



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 09:29 pm BST

PDB ID : 6RQF / pdb_00006rqf
EMDB ID : EMD-4981
Title : 3.6 Angstrom cryo-EM structure of the dimeric cytochrome b6f complex from *Spinacia oleracea* with natively bound thylakoid lipids and plastoquinone molecules
Authors : Malone, L.A.; Qian, P.; Mayneord, G.E.; Hitchcock, A.; Farmer, D.; Thompson, R.; Swainsbury, D.J.K.; Ranson, N.; Hunter, C.N.; Johnson, M.P.
Deposited on : 2019-05-15
Resolution : 3.58 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

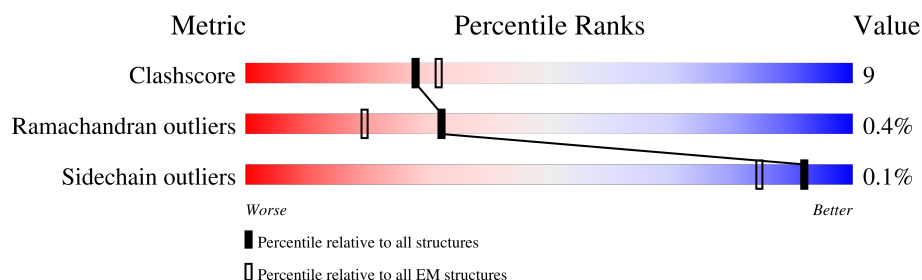
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 Å.

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



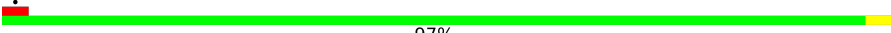
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	85% 14% .
1	I	215	84% 16%
2	B	160	91% 8% .
2	J	160	89% 9% .
3	C	285	85% 14% .
3	K	285	87% 13%
4	D	179	6% 85% 15%
4	L	179	7% 78% 22%

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Mol	Chain	Length	Quality of chain
5	E	31	 90% 10%
5	M	31	 90% 10%
6	F	36	 89% 11%
6	N	36	 97% .
7	G	37	 92% 8%
7	O	37	 97% .
8	H	29	 97% .
8	P	29	 100%

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
10	HEC	C	301	-	-	X	-
11	CLA	A	304	X	-	-	-
11	CLA	I	304	X	-	-	-
13	PL9	A	306	-	-	X	-
13	PL9	I	306	-	-	X	-
17	FES	D	201	-	-	X	-
17	FES	L	201	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 16359 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	215	Total	C	N	O	S	0	0
			1705	1131	272	290	12		
1	A	215	Total	C	N	O	S	0	0
			1705	1131	272	290	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	160	Total	C	N	O	S	0	0
			1234	825	194	210	5		
2	B	160	Total	C	N	O	S	0	0
			1234	825	194	210	5		

- Molecule 3 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	285	Total	C	N	O	S	0	0
			2209	1418	375	410	6		
3	C	285	Total	C	N	O	S	0	0
			2209	1418	375	410	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	179	Total	C	N	O	S	0	0
			1333	850	225	251	7		
4	D	179	Total	C	N	O	S	0	0
			1333	850	225	251	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	31	Total	C	N	O	S	0	0
			243	167	36	39	1		
5	E	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	N	36	Total	C	N	O	S	0	0
			264	171	44	48	1		
6	F	36	Total	C	N	O	S	0	0
			264	171	44	48	1		

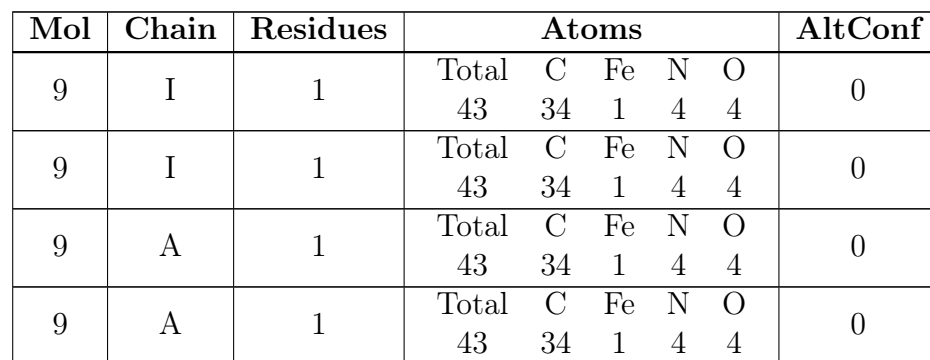
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	37	Total	C	N	O	S	0	0
			294	199	45	49	1		
7	G	37	Total	C	N	O	S	0	0
			294	199	45	49	1		

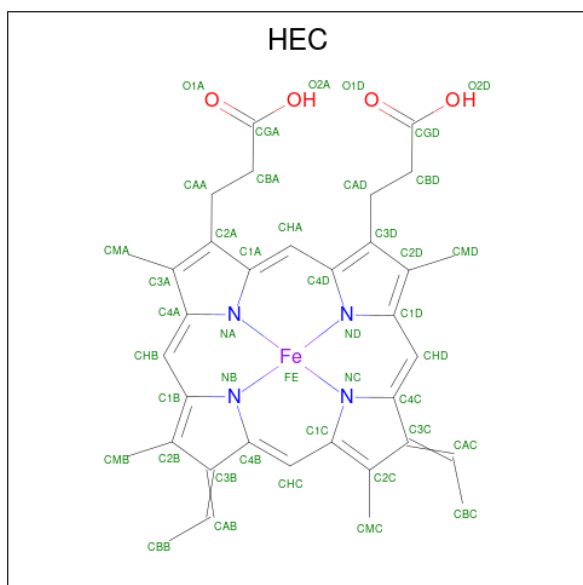
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

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

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

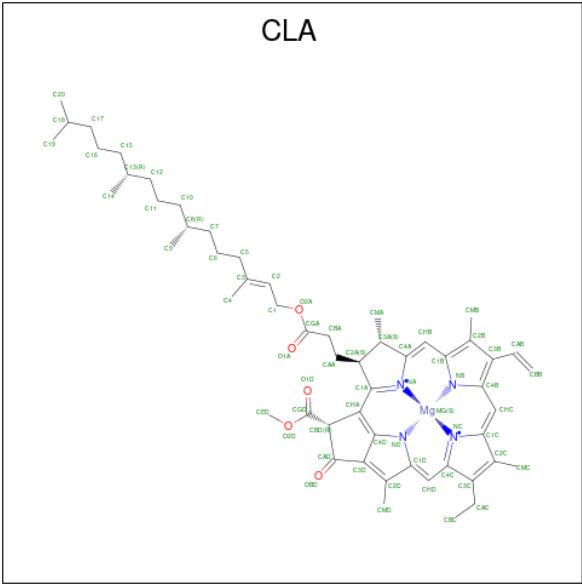


- Molecule 10 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



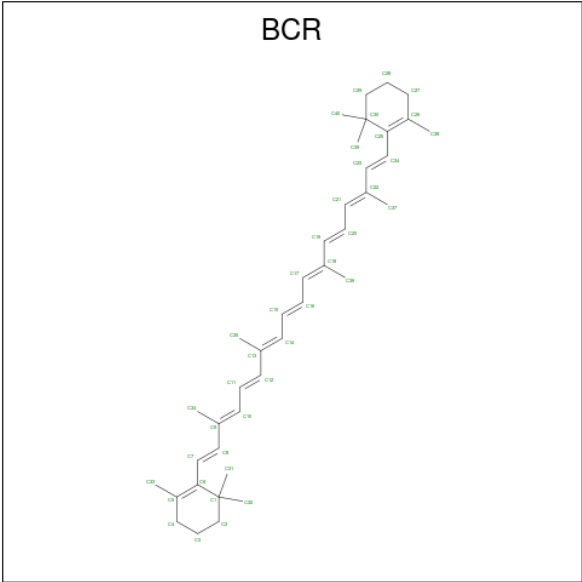
Mol	Chain	Residues	Atoms					AltConf
10	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



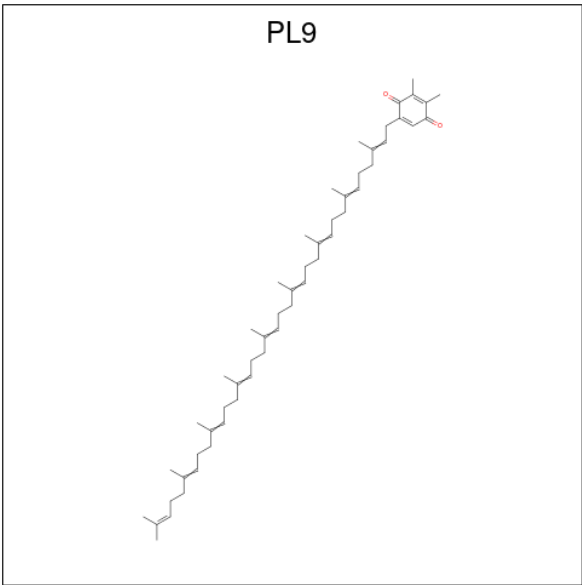
Mol	Chain	Residues	Atoms					AltConf
11	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
12	I	1	Total	C	0
			40	40	
12	H	1	Total	C	0
			40	40	

- Molecule 13 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



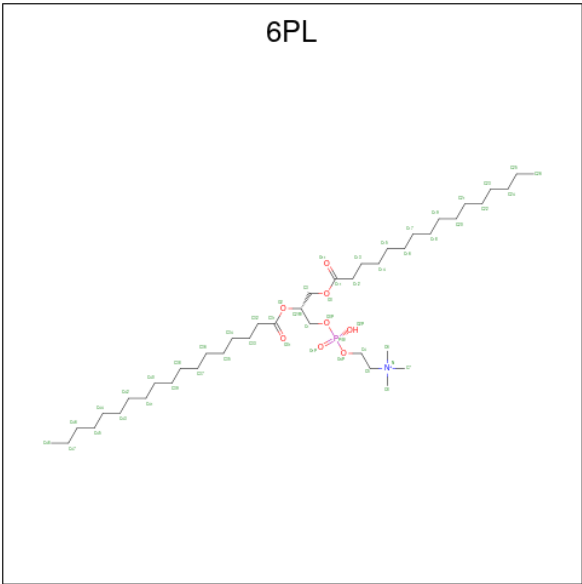
Mol	Chain	Residues	Atoms			AltConf
13	I	1	Total	C	O	0
			55	53	2	

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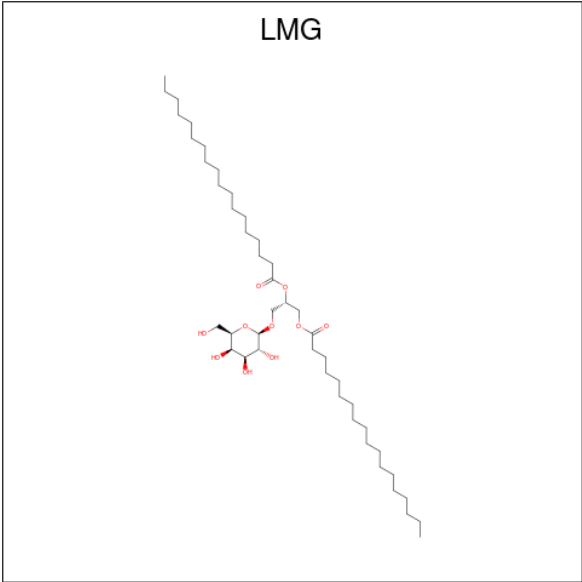
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			55	53	2	
13	A	1	Total	C	O	0
			55	53	2	

- Molecule 14 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C₄₂H₈₅NO₈P).



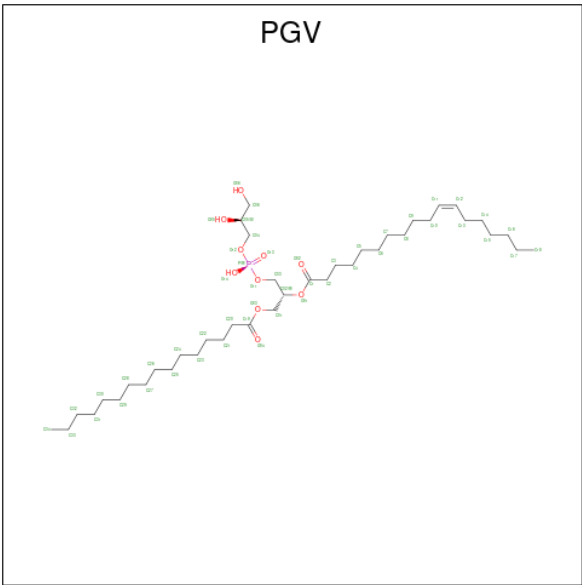
Mol	Chain	Residues	Atoms					AltConf
14	I	1	Total	C	N	O	P	0
			52	42	1	8	1	
14	N	1	Total	C	N	O	P	0
			52	42	1	8	1	
14	E	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 15 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
15	J	1	Total	C	O	0
			55	45	10	
15	F	1	Total	C	O	0
			55	45	10	

- Molecule 16 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



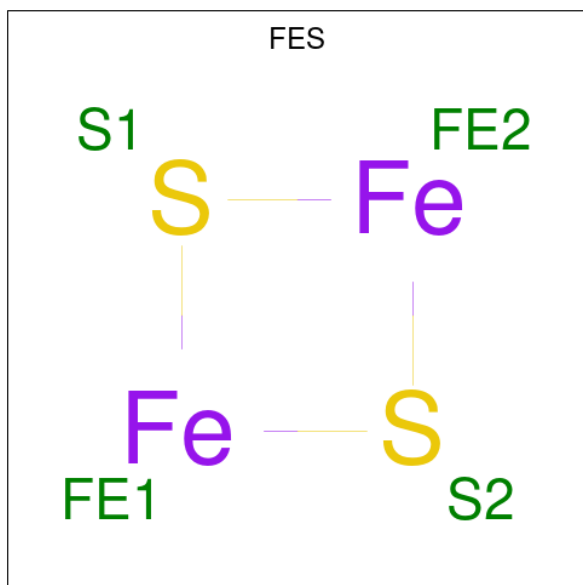
Mol	Chain	Residues	Atoms				AltConf
16	J	1	Total	C	O	P	0
			51	40	10	1	

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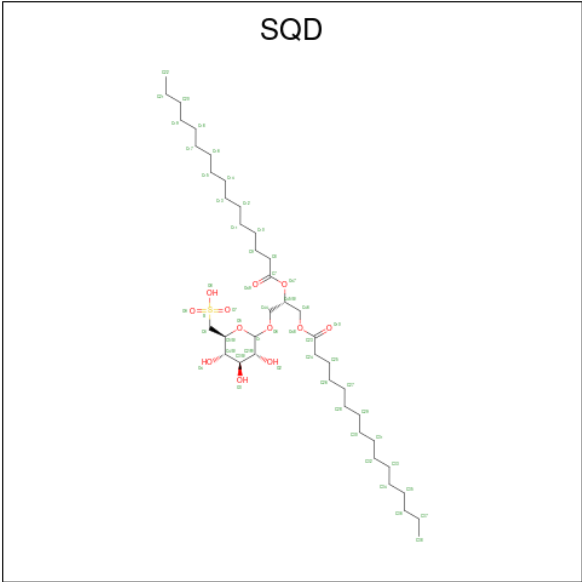
Mol	Chain	Residues	Atoms				AltConf
16	K	1	Total	C	O	P	0
			51	40	10	1	
16	A	1	Total	C	O	P	0
			45	34	10	1	
16	B	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).

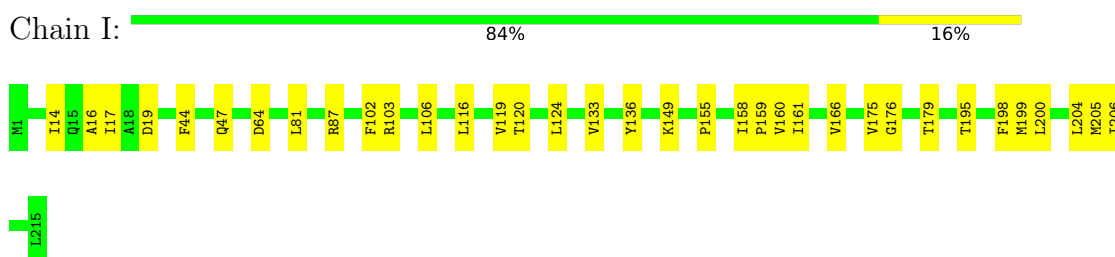


Mol	Chain	Residues	Atoms				AltConf
18	L	1	Total	C	O	S	0
			54	41	12	1	
18	A	1	Total	C	O	S	0
			54	41	12	1	
18	C	1	Total	C	O	S	0
			54	41	12	1	

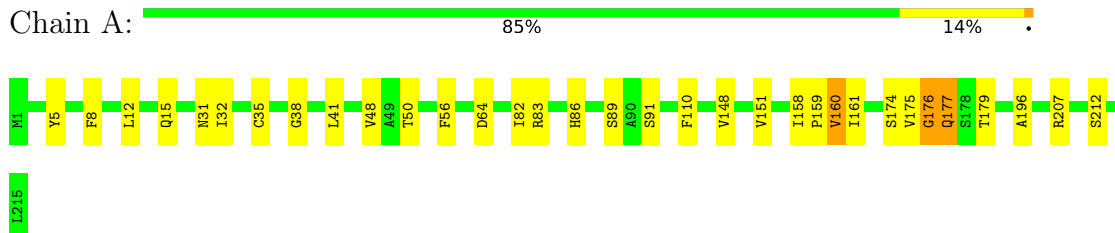
3 Residue-property plots [i](#)

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

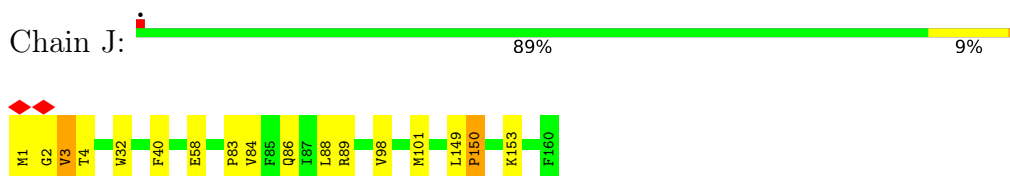
- Molecule 1: Cytochrome b6



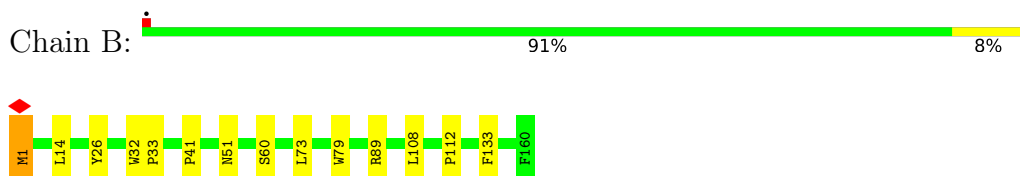
- Molecule 1: Cytochrome b6




- Molecule 2: Cytochrome b6-f complex subunit 4

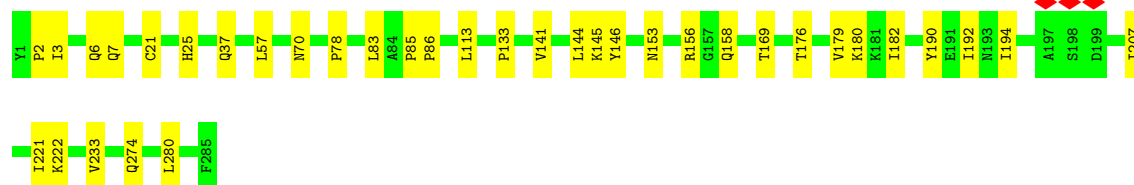


- Molecule 2: Cytochrome b6-f complex subunit 4




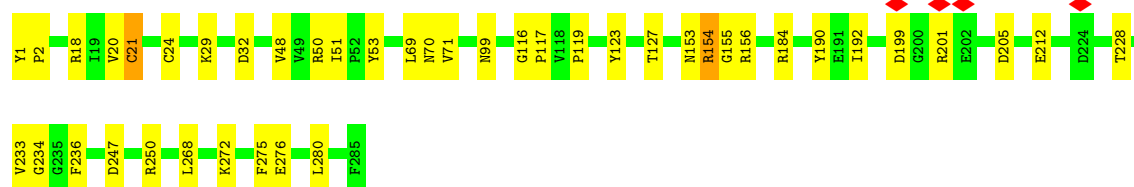
- Molecule 3: Cytochrome f

Chain K:  87% 13%




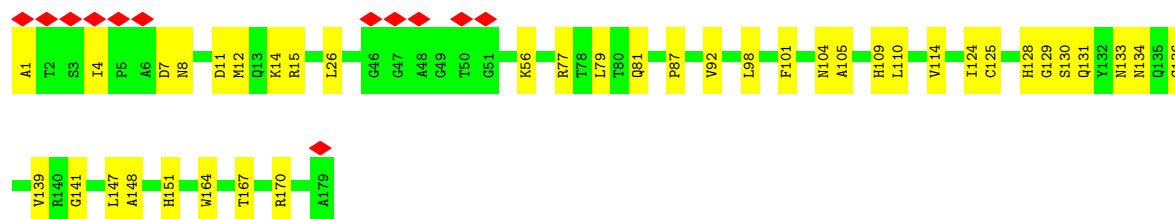
- Molecule 3: Cytochrome f

Chain C:  85% 14%




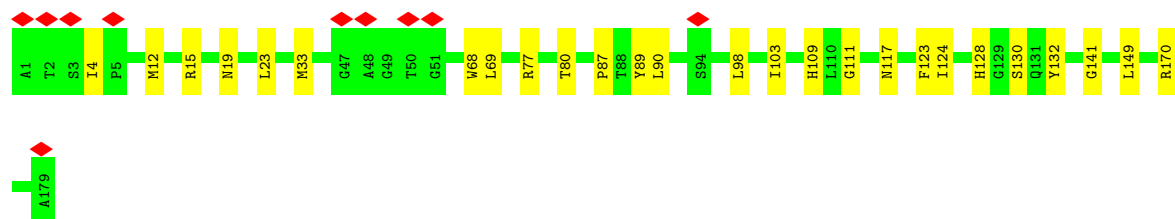
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain L:  7% 78% 22%



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

Chain D:  6% 85% 15%




- Molecule 5: Cytochrome b6-f complex subunit 6

Chain M:  90% 10%



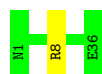
- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:  90% 10%




- Molecule 6: Cytochrome b6-f complex subunit 7

Chain N:  97% .



