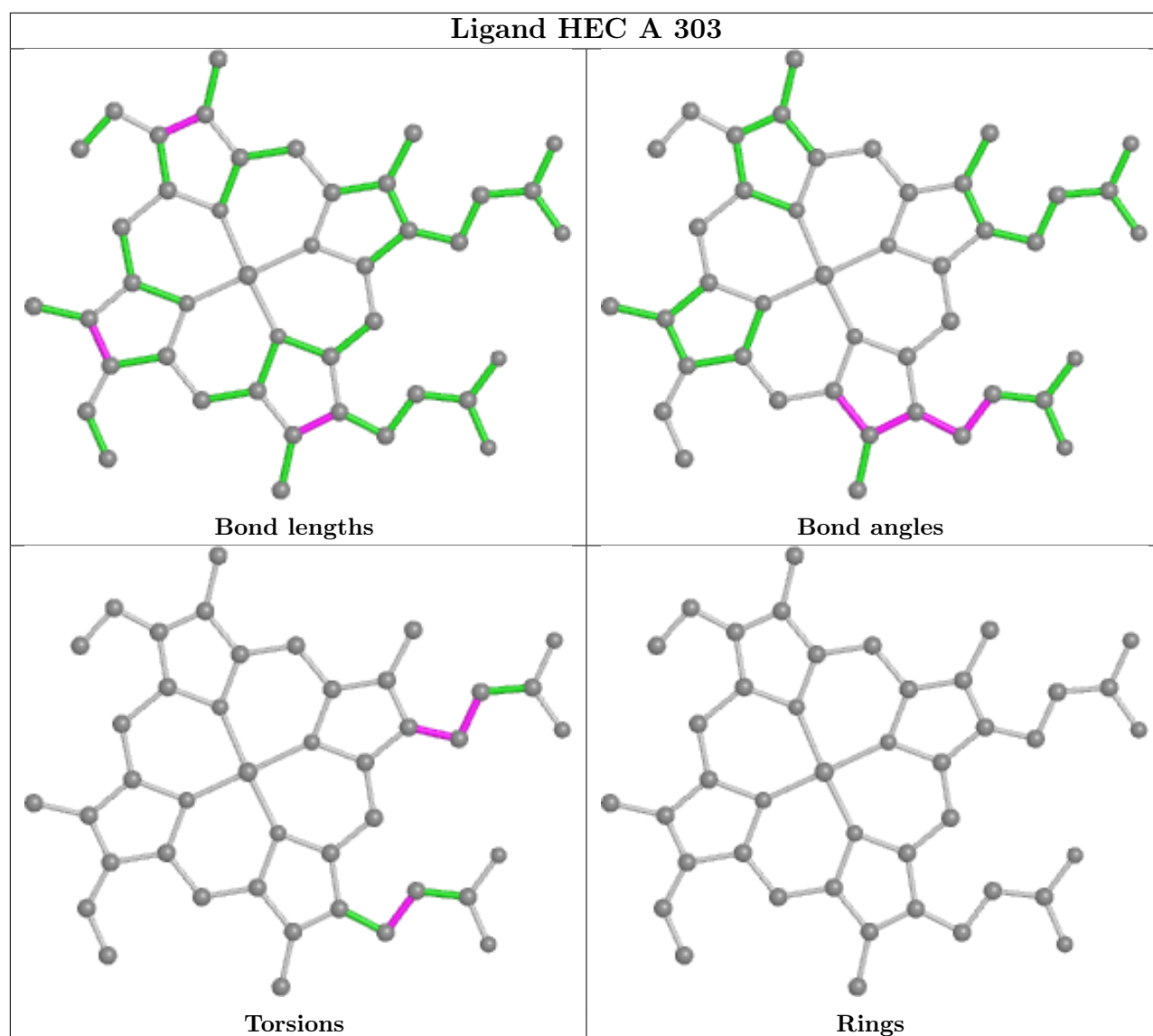












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



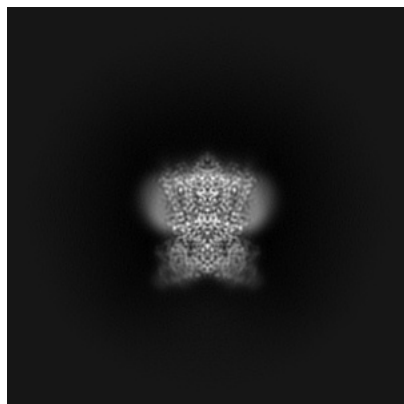
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15027. These allow visual inspection of the internal detail of the map and identification of artifacts.

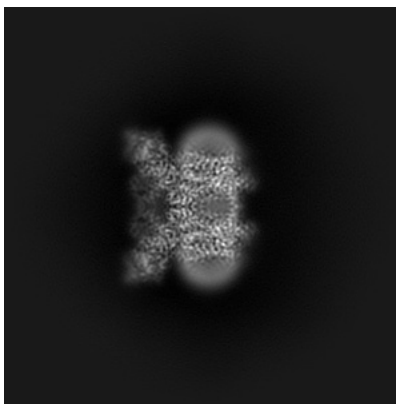
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

