



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:24 AM UTC

PDB ID : 7ZXY / pdb_00007zxy
EMDB ID : EMD-15017
Title : 3.15 Angstrom cryo-EM structure of the dimeric cytochrome b6f complex from Synechocystis sp. PCC 6803 with natively bound plastoquinone and lipid molecules.
Authors : Malone, L.A.; Procter, M.S.; Farmer, D.F.; Swainsbury, D.J.K.; Hawkings, F.R.; Pastorelli, F.; Emrich-Mills, T.Z.; Siebert, A.; Hunter, C.N.; Hitchcock, A.; Johnson, M.P.
Deposited on : 2022-05-23
Resolution : 3.15 Å(reported)

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<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)

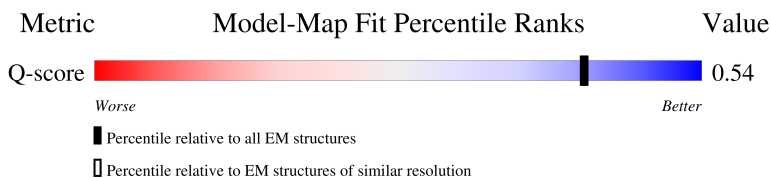
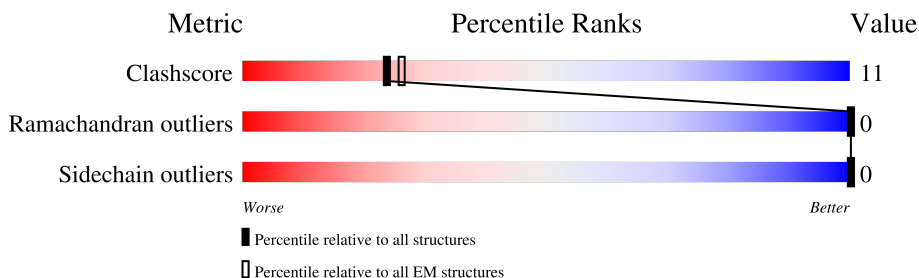
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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	14486 (2.65 - 3.65)

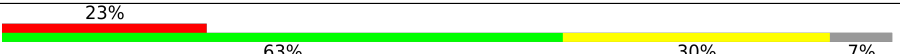
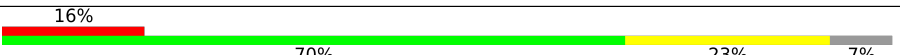
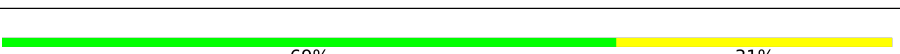
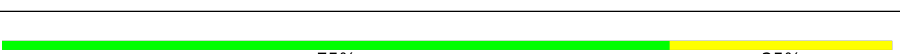
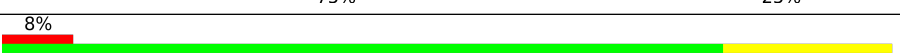
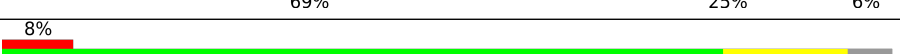
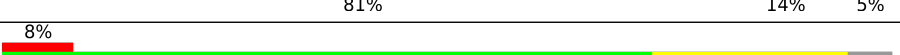
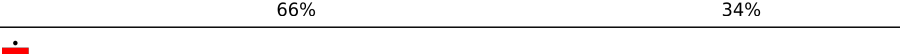
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	222	
1	I	222	
2	B	160	

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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	284	
3	K	284	
4	D	180	
4	L	180	
5	E	32	
5	M	32	
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
12	CLA	B	201	X	-	-	-
12	CLA	J	201	X	-	-	-
15	FES	D	201	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 15606 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	220	Total	C	N	O	S	0	0
			1750	1161	281	297	11		
1	I	220	Total	C	N	O	S	0	0
			1750	1161	281	297	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	158	Total	C	N	O	S	0	0
			1211	811	189	204	7		
2	J	159	Total	C	N	O	S	0	0
			1223	820	190	206	7		

- Molecule 3 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	279	Total	C	N	O	S	0	0
			2116	1356	352	403	5		
3	K	279	Total	C	N	O	S	0	0
			2116	1356	352	403	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1248	789	213	240	6		
4	L	168	Total	C	N	O	S	0	0
			1248	789	213	240	6		

- Molecule 5 is a protein called Cytochrome B6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	32	Total	C	N	O	S	0	0
			239	165	36	37	1		
5	M	32	Total	C	N	O	S	0	0
			239	165	36	37	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
			267	175	40	49	3		
6	N	34	Total	C	N	O	S	0	0
			248	165	38	42	3		

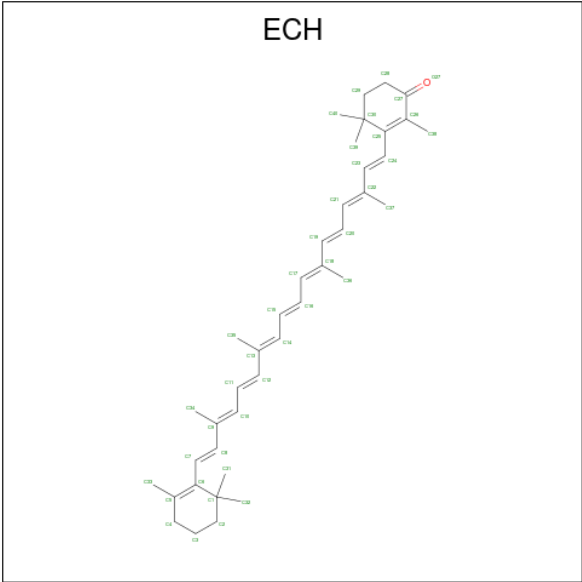
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	35	Total	C	N	O	S	0	0
			270	184	42	43	1		
7	O	35	Total	C	N	O	S	0	0
			270	184	42	43	1		

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

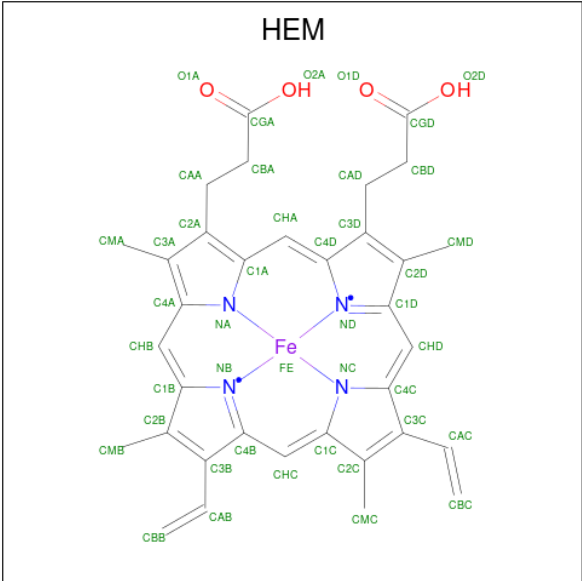
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	29	Total	C	N	O	S	0	0
			235	159	36	38	2		
8	P	29	Total	C	N	O	S	0	0
			235	159	36	38	2		

- Molecule 9 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O		0
			41	40	1		
9	I	1	Total	C	O		0
			41	40	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



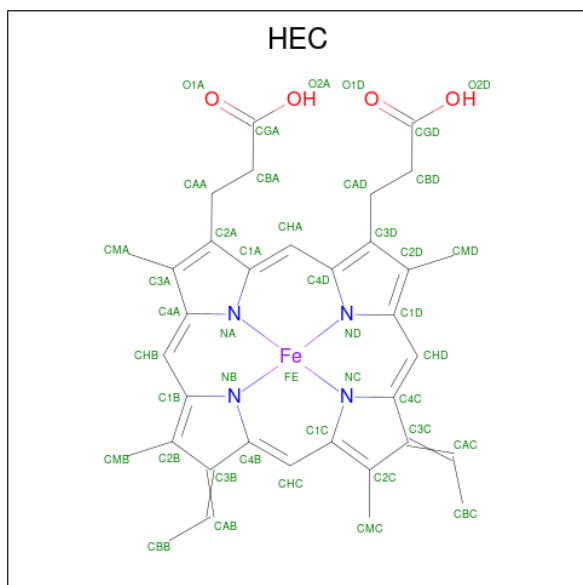
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 11 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltCon
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	J	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 13 is (1R)-2-{\{[(2S)-2,3-DIHYDROXYPROPYL]OXY\}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



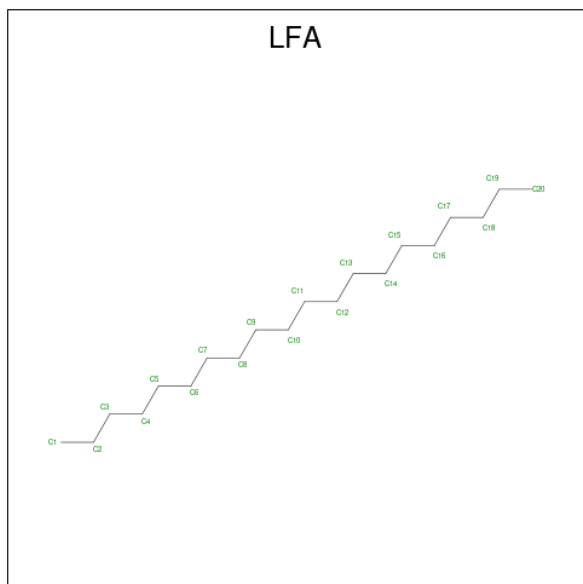
Mol	Chain	Residues	Atoms				AltCon
13	B	1	Total	C	O	P	0
			45	34	10	1	

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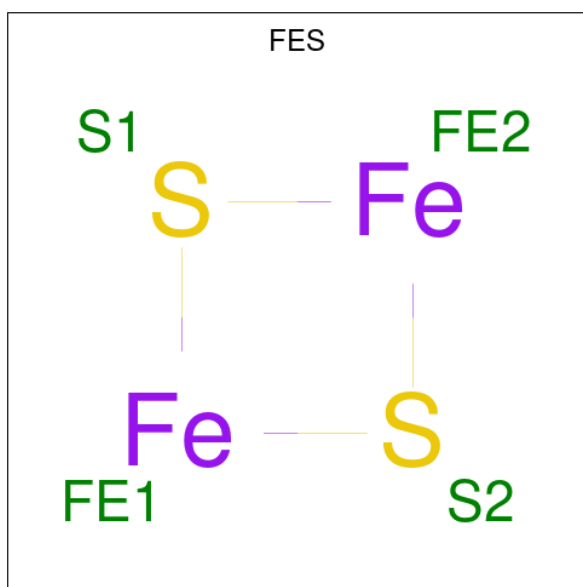
Mol	Chain	Residues	Atoms				AltConf
13	B	1	Total	C	O	P	0
			44	33	10	1	
13	C	1	Total	C	O	P	0
			51	40	10	1	
13	I	1	Total	C	O	P	0
			51	40	10	1	
13	J	1	Total	C	O	P	0
			51	40	10	1	
13	J	1	Total	C	O	P	0
			44	33	10	1	
13	J	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 14 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		AltConf
14	C	1	Total	C	0
			20	20	
14	E	1	Total	C	0
			20	20	

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



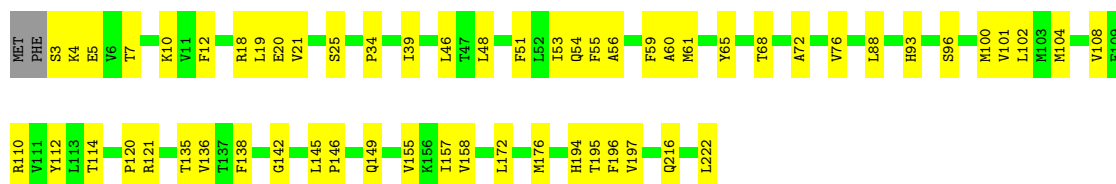
Mol	Chain	Residues	Atoms			AltConf
15	D	1	Total	Fe	S	0
			4	2	2	
15	L	1	Total	Fe	S	0
			4	2	2	

3 Residue-property plots [i](#)

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

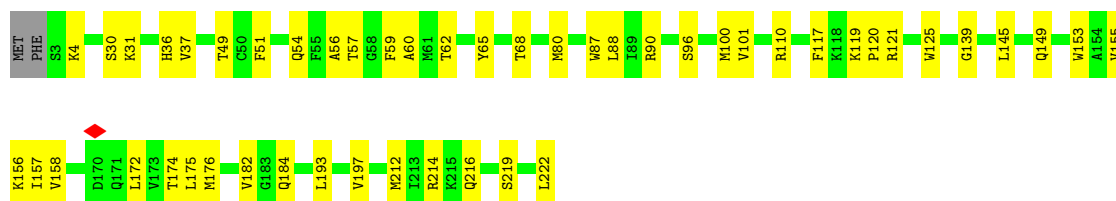
• Molecule 1: Cytochrome b6

Chain A:  73% 26%



• Molecule 1: Cytochrome b6

Chain I:  77% 22%



• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:  78% 21%

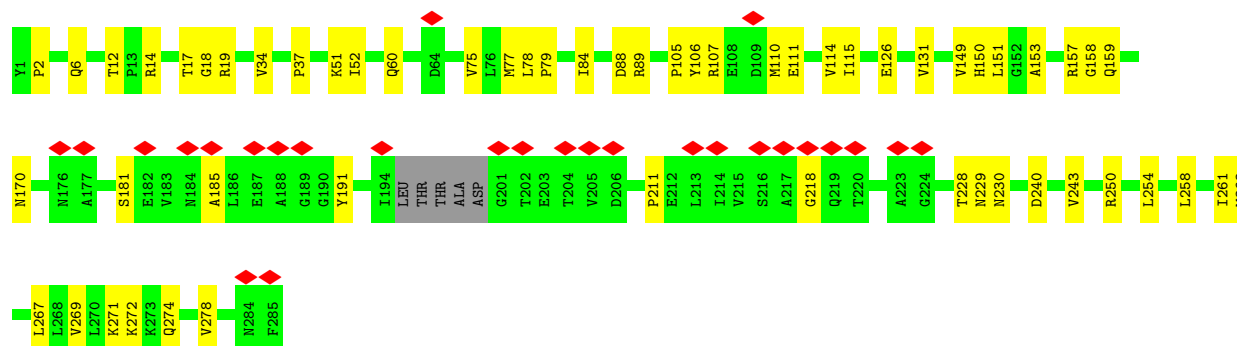
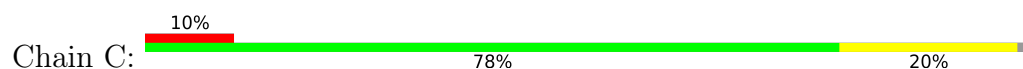


• Molecule 2: Cytochrome b6-f complex subunit 4

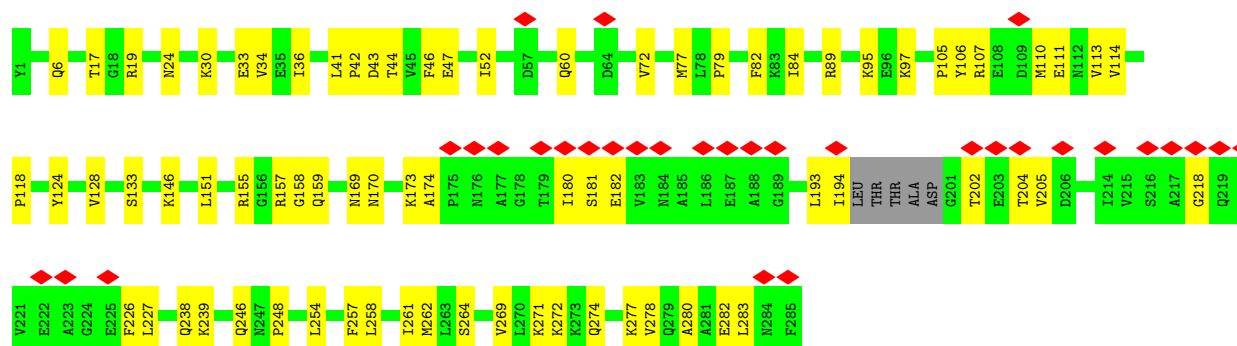
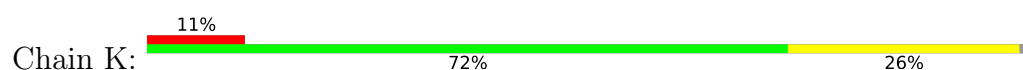
Chain J:  81% 19%



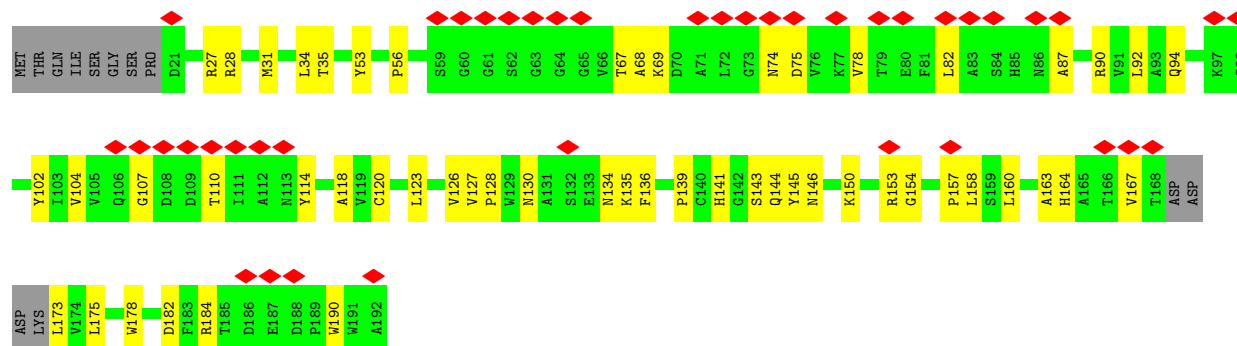
• Molecule 3: Cytochrome f



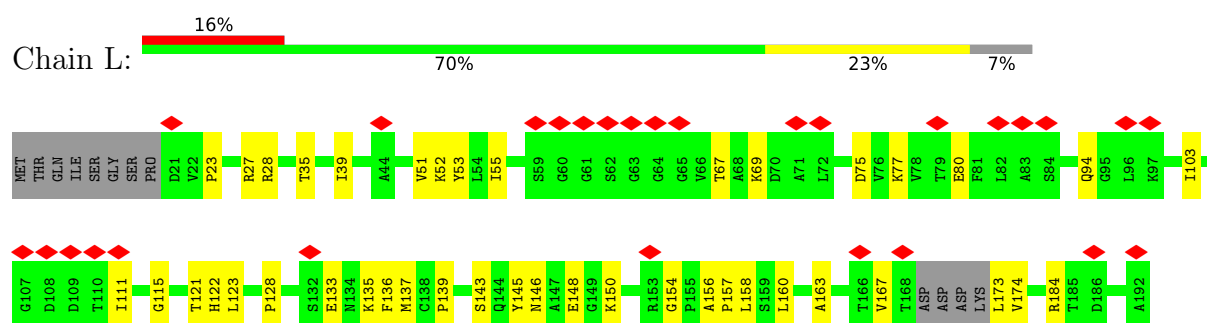
• Molecule 3: Cytochrome f



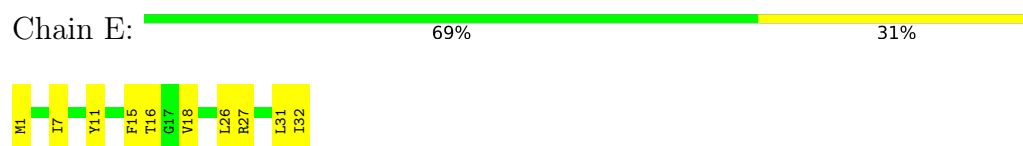
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 2



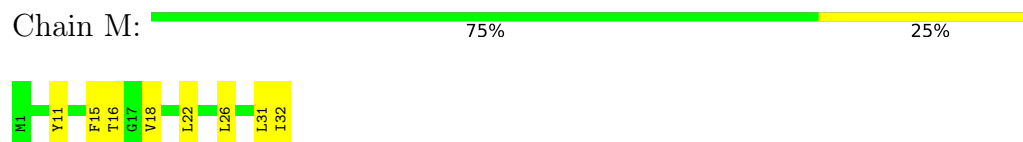
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 2



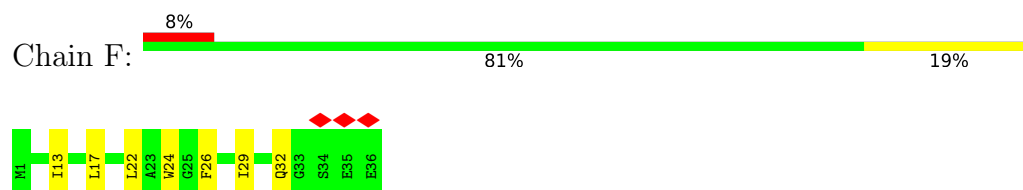
- Molecule 5: Cytochrome B6



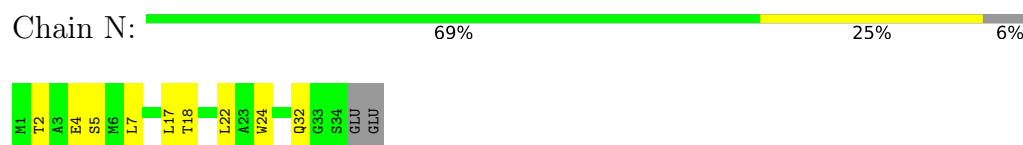
- Molecule 5: Cytochrome B6



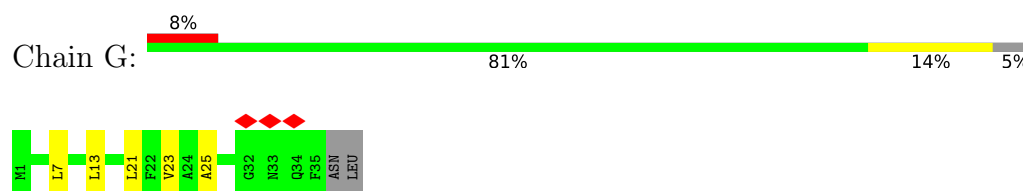
- Molecule 6: Cytochrome b6-f complex subunit 7



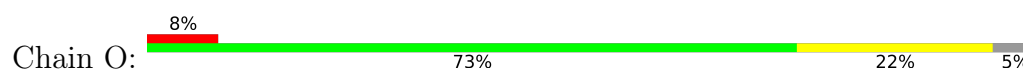
- Molecule 6: Cytochrome b6-f complex subunit 7



- Molecule 7: Cytochrome b6-f complex subunit 5

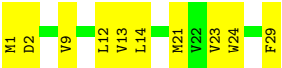


- Molecule 7: Cytochrome b6-f complex subunit 5





● 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	413442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.272	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0221	Depositor
Map size (Å)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, ECH, FES, PGV, HEM, HEC, LFA

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	0.20	0/1801	0.40	0/2454
1	I	0.17	0/1801	0.36	0/2454
2	B	0.14	0/1248	0.32	0/1705
2	J	0.13	0/1261	0.29	0/1721
3	C	0.13	0/2159	0.33	0/2935
3	K	0.14	0/2159	0.35	0/2935
4	D	0.14	0/1278	0.33	0/1746
4	L	0.13	0/1278	0.32	0/1746
5	E	0.13	0/243	0.42	0/326
5	M	0.14	0/243	0.32	0/326
6	F	0.18	0/270	0.34	0/361
6	N	0.15	0/251	0.31	0/337
7	G	0.13	0/275	0.29	0/373
7	O	0.12	0/275	0.27	0/373
8	H	0.20	0/242	0.40	0/329
8	P	0.19	0/242	0.43	0/329
All	All	0.15	0/15026	0.34	0/20450

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1750	0	1777	55	0
1	I	1750	0	1777	44	0
2	B	1211	0	1259	26	0
2	J	1223	0	1268	31	0
3	C	2116	0	2133	43	0
3	K	2116	0	2133	59	0
4	D	1248	0	1206	43	0
4	L	1248	0	1208	29	0
5	E	239	0	264	12	0
5	M	239	0	264	8	0
6	F	267	0	280	7	0
6	N	248	0	268	9	0
7	G	270	0	297	5	0
7	O	270	0	297	10	0
8	H	235	0	240	10	0
8	P	235	0	240	12	0
9	A	41	0	54	5	0
9	I	41	0	54	5	0
10	A	86	0	60	13	0
10	I	86	0	60	7	0
11	A	43	0	31	2	0
11	C	43	0	30	3	0
11	I	43	0	31	3	0
11	K	43	0	30	3	0
12	B	65	0	72	5	0
12	J	65	0	72	3	0
13	B	89	0	122	7	0
13	C	51	0	76	3	0
13	I	51	0	76	3	0
13	J	146	0	213	6	0
14	C	20	0	42	0	0
14	E	20	0	42	0	0
15	D	4	0	0	2	0
15	L	4	0	0	0	0
All	All	15606	0	15976	344	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 11.