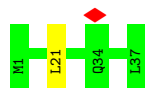
- Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:  89% 11%



- Molecule 7: Cytochrome b6-f complex subunit 5

Chain O:  97% .



- Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:  92% 8%



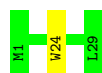
- Molecule 8: Cytochrome b6-f complex subunit 8

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:  97% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.15	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0144	Depositor
Map size (Å)	330.15002, 330.15002, 330.15002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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: PGV, PL9, SQD, 6PL, HEC, HEM, BCR, LMG, CLA, FES

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	0.43	0/1755	0.59	3/2392 (0.1%)
1	I	0.43	1/1755 (0.1%)	0.53	0/2392
2	B	0.36	0/1271	0.54	0/1743
2	J	0.38	0/1271	0.58	0/1743
3	C	0.36	1/2256 (0.0%)	0.56	1/3058 (0.0%)
3	K	0.36	1/2256 (0.0%)	0.51	0/3058
4	D	0.41	0/1369	0.59	0/1875
4	L	0.39	1/1369 (0.1%)	0.57	0/1875
5	E	0.30	0/247	0.57	0/333
5	M	0.30	0/247	0.59	0/333
6	F	0.34	0/265	0.47	0/359
6	N	0.33	0/265	0.49	0/359
7	G	0.34	0/299	0.53	0/405
7	O	0.33	0/299	0.56	0/405
8	H	0.35	0/228	0.46	0/309
8	P	0.35	0/228	0.44	0/309
All	All	0.38	4/15380 (0.0%)	0.55	4/20948 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	124	ILE	C-N	-5.86	1.20	1.34
3	K	21	CYS	C-N	5.76	1.47	1.34
3	C	20	VAL	C-N	5.32	1.46	1.34
1	I	206	ILE	C-N	5.03	1.45	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLY	N-CA-C	-8.79	91.12	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	GLN	N-CA-C	8.12	132.92	111.00
1	A	177	GLN	N-CA-CB	-5.88	100.02	110.60
3	C	21	CYS	O-C-N	5.06	130.80	122.70

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	1705	0	1736	38	0
1	I	1705	0	1736	42	0
2	B	1234	0	1288	13	0
2	J	1234	0	1288	24	0
3	C	2209	0	2254	54	0
3	K	2209	0	2252	26	0
4	D	1333	0	1304	20	0
4	L	1333	0	1304	39	0
5	E	243	0	268	9	0
5	M	243	0	268	3	0
6	F	264	0	282	3	0
6	N	264	0	282	3	0
7	G	294	0	314	2	0
7	O	294	0	314	1	0
8	H	223	0	234	2	0
8	P	223	0	234	0	0
9	A	86	0	60	3	0
9	I	86	0	60	1	0
10	A	43	0	31	7	0
10	C	43	0	32	21	0
10	I	43	0	32	5	0
10	K	43	0	29	2	0
11	A	65	0	72	2	0
11	I	65	0	72	3	0
12	H	40	0	56	1	0
12	I	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	110	0	160	41	0
13	I	55	0	80	25	0
14	E	51	0	79	10	0
14	I	52	0	84	1	0
14	N	52	0	84	3	0
15	F	55	0	86	0	0
15	J	55	0	86	1	0
16	A	45	0	62	1	0
16	B	48	0	67	0	0
16	J	51	0	76	0	0
16	K	51	0	76	1	0
17	D	4	0	0	2	0
17	L	4	0	0	3	0
18	A	54	0	78	8	0
18	C	54	0	78	10	0
18	L	54	0	77	5	0
All	All	16359	0	17031	315	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 315 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:C:21:CYS:SG	10:C:301:HEC:CAB	2.11	1.37
3:C:24:CYS:SG	10:C:301:HEC:CAC	2.19	1.31
13:A:305:PL9:H252	13:A:306:PL9:C20	1.62	1.28
3:C:24:CYS:CB	10:C:301:HEC:HBC3	1.63	1.26
1:A:175:VAL:HG23	1:A:179:THR:CG2	1.65	1.25

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	213/215 (99%)	203 (95%)	8 (4%)	2 (1%)	14	48
1	I	213/215 (99%)	204 (96%)	7 (3%)	2 (1%)	14	48
2	B	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
2	J	158/160 (99%)	149 (94%)	7 (4%)	2 (1%)	10	41
3	C	283/285 (99%)	271 (96%)	12 (4%)	0	100	100
3	K	283/285 (99%)	273 (96%)	10 (4%)	0	100	100
4	D	177/179 (99%)	164 (93%)	13 (7%)	0	100	100
4	L	177/179 (99%)	163 (92%)	13 (7%)	1 (1%)	22	55
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
5	M	29/31 (94%)	29 (100%)	0	0	100	100
6	F	34/36 (94%)	34 (100%)	0	0	100	100
6	N	34/36 (94%)	34 (100%)	0	0	100	100
7	G	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
7	O	35/37 (95%)	34 (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
All	All	1912/1944 (98%)	1824 (95%)	81 (4%)	7 (0%)	32	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	160	VAL
1	A	160	VAL
4	L	129	GLY
2	J	150	PRO
1	A	174	SER

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	A	186/186 (100%)	186 (100%)	0	100	100
1	I	186/186 (100%)	186 (100%)	0	100	100
2	B	135/135 (100%)	134 (99%)	1 (1%)	81	90
2	J	135/135 (100%)	135 (100%)	0	100	100
3	C	242/242 (100%)	241 (100%)	1 (0%)	89	95
3	K	242/242 (100%)	242 (100%)	0	100	100
4	D	141/141 (100%)	141 (100%)	0	100	100
4	L	141/141 (100%)	141 (100%)	0	100	100
5	E	26/26 (100%)	26 (100%)	0	100	100
5	M	26/26 (100%)	26 (100%)	0	100	100
6	F	26/26 (100%)	26 (100%)	0	100	100
6	N	26/26 (100%)	26 (100%)	0	100	100
7	G	31/31 (100%)	31 (100%)	0	100	100
7	O	31/31 (100%)	31 (100%)	0	100	100
8	H	24/24 (100%)	24 (100%)	0	100	100
8	P	24/24 (100%)	24 (100%)	0	100	100
All	All	1622/1622 (100%)	1620 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1	MET
3	C	154	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	GLN
3	C	23	ASN
4	D	117	ASN
3	K	168	ASN
4	L	104	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 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$
14	6PL	I	307	-	51,51,51	1.61	4 (7%)	57,59,59	1.36	4 (7%)
10	HEC	A	303	-	32,50,50	2.20	4 (12%)	24,82,82	2.01	4 (16%)
9	HEM	A	301	1	41,50,50	1.47	4 (9%)	45,82,82	1.52	8 (17%)
17	FES	L	201	4	0,4,4	-	-	-		
10	HEC	I	303	1	32,50,50	2.33	4 (12%)	24,82,82	1.74	4 (16%)
16	PGV	J	202	-	50,50,50	0.93	2 (4%)	53,56,56	0.94	2 (3%)
14	6PL	N	101	-	51,51,51	1.59	4 (7%)	57,59,59	1.51	5 (8%)
13	PL9	A	306	-	55,55,55	0.70	1 (1%)	68,69,69	0.60	1 (1%)
11	CLA	I	304	-	65,73,73	1.44	9 (13%)	76,113,113	1.48	8 (10%)
16	PGV	K	302	-	50,50,50	0.92	2 (4%)	53,56,56	0.96	2 (3%)
15	LMG	J	201	-	55,55,55	0.84	1 (1%)	63,63,63	1.41	8 (12%)
10	HEC	C	301	3	32,50,50	1.60	5 (15%)	24,82,82	1.28	1 (4%)
9	HEM	A	302	1	41,50,50	1.44	5 (12%)	45,82,82	1.51	8 (17%)
12	BCR	H	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.20	7 (12%)
9	HEM	I	301	1	41,50,50	1.44	4 (9%)	45,82,82	1.33	4 (8%)
16	PGV	B	201	-	47,47,50	0.94	2 (4%)	50,53,56	1.02	3 (6%)
18	SQD	L	202	-	53,54,54	0.97	5 (9%)	62,65,65	1.46	10 (16%)
16	PGV	A	308	-	44,44,50	0.98	2 (4%)	47,50,56	1.06	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	SQD	A	307	-	53,54,54	0.37	1 (1%)	62,65,65	0.42	1 (1%)
12	BCR	I	305	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	6 (10%)
13	PL9	I	306	-	55,55,55	0.60	1 (1%)	68,69,69	1.76	21 (30%)
13	PL9	A	305	-	55,55,55	0.69	1 (1%)	68,69,69	0.58	1 (1%)
14	6PL	E	101	-	50,50,51	1.62	4 (8%)	56,58,59	1.42	4 (7%)
10	HEC	K	301	3	32,50,50	2.11	4 (12%)	24,82,82	2.06	7 (29%)
11	CLA	A	304	-	65,73,73	1.49	9 (13%)	76,113,113	1.42	9 (11%)
15	LMG	F	101	-	55,55,55	0.79	2 (3%)	63,63,63	1.37	8 (12%)
18	SQD	C	302	-	53,54,54	0.37	1 (1%)	62,65,65	0.43	1 (1%)
17	FES	D	201	4	0,4,4	-	-	-	-	-
9	HEM	I	302	1	41,50,50	1.54	4 (9%)	45,82,82	1.24	4 (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
14	6PL	I	307	-	-	14/55/55/55	-
10	HEC	A	303	-	-	5/10/54/54	-
9	HEM	A	301	1	-	5/12/54/54	-
17	FES	L	201	4	-	-	0/1/1/1
10	HEC	I	303	1	-	4/10/54/54	-
16	PGV	J	202	-	-	17/55/55/55	-
14	6PL	N	101	-	-	17/55/55/55	-
13	PL9	A	306	-	-	32/53/73/73	0/1/1/1
11	CLA	I	304	-	1/1/15/20	8/37/115/115	-
16	PGV	K	302	-	-	13/55/55/55	-
15	LMG	J	201	-	-	30/50/70/70	0/1/1/1
10	HEC	C	301	3	-	2/10/54/54	-
9	HEM	A	302	1	-	2/12/54/54	-
12	BCR	H	101	-	-	11/29/63/63	0/2/2/2
9	HEM	I	301	1	-	1/12/54/54	-
16	PGV	B	201	-	-	13/52/52/55	-
18	SQD	L	202	-	-	22/49/69/69	0/1/1/1
16	PGV	A	308	-	-	12/49/49/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	SQD	A	307	-	-	21/49/69/69	0/1/1/1
12	BCR	I	305	-	-	16/29/63/63	0/2/2/2
13	PL9	I	306	-	-	22/53/73/73	0/1/1/1
13	PL9	A	305	-	-	34/53/73/73	0/1/1/1
14	6PL	E	101	-	-	19/54/54/55	-
10	HEC	K	301	3	-	0/10/54/54	-
11	CLA	A	304	-	1/1/15/20	14/37/115/115	-
15	LMG	F	101	-	-	21/50/70/70	0/1/1/1
18	SQD	C	302	-	-	20/49/69/69	0/1/1/1
17	FES	D	201	4	-	-	0/1/1/1
9	HEM	I	302	1	-	1/12/54/54	-

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	303	HEC	C3C-C2C	-8.19	1.32	1.40
10	A	303	HEC	C3C-C2C	-7.48	1.32	1.40
11	A	304	CLA	C4B-NB	7.14	1.41	1.35
14	I	307	6PL	O11-C11	7.06	1.43	1.22
14	E	101	6PL	O31-C31	7.06	1.43	1.22

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	101	6PL	O2-C31-O31	-6.46	108.08	123.70
11	I	304	CLA	C4A-NA-C1A	6.33	109.55	106.71
11	A	304	CLA	C4A-NA-C1A	6.10	109.45	106.71
14	N	101	6PL	O3-C11-O11	-5.85	108.83	123.59
14	E	101	6PL	O2-C31-O31	-5.85	109.57	123.70

All (2) chirality outliers are listed below:

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

5 of 376 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	301	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	A	301	HEM	C2A-CAA-CBA-CGA
11	A	304	CLA	CHA-CBD-CGD-O1D
11	A	304	CLA	CHA-CBD-CGD-O2D
12	I	305	BCR	C1-C6-C7-C8

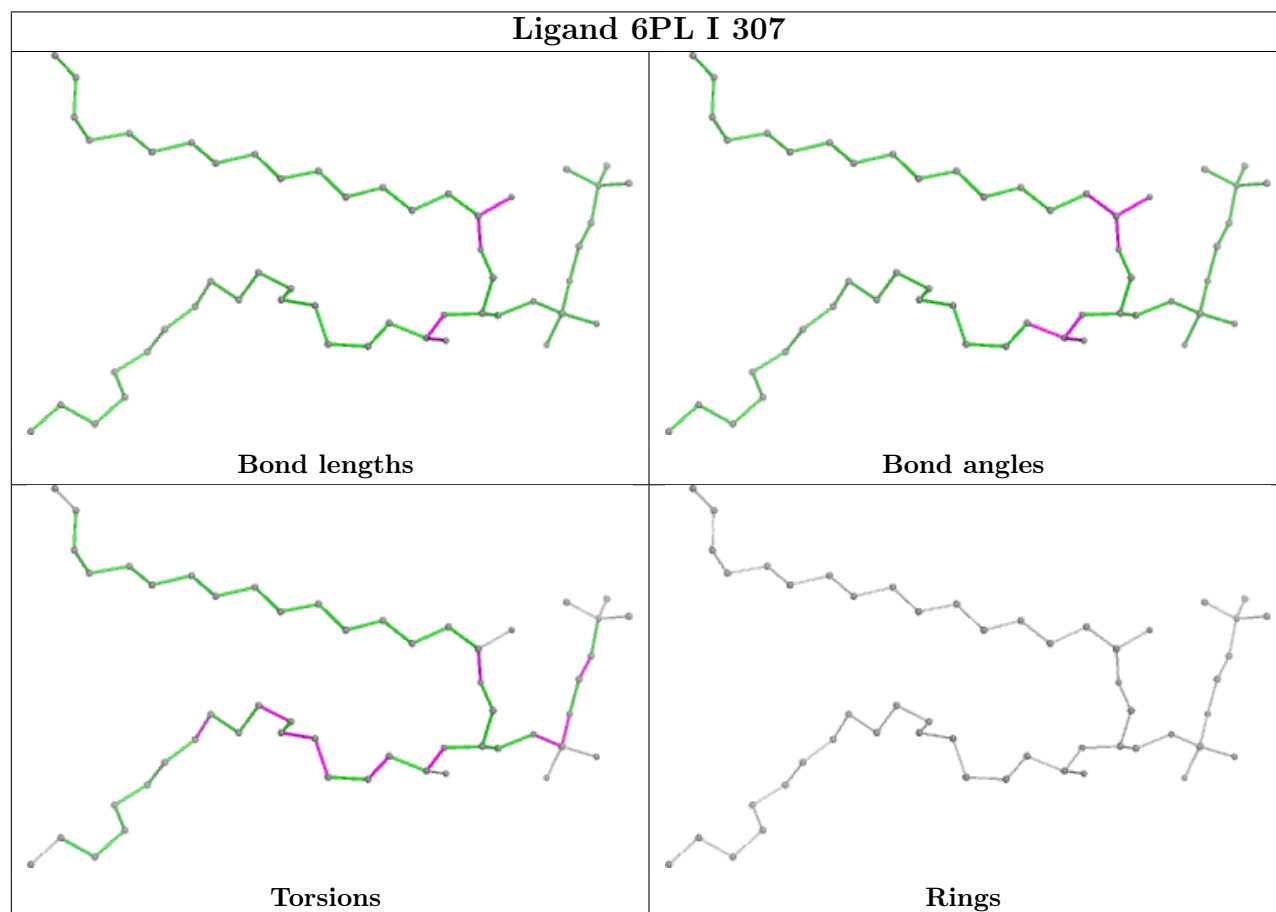
There are no ring outliers.

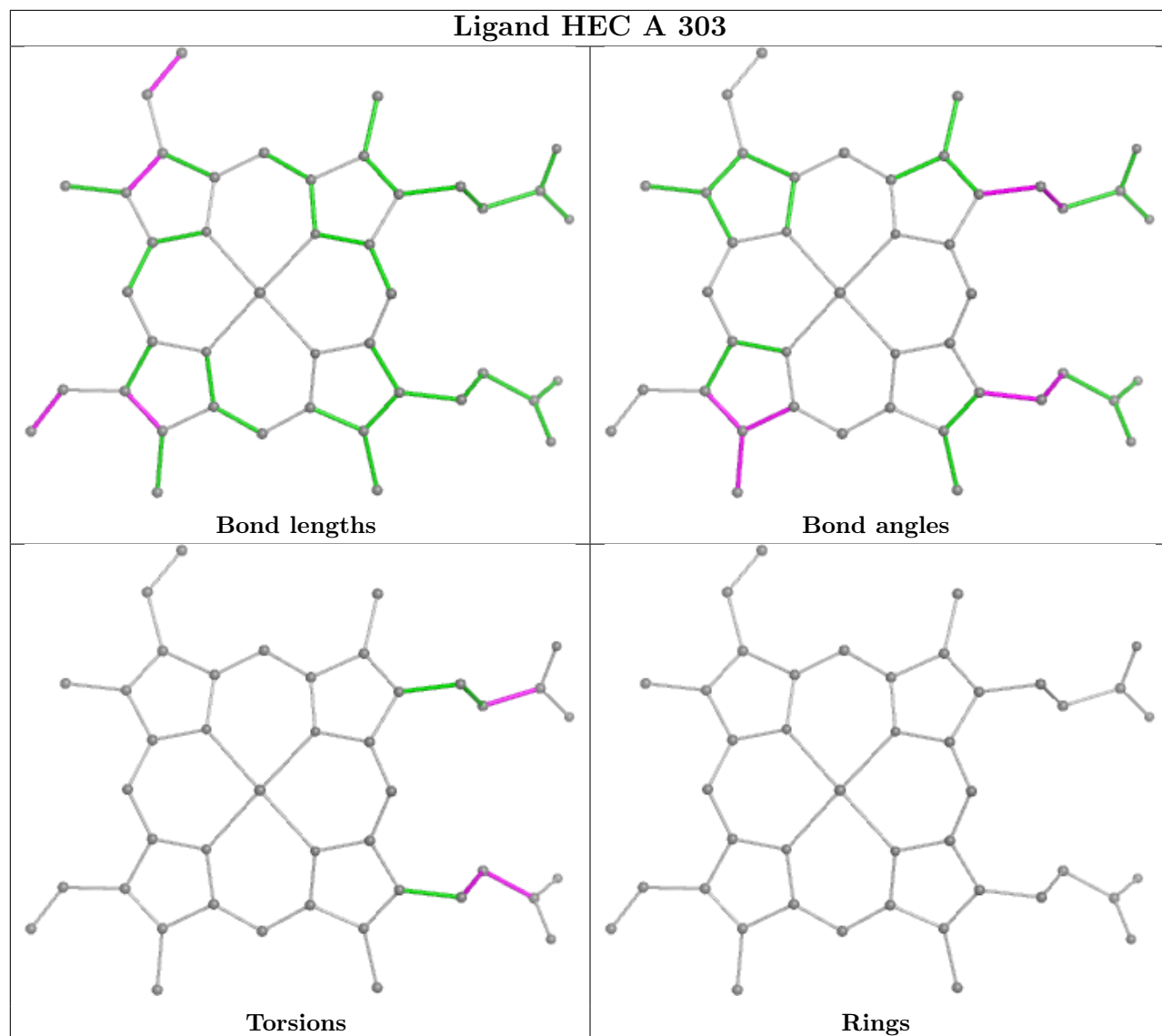
24 monomers are involved in 149 short contacts:

