



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 04:50 AM UTC

PDB ID : 9ES9 / pdb_00009es9
EMDB ID : EMD-19940
Title : Cryo-EM structure of Spinacia oleracea cytochrome b6f complex with inhibitor DBMIB bound at plastoquinol oxidation site
Authors : Pietras, R.; Pintscher, S.; Mielecki, B.; Szwalec, M.; Wojcik-Augustyn, A.; Indyka, P.; Rawski, M.; Koziej, L.; Jaciuk, M.; Wazny, G.; Glatt, S.; Osyczka, A.
Deposited on : 2024-03-25
Resolution : 2.33 Å(reported)
Based on initial model : 7ZYV

This is a Full wwPDB EM Validation 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)

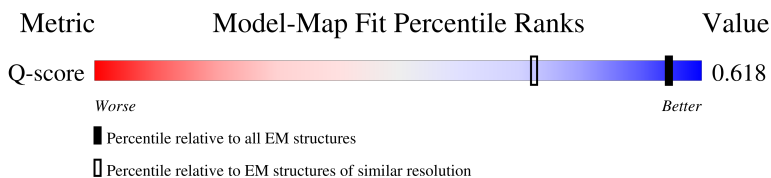
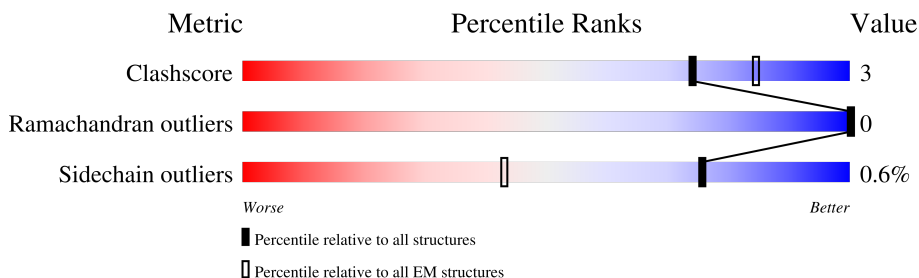
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

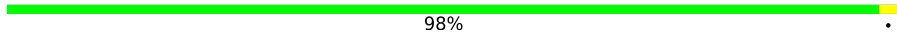
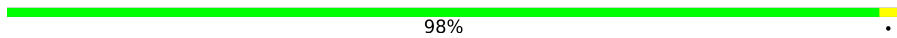
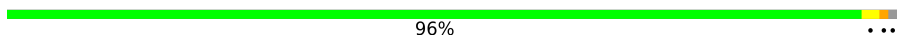
The reported resolution of this entry is 2.33 Å.

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	4434 (1.83 - 2.83)

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	 98%
1	I	215	 98%
2	B	160	 96%

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	J	160	
3	C	320	
3	K	320	
4	D	230	
4	L	230	
5	E	31	
5	M	31	
6	F	131	
6	N	131	
7	G	37	
7	O	37	
8	H	29	
8	P	29	
9	Q	103	
9	R	103	

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
15	CLA	B	201	X	-	-	-
15	CLA	J	201	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 16450 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	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
			1226	820	193	209	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	279	Total	C	N	O	S	0	0
			2168	1396	366	400	6		
3	K	279	Total	C	N	O	S	0	0
			2168	1396	366	400	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	179	Total	C	N	O	S	0	0
			1334	850	225	252	7		
4	L	179	Total	C	N	O	S	0	0
			1334	850	225	252	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	37	Total	C	N	O	S	1	0
			280	183	46	50	1		
6	N	37	Total	C	N	O	S	1	0
			280	183	46	50	1		

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

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

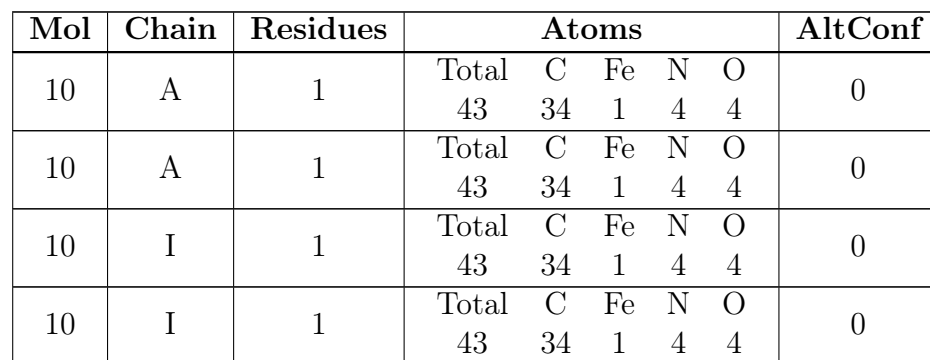
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

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

- Molecule 9 is a protein called Thylakoid soluble phosphoprotein.

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

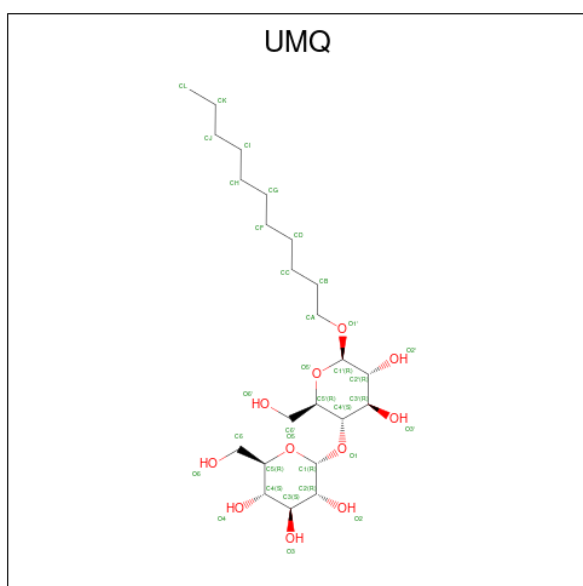
- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



- # HEC

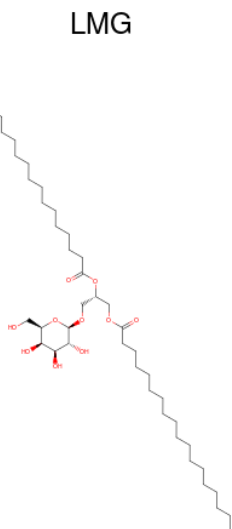
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	I	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	K	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 12 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).



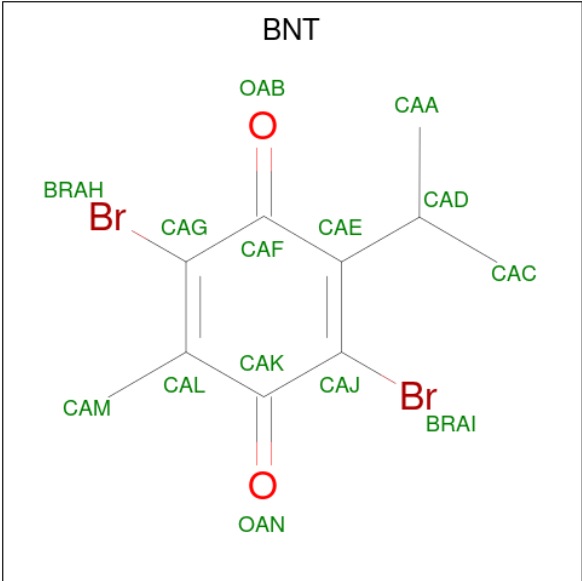
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			34	23	11	
12	H	1	Total	C	O	0
			34	23	11	
12	I	1	Total	C	O	0
			34	23	11	
12	P	1	Total	C	O	0
			34	23	11	

- Molecule 13 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			55	45	10	
13	I	1	Total	C	O	0
			55	45	10	

- Molecule 14 is 2,5-DIBROMO-3-ISOPROPYL-6-METHYLBENZO-1,4-QUINONE (CCD ID: BNT) (formula: $C_{10}H_{10}Br_2O_2$) (labeled as "Ligand of Interest" by depositor).



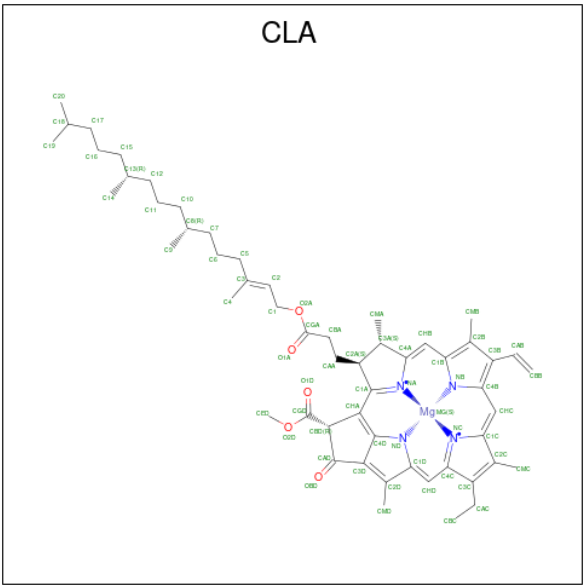
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total 14	Br 2	C 10	O 2	0

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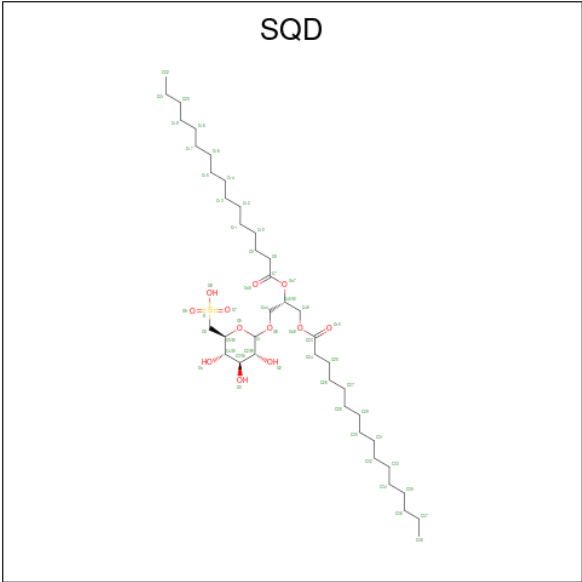
Mol	Chain	Residues	Atoms				AltConf
			Total	Br	C	O	
14	I	1	14	2	10	2	0

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



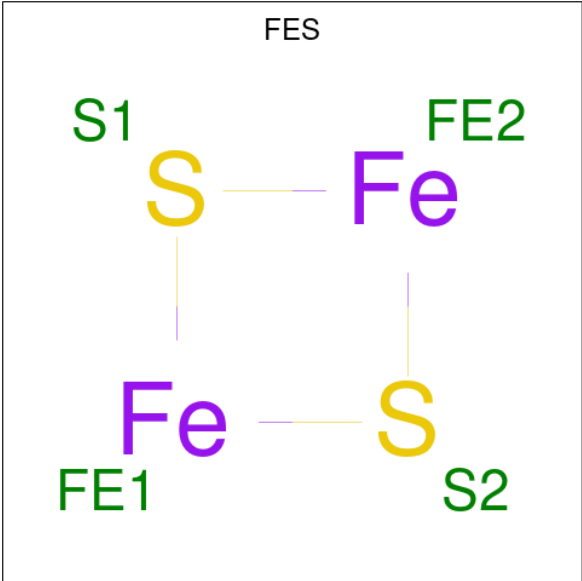
Mol	Chain	Residues	Atoms				AltConf
			Total	C	Mg	N	O
15	B	1	65	55	1	4	5
15	J	1	65	55	1	4	5

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



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

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



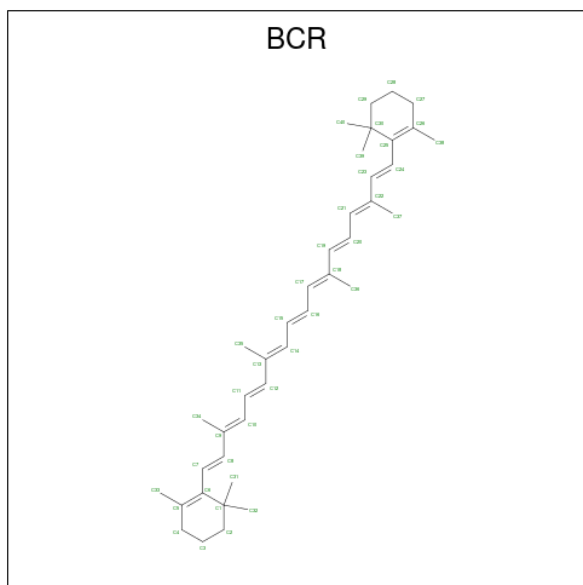
Mol	Chain	Residues	Atoms			AltConf
17	D	1	Total	Fe	S	0
			4	2	2	

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

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
18	H	1	Total	C	0
			40	40	
18	P	1	Total	C	0
			40	40	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	A	29	Total	O	0
			29	29	
19	B	16	Total	O	0
			16	16	
19	C	48	Total	O	0
			48	48	
19	D	6	Total	O	0
			6	6	
19	G	1	Total	O	0
			1	1	
19	H	3	Total	O	0
			3	3	

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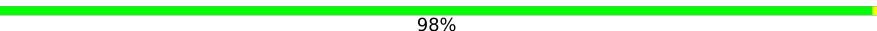
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Mol	Chain	Residues	Atoms		AltConf
19	I	29	Total 29	O 29	0
19	J	16	Total 16	O 16	0
19	K	48	Total 48	O 48	0
19	L	6	Total 6	O 6	0
19	O	1	Total 1	O 1	0
19	P	3	Total 3	O 3	0

3 Residue-property plots

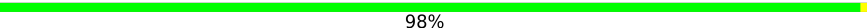
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

Chain A:  98%

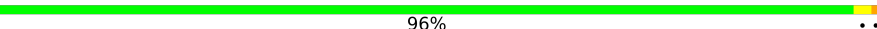


- Molecule 1: Cytochrome b6

Chain I:  98%



- Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:  96%



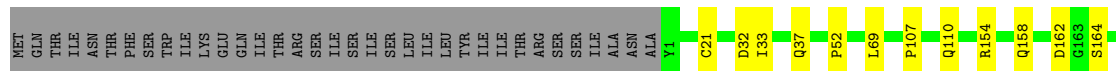
- Molecule 2: Cytochrome b6-f complex subunit 4

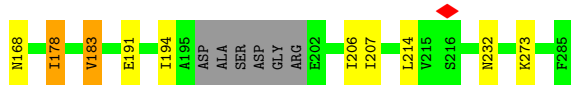
Chain J:  96%



- Molecule 3: Cytochrome f

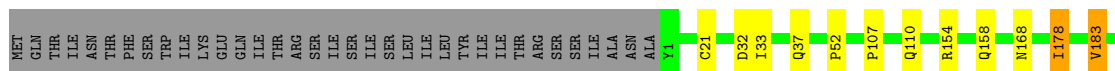
Chain C:  80% 6% 13%





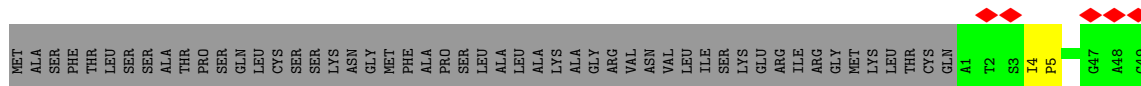
- Molecule 3: Cytochrome f

Chain K: 81% 5% 13%



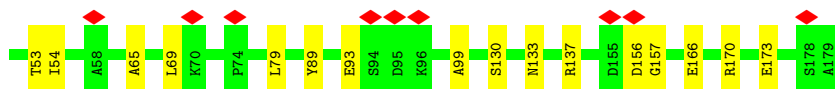
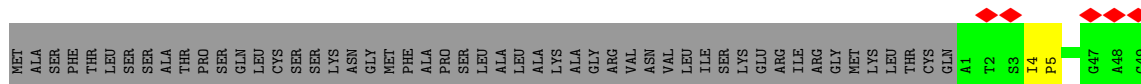
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain D: 6% 69% 9% 22%



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

Chain L: 6% 70% 8% 22%



- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: Cytochrome b6-f complex subunit 6

Chain M: 100%

There are no outlier residues recorded for this chain.

- Molecule 6: cytochrome b6-f complex subunit 7

Chain F:  28% 72%

MET ALA THR ALA VAL ALA SER THR THR SER SER ALA ALA VAL PRO ILE SER GLY SER ARG GLN ARG LYS MET ASN LYS THR VAL THR MET SER GLY VAL ASN SER TYR GLY GLY LEU LYS ALA ASN ASN ALA VAL LEU GLY LEU GLN ALA VAL CYS THR GLN CYS

PHE ALA ASN VAL VAL SER SER LEU ARG THR THR LYS LYS ARG SER GLY GLY GLY GLY ALA GLY GLY MET ASN LYS THR THR THR CYS N1 A37 GLU

- Molecule 6: cytochrome b6-f complex subunit 7

Chain N:  28% 72%

MET ALA THR ALA VAL ALA SER THR THR SER SER ALA ALA VAL PRO ILE SER GLY SER ARG GLN ARG LYS MET ASN LYS THR VAL THR MET SER GLY VAL ASN SER TYR GLY GLY LEU LYS ALA ASN ASN ALA VAL LEU GLY LEU GLN ALA VAL CYS THR GLN CYS

PHE ALA ASN VAL VAL SER SER LEU ARG THR THR LYS LYS ARG SER GLY GLY GLY GLY ALA GLY GLY MET ASN LYS THR THR THR CYS N1 A37 GLU

- Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:  86% 11%

H1 R31 G32 D33 GLN LEU ASP LEU

- Molecule 7: Cytochrome b6-f complex subunit 5

Chain O:  86% 11%

H1 R31 G32 D33 GLN LEU ASP LEU

- Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:  93% 7%

H1 D2 L29

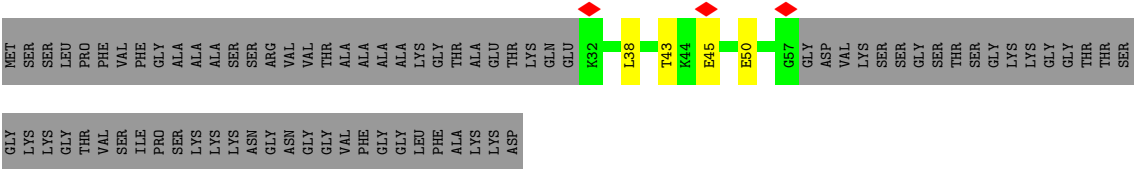
- Molecule 8: Cytochrome b6-f complex subunit 8

Chain P:  93% 7%

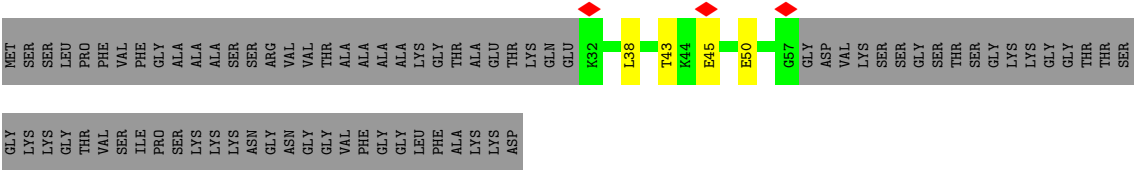
H1 D2 L29

- Molecule 9: Thylakoid soluble phosphoprotein

Chain Q:  21% 75%



● Molecule 9: Thylakoid soluble phosphoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	389849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.34	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	1.838	Depositor
Minimum map value	-0.572	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.204	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.14	0/1747	0.23	0/2382
1	I	0.14	0/1747	0.23	0/2382
2	B	0.15	0/1263	0.24	0/1733
2	J	0.15	0/1263	0.24	0/1733
3	C	0.12	0/2214	0.25	0/2999
3	K	0.13	0/2214	0.25	0/2999
4	D	0.11	0/1370	0.25	0/1875
4	L	0.11	0/1370	0.25	0/1875
5	E	0.15	0/247	0.17	0/333
5	M	0.15	0/247	0.17	0/333
6	F	0.14	0/282	0.17	0/382
6	N	0.14	0/282	0.17	0/382
7	G	0.16	0/266	0.19	0/360
7	O	0.16	0/266	0.19	0/360
8	H	0.17	0/227	0.19	0/309
8	P	0.16	0/227	0.19	0/309
9	Q	0.15	0/224	0.22	0/301
9	R	0.15	0/224	0.22	0/301
All	All	0.13	0/15680	0.24	0/21348

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	0	1724	2	0
1	I	1697	0	1724	2	0
2	B	1226	0	1276	5	0
2	J	1226	0	1276	5	0
3	C	2168	0	2218	17	0
3	K	2168	0	2218	15	0
4	D	1334	0	1304	14	0
4	L	1334	0	1304	13	0
5	E	243	0	268	0	0
5	M	243	0	268	0	0
6	F	280	0	295	0	0
6	N	280	0	295	0	0
7	G	261	0	280	1	0
7	O	261	0	280	1	0
8	H	222	0	234	2	0
8	P	222	0	234	2	0
9	Q	219	0	216	3	0
9	R	219	0	216	3	0
10	A	86	0	60	9	0
10	I	86	0	60	9	0
11	A	43	0	31	1	0
11	C	43	0	31	2	0
11	I	43	0	31	1	0
11	K	43	0	31	2	0
12	A	34	0	44	0	0
12	H	34	0	44	1	0
12	I	34	0	44	0	0
12	P	34	0	44	1	0
13	A	55	0	86	1	0
13	I	55	0	86	1	0
14	A	14	0	10	1	0
14	I	14	0	10	1	0
15	B	65	0	72	0	0
15	J	65	0	72	0	0
16	D	54	0	78	0	0
16	L	54	0	78	0	0
17	D	4	0	0	1	0
17	L	4	0	0	1	0
18	H	40	0	56	0	0
18	P	40	0	56	1	0
19	A	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	16	0	0	2	0
19	C	48	0	0	2	0
19	D	6	0	0	0	0
19	G	1	0	0	0	0
19	H	3	0	0	0	0
19	I	29	0	0	1	0
19	J	16	0	0	2	0
19	K	48	0	0	2	0
19	L	6	0	0	0	0
19	O	1	0	0	0	0
19	P	3	0	0	0	0
All	All	16450	0	16654	106	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 3.