All (344) 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)
4:D:69:LYS:HB2	4:D:94:GLN:HB3	1.54	0.90
1:A:56:ALA:O	1:A:59:PHE:HB3	1.84	0.77
3:K:159:GLN:HG3	3:K:170:ASN:HB3	1.66	0.76
4:D:120:CYS:HB3	15:D:201:FES:S1	2.27	0.74
3:K:30:LYS:HB2	3:K:155:ARG:NH2	2.03	0.74
2:B:39:MET:HE3	3:C:272:LYS:HD2	1.70	0.72
2:J:39:MET:HE3	3:K:272:LYS:HD3	1.71	0.72
3:C:12:THR:HG22	3:C:14:ARG:H	1.55	0.71
4:D:164:HIS:O	4:D:175:LEU:HA	1.90	0.71
1:A:59:PHE:HE1	1:I:197:VAL:HG22	1.56	0.71
4:L:160:LEU:O	4:L:184:ARG:NH1	2.24	0.70
4:D:69:LYS:NZ	4:D:75:ASP:OD1	2.21	0.70
3:K:19:ARG:NH2	3:K:24:ASN:OD1	2.25	0.69
1:A:3:SER:N	1:A:7:THR:HG1	1.90	0.69
3:K:6:GLN:HE21	3:K:106:TYR:HA	1.55	0.69
4:D:78:VAL:HG21	4:D:167:VAL:HG21	1.76	0.68
4:L:167:VAL:HB	4:L:173:LEU:HA	1.75	0.68
3:C:2:PRO:HB2	3:C:115:ILE:HD12	1.75	0.67
3:C:271:LYS:HB2	4:D:35:THR:HG21	1.76	0.67
4:D:90:ARG:HG2	4:D:104:VAL:HG22	1.75	0.67
12:J:201:CLA:HHC	12:J:201:CLA:HBB1	1.76	0.67
1:A:110:ARG:NH2	10:A:303:HEM:O2A	2.28	0.67
2:B:145:ALA:HA	13:B:203:PGV:H31	1.77	0.67
1:A:39:ILE:HG12	9:A:301:ECH:H32A	1.76	0.67
12:B:201:CLA:HBB1	13:B:202:PGV:H81	1.75	0.67
3:C:159:GLN:HG3	3:C:170:ASN:HB3	1.76	0.66
1:A:149:GLN:NE2	2:B:70:ALA:O	2.29	0.66
1:A:157:ILE:HD12	4:L:123:LEU:HG	1.78	0.66
5:E:26:LEU:HB3	5:E:32:ILE:HG12	1.78	0.66
1:A:59:PHE:CE1	1:I:197:VAL:HG22	2.31	0.65
3:K:34:VAL:HB	3:K:151:LEU:HD22	1.79	0.64
3:K:41:LEU:HD22	3:K:248:PRO:HG3	1.78	0.64
3:K:60:GLN:NE2	11:K:301:HEC:O1A	2.29	0.64
3:K:84:ILE:HG12	3:K:114:VAL:HG11	1.79	0.64
4:L:69:LYS:HB2	4:L:94:GLN:HB2	1.80	0.64
4:D:143:SER:HA	4:D:154:GLY:HA3	1.79	0.63
1:A:88:LEU:HD21	13:C:303:PGV:H72	1.81	0.63
4:L:143:SER:HA	4:L:154:GLY:HA3	1.80	0.62
4:D:144:GLN:HB2	4:D:153:ARG:HB2	1.80	0.62
9:I:301:ECH:H32B	8:P:19:ILE:HG12	1.80	0.62
6:N:4:GLU:HG2	6:N:5:SER:H	1.63	0.62
1:A:46:LEU:HD11	2:B:43:CYS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:TYR:OH	3:C:271:LYS:NZ	2.33	0.61
3:K:30:LYS:HB2	3:K:155:ARG:HH21	1.65	0.61
4:L:136:PHE:HB2	4:L:145:TYR:HB2	1.83	0.61
3:K:43:ASP:O	3:K:89:ARG:NH2	2.33	0.61
3:K:271:LYS:NZ	3:K:274:GLN:OE1	2.34	0.61
3:K:278:VAL:HG21	4:L:28:ARG:HD3	1.82	0.61
10:A:303:HEM:HBC2	10:A:303:HEM:HMC2	1.83	0.60
3:C:79:PRO:HD3	3:C:149:VAL:HG22	1.83	0.60
2:B:2:SER:OG	2:B:3:ILE:N	2.35	0.60
1:A:48:LEU:HD23	11:A:304:HEC:HBC3	1.83	0.60
1:A:93:HIS:HE1	10:A:302:HEM:NB	1.98	0.59
2:B:84:THR:HB	2:B:101:MET:HG3	1.83	0.59
8:H:9:VAL:O	8:H:13:VAL:HG23	2.02	0.59
3:K:180:ILE:HG21	3:K:193:LEU:HB3	1.84	0.59
10:A:303:HEM:HBB2	10:A:303:HEM:HMB2	1.84	0.59
10:I:304:HEM:HBC2	10:I:304:HEM:HMC2	1.85	0.59
4:D:164:HIS:CE1	4:D:178:TRP:HA	2.37	0.59
5:E:16:THR:OG1	6:F:24:TRP:NE1	2.35	0.59
1:A:104:MET:HE2	10:A:303:HEM:HAB	1.84	0.59
2:J:50:LEU:HD11	8:P:15:PHE:HB2	1.85	0.59
2:B:56:ILE:HD12	3:C:254:LEU:HD13	1.85	0.58
3:K:157:ARG:HB2	3:K:169:ASN:HD22	1.68	0.58
2:B:86:GLN:NE2	2:B:154:SER:OG	2.37	0.58
4:D:69:LYS:O	4:D:94:GLN:N	2.37	0.58
4:D:56:PRO:HG2	1:I:174:THR:HG22	1.85	0.58
3:K:174:ALA:HB2	3:K:227:LEU:HD11	1.86	0.58
3:C:60:GLN:NE2	11:C:301:HEC:O2A	2.37	0.57
4:D:82:LEU:HD13	4:D:110:THR:HB	1.87	0.57
4:L:115:GLY:N	4:L:163:ALA:O	2.33	0.57
4:D:120:CYS:CB	15:D:201:FES:S1	2.88	0.57
2:B:86:GLN:HE22	2:B:89:ARG:HH21	1.53	0.57
3:K:36:ILE:HD11	3:K:46:PHE:HE2	1.69	0.57
1:A:34:PRO:HG3	2:B:24:HIS:O	2.05	0.57
10:I:303:HEM:HMC1	10:I:303:HEM:HBC2	1.87	0.56
1:I:30:SER:OG	1:I:31:LYS:NZ	2.39	0.56
10:I:303:HEM:HBB2	10:I:303:HEM:HMB2	1.87	0.56
4:L:67:THR:HA	4:L:174:VAL:HA	1.88	0.56
2:B:91:LEU:HD12	2:B:97:GLY:HA2	1.87	0.55
2:J:2:SER:HB3	3:K:283:LEU:HB2	1.88	0.55
3:C:34:VAL:HB	3:C:151:LEU:HD22	1.87	0.55
3:K:262:MET:HE1	5:M:11:TYR:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:PRO:HB3	3:C:111:GLU:HA	1.89	0.54
3:K:107:ARG:HB3	3:K:110:MET:HB3	1.88	0.54
1:I:56:ALA:O	1:I:59:PHE:HB3	2.08	0.54
13:J:204:PGV:H251	7:O:11:LEU:HD11	1.90	0.54
5:E:15:PHE:HA	5:E:18:VAL:HG22	1.89	0.54
1:I:172:LEU:O	1:I:176:MET:HG3	2.08	0.54
3:K:77:MET:HG2	3:K:113:VAL:HG13	1.88	0.54
9:I:301:ECH:H37B	7:O:23:VAL:HG21	1.90	0.53
4:D:74:ASN:ND2	4:D:75:ASP:O	2.41	0.53
3:C:185:ALA:HA	3:C:191:TYR:HA	1.90	0.53
6:N:7:LEU:HD11	7:O:11:LEU:HD12	1.90	0.53
1:I:87:TRP:HE1	13:I:302:PGV:H042	1.74	0.53
2:J:45:LEU:HB3	3:K:261:ILE:HG23	1.90	0.53
2:B:123:PRO:HB3	2:B:130:MET:SD	2.49	0.53
1:I:59:PHE:O	1:I:62:THR:OG1	2.21	0.53
1:A:4:LYS:HE2	1:A:7:THR:HG21	1.90	0.52
5:E:26:LEU:HG	5:E:31:LEU:HD23	1.91	0.52
11:I:305:HEC:HBC3	2:J:44:ILE:HD11	1.91	0.52
5:E:1:MET:HE1	6:F:13:ILE:HD11	1.90	0.52
4:D:146:ASN:OD1	4:D:150:LYS:N	2.42	0.52
3:C:150:HIS:ND1	3:C:240:ASP:OD1	2.42	0.52
2:J:123:PRO:HD2	7:O:25:ALA:HB1	1.92	0.52
4:L:157:PRO:HG2	4:L:158:LEU:HD12	1.91	0.52
2:J:89:ARG:NH2	2:J:149:PHE:O	2.41	0.52
3:C:84:ILE:HG12	3:C:114:VAL:HG21	1.92	0.52
1:I:65:TYR:OH	1:I:145:LEU:O	2.20	0.52
1:A:102:LEU:HD21	7:G:13:LEU:HD12	1.92	0.51
1:I:4:LYS:H	1:I:4:LYS:HD2	1.76	0.51
1:I:4:LYS:O	2:J:32:TRP:NE1	2.35	0.51
2:J:35:ASP:OD1	8:P:26:ARG:NH1	2.44	0.51
3:K:105:PRO:HB3	3:K:111:GLU:HA	1.92	0.51
3:K:278:VAL:O	3:K:282:GLU:HG2	2.10	0.51
1:A:60:ALA:HB1	4:D:53:TYR:CE1	2.46	0.51
3:C:262:MET:HE1	5:E:11:TYR:CE2	2.46	0.51
5:M:15:PHE:HA	5:M:18:VAL:HG22	1.93	0.51
4:L:77:LYS:HB3	4:L:80:GLU:HG3	1.92	0.51
3:C:181:SER:HA	3:C:218:GLY:H	1.75	0.51
3:K:262:MET:HE1	5:M:11:TYR:CE2	2.46	0.50
1:I:139:GLY:HA3	2:J:80:TYR:OH	2.12	0.50
13:J:204:PGV:H262	7:O:7:LEU:HD22	1.93	0.50
1:A:19:LEU:HD11	1:I:212:MET:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:135:LYS:NZ	4:D:144:GLN:OE1	2.34	0.50
13:J:204:PGV:H242	7:O:7:LEU:HD13	1.92	0.50
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.93	0.50
2:J:58:ASP:OD1	3:K:146:LYS:NZ	2.37	0.50
1:A:54:GLN:NE2	1:A:96:SER:HB3	2.27	0.50
4:L:121:THR:OG1	4:L:158:LEU:O	2.27	0.50
4:D:87:ALA:HA	4:D:107:GLY:HA2	1.93	0.49
3:K:180:ILE:HD13	3:K:193:LEU:HB3	1.93	0.49
3:C:258:LEU:HD22	8:H:14:LEU:HD22	1.94	0.49
1:I:68:THR:HA	1:I:184:GLN:HE22	1.76	0.49
8:H:21:MET:HE2	8:H:21:MET:HA	1.95	0.49
1:A:112:TYR:OH	2:B:115:GLU:OE2	2.24	0.49
1:I:88:LEU:HD21	13:I:302:PGV:H261	1.95	0.49
2:J:132:VAL:HG11	13:J:202:PGV:H212	1.94	0.49
3:K:19:ARG:HG3	3:K:238:GLN:HE22	1.78	0.49
10:I:304:HEM:HMB1	10:I:304:HEM:HBB2	1.94	0.49
3:K:46:PHE:HE1	3:K:133:SER:HB3	1.77	0.49
2:J:77:PRO:HB2	2:J:81:LEU:HB2	1.95	0.49
3:C:262:MET:HE1	5:E:11:TYR:HE2	1.76	0.48
1:I:54:GLN:NE2	1:I:96:SER:HB3	2.29	0.48
3:K:41:LEU:HB2	3:K:44:THR:HG21	1.95	0.48
1:A:216:GLN:HG2	2:B:22:MET:HE3	1.96	0.48
4:L:122:HIS:HB2	4:L:156:ALA:HA	1.96	0.48
1:I:49:THR:OG1	11:I:305:HEC:HBC2	2.13	0.48
1:I:193:LEU:HA	1:I:197:VAL:HB	1.94	0.48
3:K:52:ILE:HG22	3:K:155:ARG:HD2	1.96	0.48
3:C:158:GLY:H	11:C:301:HEC:C3D	2.27	0.48
2:B:30:PRO:HG2	2:B:34:ASN:OD1	2.13	0.48
2:J:105:PRO:HG2	12:J:201:CLA:H102	1.94	0.48
1:I:60:ALA:HB1	4:L:53:TYR:CE1	2.48	0.48
1:A:76:VAL:HG21	1:A:146:PRO:HA	1.95	0.48
5:M:16:THR:OG1	6:N:24:TRP:NE1	2.43	0.48
3:C:107:ARG:HB3	3:C:110:MET:HB3	1.96	0.47
4:L:133:GLU:OE1	4:L:137:MET:HE1	2.13	0.47
1:A:54:GLN:HB3	10:A:302:HEM:CHC	2.44	0.47
4:D:128:PRO:HD2	4:D:139:PRO:HD3	1.95	0.47
3:K:42:PRO:HD3	3:K:246:GLN:O	2.14	0.47
10:A:302:HEM:HBB2	10:A:302:HEM:HMB1	1.97	0.47
6:F:17:LEU:HD11	8:H:12:LEU:HB3	1.96	0.47
1:A:54:GLN:HE21	1:A:96:SER:HB3	1.79	0.47
3:C:267:LEU:HB3	4:D:35:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:PRO:O	1:I:216:GLN:NE2	2.33	0.47
3:K:193:LEU:HB2	3:K:205:VAL:HG13	1.95	0.47
3:C:278:VAL:HG21	4:D:28:ARG:HD3	1.97	0.47
1:A:197:VAL:HG22	1:I:59:PHE:CE1	2.50	0.47
3:C:229:ASN:OD1	3:C:230:ASN:N	2.48	0.47
4:D:127:VAL:HG11	4:D:145:TYR:HE2	1.80	0.47
3:K:33:GLU:HA	3:K:239:LYS:HD2	1.97	0.47
1:I:120:PRO:HD2	1:I:121:ARG:HH11	1.80	0.46
4:L:69:LYS:O	4:L:94:GLN:N	2.41	0.46
4:D:120:CYS:SG	4:D:145:TYR:OH	2.71	0.46
4:L:135:LYS:HE2	4:L:137:MET:HE2	1.97	0.46
1:A:138:PHE:CE2	10:A:302:HEM:C1C	3.04	0.46
2:B:104:ILE:HA	13:B:202:PGV:H12	1.98	0.46
4:L:103:ILE:HD13	4:L:173:LEU:HD11	1.97	0.46
2:B:4:ILE:HG13	2:B:28:GLY:HA2	1.98	0.46
2:J:104:ILE:HB	2:J:105:PRO:HD3	1.97	0.46
6:N:17:LEU:HD11	8:P:12:LEU:HB3	1.97	0.46
4:D:118:ALA:HB1	4:D:126:VAL:HG13	1.98	0.46
4:L:148:GLU:OE2	4:L:184:ARG:HG2	2.16	0.46
4:D:136:PHE:HB2	4:D:145:TYR:HB2	1.98	0.46
1:I:156:LYS:HA	1:I:182:VAL:HG21	1.98	0.46
1:A:104:MET:HE1	1:A:135:THR:OG1	2.16	0.45
9:I:301:ECH:H20	9:I:301:ECH:H36	1.71	0.45
2:J:89:ARG:HH21	2:J:154:SER:HB3	1.81	0.45
3:C:274:GLN:HG3	5:E:32:ILE:HA	1.99	0.45
3:K:274:GLN:HG3	4:L:23:PRO:HG2	1.97	0.45
1:A:5:GLU:OE2	1:A:25:SER:HB3	2.16	0.45
1:A:68:THR:O	1:A:72:ALA:N	2.48	0.45
9:A:301:ECH:H20	9:A:301:ECH:H36	1.71	0.45
2:B:108:LEU:HD23	13:B:202:PGV:H91	1.98	0.45
9:I:301:ECH:H2A	8:P:22:VAL:HG21	1.98	0.45
3:K:182:GLU:O	3:K:193:LEU:HD23	2.16	0.45
3:C:157:ARG:NE	11:C:301:HEC:O1D	2.41	0.45
2:J:49:GLY:HA3	8:P:14:LEU:HD21	1.99	0.45
4:D:167:VAL:HB	4:D:173:LEU:HA	1.99	0.45
1:I:125:TRP:NE1	2:J:108:LEU:O	2.33	0.45
2:J:71:THR:O	3:K:17:THR:OG1	2.31	0.45
1:A:10:LYS:HA	1:A:10:LYS:HD3	1.77	0.45
1:A:136:VAL:HG21	12:B:201:CLA:H11	1.97	0.45
5:E:7:ILE:HG22	8:H:9:VAL:HG11	1.99	0.45
3:K:269:VAL:HG11	8:P:24:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:27:ARG:HB3	5:M:31:LEU:HD12	1.99	0.45
4:D:31:MET:O	4:D:35:THR:HG23	2.16	0.45
2:J:82:TYR:HB3	2:J:144:GLY:HA2	1.99	0.45
10:A:302:HEM:HMC1	10:A:302:HEM:HBC2	1.98	0.45
1:I:4:LYS:HD2	1:I:4:LYS:N	2.31	0.45
3:K:158:GLY:H	11:K:301:HEC:C3D	2.30	0.45
3:C:88:ASP:OD1	3:C:89:ARG:N	2.49	0.44
3:K:194:ILE:HD12	3:K:204:THR:HA	1.99	0.44
3:K:194:ILE:HG13	3:K:202:THR:HG23	1.99	0.44
4:D:31:MET:HE3	4:D:35:THR:CG2	2.48	0.44
5:E:27:ARG:HG3	5:E:32:ILE:HG13	1.98	0.44
3:K:97:LYS:HE3	3:K:97:LYS:HB2	1.80	0.44
4:L:111:ILE:HG21	4:L:173:LEU:HD13	1.99	0.44
3:C:269:VAL:HG11	8:H:24:TRP:CE3	2.53	0.44
2:J:114:ILE:HG23	13:J:202:PGV:H31	1.98	0.44
4:L:35:THR:O	4:L:39:ILE:HG13	2.17	0.44
1:A:120:PRO:HD2	1:A:121:ARG:NH1	2.32	0.44
4:D:182:ASP:OD1	4:D:184:ARG:NE	2.48	0.44
1:I:149:GLN:HG2	2:J:72:PRO:HG3	2.00	0.44
1:A:142:GLY:HA3	1:A:194:HIS:CE1	2.53	0.44
3:C:14:ARG:NE	3:C:18:GLY:HA2	2.33	0.44
3:C:51:LYS:HG2	3:C:126:GLU:HB3	1.99	0.44
4:D:130:ASN:O	4:D:134:ASN:N	2.51	0.44
3:C:6:GLN:NE2	3:C:106:TYR:HA	2.32	0.44
1:I:110:ARG:HG2	7:O:21:LEU:HD21	2.00	0.44
1:A:104:MET:O	1:A:108:VAL:HG23	2.18	0.44
3:C:274:GLN:HB2	5:E:32:ILE:HG22	2.00	0.44
4:D:123:LEU:HD12	4:D:141:HIS:HE1	1.83	0.44
12:J:201:CLA:H3A	12:J:201:CLA:HBA2	1.60	0.44
1:A:114:THR:HA	1:A:222:LEU:HD21	2.00	0.44
3:C:267:LEU:HD13	4:D:34:LEU:HG	2.00	0.44
1:I:57:THR:HG23	13:I:302:PGV:H311	2.00	0.43
2:J:108:LEU:HA	2:J:108:LEU:HD12	1.84	0.43
1:A:61:MET:HE3	10:A:302:HEM:HBA1	2.00	0.43
1:A:145:LEU:N	1:A:146:PRO:HD2	2.32	0.43
11:A:304:HEC:CBC	11:A:304:HEC:HHH	2.48	0.43
3:C:250:ARG:HH21	13:C:303:PGV:H042	1.83	0.43
3:K:79:PRO:HG2	3:K:82:PHE:CE1	2.53	0.43
3:C:78:LEU:HD13	3:C:131:VAL:HG13	2.00	0.43
3:K:118:PRO:HB3	11:K:301:HEC:HMA1	2.00	0.43
6:N:22:LEU:HD13	8:P:23:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HA	13:C:303:PGV:H161	2.01	0.43
4:D:160:LEU:O	4:D:184:ARG:NH1	2.38	0.43
3:K:79:PRO:HG2	3:K:82:PHE:CD1	2.53	0.43
1:A:51:PHE:O	1:A:55:PHE:N	2.50	0.43
1:I:222:LEU:HB2	7:O:28:GLN:OE1	2.19	0.43
4:L:51:VAL:O	4:L:55:ILE:HG13	2.17	0.43
3:C:75:VAL:HG23	3:C:115:ILE:HG22	2.01	0.43
1:I:155:VAL:HA	1:I:158:VAL:HG22	2.01	0.43
4:L:128:PRO:HD3	4:L:139:PRO:HD3	2.00	0.43
1:I:153:TRP:CD1	2:J:72:PRO:HD3	2.54	0.43
3:K:264:SER:OG	4:L:39:ILE:HG12	2.19	0.43
1:I:214:ARG:HB2	11:I:305:HEC:O1D	2.19	0.43
9:I:301:ECH:H35	6:N:22:LEU:HD21	2.00	0.43
2:J:56:ILE:HD12	3:K:254:LEU:HD13	1.99	0.43
12:B:201:CLA:C1C	13:B:202:PGV:H102	2.49	0.43
3:C:211:PRO:HB2	3:C:228:THR:HB	2.01	0.43
3:K:72:VAL:HG21	3:K:124:TYR:O	2.19	0.43
3:K:180:ILE:HG22	3:K:182:GLU:H	1.84	0.42
6:N:32:GLN:CD	8:P:24:TRP:HE1	2.27	0.42
1:A:104:MET:HE2	10:A:303:HEM:CAB	2.49	0.42
3:C:52:ILE:HG12	3:C:153:ALA:HB1	2.01	0.42
1:I:36:HIS:NE2	1:I:219:SER:O	2.50	0.42
3:K:181:SER:HA	3:K:218:GLY:H	1.84	0.42
6:N:2:THR:HG22	8:P:4:LEU:HB2	2.01	0.42
4:D:102:TYR:OH	4:D:127:VAL:O	2.34	0.42
4:L:67:THR:OG1	4:L:75:ASP:OD2	2.27	0.42
3:C:6:GLN:HE21	3:C:115:ILE:CD1	2.33	0.42
4:D:157:PRO:HB2	4:D:158:LEU:HD12	2.02	0.42
3:K:277:LYS:NZ	5:M:32:ILE:OXT	2.44	0.42
1:A:51:PHE:HB2	1:A:100:MET:CE	2.49	0.42
1:A:65:TYR:OH	1:A:145:LEU:O	2.28	0.42
1:A:196:PHE:CZ	10:I:303:HEM:HBB2	2.54	0.42
1:I:37:VAL:O	8:P:26:ARG:NH2	2.52	0.42
9:A:301:ECH:H15	9:A:301:ECH:H35	1.90	0.42
13:B:202:PGV:H101	13:B:202:PGV:H132	1.69	0.42
4:D:92:LEU:HD11	2:J:69:PHE:HB3	2.02	0.42
2:B:46:GLY:O	2:B:50:LEU:HG	2.19	0.42
2:J:2:SER:N	3:K:280:ALA:HA	2.35	0.42
2:B:45:LEU:HB3	3:C:261:ILE:HG23	2.01	0.42
4:D:114:TYR:HA	4:D:163:ALA:O	2.20	0.42
1:A:155:VAL:HA	1:A:158:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:301:ECH:H21	9:A:301:ECH:H24	1.77	0.41
12:B:201:CLA:H93	12:B:201:CLA:H111	1.92	0.41
3:C:14:ARG:CD	3:C:77:MET:HE1	2.51	0.41
1:I:175:LEU:HD23	1:I:175:LEU:HA	1.95	0.41
13:J:202:PGV:H151	13:J:202:PGV:H12	1.82	0.41
4:L:146:ASN:OD1	4:L:150:LYS:N	2.52	0.41
3:K:173:LYS:HG2	3:K:226:PHE:HD1	1.86	0.41
3:K:193:LEU:HD12	3:K:227:LEU:HD23	2.00	0.41
3:K:257:PHE:CE2	3:K:261:ILE:HD11	2.55	0.41
1:A:195:THR:HG22	10:A:302:HEM:HMB2	2.01	0.41
1:A:196:PHE:CE1	10:I:303:HEM:HBB2	2.56	0.41
12:B:201:CLA:H61	12:B:201:CLA:H2	1.74	0.41
1:I:80:MET:HE3	1:I:80:MET:HB3	1.88	0.41
3:K:105:PRO:C	3:K:107:ARG:H	2.29	0.41
1:A:20:GLU:O	1:A:20:GLU:HG3	2.20	0.41
2:B:82:TYR:HB3	2:B:144:GLY:HA2	2.03	0.41
1:I:51:PHE:HB2	1:I:100:MET:CE	2.51	0.41
1:I:193:LEU:HD23	1:I:197:VAL:HG21	2.02	0.41
1:A:54:GLN:HB3	10:A:302:HEM:HHC	2.01	0.41
4:D:67:THR:OG1	4:D:68:ALA:N	2.52	0.41
8:H:1:MET:HB3	8:H:2:ASP:H	1.76	0.41
1:I:157:ILE:HG13	2:J:75:ILE:HD12	2.02	0.41
2:J:123:PRO:HB3	2:J:130:MET:SD	2.60	0.41
1:A:110:ARG:HG2	7:G:21:LEU:HD21	2.03	0.41
5:M:22:LEU:O	5:M:26:LEU:HG	2.21	0.41
1:A:172:LEU:O	1:A:176:MET:HG3	2.20	0.41
3:C:17:THR:HG23	3:C:19:ARG:H	1.85	0.41
4:D:92:LEU:HA	4:D:102:TYR:HA	2.02	0.41
4:D:158:LEU:HD23	4:D:190:TRP:CG	2.56	0.41
7:G:7:LEU:HD23	7:G:7:LEU:HA	1.90	0.41
2:J:79:TRP:CD1	7:O:6:LEU:HD21	2.56	0.41
6:N:18:THR:OG1	7:O:16:VAL:HG21	2.21	0.41
1:A:197:VAL:HG22	1:I:59:PHE:HE1	1.85	0.41
3:K:47:GLU:HB2	3:K:128:VAL:HG13	2.03	0.41
2:B:86:GLN:HE22	2:B:89:ARG:NH2	2.19	0.40
3:C:37:PRO:O	3:C:243:VAL:HG23	2.20	0.40
6:F:22:LEU:HD23	8:H:23:VAL:HG21	2.02	0.40
1:I:117:PHE:HB3	1:I:125:TRP:CE3	2.56	0.40
1:A:4:LYS:O	2:B:32:TRP:NE1	2.48	0.40
13:B:202:PGV:H261	13:B:202:PGV:H232	1.88	0.40
4:D:27:ARG:HB3	5:E:31:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:26:PHE:CZ	8:H:29:PHE:HB3	2.56	0.40
3:K:254:LEU:O	3:K:258:LEU:HG	2.21	0.40
5:M:11:TYR:CD2	8:P:13:VAL:HG11	2.56	0.40
1:A:12:PHE:CZ	1:A:21:VAL:HG23	2.56	0.40
3:C:110:MET:O	3:C:110:MET:HG2	2.22	0.40
4:D:150:LYS:HB2	4:D:184:ARG:HB3	2.02	0.40
1:I:90:ARG:NE	10:I:303:HEM:O1D	2.51	0.40
3:K:95:LYS:HB2	3:K:95:LYS:HE3	1.72	0.40
4:L:52:LYS:HD2	4:L:52:LYS:HA	1.80	0.40
1:A:101:VAL:HG21	2:B:80:TYR:CE1	2.57	0.40
1:A:18:ARG:HH12	1:I:119:LYS:HD2	1.87	0.40
9:A:301:ECH:H37B	7:G:23:VAL:HG21	2.02	0.40
6:F:17:LEU:CD1	8:H:12:LEU:HB3	2.51	0.40
6:F:29:ILE:O	6:F:32:GLN:HG2	2.21	0.40
1:I:101:VAL:HG11	2:J:80:TYR:CG	2.57	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	218/222 (98%)	210 (96%)	8 (4%)	0	100	100
1	I	218/222 (98%)	212 (97%)	6 (3%)	0	100	100
2	B	156/160 (98%)	149 (96%)	7 (4%)	0	100	100
2	J	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
3	C	275/284 (97%)	266 (97%)	9 (3%)	0	100	100
3	K	275/284 (97%)	262 (95%)	13 (5%)	0	100	100
4	D	164/180 (91%)	155 (94%)	9 (6%)	0	100	100
4	L	164/180 (91%)	162 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	30/32 (94%)	30 (100%)	0	0	100	100
5	M	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
6	F	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
6	N	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
7	G	33/37 (89%)	33 (100%)	0	0	100	100
7	O	33/37 (89%)	33 (100%)	0	0	100	100
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	1873/1960 (96%)	1808 (96%)	65 (4%)	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	190/192 (99%)	190 (100%)	0	100	100
1	I	190/192 (99%)	190 (100%)	0	100	100
2	B	126/128 (98%)	126 (100%)	0	100	100
2	J	127/128 (99%)	127 (100%)	0	100	100
3	C	226/230 (98%)	226 (100%)	0	100	100
3	K	226/230 (98%)	226 (100%)	0	100	100
4	D	131/142 (92%)	131 (100%)	0	100	100
4	L	131/142 (92%)	131 (100%)	0	100	100
5	E	23/23 (100%)	23 (100%)	0	100	100
5	M	23/23 (100%)	23 (100%)	0	100	100
6	F	27/27 (100%)	27 (100%)	0	100	100
6	N	25/27 (93%)	25 (100%)	0	100	100
7	G	28/30 (93%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	O	28/30 (93%)	28 (100%)	0	100	100
8	H	26/26 (100%)	26 (100%)	0	100	100
8	P	26/26 (100%)	26 (100%)	0	100	100
All	All	1553/1596 (97%)	1553 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	54	GLN
2	B	86	GLN
2	B	122	ASN
3	C	6	GLN
3	C	143	ASN
3	C	274	GLN
4	D	29	GLN
4	D	74	ASN
1	I	54	GLN
2	J	86	GLN
3	K	6	GLN
3	K	143	ASN
3	K	159	GLN
3	K	169	ASN
3	K	246	GLN
4	L	94	GLN
4	L	164	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 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	LFA	E	101	-	19,19,19	0.11	0	18,18,18	1.36	0
13	PGV	B	203	-	43,43,50	0.79	1 (2%)	46,49,56	1.03	3 (6%)
12	CLA	J	201	-	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
11	HEC	C	301	3	46,50,50	1.83	7 (15%)	58,82,82	1.72	5 (8%)
10	HEM	I	304	1	50,50,50	1.41	6 (12%)	67,82,82	1.07	5 (7%)
13	PGV	I	302	-	50,50,50	0.74	1 (2%)	53,56,56	0.99	3 (5%)
11	HEC	A	304	1	46,50,50	1.86	6 (13%)	58,82,82	1.13	2 (3%)
10	HEM	I	303	1	50,50,50	1.38	7 (14%)	67,82,82	1.13	5 (7%)
11	HEC	I	305	1	46,50,50	1.88	7 (15%)	58,82,82	1.08	2 (3%)
12	CLA	B	201	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
13	PGV	B	202	-	44,44,50	0.77	1 (2%)	47,50,56	1.01	3 (6%)
13	PGV	J	203	-	43,43,50	0.79	2 (4%)	46,49,56	1.04	3 (6%)
9	ECH	I	301	-	42,42,42	0.87	2 (4%)	55,58,58	2.02	14 (25%)
11	HEC	K	301	3	46,50,50	1.83	6 (13%)	58,82,82	1.75	4 (6%)
10	HEM	A	302	1	50,50,50	1.45	8 (16%)	67,82,82	1.10	5 (7%)
13	PGV	J	204	-	50,50,50	0.72	2 (4%)	53,56,56	1.00	3 (5%)
9	ECH	A	301	-	42,42,42	1.05	3 (7%)	55,58,58	2.04	12 (21%)
15	FES	D	201	4	0,4,4	-	-	-	-	-
10	HEM	A	303	1	50,50,50	1.41	6 (12%)	67,82,82	1.04	4 (5%)
14	LFA	C	302	-	19,19,19	0.12	0	18,18,18	1.38	0
13	PGV	C	303	-	50,50,50	0.73	1 (2%)	53,56,56	1.01	3 (5%)
15	FES	L	201	4	0,4,4	-	-	-	-	-
13	PGV	J	202	-	50,50,50	0.73	1 (2%)	53,56,56	1.01	3 (5%)