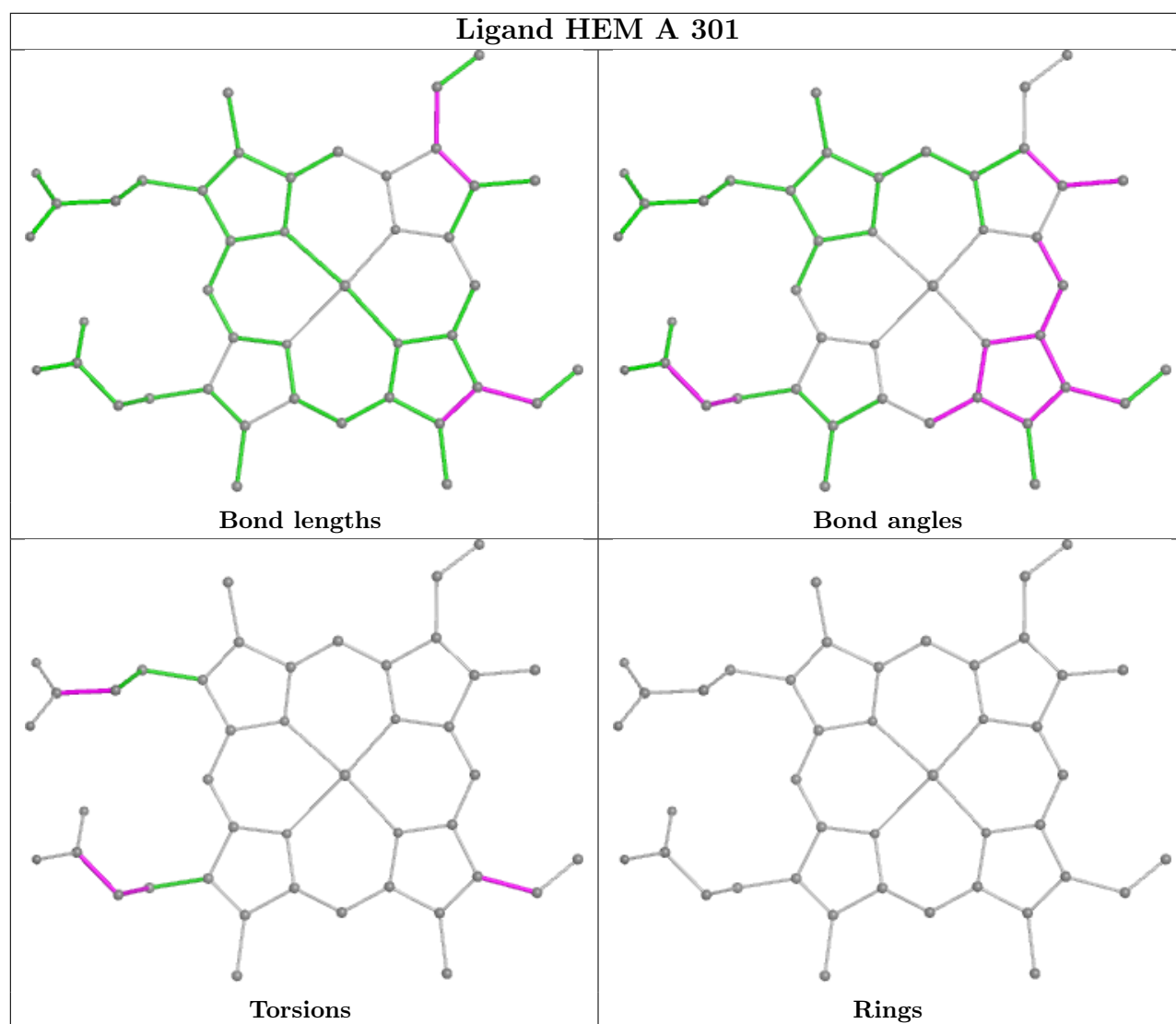
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	I	307	6PL	1	0
10	A	303	HEC	7	0
9	A	301	HEM	1	0
17	L	201	FES	3	0
10	I	303	HEC	5	0
14	N	101	6PL	3	0
13	A	306	PL9	34	0
11	I	304	CLA	3	0
16	K	302	PGV	1	0
15	J	201	LMG	1	0
10	C	301	HEC	21	0
9	A	302	HEM	2	0
12	H	101	BCR	1	0
18	L	202	SQD	5	0
16	A	308	PGV	1	0
18	A	307	SQD	8	0
13	I	306	PL9	25	0
13	A	305	PL9	16	0
14	E	101	6PL	10	0
10	K	301	HEC	2	0
11	A	304	CLA	2	0
18	C	302	SQD	10	0
17	D	201	FES	2	0
9	I	302	HEM	1	0

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

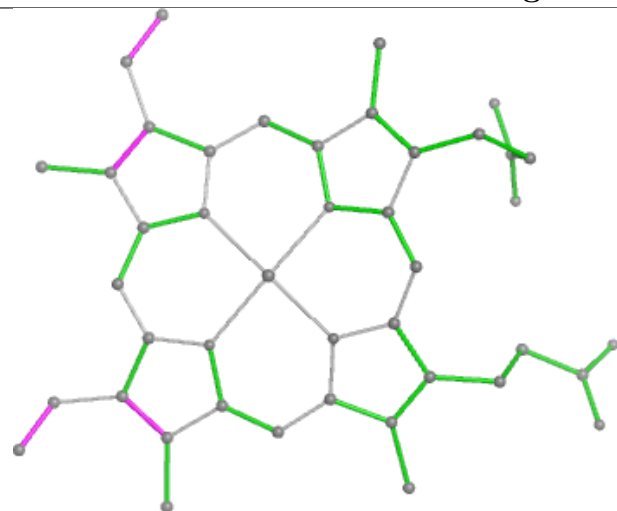
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



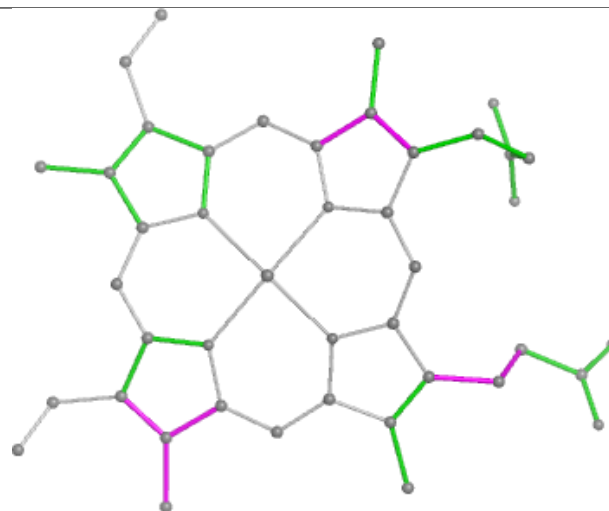




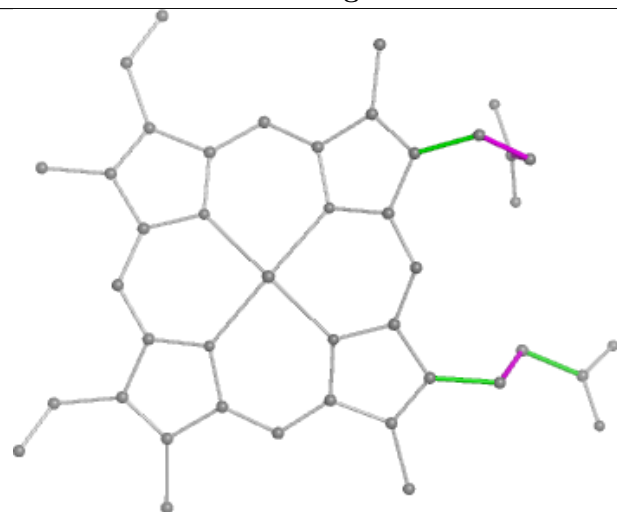
Ligand HEC I 303



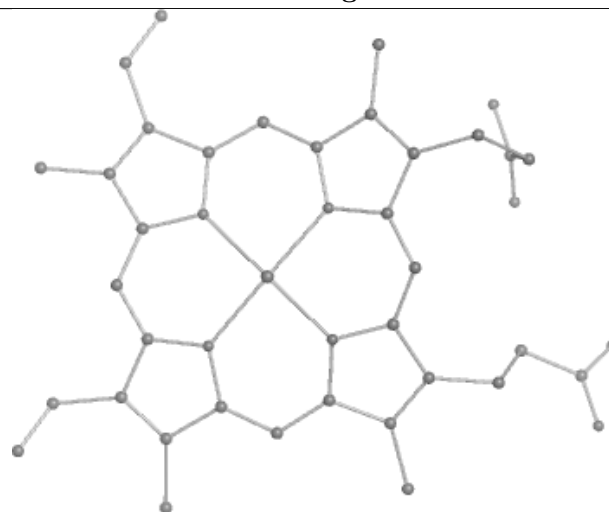
Bond lengths



Bond angles

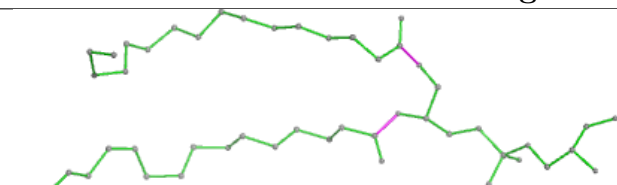


Torsions

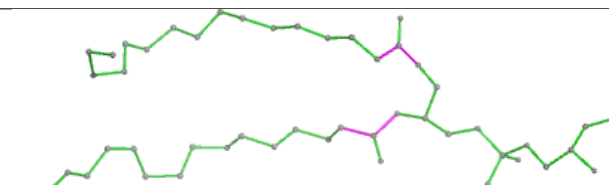


Rings

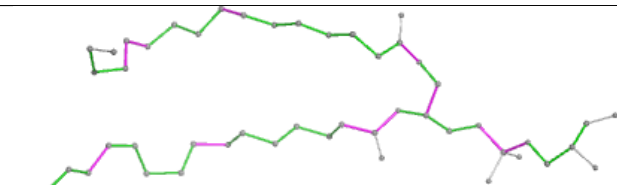
Ligand PGV J 202



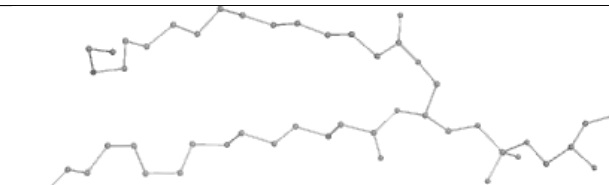
Bond lengths



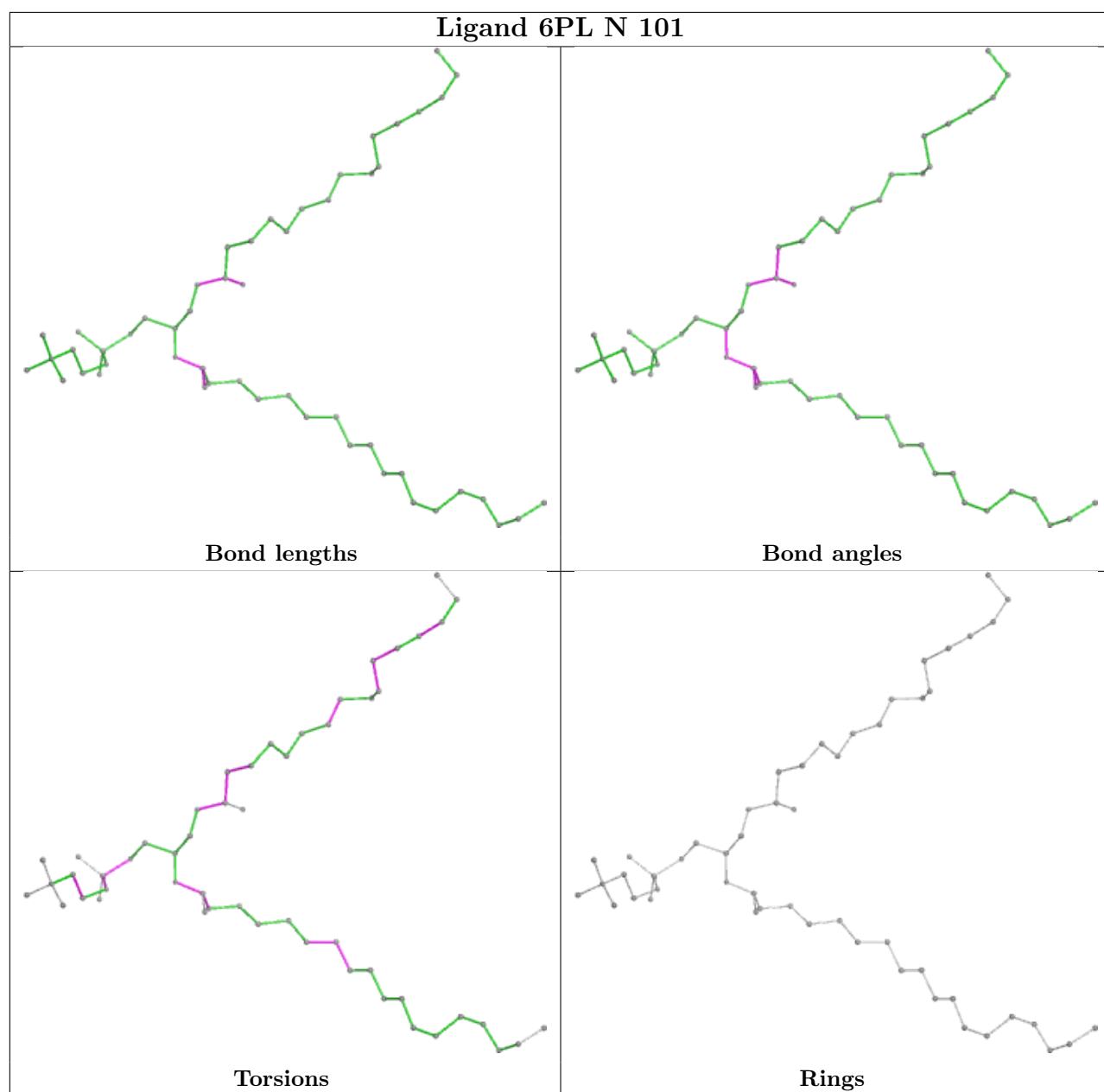
Bond angles

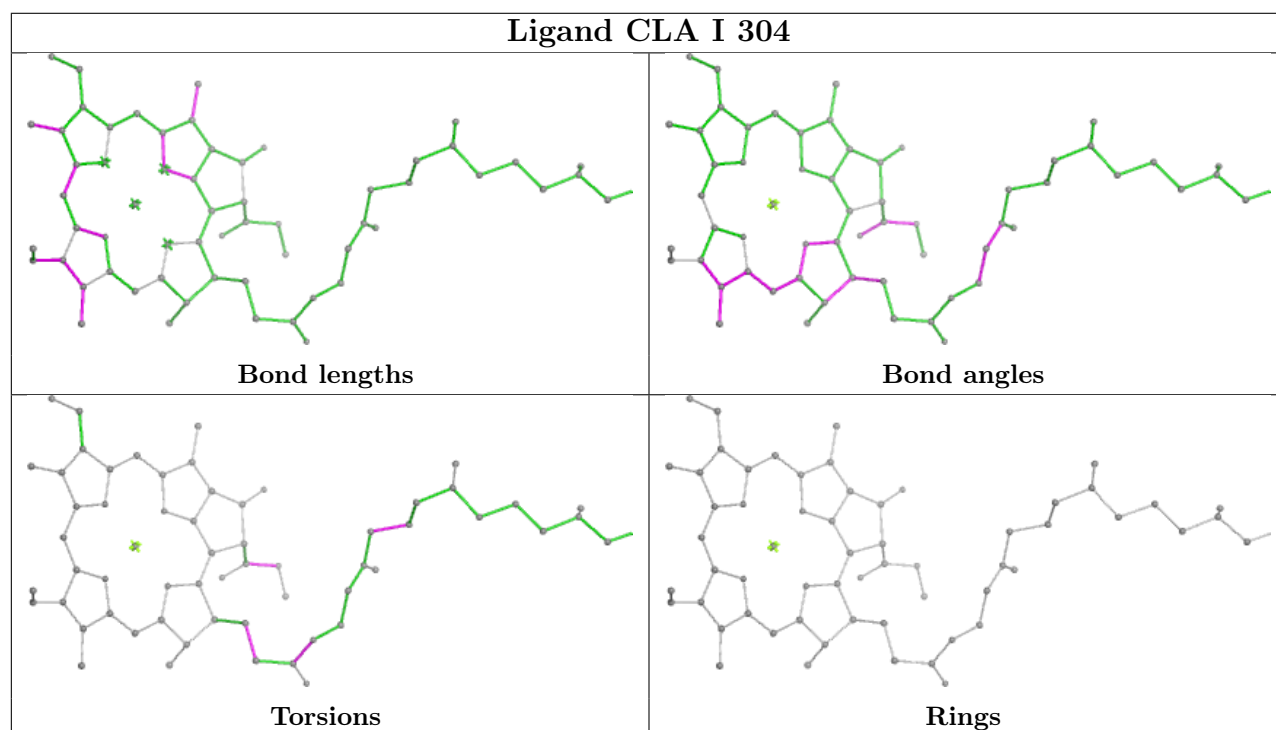
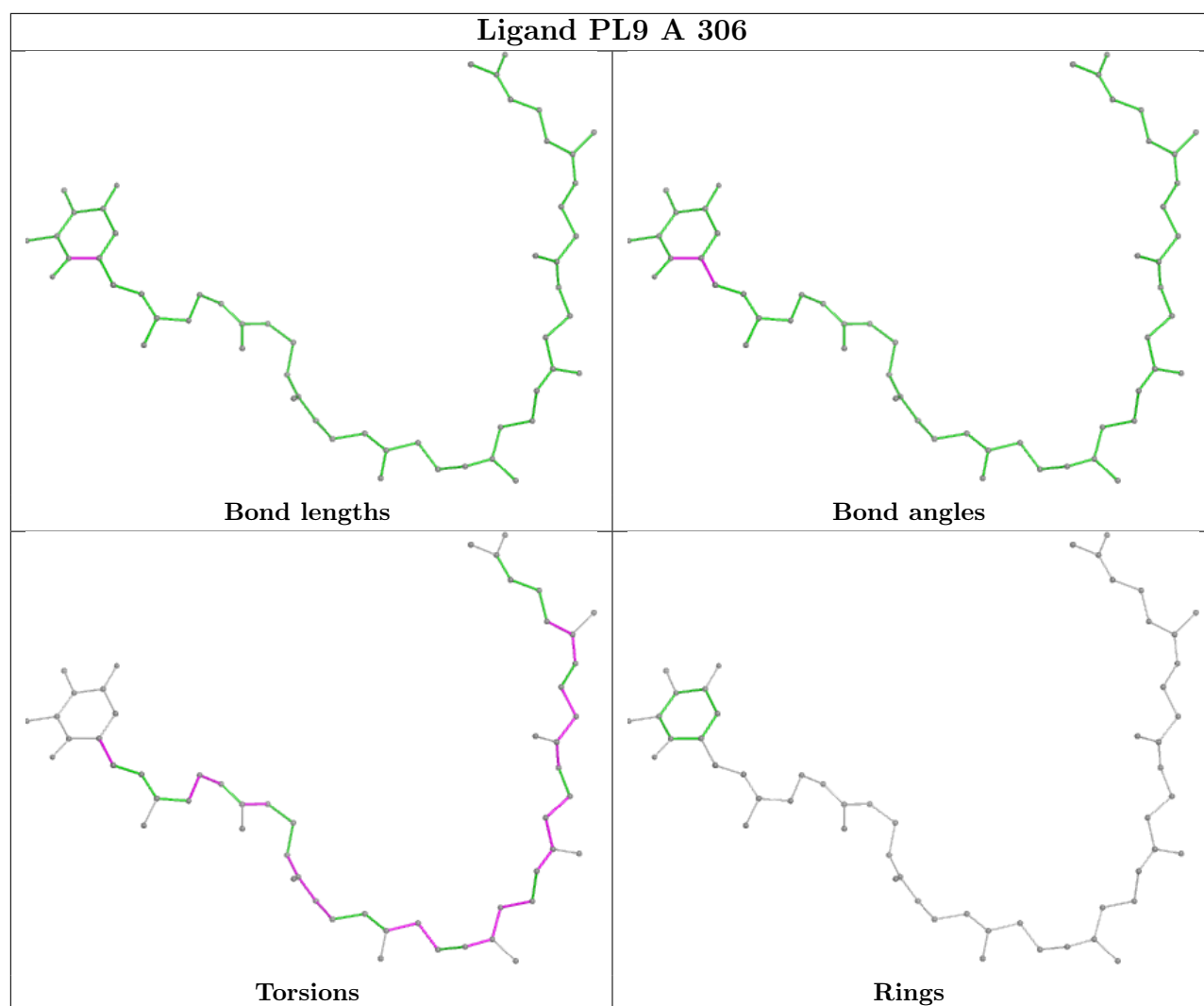