All (106) 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)
2:J:35:ASP:OD2	19:J:301:HOH:O	2.00	0.80
2:B:35:ASP:OD2	19:B:301:HOH:O	1.99	0.79
4:D:4:ILE:HD12	4:D:5:PRO:HD2	1.65	0.79
4:L:4:ILE:HD12	4:L:5:PRO:HD2	1.65	0.77
2:J:35:ASP:OD1	19:J:302:HOH:O	2.02	0.76
2:B:35:ASP:OD1	19:B:302:HOH:O	2.02	0.75
3:K:21:CYS:HB2	11:K:301:HEC:HAB	1.71	0.72
3:C:21:CYS:HB2	11:C:301:HEC:HAB	1.71	0.72
3:K:168:ASN:OD1	19:K:401:HOH:O	2.07	0.71
3:C:168:ASN:OD1	19:C:401:HOH:O	2.09	0.71
3:C:273:LYS:O	19:C:402:HOH:O	2.10	0.70
4:D:137:ARG:NH1	4:D:170:ARG:O	2.25	0.70
3:K:273:LYS:O	19:K:402:HOH:O	2.10	0.70
3:C:158:GLN:NE2	3:C:232:ASN:OD1	2.26	0.69
3:K:158:GLN:NE2	3:K:232:ASN:OD1	2.26	0.69
4:L:137:ARG:NH1	4:L:170:ARG:O	2.25	0.69
4:L:133:ASN:OD1	4:L:137:ARG:N	2.29	0.66
4:D:133:ASN:OD1	4:D:137:ARG:N	2.29	0.65
13:A:305:LMG:O5	13:A:305:LMG:O9	2.16	0.64
13:I:305:LMG:O5	13:I:305:LMG:O9	2.16	0.63
10:A:302:HEM:HMB1	10:A:302:HEM:HBB2	1.81	0.62
10:I:302:HEM:HMC1	10:I:302:HEM:HBC2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:302:HEM:HMC1	10:A:302:HEM:HBC2	1.82	0.61
10:I:301:HEM:HMC1	10:I:301:HEM:HBC2	1.82	0.61
10:A:301:HEM:HMC1	10:A:301:HEM:HBC2	1.82	0.61
10:I:302:HEM:HBB2	10:I:302:HEM:HMB1	1.81	0.60
2:J:58:GLU:OE2	3:K:37:GLN:NE2	2.35	0.60
10:A:301:HEM:HMB1	10:A:301:HEM:HBB2	1.83	0.60
2:B:58:GLU:OE2	3:C:37:GLN:NE2	2.35	0.59
4:L:130:SER:OG	17:L:202:FES:S2	2.54	0.59
10:I:301:HEM:HMB1	10:I:301:HEM:HBB2	1.83	0.58
3:K:107:PRO:O	3:K:110:GLN:NE2	2.37	0.58
3:C:107:PRO:O	3:C:110:GLN:NE2	2.37	0.57
4:L:53:THR:HG22	4:L:54:ILE:H	1.71	0.56
4:D:4:ILE:CD1	4:D:5:PRO:HD2	2.36	0.55
3:C:183:VAL:HG22	3:C:191:GLU:HB2	1.89	0.55
4:L:4:ILE:CD1	4:L:5:PRO:HD2	2.36	0.55
4:D:53:THR:HG22	4:D:54:ILE:H	1.71	0.55
2:B:121:GLN:N	9:Q:50:GLU:OE2	2.37	0.55
3:K:183:VAL:HG22	3:K:191:GLU:HB2	1.89	0.55
2:J:121:GLN:N	9:R:50:GLU:OE2	2.36	0.53
9:R:45:GLU:OE1	9:R:45:GLU:N	2.37	0.53
4:L:93:GLU:OE2	4:L:99:ALA:N	2.42	0.53
10:A:302:HEM:HBC2	10:A:302:HEM:CMC	2.38	0.53
4:D:65:ALA:O	4:D:69:LEU:HD23	2.09	0.53
10:I:302:HEM:HBC2	10:I:302:HEM:CMC	2.38	0.52
4:D:93:GLU:OE2	4:D:99:ALA:N	2.42	0.52
4:L:65:ALA:O	4:L:69:LEU:HD23	2.09	0.52
10:I:302:HEM:HBB2	10:I:302:HEM:CMB	2.40	0.52
10:A:301:HEM:HBC2	10:A:301:HEM:CMC	2.40	0.51
10:I:301:HEM:HBC2	10:I:301:HEM:CMC	2.40	0.51
10:A:302:HEM:HBB2	10:A:302:HEM:CMB	2.40	0.51
4:D:166:GLU:OE1	4:D:166:GLU:N	2.41	0.51
10:A:302:HEM:HBA1	10:A:302:HEM:HHA	1.93	0.51
10:I:301:HEM:HBB2	10:I:301:HEM:CMB	2.42	0.50
4:L:156:ASP:OD1	4:L:157:GLY:N	2.45	0.50
9:Q:45:GLU:OE1	9:Q:45:GLU:N	2.37	0.50
7:G:31:ARG:NH2	9:Q:43:THR:OG1	2.45	0.49
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	2.42	0.49
4:D:156:ASP:OD1	4:D:157:GLY:N	2.45	0.49
10:I:302:HEM:HBA1	10:I:302:HEM:HHA	1.93	0.49
8:H:2:ASP:OD2	12:H:102:UMQ:O4	2.27	0.49
4:D:173:GLU:OE1	4:D:173:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:173:GLU:N	4:L:173:GLU:OE1	2.46	0.49
4:L:166:GLU:OE1	4:L:166:GLU:N	2.41	0.48
3:C:206:ILE:C	3:C:207:ILE:HD12	2.38	0.48
2:B:118:ASN:OD1	2:B:119:LYS:N	2.47	0.48
3:K:178:ILE:HD12	3:K:178:ILE:O	2.13	0.48
3:K:206:ILE:C	3:K:207:ILE:HD12	2.38	0.48
3:C:178:ILE:HD12	3:C:178:ILE:O	2.13	0.47
2:J:118:ASN:OD1	2:J:119:LYS:N	2.47	0.47
1:A:210:GLY:O	19:A:401:HOH:O	2.21	0.46
1:I:210:GLY:O	19:I:401:HOH:O	2.21	0.46
8:P:2:ASP:OD2	12:P:102:UMQ:O4	2.27	0.46
1:I:52:PHE:O	1:I:55:THR:OG1	2.34	0.46
7:O:31:ARG:NH2	9:R:43:THR:OG1	2.49	0.46
3:C:162:ASP:CG	3:C:164:SER:HG	2.25	0.45
3:C:194:ILE:HD12	3:C:194:ILE:O	2.17	0.45
1:A:52:PHE:O	1:A:55:THR:OG1	2.34	0.45
14:I:306:BNT:BRAI	14:I:306:BNT:HAA3	2.72	0.45
8:H:29:LEU:C	8:H:29:LEU:HD23	2.42	0.45
14:A:306:BNT:BRAI	14:A:306:BNT:HAA3	2.72	0.45
8:P:29:LEU:C	8:P:29:LEU:HD23	2.42	0.44
11:C:301:HEC:CMC	11:C:301:HEC:HBC3	2.47	0.44
11:K:301:HEC:CMC	11:K:301:HEC:HBC3	2.48	0.44
4:L:79:LEU:HD21	4:L:89:TYR:CE2	2.53	0.44
3:K:194:ILE:HD12	3:K:194:ILE:O	2.17	0.44
3:C:52:PRO:O	3:C:154:ARG:NH1	2.51	0.43
11:A:303:HEC:HMC3	11:A:303:HEC:CBC	2.49	0.43
4:D:79:LEU:HD21	4:D:89:TYR:CE2	2.53	0.43
3:C:206:ILE:HD12	3:C:206:ILE:N	2.34	0.43
3:K:206:ILE:HD12	3:K:206:ILE:N	2.34	0.43
11:I:303:HEC:HMC3	11:I:303:HEC:CBC	2.49	0.43
3:K:52:PRO:O	3:K:154:ARG:NH1	2.51	0.42
4:D:130:SER:OG	17:D:202:FES:S2	2.54	0.42
3:C:194:ILE:HD12	3:C:194:ILE:C	2.45	0.42
3:K:32:ASP:OD1	3:K:33:ILE:N	2.53	0.42
3:K:214:LEU:H	3:K:214:LEU:HD23	1.86	0.41
3:C:32:ASP:OD1	3:C:33:ILE:N	2.53	0.41
4:D:167:THR:HG22	4:D:168:ASP:N	2.36	0.41
3:C:214:LEU:HD23	3:C:214:LEU:H	1.86	0.41
4:D:53:THR:HG22	4:D:54:ILE:N	2.35	0.41
3:K:194:ILE:HD12	3:K:194:ILE:C	2.45	0.41
4:L:53:THR:HG22	4:L:54:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:LEU:HD12	3:C:69:LEU:N	2.36	0.40
18:P:101:BCR:H20C	18:P:101:BCR:H361	1.91	0.40

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%)	206 (97%)	6 (3%)	0	100	100
1	I	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
2	B	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
2	J	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
3	C	275/320 (86%)	265 (96%)	10 (4%)	0	100	100
3	K	275/320 (86%)	265 (96%)	10 (4%)	0	100	100
4	D	177/230 (77%)	167 (94%)	10 (6%)	0	100	100
4	L	177/230 (77%)	167 (94%)	10 (6%)	0	100	100
5	E	29/31 (94%)	29 (100%)	0	0	100	100
5	M	29/31 (94%)	29 (100%)	0	0	100	100
6	F	36/131 (28%)	36 (100%)	0	0	100	100
6	N	36/131 (28%)	36 (100%)	0	0	100	100
7	G	31/37 (84%)	31 (100%)	0	0	100	100
7	O	31/37 (84%)	31 (100%)	0	0	100	100
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	27 (100%)	0	0	100	100
9	Q	24/103 (23%)	23 (96%)	1 (4%)	0	100	100
9	R	24/103 (23%)	23 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1936/2512 (77%)	1874 (97%)	62 (3%)	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%)	184 (100%)	1 (0%)	81	88
1	I	185/186 (100%)	184 (100%)	1 (0%)	81	88
2	B	134/135 (99%)	133 (99%)	1 (1%)	76	84
2	J	134/135 (99%)	133 (99%)	1 (1%)	76	84
3	C	238/275 (86%)	236 (99%)	2 (1%)	73	82
3	K	238/275 (86%)	236 (99%)	2 (1%)	73	82
4	D	141/183 (77%)	141 (100%)	0	100	100
4	L	141/183 (77%)	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	27/90 (30%)	27 (100%)	0	100	100
6	N	27/90 (30%)	27 (100%)	0	100	100
7	G	27/31 (87%)	27 (100%)	0	100	100
7	O	27/31 (87%)	27 (100%)	0	100	100
8	H	24/24 (100%)	24 (100%)	0	100	100
8	P	24/24 (100%)	24 (100%)	0	100	100
9	Q	24/78 (31%)	23 (96%)	1 (4%)	26	34
9	R	24/78 (31%)	23 (96%)	1 (4%)	26	34
All	All	1652/2056 (80%)	1642 (99%)	10 (1%)	76	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
2	B	119	LYS
3	C	178	ILE
3	C	183	VAL
1	I	75	GLU
2	J	119	LYS
3	K	178	ILE
3	K	183	VAL
9	Q	38	LEU
9	R	38	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	142	HIS
4	L	8	ASN
9	Q	47	GLN
9	R	47	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	BNT	A	306	-	12,14,14	0.70	0	13,21,21	1.00	1 (7%)
17	FES	L	202	4	0,4,4	-	-	-		
10	HEM	A	301	1	50,50,50	1.42	7 (14%)	67,82,82	1.12	5 (7%)
13	LMG	I	305	-	55,55,55	0.49	0	63,63,63	0.60	0
12	UMQ	P	102	-	35,35,35	0.54	0	46,46,46	0.64	0
11	HEC	C	301	3	46,50,50	1.83	5 (10%)	58,82,82	1.86	4 (6%)
16	SQD	D	201	-	52,54,54	1.54	6 (11%)	62,65,65	1.35	7 (11%)
10	HEM	I	302	1	50,50,50	1.40	6 (12%)	67,82,82	1.11	5 (7%)
12	UMQ	A	304	-	35,35,35	0.54	0	46,46,46	0.62	0
12	UMQ	H	102	-	35,35,35	0.54	0	46,46,46	0.64	0
14	BNT	I	306	-	12,14,14	0.70	0	13,21,21	1.01	1 (7%)
16	SQD	L	201	-	52,54,54	1.54	6 (11%)	62,65,65	1.36	8 (12%)
11	HEC	I	303	1	46,50,50	1.83	5 (10%)	58,82,82	1.56	4 (6%)
11	HEC	K	301	3	46,50,50	1.83	5 (10%)	58,82,82	1.86	4 (6%)
15	CLA	J	201	19	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
17	FES	D	202	4	0,4,4	-	-	-		
10	HEM	I	301	1	50,50,50	1.42	7 (14%)	67,82,82	1.12	5 (7%)
18	BCR	P	101	-	41,41,41	0.30	0	56,56,56	0.64	1 (1%)
13	LMG	A	305	-	55,55,55	0.49	0	63,63,63	0.60	0
10	HEM	A	302	1	50,50,50	1.40	6 (12%)	67,82,82	1.11	5 (7%)
15	CLA	B	201	19	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
12	UMQ	I	304	-	35,35,35	0.54	0	46,46,46	0.62	0
11	HEC	A	303	1	46,50,50	1.83	5 (10%)	58,82,82	1.56	4 (6%)
18	BCR	H	101	-	41,41,41	0.30	0	56,56,56	0.64	1 (1%)

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	BNT	A	306	-	-	0/4/28/28	0/1/1/1
17	FES	L	202	4	-	-	0/1/1/1
10	HEM	A	301	1	-	2/14/54/54	-
13	LMG	I	305	-	-	19/50/70/70	0/1/1/1
12	UMQ	P	102	-	-	1/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEC	C	301	3	-	6/14/54/54	-
16	SQD	D	201	-	-	15/49/69/69	0/1/1/1
10	HEM	I	302	1	-	2/14/54/54	-
12	UMQ	A	304	-	-	6/20/60/60	0/2/2/2
12	UMQ	H	102	-	-	1/20/60/60	0/2/2/2
14	BNT	I	306	-	-	0/4/28/28	0/1/1/1
16	SQD	L	201	-	-	15/49/69/69	0/1/1/1
11	HEC	I	303	1	-	4/14/54/54	-
15	CLA	J	201	19	1/1/15/20	12/39/115/115	-
11	HEC	K	301	3	-	6/14/54/54	-
17	FES	D	202	4	-	-	0/1/1/1
10	HEM	I	301	1	-	2/14/54/54	-
18	BCR	P	101	-	-	4/29/63/63	0/2/2/2
13	LMG	A	305	-	-	19/50/70/70	0/1/1/1
10	HEM	A	302	1	-	2/14/54/54	-
15	CLA	B	201	19	1/1/15/20	12/39/115/115	-
12	UMQ	I	304	-	-	6/20/60/60	0/2/2/2
11	HEC	A	303	1	-	4/14/54/54	-
18	BCR	H	101	-	-	4/29/63/63	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	303	HEC	CAC-C3C	6.20	1.55	1.35
11	I	303	HEC	CAC-C3C	6.20	1.55	1.35
11	K	301	HEC	CAC-C3C	6.19	1.55	1.35
11	C	301	HEC	CAC-C3C	6.19	1.55	1.35
11	A	303	HEC	CAB-C3B	6.10	1.54	1.35
11	I	303	HEC	CAB-C3B	6.10	1.54	1.35
11	C	301	HEC	CAB-C3B	6.09	1.54	1.35
11	K	301	HEC	CAB-C3B	6.09	1.54	1.35
11	K	301	HEC	C3D-C2D	5.65	1.53	1.38
11	C	301	HEC	C3D-C2D	5.65	1.53	1.38
11	A	303	HEC	C3D-C2D	5.61	1.53	1.38
11	I	303	HEC	C3D-C2D	5.61	1.53	1.38
16	D	201	SQD	O48-C23	4.67	1.47	1.33
16	L	201	SQD	O48-C23	4.66	1.46	1.33
16	D	201	SQD	O47-C45	-3.78	1.37	1.46
16	L	201	SQD	O47-C45	-3.78	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	201	CLA	C1D-ND	3.44	1.42	1.37
15	J	201	CLA	C1D-ND	3.44	1.42	1.37
10	A	301	HEM	FE-NB	3.29	2.05	1.94
10	I	301	HEM	FE-NB	3.29	2.05	1.94
16	L	201	SQD	O47-C7	3.26	1.43	1.34
16	D	201	SQD	O47-C7	3.26	1.43	1.34
10	A	301	HEM	FE-ND	3.23	2.04	1.94
10	I	301	HEM	FE-ND	3.23	2.04	1.94
10	A	302	HEM	FE-NB	3.12	2.04	1.94
10	I	302	HEM	FE-NB	3.12	2.04	1.94
10	A	302	HEM	FE-NA	3.11	2.05	1.95
10	I	302	HEM	FE-NA	3.11	2.05	1.95
10	A	302	HEM	FE-NC	3.09	2.05	1.95
10	I	302	HEM	FE-NC	3.09	2.05	1.95
16	D	201	SQD	O5-C1	3.07	1.49	1.41
10	A	301	HEM	FE-NC	3.06	2.05	1.95
10	I	301	HEM	FE-NC	3.06	2.05	1.95
10	A	301	HEM	FE-NA	3.05	2.05	1.95
10	I	301	HEM	FE-NA	3.05	2.05	1.95
16	L	201	SQD	O5-C1	3.03	1.49	1.41
10	A	301	HEM	CAC-C3C	2.98	1.55	1.47
10	I	301	HEM	CAC-C3C	2.98	1.55	1.47
10	A	302	HEM	CAB-C3B	2.96	1.55	1.47
10	I	302	HEM	CAB-C3B	2.96	1.55	1.47
16	D	201	SQD	C24-C23	2.96	1.59	1.50
10	A	301	HEM	CAB-C3B	2.95	1.55	1.47
10	I	301	HEM	CAB-C3B	2.95	1.55	1.47
10	A	302	HEM	FE-ND	2.94	2.04	1.94
10	I	302	HEM	FE-ND	2.94	2.04	1.94
16	L	201	SQD	C24-C23	2.93	1.59	1.50
10	A	302	HEM	CAC-C3C	2.88	1.55	1.47
10	I	302	HEM	CAC-C3C	2.88	1.55	1.47
15	B	201	CLA	C4B-NB	2.87	1.41	1.37
15	J	201	CLA	C4B-NB	2.87	1.41	1.37
15	B	201	CLA	C1B-C2B	2.80	1.49	1.43
15	J	201	CLA	C1B-C2B	2.80	1.49	1.43
11	K	301	HEC	C3B-C2B	-2.19	1.33	1.41
11	C	301	HEC	C3B-C2B	-2.18	1.33	1.41
15	B	201	CLA	CHC-C1C	2.18	1.42	1.38
15	J	201	CLA	CHC-C1C	2.18	1.42	1.38
11	A	303	HEC	C3B-C2B	-2.15	1.33	1.41
11	I	303	HEC	C3B-C2B	-2.15	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	201	CLA	C3B-C4B	2.08	1.48	1.42
15	J	201	CLA	C3B-C4B	2.08	1.48	1.42
15	B	201	CLA	CMB-C2B	-2.08	1.46	1.50
15	J	201	CLA	CMB-C2B	-2.08	1.46	1.50
15	B	201	CLA	CMD-C2D	-2.05	1.46	1.50
15	J	201	CLA	CMD-C2D	-2.05	1.46	1.50
11	K	301	HEC	C3C-C2C	-2.04	1.34	1.41
16	D	201	SQD	O9-S	2.04	1.50	1.45
16	L	201	SQD	O9-S	2.03	1.50	1.45
11	C	301	HEC	C3C-C2C	-2.03	1.34	1.41
15	B	201	CLA	MG-NB	-2.03	2.01	2.05
15	J	201	CLA	MG-NB	-2.03	2.01	2.05
11	A	303	HEC	C3C-C2C	-2.02	1.34	1.41
11	I	303	HEC	C3C-C2C	-2.02	1.34	1.41
10	A	301	HEM	CMD-C2D	2.02	1.54	1.50
10	I	301	HEM	CMD-C2D	2.02	1.54	1.50

