



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 11:43 AM UTC

PDB ID : 7QRM / pdb_00007qrm
EMDB ID : EMD-14123
Title : Cryo-EM structure of catalytically active *Spinacia oleracea* cytochrome b6f in complex with endogenous plastoquinones at 2.7 Å resolution
Authors : Sarewicz, M.; Szwalec, M.; Indyka, P.; Rawski, M.; Pintscher, S.; Pietras, R.; Mielecki, B.; Jaciuk, M.; Glatt, S.; Osyczka, A.
Deposited on : 2022-01-11
Resolution : 2.70 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

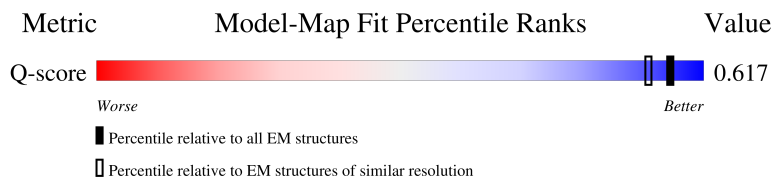
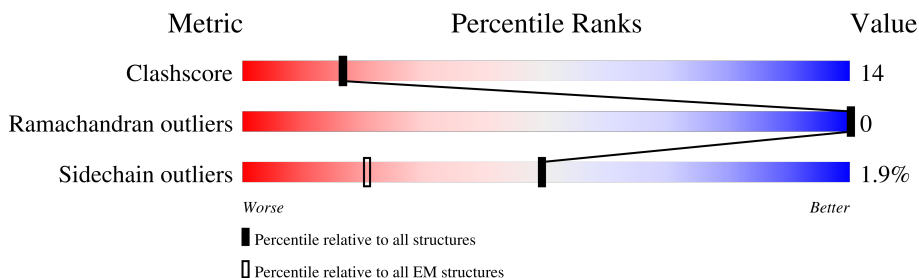
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	
1	I	215	
2	B	160	
2	J	160	

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Mol	Chain	Length	Quality of chain
3	C	320	
3	K	320	
4	D	230	
4	L	230	
5	E	31	
5	M	31	
6	F	36	
6	N	36	
7	G	37	
7	O	37	
8	H	29	
8	P	29	

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
11	CLA	A	304	X	-	-	-
11	CLA	J	201	X	-	-	-
12	PL9	J	202	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 17012 atoms, of which 676 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	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
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
3	C	285	Total	C	N	O	S	0	0
			2209	1418	375	410	6		
3	K	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	D	167	Total	C	N	O	S	0	0
			1263	809	213	234	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	36	Total	C	N	O	S	0	0
			264	171	44	48	1		
6	N	36	Total	C	N	O	S	0	0
			264	171	44	48	1		

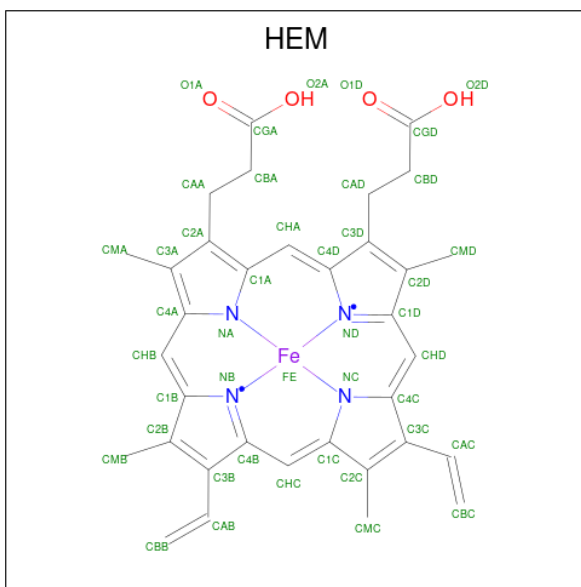
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	31	Total	C	N	O	S	0	0
			249	172	38	38	1		
7	O	31	Total	C	N	O	S	0	0
			249	172	38	38	1		

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

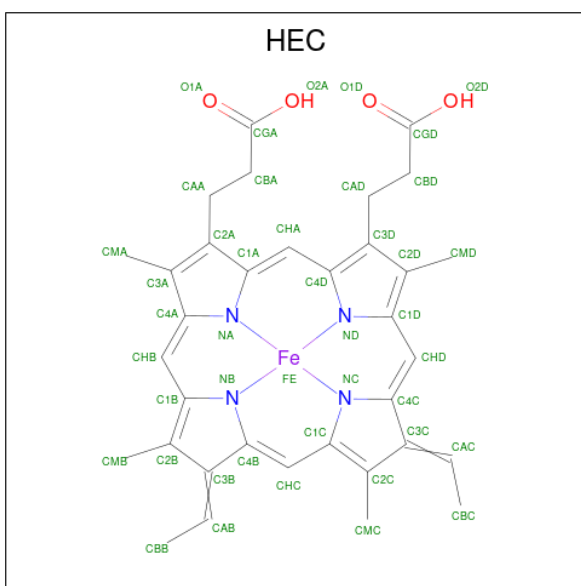
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	29	Total	C	N	O	S	0	0
			222	150	34	36	2		
8	P	29	Total	C	N	O	S	0	0
			223	150	34	37	2		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



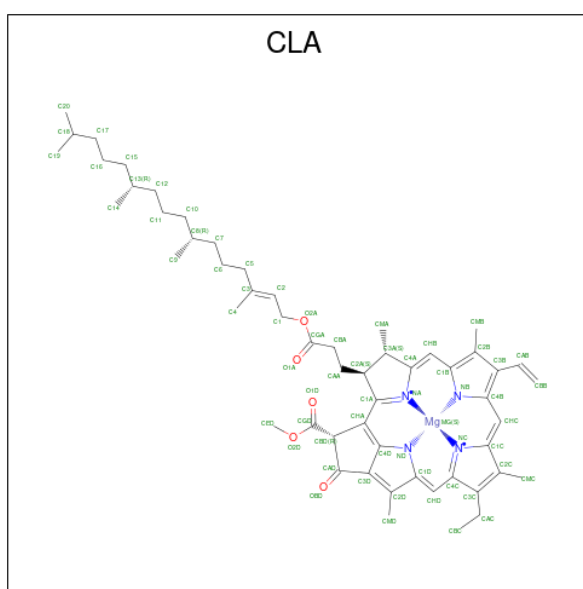
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



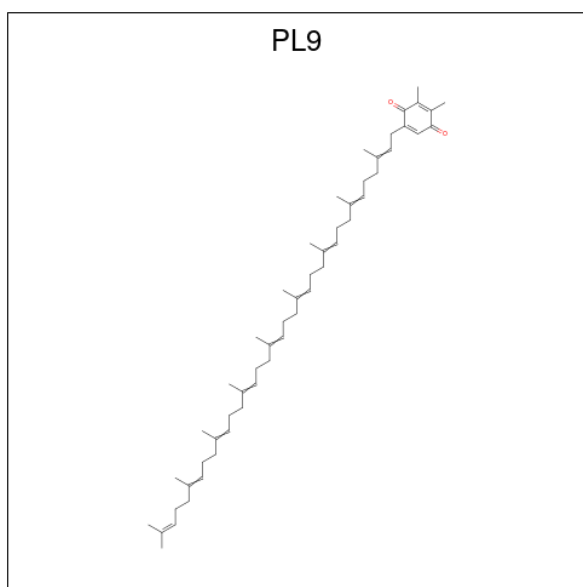
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



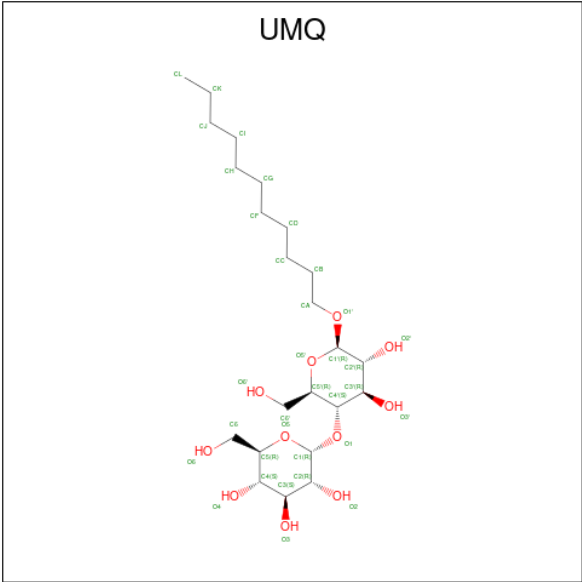
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 12 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



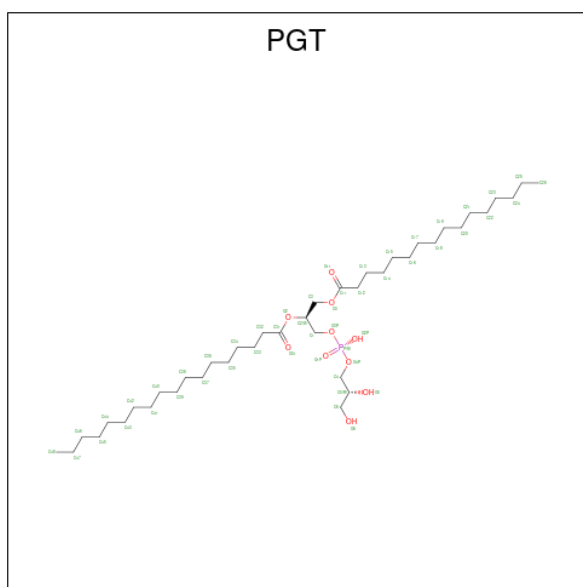
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O		0
			55	53	2		
12	B	1	Total	C	O		0
			55	53	2		
12	D	1	Total	C	O		0
			55	53	2		
12	I	1	Total	C	H	O	0
			135	53	80	2	
12	I	1	Total	C	O		0
			55	53	2		
12	J	1	Total	C	O		0
			55	53	2		
12	J	1	Total	C	O		0
			55	53	2		

- Molecule 13 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



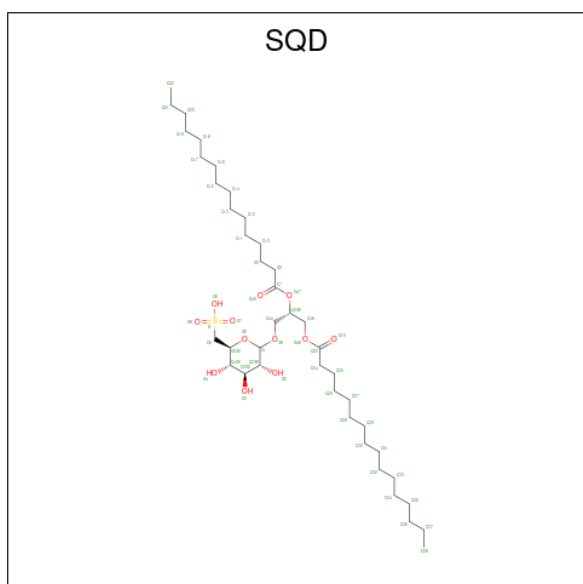
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	H	O	0
			78	23	44	11	
13	A	1	Total	C	H	O	0
			78	23	44	11	
13	B	1	Total	C	H	O	0
			78	23	44	11	
13	B	1	Total	C	H	O	0
			78	23	44	11	
13	H	1	Total	C	H	O	0
			78	23	44	11	
13	I	1	Total	C	H	O	0
			78	23	44	11	
13	I	1	Total	C	H	O	0
			78	23	44	11	
13	J	1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

- Molecule 14 is (1S)-2-{{{[(2R)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(palmitoyloxy)methyl]ethyl stearate (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



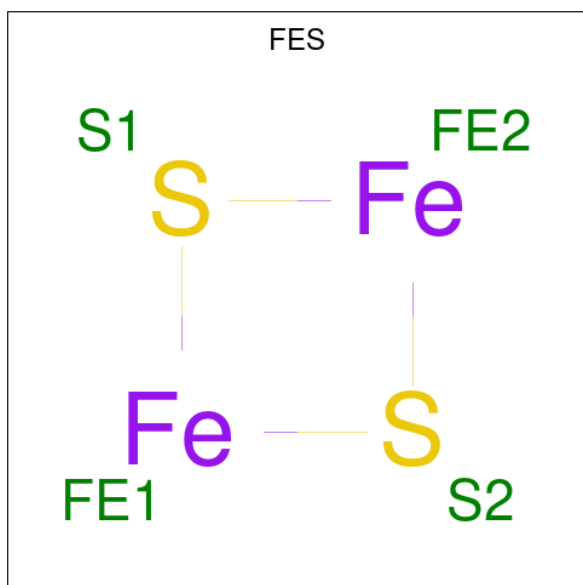
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	H	O	P	0
			129	40	78	10	1	
14	D	1	Total	C	O	P		0
			51	40	10	1		
14	I	1	Total	C	H	O	P	0
			129	40	78	10	1	
14	L	1	Total	C	O	P		0
			51	40	10	1		

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



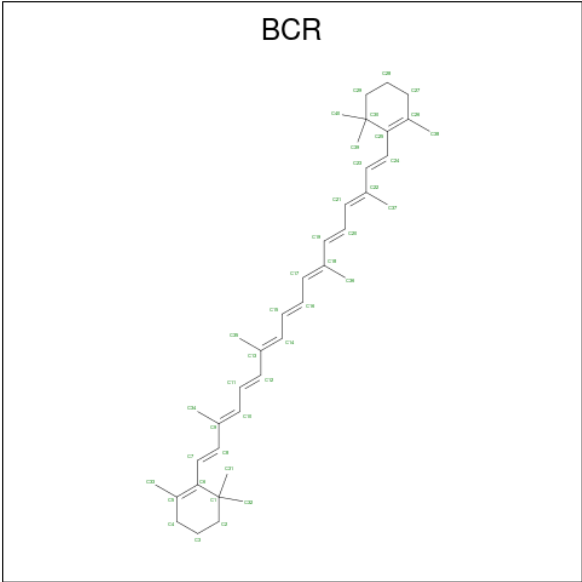
Mol	Chain	Residues	Atoms				AltConf
15	D	1	Total	C	O	S	0
			54	41	12	1	
15	K	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$) (labeled as "Ligand of Interest" by depositor).

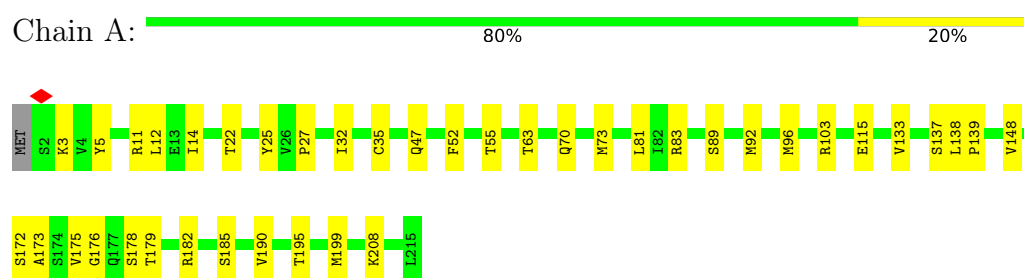


Mol	Chain	Residues	Atoms		AltConf
17	F	1	Total	C	0
			40	40	
17	P	1	Total	C	0
			40	40	

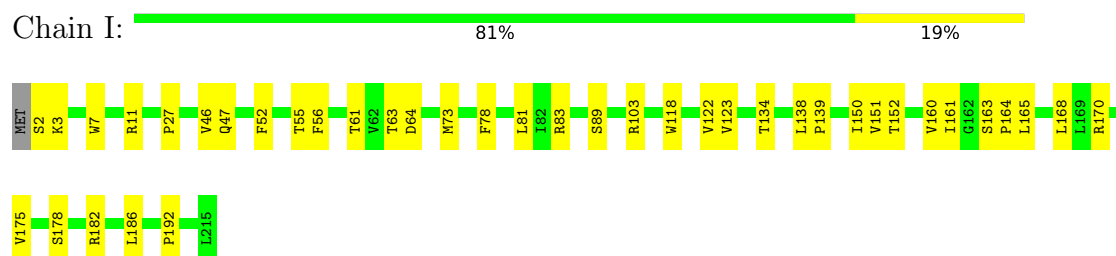
3 Residue-property plots

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.