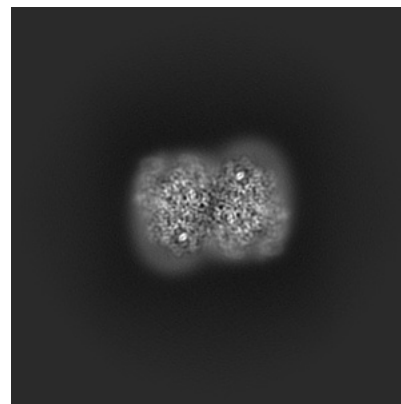
#### 6.1.1 Primary map



X

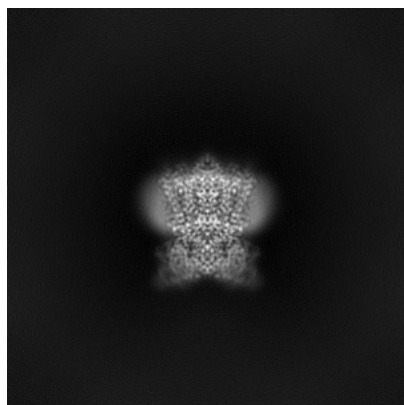


Y

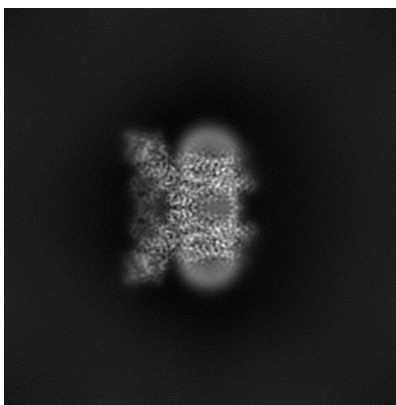


Z

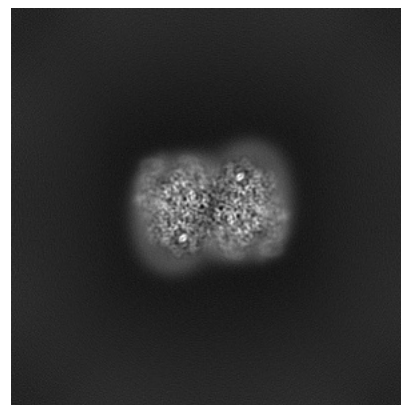
#### 6.1.2 Raw map



X



Y

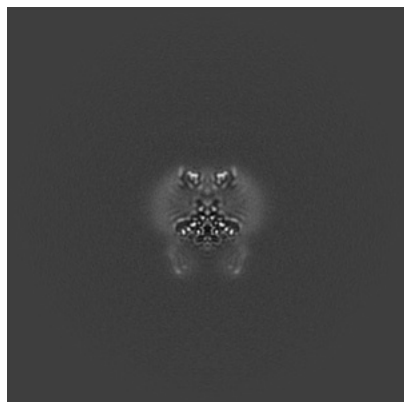


Z

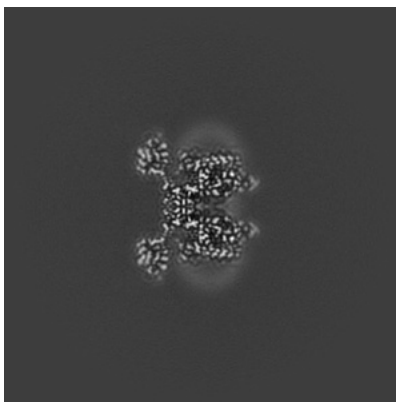
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