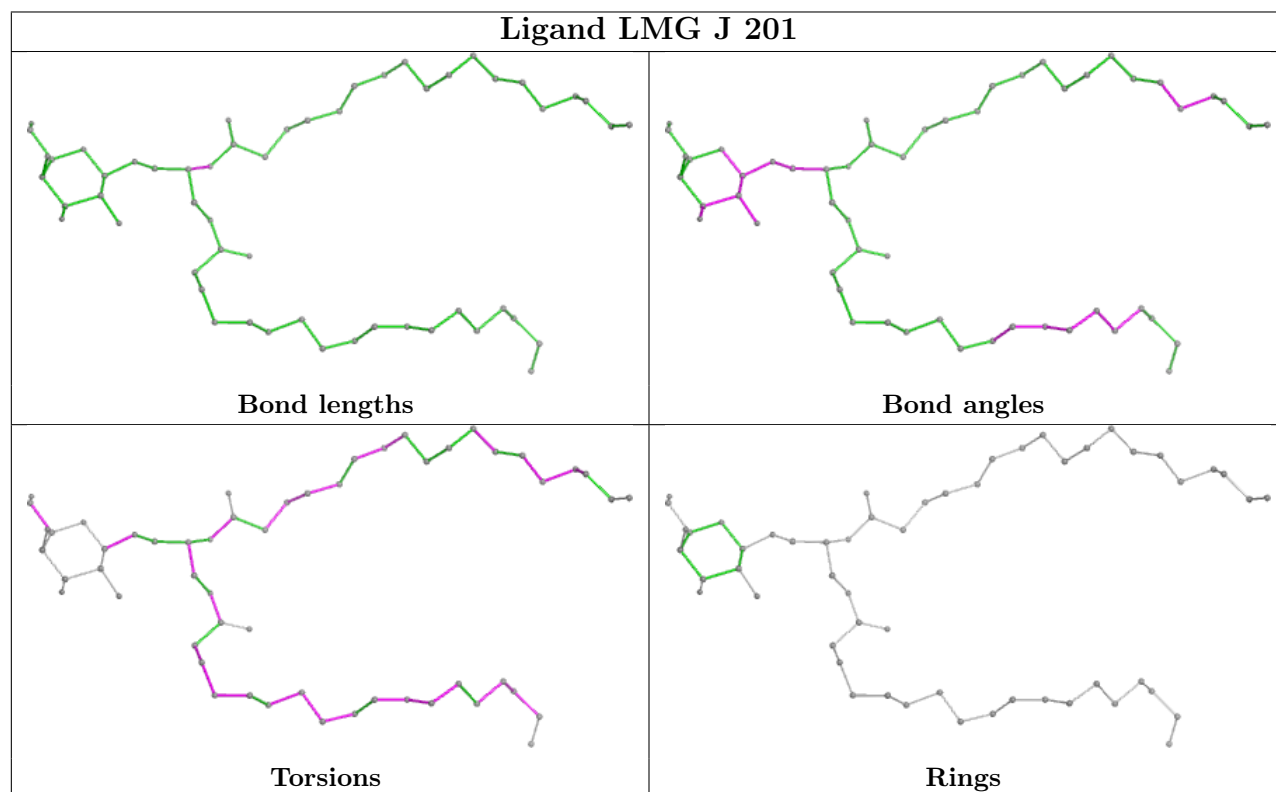
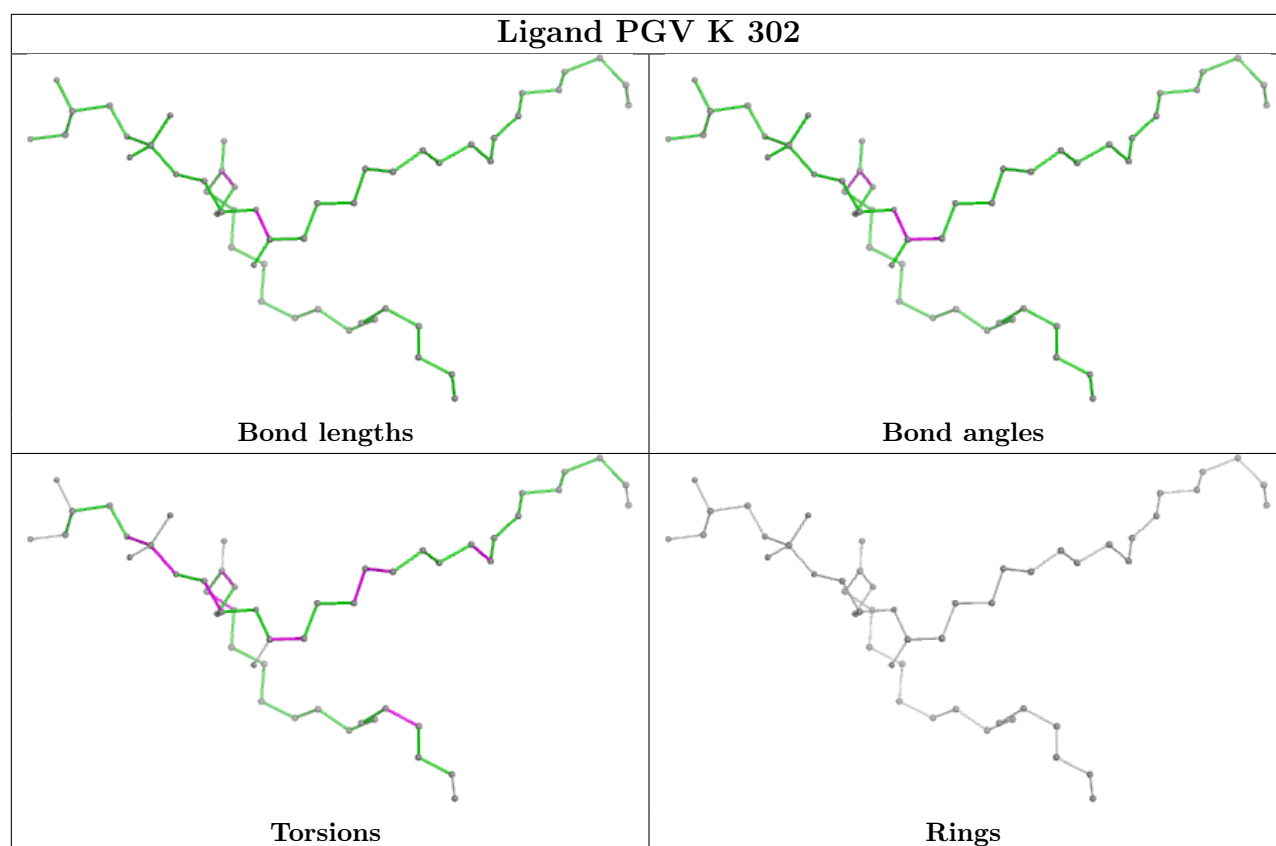
Torsions

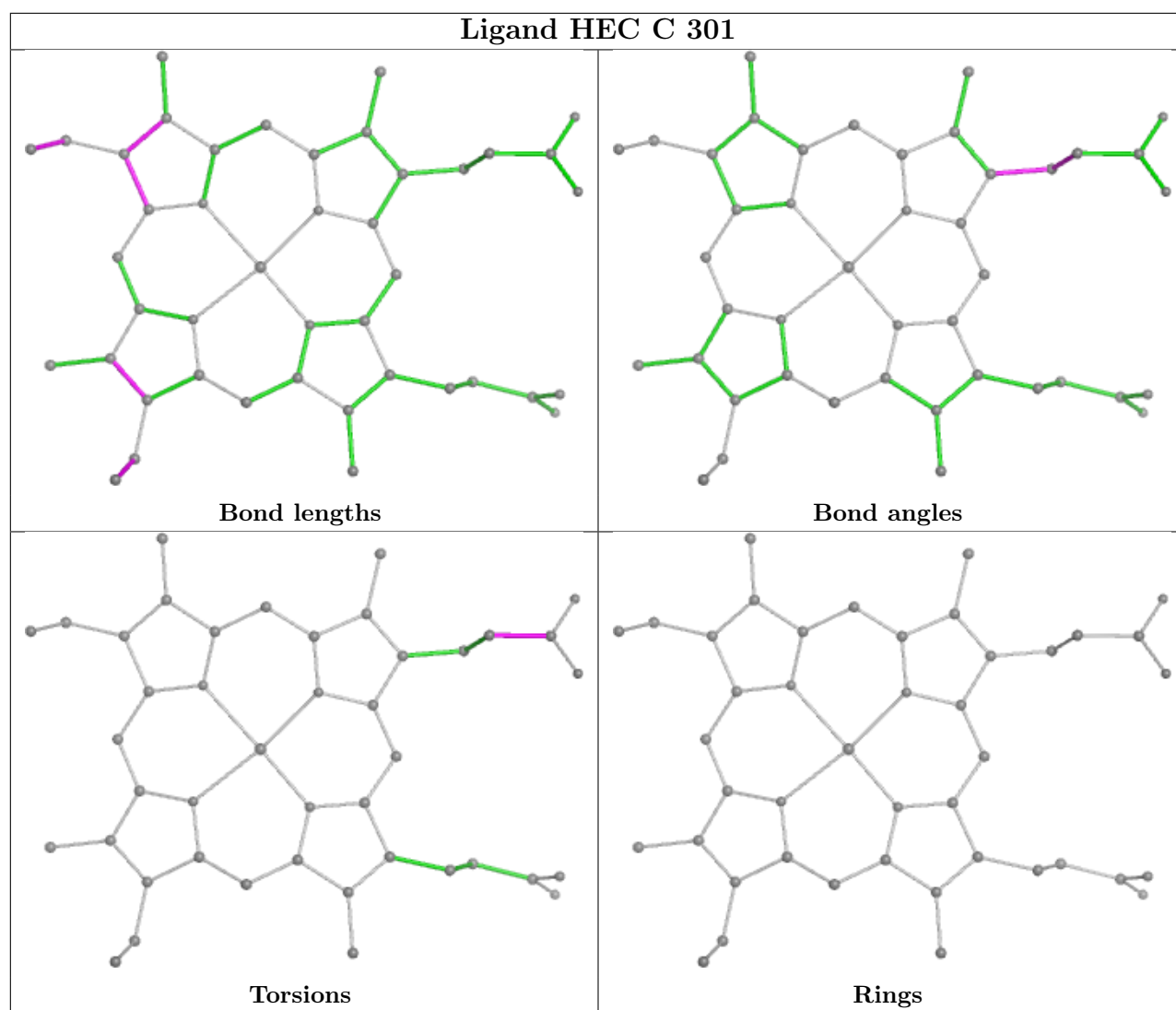


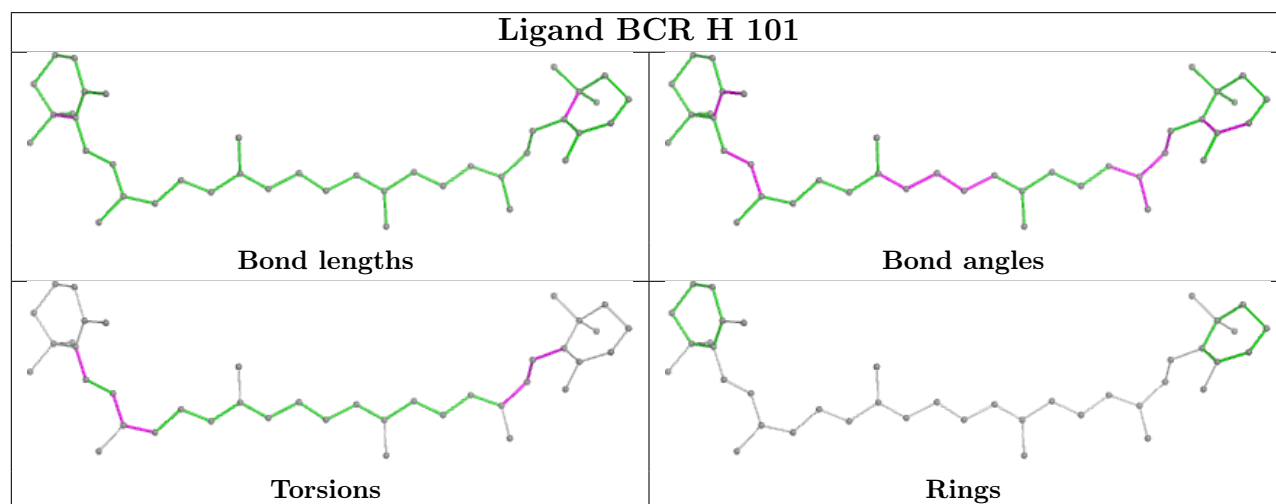
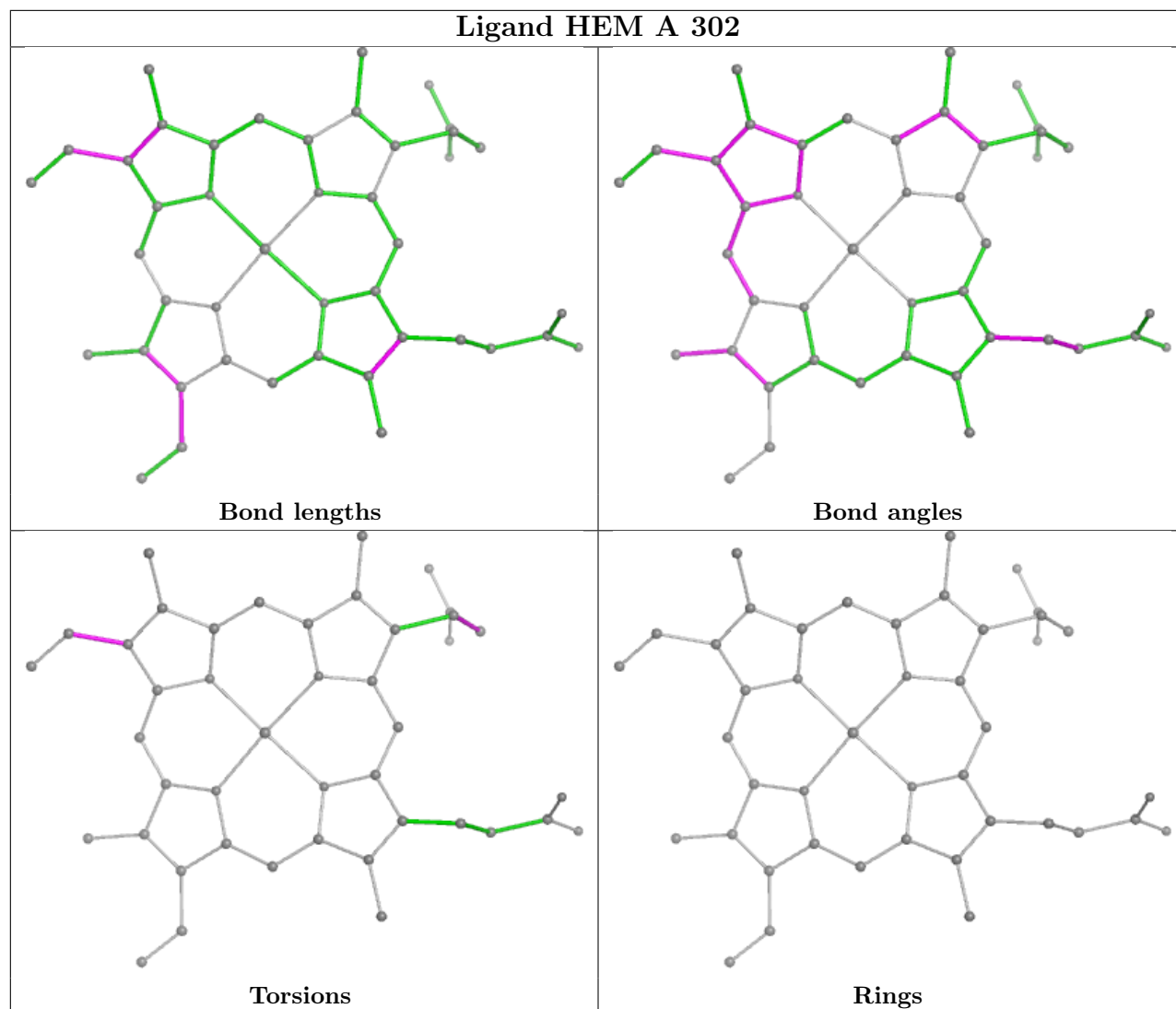
Rings