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	LFA	E	101	-	-	4/17/17/17	-
13	PGV	B	203	-	-	18/48/48/55	-
12	CLA	J	201	-	1/1/15/20	10/39/115/115	-
11	HEC	C	301	3	-	4/14/54/54	-
10	HEM	I	304	1	-	1/14/54/54	-
13	PGV	I	302	-	-	16/55/55/55	-
11	HEC	A	304	1	-	4/14/54/54	-
10	HEM	I	303	1	-	4/14/54/54	-
11	HEC	I	305	1	-	4/14/54/54	-
12	CLA	B	201	-	1/1/15/20	13/39/115/115	-
13	PGV	B	202	-	-	16/49/49/55	-
13	PGV	J	203	-	-	22/48/48/55	-
9	ECH	I	301	-	-	8/29/66/66	0/2/2/2
11	HEC	K	301	3	-	7/14/54/54	-
10	HEM	A	302	1	-	3/14/54/54	-
13	PGV	J	204	-	-	20/55/55/55	-
9	ECH	A	301	-	-	8/29/66/66	0/2/2/2
15	FES	D	201	4	-	-	0/1/1/1
10	HEM	A	303	1	-	0/14/54/54	-
14	LFA	C	302	-	-	6/17/17/17	-
13	PGV	C	303	-	-	17/55/55/55	-
15	FES	L	201	4	-	-	0/1/1/1
13	PGV	J	202	-	-	13/55/55/55	-

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	304	HEC	CAB-C3B	6.37	1.55	1.35
11	I	305	HEC	CAB-C3B	6.30	1.55	1.35
11	I	305	HEC	CAC-C3C	6.25	1.55	1.35
11	A	304	HEC	CAC-C3C	6.24	1.55	1.35
11	C	301	HEC	CAC-C3C	6.12	1.54	1.35
11	K	301	HEC	CAB-C3B	6.11	1.54	1.35
11	K	301	HEC	CAC-C3C	6.09	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	301	HEC	CAB-C3B	5.99	1.54	1.35
11	K	301	HEC	C3D-C2D	5.74	1.53	1.38
11	C	301	HEC	C3D-C2D	5.73	1.53	1.38
11	I	305	HEC	CBC-CAC	-4.29	1.33	1.49
11	I	305	HEC	CBB-CAB	-4.16	1.34	1.49
11	A	304	HEC	CBC-CAC	-4.15	1.34	1.49
11	A	304	HEC	CBB-CAB	-4.14	1.34	1.49
10	A	302	HEM	FE-ND	3.94	2.07	1.94
12	J	201	CLA	C1D-ND	3.52	1.42	1.37
12	B	201	CLA	C1D-ND	3.50	1.42	1.37
10	A	303	HEM	FE-NB	3.40	2.05	1.94
10	I	304	HEM	FE-ND	3.36	2.05	1.94
12	J	201	CLA	C4B-NB	3.30	1.42	1.37
10	A	303	HEM	FE-NC	3.28	2.06	1.95
10	I	304	HEM	FE-NC	3.24	2.05	1.95
10	A	302	HEM	FE-NC	3.22	2.05	1.95
10	A	302	HEM	FE-NA	3.19	2.05	1.95
10	I	303	HEM	FE-ND	3.13	2.04	1.94
10	A	303	HEM	FE-ND	3.12	2.04	1.94
10	I	304	HEM	FE-NB	3.09	2.04	1.94
10	I	303	HEM	FE-NC	3.07	2.05	1.95
12	B	201	CLA	C4B-NB	3.07	1.41	1.37
10	A	302	HEM	FE-NB	3.04	2.04	1.94
10	I	303	HEM	CAC-C3C	3.01	1.55	1.47
10	I	304	HEM	CAC-C3C	3.01	1.55	1.47
10	I	304	HEM	CAB-C3B	3.00	1.55	1.47
10	A	303	HEM	CAB-C3B	2.98	1.55	1.47
10	A	302	HEM	CAB-C3B	2.97	1.55	1.47
10	A	303	HEM	CAC-C3C	2.97	1.55	1.47
10	A	302	HEM	CAC-C3C	2.96	1.55	1.47
10	I	304	HEM	FE-NA	2.96	2.04	1.95
10	I	303	HEM	FE-NA	2.95	2.04	1.95
10	I	303	HEM	CAB-C3B	2.94	1.55	1.47
10	I	303	HEM	FE-NB	2.90	2.03	1.94
9	A	301	ECH	C30-C25	-2.90	1.50	1.53
9	A	301	ECH	C1-C6	-2.88	1.50	1.53
10	A	303	HEM	FE-NA	2.87	2.04	1.95
9	A	301	ECH	C25-C26	-2.68	1.32	1.35
12	B	201	CLA	C1B-C2B	2.62	1.49	1.43
12	J	201	CLA	C3B-C4B	2.61	1.50	1.42
12	J	201	CLA	C1B-C2B	2.57	1.49	1.43
9	I	301	ECH	C30-C25	-2.43	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	201	CLA	C3B-C4B	2.37	1.49	1.42
13	J	204	PGV	P-O12	2.29	1.68	1.59
13	B	203	PGV	P-O12	2.27	1.68	1.59
13	J	203	PGV	P-O12	2.27	1.68	1.59
12	J	201	CLA	CHC-C1C	2.26	1.43	1.38
12	B	201	CLA	CHC-C1C	2.24	1.43	1.38
11	A	304	HEC	C3C-C2C	-2.21	1.33	1.41
11	K	301	HEC	C3B-C2B	-2.19	1.33	1.41
13	J	202	PGV	P-O12	2.19	1.68	1.59
13	C	303	PGV	P-O12	2.18	1.67	1.59
13	I	302	PGV	P-O12	2.13	1.67	1.59
12	J	201	CLA	CMD-C2D	-2.13	1.46	1.50
10	A	302	HEM	CMC-C2C	2.12	1.55	1.50
9	I	301	ECH	C1-C6	-2.12	1.51	1.53
13	B	202	PGV	P-O12	2.11	1.67	1.59
12	B	201	CLA	CMB-C2B	-2.11	1.46	1.50
12	B	201	CLA	MG-NB	-2.10	2.01	2.05
12	J	201	CLA	CMB-C2B	-2.08	1.46	1.50
11	I	305	HEC	CMB-C2B	2.08	1.55	1.50
11	C	301	HEC	CMC-C2C	2.07	1.55	1.50
11	A	304	HEC	CMB-C2B	2.06	1.55	1.50
12	B	201	CLA	CMD-C2D	-2.06	1.46	1.50
11	C	301	HEC	C3B-C2B	-2.06	1.34	1.41
11	K	301	HEC	C3C-C2C	-2.05	1.34	1.41
13	J	204	PGV	P-O11	2.04	1.67	1.59
10	I	303	HEM	CMC-C2C	2.04	1.54	1.50
11	I	305	HEC	CMC-C2C	2.03	1.54	1.50
11	I	305	HEC	C3D-C2D	-2.02	1.33	1.38
11	C	301	HEC	C3C-C2C	-2.01	1.34	1.41
11	C	301	HEC	CMB-C2B	2.01	1.54	1.50
11	K	301	HEC	CMC-C2C	2.00	1.54	1.50
13	J	203	PGV	P-O11	2.00	1.67	1.59
10	A	302	HEM	C2A-C3A	-2.00	1.33	1.38