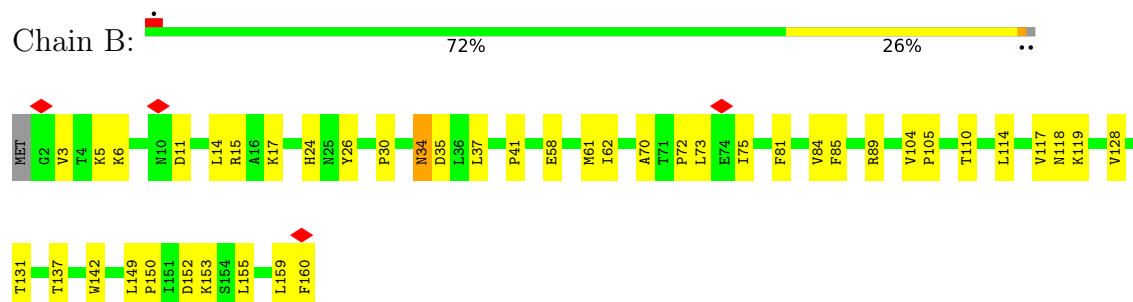
• Molecule 1: Cytochrome b6



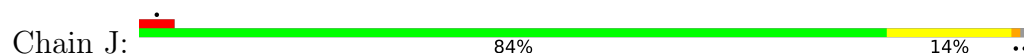
• Molecule 1: Cytochrome b6

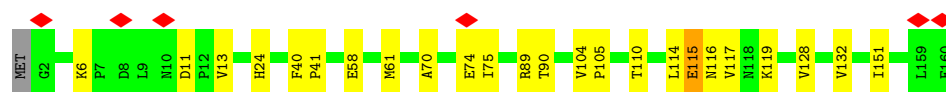


• Molecule 2: Cytochrome b6-f complex subunit 4

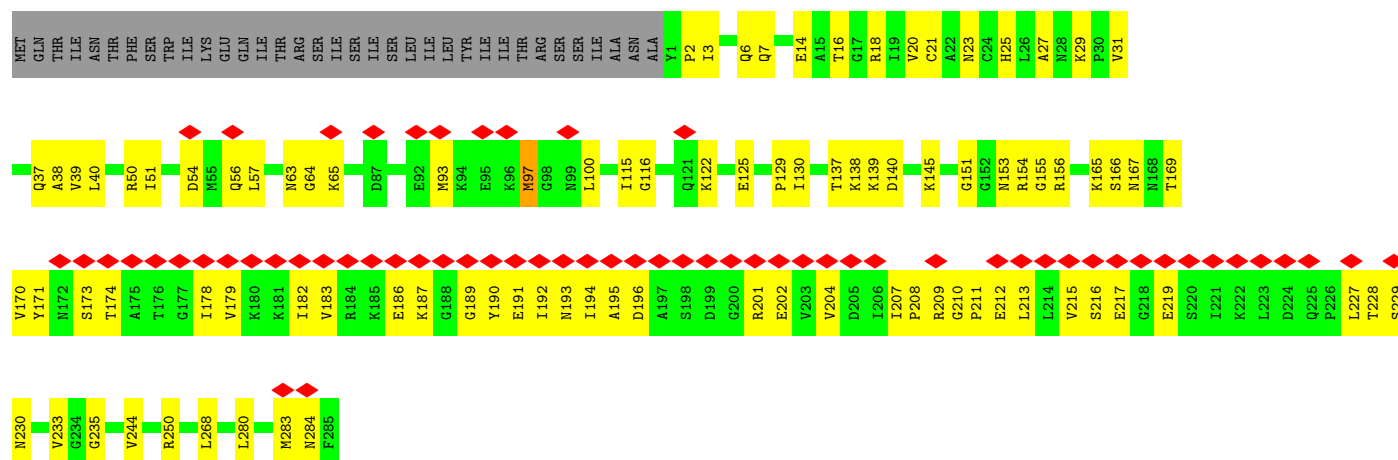


• Molecule 2: Cytochrome b6-f complex subunit 4

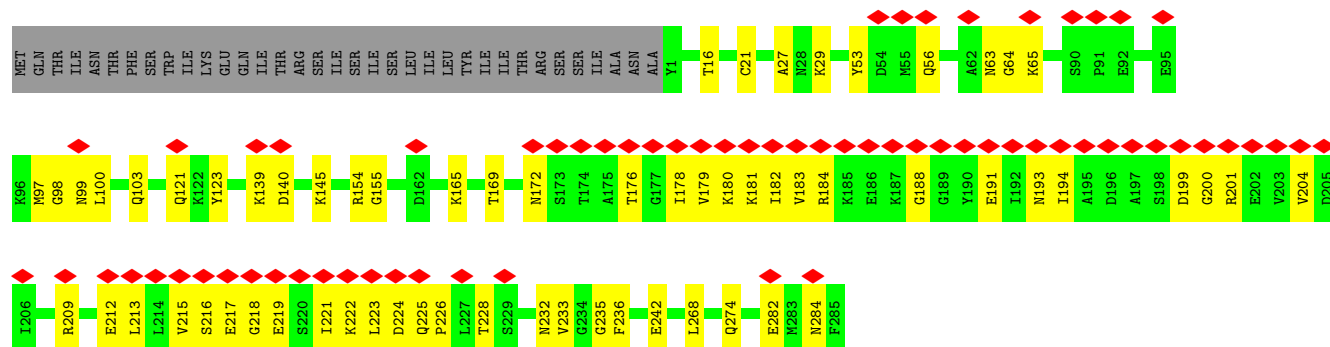




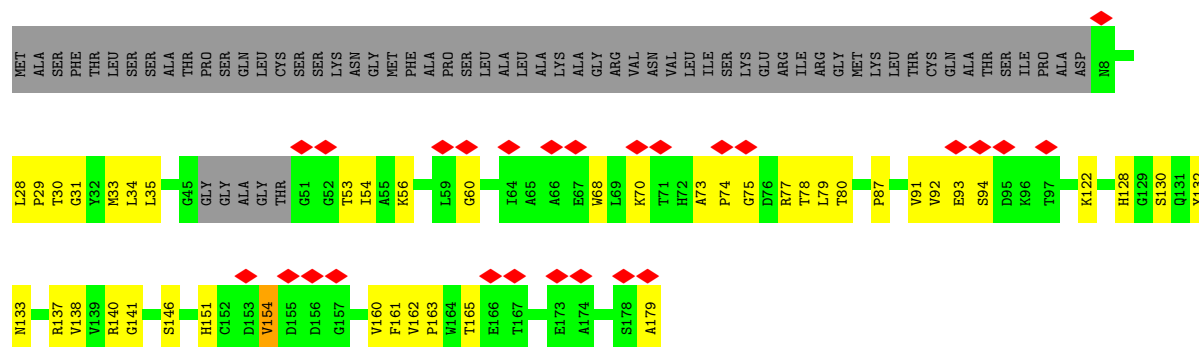
• Molecule 3: Cytochrome f



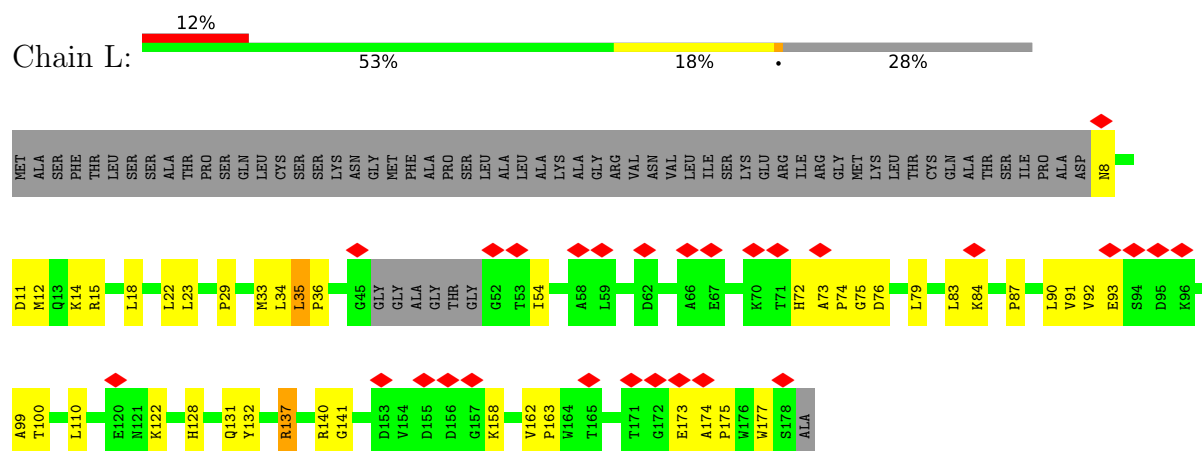
• Molecule 3: Cytochrome f



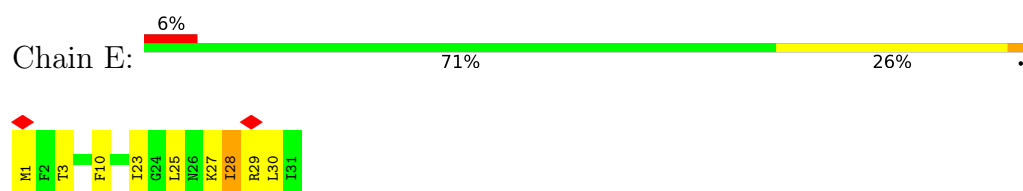
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic



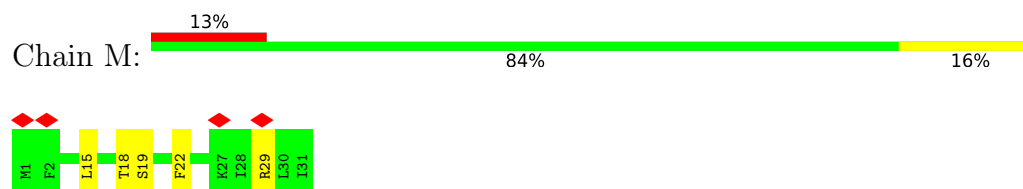
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic



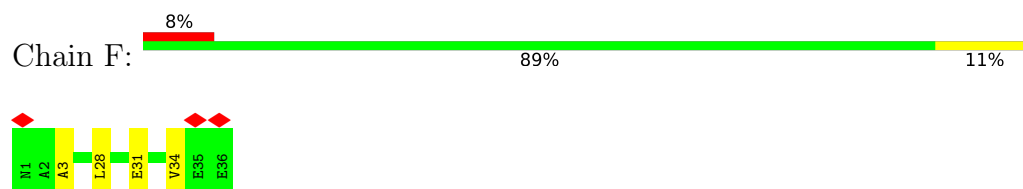
- Molecule 5: Cytochrome b6-f complex subunit 6



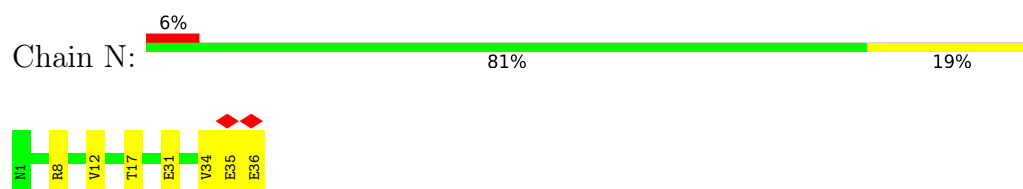
- Molecule 5: Cytochrome b6-f complex subunit 6



- Molecule 6: Cytochrome b6-f complex subunit 7

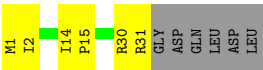


- Molecule 6: Cytochrome b6-f complex subunit 7



- Molecule 7: Cytochrome b6-f complex subunit 5

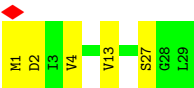
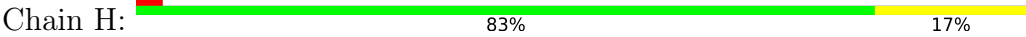




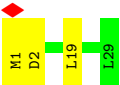
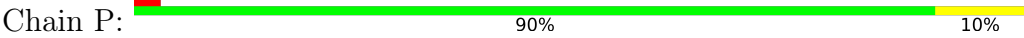
● Molecule 7: Cytochrome b6-f complex subunit 5



● Molecule 8: Cytochrome b6-f complex subunit 8



● Molecule 8: Cytochrome b6-f complex subunit 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97597	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; 2 iteration in global CTF refinement, with an anisotropic mag. 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	2.202	Depositor
Minimum map value	-0.958	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: UMQ, SQD, BCR, PGT, CLA, HEM, FES, HEC, PL9

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	0.22	0/1747	0.47	1/2382 (0.0%)
1	I	0.21	0/1747	0.44	0/2382
2	B	0.23	0/1262	0.53	3/1733 (0.2%)
2	J	0.18	0/1263	0.35	0/1733
3	C	0.18	0/2256	0.37	0/3058
3	K	0.16	0/2256	0.36	0/3058
4	D	0.16	0/1297	0.43	0/1774
4	L	0.15	0/1288	0.38	0/1762
5	E	0.21	0/247	0.49	0/333
5	M	0.14	0/247	0.30	0/333
6	F	0.23	0/265	0.41	0/359
6	N	0.19	0/265	0.35	0/359
7	G	0.16	0/254	0.35	0/344
7	O	0.17	0/254	0.38	0/344
8	H	0.15	0/227	0.36	0/309
8	P	0.16	0/228	0.30	0/309
All	All	0.19	0/15103	0.41	4/20572 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LEU	N-CA-C	6.64	121.45	112.88
2	B	34	ASN	N-CA-C	5.84	118.15	111.02
2	B	11	ASP	CA-C-N	5.38	125.20	119.28
2	B	11	ASP	C-N-CA	5.38	125.20	119.28

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	1725	35	0
1	I	1697	0	1724	43	0
2	B	1225	0	1276	38	0
2	J	1226	0	1276	27	0
3	C	2209	0	2253	92	0
3	K	2209	0	2253	66	0
4	D	1263	0	1235	39	0
4	L	1254	0	1227	38	0
5	E	243	0	268	5	0
5	M	243	0	268	6	0
6	F	264	0	282	6	0
6	N	264	0	282	6	0
7	G	249	0	273	7	0
7	O	249	0	273	7	0
8	H	222	0	234	8	0
8	P	223	0	234	2	0
9	A	86	0	60	10	0
9	I	86	0	60	9	0
10	A	43	0	32	5	0
10	C	43	0	29	4	0
10	I	43	0	31	3	0
10	K	43	0	31	4	0
11	A	65	0	72	6	0
11	J	65	0	72	12	0
12	A	55	0	80	6	0
12	B	55	0	80	13	0
12	D	55	0	80	4	0
12	I	110	80	160	16	0
12	J	110	0	160	37	0
13	A	68	88	88	1	0
13	B	68	88	88	1	0
13	H	34	44	44	1	0
13	I	68	88	88	0	0
13	J	68	88	88	3	0
13	P	34	44	44	0	0
14	A	51	78	78	1	0
14	D	51	0	78	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	51	78	78	2	0
14	L	51	0	78	3	0
15	D	54	0	77	3	0
15	K	54	0	77	1	0
16	D	4	0	0	1	0
16	L	4	0	0	0	0
17	F	40	0	56	3	0
17	P	40	0	56	2	0
All	All	16336	676	17048	470	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 470 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)
1:A:35:CYS:SG	10:A:303:HEC:HBB2	1.77	1.23
3:C:211:PRO:HB2	3:C:228:THR:HG21	1.30	1.13
3:K:182:ILE:HG23	3:K:184:ARG:HH12	1.18	1.03
3:C:173:SER:HB3	3:C:227:LEU:HD11	1.39	1.03
10:I:2004:HEC:HBD1	10:I:2004:HEC:HHA	1.38	1.01

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%)	203 (96%)	9 (4%)	0	100	100
1	I	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
3	C	283/320 (88%)	265 (94%)	18 (6%)	0	100	100
3	K	283/320 (88%)	274 (97%)	9 (3%)	0	100	100
4	D	163/230 (71%)	153 (94%)	10 (6%)	0	100	100
4	L	161/230 (70%)	149 (92%)	12 (8%)	0	100	100
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	34/36 (94%)	34 (100%)	0	0	100	100
6	N	34/36 (94%)	34 (100%)	0	0	100	100
7	G	29/37 (78%)	28 (97%)	1 (3%)	0	100	100
7	O	29/37 (78%)	27 (93%)	2 (7%)	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	1866/2116 (88%)	1780 (95%)	86 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	185/186 (100%)	183 (99%)	2 (1%)	65	85
1	I	185/186 (100%)	184 (100%)	1 (0%)	81	92
2	B	134/135 (99%)	129 (96%)	5 (4%)	30	59
2	J	134/135 (99%)	129 (96%)	5 (4%)	30	59
3	C	242/275 (88%)	238 (98%)	4 (2%)	53	79
3	K	242/275 (88%)	241 (100%)	1 (0%)	84	93
4	D	135/183 (74%)	132 (98%)	3 (2%)	45	74
4	L	135/183 (74%)	132 (98%)	3 (2%)	45	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	26/26 (100%)	21 (81%)	5 (19%)	1	4
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	26/31 (84%)	26 (100%)	0	100	100
7	O	26/31 (84%)	25 (96%)	1 (4%)	29	58
8	H	24/24 (100%)	24 (100%)	0	100	100
8	P	24/24 (100%)	24 (100%)	0	100	100
All	All	1596/1772 (90%)	1566 (98%)	30 (2%)	49	77

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	23	ILE
4	L	122	LYS
5	E	28	ILE
7	O	30	ARG
2	J	119	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	K	193	ASN
3	K	225	GLN
4	L	121	ASN
4	L	117	ASN
2	J	116	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

37 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	B	302	-	35,35,35	1.18	2 (5%)	46,46,46	1.07	2 (4%)
12	PL9	D	202	-	55,55,55	1.14	5 (9%)	68,69,69	1.50	14 (20%)
14	PGT	A	308	-	50,50,50	0.89	4 (8%)	53,56,56	1.04	2 (3%)
13	UMQ	I	2005	-	35,35,35	1.13	1 (2%)	46,46,46	0.84	1 (2%)
9	HEM	A	302	1	50,50,50	1.44	7 (14%)	67,82,82	1.14	6 (8%)
14	PGT	L	801	-	50,50,50	0.88	4 (8%)	53,56,56	1.09	2 (3%)
16	FES	D	203	4	0,4,4	-	-	-	-	-
9	HEM	A	301	1	50,50,50	1.45	8 (16%)	67,82,82	1.20	5 (7%)
12	PL9	I	2001	-	55,55,55	0.88	2 (3%)	68,69,69	1.65	11 (16%)
13	UMQ	J	205	-	35,35,35	1.21	4 (11%)	46,46,46	1.04	5 (10%)
12	PL9	I	2008	-	55,55,55	1.04	4 (7%)	68,69,69	1.53	12 (17%)
13	UMQ	P	102	-	35,35,35	1.14	2 (5%)	46,46,46	0.74	0
11	CLA	J	201	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
13	UMQ	A	306	-	35,35,35	1.14	2 (5%)	46,46,46	0.87	0
17	BCR	P	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	9 (16%)
13	UMQ	J	204	-	35,35,35	1.15	3 (8%)	46,46,46	0.75	1 (2%)
10	HEC	K	301	3	46,50,50	1.82	5 (10%)	58,82,82	1.98	4 (6%)
13	UMQ	A	307	-	35,35,35	1.15	3 (8%)	46,46,46	0.85	1 (2%)
15	SQD	K	302	-	52,54,54	0.99	5 (9%)	62,65,65	1.40	9 (14%)
12	PL9	A	305	-	55,55,55	0.98	4 (7%)	68,69,69	1.54	12 (17%)
10	HEC	A	303	-	46,50,50	2.51	24 (52%)	58,82,82	2.07	20 (34%)
12	PL9	J	203	-	55,55,55	1.08	4 (7%)	68,69,69	1.54	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HEC	I	2004	1	46,50,50	1.83	6 (13%)	58,82,82	2.03	6 (10%)
9	HEM	I	2002	1	50,50,50	1.44	7 (14%)	67,82,82	1.16	5 (7%)
13	UMQ	H	201	-	35,35,35	1.13	0	46,46,46	0.74	0
12	PL9	J	202	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
14	PGT	I	2007	-	50,50,50	0.90	4 (8%)	53,56,56	1.07	2 (3%)
13	UMQ	I	2006	-	35,35,35	1.13	2 (5%)	46,46,46	1.01	2 (4%)
16	FES	L	802	4	0,4,4	-	-	-	-	-
14	PGT	D	204	-	50,50,50	0.88	4 (8%)	53,56,56	1.09	2 (3%)
13	UMQ	B	303	-	35,35,35	1.19	3 (8%)	46,46,46	0.86	1 (2%)
17	BCR	F	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	7 (12%)
10	HEC	C	301	3	46,50,50	1.82	5 (10%)	58,82,82	2.02	6 (10%)
11	CLA	A	304	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
15	SQD	D	201	-	52,54,54	0.98	5 (9%)	62,65,65	1.47	8 (12%)
12	PL9	B	301	-	55,55,55	1.08	4 (7%)	68,69,69	1.54	13 (19%)
9	HEM	I	2003	1	50,50,50	1.43	7 (14%)	67,82,82	1.15	6 (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	B	302	-	-	11/20/60/60	0/2/2/2
12	PL9	D	202	-	-	21/53/73/73	0/1/1/1
14	PGT	A	308	-	-	29/55/55/55	-
13	UMQ	I	2005	-	-	8/20/60/60	0/2/2/2
9	HEM	A	302	1	-	2/14/54/54	-
14	PGT	L	801	-	-	25/55/55/55	-
16	FES	D	203	4	-	-	0/1/1/1
9	HEM	A	301	1	-	2/14/54/54	-
12	PL9	I	2001	-	-	29/53/73/73	0/1/1/1
13	UMQ	J	205	-	-	12/20/60/60	0/2/2/2
12	PL9	I	2008	-	-	22/53/73/73	0/1/1/1
13	UMQ	P	102	-	-	6/20/60/60	0/2/2/2
11	CLA	J	201	-	1/1/15/20	16/39/115/115	-
13	UMQ	A	306	-	-	7/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	P	101	-	-	9/29/63/63	0/2/2/2
13	UMQ	J	204	-	-	13/20/60/60	0/2/2/2
10	HEC	K	301	3	-	8/14/54/54	-
13	UMQ	A	307	-	-	14/20/60/60	0/2/2/2
15	SQD	K	302	-	-	18/49/69/69	0/1/1/1
12	PL9	A	305	-	-	23/53/73/73	0/1/1/1
10	HEC	A	303	-	-	5/14/54/54	-
12	PL9	J	203	-	-	20/53/73/73	0/1/1/1
10	HEC	I	2004	1	-	9/14/54/54	-
9	HEM	I	2002	1	-	1/14/54/54	-
13	UMQ	H	201	-	-	3/20/60/60	0/2/2/2
12	PL9	J	202	-	-	23/53/73/73	0/1/1/1
14	PGT	I	2007	-	-	23/55/55/55	-
13	UMQ	I	2006	-	-	11/20/60/60	0/2/2/2
16	FES	L	802	4	-	-	0/1/1/1
14	PGT	D	204	-	-	36/55/55/55	-
13	UMQ	B	303	-	-	6/20/60/60	0/2/2/2
17	BCR	F	101	-	-	6/29/63/63	0/2/2/2
11	CLA	A	304	-	1/1/15/20	17/39/115/115	-
10	HEC	C	301	3	-	11/14/54/54	-
15	SQD	D	201	-	-	24/49/69/69	0/1/1/1
12	PL9	B	301	-	-	23/53/73/73	0/1/1/1
9	HEM	I	2003	1	-	2/14/54/54	-

The worst 5 of 165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	2004	HEC	CAB-C3B	6.19	1.55	1.35
10	I	2004	HEC	CAC-C3C	6.16	1.55	1.35
10	K	301	HEC	CAB-C3B	6.14	1.54	1.35
10	C	301	HEC	CAB-C3B	6.11	1.54	1.35
10	K	301	HEC	CAC-C3C	6.10	1.54	1.35

The worst 5 of 211 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	301	HEC	CBC-CAC-C3C	-9.30	108.86	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	301	HEC	CBC-CAC-C3C	-9.19	109.06	127.43
10	C	301	HEC	CBB-CAB-C3B	-8.96	109.52	127.43
10	K	301	HEC	CBB-CAB-C3B	-8.69	110.07	127.43
10	I	2004	HEC	CBB-CAB-C3B	-8.66	110.13	127.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	304	CLA	ND
11	J	201	CLA	ND

5 of 495 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	302	HEM	C1A-C2A-CAA-CBA
9	I	2003	HEM	C1A-C2A-CAA-CBA
10	C	301	HEC	C2B-C3B-CAB-CBB
10	C	301	HEC	C4B-C3B-CAB-CBB
10	C	301	HEC	C2C-C3C-CAC-CBC

There are no ring outliers.