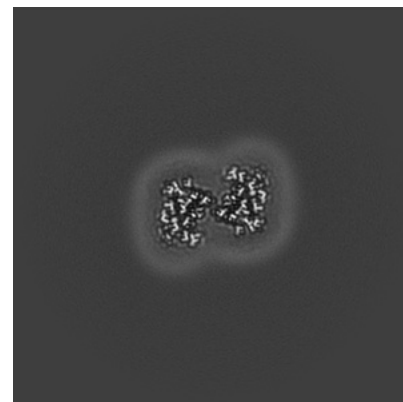
### 6.2.1 Primary map



X Index: 186

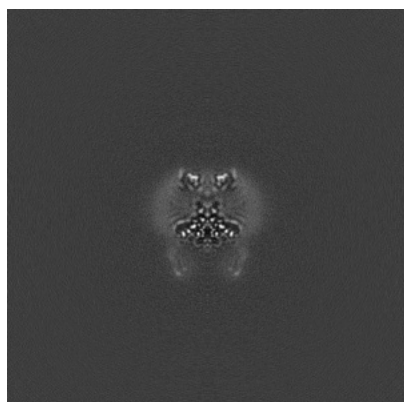


Y Index: 186

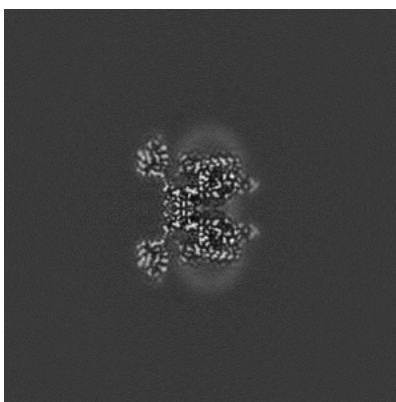


Z Index: 186

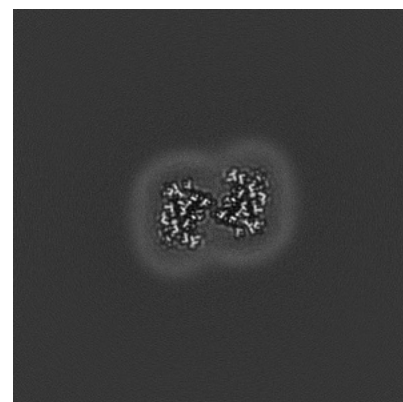
### 6.2.2 Raw map



X Index: 186



Y Index: 186

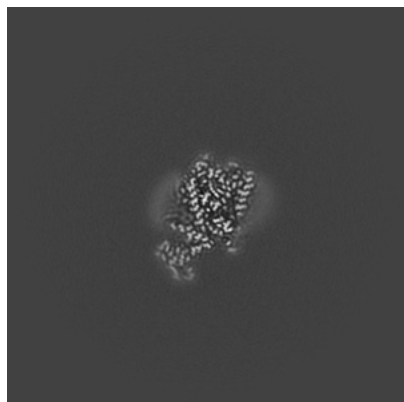


Z Index: 186

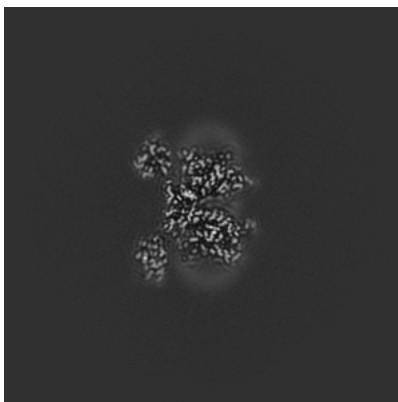
The images above show central slices of the map in three orthogonal directions.