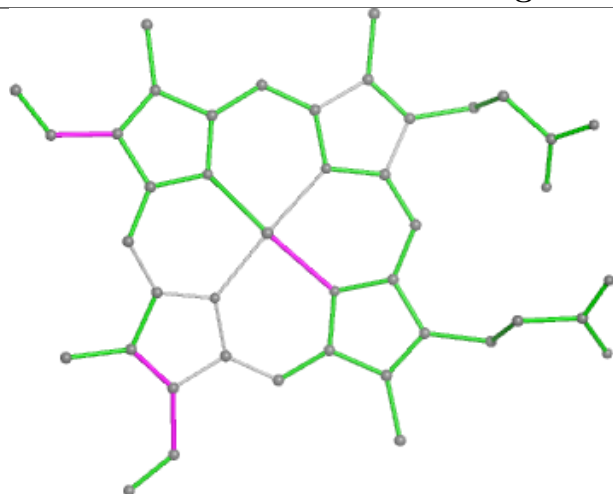




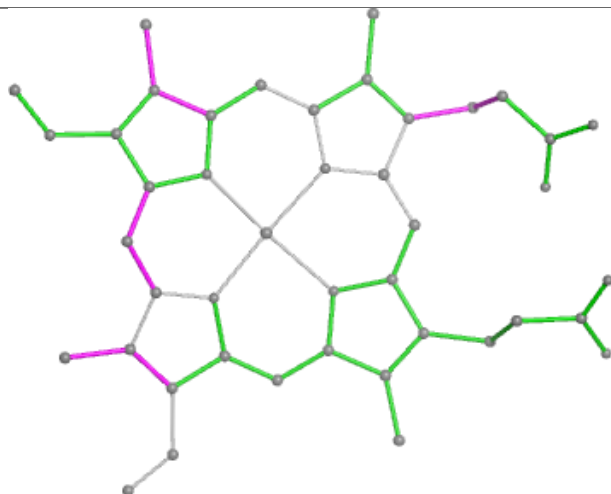




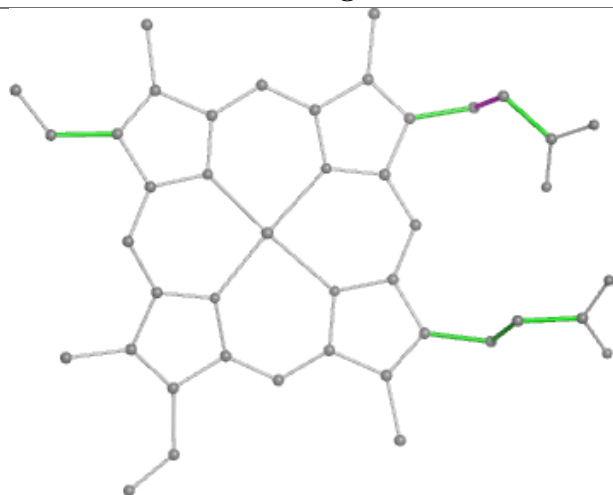
Ligand HEM I 301



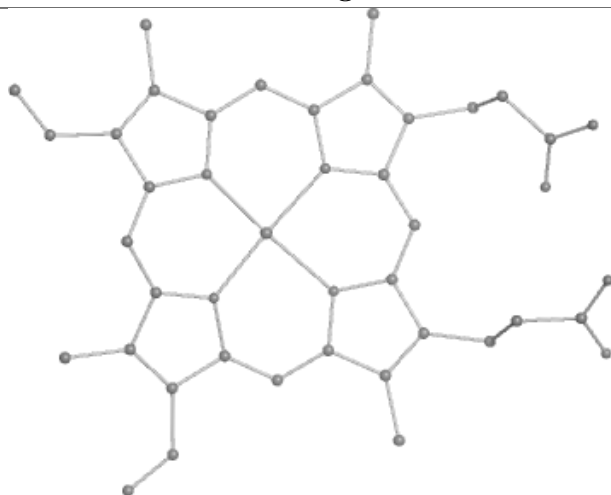
Bond lengths



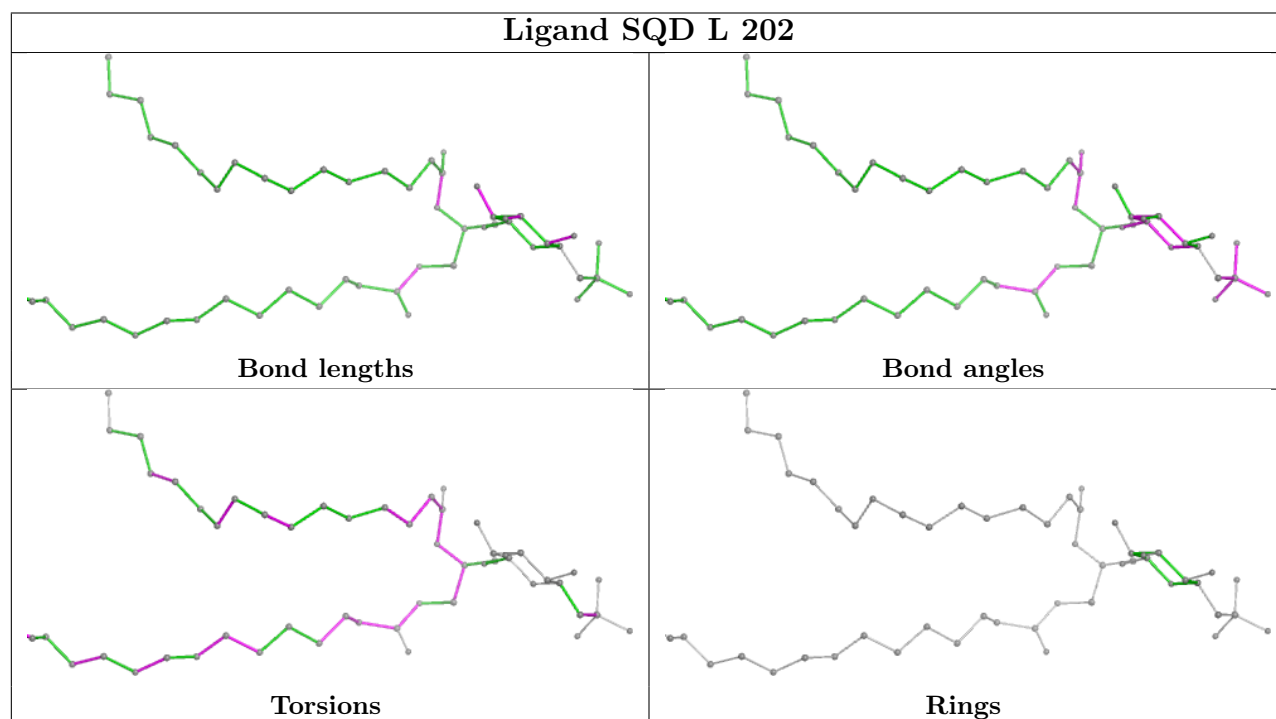
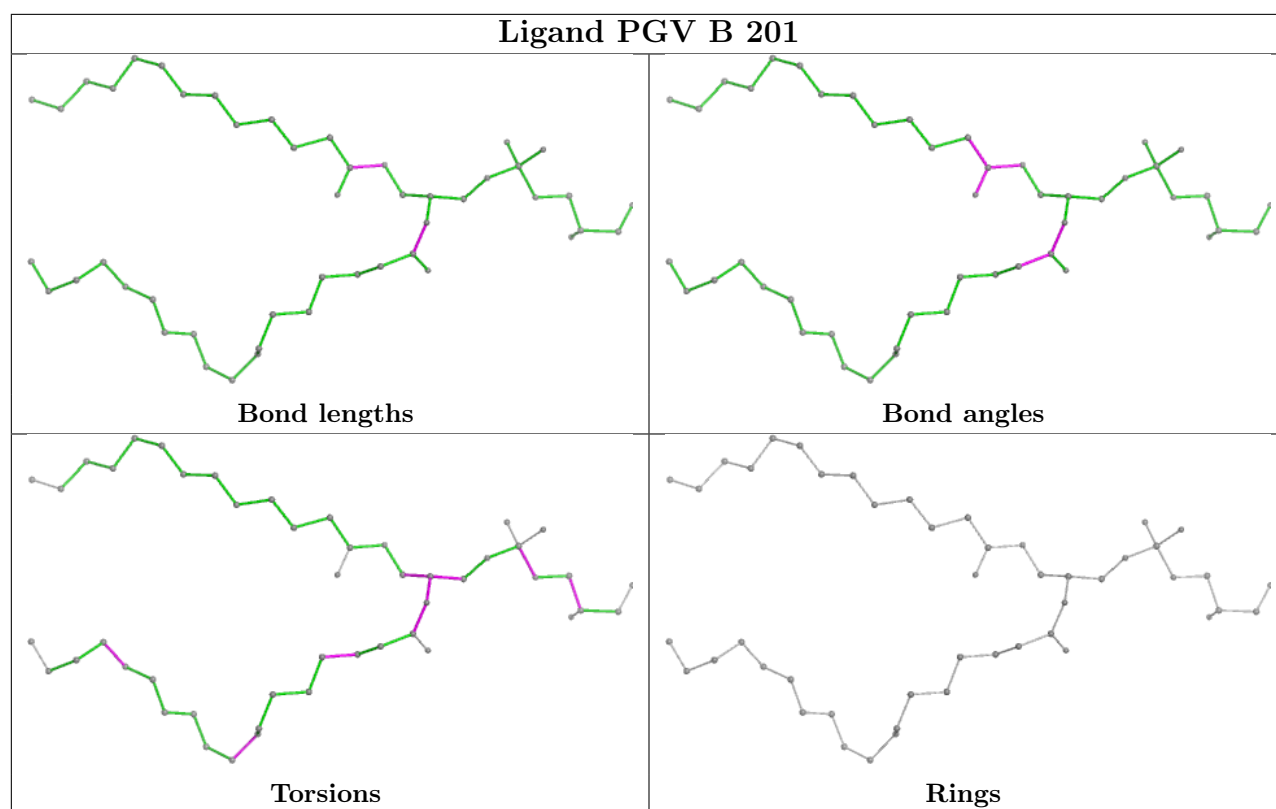
Bond angles

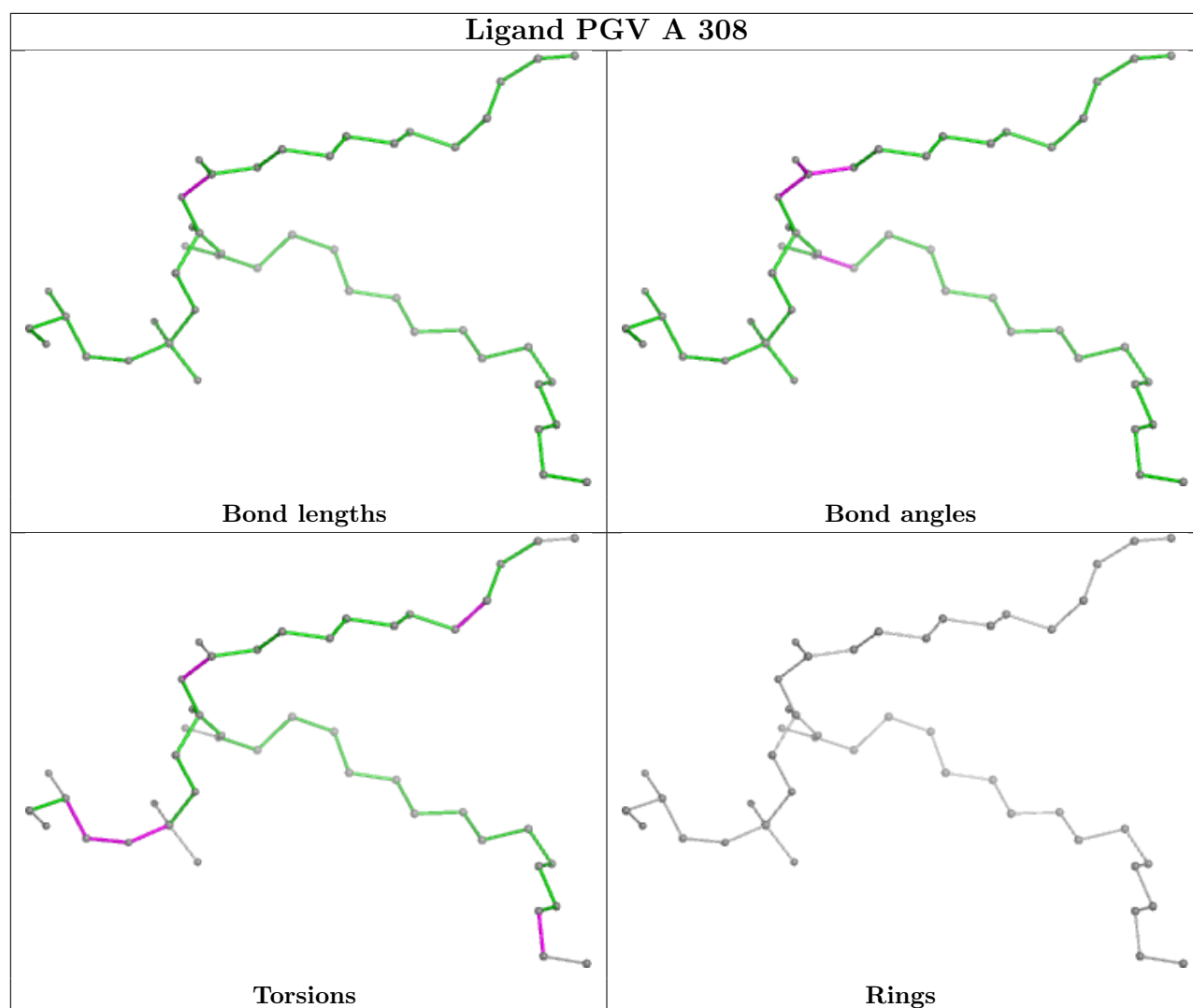


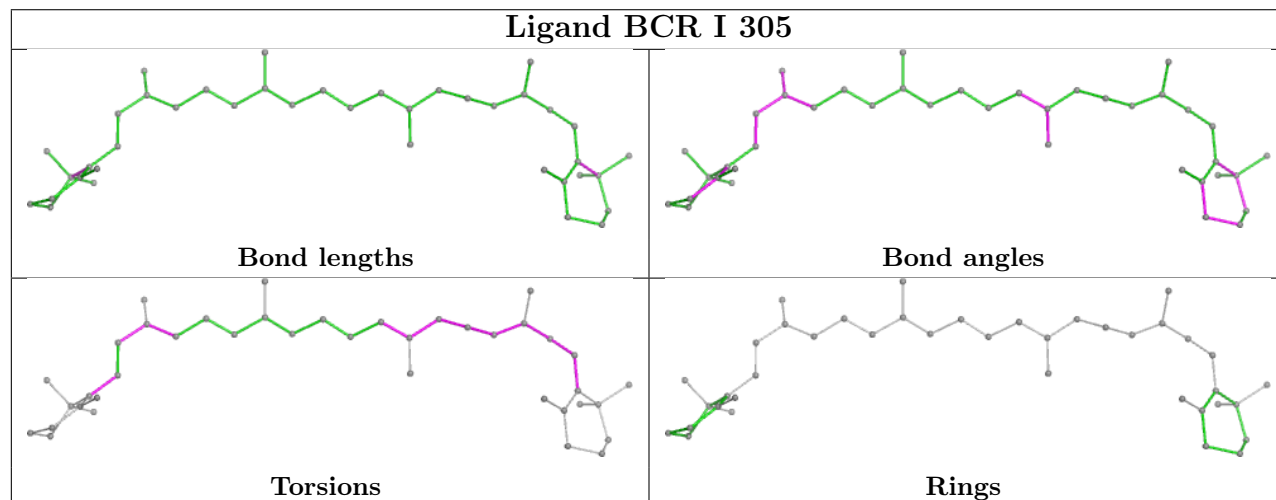
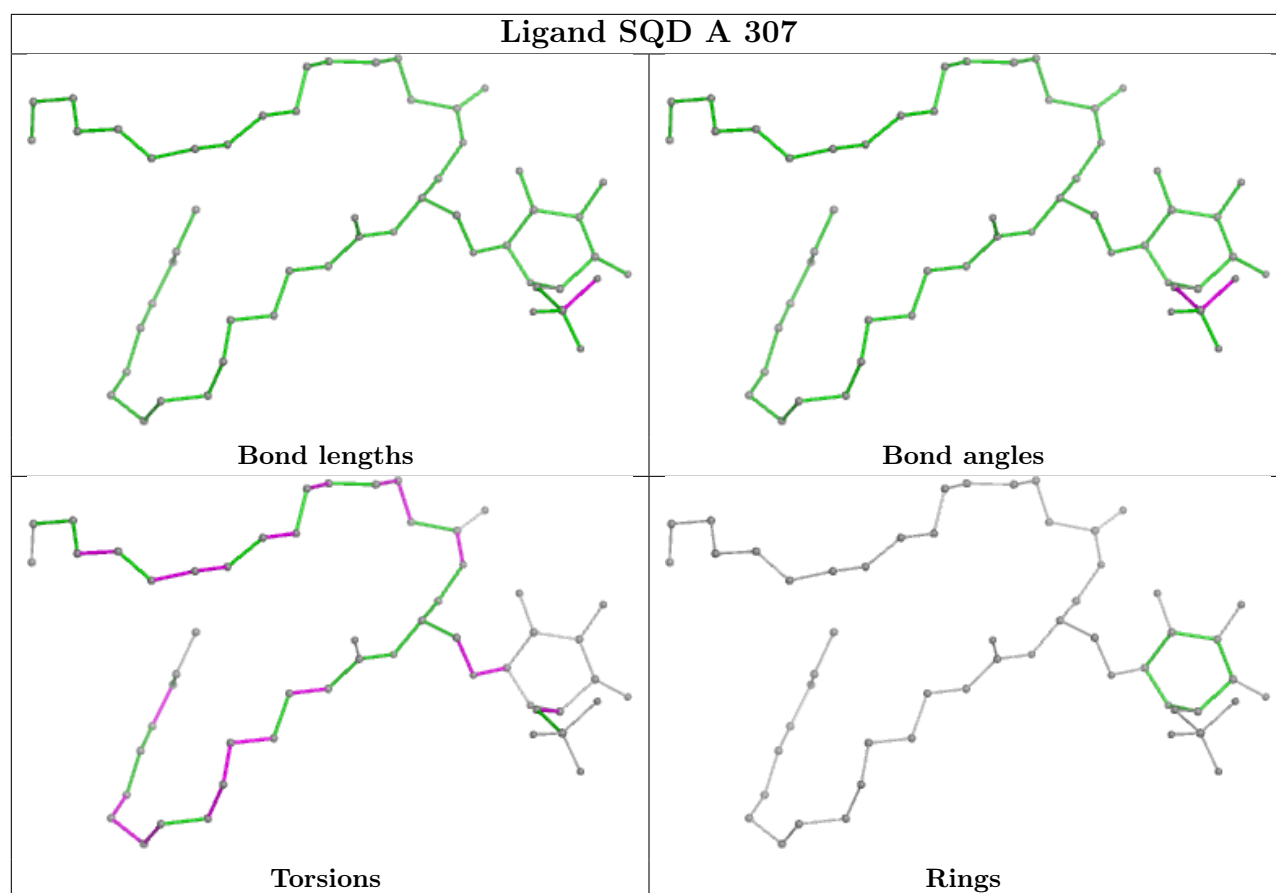
Torsions

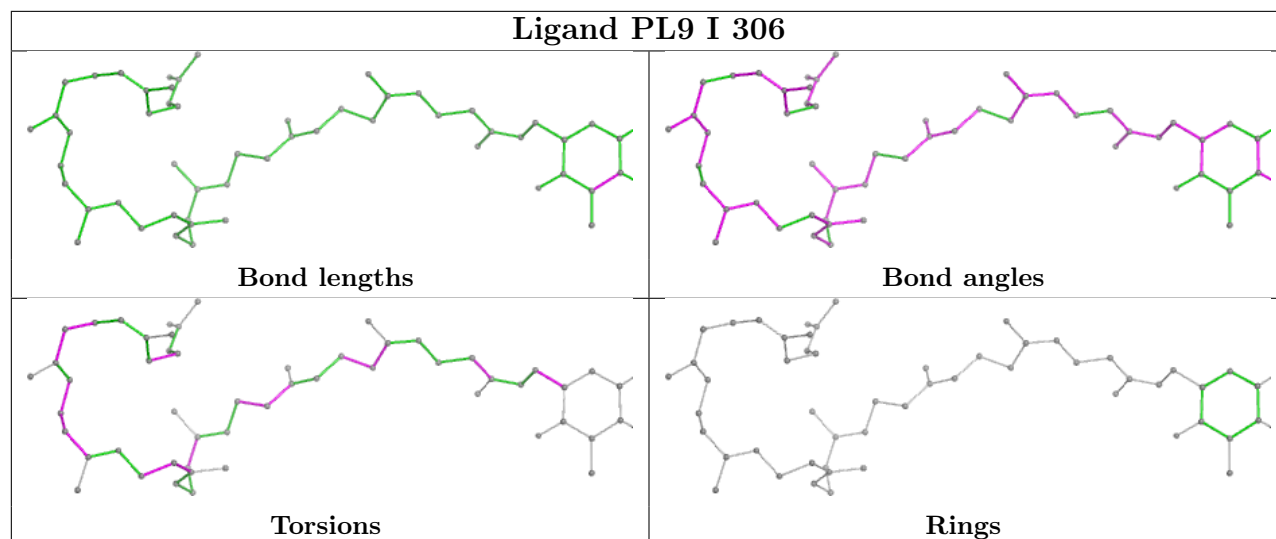
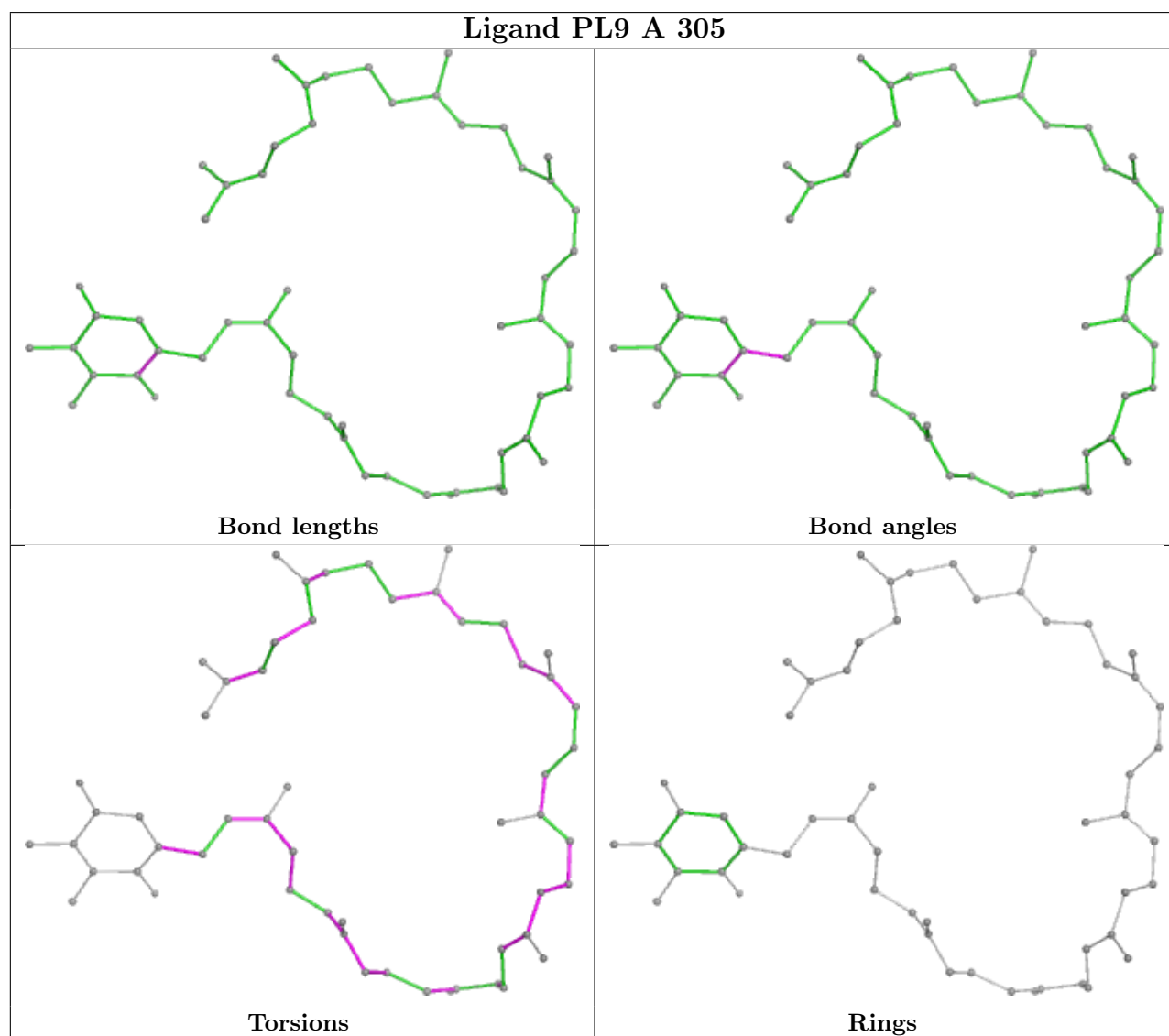