30 monomers are involved in 142 short contacts:

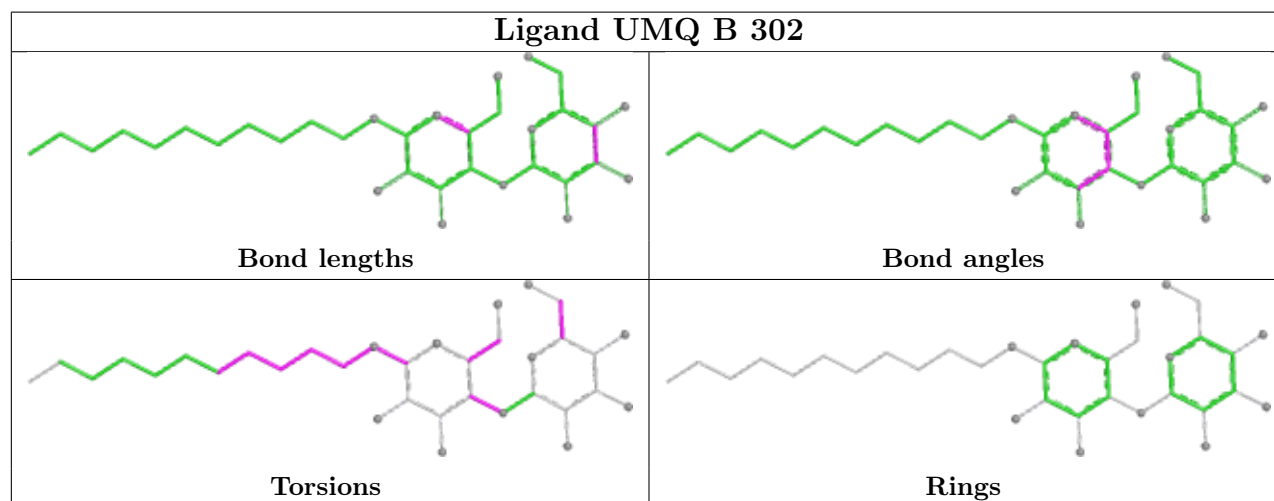
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	302	UMQ	1	0
12	D	202	PL9	4	0
14	A	308	PGT	1	0
9	A	302	HEM	6	0
14	L	801	PGT	3	0
16	D	203	FES	1	0
9	A	301	HEM	4	0
12	I	2001	PL9	1	0
13	J	205	UMQ	3	0
12	I	2008	PL9	15	0
11	J	201	CLA	12	0
13	A	306	UMQ	1	0
17	P	101	BCR	2	0
10	K	301	HEC	4	0
15	K	302	SQD	1	0
12	A	305	PL9	6	0
10	A	303	HEC	5	0
12	J	203	PL9	10	0

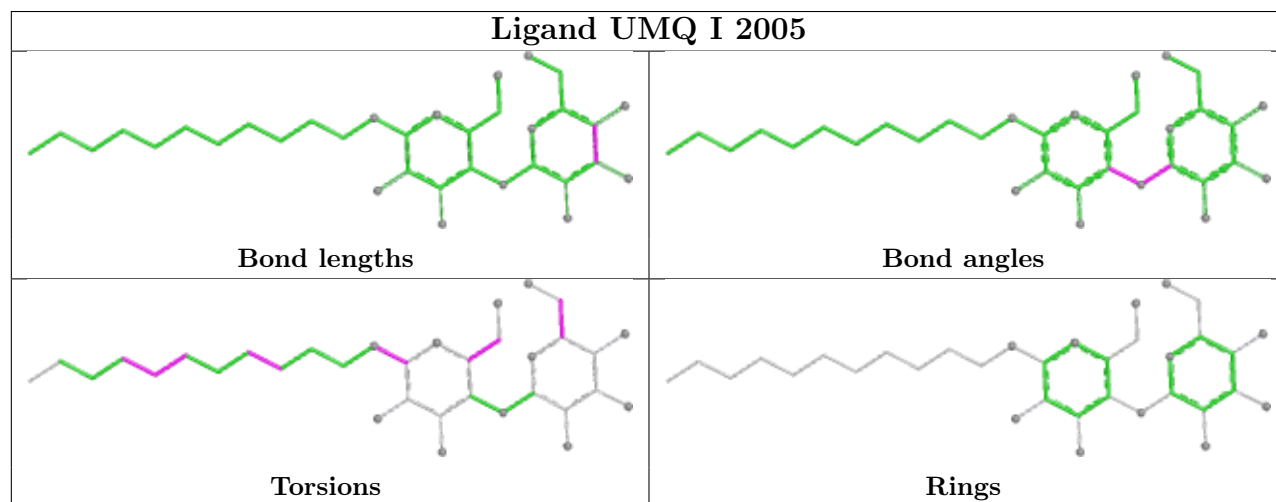
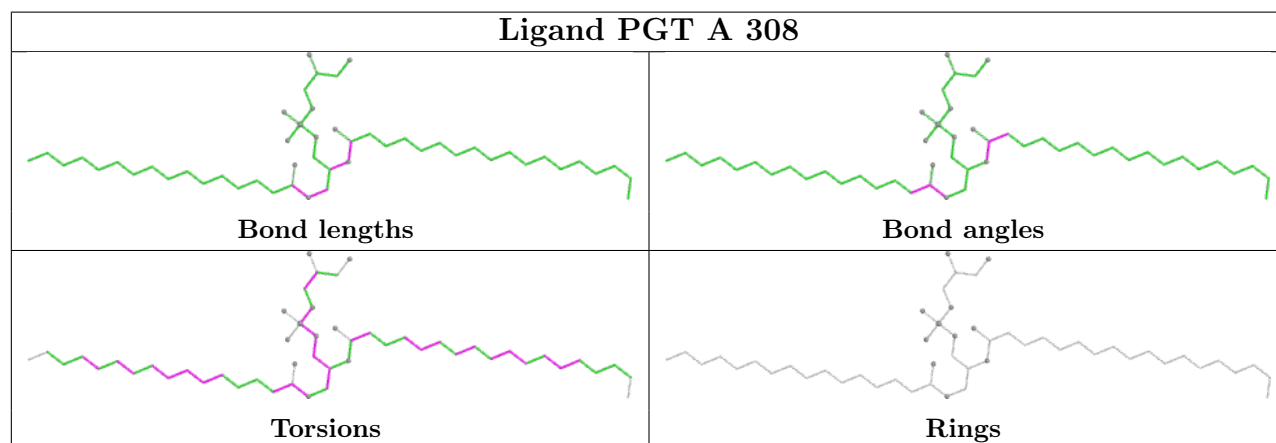
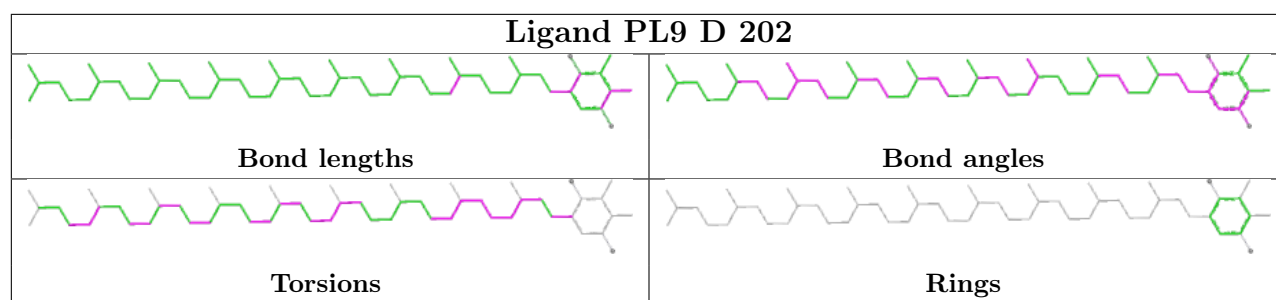
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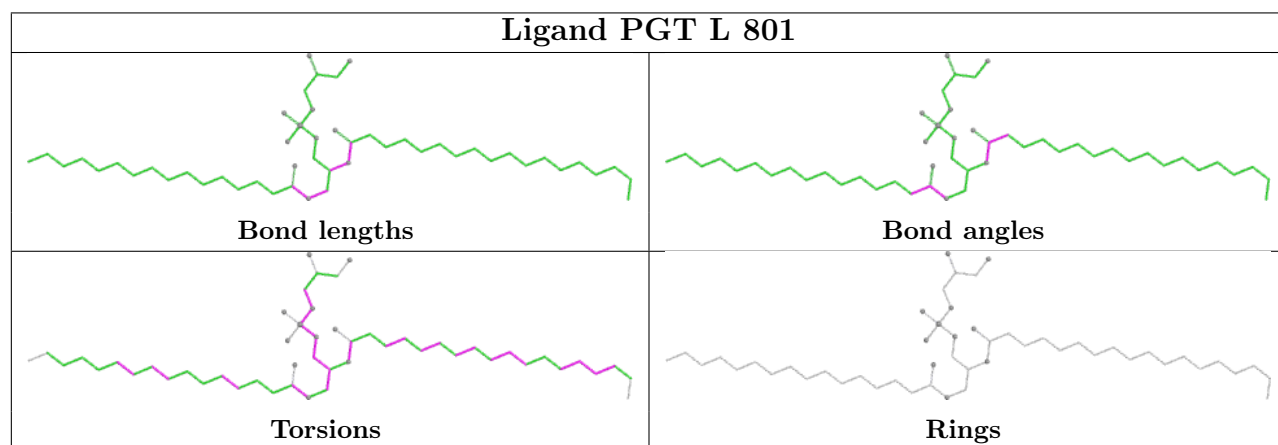
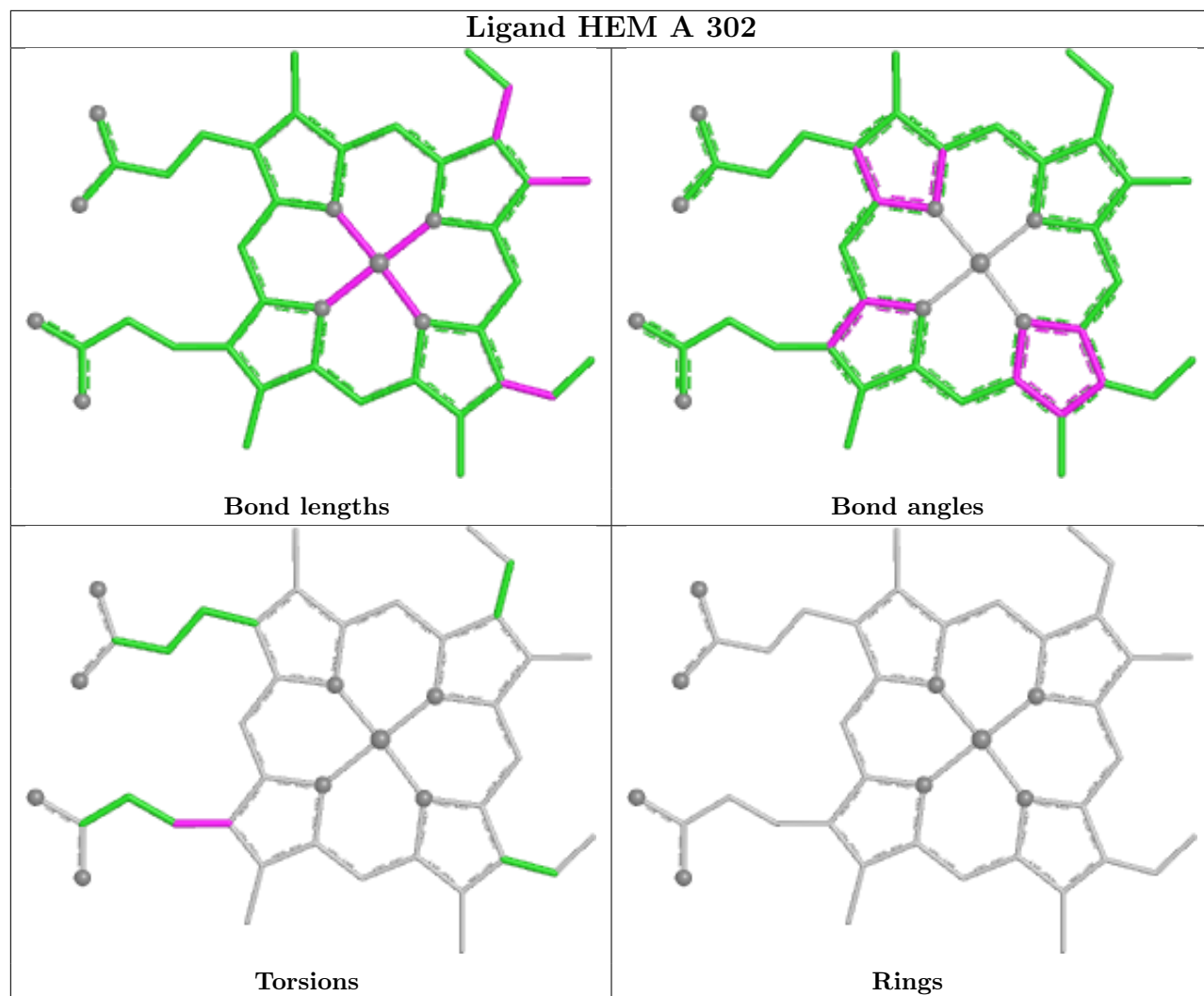
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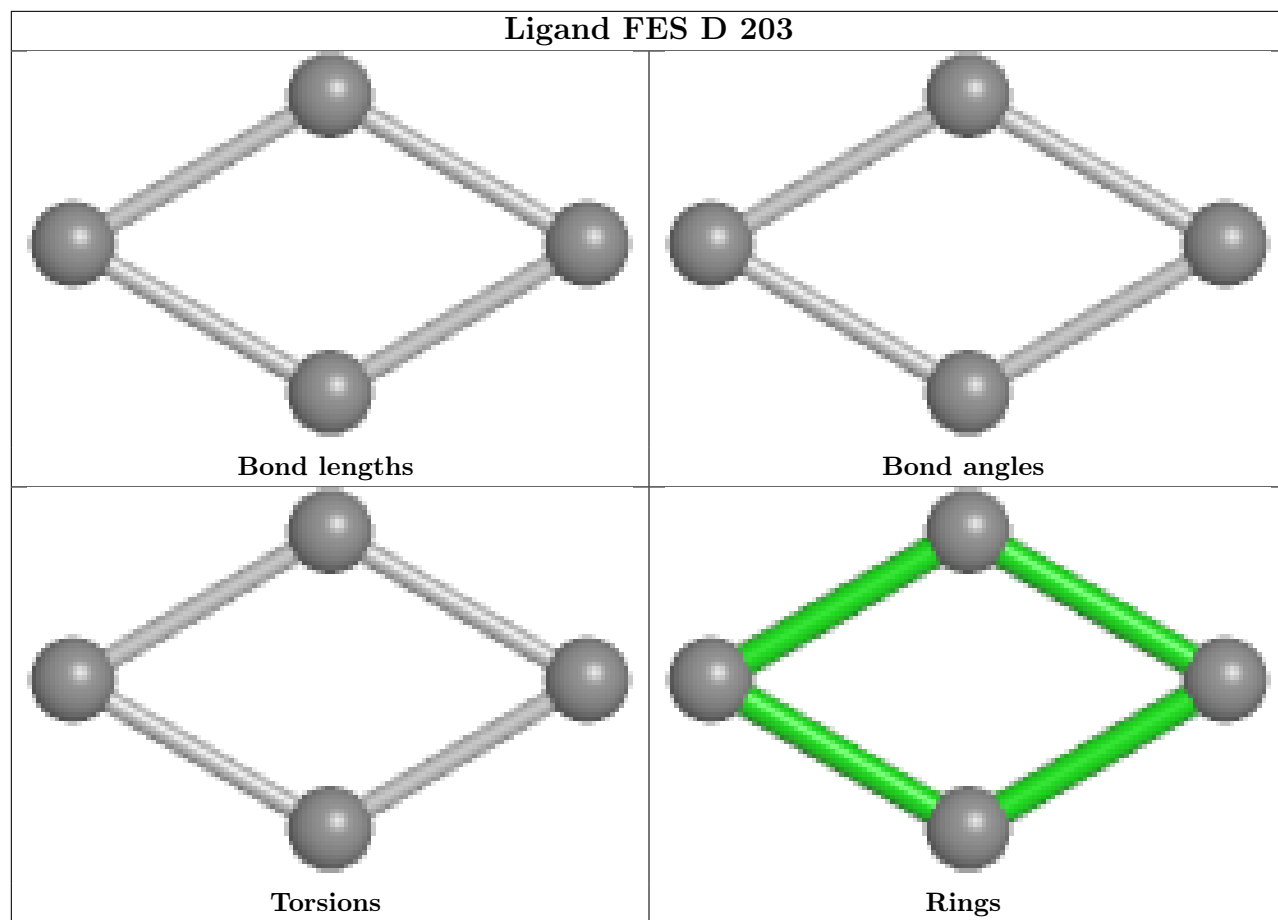
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	2004	HEC	3	0
9	I	2002	HEM	4	0
13	H	201	UMQ	1	0
12	J	202	PL9	27	0
14	I	2007	PGT	2	0
14	D	204	PGT	4	0
17	F	101	BCR	3	0
10	C	301	HEC	4	0
11	A	304	CLA	6	0
15	D	201	SQD	3	0
12	B	301	PL9	13	0
9	I	2003	HEM	5	0