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	301	HEC	CBB-CAB-C3B	-8.58	110.28	127.43
11	K	301	HEC	CBB-CAB-C3B	-8.57	110.31	127.43
11	A	303	HEC	CBB-CAB-C3B	-8.44	110.56	127.43
11	I	303	HEC	CBB-CAB-C3B	-8.44	110.56	127.43
11	C	301	HEC	CBC-CAC-C3C	-7.83	111.79	127.43
11	K	301	HEC	CBC-CAC-C3C	-7.81	111.83	127.43
15	B	201	CLA	C4A-NA-C1A	6.44	109.61	106.68
15	J	201	CLA	C4A-NA-C1A	6.44	109.61	106.68
16	L	201	SQD	O9-S-O7	-3.87	101.25	113.82
16	D	201	SQD	O47-C7-C8	3.83	119.78	111.48
16	L	201	SQD	O47-C7-C8	3.83	119.77	111.48
16	D	201	SQD	O9-S-O7	-3.83	101.37	113.82
11	A	303	HEC	C4D-ND-C1D	3.46	111.46	105.82
11	I	303	HEC	C4D-ND-C1D	3.46	111.46	105.82
11	K	301	HEC	C4D-ND-C1D	3.44	111.42	105.82
11	C	301	HEC	C4D-ND-C1D	3.42	111.40	105.82
16	L	201	SQD	O9-S-C6	3.39	111.81	106.76
16	D	201	SQD	O9-S-C6	3.31	111.70	106.76
15	B	201	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
15	J	201	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
16	L	201	SQD	O7-S-C6	3.12	111.41	106.76
16	D	201	SQD	O7-S-C6	3.11	111.40	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	201	SQD	O48-C23-C24	2.87	120.58	111.83
16	D	201	SQD	O48-C23-C24	2.85	120.52	111.83
15	B	201	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	J	201	CLA	C3B-C4B-NB	-2.70	108.12	110.53
16	D	201	SQD	O6-C1-C2	2.56	112.17	108.27
16	L	201	SQD	O6-C1-C2	2.52	112.10	108.27
10	A	302	HEM	C4D-ND-C1D	2.49	108.15	105.21
10	I	302	HEM	C4D-ND-C1D	2.49	108.15	105.21
10	A	301	HEM	C4D-ND-C1D	2.45	108.11	105.21
10	I	301	HEM	C4D-ND-C1D	2.45	108.11	105.21
15	B	201	CLA	CHB-C4A-NA	2.38	127.83	124.40
15	J	201	CLA	CHB-C4A-NA	2.38	127.83	124.40
10	A	302	HEM	C3B-C2B-C1B	2.37	108.19	106.41
10	I	302	HEM	C3B-C2B-C1B	2.37	108.19	106.41
10	A	302	HEM	C3D-C4D-ND	-2.36	107.58	110.17
10	I	302	HEM	C3D-C4D-ND	-2.36	107.58	110.17
11	A	303	HEC	CBC-CAC-C3C	-2.33	122.78	127.43
11	I	303	HEC	CBC-CAC-C3C	-2.33	122.78	127.43
11	A	303	HEC	C2A-C1A-NA	-2.32	108.08	110.32
11	I	303	HEC	C2A-C1A-NA	-2.32	108.08	110.32
10	A	302	HEM	C1B-NB-C4B	2.30	107.93	105.21
10	I	302	HEM	C1B-NB-C4B	2.30	107.93	105.21
18	H	101	BCR	C2-C1-C6	2.29	113.76	110.44
18	P	101	BCR	C2-C1-C6	2.29	113.76	110.44
10	A	301	HEM	C1B-NB-C4B	2.28	107.90	105.21
10	I	301	HEM	C1B-NB-C4B	2.28	107.90	105.21
14	I	306	BNT	BRAI-CAJ-CAK	-2.27	112.10	116.16
10	A	301	HEM	C3D-C4D-ND	-2.26	107.69	110.17
10	I	301	HEM	C3D-C4D-ND	-2.26	107.69	110.17
14	A	306	BNT	BRAI-CAJ-CAK	-2.25	112.14	116.16
16	L	201	SQD	O8-S-C6	2.21	110.24	105.97
16	D	201	SQD	O8-S-C6	2.21	110.24	105.97
10	A	301	HEM	C2A-C1A-NA	-2.20	107.71	110.15
10	I	301	HEM	C2A-C1A-NA	-2.20	107.71	110.15
10	A	301	HEM	C3B-C2B-C1B	2.19	108.05	106.41
10	I	301	HEM	C3B-C2B-C1B	2.19	108.05	106.41
11	C	301	HEC	C2A-C1A-NA	-2.16	108.24	110.32
11	K	301	HEC	C2A-C1A-NA	-2.13	108.27	110.32
10	A	302	HEM	C2A-C1A-NA	-2.08	107.84	110.15
10	I	302	HEM	C2A-C1A-NA	-2.08	107.84	110.15
15	B	201	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
15	J	201	CLA	O2A-CGA-O1A	-2.02	118.56	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	201	SQD	C1-O5-C5	-2.00	109.81	113.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	B	201	CLA	ND
15	J	201	CLA	ND

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	302	HEM	C1A-C2A-CAA-CBA
10	I	302	HEM	C1A-C2A-CAA-CBA
11	A	303	HEC	C2B-C3B-CAB-CBB
11	A	303	HEC	C4B-C3B-CAB-CBB
11	C	301	HEC	C2B-C3B-CAB-CBB
11	C	301	HEC	C4B-C3B-CAB-CBB
11	C	301	HEC	C2C-C3C-CAC-CBC
11	C	301	HEC	C4C-C3C-CAC-CBC
11	I	303	HEC	C2B-C3B-CAB-CBB
11	I	303	HEC	C4B-C3B-CAB-CBB
11	K	301	HEC	C2B-C3B-CAB-CBB
11	K	301	HEC	C4B-C3B-CAB-CBB
11	K	301	HEC	C2C-C3C-CAC-CBC
11	K	301	HEC	C4C-C3C-CAC-CBC
12	A	304	UMQ	O5'-C1'-O1'-CA
12	I	304	UMQ	O5'-C1'-O1'-CA
13	A	305	LMG	O9-C10-O7-C8
13	I	305	LMG	O9-C10-O7-C8
15	B	201	CLA	C1A-C2A-CAA-CBA
15	J	201	CLA	C1A-C2A-CAA-CBA
16	D	201	SQD	O6-C44-C45-O47
16	L	201	SQD	O6-C44-C45-O47
13	A	305	LMG	O10-C28-O8-C9
13	I	305	LMG	O10-C28-O8-C9
13	A	305	LMG	C29-C28-O8-C9
13	I	305	LMG	C29-C28-O8-C9
15	B	201	CLA	C3-C5-C6-C7
15	J	201	CLA	C3-C5-C6-C7
13	A	305	LMG	C11-C10-O7-C8
13	I	305	LMG	C11-C10-O7-C8
16	D	201	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
16	L	201	SQD	C24-C23-O48-C46
16	D	201	SQD	O10-C23-O48-C46
16	L	201	SQD	O10-C23-O48-C46
12	A	304	UMQ	O5'-C5'-C6'-O6'
12	I	304	UMQ	O5'-C5'-C6'-O6'
12	A	304	UMQ	C4'-C5'-C6'-O6'
12	I	304	UMQ	C4'-C5'-C6'-O6'
12	A	304	UMQ	O5-C5-C6-O6
12	I	304	UMQ	O5-C5-C6-O6
12	A	304	UMQ	C4-C5-C6-O6
12	I	304	UMQ	C4-C5-C6-O6
15	B	201	CLA	C8-C10-C11-C12
15	J	201	CLA	C8-C10-C11-C12
13	A	305	LMG	O6-C5-C6-O5
13	I	305	LMG	O6-C5-C6-O5
13	A	305	LMG	C4-C5-C6-O5
13	I	305	LMG	C4-C5-C6-O5
10	A	302	HEM	C3A-C2A-CAA-CBA
10	I	302	HEM	C3A-C2A-CAA-CBA
13	A	305	LMG	C2-C1-O1-C7
13	I	305	LMG	C2-C1-O1-C7
10	A	301	HEM	C2A-CAA-CBA-CGA
10	I	301	HEM	C2A-CAA-CBA-CGA
15	B	201	CLA	C2A-CAA-CBA-CGA
15	J	201	CLA	C2A-CAA-CBA-CGA
13	A	305	LMG	O6-C1-O1-C7
13	I	305	LMG	O6-C1-O1-C7
16	D	201	SQD	C25-C26-C27-C28
16	L	201	SQD	C25-C26-C27-C28
12	H	102	UMQ	CF-CG-CH-CI
12	P	102	UMQ	CF-CG-CH-CI
15	B	201	CLA	C3A-C2A-CAA-CBA
15	J	201	CLA	C3A-C2A-CAA-CBA
13	A	305	LMG	C11-C12-C13-C14
13	I	305	LMG	C11-C12-C13-C14
16	D	201	SQD	C9-C10-C11-C12
16	L	201	SQD	C9-C10-C11-C12
18	H	101	BCR	C7-C8-C9-C34
18	P	101	BCR	C7-C8-C9-C34
16	D	201	SQD	C33-C34-C35-C36
16	L	201	SQD	C33-C34-C35-C36
13	A	305	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
13	I	305	LMG	C34-C35-C36-C37
15	B	201	CLA	CBA-CGA-O2A-C1
15	J	201	CLA	CBA-CGA-O2A-C1
13	I	305	LMG	C15-C16-C17-C18
13	A	305	LMG	C15-C16-C17-C18
16	D	201	SQD	O6-C44-C45-C46
16	L	201	SQD	O6-C44-C45-C46
13	I	305	LMG	C35-C36-C37-C38
13	A	305	LMG	C35-C36-C37-C38
13	A	305	LMG	C28-C29-C30-C31
13	I	305	LMG	C28-C29-C30-C31
15	B	201	CLA	O1A-CGA-O2A-C1
15	J	201	CLA	O1A-CGA-O2A-C1
16	D	201	SQD	C30-C31-C32-C33
16	L	201	SQD	C30-C31-C32-C33
13	A	305	LMG	C41-C42-C43-C44
13	I	305	LMG	C41-C42-C43-C44
13	A	305	LMG	C40-C41-C42-C43
13	I	305	LMG	C40-C41-C42-C43
13	I	305	LMG	C22-C23-C24-C25
13	A	305	LMG	C22-C23-C24-C25
16	D	201	SQD	C15-C16-C17-C18
16	L	201	SQD	C15-C16-C17-C18
11	A	303	HEC	C3D-CAD-CBD-CGD
11	I	303	HEC	C3D-CAD-CBD-CGD
18	H	101	BCR	C7-C8-C9-C10
18	P	101	BCR	C7-C8-C9-C10
16	D	201	SQD	O47-C45-C46-O48
16	D	201	SQD	C17-C18-C19-C20
16	L	201	SQD	C17-C18-C19-C20
11	A	303	HEC	C1A-C2A-CAA-CBA
11	I	303	HEC	C1A-C2A-CAA-CBA
16	L	201	SQD	O47-C45-C46-O48
18	H	101	BCR	C11-C10-C9-C34
18	P	101	BCR	C11-C10-C9-C34
18	H	101	BCR	C11-C10-C9-C8
18	P	101	BCR	C11-C10-C9-C8
16	L	201	SQD	C19-C20-C21-C22
16	D	201	SQD	C19-C20-C21-C22
13	A	305	LMG	C21-C22-C23-C24
13	I	305	LMG	C21-C22-C23-C24
11	C	301	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	K	301	HEC	CAA-CBA-CGA-O2A
13	A	305	LMG	C39-C40-C41-C42
13	I	305	LMG	C39-C40-C41-C42
13	A	305	LMG	C37-C38-C39-C40
13	I	305	LMG	C37-C38-C39-C40
12	A	304	UMQ	CD-CF-CG-CH
12	I	304	UMQ	CD-CF-CG-CH
15	B	201	CLA	C5-C6-C7-C8
15	J	201	CLA	C5-C6-C7-C8
15	B	201	CLA	C12-C13-C15-C16
15	J	201	CLA	C12-C13-C15-C16
11	C	301	HEC	CAA-CBA-CGA-O1A
11	K	301	HEC	CAA-CBA-CGA-O1A
16	L	201	SQD	C26-C27-C28-C29
15	B	201	CLA	C4-C3-C5-C6
15	J	201	CLA	C4-C3-C5-C6
16	D	201	SQD	C26-C27-C28-C29
16	L	201	SQD	C44-C45-C46-O48
15	B	201	CLA	C13-C15-C16-C17
15	J	201	CLA	C13-C15-C16-C17
16	D	201	SQD	C12-C13-C14-C15
16	L	201	SQD	C12-C13-C14-C15
16	D	201	SQD	C44-C45-C46-O48
10	A	301	HEM	CAA-CBA-CGA-O2A
10	I	301	HEM	CAA-CBA-CGA-O2A
15	B	201	CLA	CAA-CBA-CGA-O2A
15	J	201	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

17 monomers are involved in 33 short contacts:

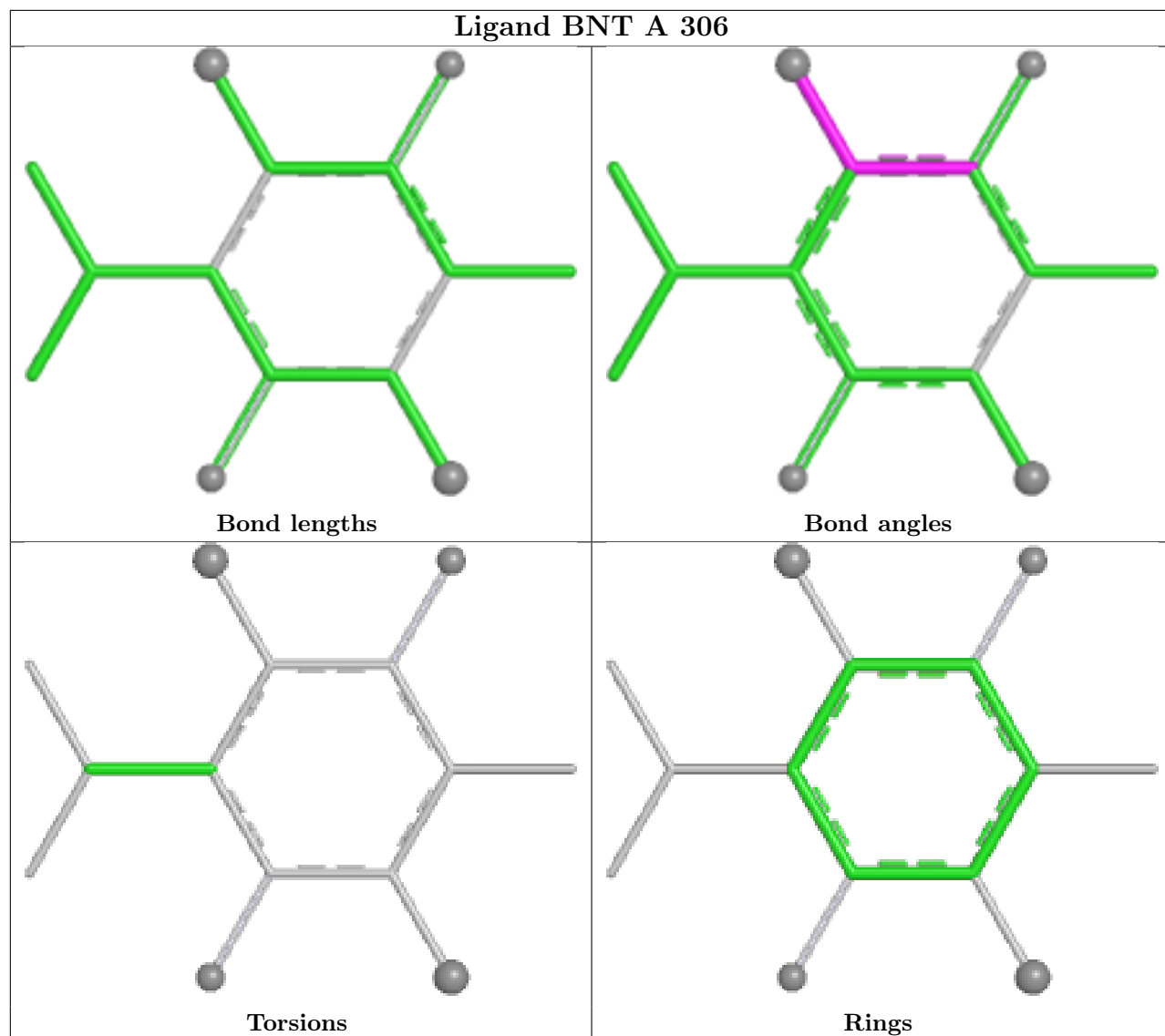
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	306	BNT	1	0
17	L	202	FES	1	0
10	A	301	HEM	4	0
13	I	305	LMG	1	0
12	P	102	UMQ	1	0
11	C	301	HEC	2	0
10	I	302	HEM	5	0
12	H	102	UMQ	1	0
14	I	306	BNT	1	0
11	I	303	HEC	1	0