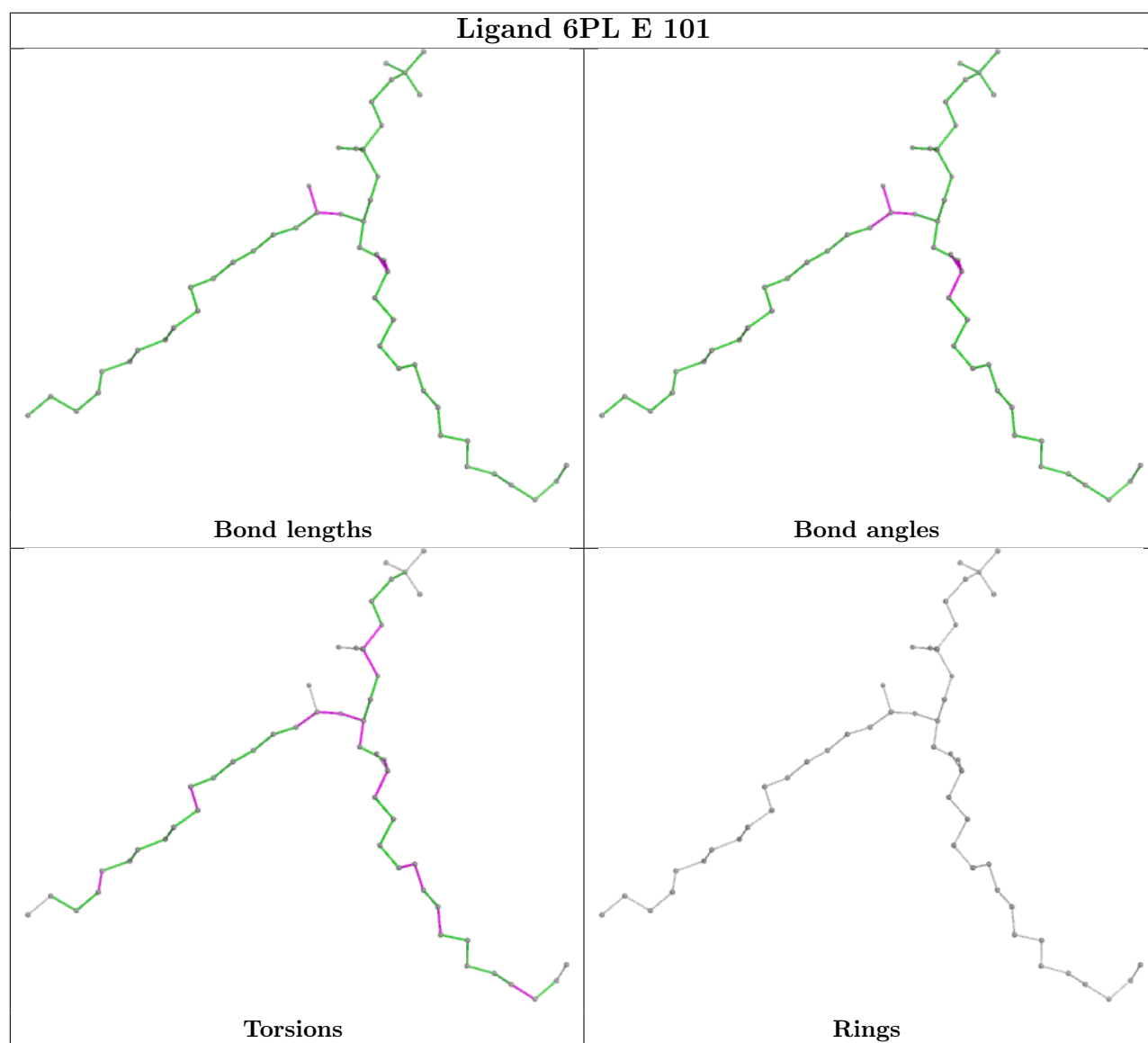
Rings

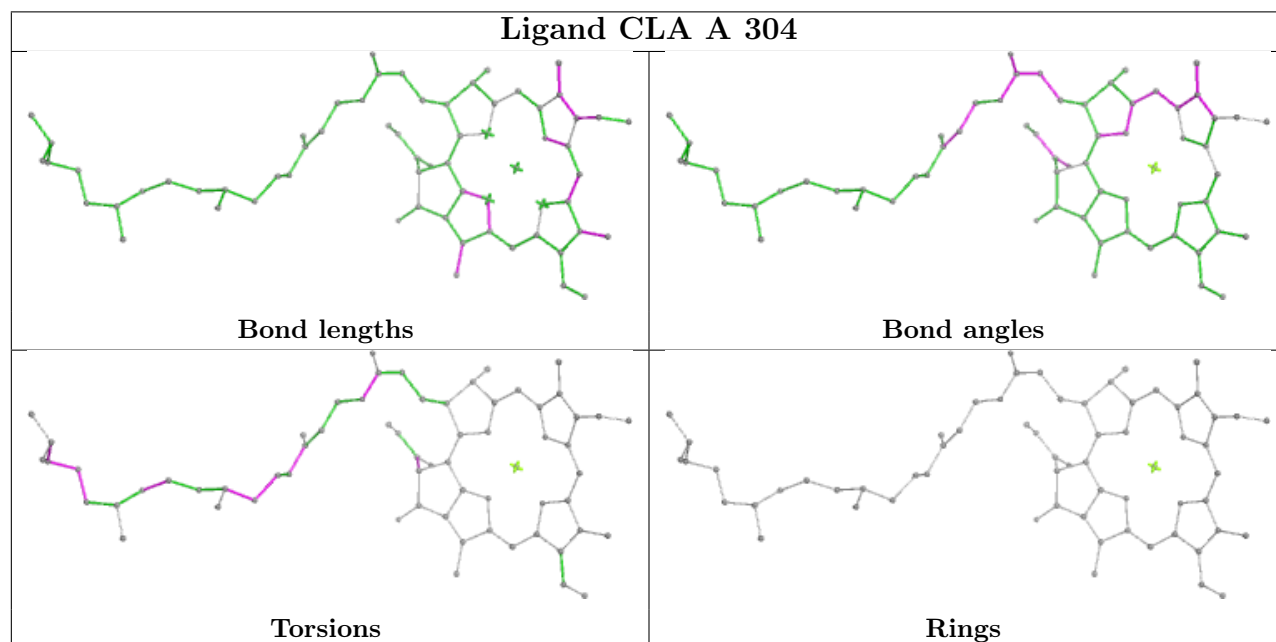
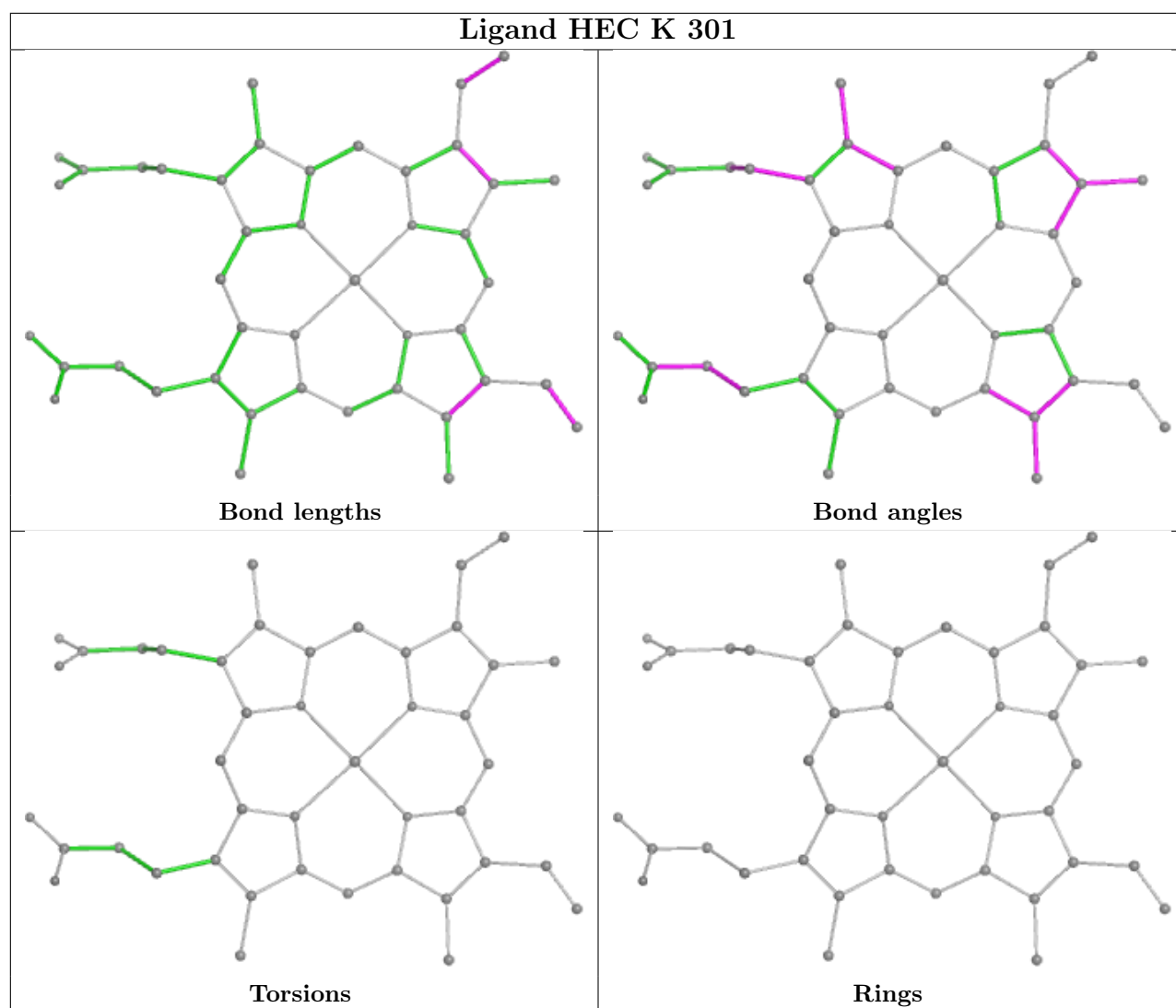


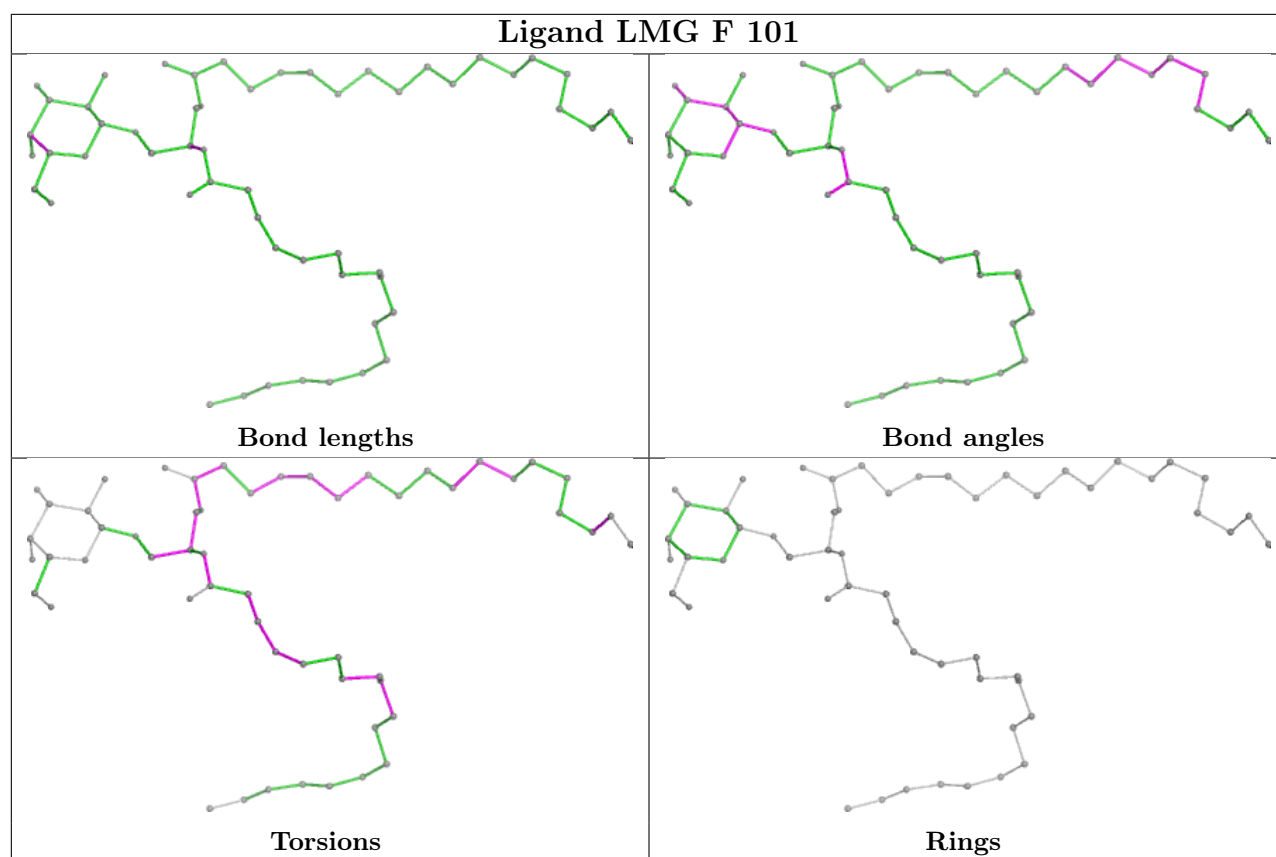


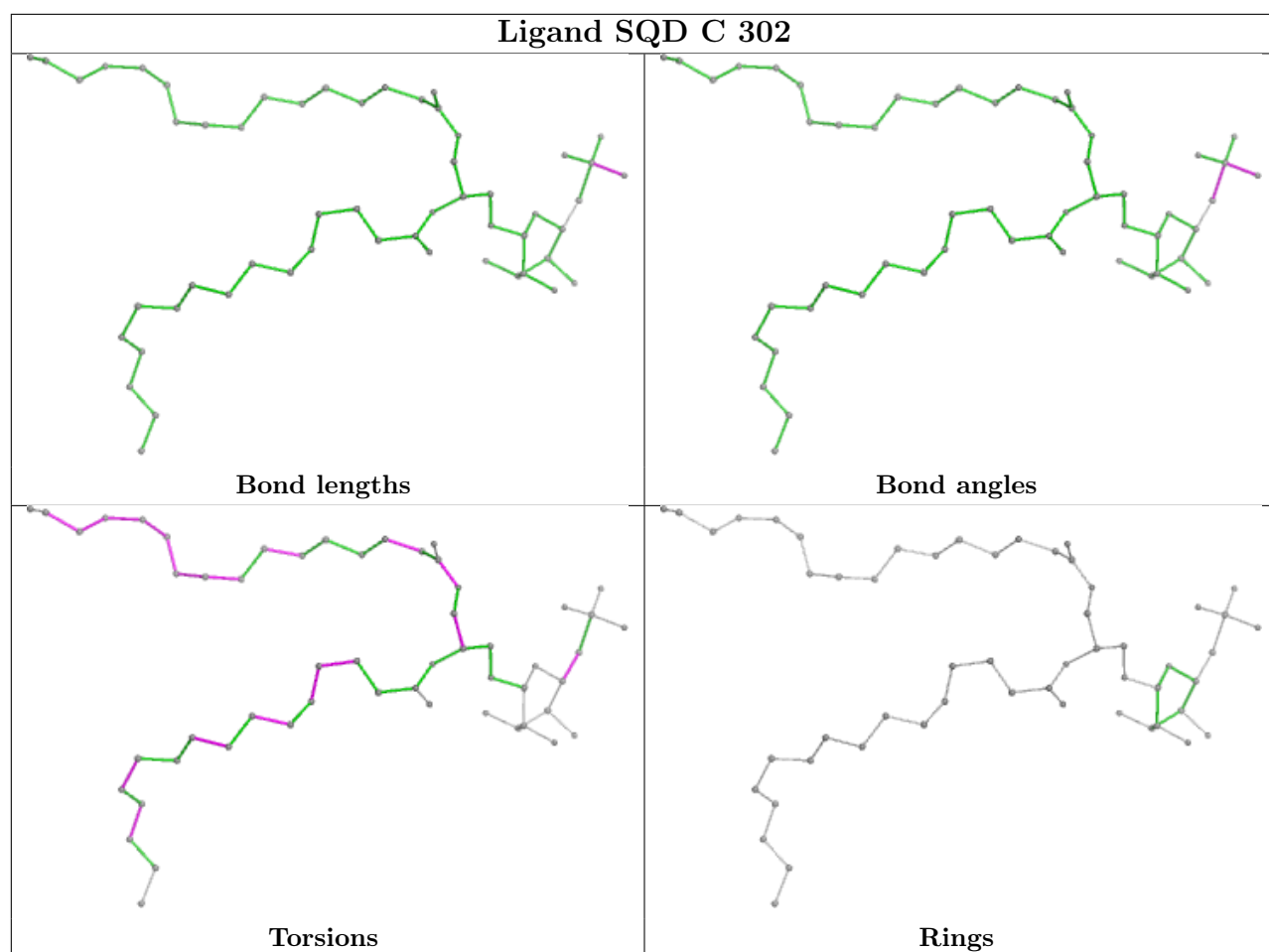


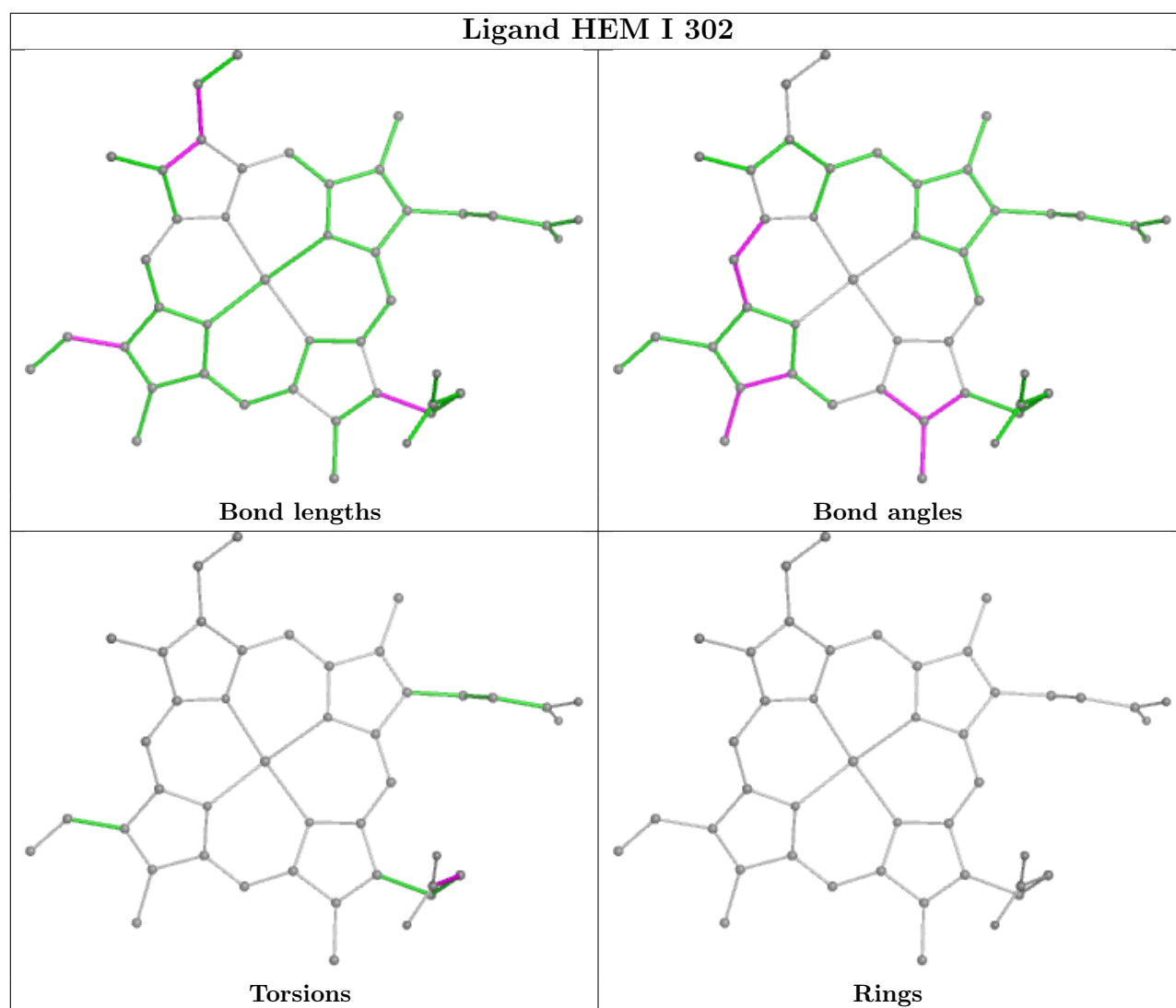
Ligand PL9 I 306**Ligand PL9 A 305**











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.