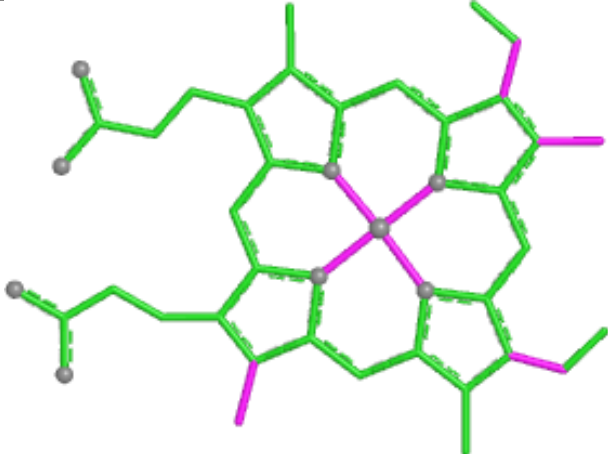
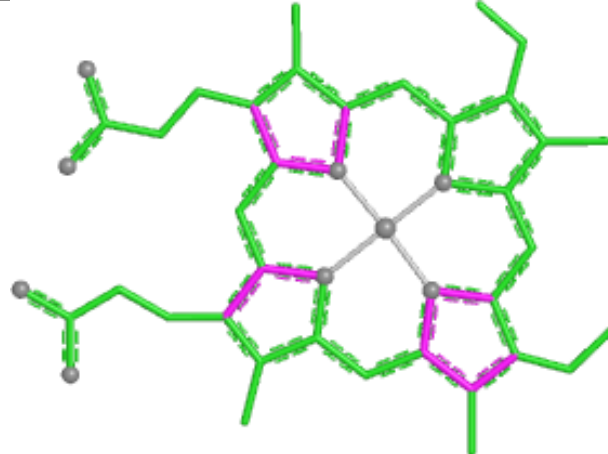
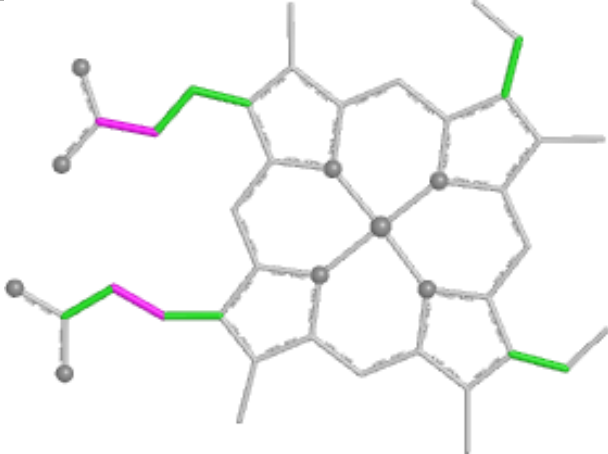
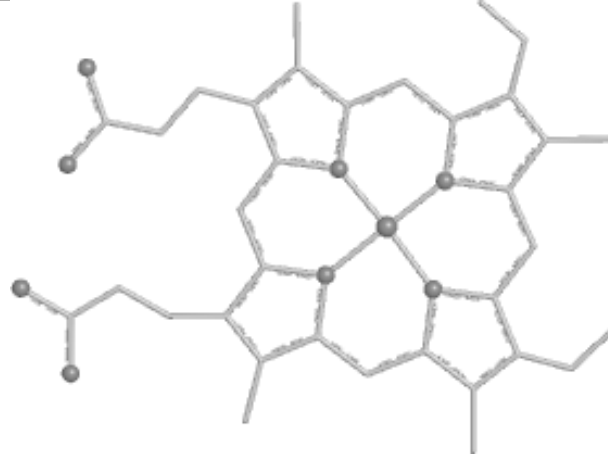
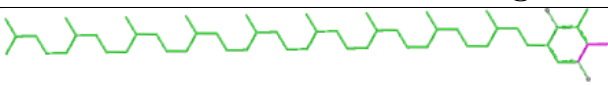
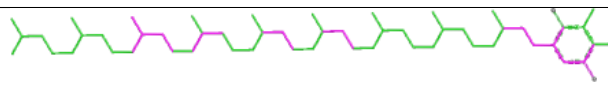
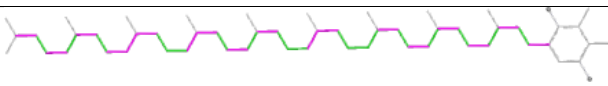
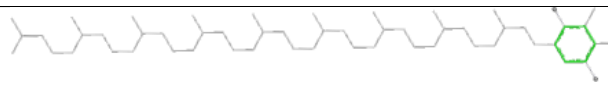
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

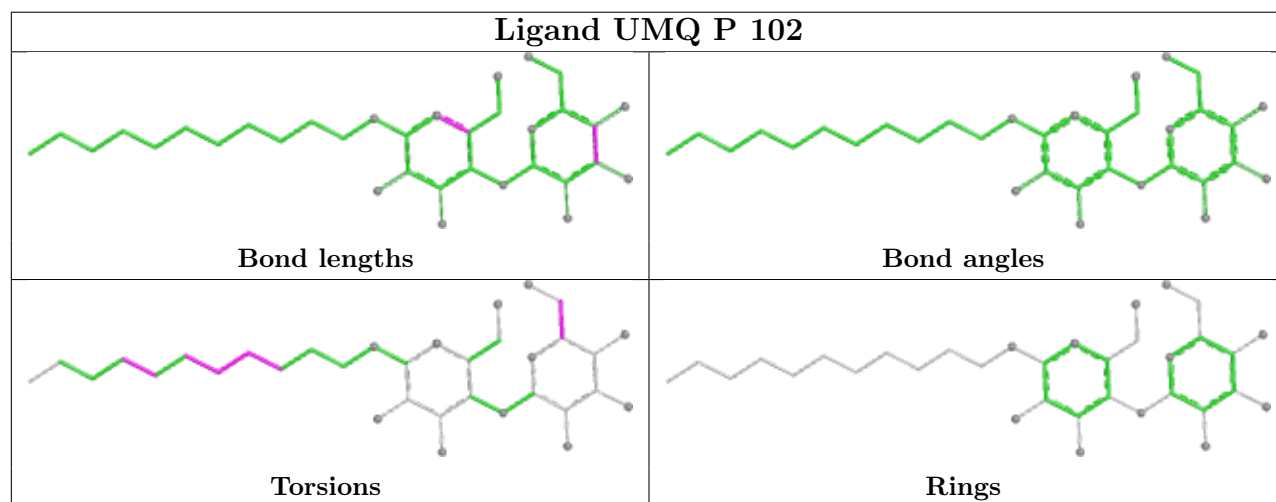
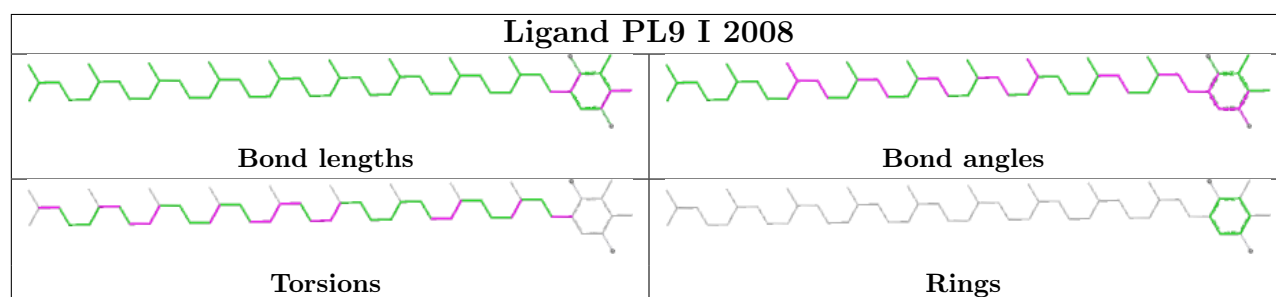
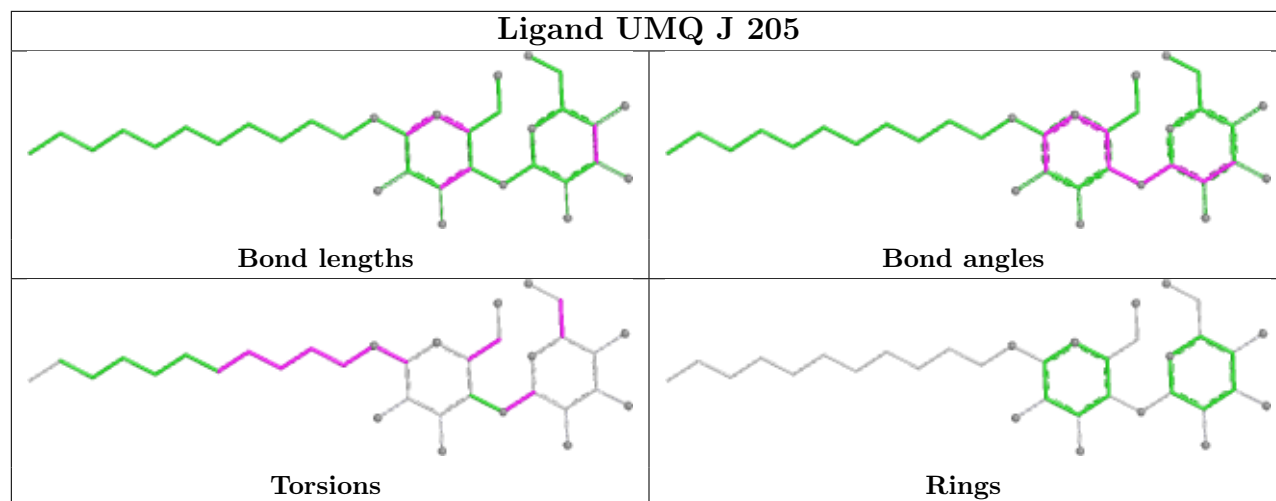


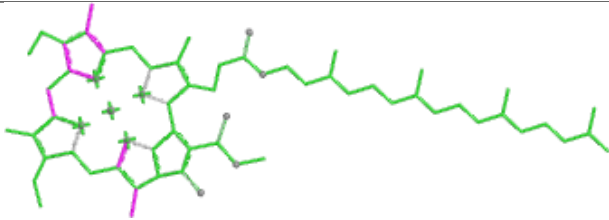
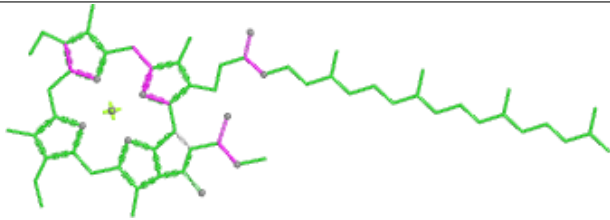
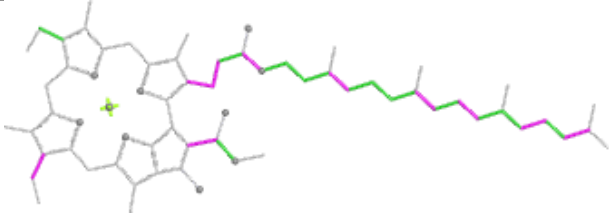
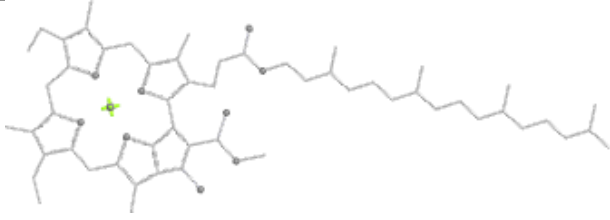


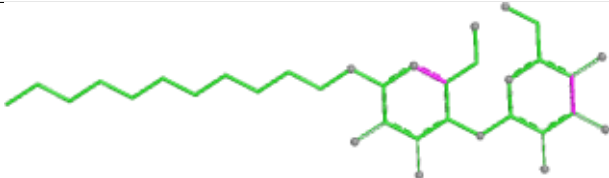
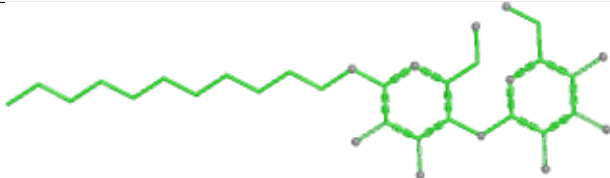
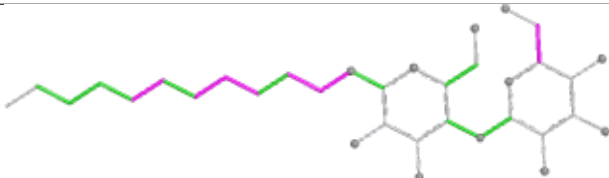
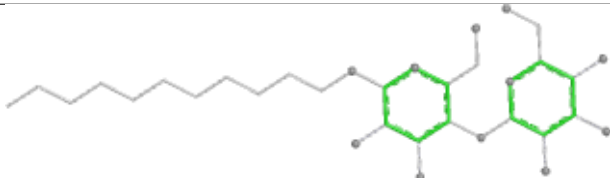


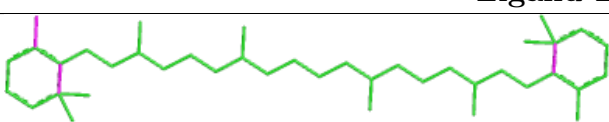
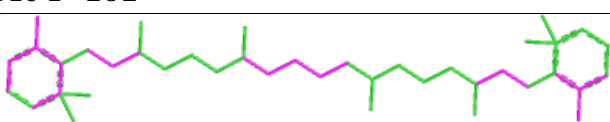
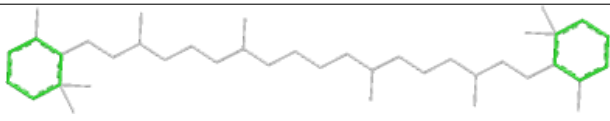


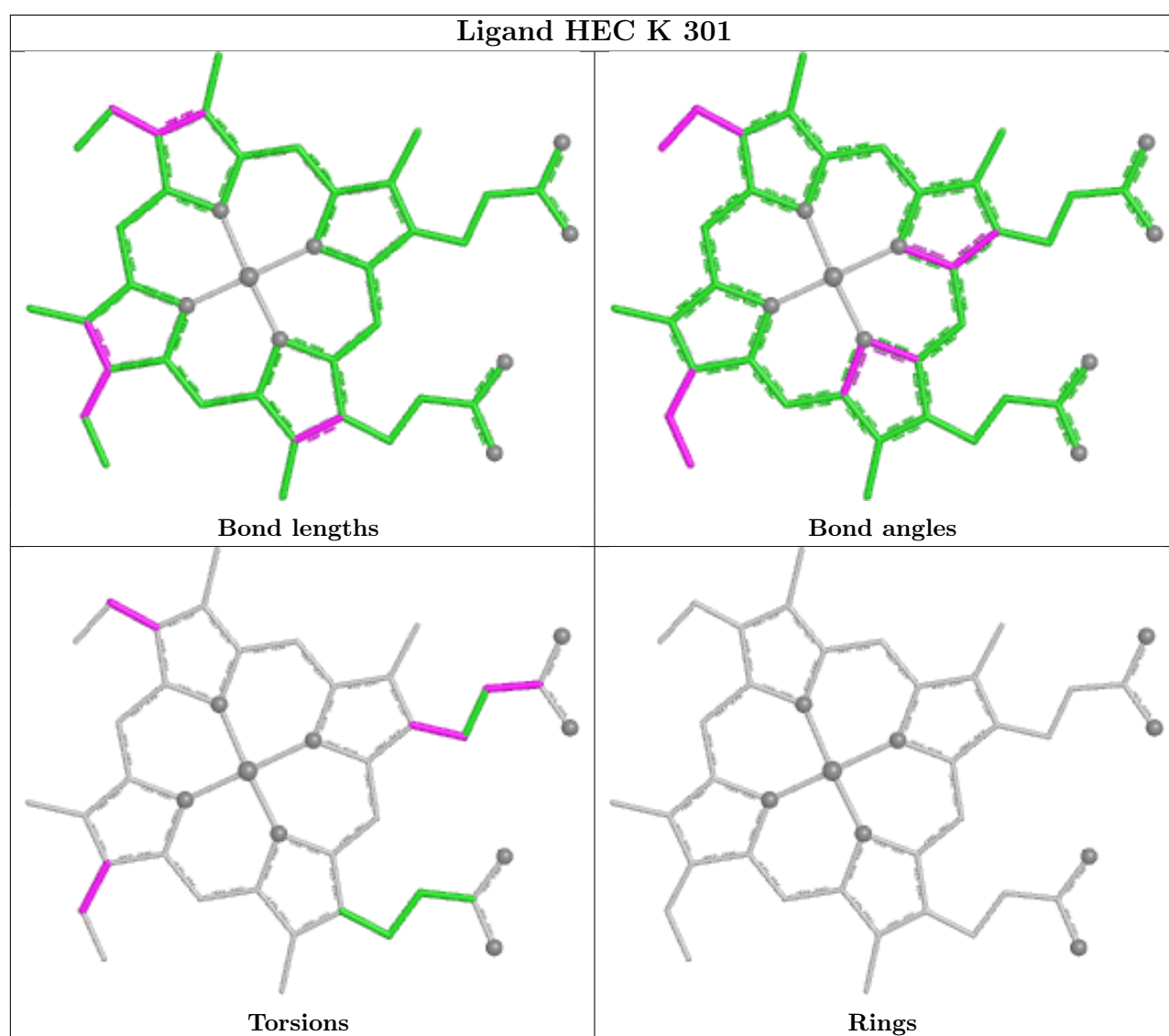
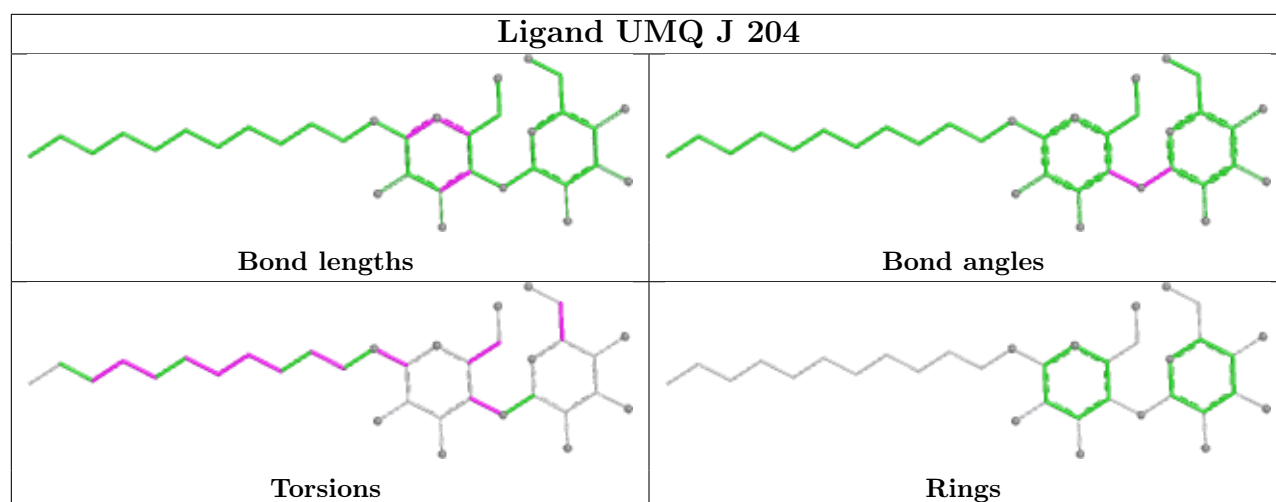
Ligand HEM A 301	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand PL9 I 2001	
	