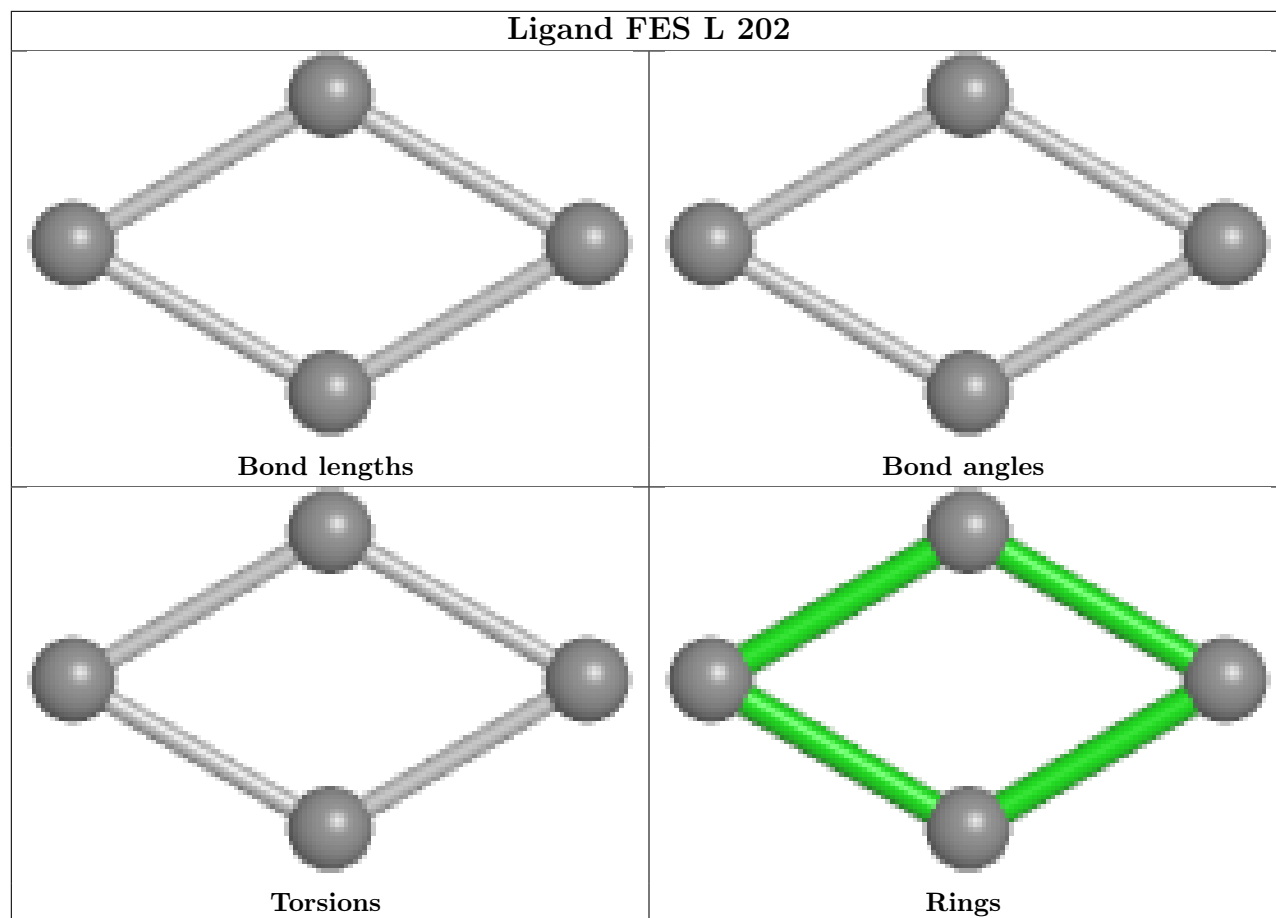
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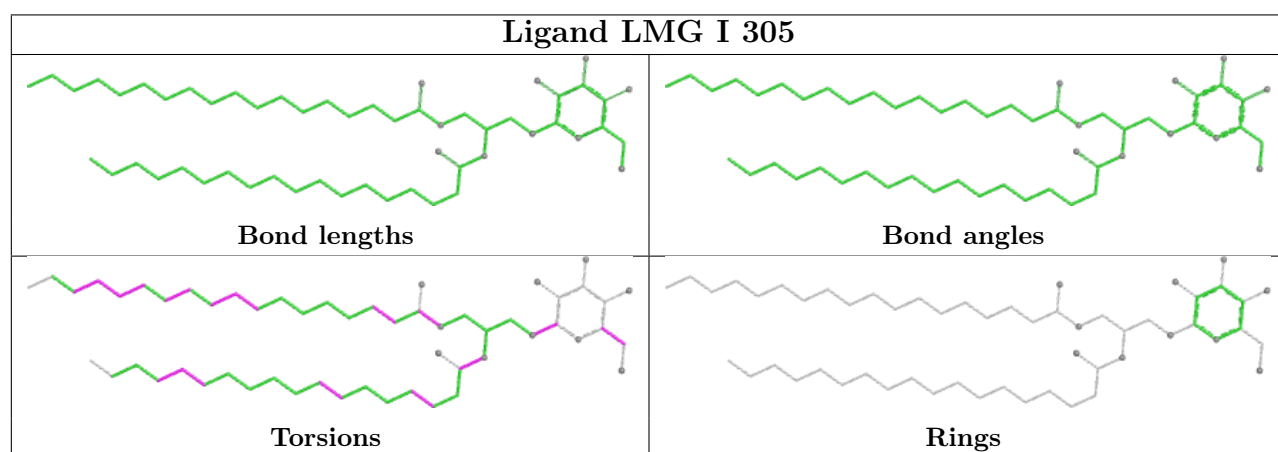
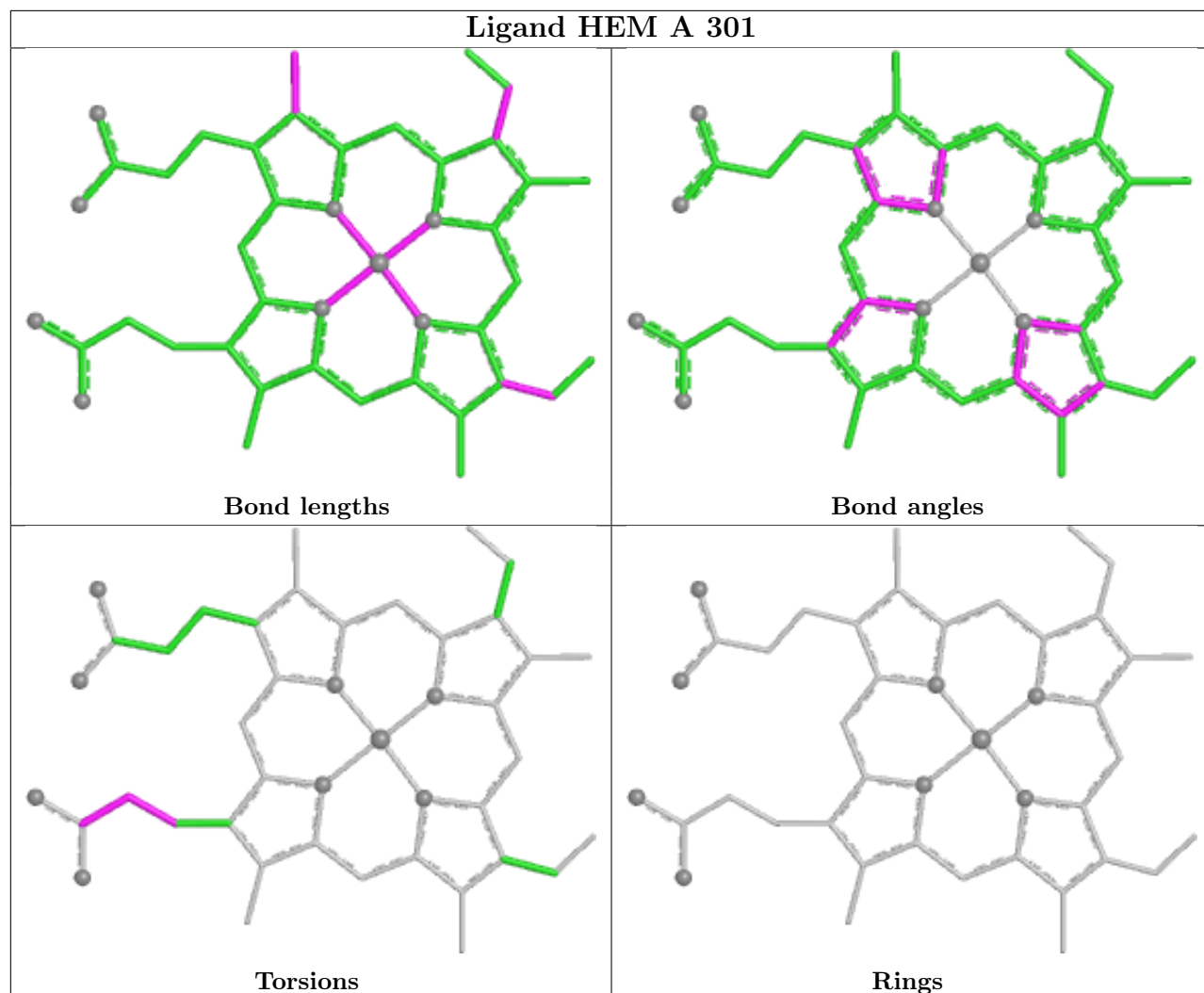
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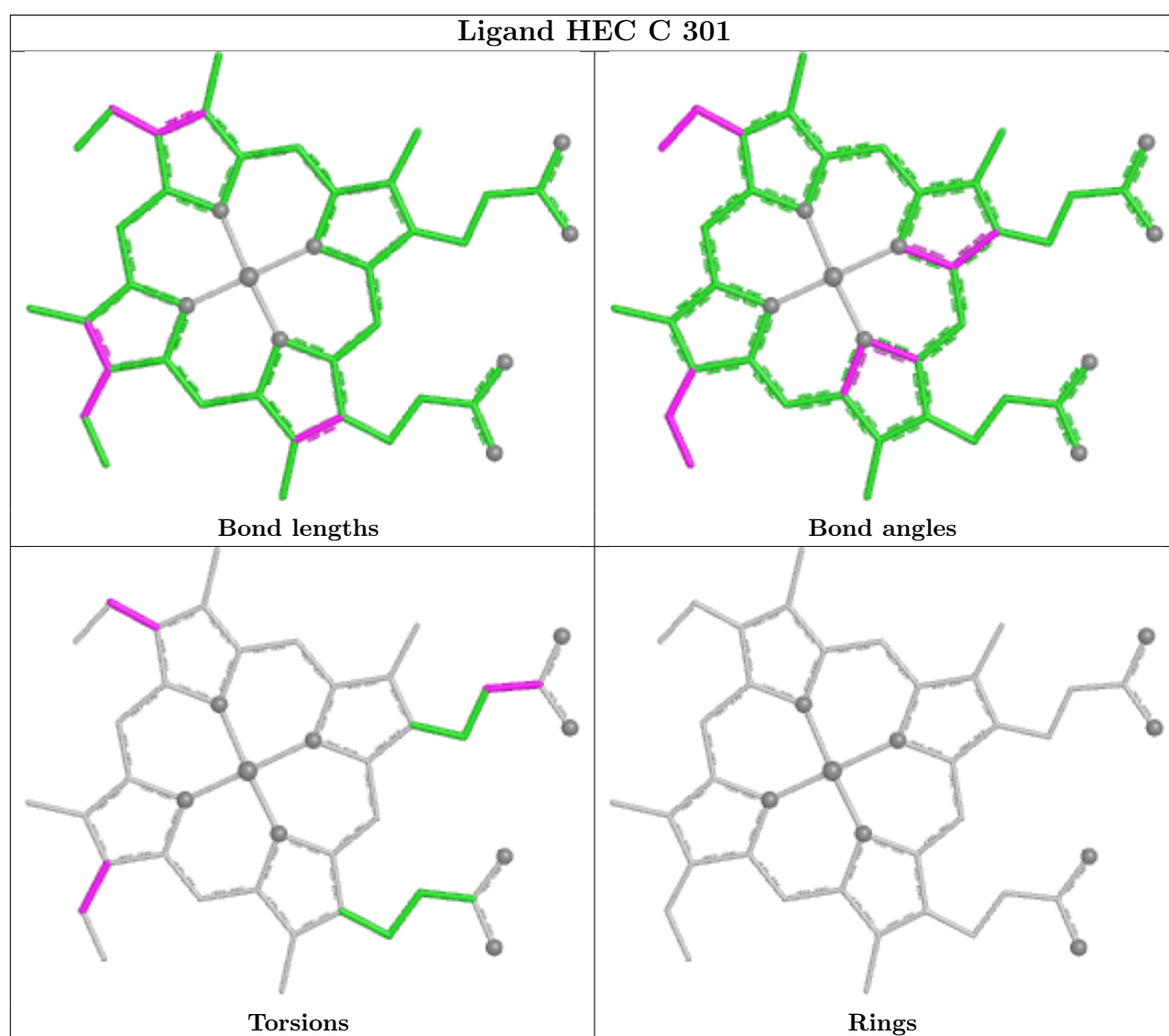
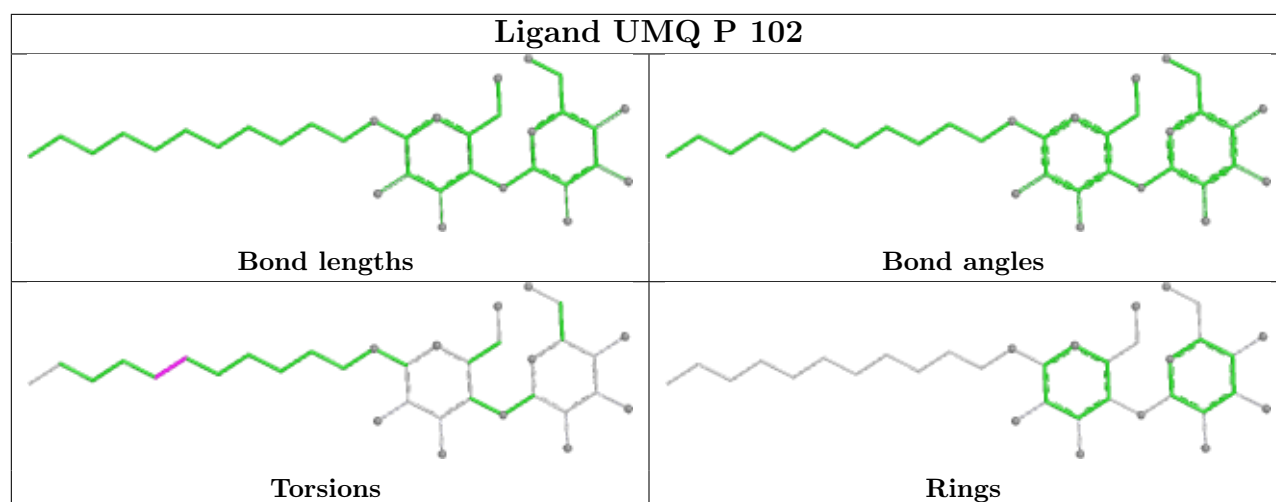
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	301	HEC	2	0
17	D	202	FES	1	0
10	I	301	HEM	4	0
18	P	101	BCR	1	0
13	A	305	LMG	1	0
10	A	302	HEM	5	0
11	A	303	HEC	1	0

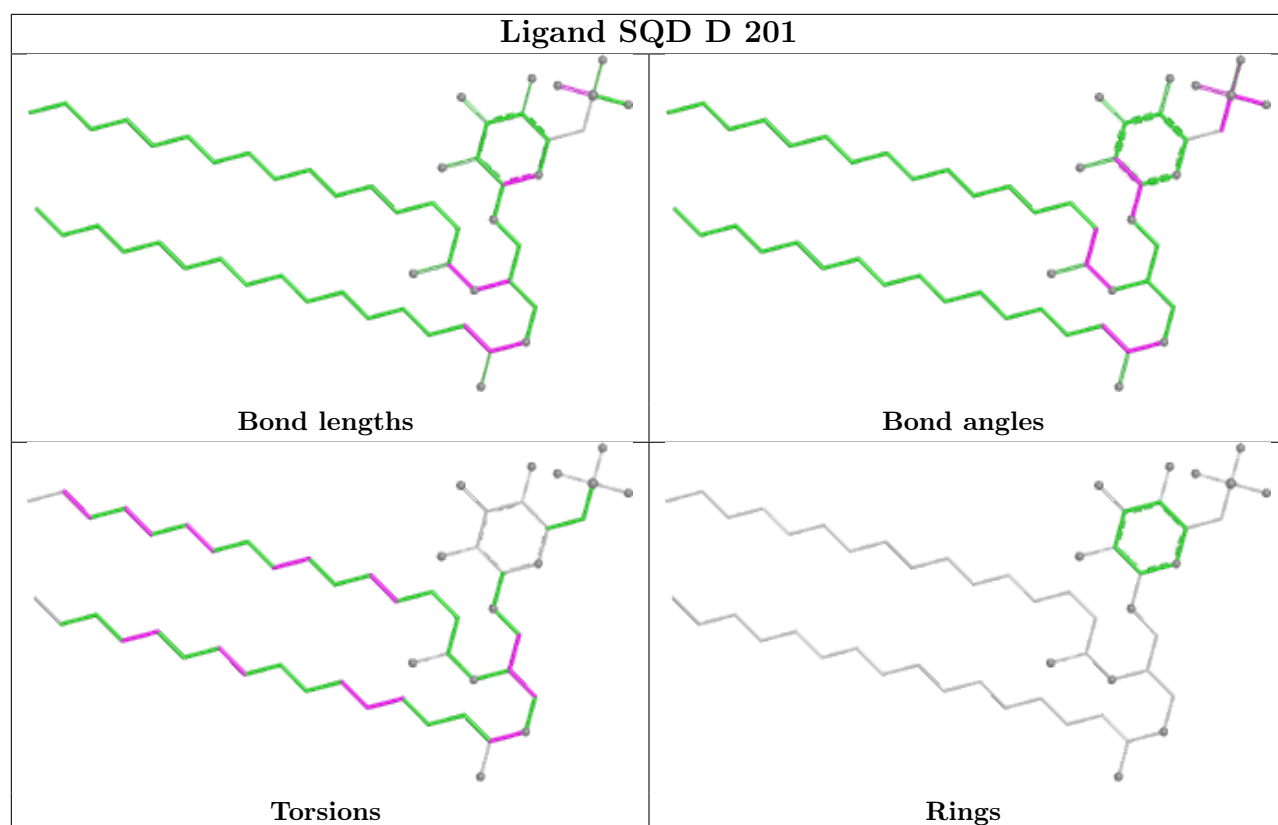
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