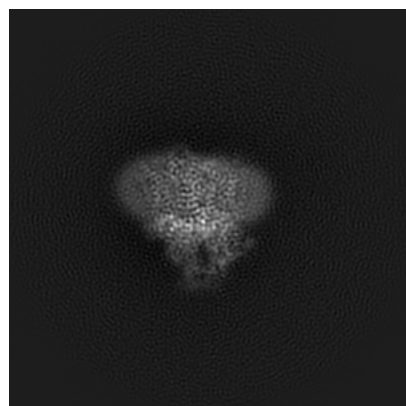
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4981. These allow visual inspection of the internal detail of the map and identification of artifacts.

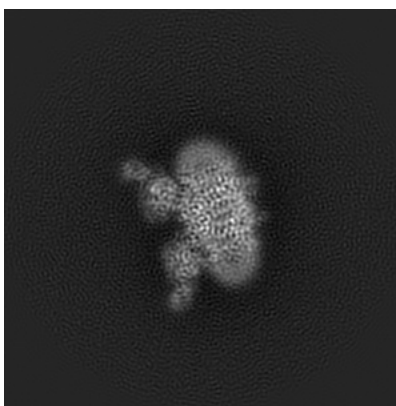
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

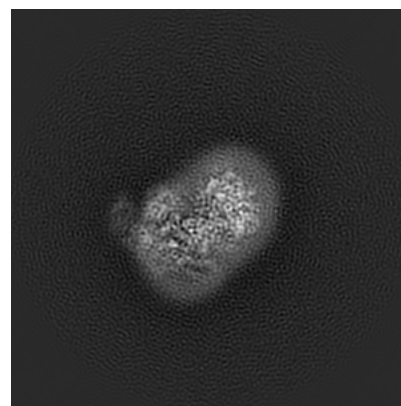
6.1.1 Primary map



X

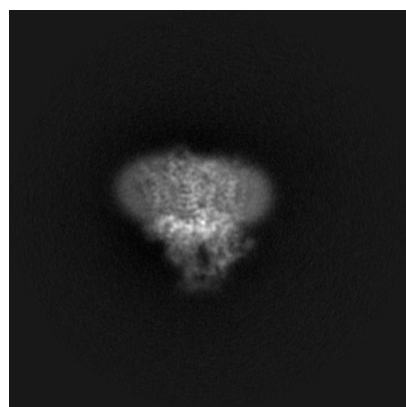


Y

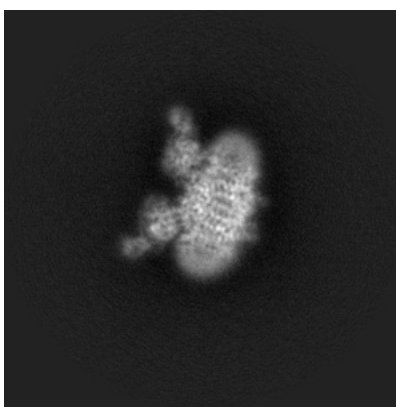


Z

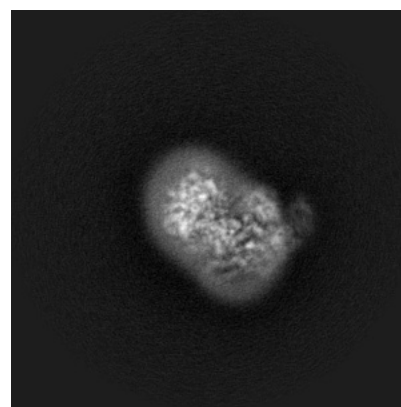
6.1.2 Raw map



X



Y

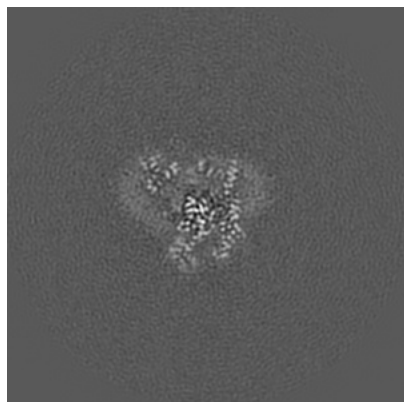


Z

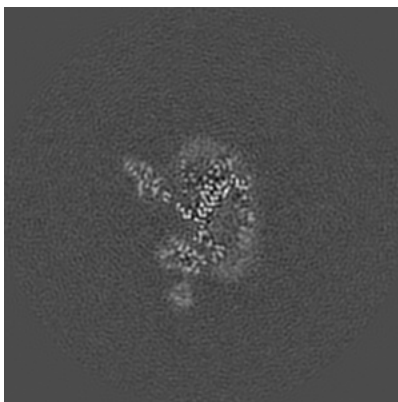
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

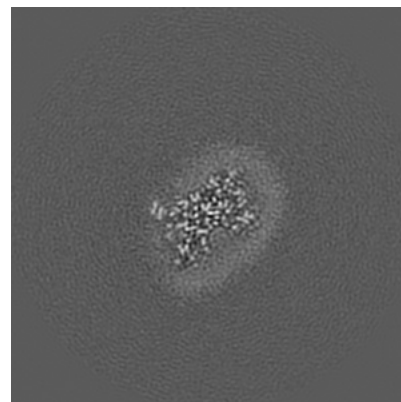
6.2.1 Primary map



X Index: 155

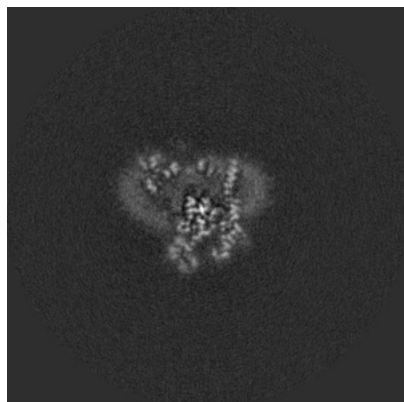


Y Index: 155

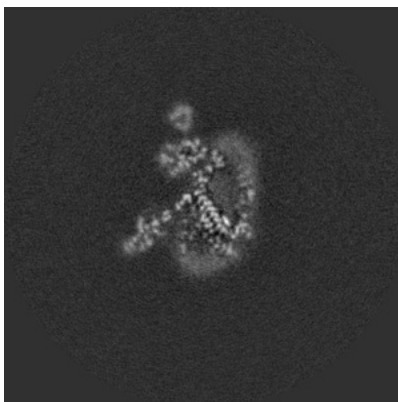


Z Index: 155

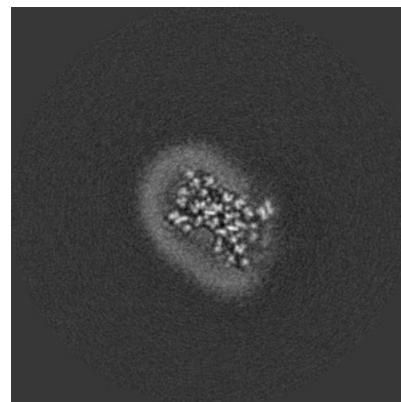
6.2.2 Raw map



X Index: 155



Y Index: 155

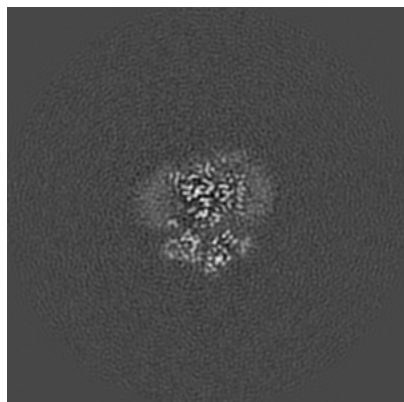


Z Index: 155

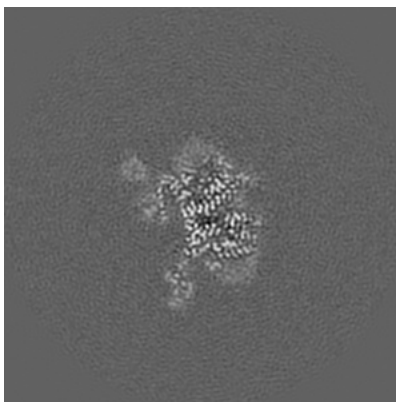
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

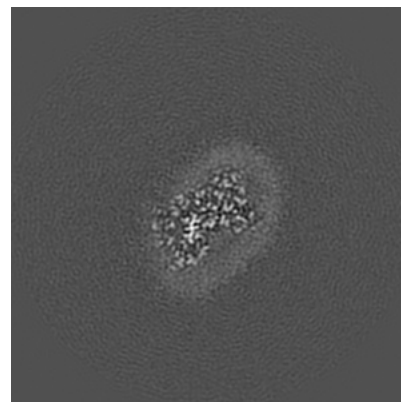
6.3.1 Primary map



X Index: 170

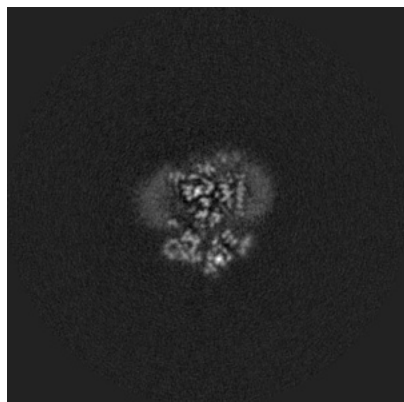


Y Index: 141

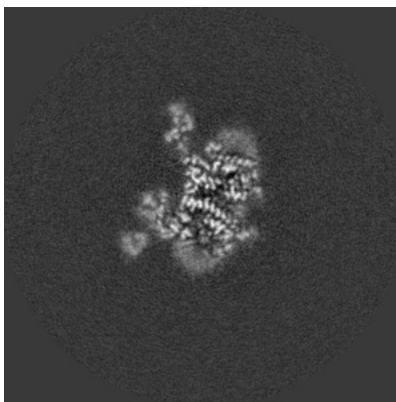


Z Index: 157

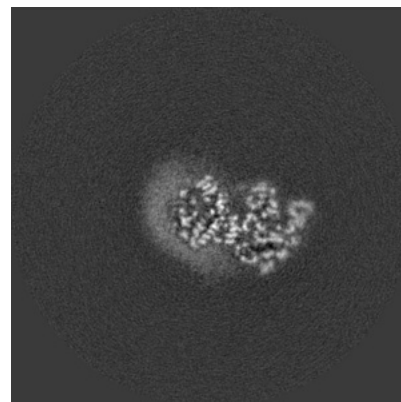
6.3.2 Raw map



X Index: 140



Y Index: 141

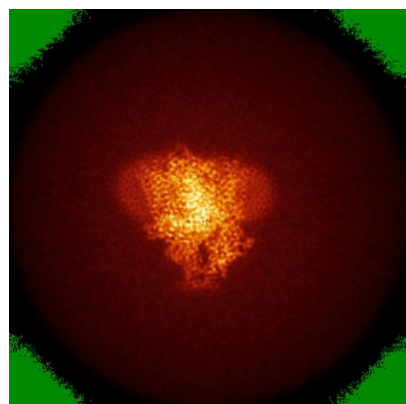


Z Index: 142

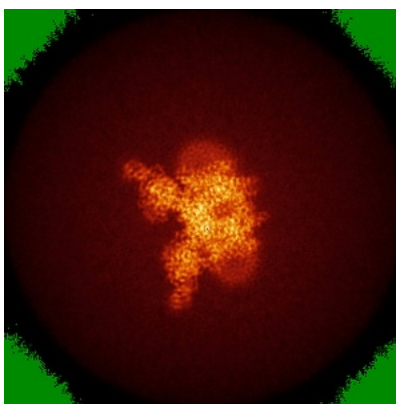
The images above show the largest variance slices of the map in three orthogonal directions.

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

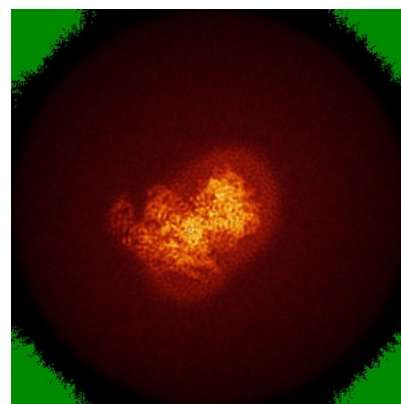
6.4.1 Primary map



X



Y

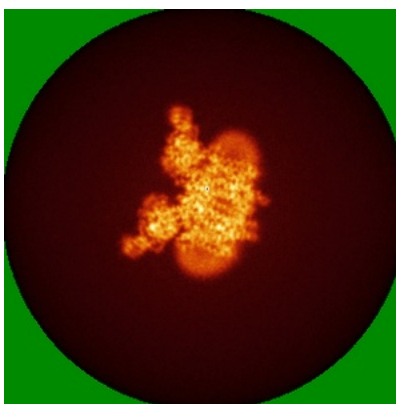


Z

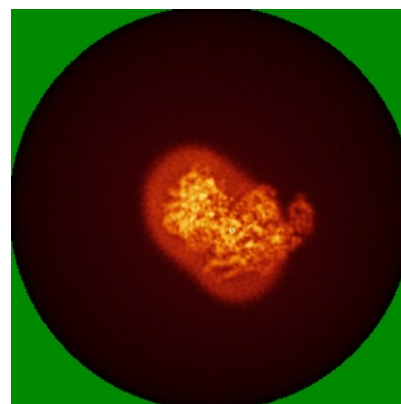
6.4.2 Raw map



X



Y



Z

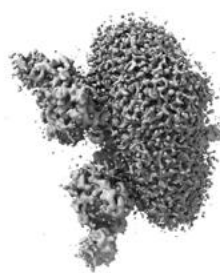
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



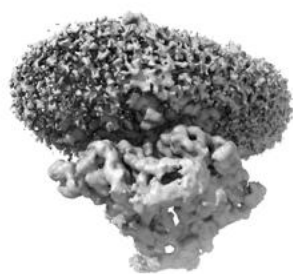
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0144. 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



X



Y



Z

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

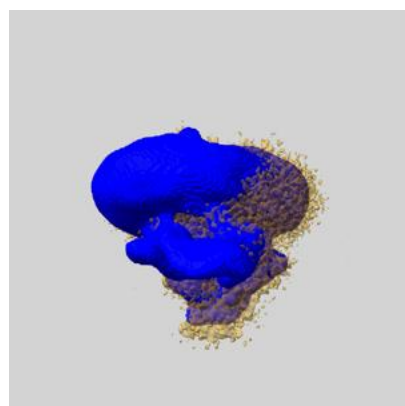
6.6 Mask visualisation [i](#)

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

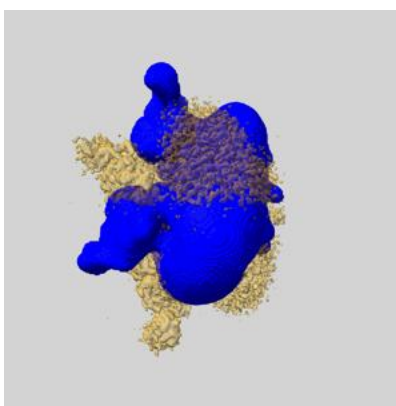
A mask typically either:

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

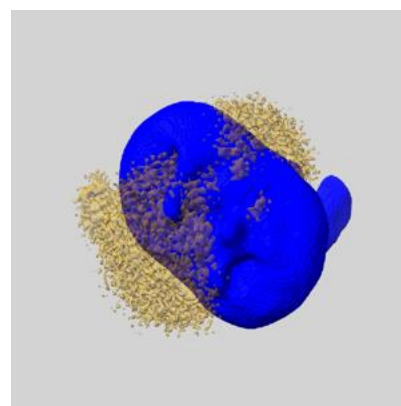
6.6.1 emd_4981_msk_1.map [i](#)