Bond lengths	Bond angles
	
Torsions	Rings

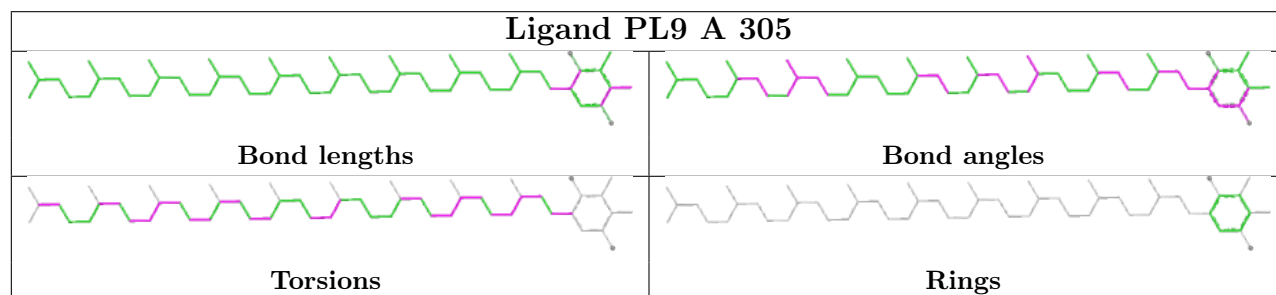
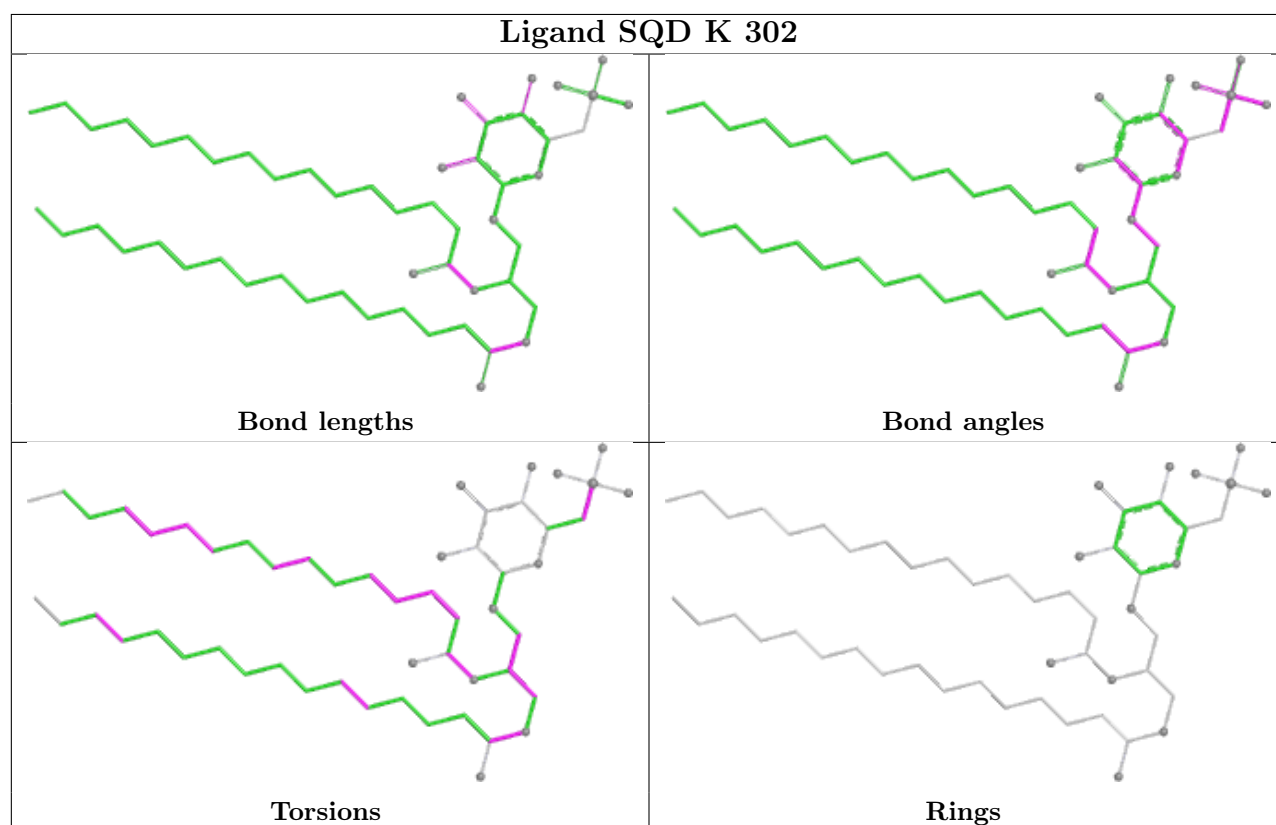
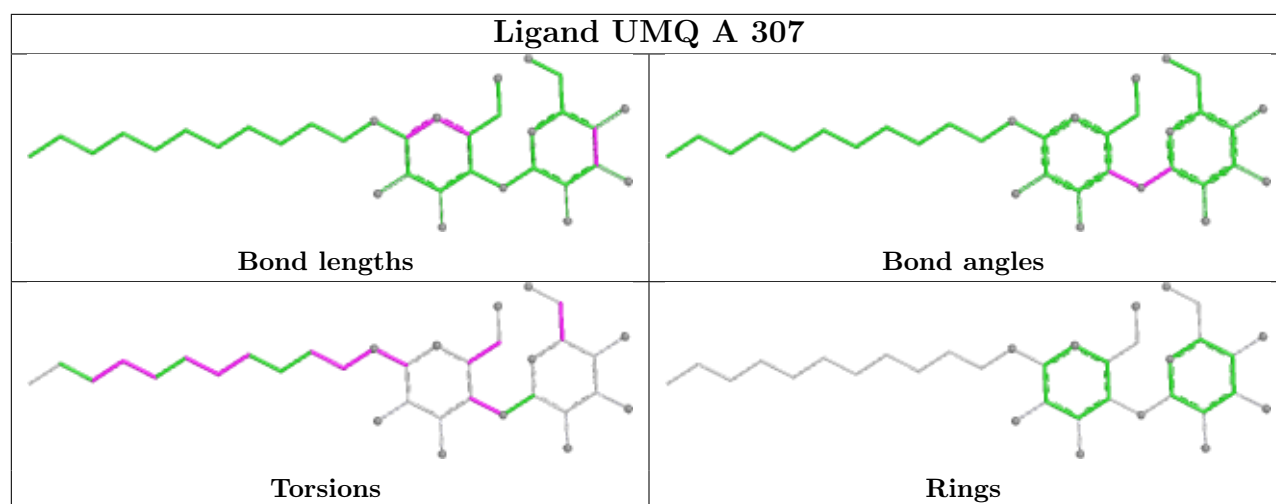


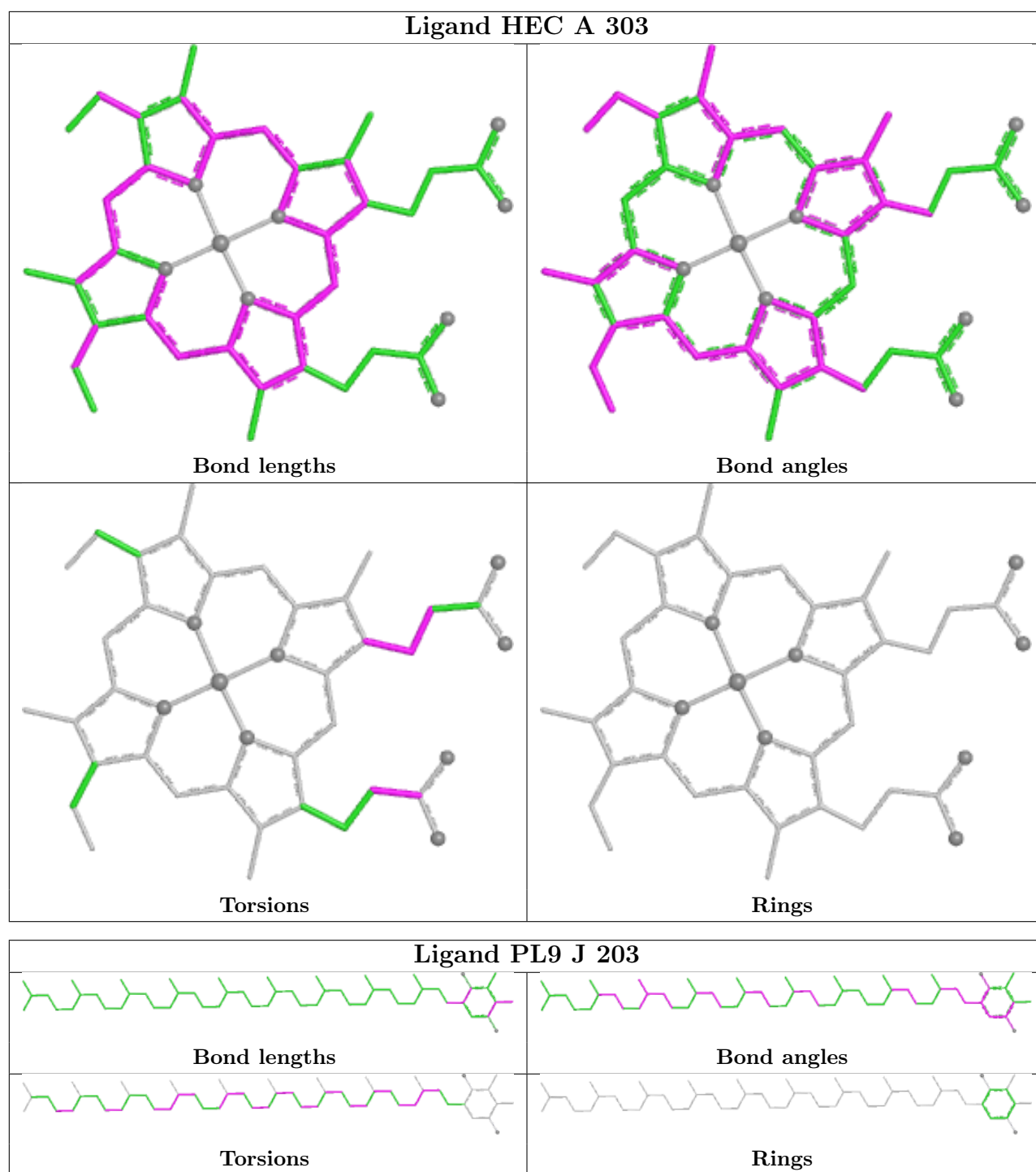
Ligand CLA J 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

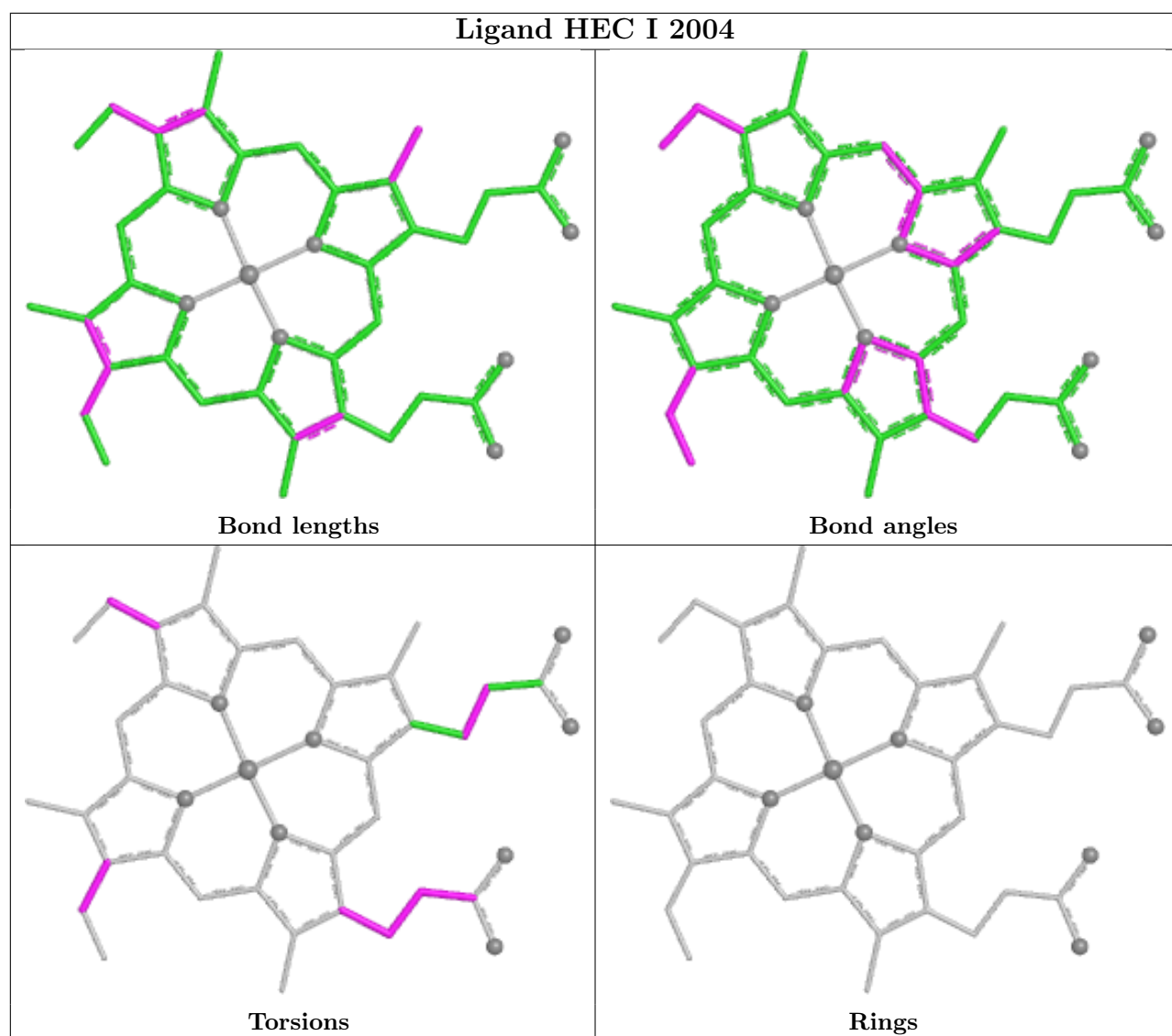
Ligand UMQ A 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR P 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