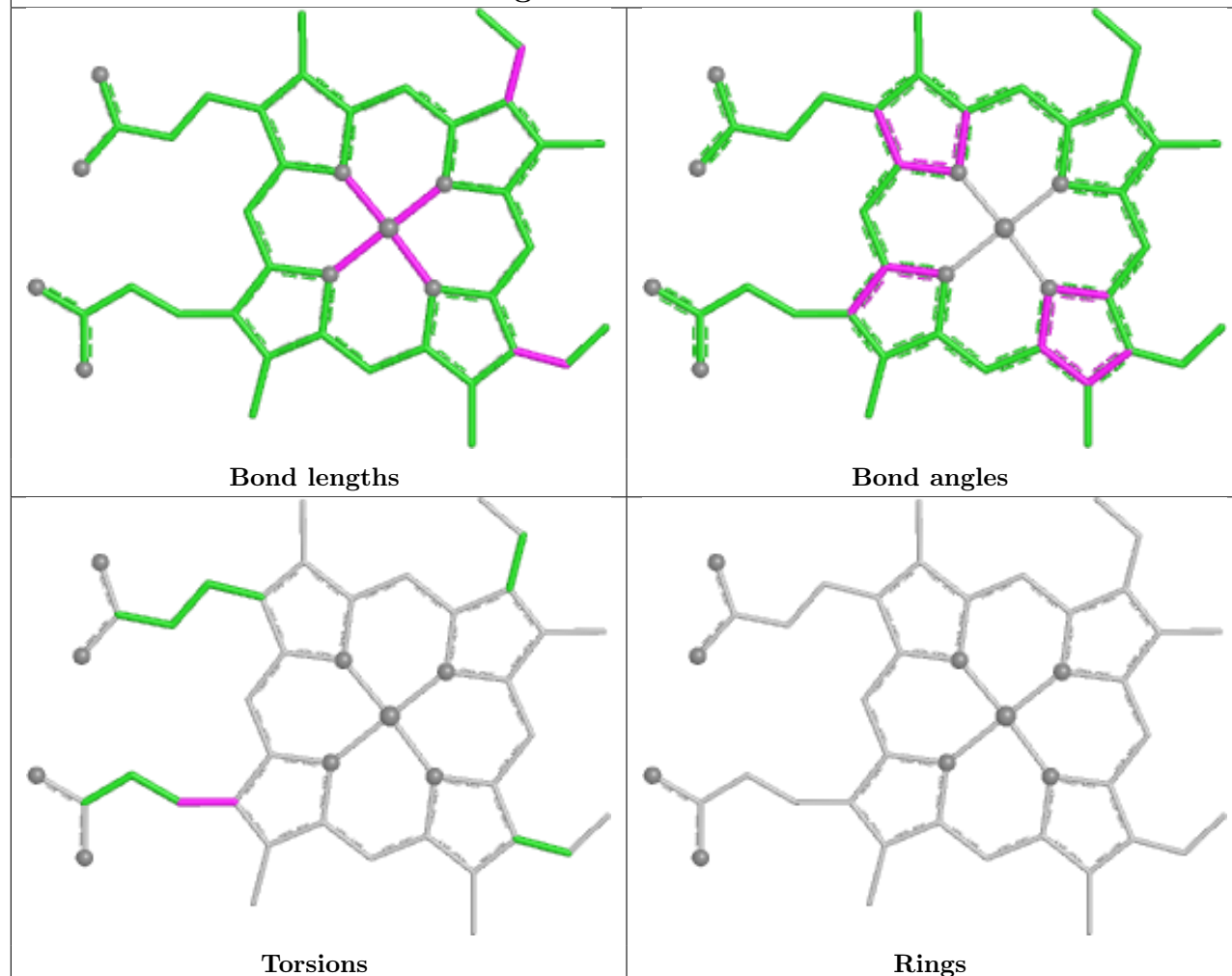




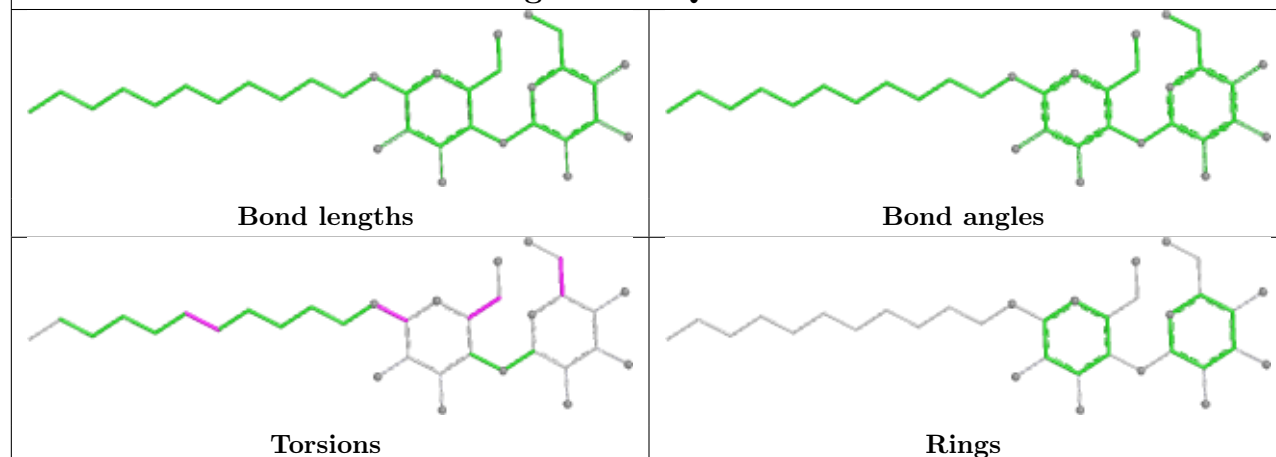


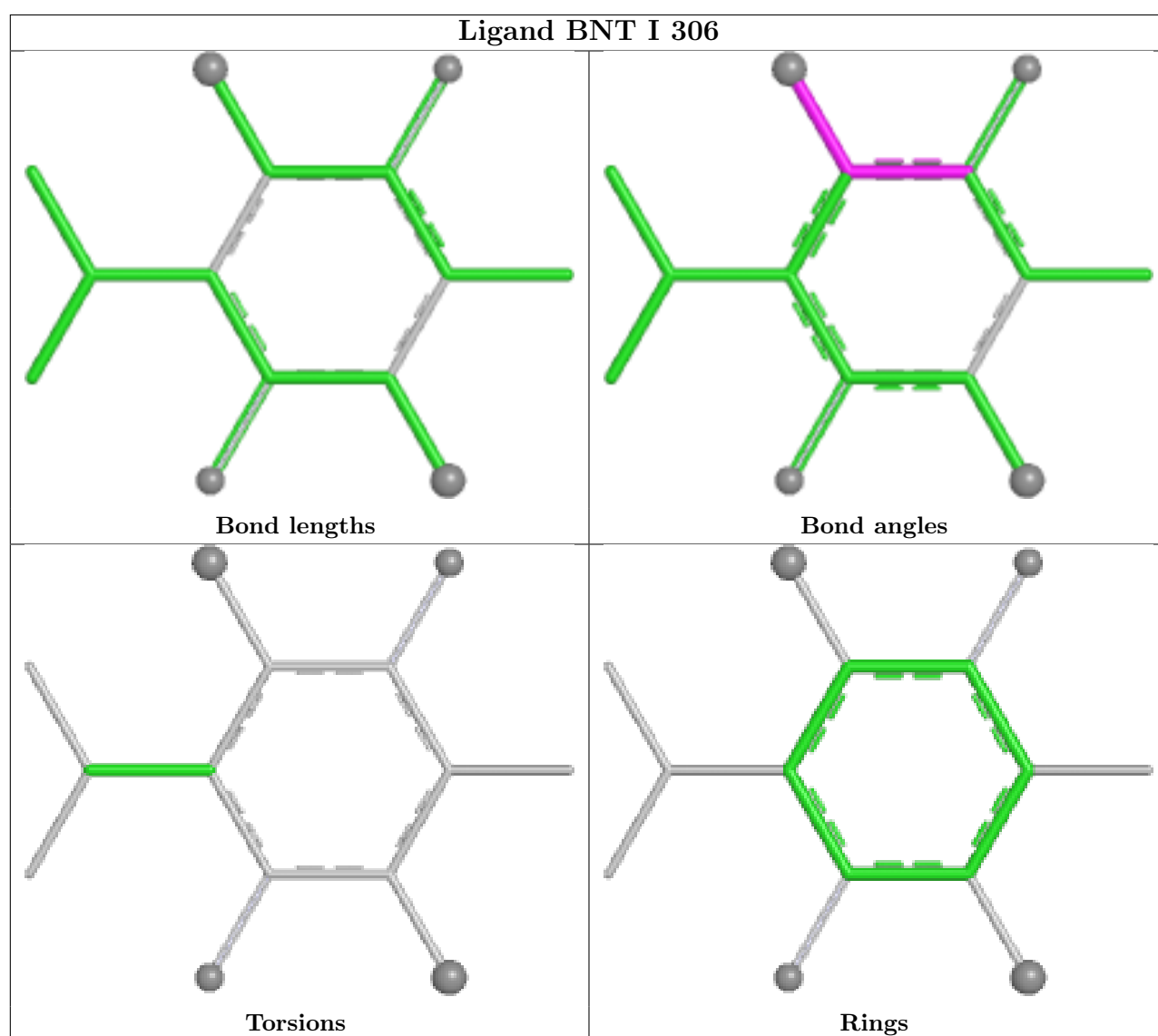
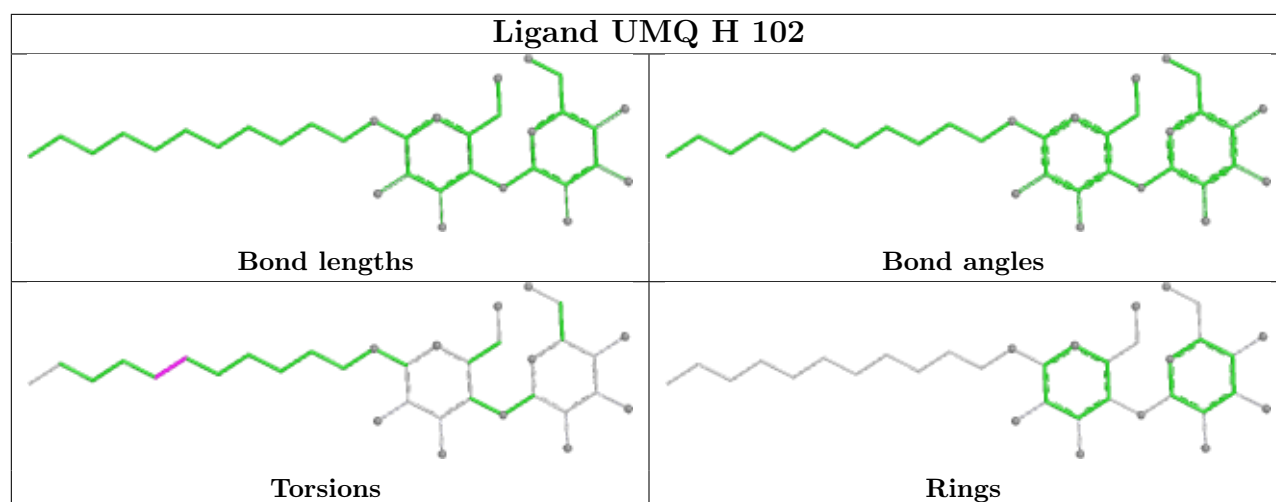