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

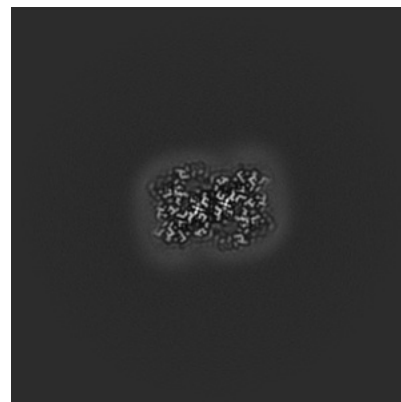
### 6.3.1 Primary map



X Index: 205

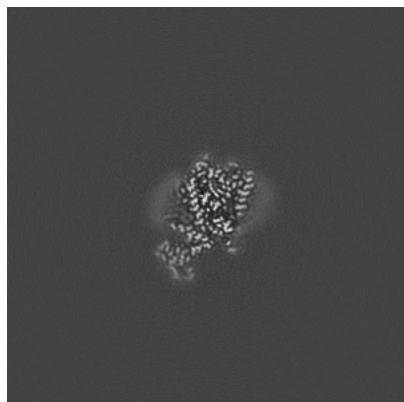


Y Index: 189

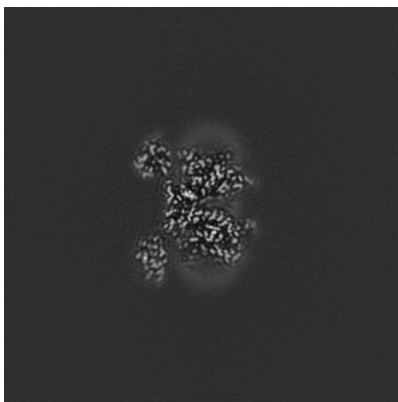


Z Index: 173

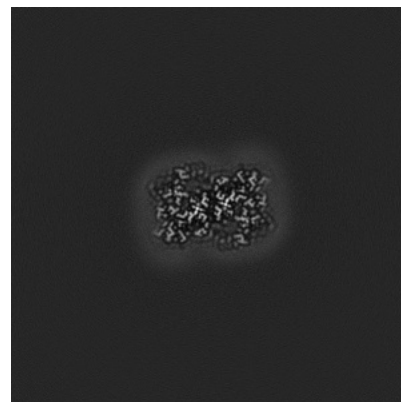
### 6.3.2 Raw map



X Index: 205



Y Index: 189

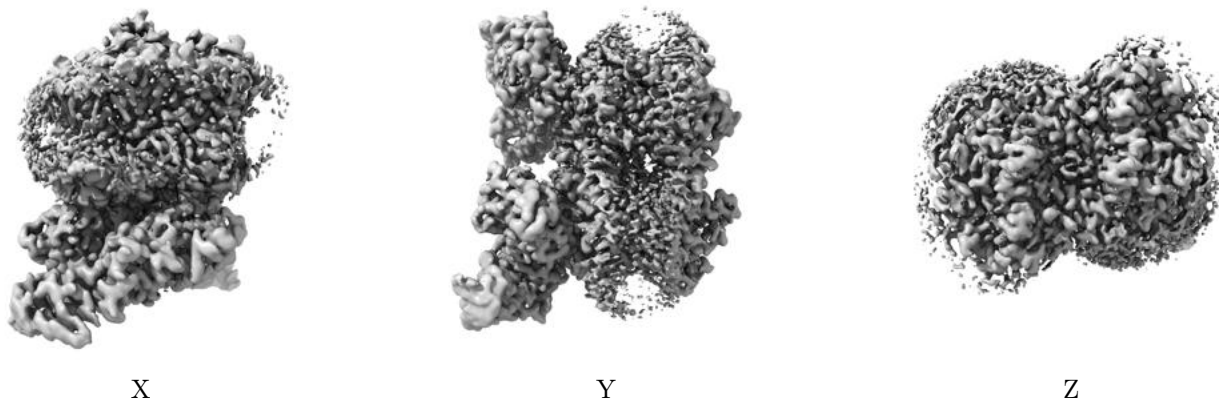


Z Index: 173

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

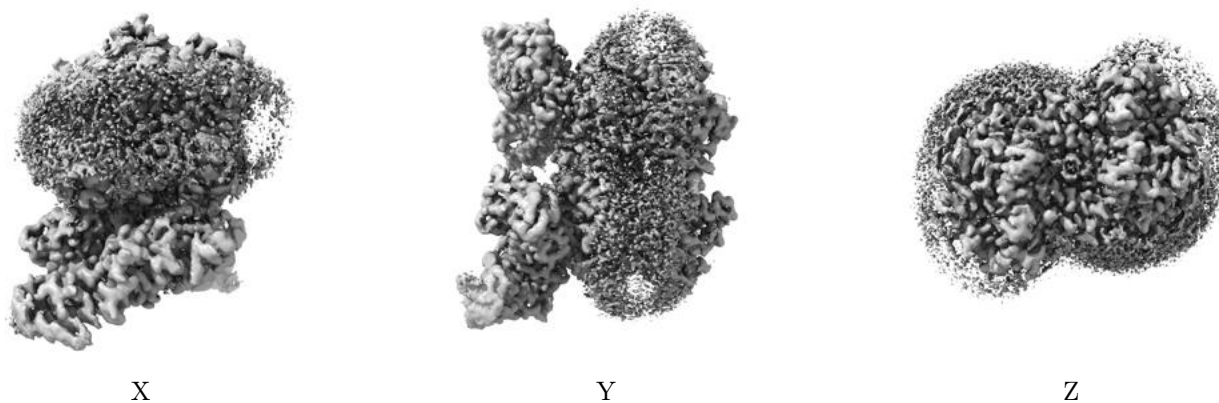
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.208. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

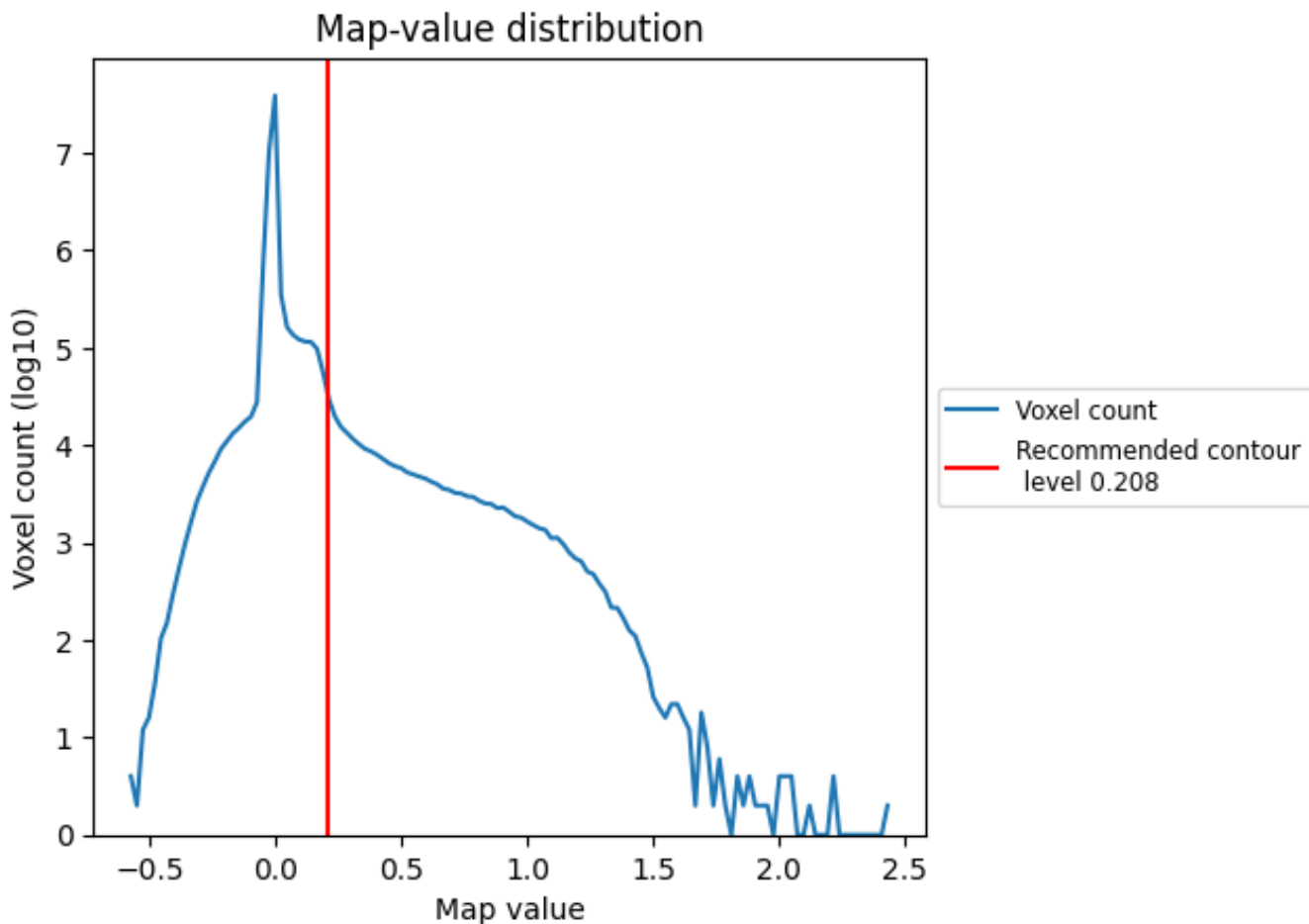
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