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	301	HEC	CBB-CAB-C3B	-7.90	111.65	127.43
11	C	301	HEC	CBC-CAC-C3C	-7.48	112.49	127.43
11	K	301	HEC	CBC-CAC-C3C	-6.71	114.02	127.43
12	B	201	CLA	C4A-NA-C1A	6.47	109.63	106.68
11	C	301	HEC	CBB-CAB-C3B	-6.31	114.81	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	201	CLA	C4A-NA-C1A	6.05	109.44	106.68
9	A	301	ECH	C20-C21-C22	-5.48	119.60	127.28
9	I	301	ECH	C20-C21-C22	-4.98	120.30	127.28
9	I	301	ECH	C24-C23-C22	-4.82	119.10	126.23
9	I	301	ECH	C15-C14-C13	-4.66	120.74	127.28
9	I	301	ECH	C16-C17-C18	-4.63	120.79	127.28
9	A	301	ECH	C15-C14-C13	-4.53	120.92	127.28
9	A	301	ECH	C7-C8-C9	-4.46	119.64	126.23
9	A	301	ECH	C33-C5-C6	-4.27	119.83	124.48
9	I	301	ECH	C33-C5-C6	-4.24	119.86	124.48
9	A	301	ECH	C24-C23-C22	-4.21	120.00	126.23
9	I	301	ECH	C7-C8-C9	-3.91	120.46	126.23
9	A	301	ECH	C28-C27-C26	-3.81	115.22	118.64
9	A	301	ECH	C16-C17-C18	-3.70	122.08	127.28
11	C	301	HEC	C4D-ND-C1D	3.50	111.53	105.82
11	K	301	HEC	C4D-ND-C1D	3.43	111.41	105.82
9	I	301	ECH	C11-C10-C9	-3.28	122.68	127.28
9	I	301	ECH	C28-C27-C26	-3.22	115.75	118.64
12	J	201	CLA	C3B-C4B-NB	-3.16	107.71	110.53
9	A	301	ECH	C23-C24-C25	-3.11	118.70	127.00
12	B	201	CLA	C3B-C4B-NB	-2.92	107.92	110.53
9	I	301	ECH	C23-C24-C25	-2.91	119.23	127.00
12	B	201	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
12	J	201	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
13	J	202	PGV	O14-P-O13	2.78	125.38	112.44
13	J	204	PGV	O14-P-O13	2.74	125.20	112.44
13	B	202	PGV	O14-P-O13	2.73	125.14	112.44
13	J	203	PGV	O14-P-O13	2.73	125.13	112.44
13	B	203	PGV	O14-P-O13	2.72	125.12	112.44
9	A	301	ECH	C11-C10-C9	-2.71	123.48	127.28
13	C	303	PGV	O14-P-O13	2.71	125.05	112.44
13	I	302	PGV	O14-P-O13	2.71	125.03	112.44
9	A	301	ECH	C8-C7-C6	-2.65	119.91	127.00
11	C	301	HEC	C2A-C1A-NA	-2.61	107.80	110.32
11	A	304	HEC	C2A-C1A-NA	-2.54	107.87	110.32
9	I	301	ECH	C8-C7-C6	-2.52	120.27	127.00
13	I	302	PGV	P-O12-C04	-2.52	106.93	121.35
13	B	202	PGV	P-O12-C04	-2.51	106.94	121.35
13	C	303	PGV	P-O12-C04	-2.51	106.98	121.35
13	J	204	PGV	P-O12-C04	-2.50	107.00	121.35
13	J	202	PGV	P-O12-C04	-2.50	107.02	121.35
9	I	301	ECH	C29-C30-C25	-2.49	106.82	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	301	HEC	C2A-C1A-NA	-2.49	107.92	110.32
10	I	303	HEM	C4D-ND-C1D	2.47	108.13	105.21
12	B	201	CLA	CHB-C4A-NA	2.44	127.92	124.40
13	J	203	PGV	P-O12-C04	-2.44	107.38	121.35
13	B	203	PGV	P-O12-C04	-2.43	107.45	121.35
10	I	303	HEM	C3D-C4D-ND	-2.38	107.56	110.17
11	I	305	HEC	C2A-C1A-NA	-2.36	108.04	110.32
13	B	203	PGV	P-O11-C03	-2.35	107.89	121.35
13	C	303	PGV	P-O11-C03	-2.33	108.03	121.35
13	J	203	PGV	P-O11-C03	-2.32	108.07	121.35
10	I	304	HEM	C4D-ND-C1D	2.31	107.94	105.21
13	J	202	PGV	P-O11-C03	-2.29	108.22	121.35
9	I	301	ECH	C28-C29-C30	-2.29	109.86	113.21
11	I	305	HEC	CHD-C4C-NC	2.28	126.93	124.45
10	A	302	HEM	C4D-ND-C1D	2.28	107.90	105.21
13	I	302	PGV	P-O11-C03	-2.27	108.32	121.35
13	J	204	PGV	P-O11-C03	-2.27	108.36	121.35
12	J	201	CLA	CHB-C4A-NA	2.25	127.65	124.40
10	A	302	HEM	C3D-C4D-ND	-2.24	107.71	110.17
9	A	301	ECH	C15-C16-C17	-2.24	118.93	123.52
13	B	202	PGV	P-O11-C03	-2.22	108.63	121.35
10	A	303	HEM	C4D-ND-C1D	2.20	107.82	105.21
10	A	303	HEM	C3B-C2B-C1B	2.20	108.07	106.41
12	J	201	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
11	C	301	HEC	CHC-C4B-NB	2.17	126.81	124.45
9	I	301	ECH	C20-C19-C18	-2.14	120.49	126.36
10	I	304	HEM	C3D-C4D-ND	-2.13	107.83	110.17
10	I	304	HEM	C2A-C1A-NA	-2.13	107.79	110.15
9	I	301	ECH	C7-C6-C5	-2.12	116.67	121.56
10	A	302	HEM	C2A-C1A-NA	-2.11	107.81	110.15
10	I	303	HEM	C1B-NB-C4B	2.10	107.70	105.21
10	A	302	HEM	C1B-NB-C4B	2.10	107.69	105.21
10	I	303	HEM	C3B-C2B-C1B	2.10	107.99	106.41
10	I	304	HEM	C3B-C2B-C1B	2.10	107.99	106.41
12	B	201	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
10	A	302	HEM	C3B-C2B-C1B	2.07	107.97	106.41
10	A	303	HEM	C3D-C4D-ND	-2.05	107.93	110.17
10	I	303	HEM	C2A-C1A-NA	-2.04	107.89	110.15
11	A	304	HEC	CBC-CAC-C3C	-2.03	123.38	127.43
10	A	303	HEM	CBD-CAD-C3D	-2.01	106.97	112.53
10	I	304	HEM	C1B-NB-C4B	2.01	107.58	105.21
9	A	301	ECH	C8-C9-C10	2.00	122.16	119.01

All (2) chirality outliers are listed below:

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

All (198) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	301	ECH	C23-C24-C25-C26
11	A	304	HEC	C2B-C3B-CAB-CBB
11	A	304	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	305	HEC	C2B-C3B-CAB-CBB
11	I	305	HEC	C4B-C3B-CAB-CBB
11	K	301	HEC	C2B-C3B-CAB-CBB
11	K	301	HEC	C2C-C3C-CAC-CBC
11	K	301	HEC	C4C-C3C-CAC-CBC
12	J	201	CLA	C3A-C2A-CAA-CBA
13	B	202	PGV	O12-C04-C05-C06
13	B	203	PGV	C04-O12-P-O11
13	B	203	PGV	C04-O12-P-O13
13	B	203	PGV	C04-O12-P-O14
13	C	303	PGV	C03-O11-P-O13
13	C	303	PGV	C04-O12-P-O13
13	I	302	PGV	C04-O12-P-O11
13	I	302	PGV	C04-O12-P-O14
13	I	302	PGV	O12-C04-C05-C06
13	J	202	PGV	O12-C04-C05-O05
13	J	202	PGV	C2-C1-O01-C02
13	J	203	PGV	C04-O12-P-O11
13	J	203	PGV	C04-O12-P-O13
13	J	203	PGV	C04-O12-P-O14
13	J	203	PGV	O02-C1-O01-C02
13	J	204	PGV	C04-O12-P-O11
13	J	204	PGV	C04-O12-P-O14
13	J	204	PGV	C2-C1-O01-C02
13	J	203	PGV	O04-C19-O03-C01
13	B	203	PGV	O04-C19-O03-C01
13	C	303	PGV	O04-C19-O03-C01
13	J	202	PGV	O02-C1-O01-C02
13	J	204	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
12	B	201	CLA	C3-C5-C6-C7
13	B	203	PGV	C20-C19-O03-C01
13	J	203	PGV	C20-C19-O03-C01
13	J	203	PGV	C2-C1-O01-C02
13	C	303	PGV	C20-C19-O03-C01
13	B	202	PGV	O12-C04-C05-O05
13	C	303	PGV	O12-C04-C05-O05
13	J	202	PGV	O12-C04-C05-C06
12	J	201	CLA	CBA-CGA-O2A-C1
9	A	301	ECH	C7-C8-C9-C34
9	I	301	ECH	C7-C8-C9-C34
9	A	301	ECH	C7-C8-C9-C10
9	A	301	ECH	C21-C22-C23-C24
9	I	301	ECH	C7-C8-C9-C10
13	J	204	PGV	C19-C20-C21-C22
12	J	201	CLA	O1A-CGA-O2A-C1
13	C	303	PGV	C1-C2-C3-C4
12	B	201	CLA	C5-C6-C7-C8
13	B	203	PGV	O12-C04-C05-O05
13	B	203	PGV	O12-C04-C05-C06
12	B	201	CLA	C13-C15-C16-C17
13	I	302	PGV	O12-C04-C05-O05
9	A	301	ECH	C37-C22-C23-C24
9	I	301	ECH	C37-C22-C23-C24
9	I	301	ECH	C21-C22-C23-C24
10	A	302	HEM	C2A-CAA-CBA-CGA
10	I	303	HEM	C2A-CAA-CBA-CGA
13	J	203	PGV	C04-C05-C06-O06
13	J	204	PGV	C03-C02-O01-C1
13	B	202	PGV	C2-C1-O01-C02
13	B	203	PGV	C2-C1-O01-C02
13	J	204	PGV	C5-C6-C7-C8
13	B	203	PGV	C5-C6-C7-C8
13	J	203	PGV	O12-C04-C05-O05
13	J	203	PGV	O12-C04-C05-C06
13	C	303	PGV	C20-C21-C22-C23
13	J	204	PGV	C29-C30-C31-C32
9	I	301	ECH	C5-C6-C7-C8
12	J	201	CLA	C3-C5-C6-C7
11	A	304	HEC	C3D-CAD-CBD-CGD
13	B	202	PGV	O02-C1-O01-C02
13	B	203	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
13	J	204	PGV	C20-C19-O03-C01
13	J	204	PGV	C27-C28-C29-C30
13	J	203	PGV	C2-C3-C4-C5
13	I	302	PGV	C2-C1-O01-C02
14	C	302	LFA	C11-C12-C13-C14
13	B	202	PGV	O01-C02-C03-O11
13	J	203	PGV	O01-C02-C03-O11
13	B	202	PGV	C1-C2-C3-C4
13	J	203	PGV	O05-C05-C06-O06
13	J	202	PGV	C26-C27-C28-C29
12	J	201	CLA	C1A-C2A-CAA-CBA
13	J	204	PGV	C12-C13-C14-C15
13	B	202	PGV	C01-C02-C03-O11
13	J	203	PGV	C01-C02-C03-O11
13	I	302	PGV	O02-C1-O01-C02
13	J	204	PGV	O04-C19-O03-C01
13	B	203	PGV	C6-C7-C8-C9
13	C	303	PGV	O03-C01-C02-C03
13	J	204	PGV	C20-C21-C22-C23
13	J	203	PGV	C4-C5-C6-C7
13	J	203	PGV	C25-C26-C27-C28
13	B	202	PGV	C4-C5-C6-C7
13	C	303	PGV	C12-C13-C14-C15
13	J	202	PGV	O03-C01-C02-O01
14	E	101	LFA	C5-C6-C7-C8
14	C	302	LFA	C13-C14-C15-C16
13	C	303	PGV	C21-C22-C23-C24
13	B	203	PGV	C01-C02-C03-O11
12	J	201	CLA	CAA-CBA-CGA-O2A
12	J	201	CLA	C12-C13-C15-C16
13	J	202	PGV	C31-C32-C33-C34
13	C	303	PGV	C25-C26-C27-C28
13	J	202	PGV	C25-C26-C27-C28
14	E	101	LFA	C10-C11-C12-C13
13	C	303	PGV	O12-C04-C05-C06
13	I	302	PGV	C24-C25-C26-C27
12	B	201	CLA	CBD-CGD-O2D-CED
13	B	203	PGV	O01-C02-C03-O11
13	J	202	PGV	O01-C02-C03-O11
13	J	204	PGV	C1-C2-C3-C4
13	B	203	PGV	O03-C01-C02-O01
13	I	302	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
13	B	202	PGV	C2-C3-C4-C5
12	B	201	CLA	C4B-C3B-CAB-CBB
14	C	302	LFA	C2-C3-C4-C5
13	J	202	PGV	C01-C02-C03-O11
11	K	301	HEC	C4B-C3B-CAB-CBB
10	A	302	HEM	C4D-C3D-CAD-CBD
13	C	303	PGV	O03-C01-C02-O01
13	I	302	PGV	C15-C16-C17-C18
13	B	203	PGV	O03-C01-C02-C03
13	B	202	PGV	C03-O11-P-O12
13	B	202	PGV	C03-O11-P-O13
13	B	202	PGV	C03-O11-P-O14
13	B	203	PGV	C03-O11-P-O13
13	J	202	PGV	C04-O12-P-O13
13	J	203	PGV	C03-O11-P-O13
9	A	301	ECH	C23-C24-C25-C30
12	J	201	CLA	C14-C13-C15-C16
13	J	204	PGV	C4-C5-C6-C7
10	I	303	HEM	C4D-C3D-CAD-CBD
13	C	303	PGV	C28-C29-C30-C31
12	B	201	CLA	O1D-CGD-O2D-CED
13	J	202	PGV	O03-C01-C02-C03
14	C	302	LFA	C16-C17-C18-C19
12	B	201	CLA	CBA-CGA-O2A-C1
13	B	203	PGV	C27-C28-C29-C30
13	I	302	PGV	C3-C4-C5-C6
12	B	201	CLA	O1A-CGA-O2A-C1
13	J	202	PGV	C1-C2-C3-C4
14	E	101	LFA	C11-C10-C9-C8
9	A	301	ECH	C11-C10-C9-C34
9	I	301	ECH	C11-C10-C9-C34
12	B	201	CLA	C4-C3-C5-C6
13	C	303	PGV	C11-C10-C9-C8
10	A	302	HEM	C2D-C3D-CAD-CBD
12	J	201	CLA	CAA-CBA-CGA-O1A
9	A	301	ECH	C11-C10-C9-C8
9	I	301	ECH	C11-C10-C9-C8
12	B	201	CLA	C1A-C2A-CAA-CBA
12	B	201	CLA	C2B-C3B-CAB-CBB
13	J	204	PGV	C01-C02-C03-O11
13	C	303	PGV	C27-C28-C29-C30
13	I	302	PGV	C02-C03-O11-P

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Mol	Chain	Res	Type	Atoms
12	B	201	CLA	C2-C3-C5-C6
10	I	303	HEM	C2D-C3D-CAD-CBD
14	C	302	LFA	C10-C11-C12-C13
11	I	305	HEC	CAD-CBD-CGD-O1D
13	C	303	PGV	C6-C7-C8-C9
11	K	301	HEC	CAA-CBA-CGA-O2A
13	I	302	PGV	C5-C6-C7-C8
13	J	204	PGV	C2-C3-C4-C5
13	B	202	PGV	C22-C23-C24-C25
13	J	204	PGV	C22-C23-C24-C25
13	B	202	PGV	C20-C19-O03-C01
13	B	202	PGV	O04-C19-O03-C01
11	K	301	HEC	CAA-CBA-CGA-O1A
13	B	203	PGV	C19-C20-C21-C22
13	I	302	PGV	C22-C23-C24-C25
13	J	203	PGV	O03-C01-C02-O01
13	J	203	PGV	O03-C19-C20-C21
9	I	301	ECH	C23-C24-C25-C26
13	J	204	PGV	C7-C8-C9-C10
11	I	305	HEC	CAD-CBD-CGD-O2D
13	J	204	PGV	C9-C10-C11-C12
13	J	203	PGV	O03-C01-C02-C03
13	I	302	PGV	C14-C15-C16-C17
14	E	101	LFA	C11-C12-C13-C14
13	I	302	PGV	C27-C28-C29-C30
11	A	304	HEC	C1A-C2A-CAA-CBA
12	J	201	CLA	C11-C10-C8-C7
13	J	203	PGV	C23-C24-C25-C26
13	B	202	PGV	C23-C24-C25-C26
13	I	302	PGV	C1-C2-C3-C4
10	I	303	HEM	CAA-CBA-CGA-O2A
13	J	203	PGV	O04-C19-C20-C21
10	I	304	HEM	CAA-CBA-CGA-O1A
14	C	302	LFA	C11-C10-C9-C8
12	B	201	CLA	CAA-CBA-CGA-O2A
11	K	301	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

19 monomers are involved in 68 short contacts:

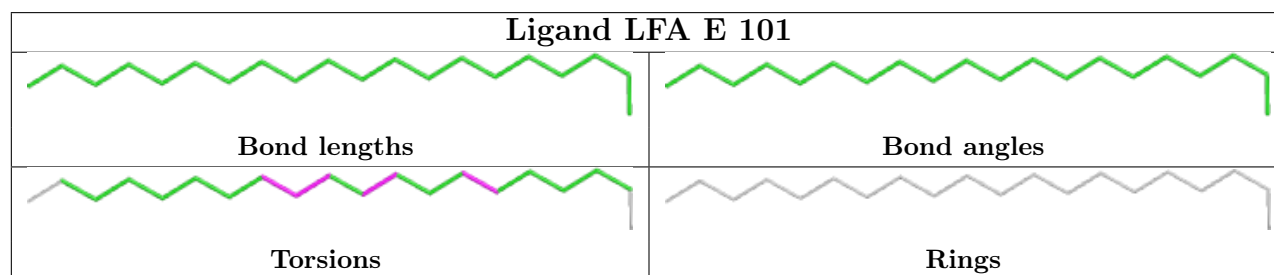
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	203	PGV	1	0

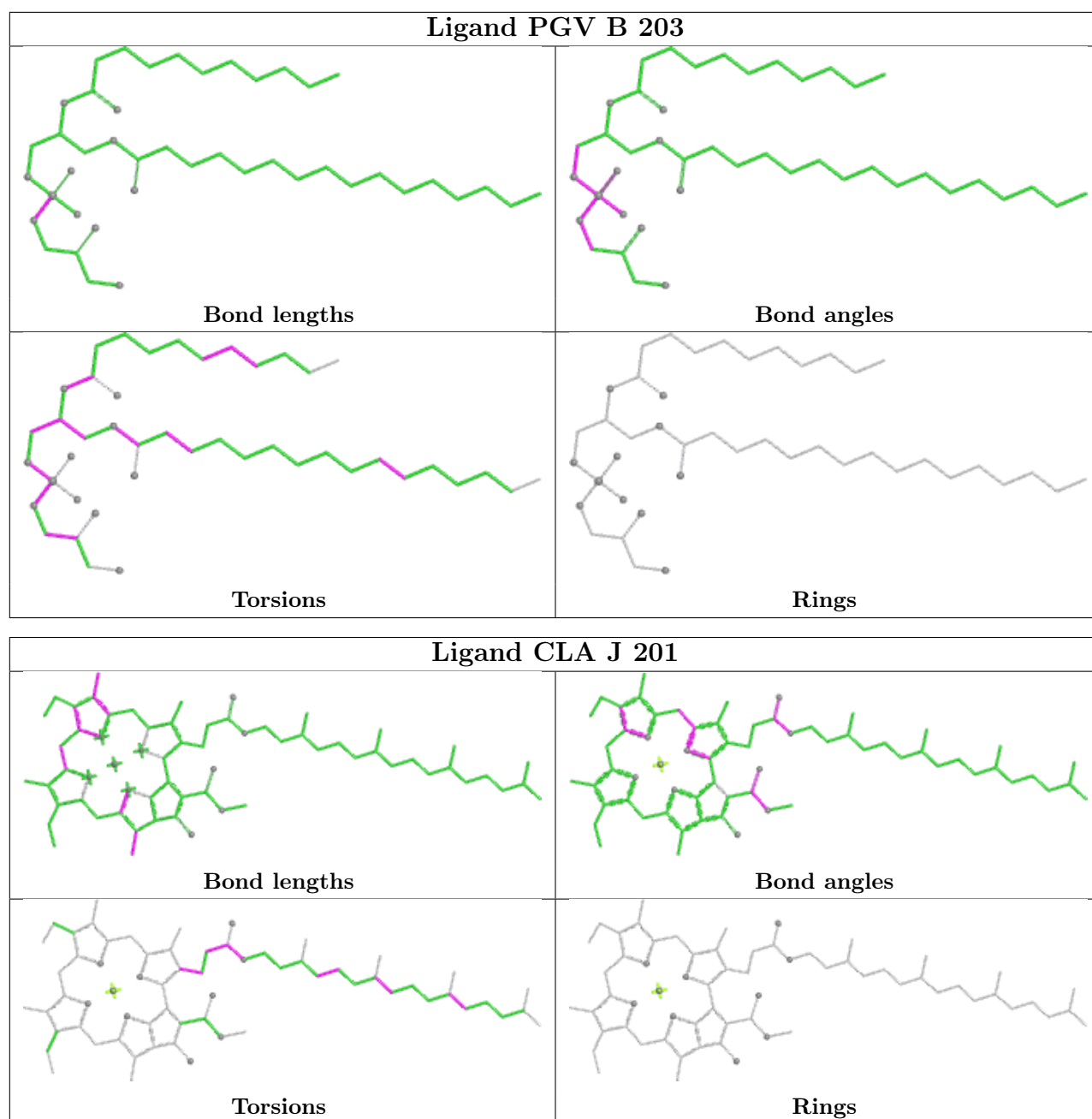
Continued on next page...

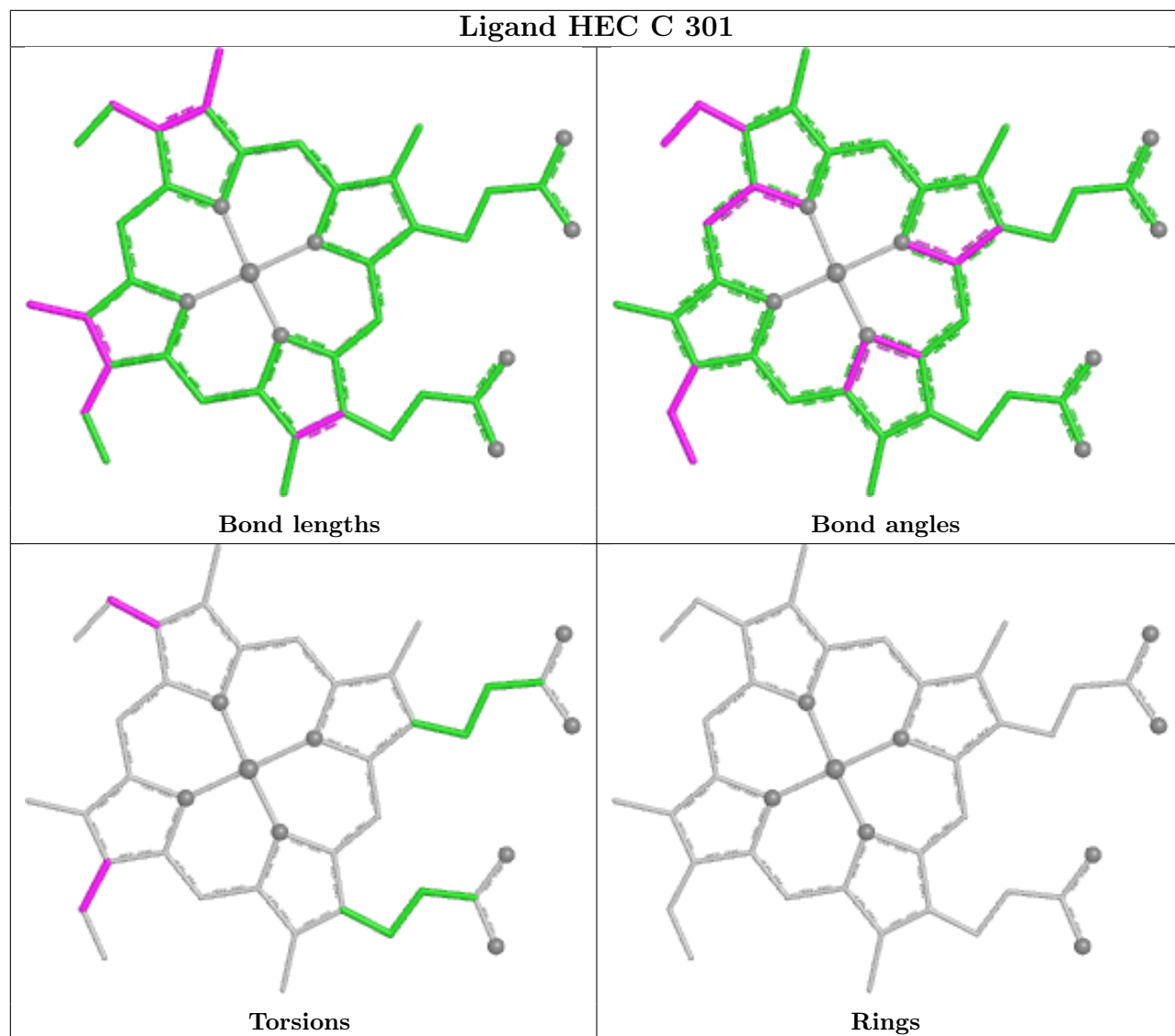
Continued from previous page...