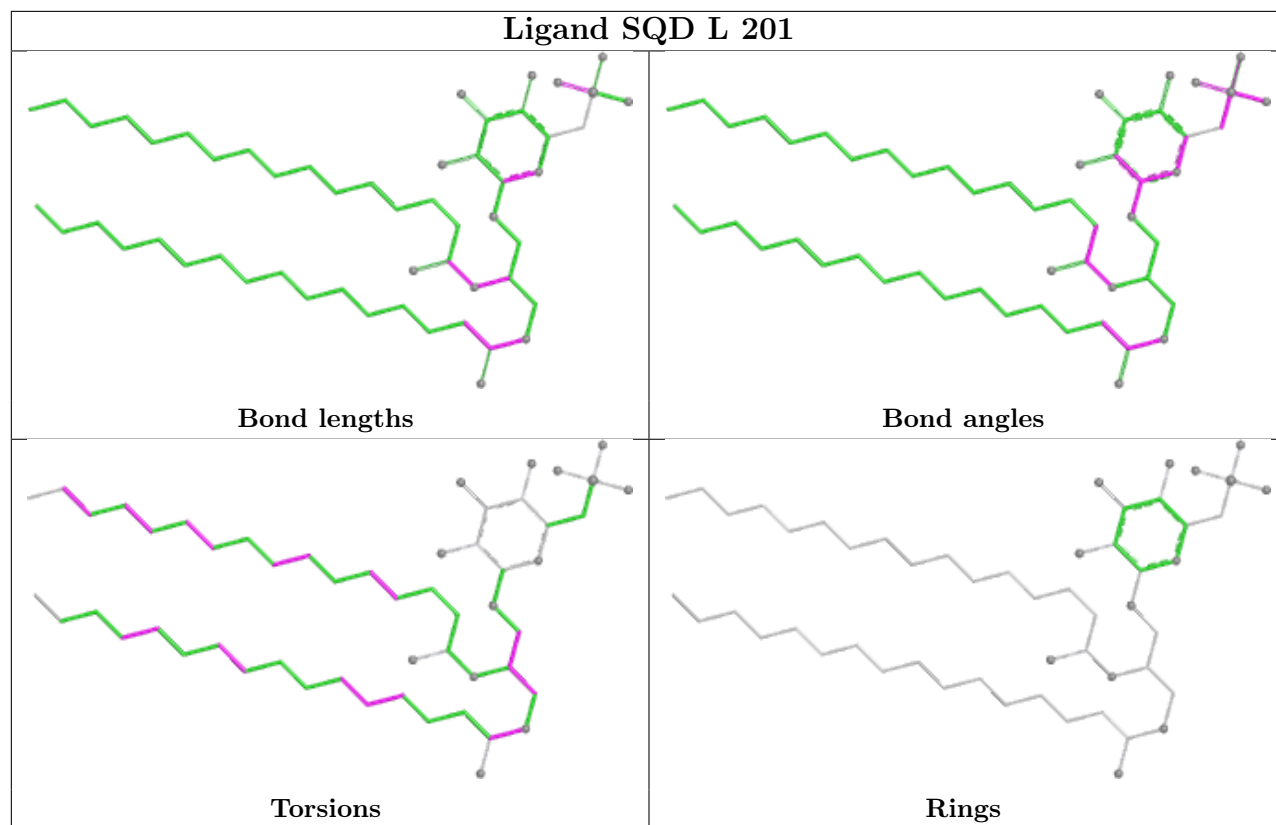
Ligand HEM I 302



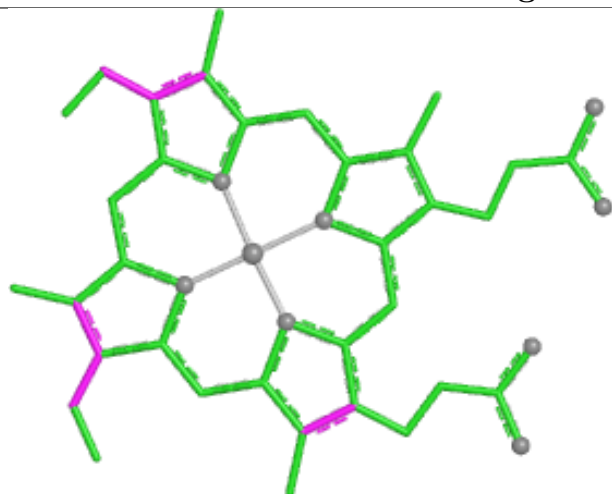
Ligand UMQ A 304



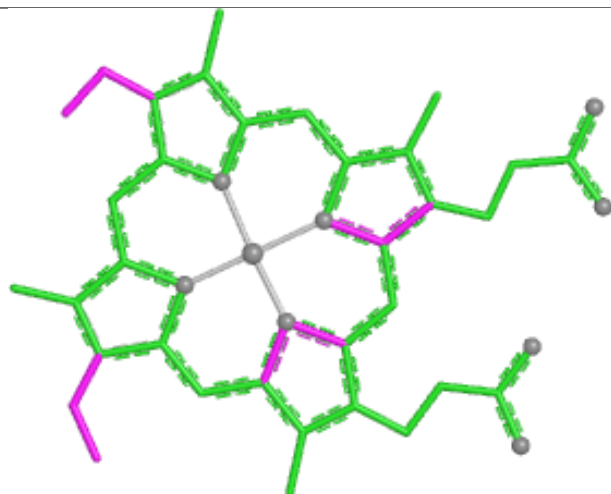




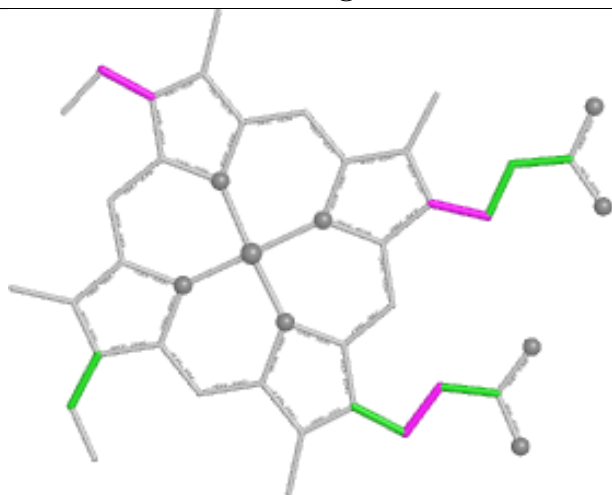
Ligand HEC I 303



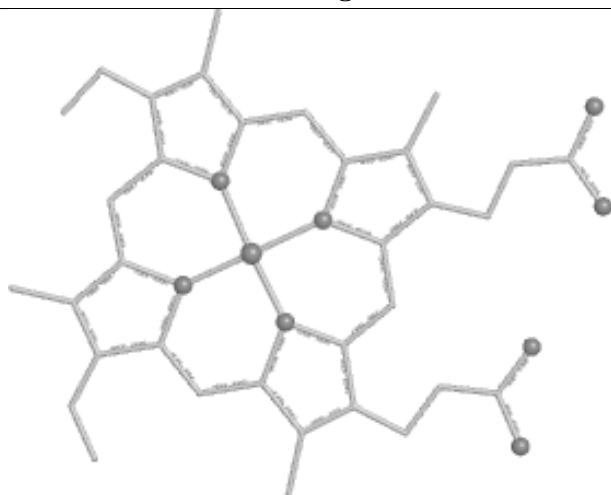
Bond lengths



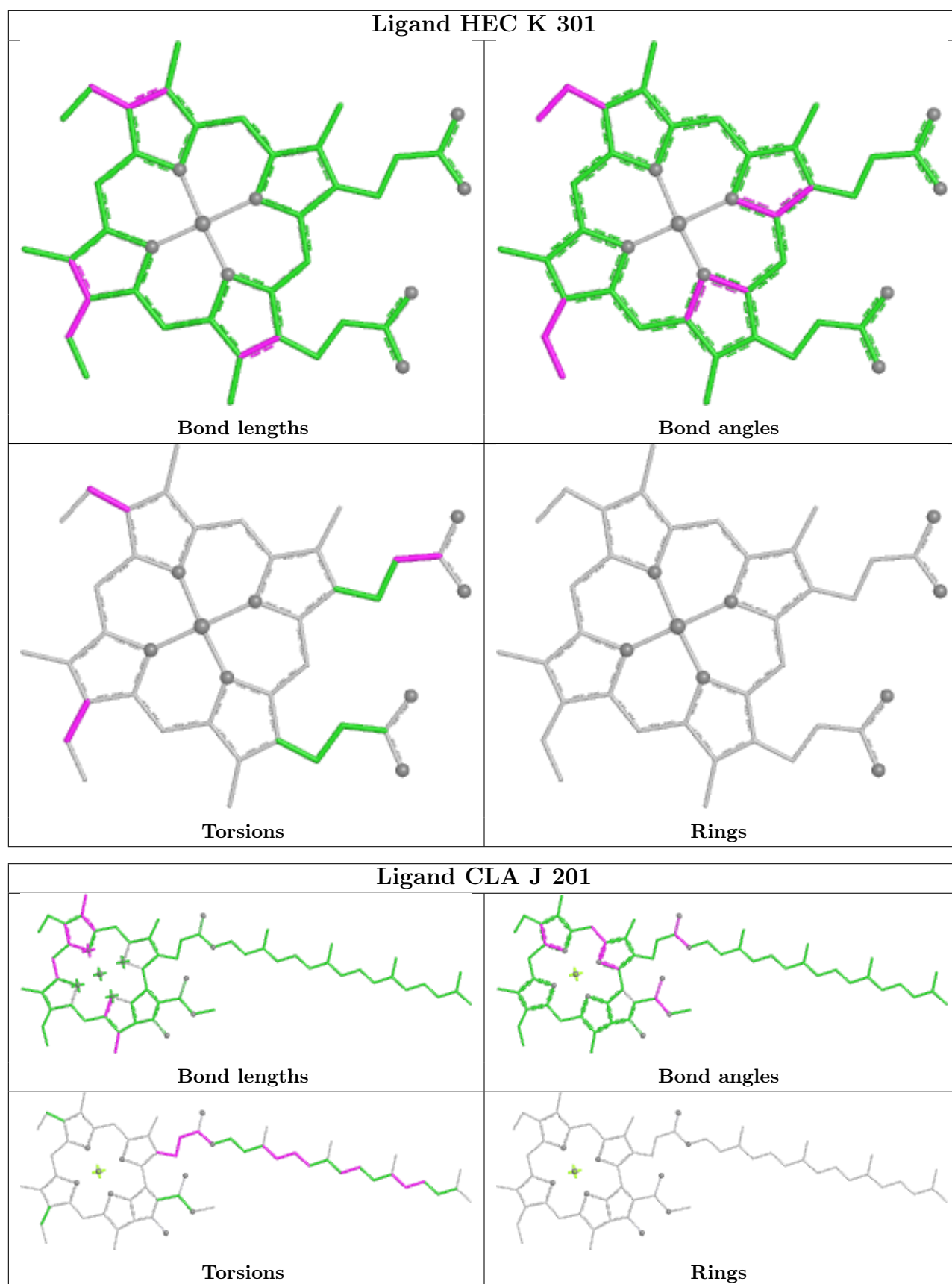
Bond angles

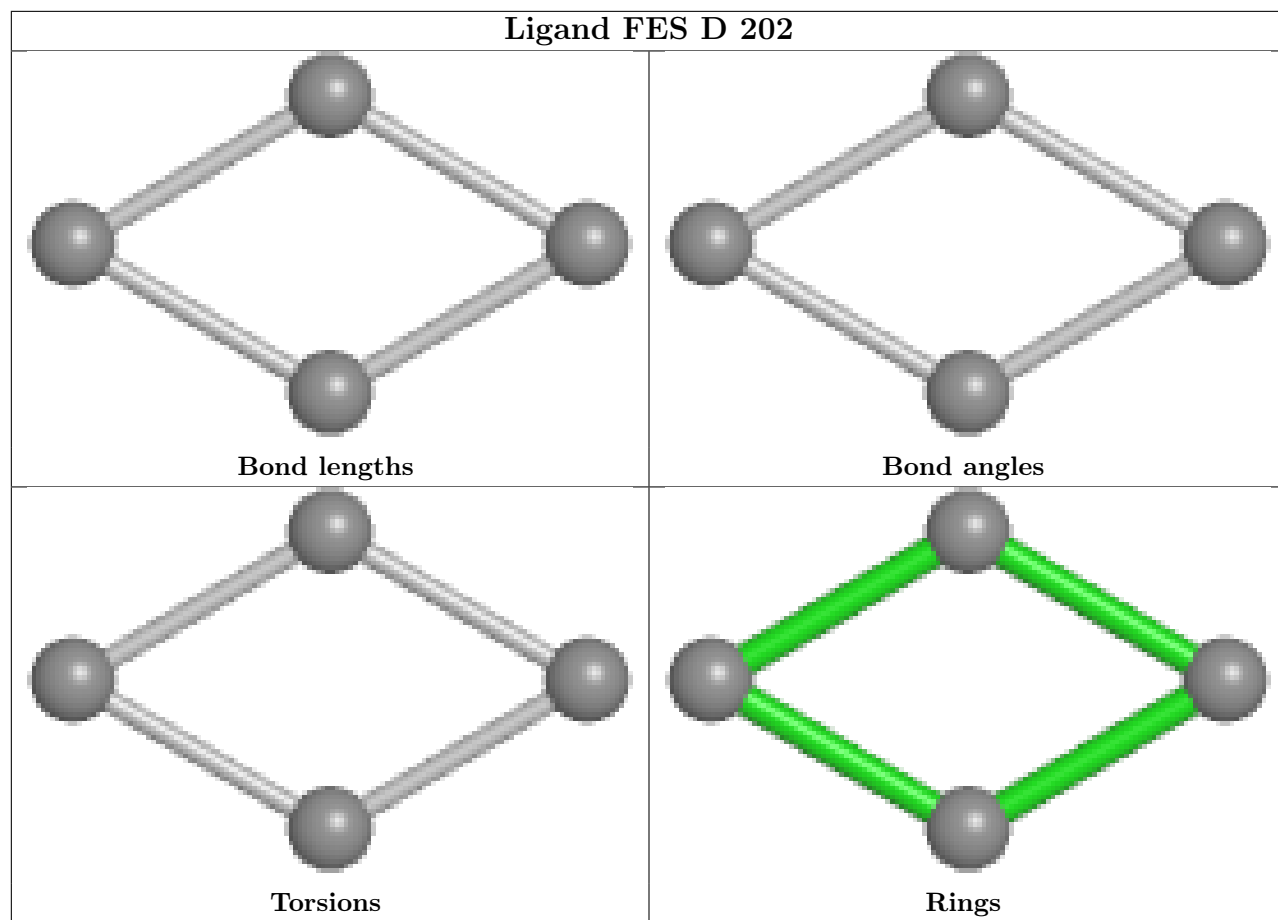


Torsions

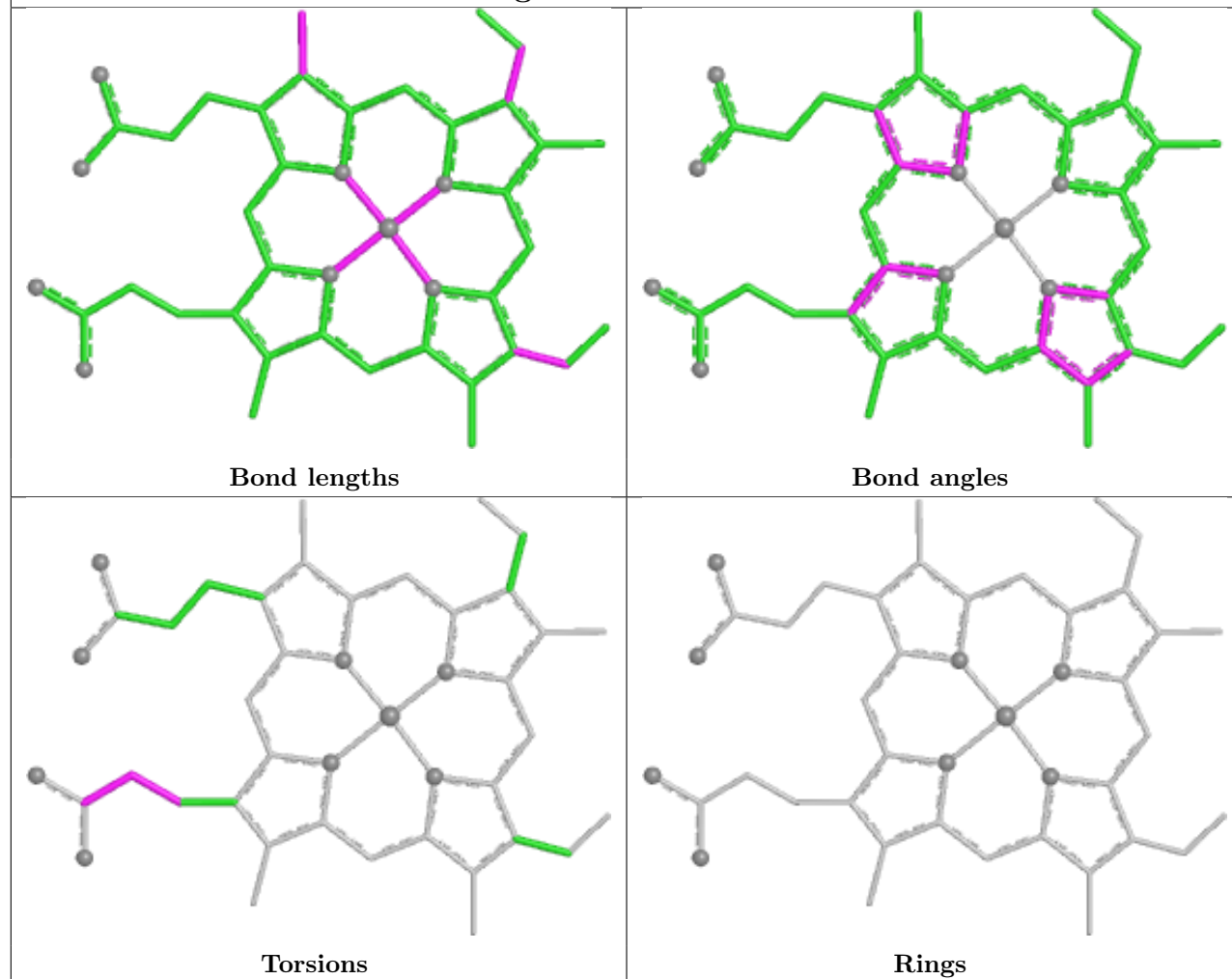


Rings

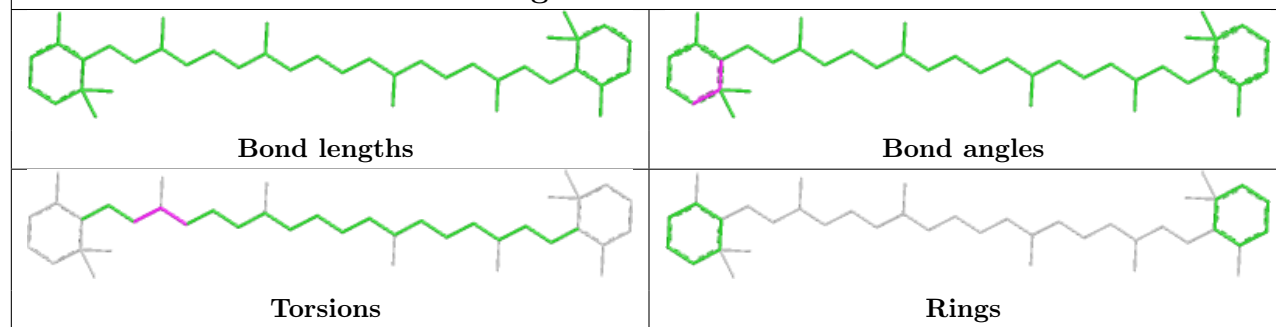


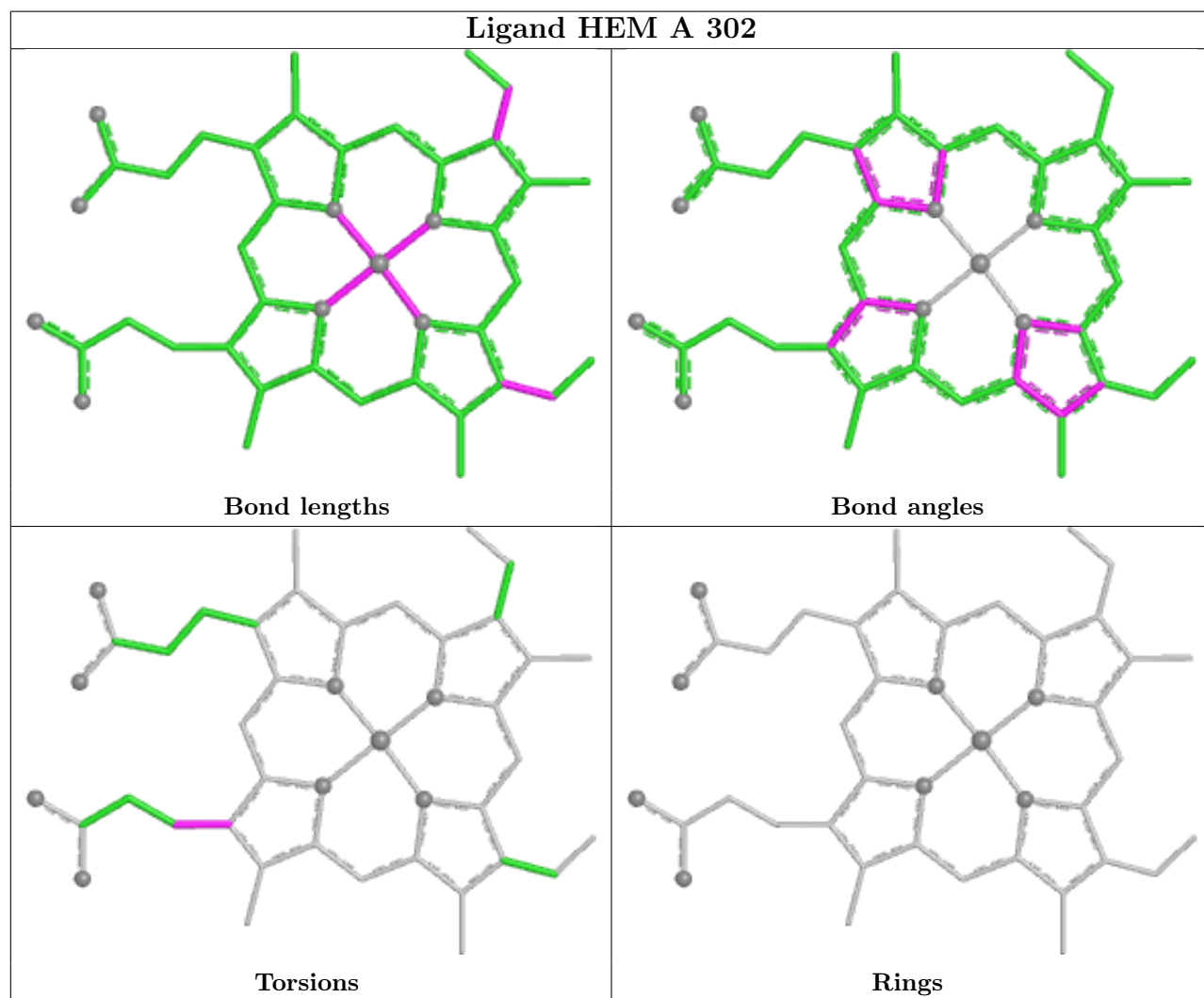
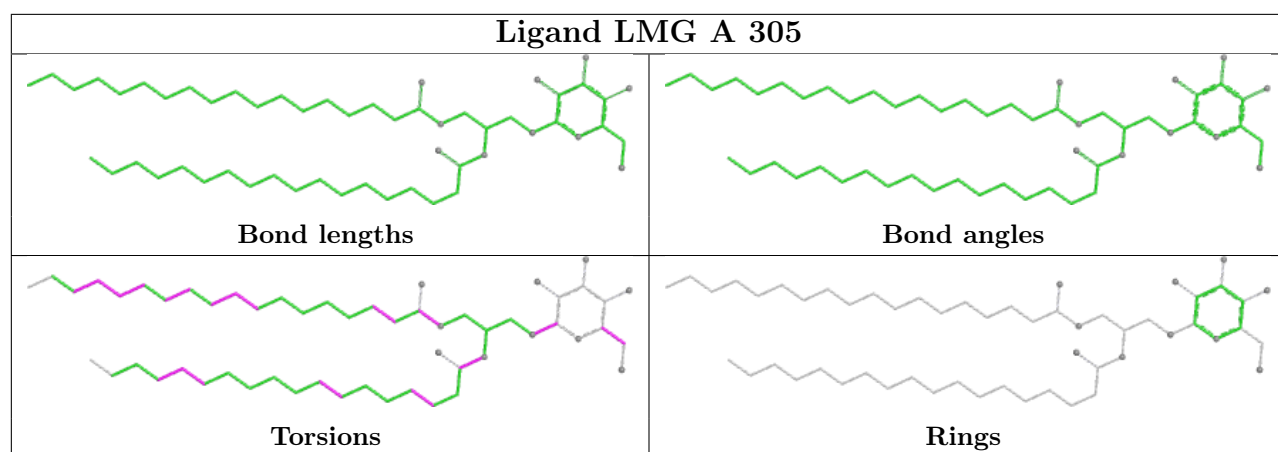


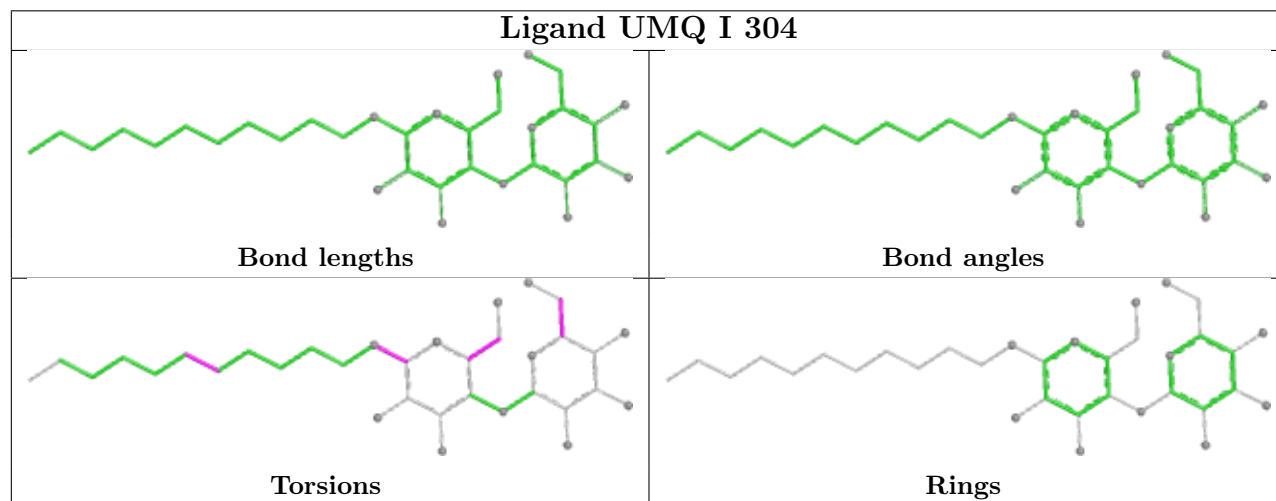
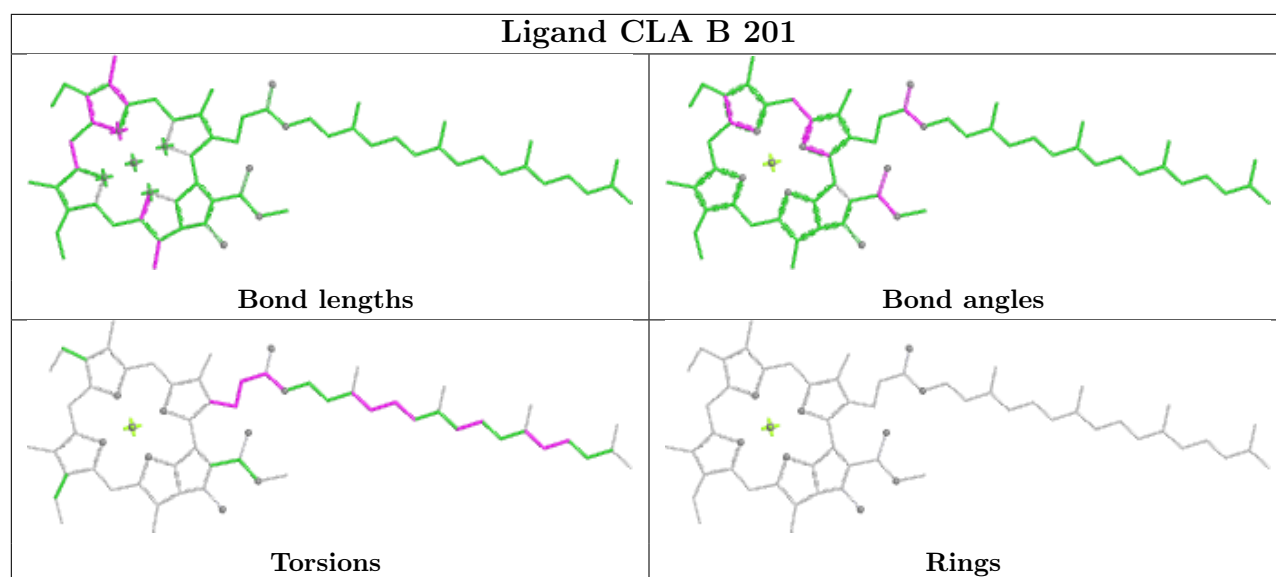
Ligand HEM I 301

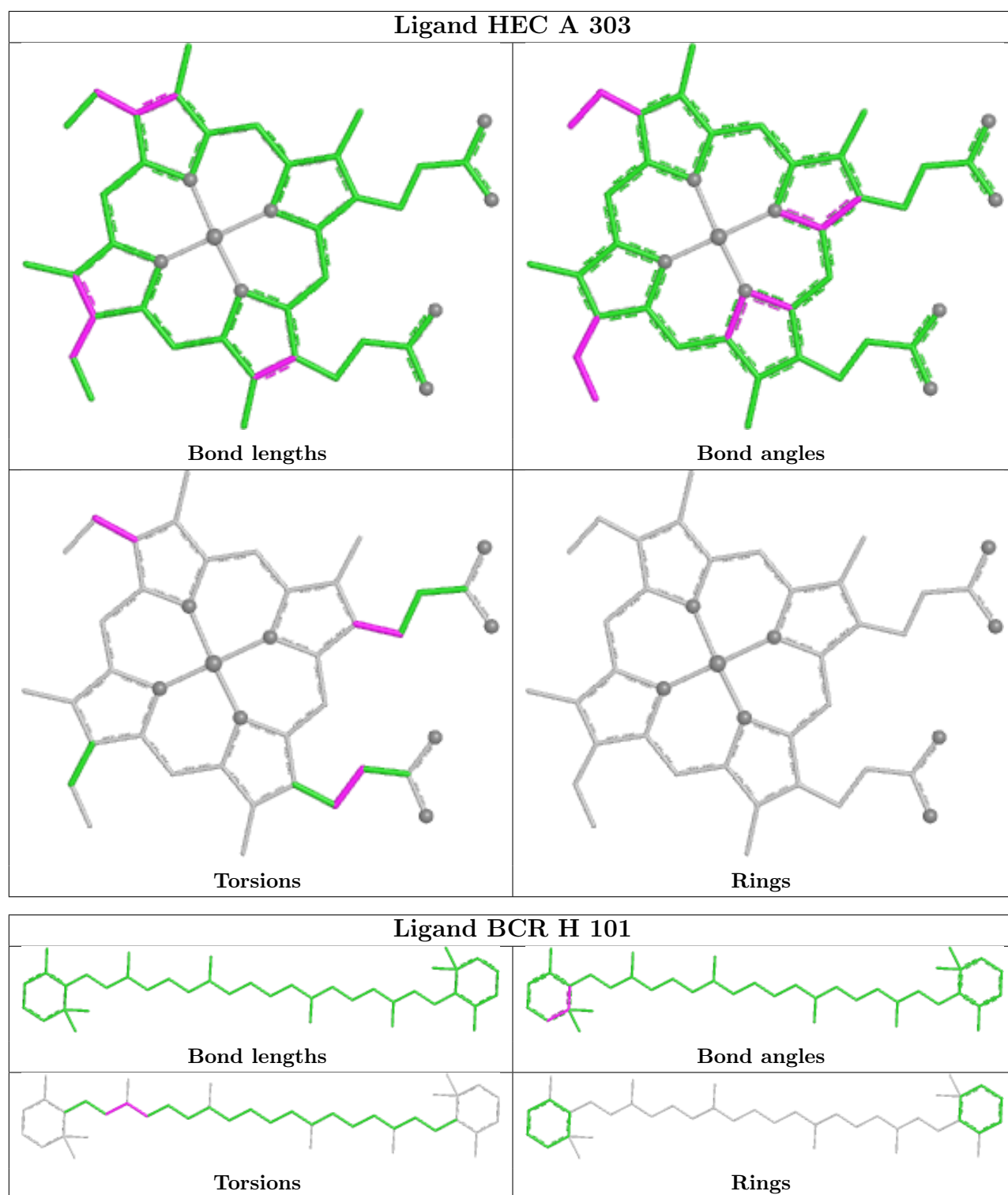


Ligand BCR P 101









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

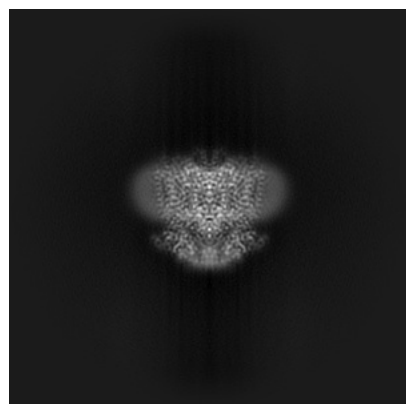
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19940. These allow visual inspection of the internal detail of the map and identification of artifacts.