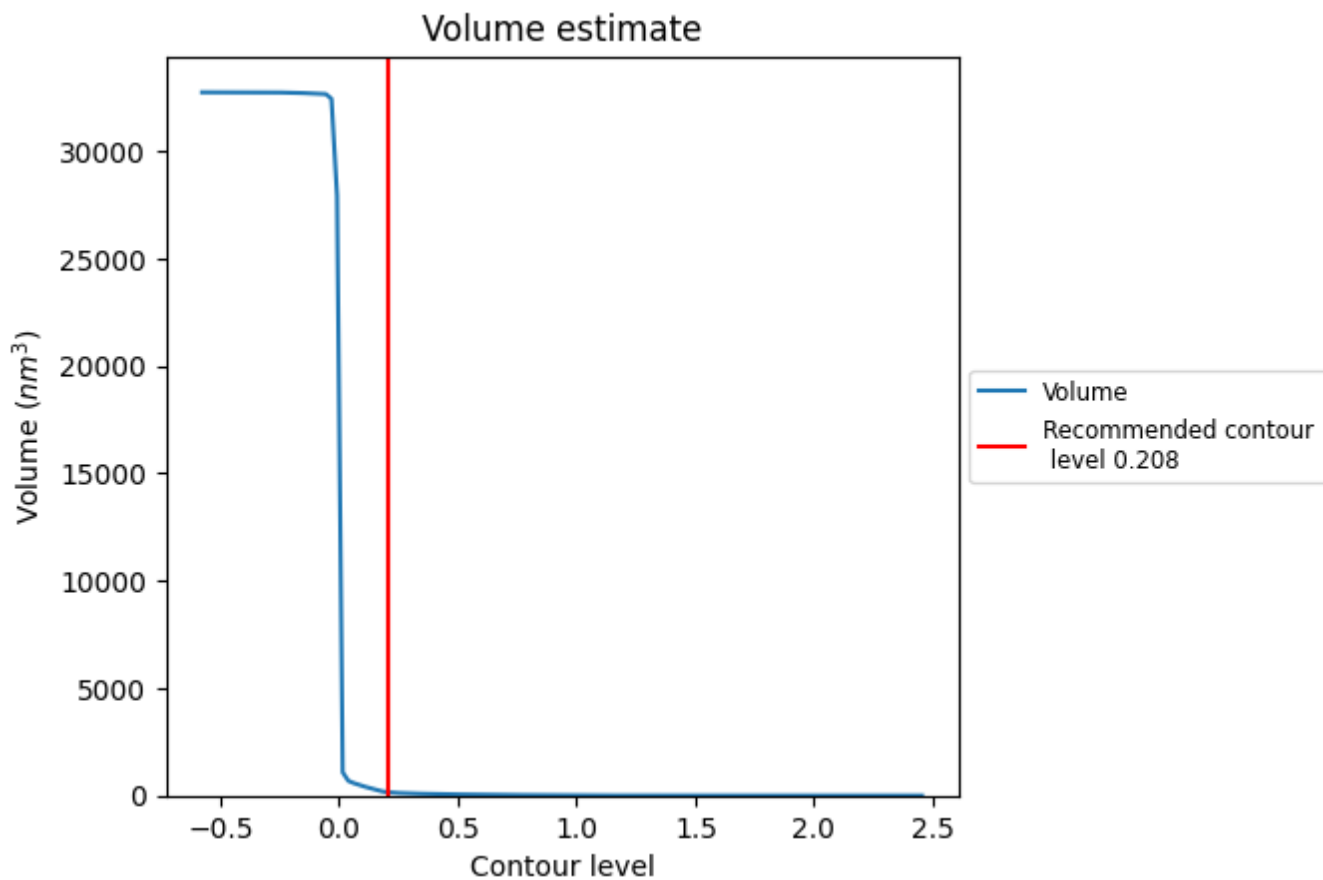
This section contains the results of statistical analysis of the map.