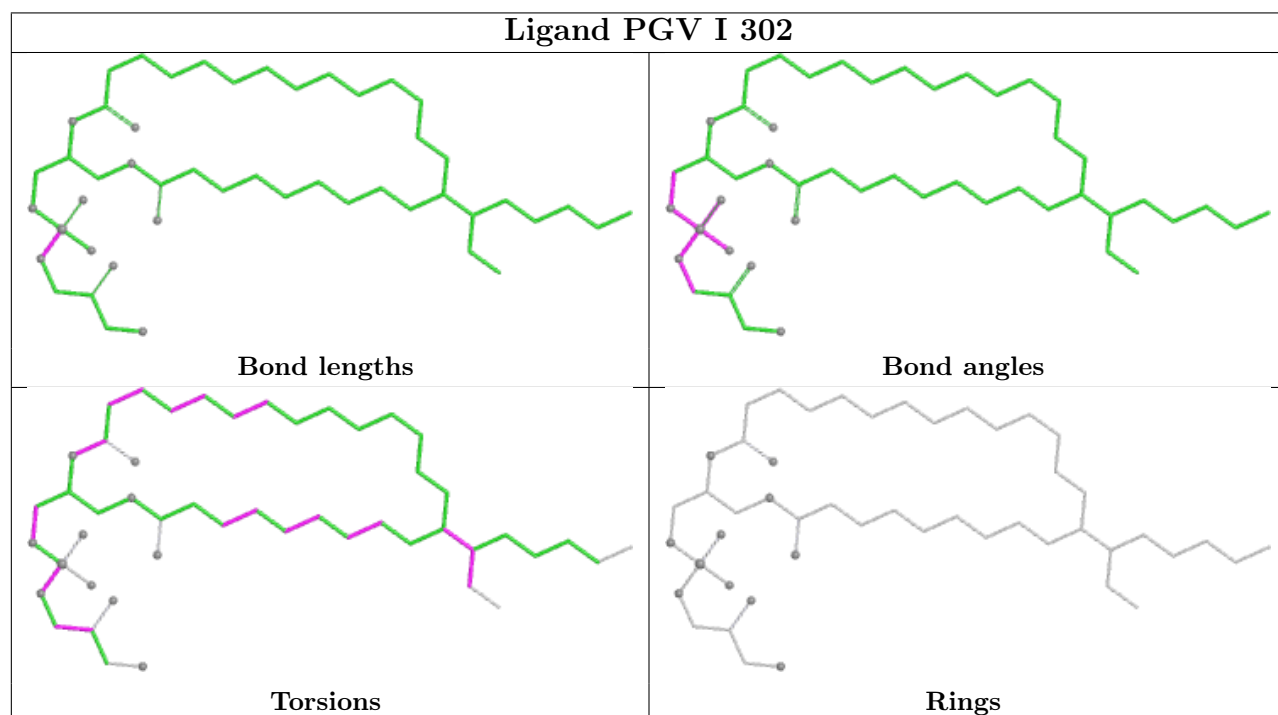
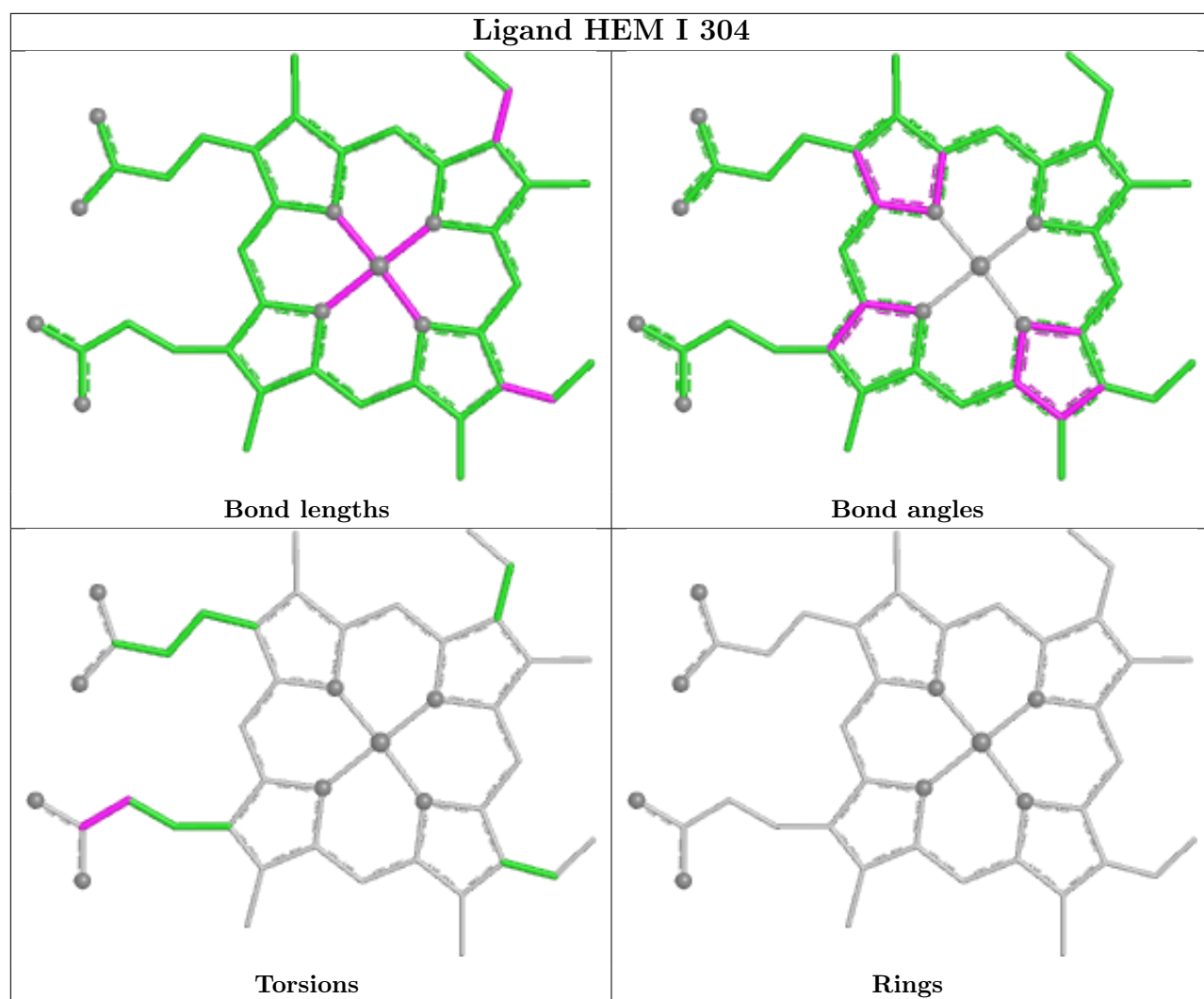
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	J	201	CLA	3	0
11	C	301	HEC	3	0
10	I	304	HEM	2	0
13	I	302	PGV	3	0
11	A	304	HEC	2	0
10	I	303	HEM	5	0
11	I	305	HEC	3	0
12	B	201	CLA	5	0
13	B	202	PGV	6	0
9	I	301	ECH	5	0
11	K	301	HEC	3	0
10	A	302	HEM	8	0
13	J	204	PGV	3	0
9	A	301	ECH	5	0
15	D	201	FES	2	0
10	A	303	HEM	5	0
13	C	303	PGV	3	0
13	J	202	PGV	3	0

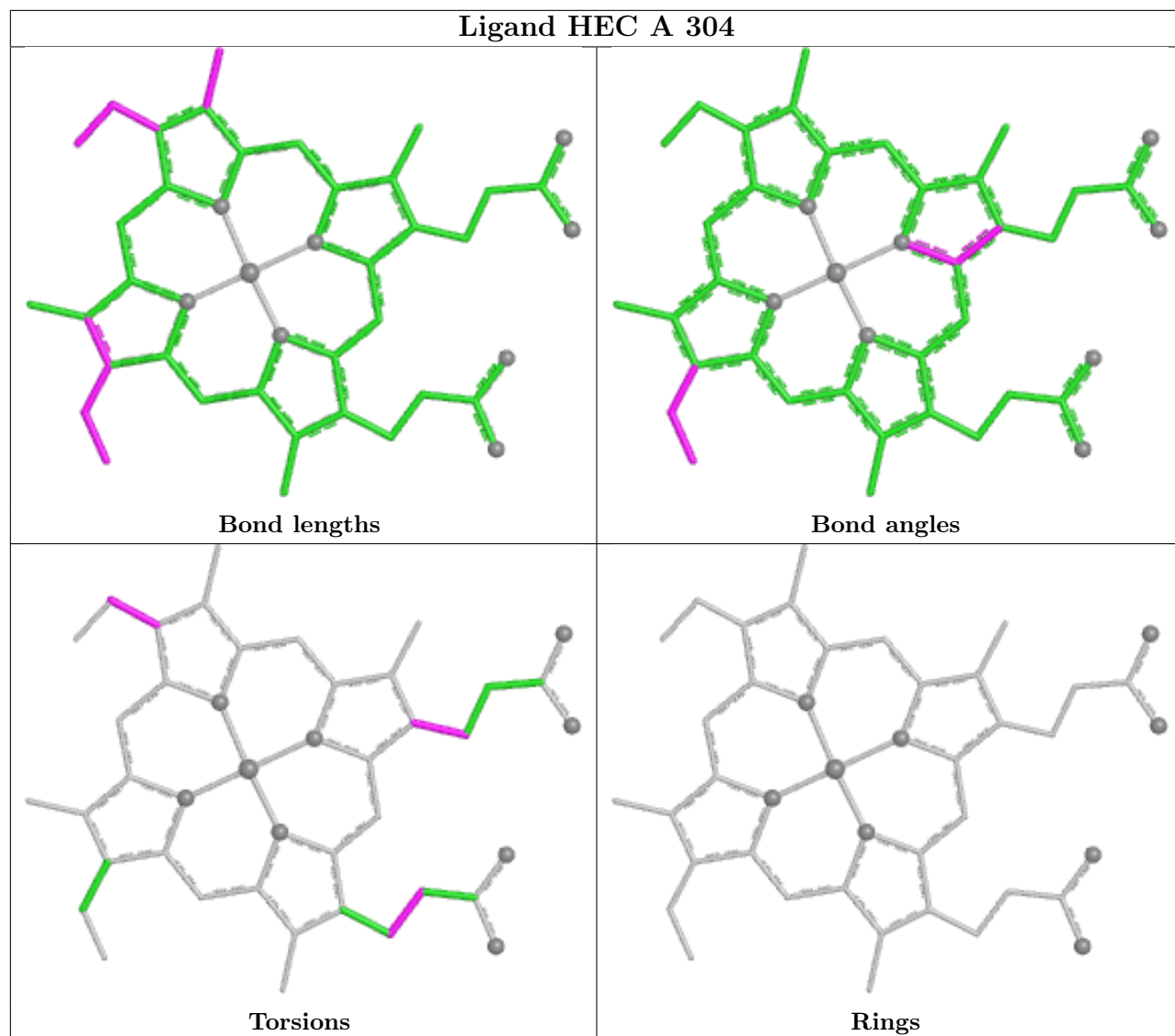
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