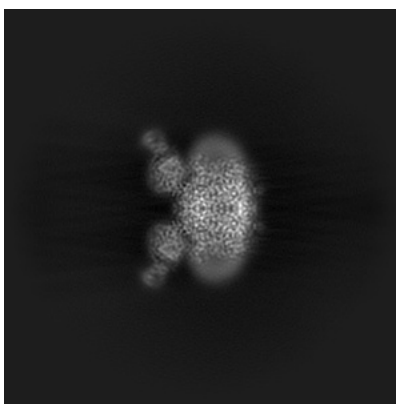
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

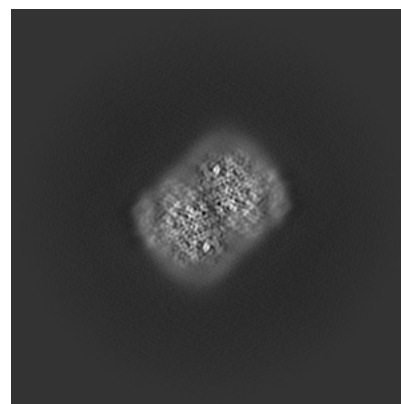
6.1.1 Primary map



X

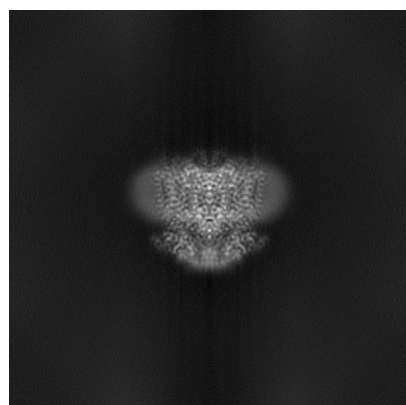


Y

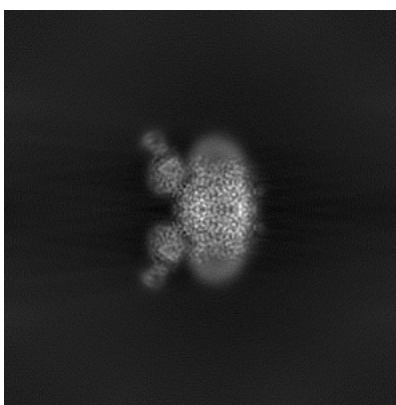


Z

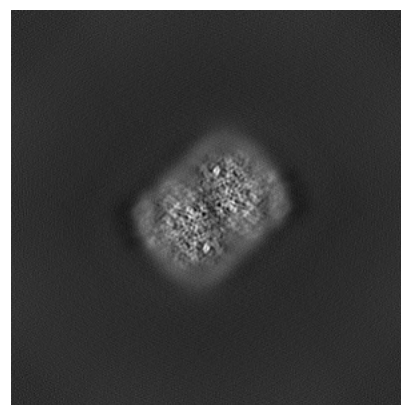
6.1.2 Raw map



X



Y

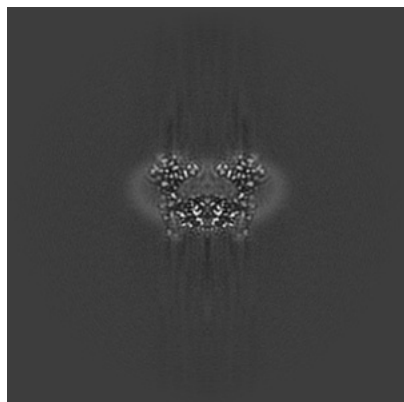


Z

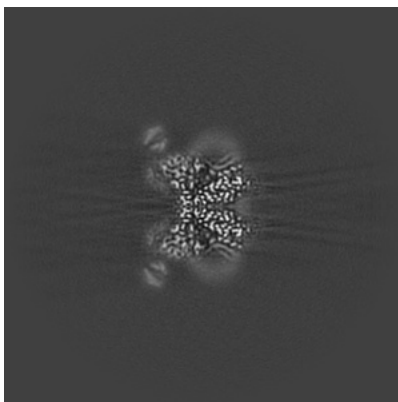
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

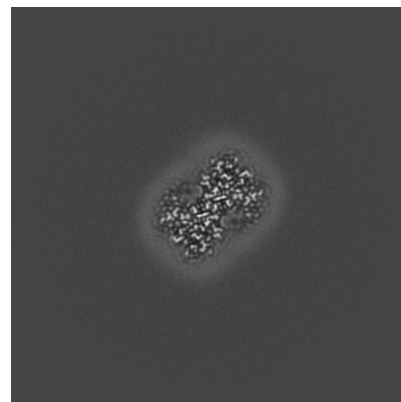
6.2.1 Primary map



X Index: 200

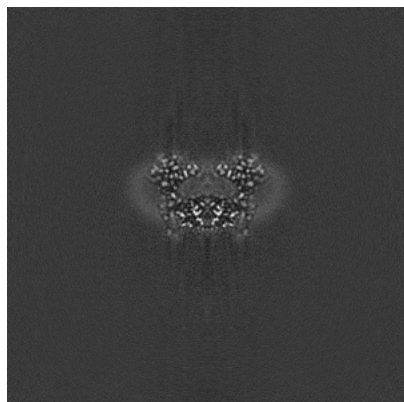


Y Index: 200

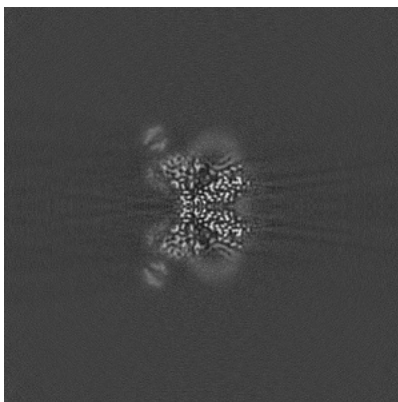


Z Index: 200

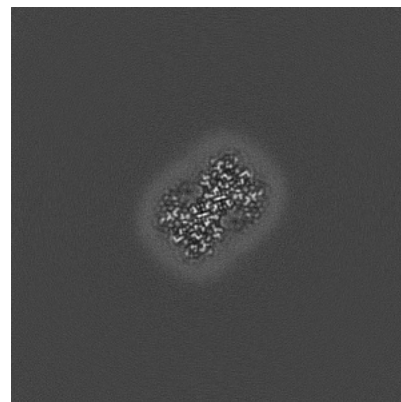
6.2.2 Raw map



X Index: 200



Y Index: 200

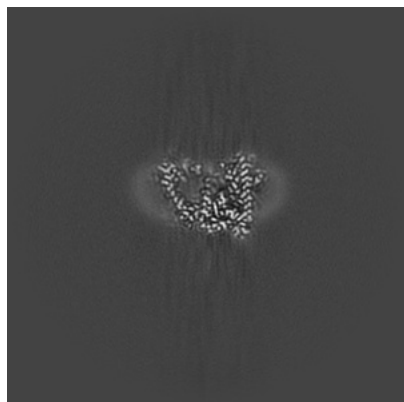


Z Index: 200

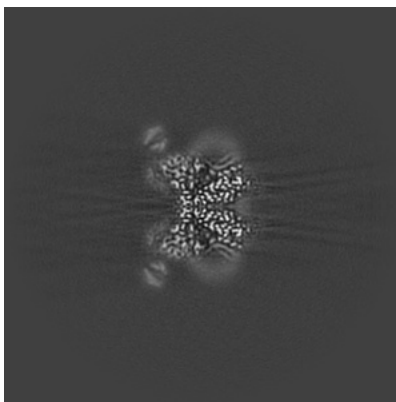
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

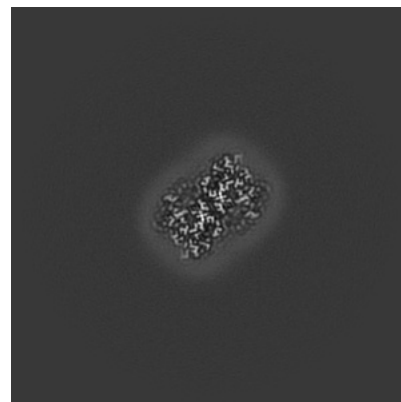
6.3.1 Primary map



X Index: 206

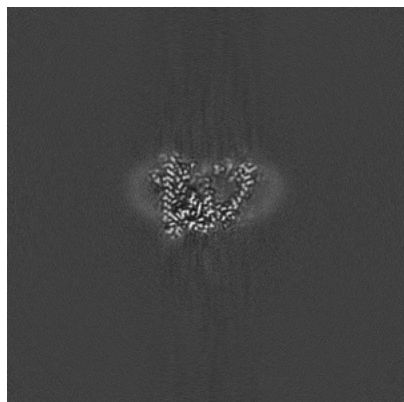


Y Index: 200

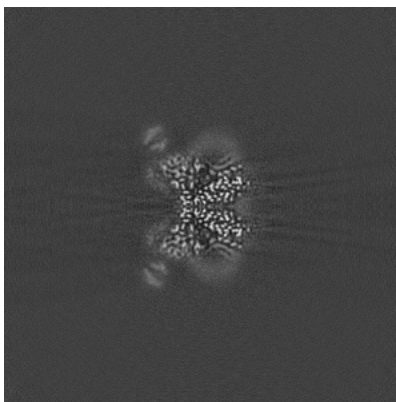


Z Index: 198

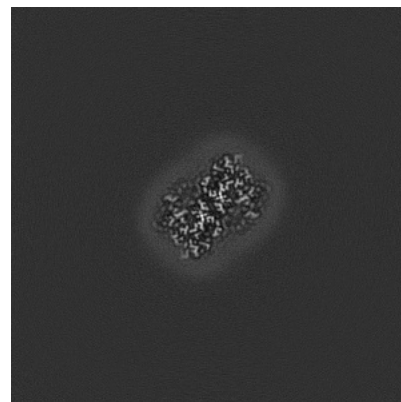
6.3.2 Raw map



X Index: 194



Y Index: 200

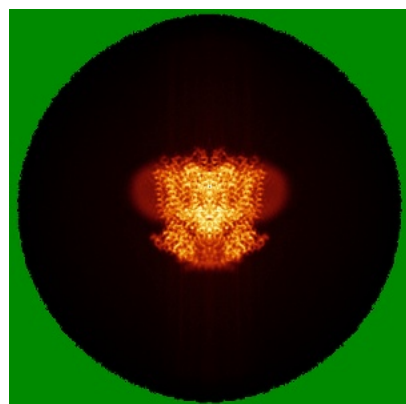


Z Index: 198

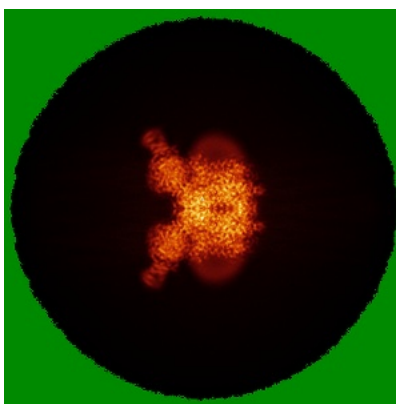
The images above show the largest variance slices of the map in three orthogonal directions.

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

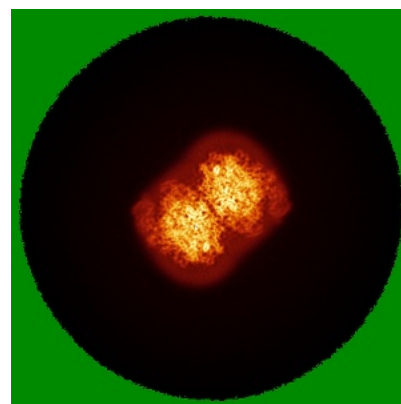
6.4.1 Primary map



X

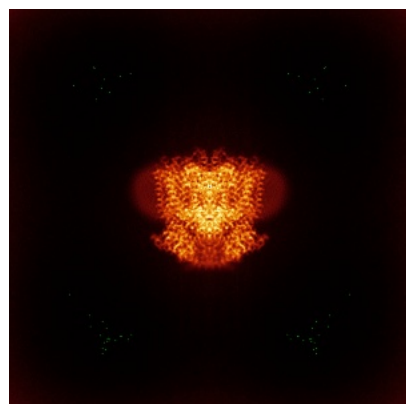


Y

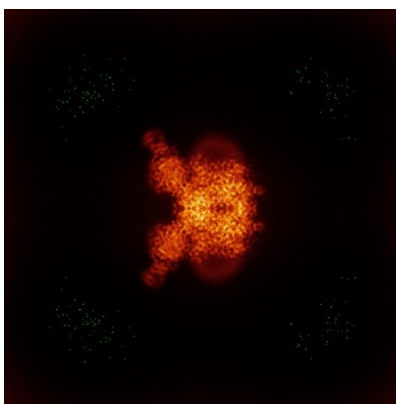


Z

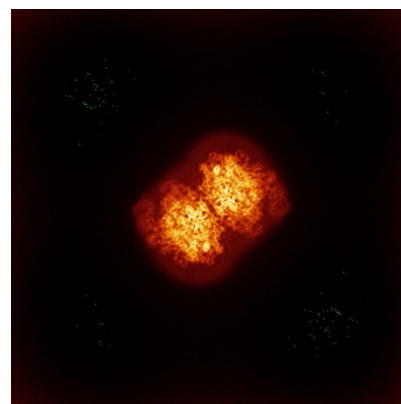
6.4.2 Raw map



X



Y

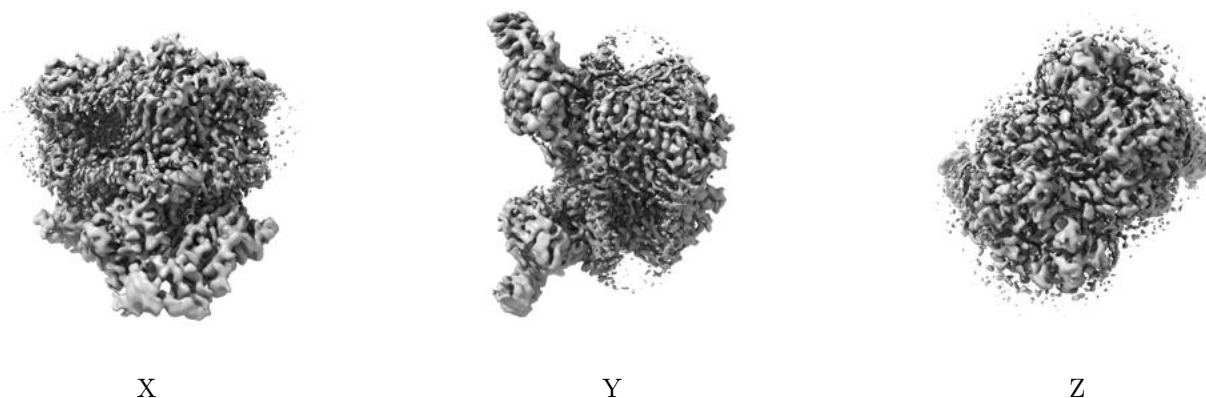


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

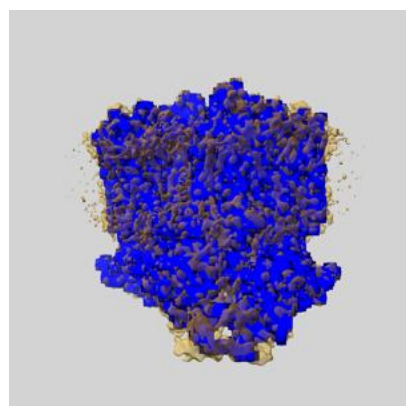
6.6 Mask visualisation [i](#)

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

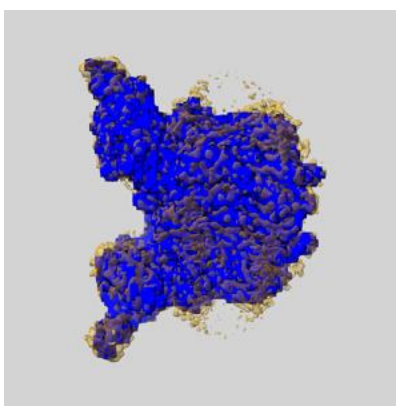
A mask typically either:

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

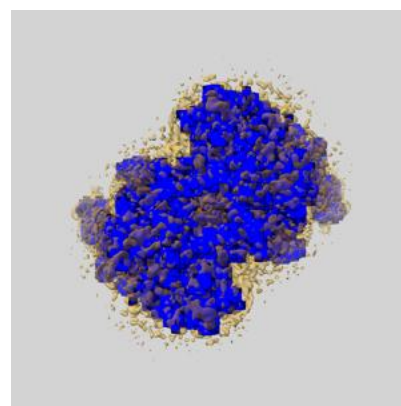
6.6.1 emd_19940_msk_2.map [i](#)



X

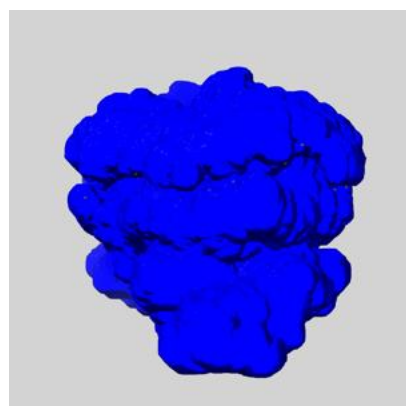


Y

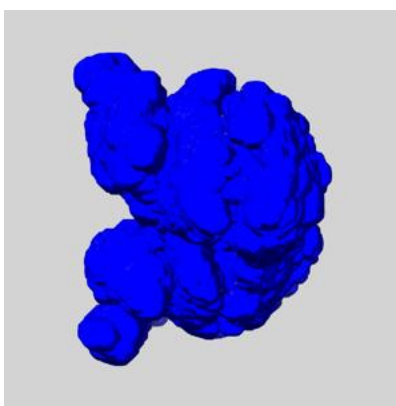


Z

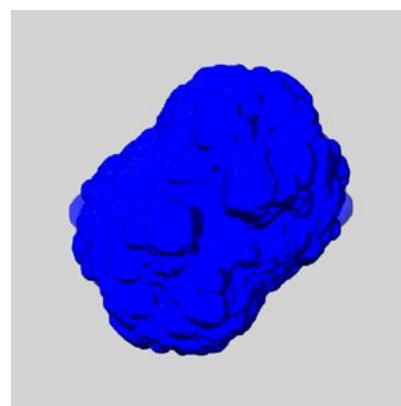
6.6.2 emd_19940_msk_1.map [i](#)