X



Y

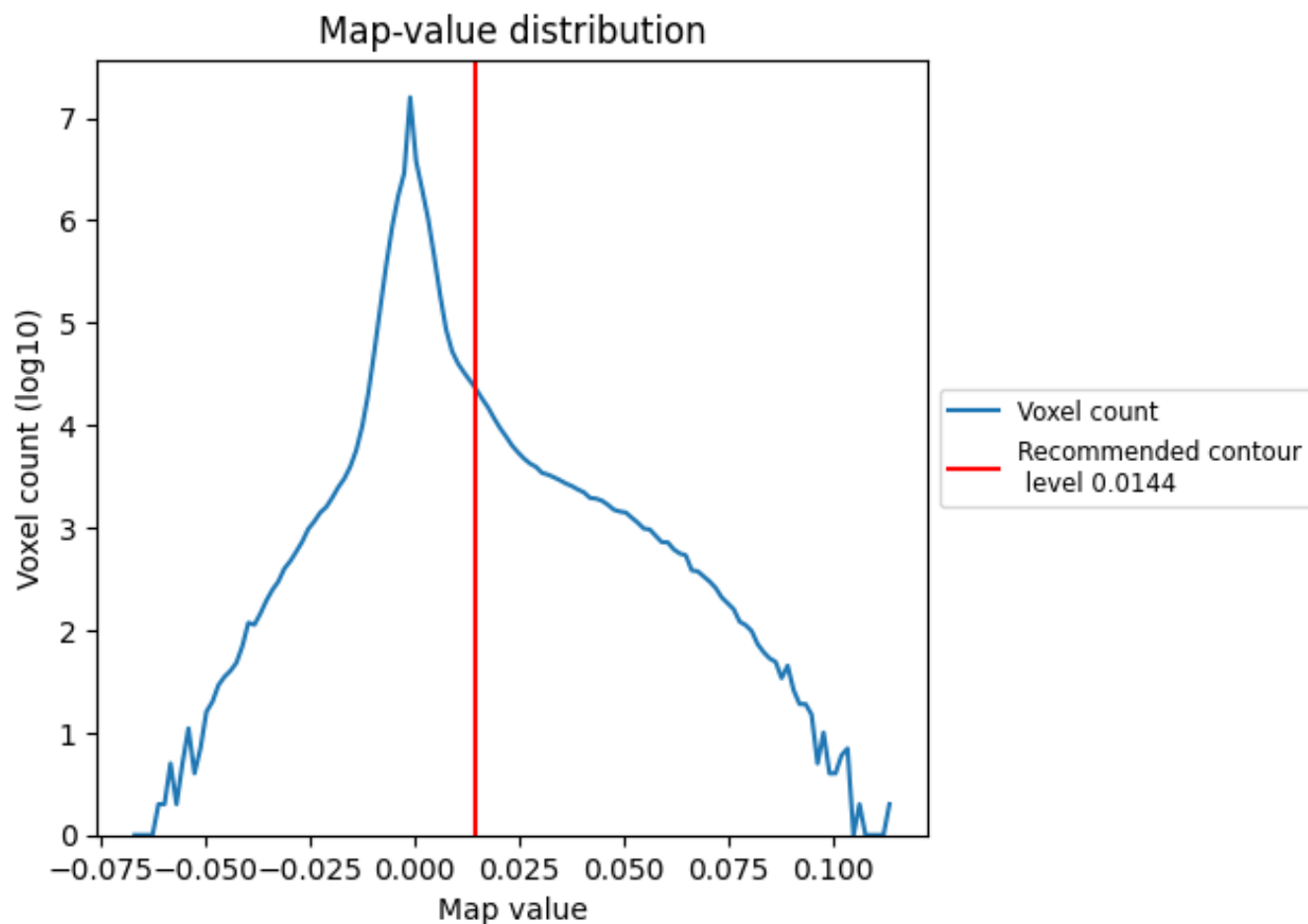


Z

7 Map analysis [i](#)

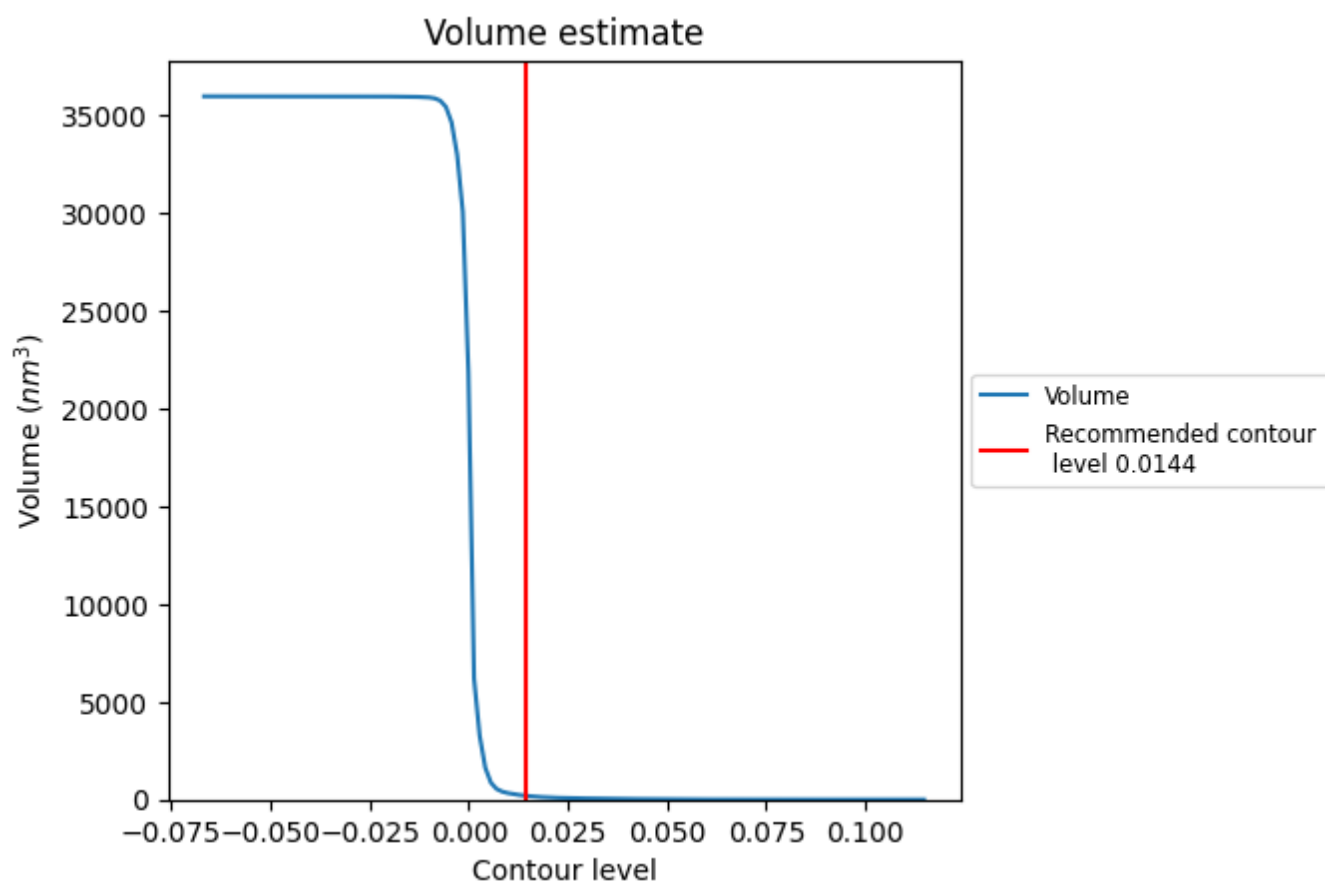
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

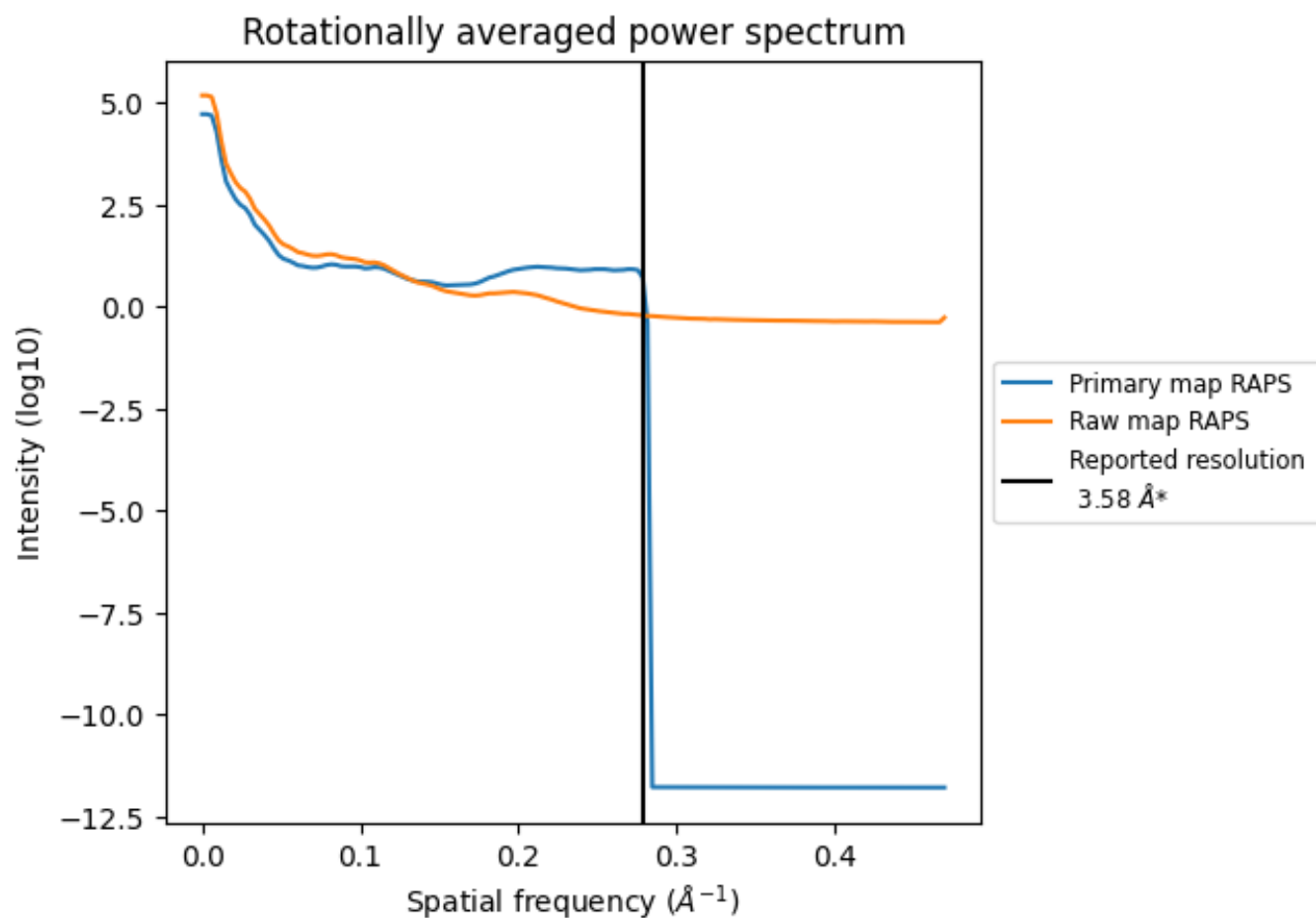
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm^3 ; this corresponds to an approximate mass of 176 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 ⓘ

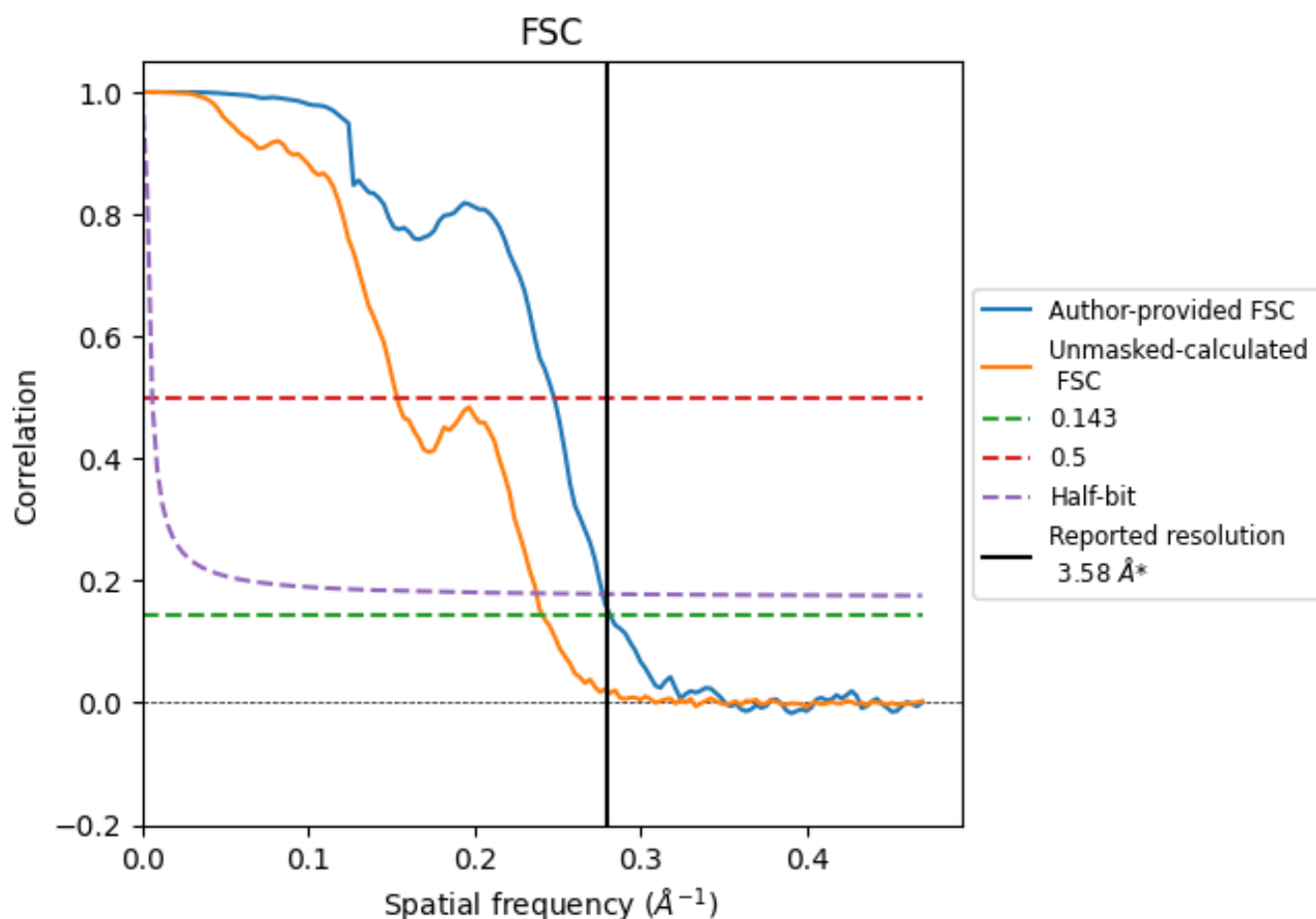


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.279 \AA^{-1}

8.2 Resolution estimates [i](#)

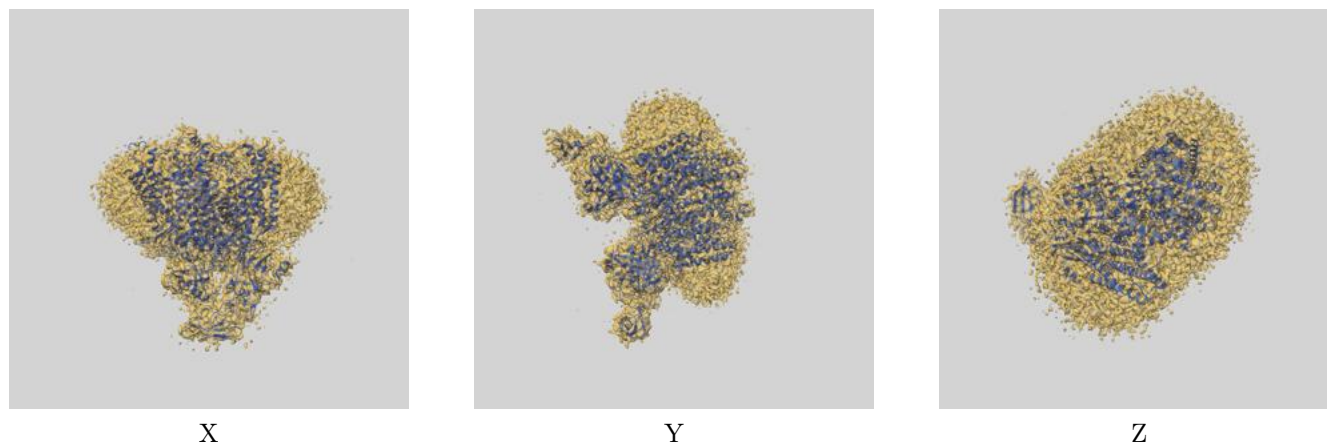
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.55	4.04	3.61
Unmasked-calculated*	4.15	6.52	4.22

*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 4.15 differs from the reported value 3.58 by more than 10 %

9 Map-model fit [i](#)

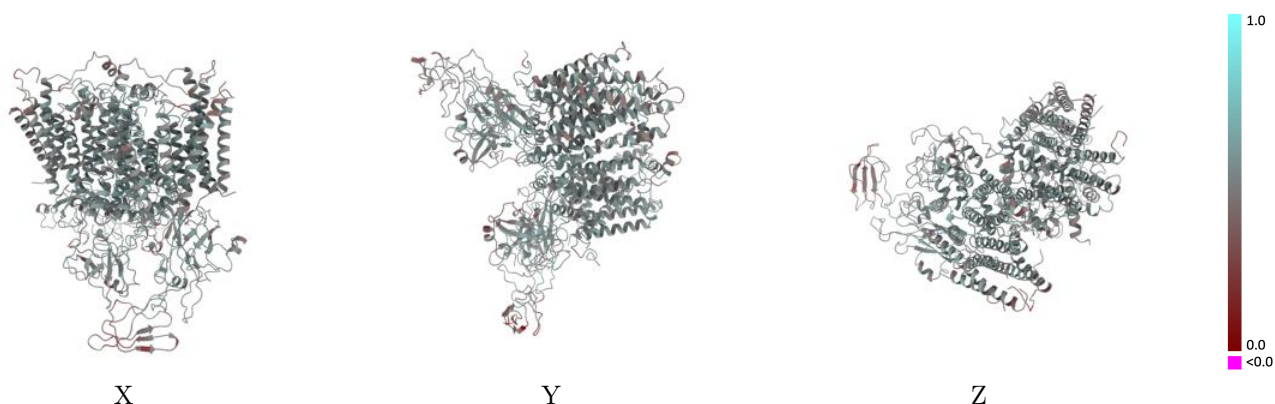
This section contains information regarding the fit between EMDB map EMD-4981 and PDB model 6RQF. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



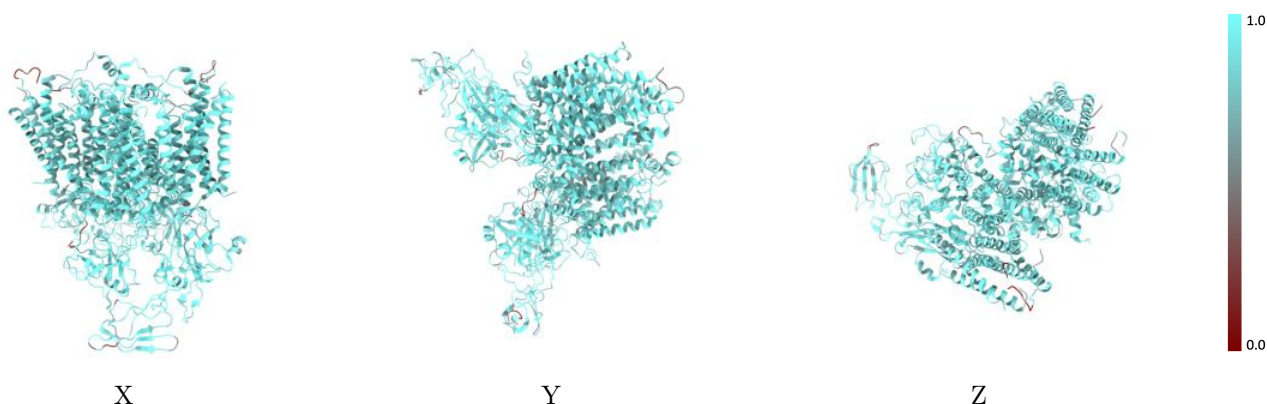
The images above show the 3D surface view of the map at the recommended contour level 0.0144 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



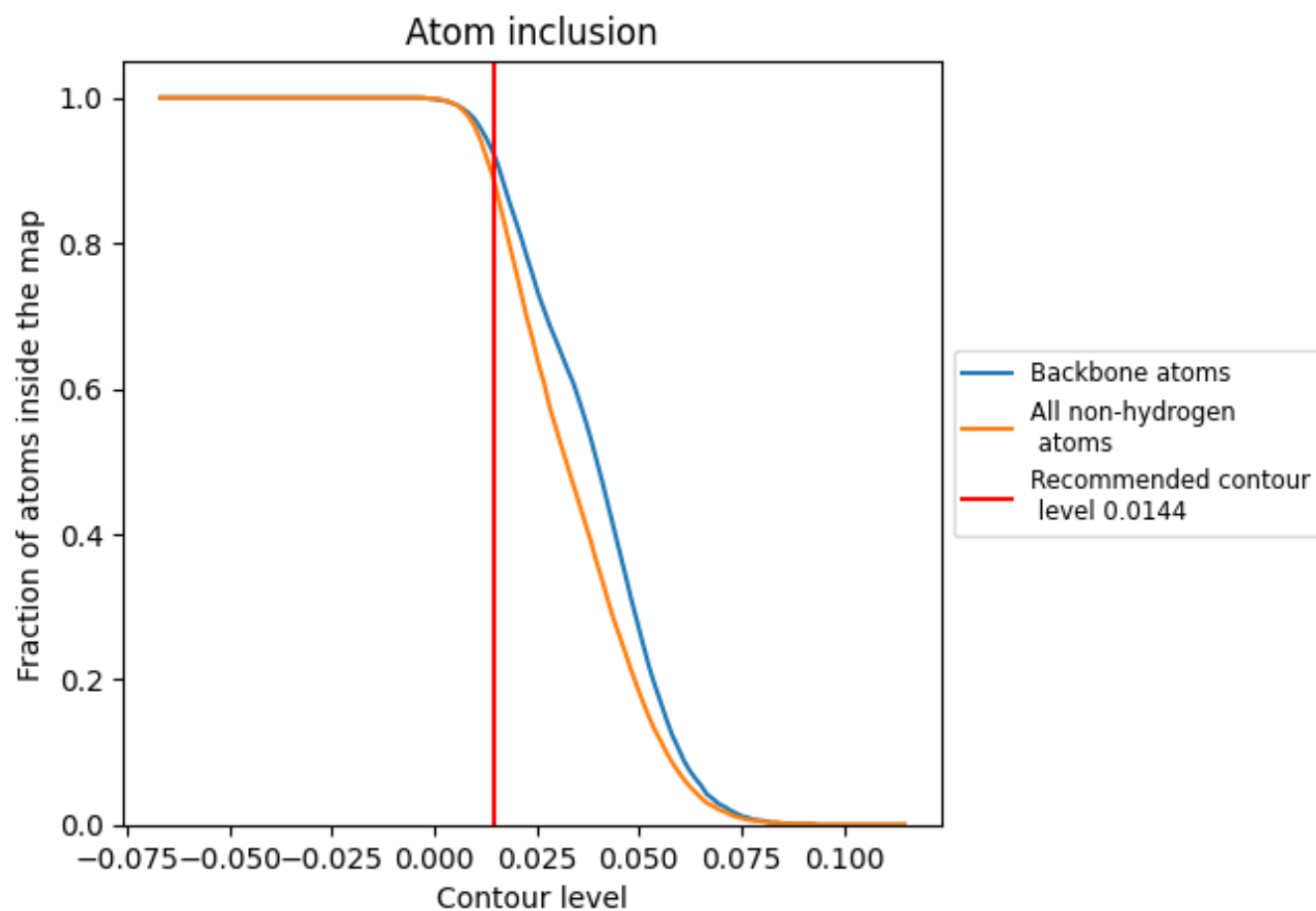
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0144).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.0144) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.5110
A	 0.9220	 0.5400
B	 0.9070	 0.5240
C	 0.8890	 0.4920
D	 0.8690	 0.4830
E	 0.8730	 0.4910
F	 0.8730	 0.4990
G	 0.8820	 0.4900
H	 0.9150	 0.5330
I	 0.9170	 0.5360
J	 0.8870	 0.5290
K	 0.8810	 0.4980
L	 0.8570	 0.4920
M	 0.8420	 0.4810
N	 0.8490	 0.5030
O	 0.8610	 0.5050
P	 0.9180	 0.5210