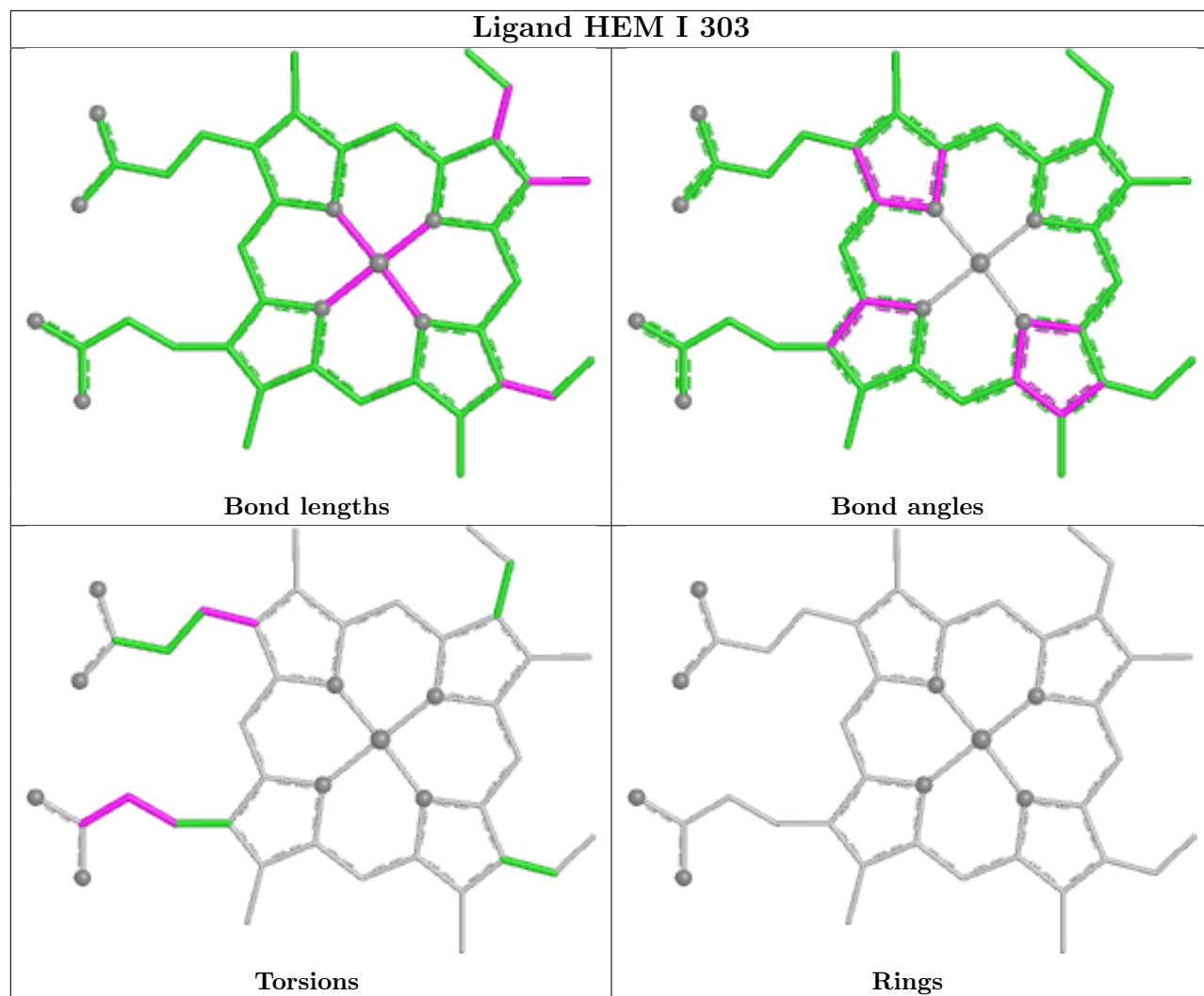




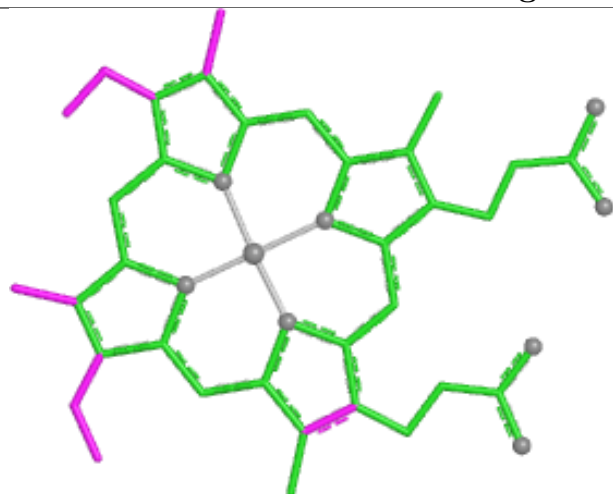




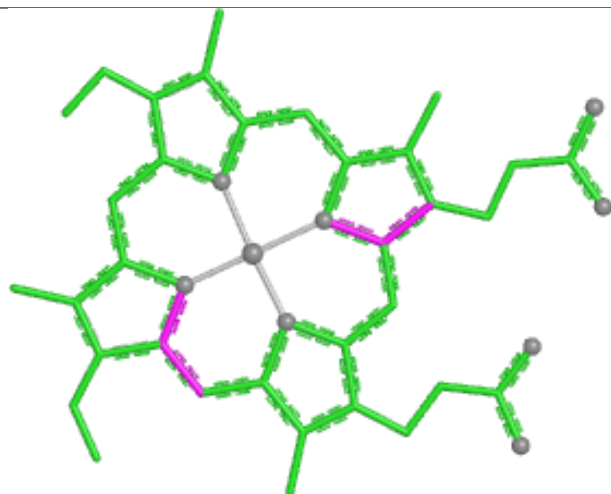
Ligand HEM I 303



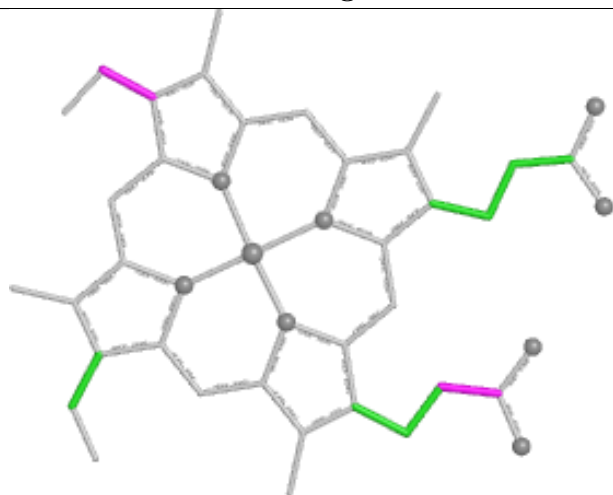
Ligand HEC I 305



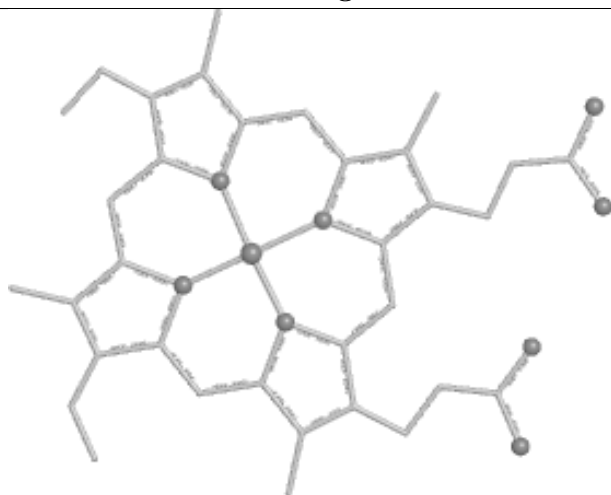
Bond lengths



Bond angles

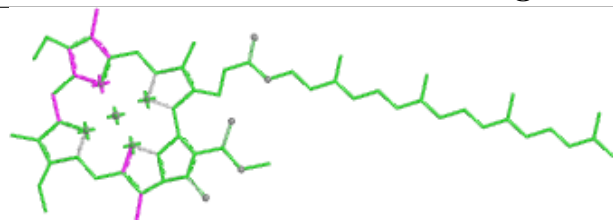


Torsions

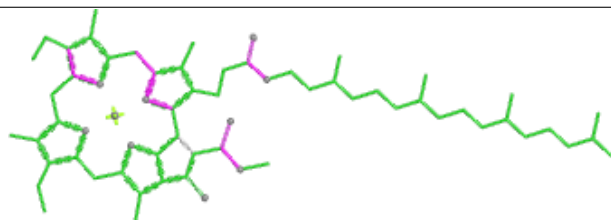


Rings

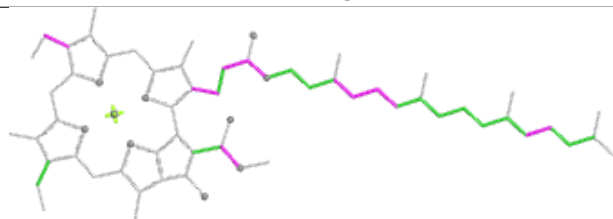
Ligand CLA B 201



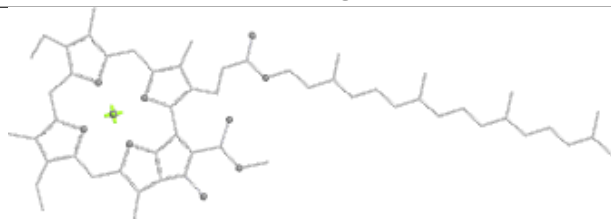
Bond lengths



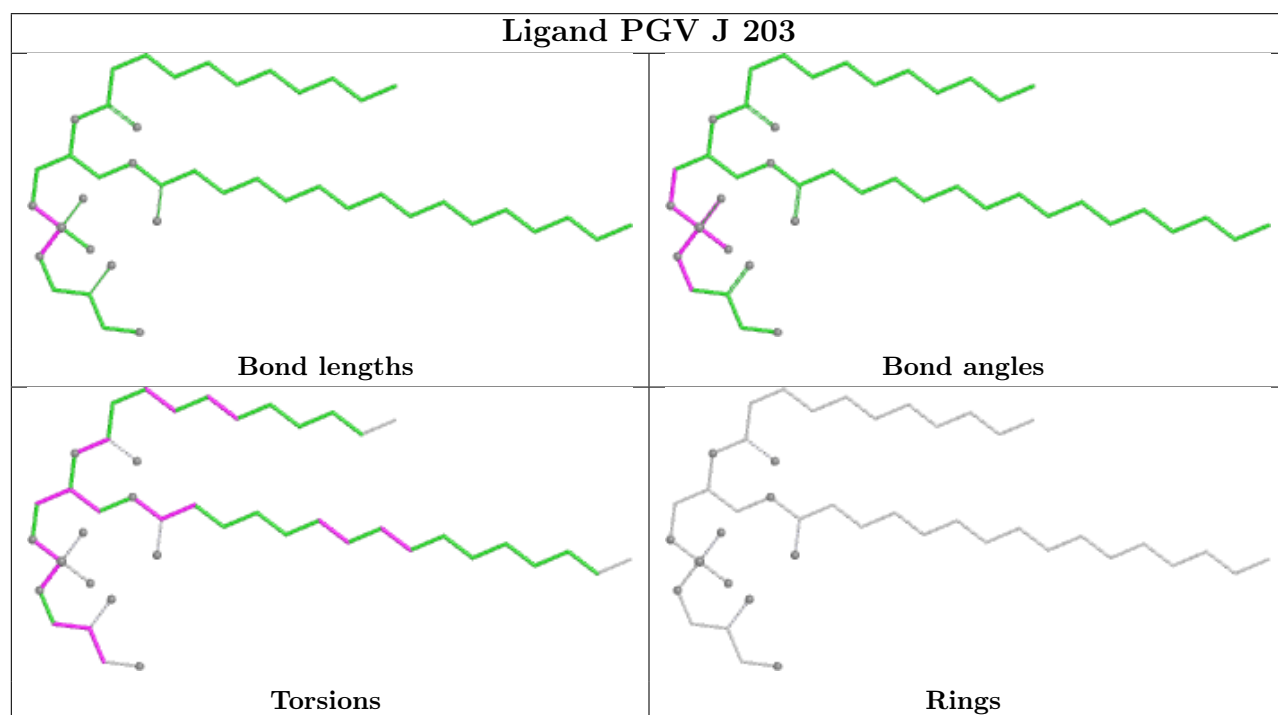
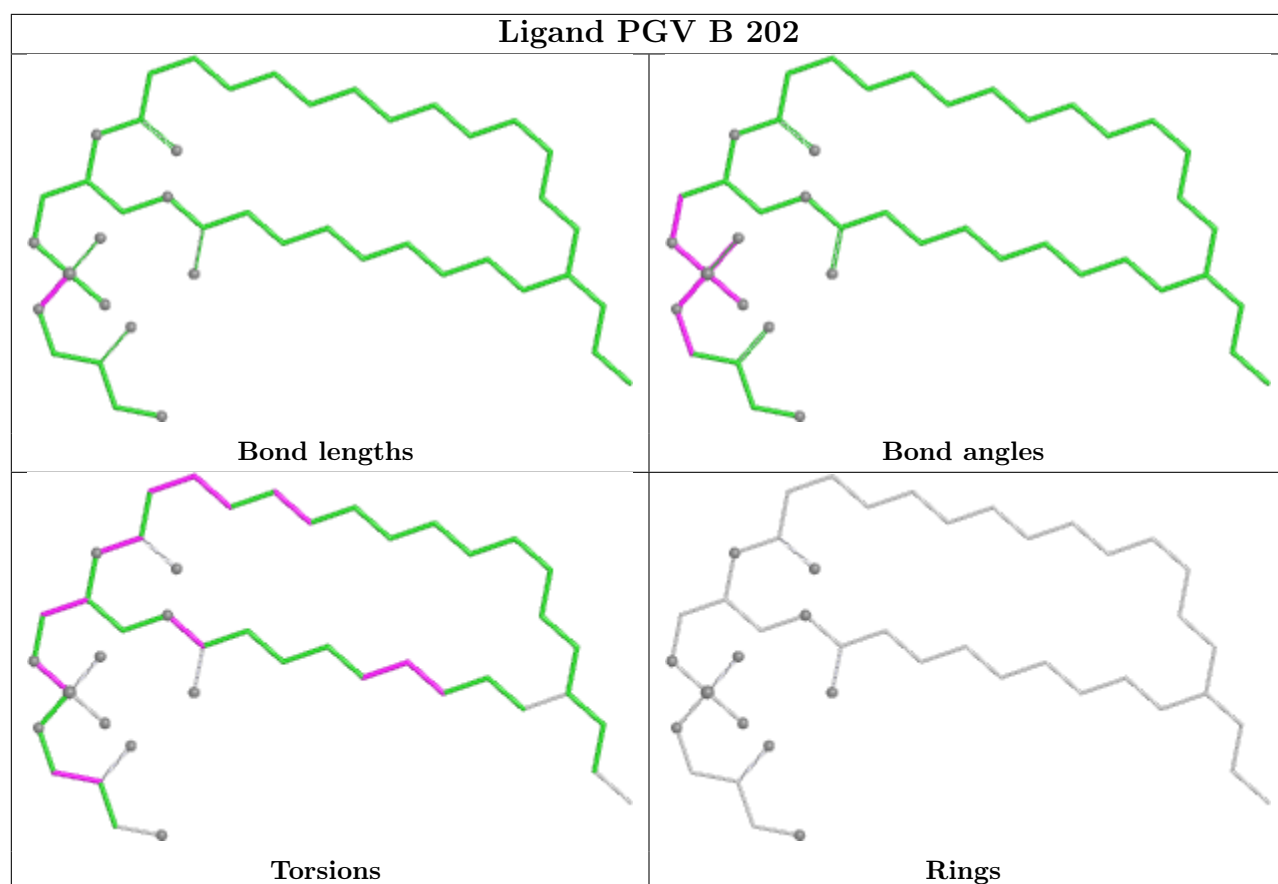
Bond angles

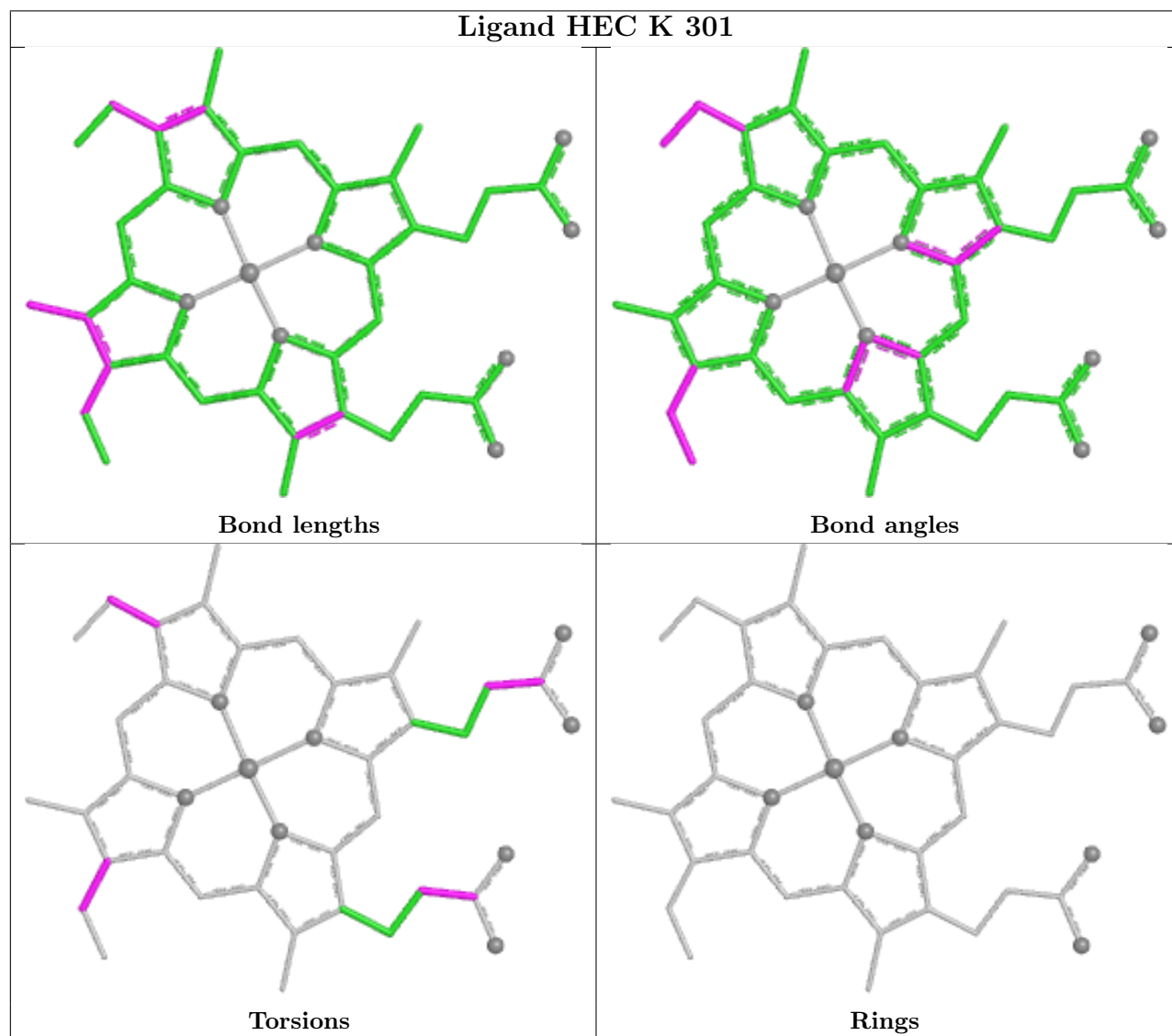
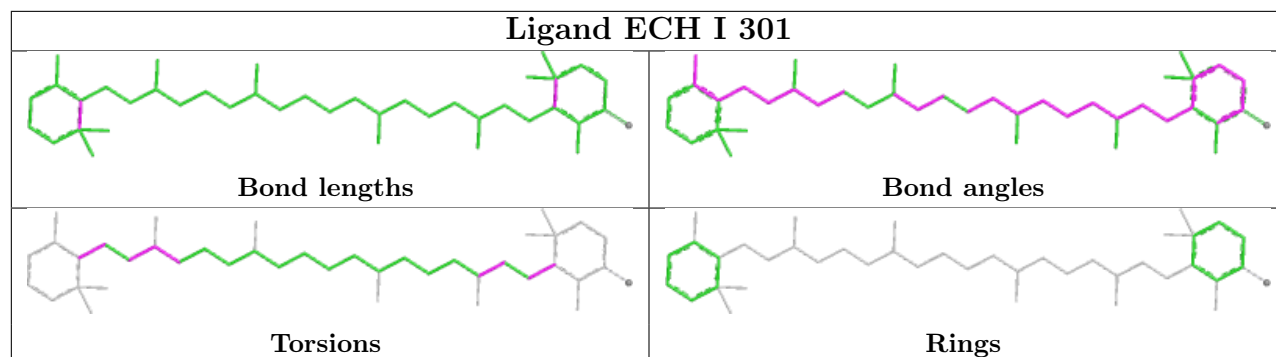


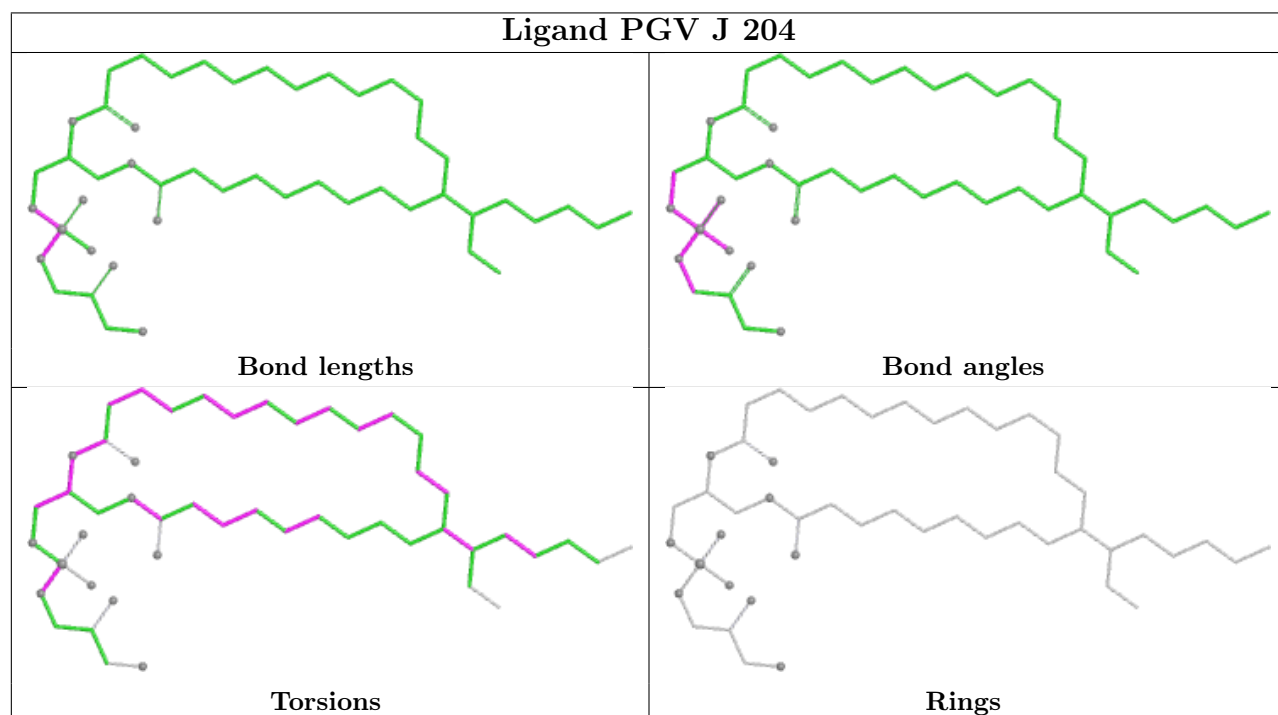
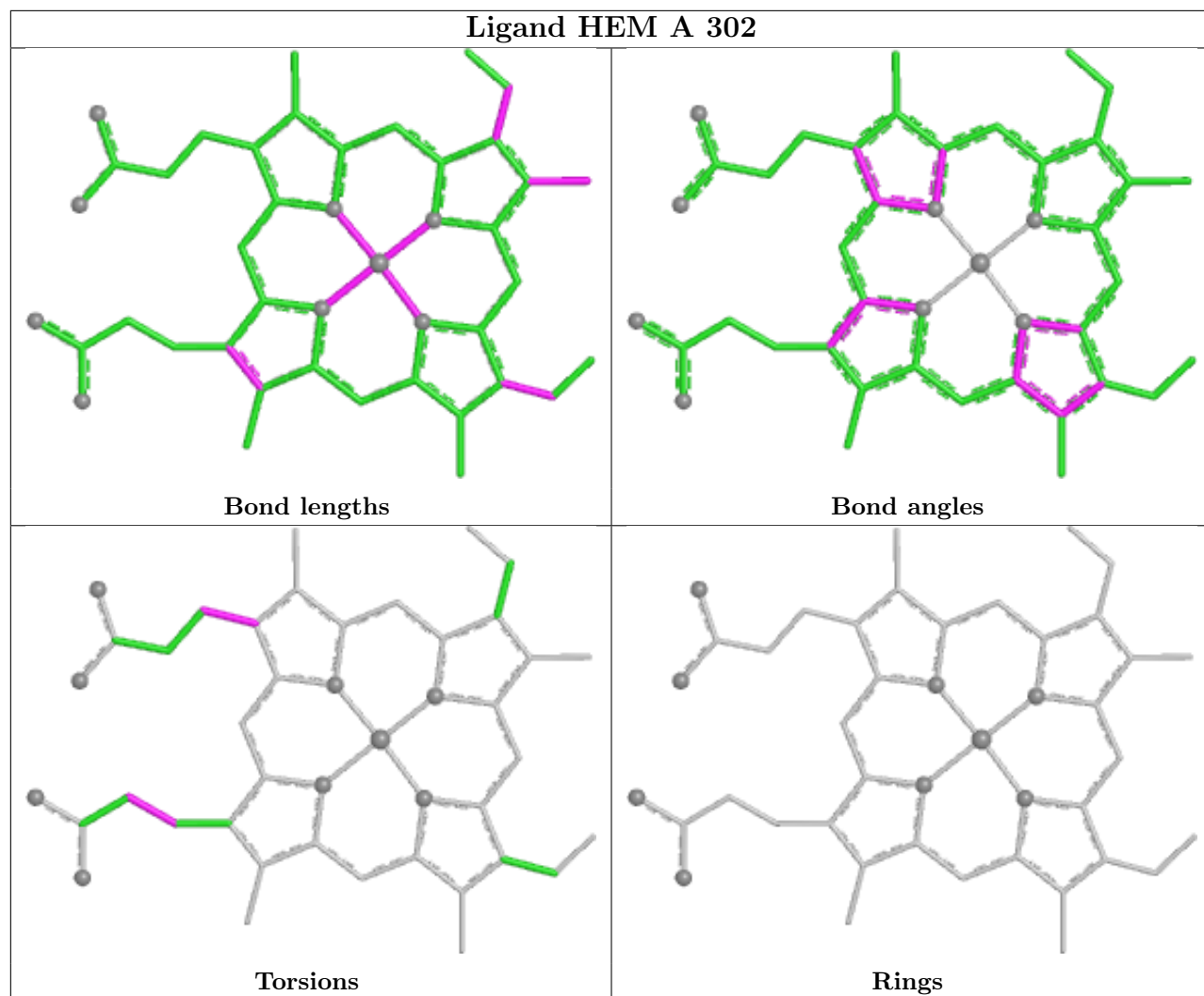
Torsions

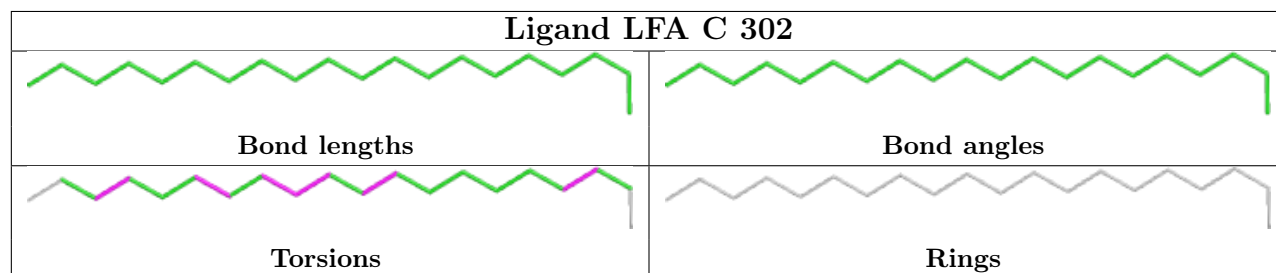
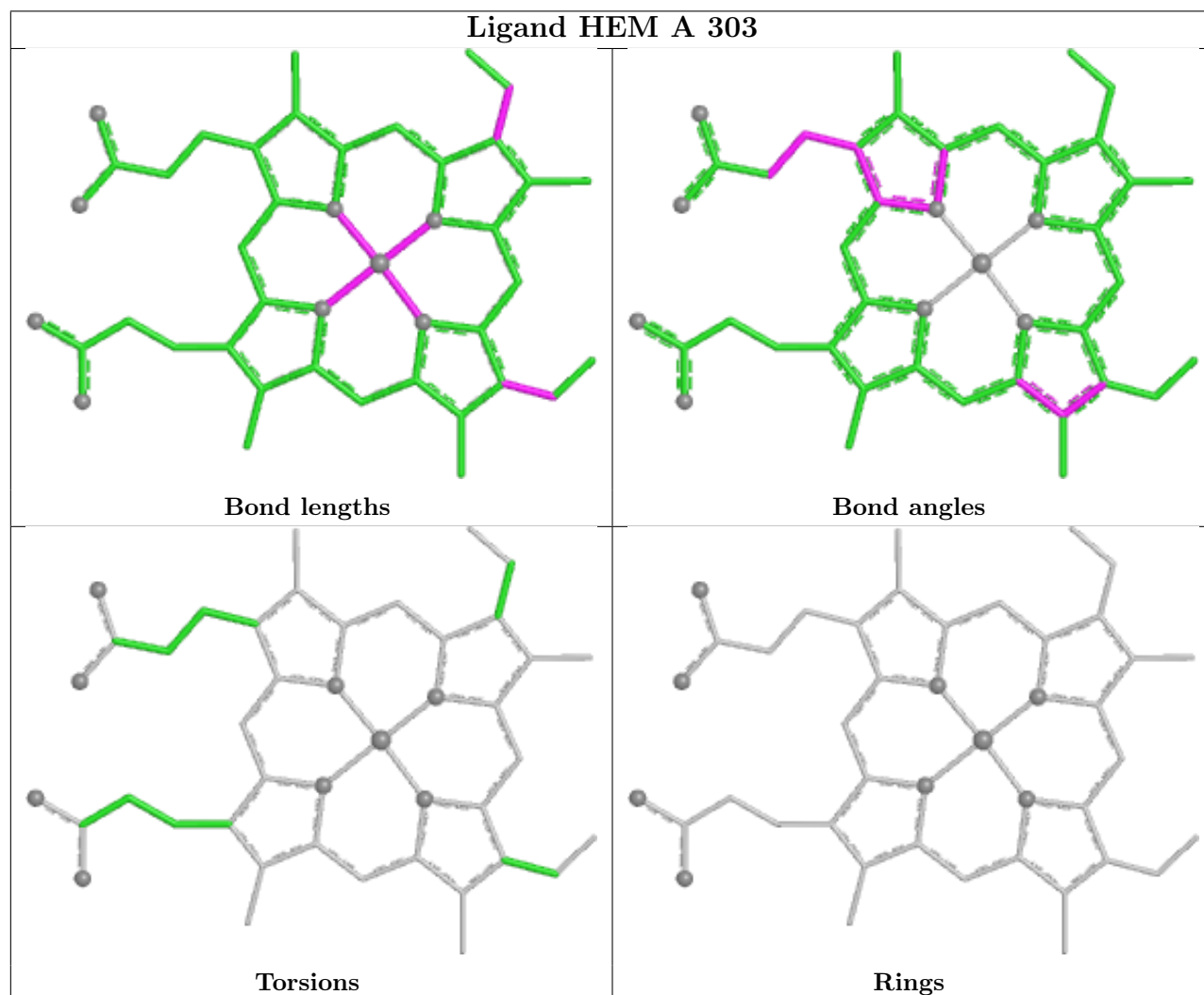
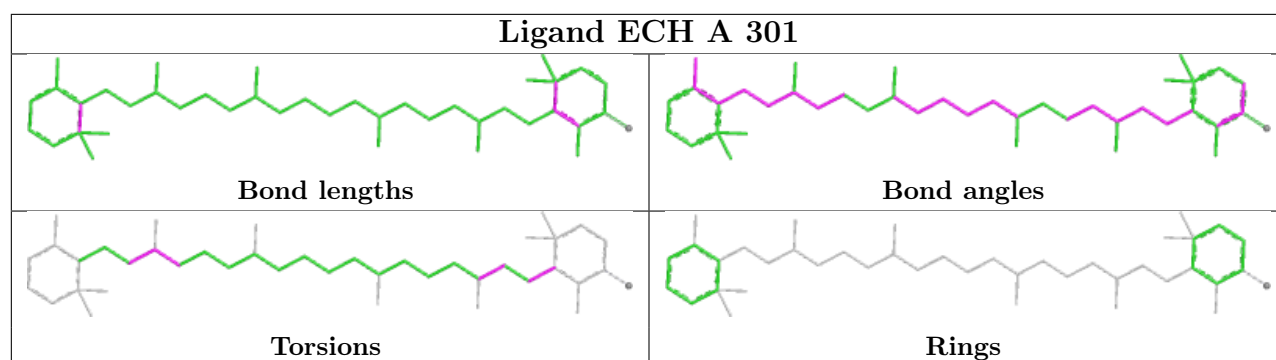