### 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.

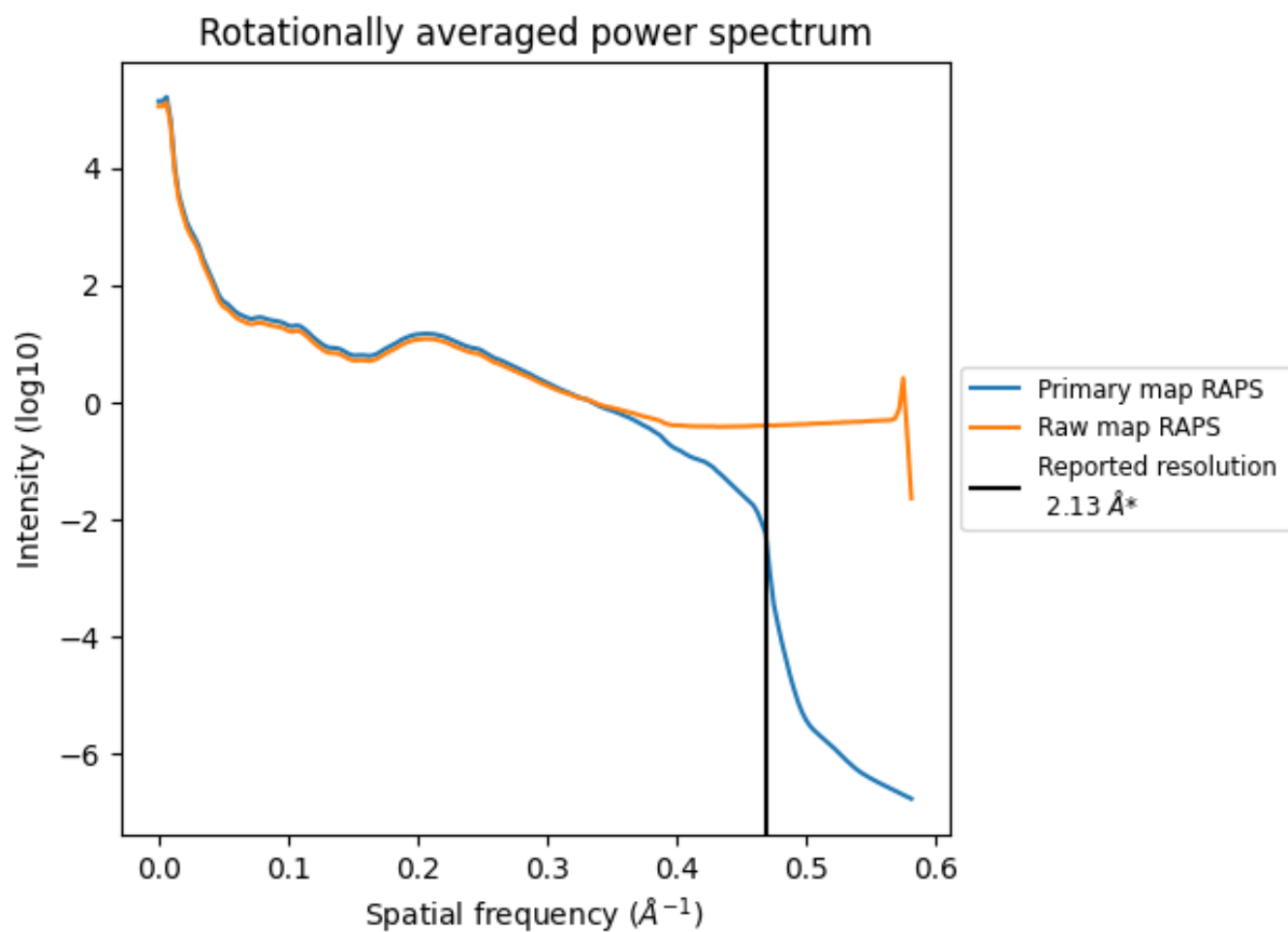
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm<sup>3</sup>; this corresponds to an approximate mass of 136 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 i

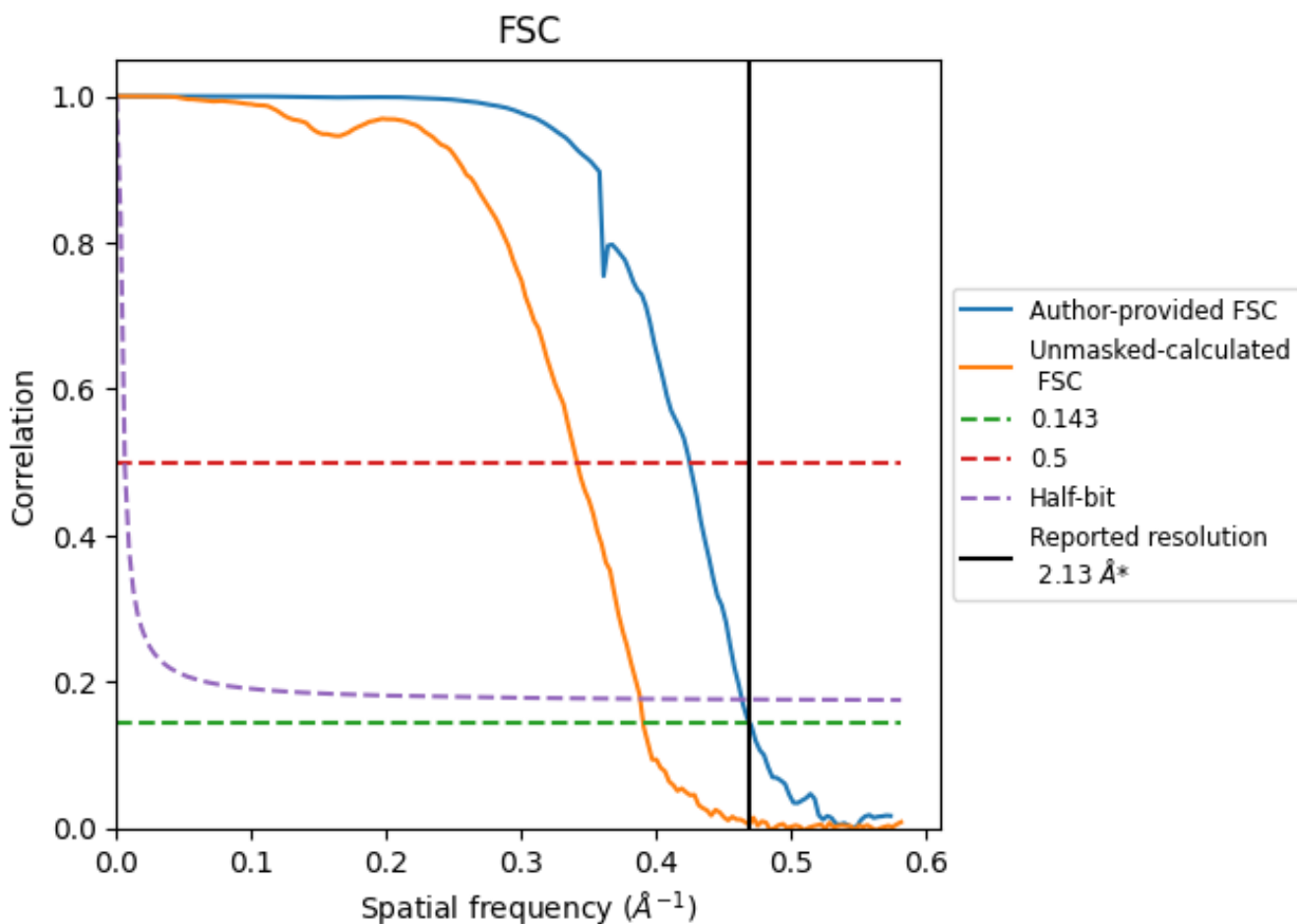


\*Reported resolution corresponds to spatial frequency of  $0.469 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.469 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