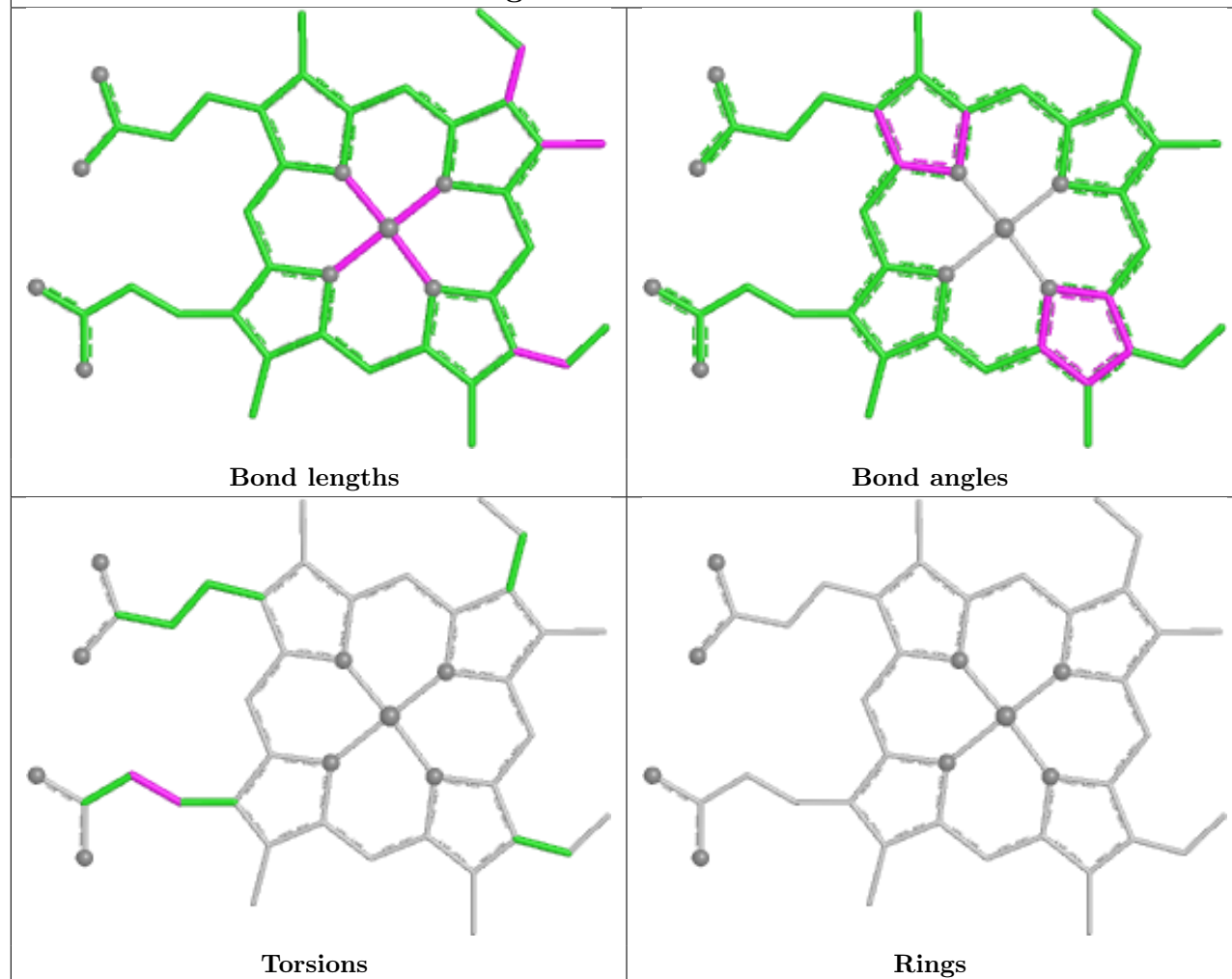




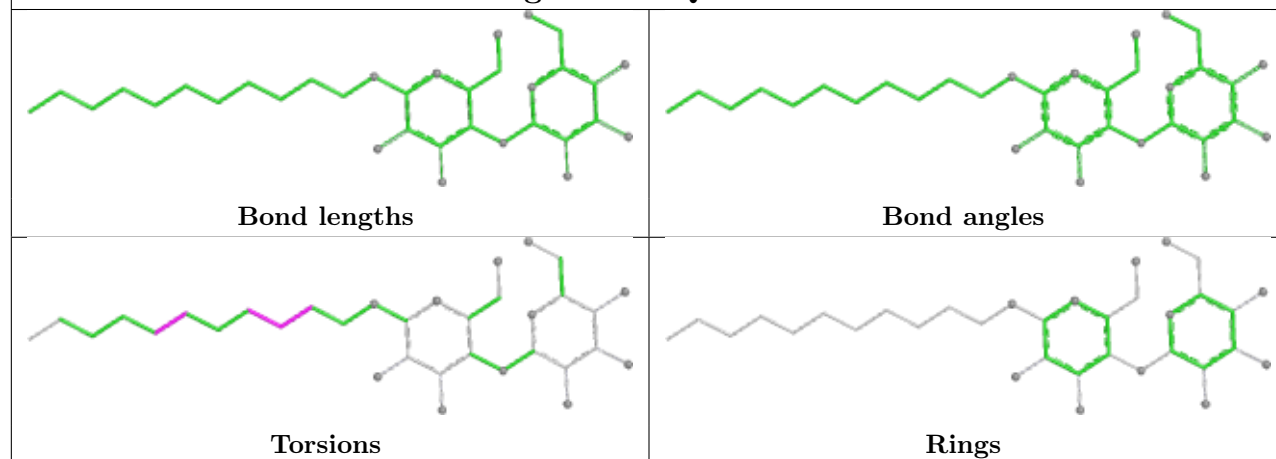


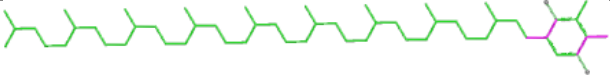
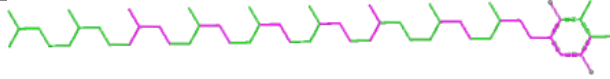
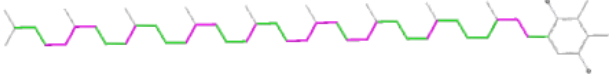
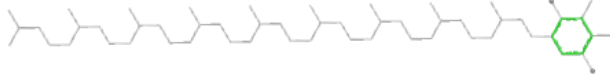
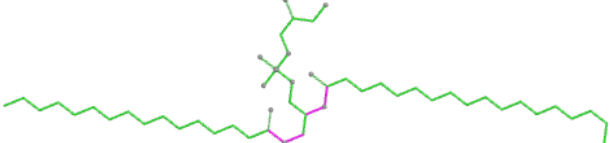
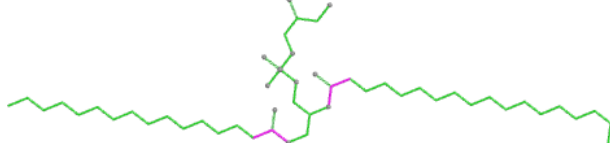
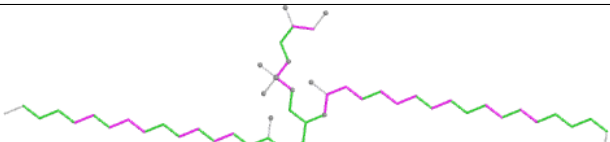
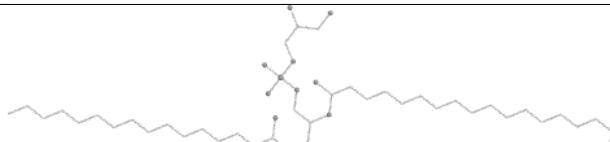
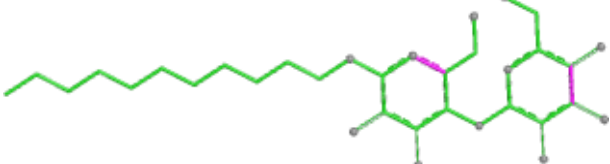
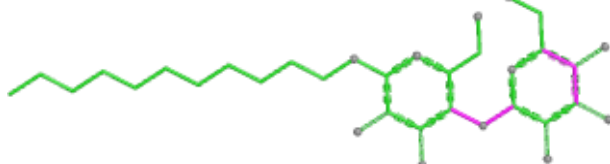
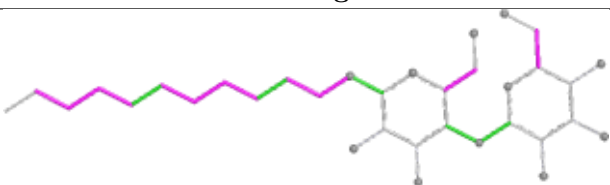
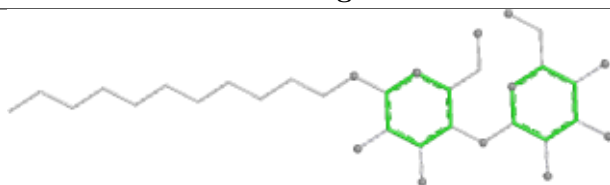


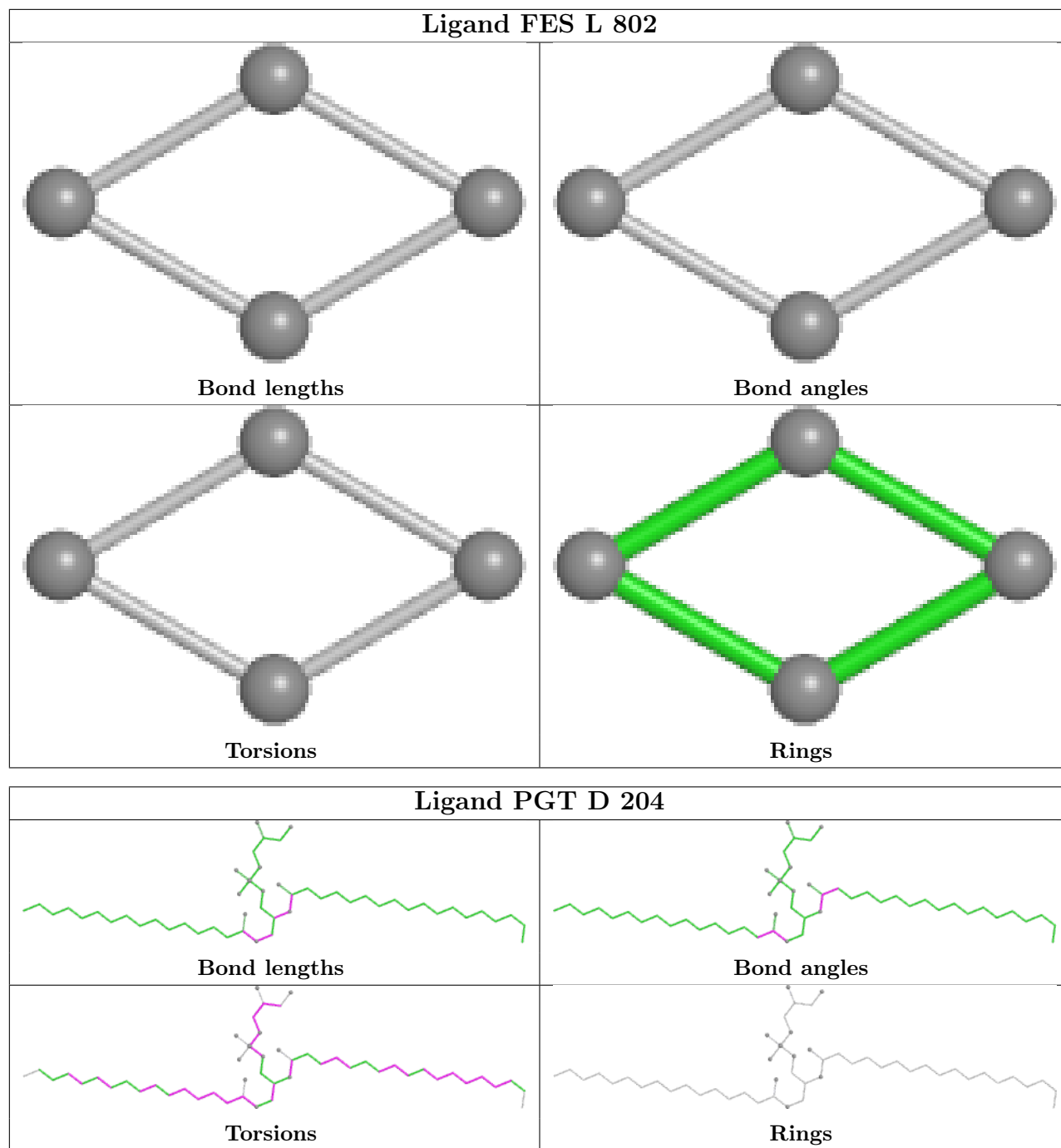
Ligand HEM I 2002

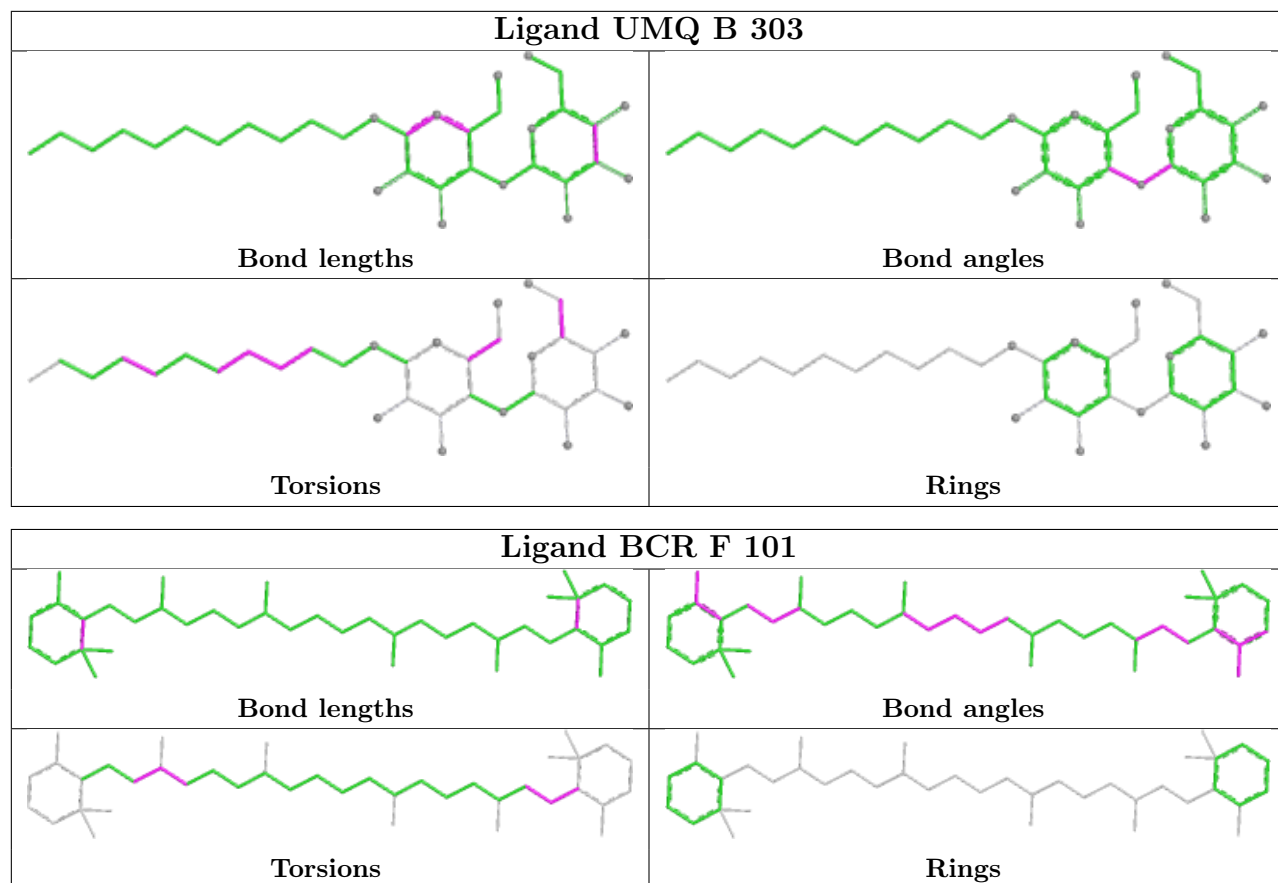


Ligand UMQ H 201

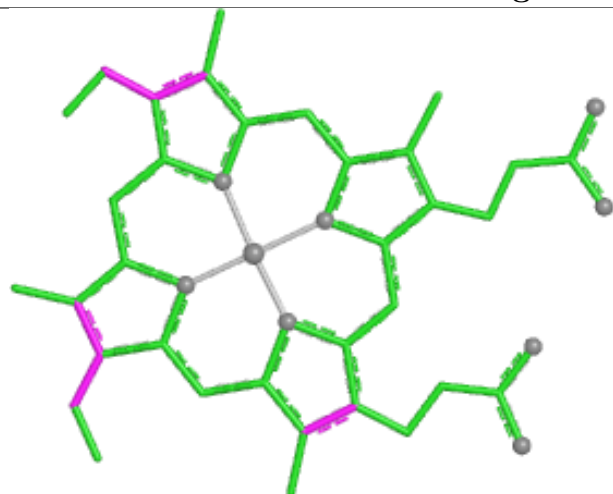


Ligand PL9 J 202	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PGT I 2007	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand UMQ I 2006	
 Bond lengths	 Bond angles
 Torsions	 Rings