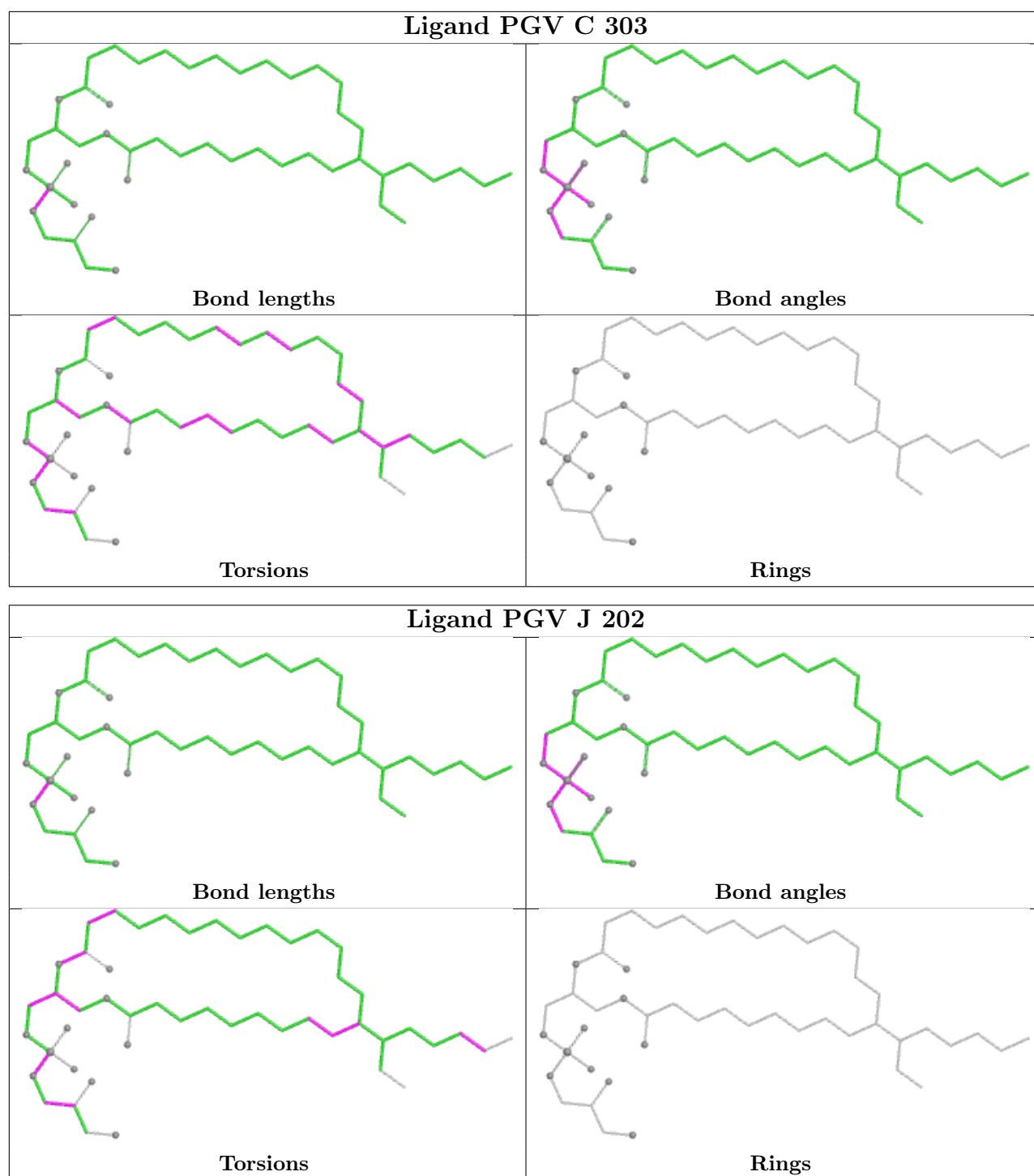
Rings











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.

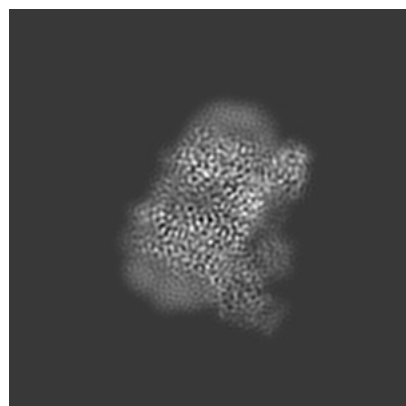
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15017. These allow visual inspection of the internal detail of the map and identification of artifacts.

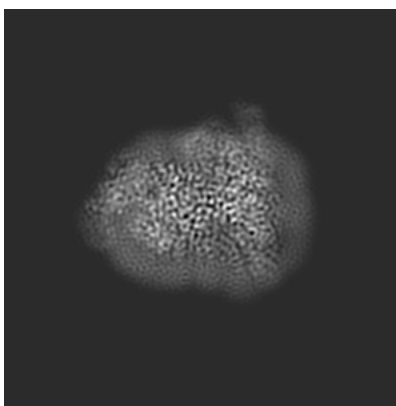
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

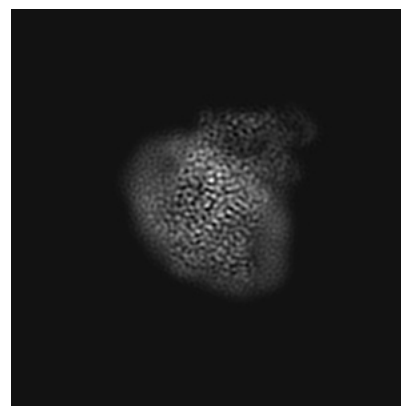
6.1.1 Primary map



X

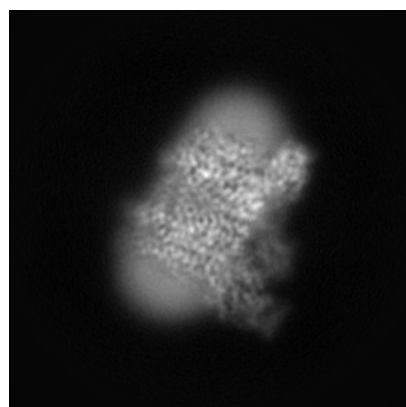


Y

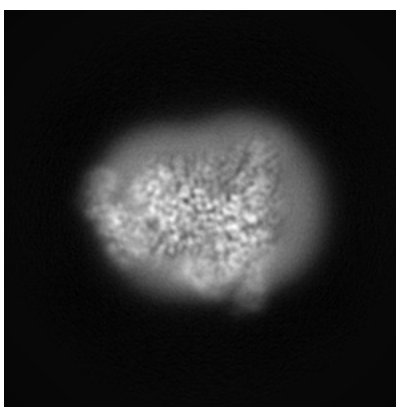


Z

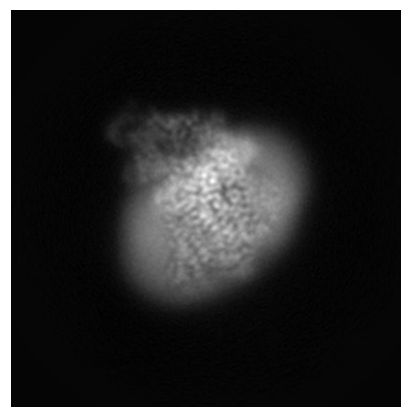
6.1.2 Raw map



X



Y

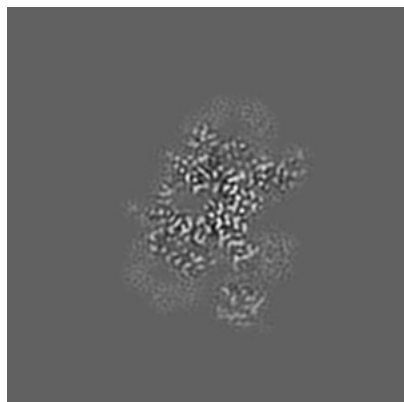


Z

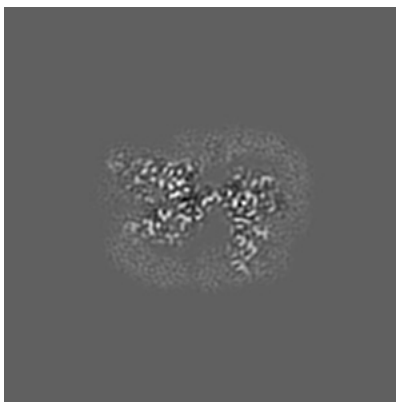
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

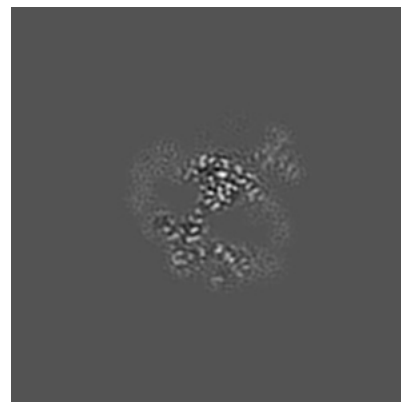
6.2.1 Primary map



X Index: 110

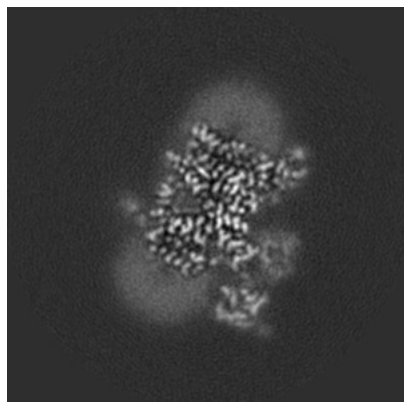


Y Index: 110

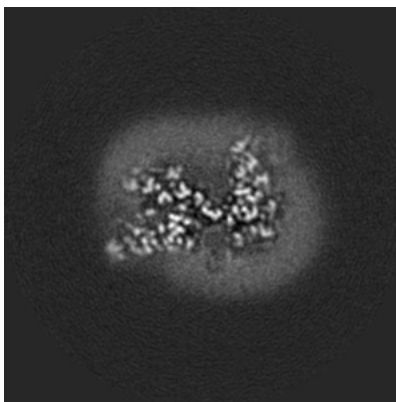


Z Index: 110

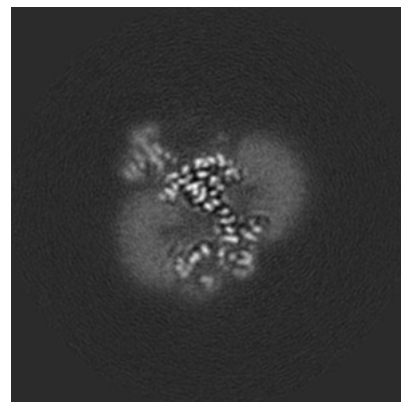
6.2.2 Raw map



X Index: 110



Y Index: 110

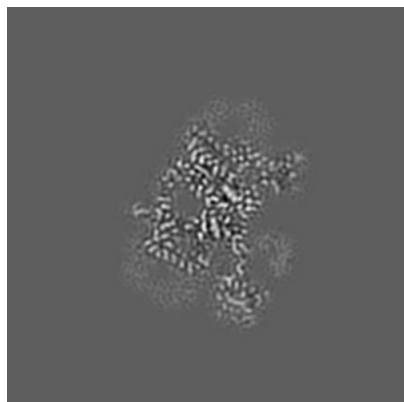


Z Index: 110

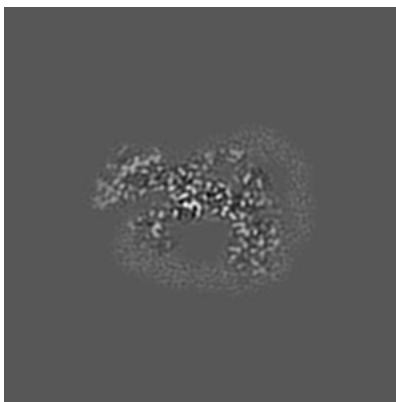
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

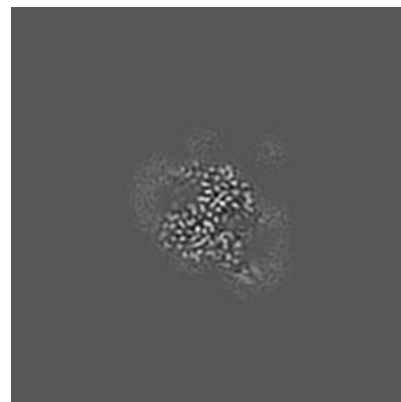
6.3.1 Primary map



X Index: 114

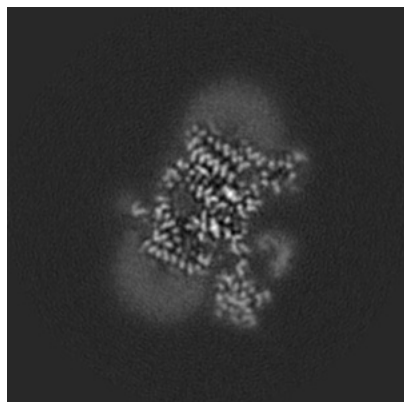


Y Index: 116

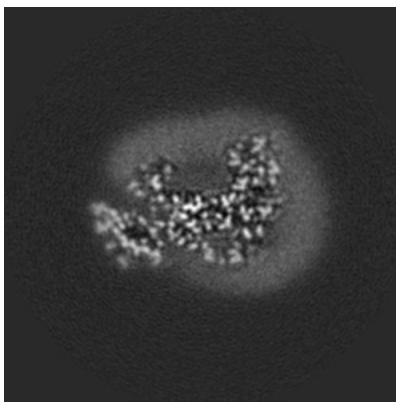


Z Index: 97

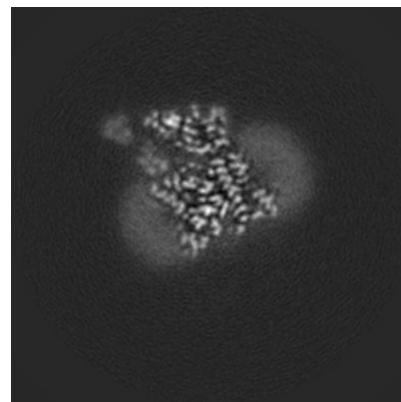
6.3.2 Raw map



X Index: 106



Y Index: 116

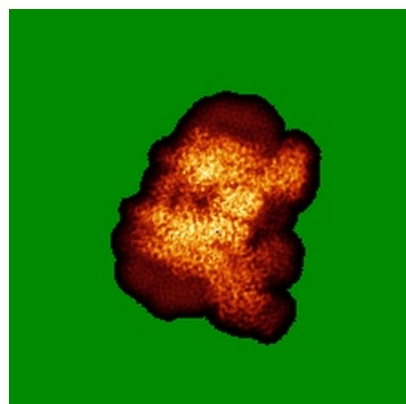


Z Index: 128

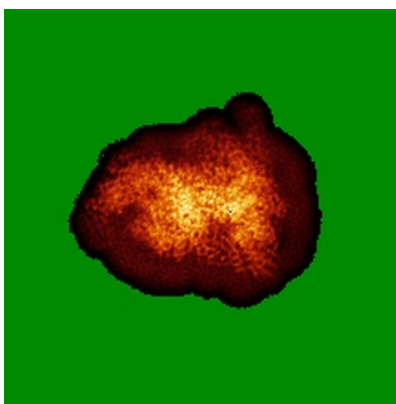
The images above show the largest variance slices of the map in three orthogonal directions.

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

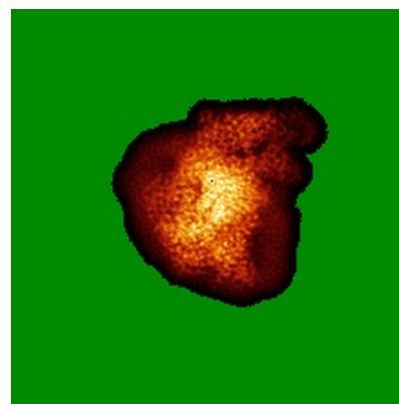
6.4.1 Primary map



X

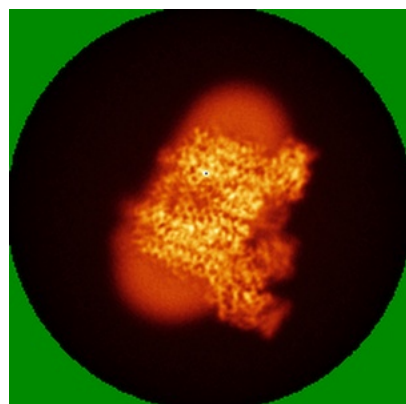


Y

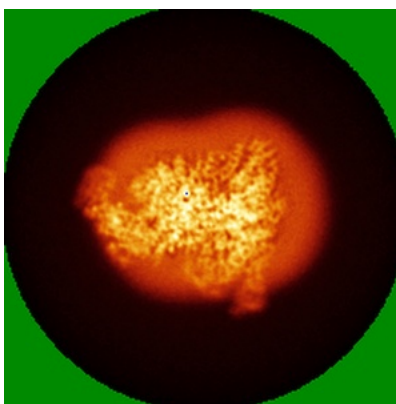


Z

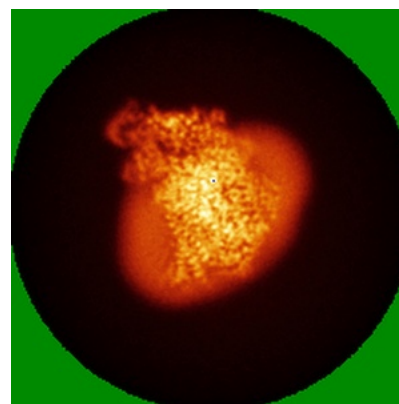
6.4.2 Raw map



X



Y

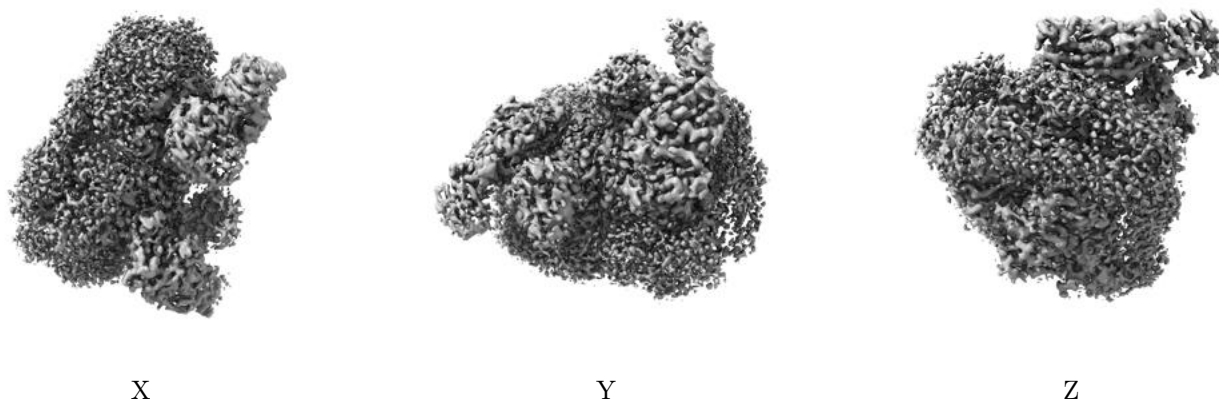


Z

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.

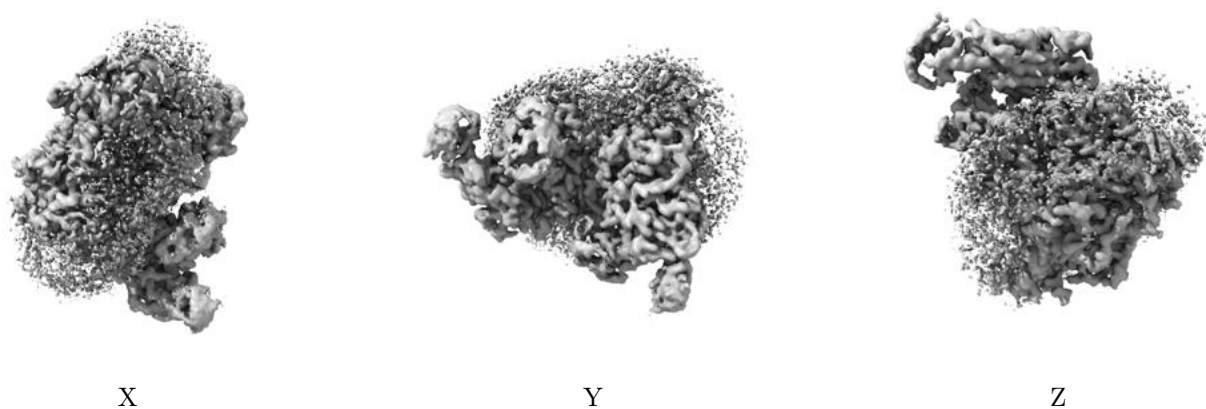
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0221. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

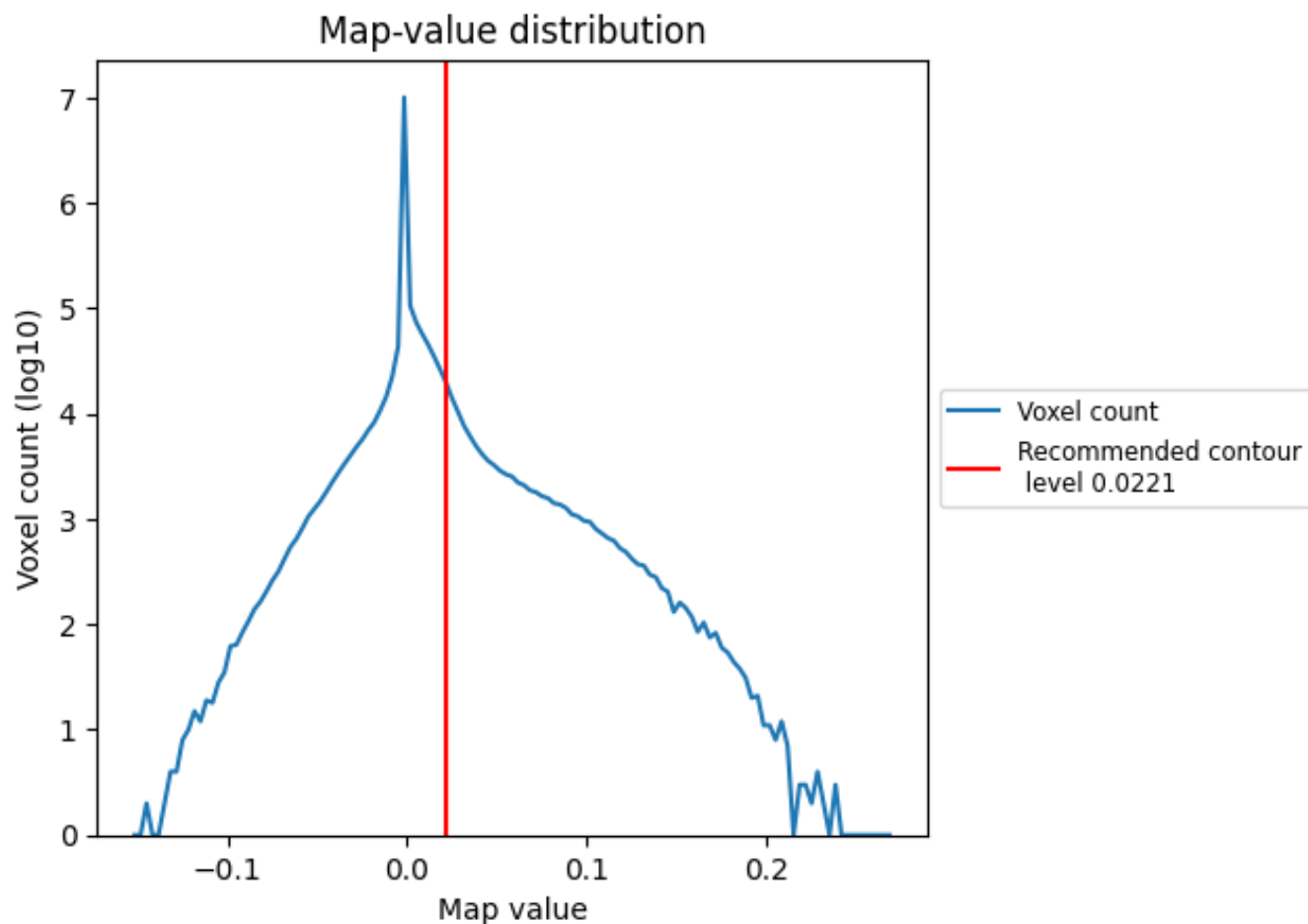
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