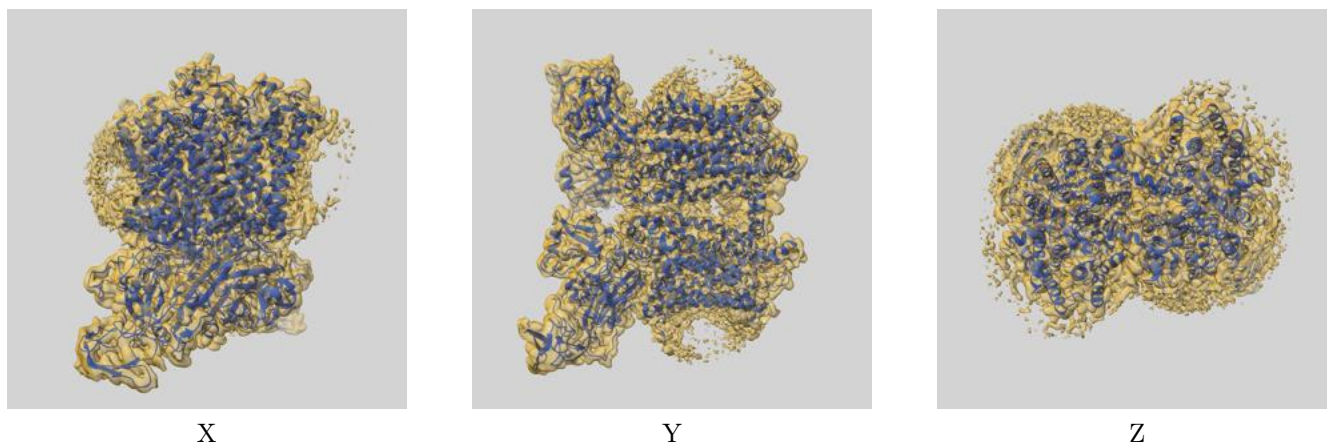
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	2.13	2.36	2.16
Unmasked-calculated*	2.56	2.93	2.58

\*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 2.56 differs from the reported value 2.13 by more than 10 %

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

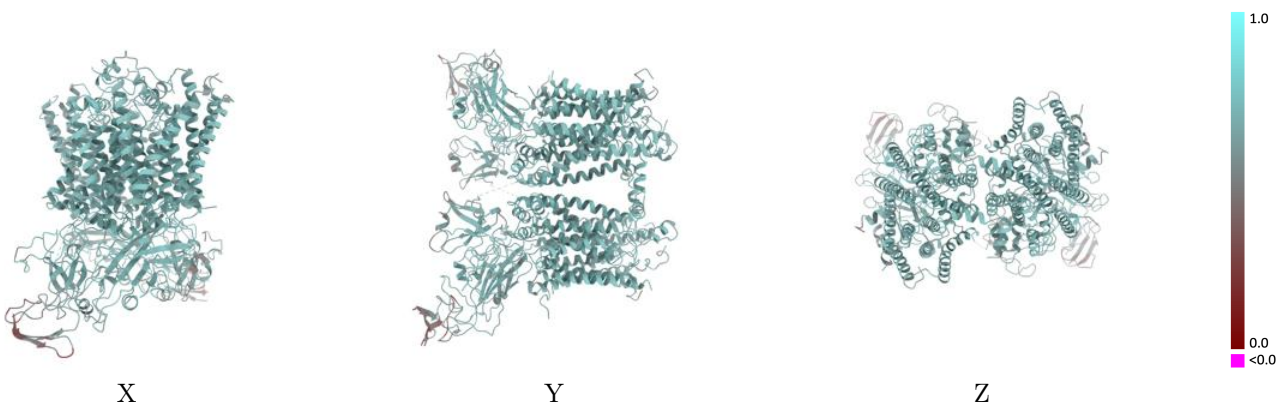
This section contains information regarding the fit between EMDB map EMD-15027 and PDB model 7ZYV. Per-residue inclusion information can be found in section 3 on page 12.