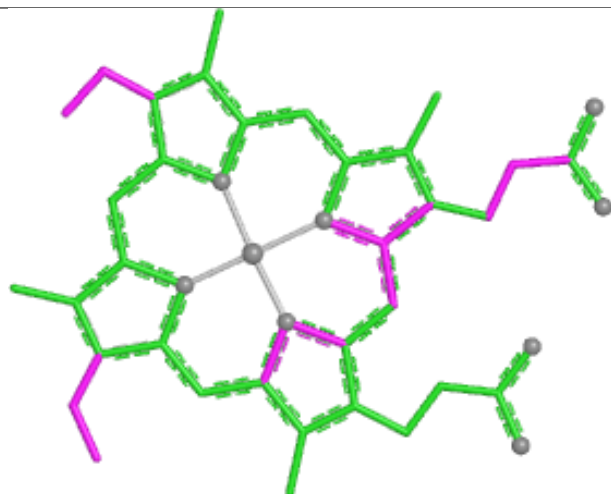




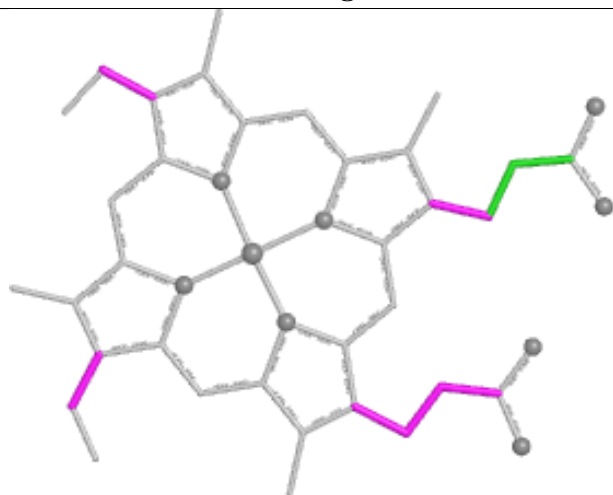
Ligand HEC C 301



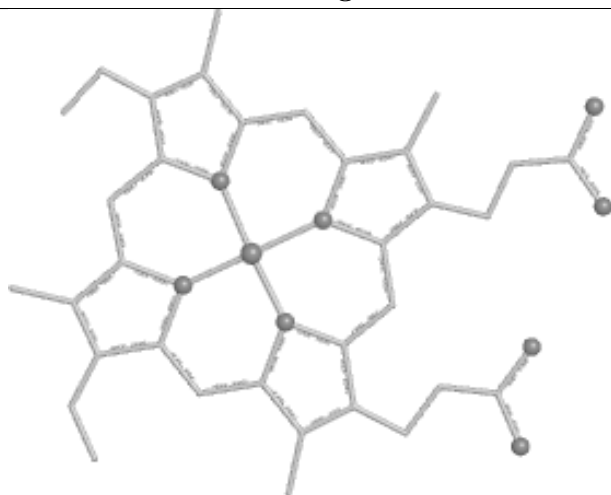
Bond lengths



Bond angles

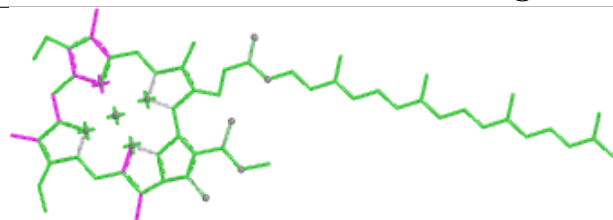


Torsions

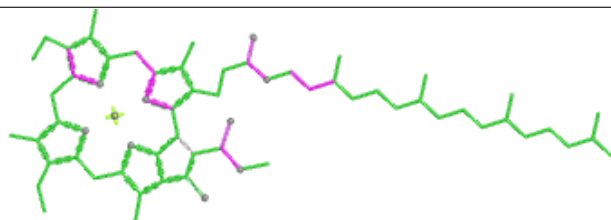


Rings

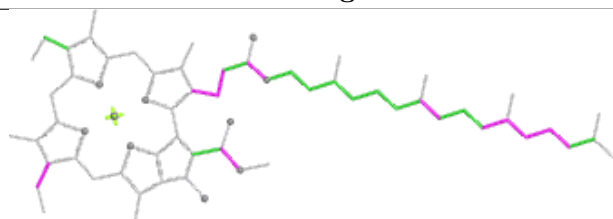
Ligand CLA A 304



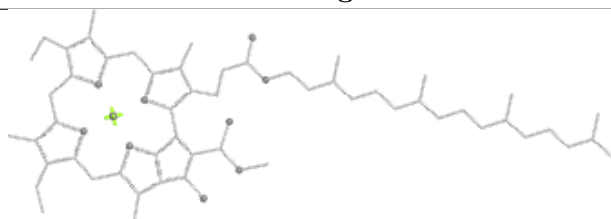
Bond lengths



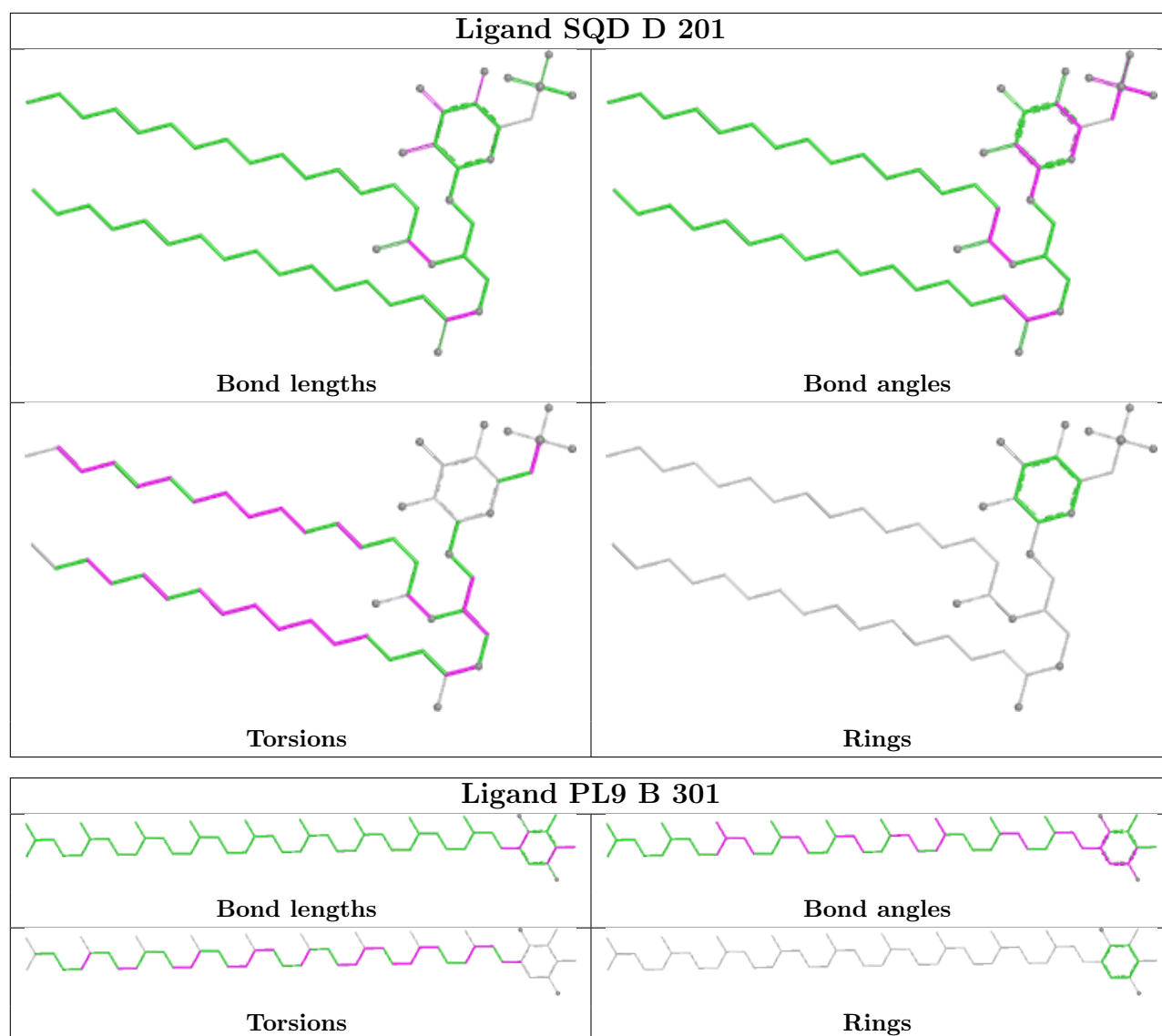
Bond angles

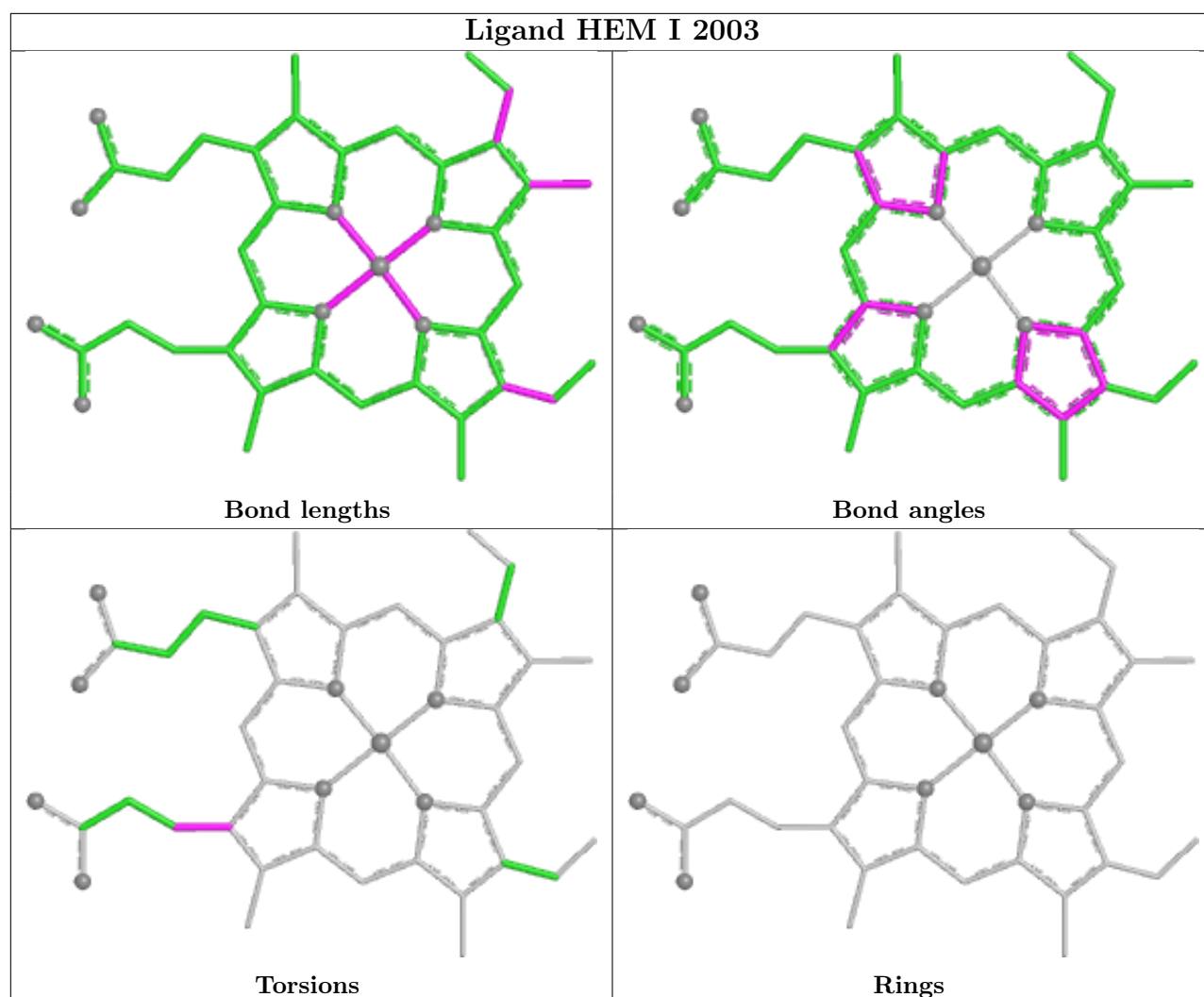


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

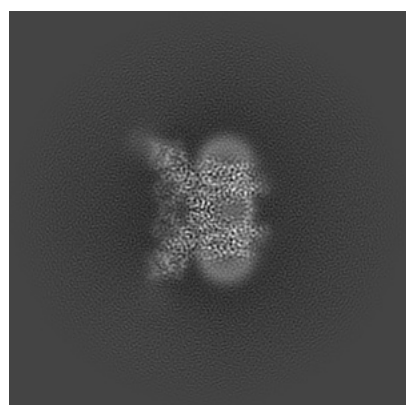
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14123. These allow visual inspection of the internal detail of the map and identification of artifacts.

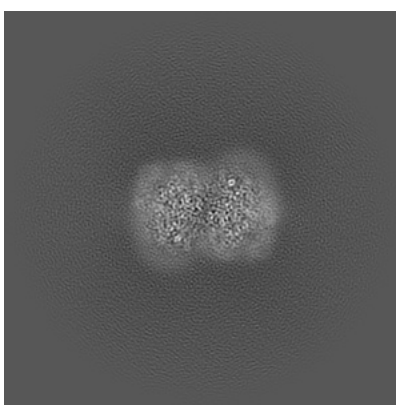
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

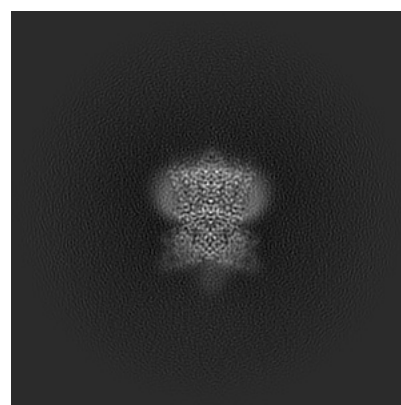
6.1.1 Primary map



X



Y

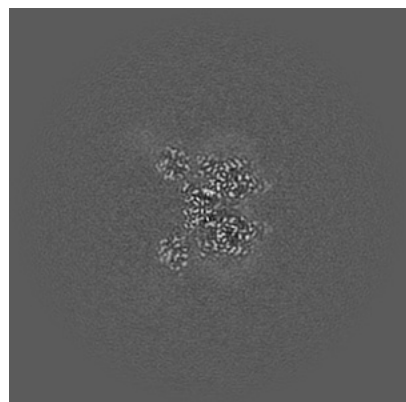


Z

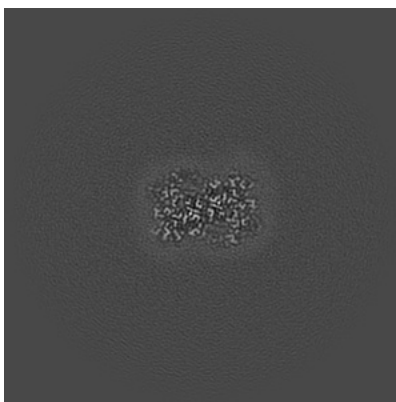
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

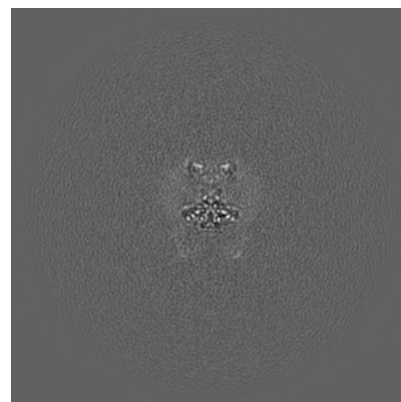
6.2.1 Primary map



X Index: 200



Y Index: 200

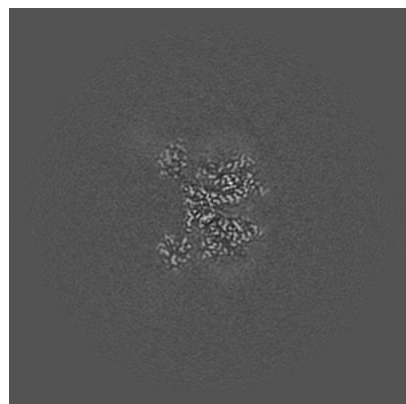


Z Index: 200

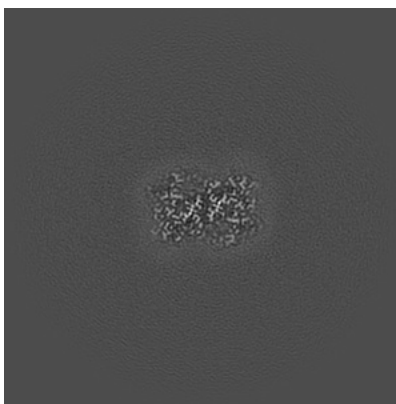
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

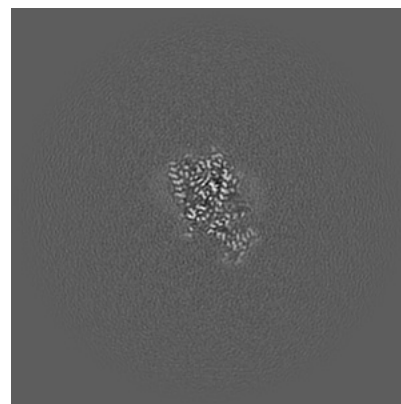
6.3.1 Primary map



X Index: 196



Y Index: 199

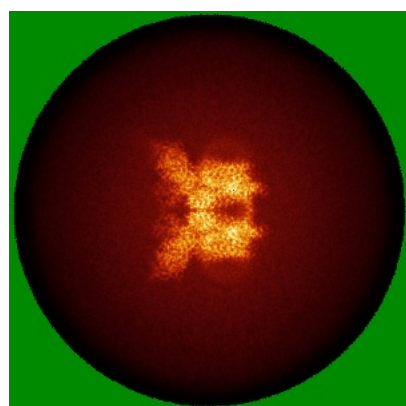


Z Index: 181

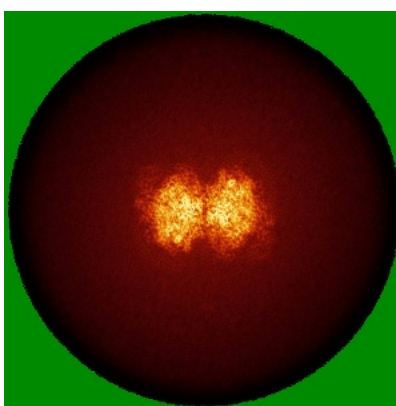
The images above show the largest variance slices of the map in three orthogonal directions.

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

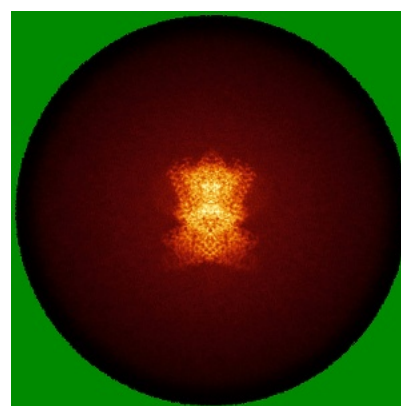
6.4.1 Primary map



X



Y

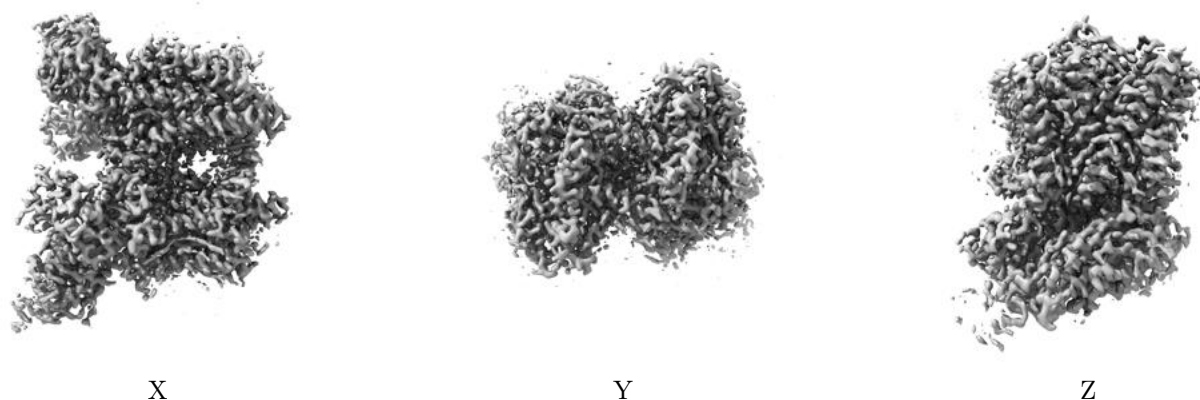


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

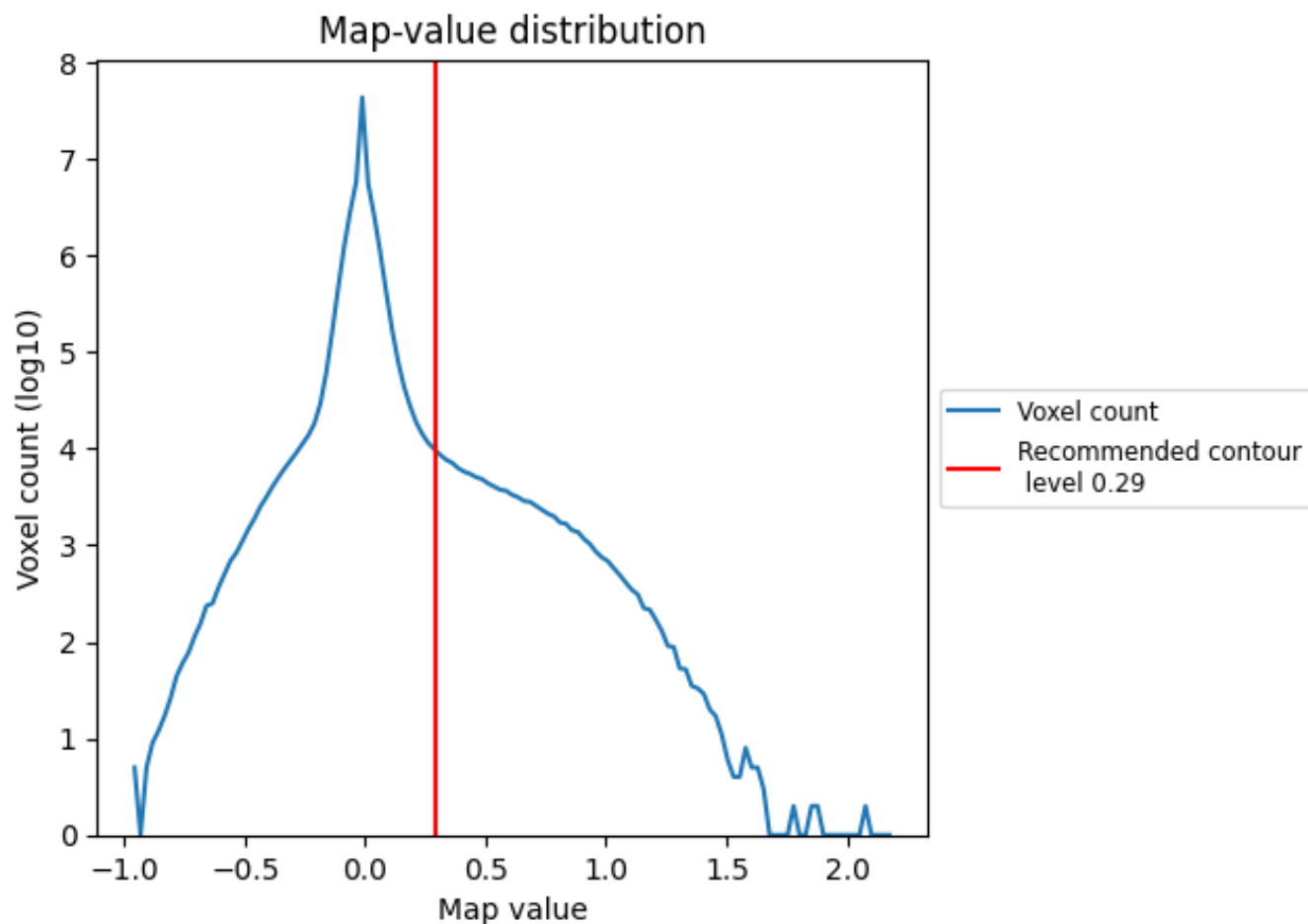
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