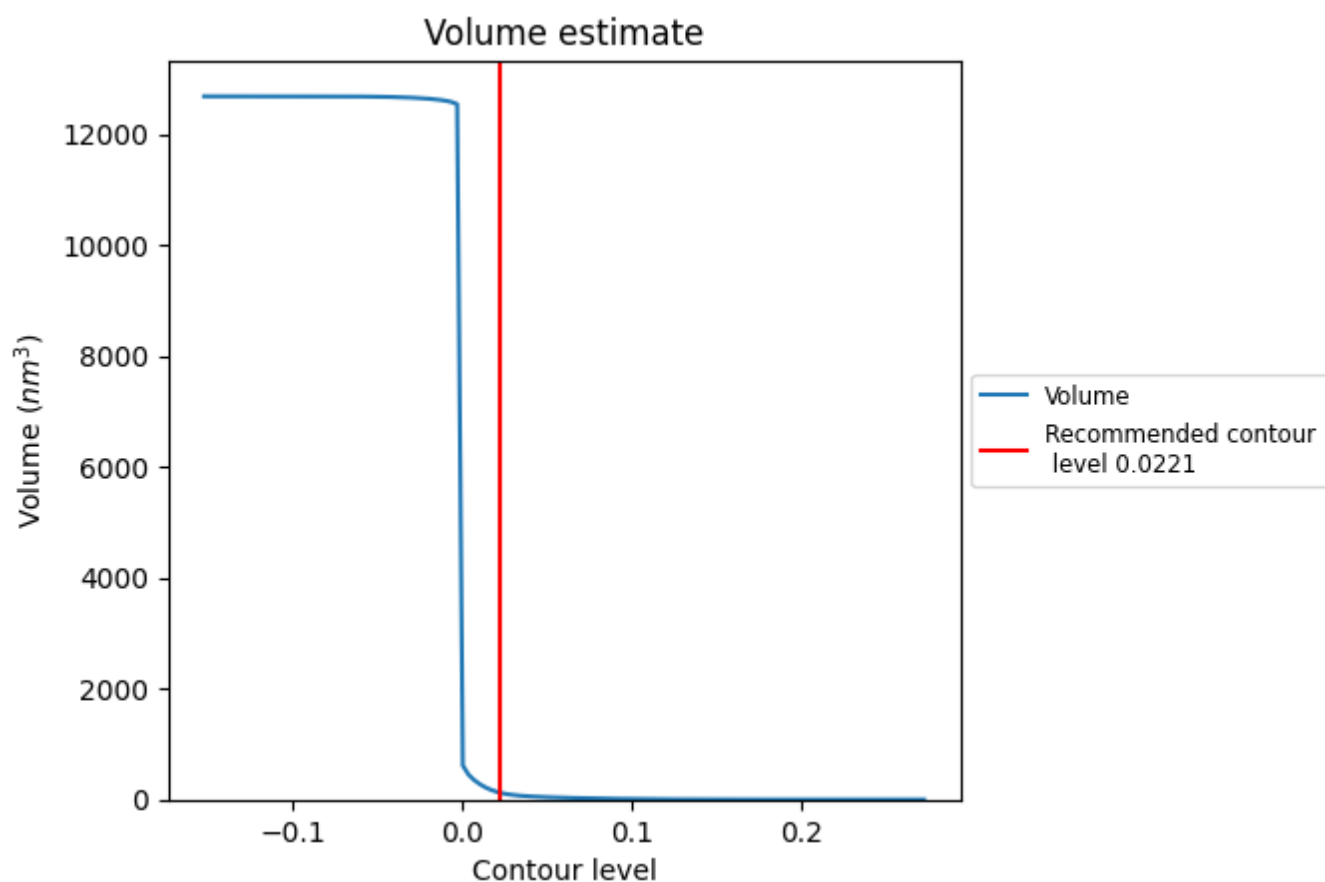
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

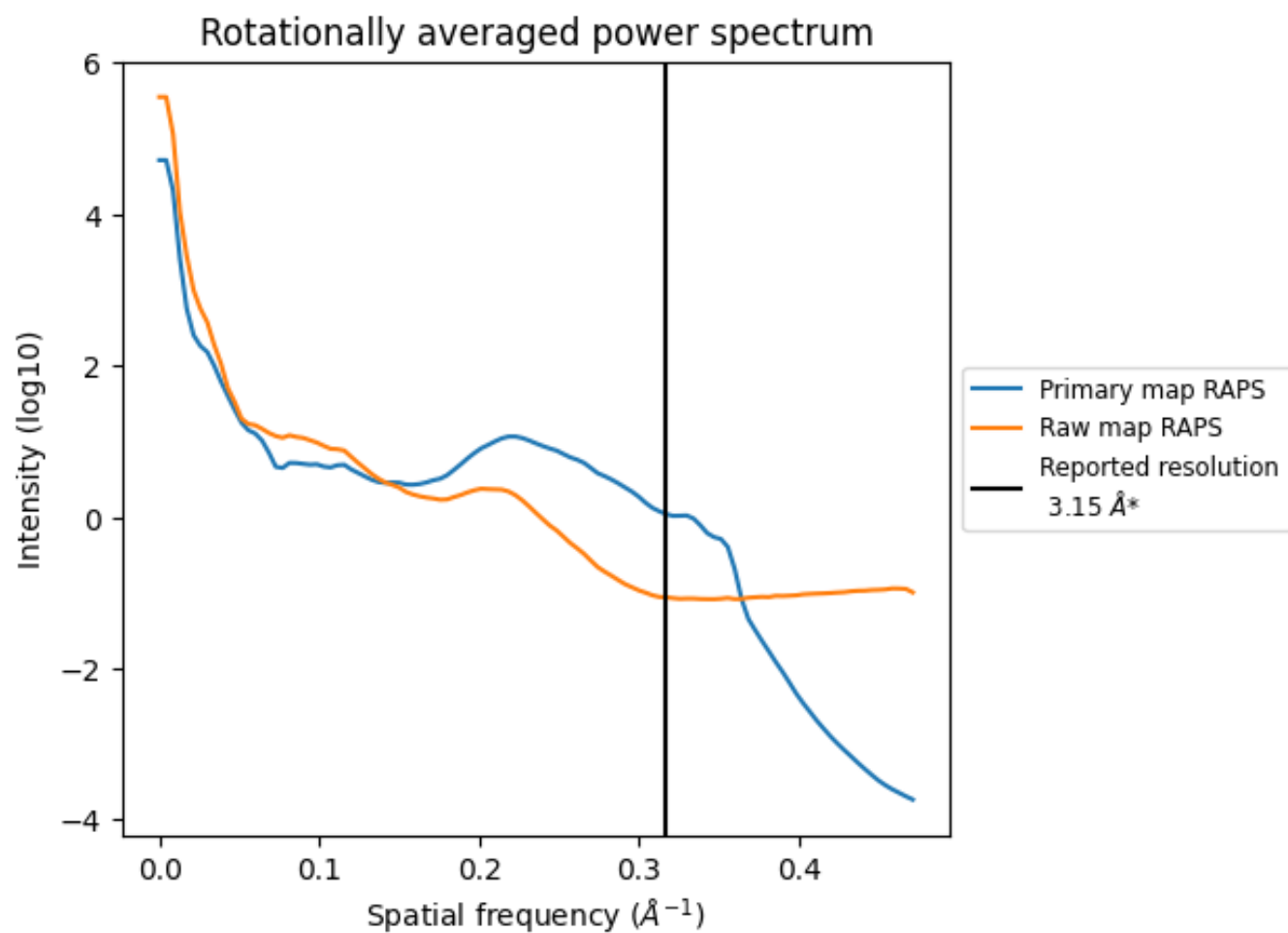
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 115 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 ⓘ

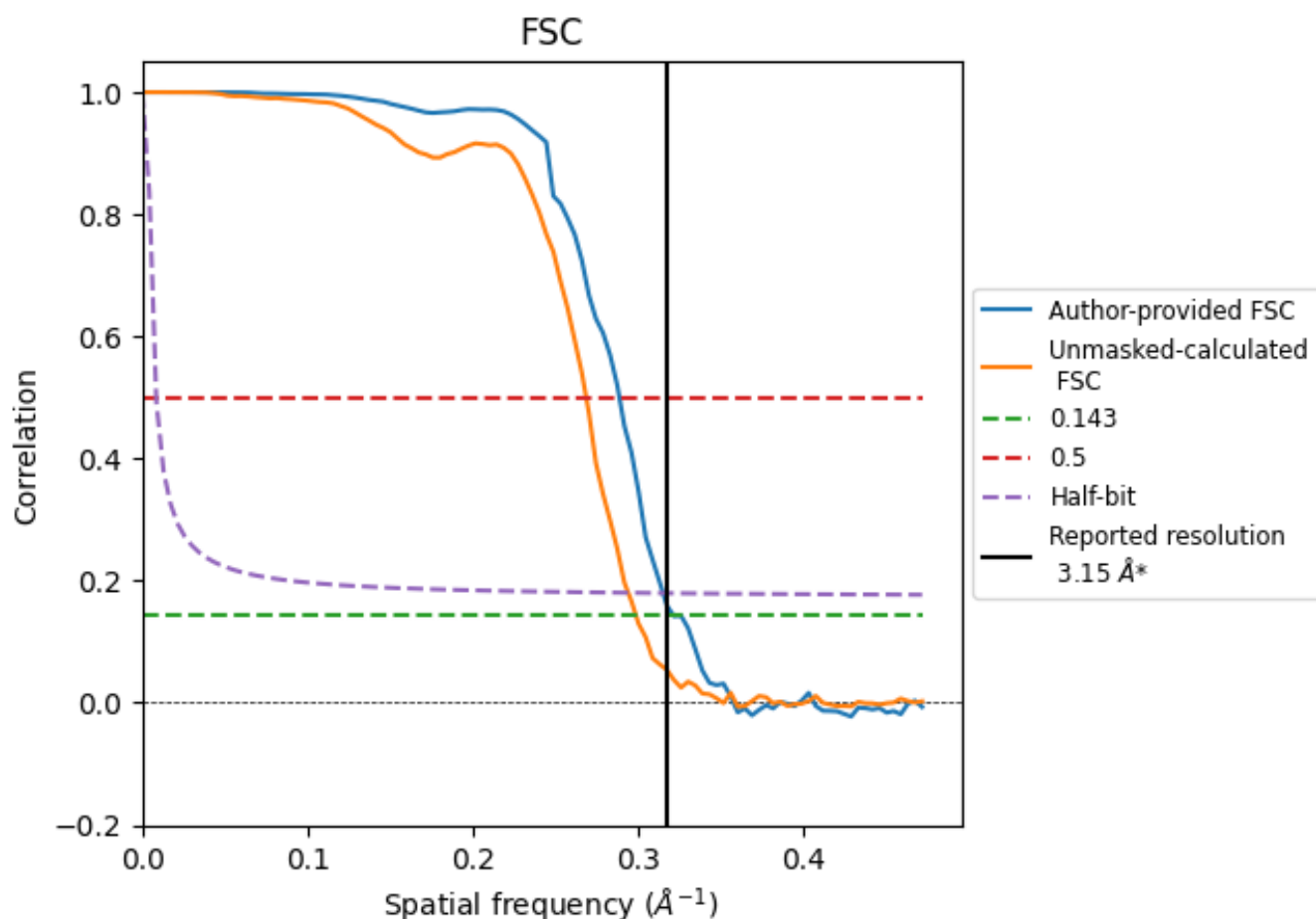


*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

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 $0.317 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

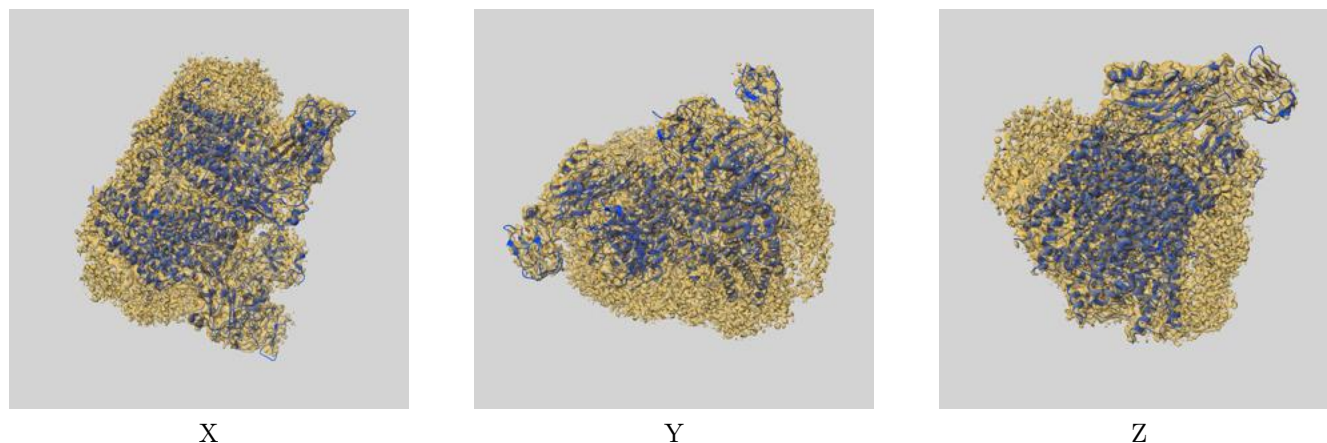
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.11	3.47	3.17
Unmasked-calculated*	3.35	3.72	3.40

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

9 Map-model fit [i](#)

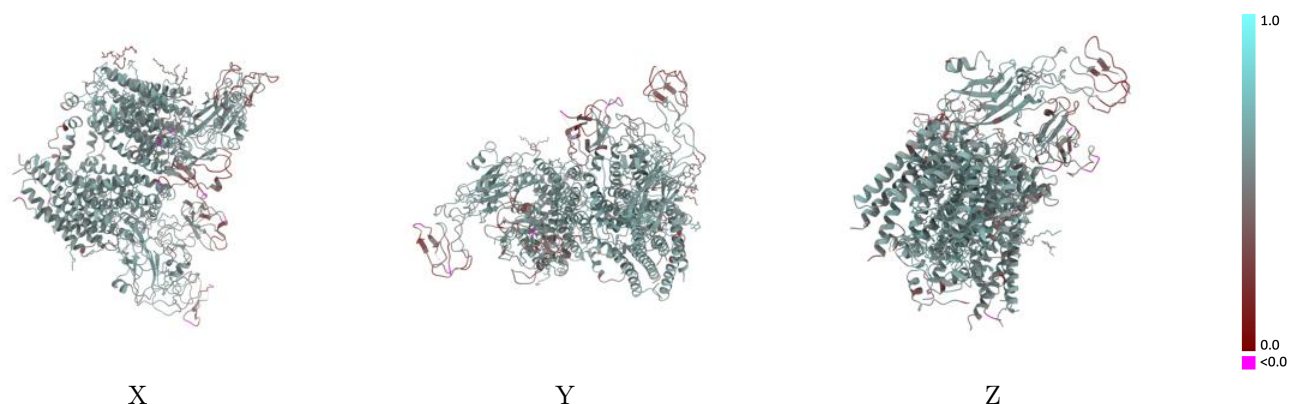
This section contains information regarding the fit between EMDB map EMD-15017 and PDB model 7ZXY. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



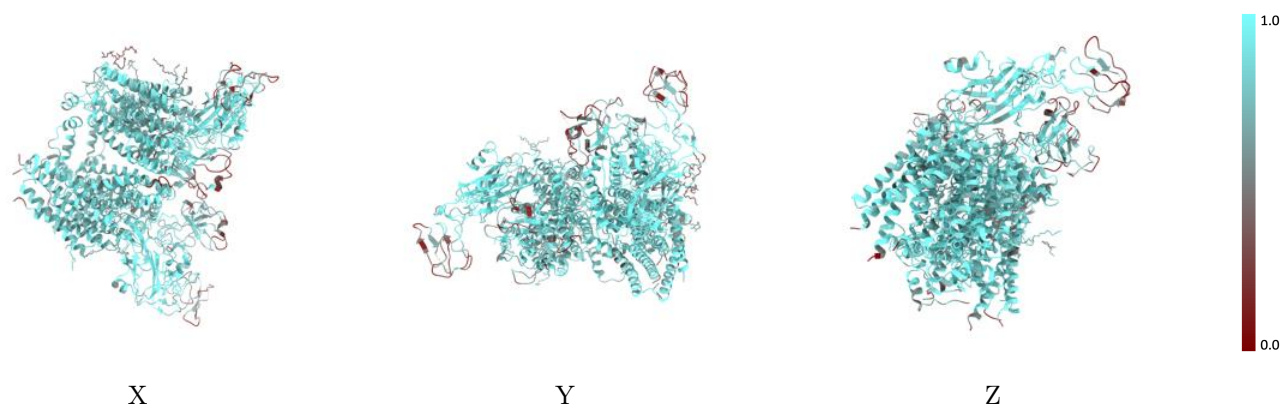
The images above show the 3D surface view of the map at the recommended contour level 0.0221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



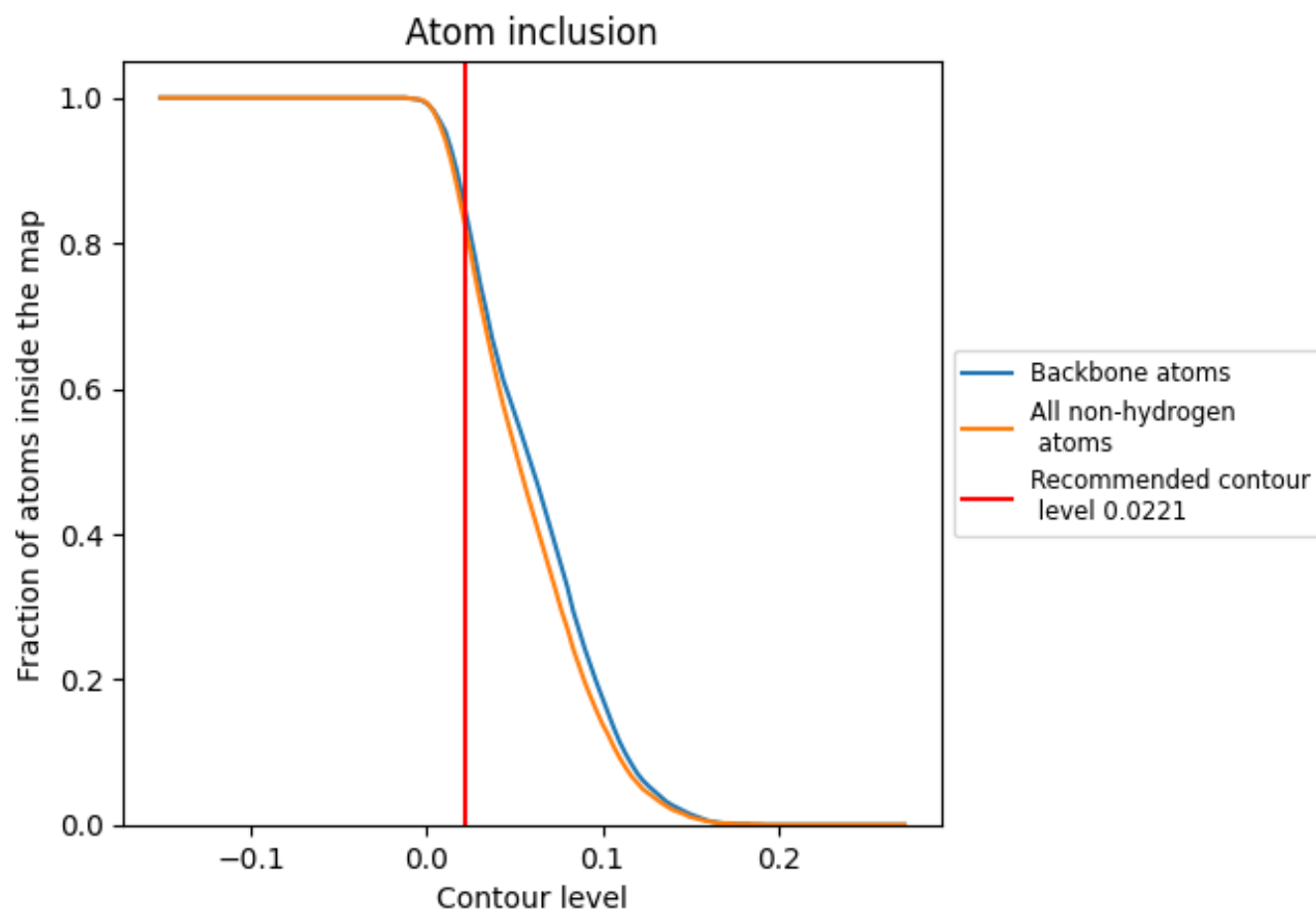
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0221).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.0221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5400
A	 0.9250	 0.5900
B	 0.8580	 0.5700
C	 0.7950	 0.5250
D	 0.6630	 0.4540
E	 0.8310	 0.5430
F	 0.8120	 0.5040
G	 0.8160	 0.5540
H	 0.8700	 0.5610
I	 0.9170	 0.5930
J	 0.8160	 0.5540
K	 0.7870	 0.5220
L	 0.7020	 0.4640
M	 0.8430	 0.5540
N	 0.8500	 0.5310
O	 0.7930	 0.5510
P	 0.8830	 0.5770