X



Y

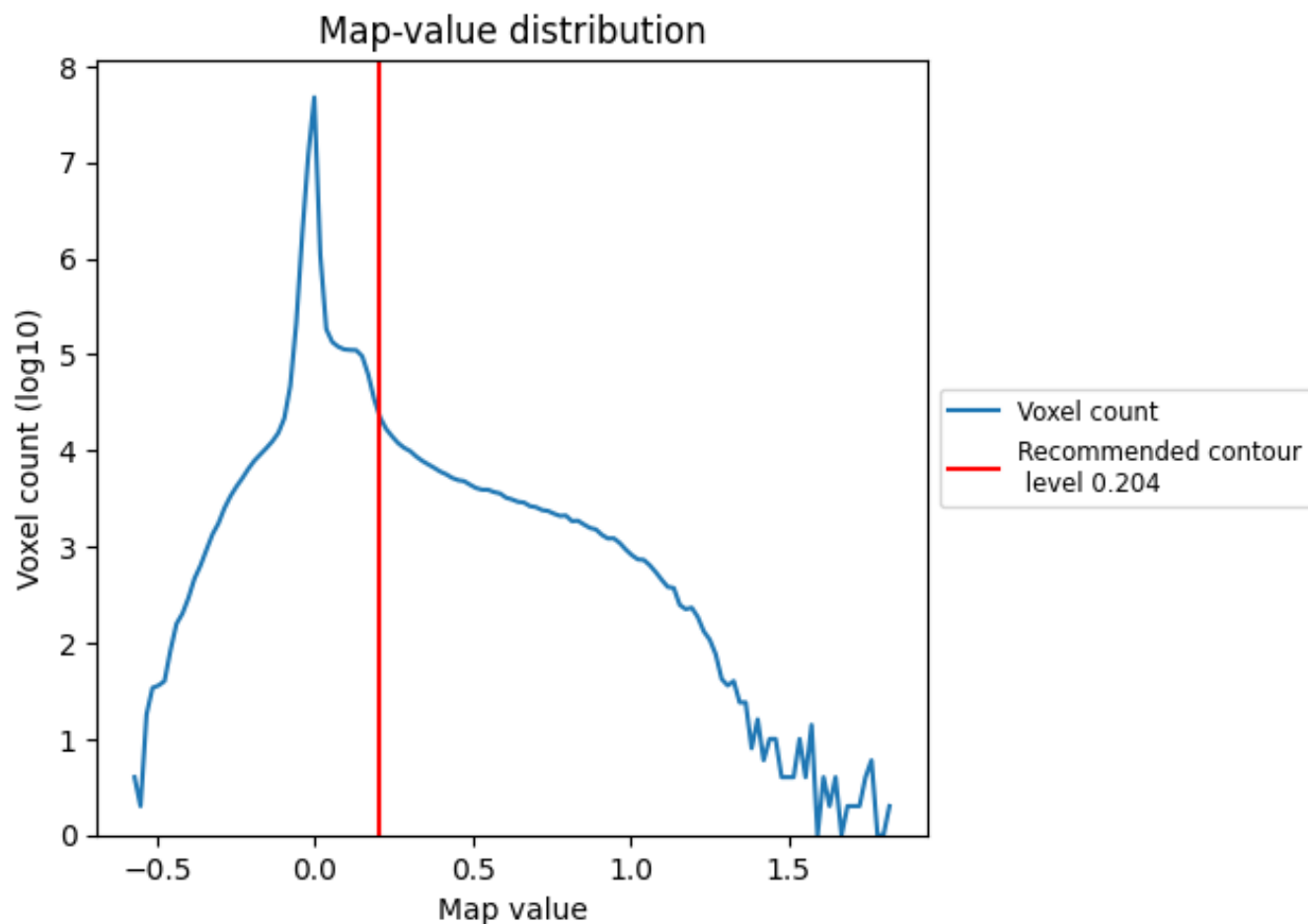


Z

7 Map analysis [i](#)

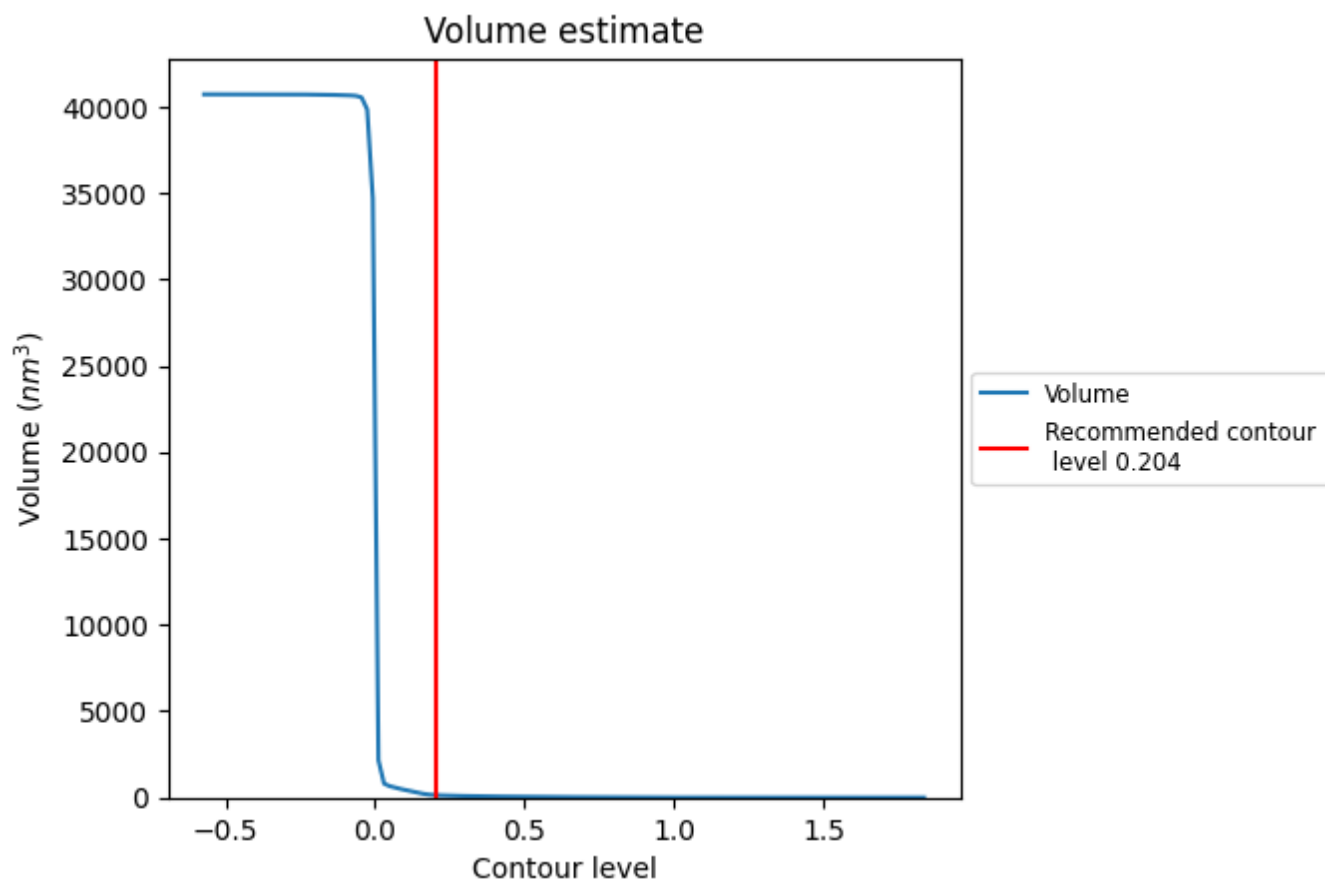
This section contains the results of statistical analysis of the map.

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.

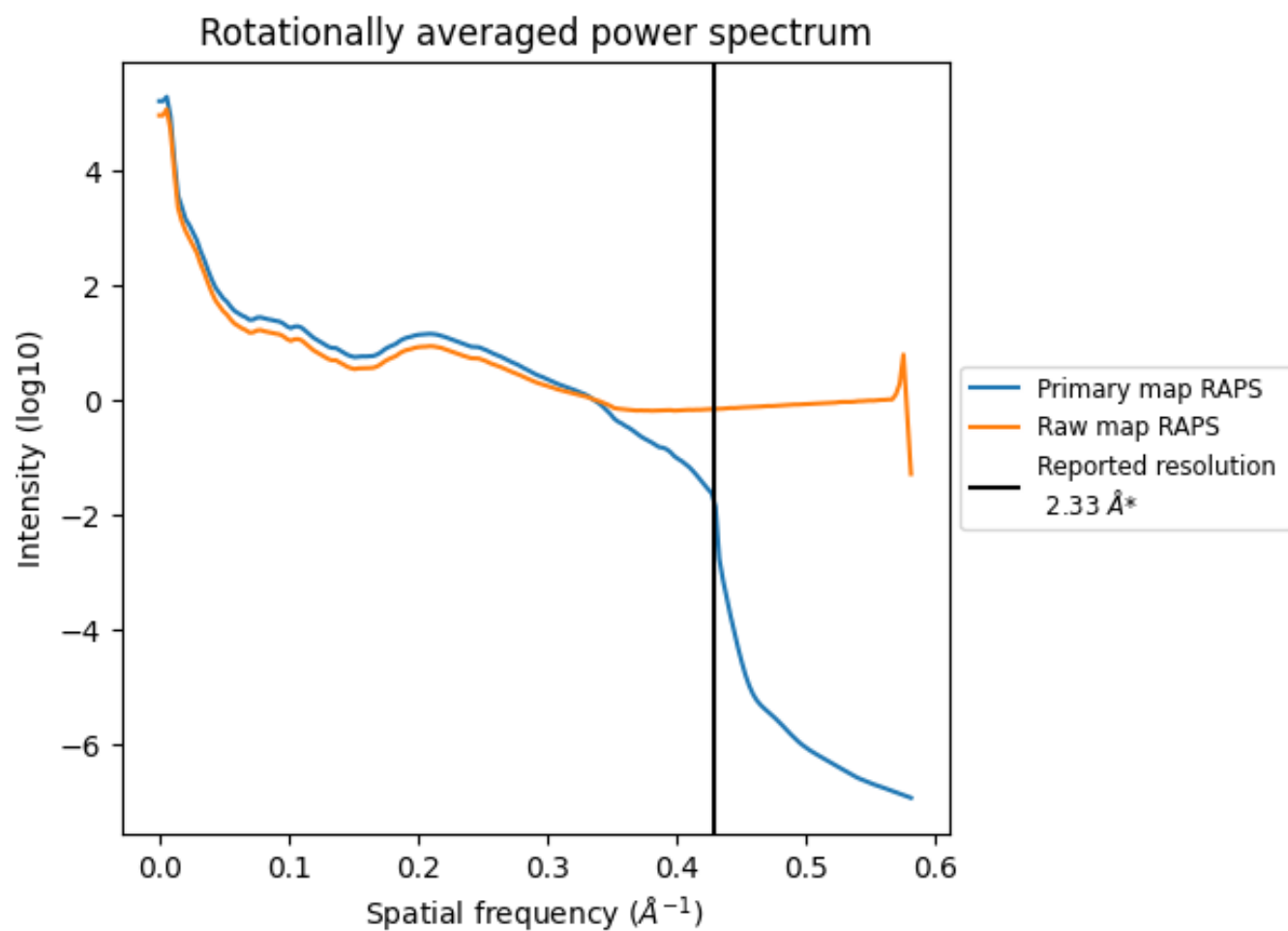
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm^3 ; this corresponds to an approximate mass of 126 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 ⓘ

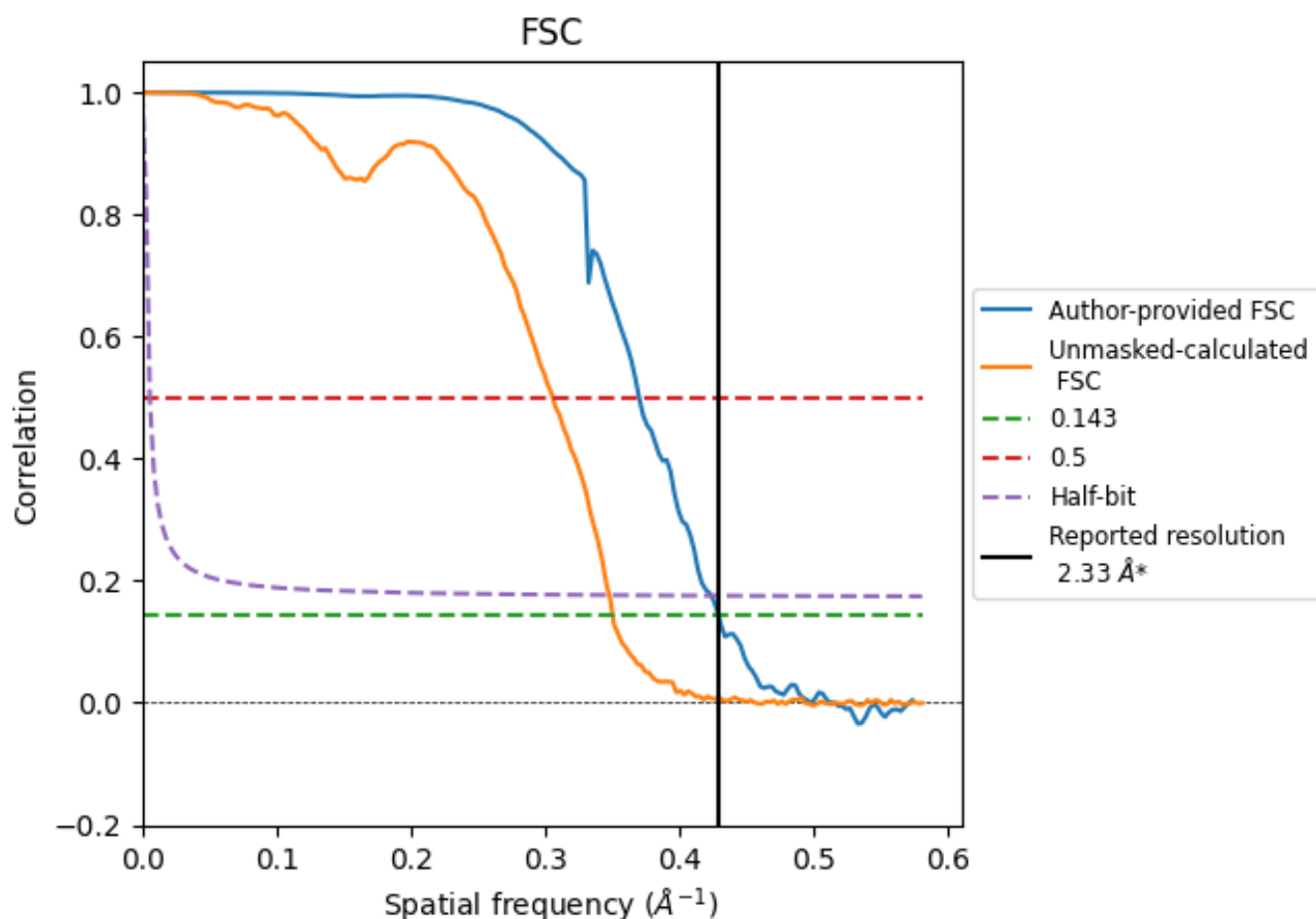


*Reported resolution corresponds to spatial frequency of 0.429 Å⁻¹

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 0.429 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

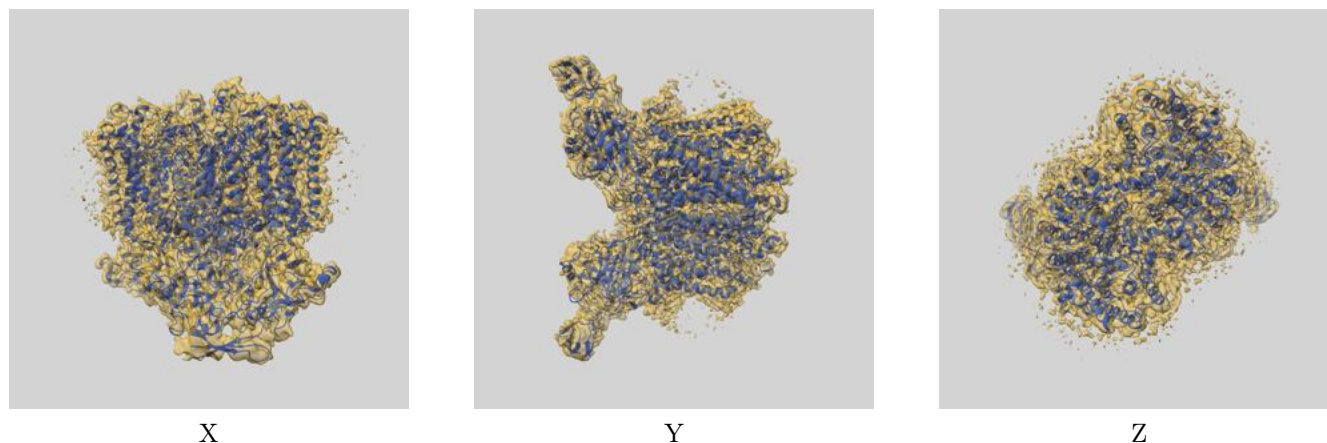
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.33	2.70	2.36
Unmasked-calculated*	2.85	3.27	2.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.85 differs from the reported value 2.33 by more than 10 %

9 Map-model fit [i](#)

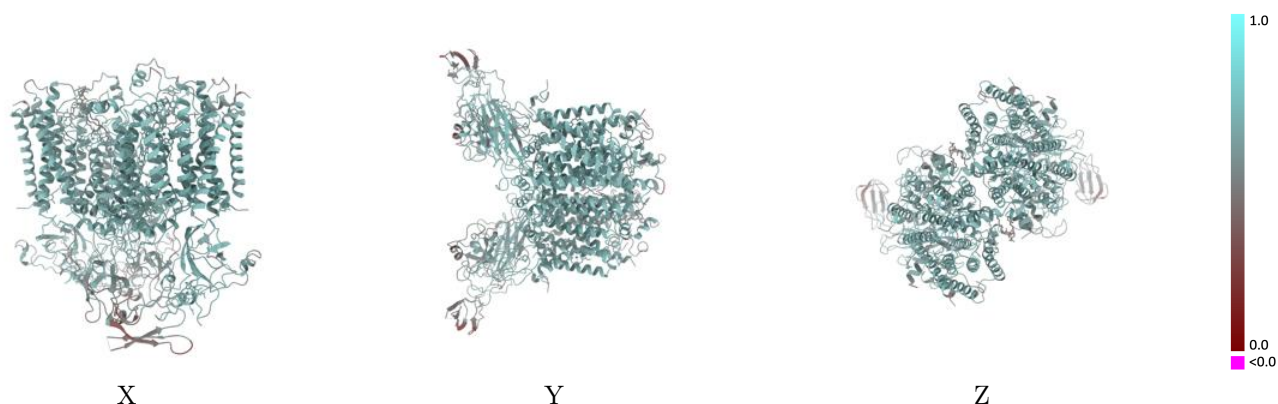
This section contains information regarding the fit between EMDB map EMD-19940 and PDB model 9ES9. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



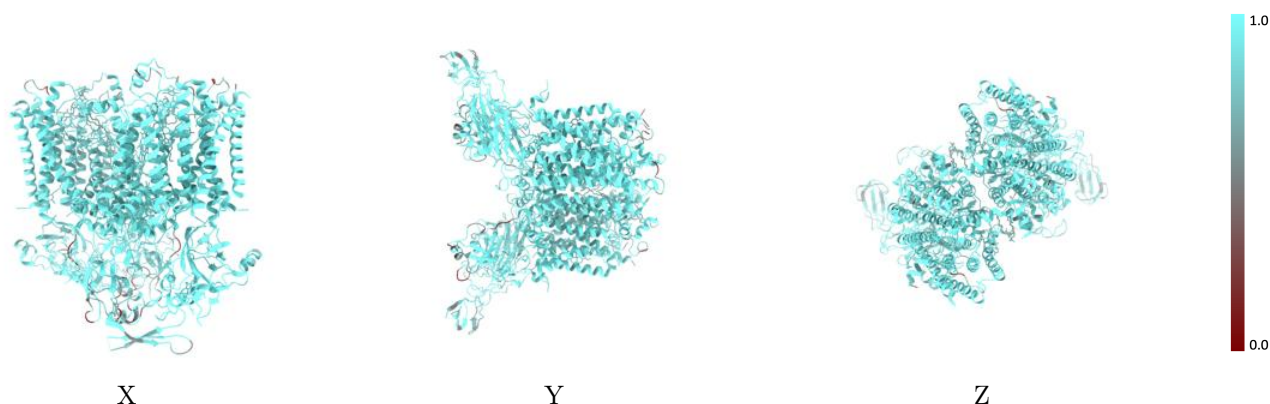
The images above show the 3D surface view of the map at the recommended contour level 0.204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



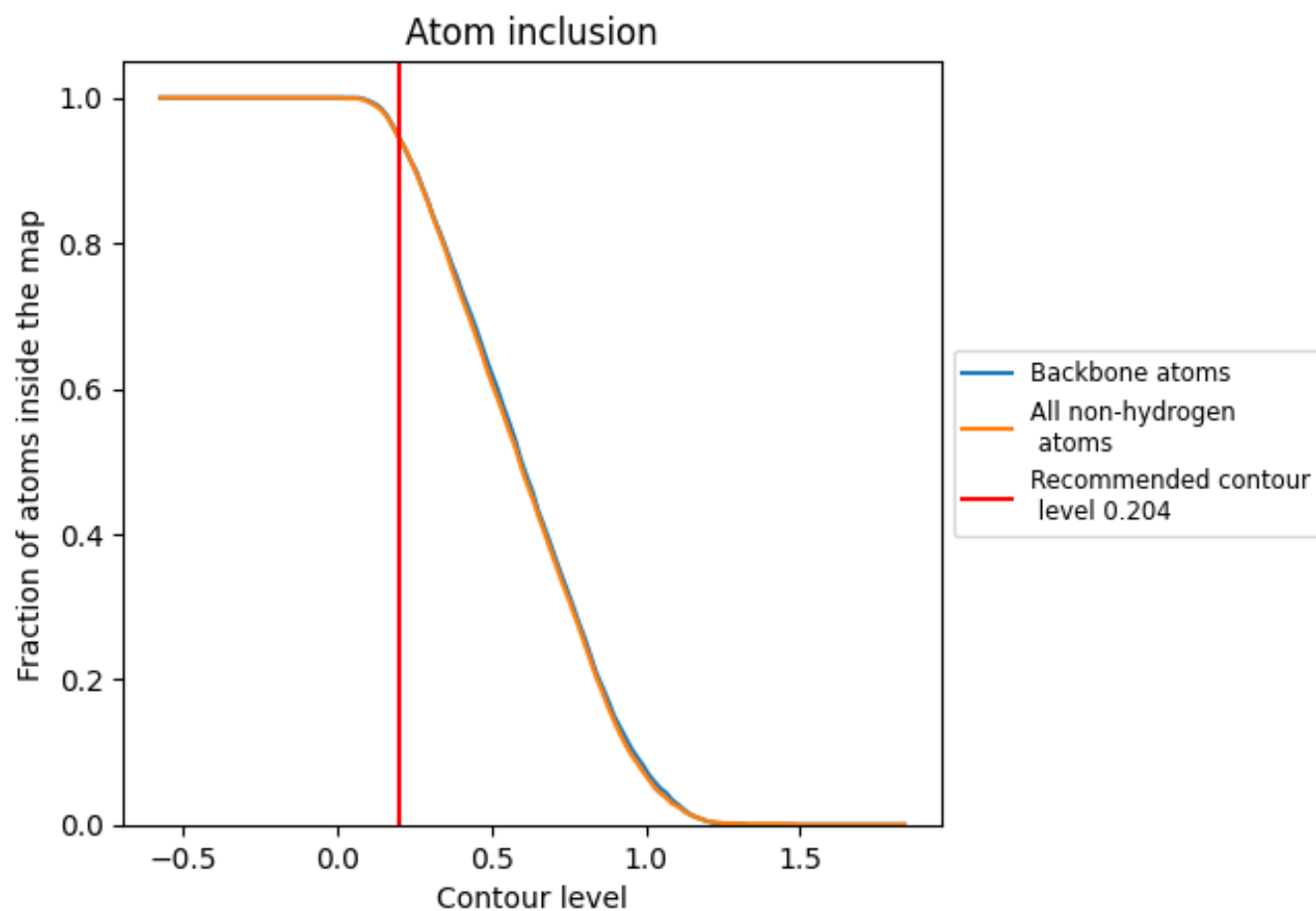
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.204).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9420	 0.6180
A	 0.9780	 0.6610
B	 0.9800	 0.6380
C	 0.9440	 0.5990
D	 0.8520	 0.5650
E	 0.9960	 0.6350
F	 0.9740	 0.6290
G	 0.9770	 0.6440
H	 0.9760	 0.6570
I	 0.9780	 0.6600
J	 0.9800	 0.6370
K	 0.9450	 0.5980
L	 0.8520	 0.5640
M	 0.9960	 0.6310
N	 0.9740	 0.6250
O	 0.9770	 0.6460
P	 0.9760	 0.6550
Q	 0.7950	 0.5340
R	 0.7950	 0.5380