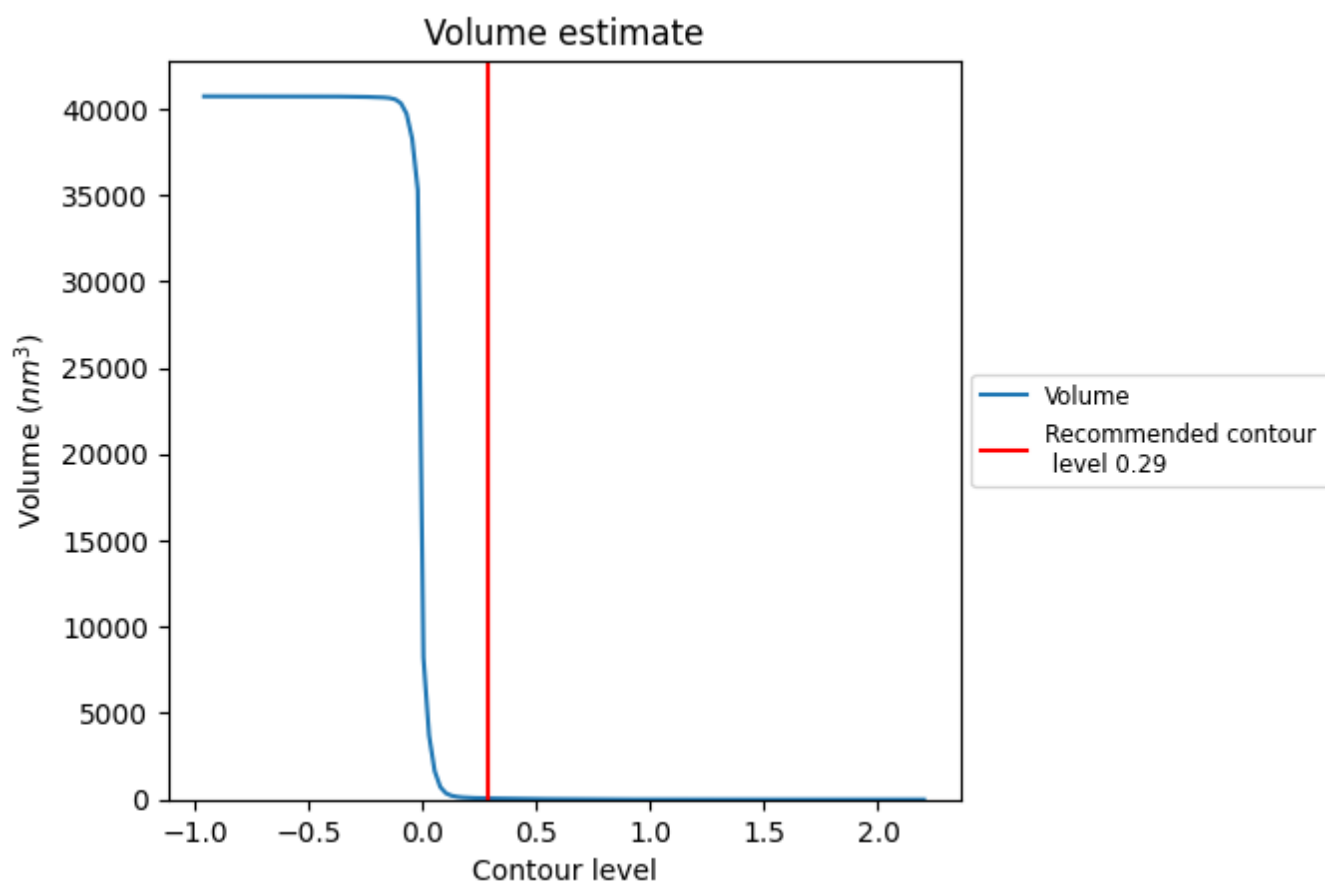
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

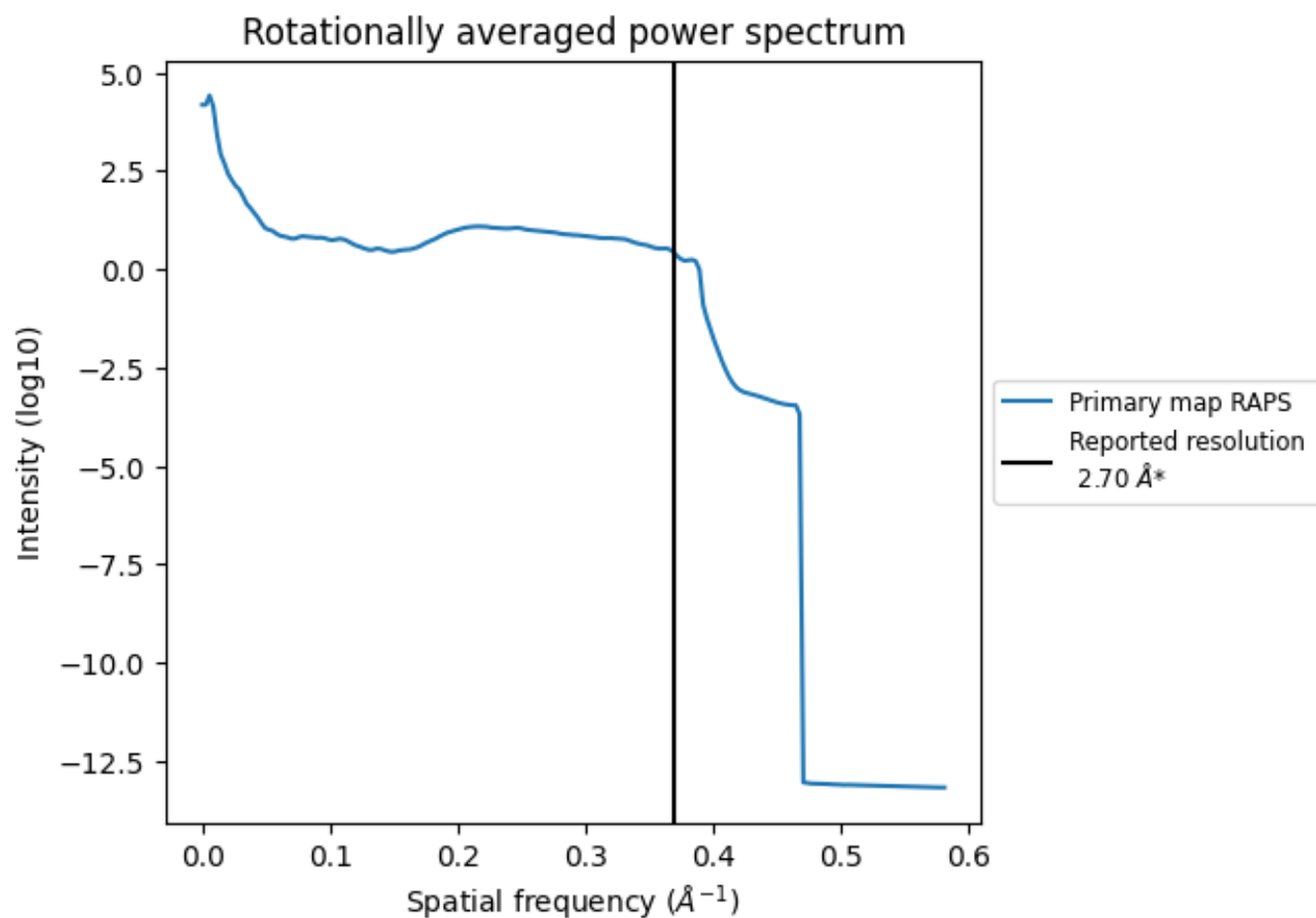
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 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 ⓘ

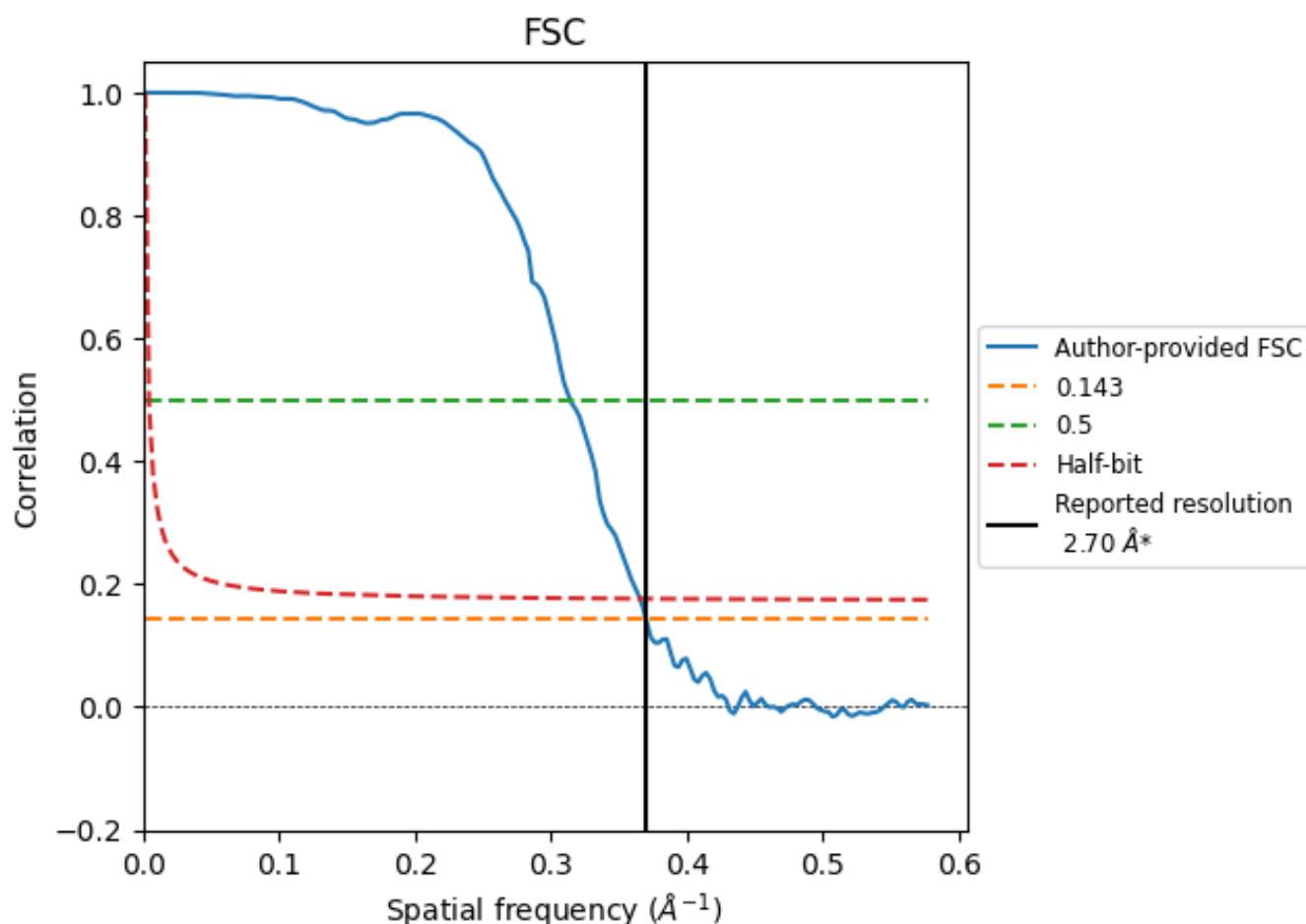


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

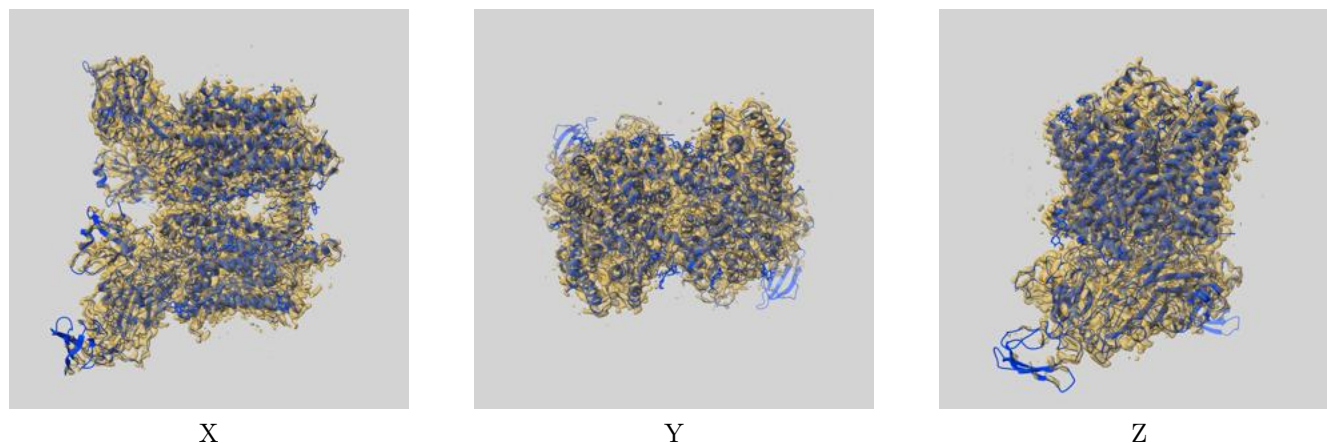
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.18	2.74
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

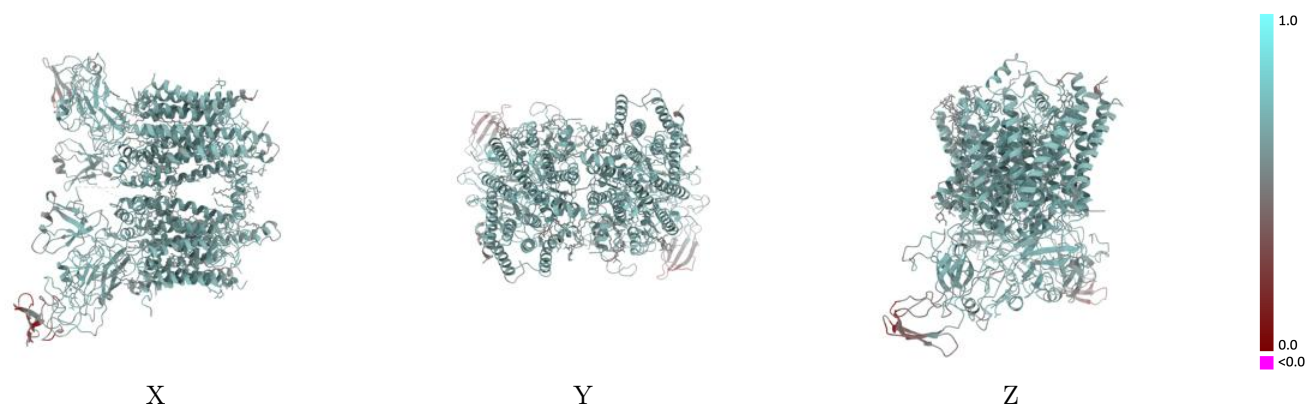
This section contains information regarding the fit between EMDB map EMD-14123 and PDB model 7QRM. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



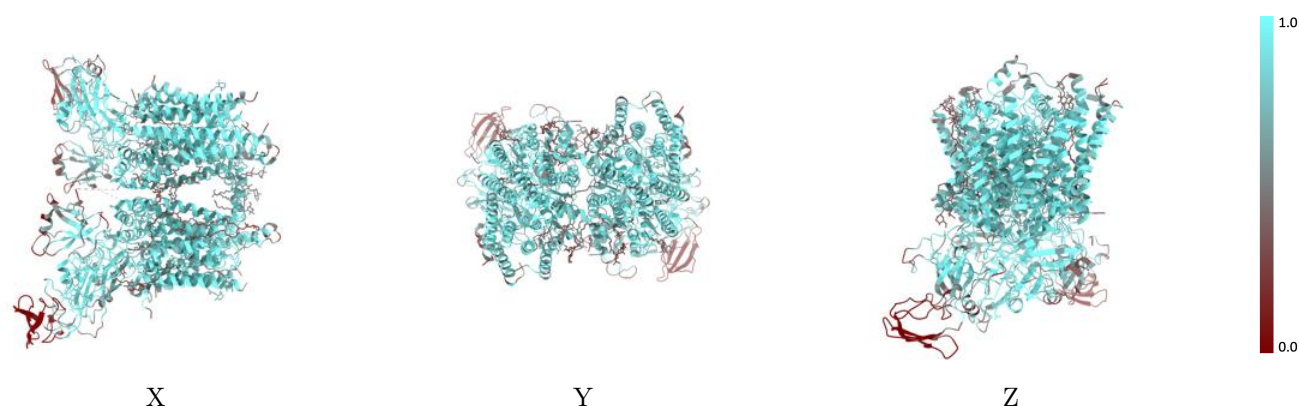
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



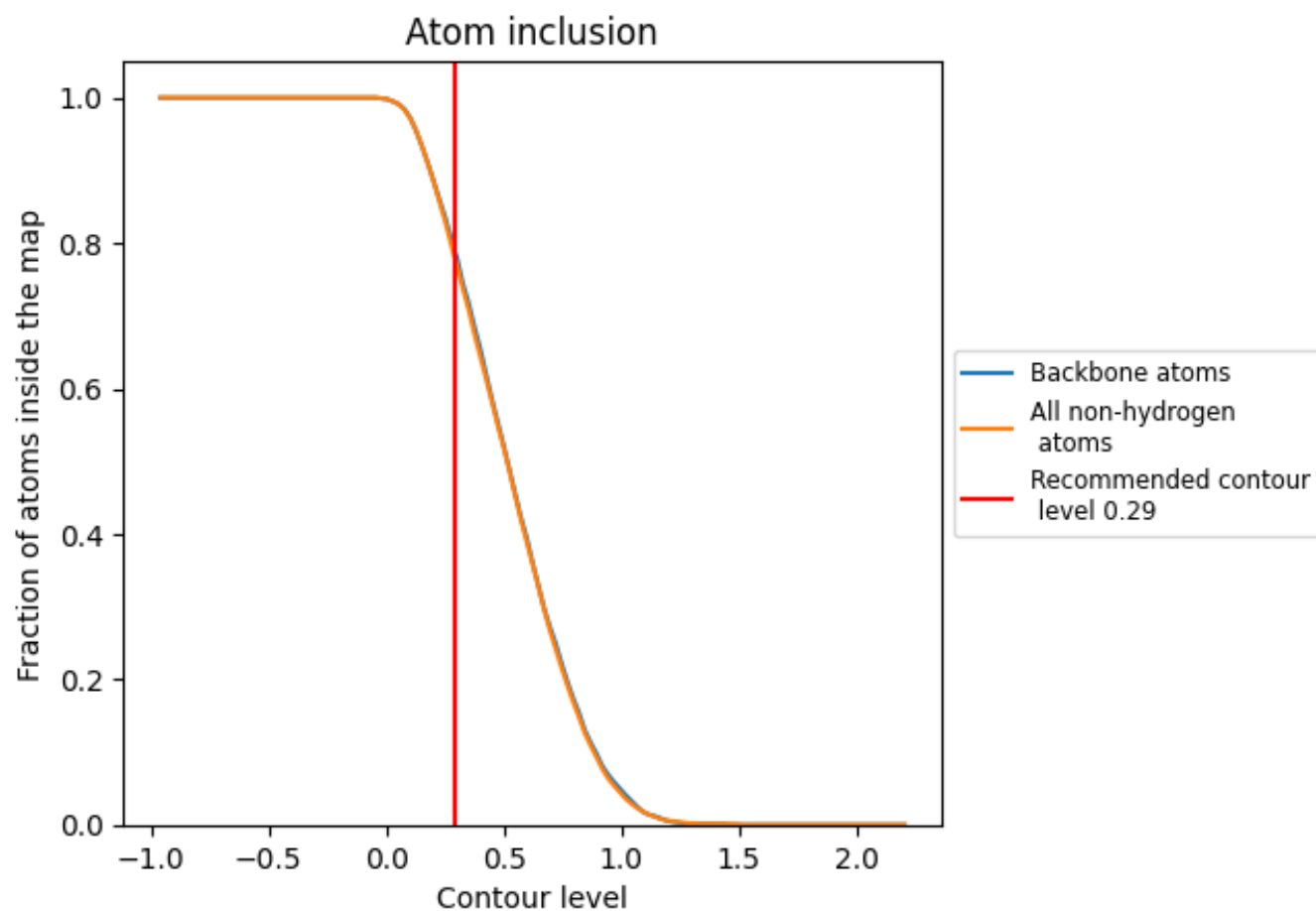
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.29).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.6170
A	0.8970	0.6530
B	0.8330	0.6280
C	0.6780	0.5800
D	0.6930	0.6040
E	0.7750	0.6100
F	0.8000	0.6200
G	0.9090	0.6330
H	0.9040	0.6470
I	0.8850	0.6500
J	0.8140	0.6260
K	0.6940	0.5840
L	0.6980	0.6020
M	0.7380	0.6110
N	0.8040	0.6090
O	0.9340	0.6500
P	0.8730	0.6400

1.0

0.0

<0.0