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



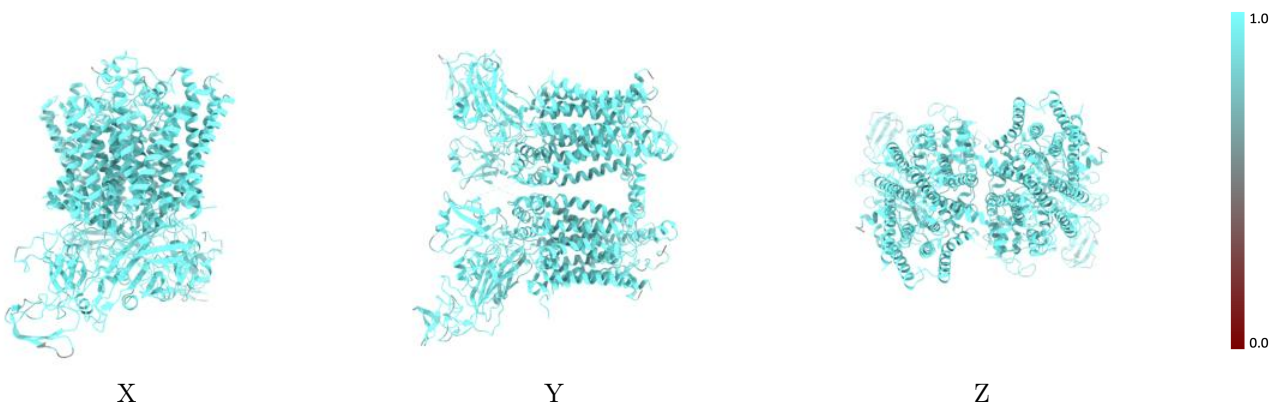
The images above show the 3D surface view of the map at the recommended contour level 0.208 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



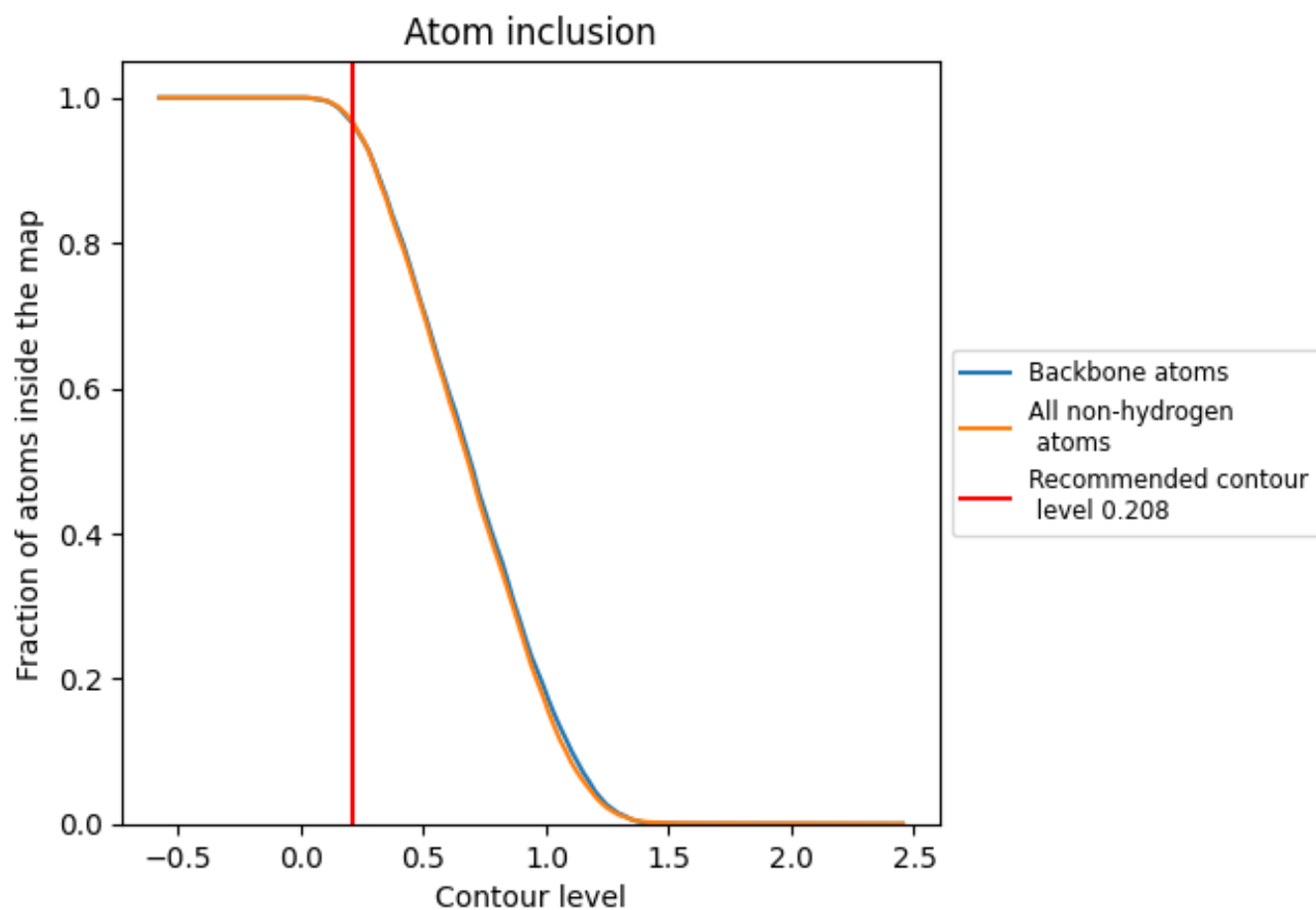
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.208).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.208) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9675	 0.6440
A	 0.9873	 0.6780
B	 0.9646	 0.6510
C	 0.9571	 0.6120
D	 0.9654	 0.6270
E	 0.9917	 0.6400
F	 0.9639	 0.6470
G	 0.9885	 0.6670
H	 0.9920	 0.6740
I	 0.9885	 0.6820
J	 0.9640	 0.6510
K	 0.9543	 0.6110
L	 0.9606	 0.6300
M	 0.9958	 0.6480
N	 0.9808	 0.6500
O	 0.9961	 0.6730
P	 0.9829	 0.6700
Q	 0.8930	 0.6110
R	 0.8884	 0.5990

